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THEORETICAL STUDIES OF SOME THIRD ROW TRANSITION METAL COMPLEXES

by

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B.S. in Chemistry

University of Michigan

(1963)

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

May, 1966

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Charles Bonner Harris

Submitted to the Department of Chemistry on May 23, 1966, in partial fulfillment of the requirements for the degree of Doctor of Philosophy

ABSTRACT

The electronic ground state of $PtCl_4^{2-}$ calculated by semiempirical molecular orbital theory is a $^1A_{1g}$ with a Pt d orbital order and occupation of $(d_{z^2})^2\ (d_{xz},d_{yz})^2(d_{xy})^2(d_{x^2-y^2})^0$. This result was obtained over a wide range of variations in the Pt valence state ionization potentials, the Pt wavefunctions, and the Wolfsberg-Helmholz factor in both the Mulliken-Wolfsberg-Helmholz and the Ballhausen-Gray approximation. The numerical dependence of the Pt-Cl bond order and the one-electron molecular orbitals of $PtCl_4^{2-}$ have been examined as functions of variations in the Pt 6s, 6p and 5d wavefunctions, the corresponding valence state ionization potentials, and the weight given to the off diagonal terms in the Hamiltonian matrix. Finally, a method is outlined for computing STO overlap integrals that accurately approximate SCF overlap integrals.

A three-dimensional, single crystal X-ray diffraction study of the structure of $K_2[Re_2Cl_8]\cdot 2H_2O$ is reported. The crystals are triclinic with $a = 6.75$, $b = 7.86$, and $c = 7.61$ A, and $\alpha = 102.0^\circ$, $\beta = 108.9^\circ$, and $\gamma = 104.8^\circ$. There is one formula unit in the cell, and the space group is $P\bar{1}$. The $[Re_2Cl_8]^{2-}$ ion therefore has a center of symmetry; its idealized point symmetry is $4/mmm$ (D_{4h}). The mean Re-Cl distance is 2.29 A, the mean Re-Re-Cl angle is 104°, the mean Cl-Re-Cl angle is 87°, and the Re-Re distance is 2.24 A. The water molecules are coordinated to K^+ ions.

The metal-metal and metal-chloride bonding in $[Re_2Cl_8]^{2-}$ is treated by "extended" Hückel Molecular Orbital Theory. The calculation suggests that the pi(π) bonding contribution to the Re-Re bond is four times that of the delta(δ) bonding and almost twice that of the sigma(σ) bonding. The Re-Re bond stabilization and the δ-bond rotational (D_{4h} to D_{4d}) barrier in $[Re_2Cl_8]^{2-}$ are calculated as

250 kcal and 50 kcal respectively by comparing a hypothetical $[ReCl_4]^{1-}$ anion (C_{4v}) with the $[Re_2Cl_8]^{2-}$ anion (D_{4h}). The ordering of the molecular orbitals is discussed with respect to the magnetic properties and the observed and calculated spectral properties.

A molecular orbital interpretation of nqr coupling constants is derived in a general manner. It is simplified by judicious assumptions and applied to some third row transition metal chlorides.

The bonding, charge distributions, spin densities and spectra of the third row MCl_6^{2-} (M = Re(IV), Os(IV), Ir(IV), and Pt(IV)) series is treated by molecular orbital theory. Specifically, the calculated nqr coupling constants, the t_{2g} spin densities and the charge transfer spectra are shown to be in good agreement with experimental results.

Thesis Supervisor: F. Albert Cotton

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CHAPTER I

GENERAL BACKGROUND AND DEVELOPMENT OF MOLECULAR ORBITAL THEORIES

General Molecular Theory

The problems of molecular physics were solved in principle with the advent of quantum mechanics in the 1920's when Schrodinger[1] presented his time-independent differential equation.

$$H\psi = E\psi \tag{1}$$

This equation accounted quantitatively for a multitude of atomic state phenomena. Exact solutions of Eq. (1) have been obtained only for H and its isoelectronic ions (e.g., He^{+}, Li^{++}, etc.) because of the mathematical difficulties inherent in the solution of the three-body problem. As a result, the solution of Eq. (1) can be arrived at for molecules only by a method of successive approximations, that is, a trial function, Φ_i, is used to calculate an energy, E^i; the function is changed and a new energy is calculated. This process of iteration is repeated until a minimum energy, E_m, the expectation value of the energy of the system in the state Φ_m, is obtained. This procedure defines the variational method and as such is subject to the limitation of the variational theorem[2] which states that the expectation energy, E_m, of the system in the state Φ_m is always greater than the actual ground-state energy, E, of the system, e.g.,

$$E_m \geq E \tag{2}$$

The difference between E_m and E is termed the correlation energy and is inherent in all molecular calculations.

Equation (1) can be simplified owing to the smallness of the ratio of the mass of an electron to that of any nucleus. The Born and Oppenheimer approximation[3] allows the wavefunction, ψ, to be separated into its electronic and nuclear coordinates ψ_e and ψ_n respectively. Thus, the total energy, E, is simply the sum of the electronic energy, E_e, associated with the electronic states, ψ_e, plus the energy of the nucleus, E_n, associated with the nuclear states, ψ_n. The determination of ψ_e is our central concern; the rest is the familiar problem of translation-vibrational-rotational motion associated with the nuclei. The validity of the Born and Oppenheimer approximation has been substantiated[4] in the case of H_2 insofar as the Born-Oppenheimer correction amounts to only 0.014 ev. of a total H_2 dissociation energy of 4.7466 ev.

Equation (3) restates the variational equivalent of our problem for electron wavefunctions, ψ_e, assuming fixed nuclear coordinates.

$$E_e = \int \psi_e^* H e \psi_e d\psi_e / \int \psi_e^* \psi_e d\tau_e \qquad (3)$$

The solution of Eq. (3), strictly speaking, is only a mathematical problem. As such, the challenge of its solution has produced a dichotomy involving purely theoretical methods on the one hand, and semiempirical methods on the other. Although purely theoretical methods play a fundamental role in our understanding of "small" molecular systems, they cannot, as yet, be applied to many molecules aside from diatomics and a few H-triatomics. Thus semiempirical methods

are a necessary and essential tool for applying molecular quantum mechanics to larger molecules. Carefully used and properly "calibrated" they have great value and utility for predicting unknown molecular properties.

Since our interest centers around calculations of transition metals, and therefore not small compounds, we will restrict this discussion to semiempirical methods. In particular the following discussion will be devoted almost entirely to the various Hückel-type[5] approaches. However, an understanding of the approximations made in Hückel theory prerequisites a rudimentary understanding of the molecular Hartree-Fock or self-consistent-field (SCF) method.[6,7]

Self-Consistent Field Theory (SCF).

The Hamiltonian operator for an n-electron problem has the form

$$H^e = \sum_i - 1/2\nabla_i^2 - \sum_i \sum_\alpha (z_\alpha/r_{i\alpha}) + \sum_i \sum_{j>i} (\phi_j\phi_j/r_{ij}) \qquad (4)$$

where the indicies run from 1 to n, the terms $-1/2\nabla_i^2$ are the kinetic energy components, the terms (z_α/r_α) are the nuclear attraction components where z_α is the charge on the α nucleus, and the terms $(\phi_j\phi_j/r_{ij})$ represent the electron-electron repulsions.

The first two terms in Eq. (4) are customarily called H_{core}; the latter being either the coulomb operator J_i or the exchange operator K_i where

$$J_i = \phi(1)\phi_i(1)/r_{ij} \qquad (5)$$

$$K_i = \phi_i(1)\phi_i(2)/r_{ij} \tag{6}$$

The $\phi_i(1)$ notation refers to electron 1 in orbital i. For molecules the LCAO-MO-SCF method is ordinarily employed to solve Schrodinger's equation using the Hamiltonian operator given by Eq. (4). A linear combination of atomic orbitals (LCAO)[8] is used to construct solutions of Molecular Orbitals (MO), ϕ_i, to Eq. (1):

$$\text{e.g.,} \qquad \phi_i = \sum_j C_j^i X_j \tag{7}$$

where the X_j are the atomic orbitals. If enough X_j's are included no error is introduced. However, one usually restricts the number of X_j's used arriving at a final solution which contains a margin of error, otherwise known as the LCAO "approximation".

If we insert Eq. (7) into Eq. (1) using Eq. (4), multiply on the left by X_i, and integrate we obtain a set of equations

$$\sum_j C_j^i (H_{ij}^e - S_{ij}\epsilon_j) = 0 \tag{8}$$

where in the notations of Eqs. (5) and (6)

$$H_{ij} = H_{ij}^{core} + \sum_j [2J_{ij} - K_{ij}] \tag{9}$$

and

$$S_{ij} = \int X_i X_j \, d\tau \tag{10}$$

Equations (8) are simultaneous linear equations for unknowns, C_{ij}, and a non-trivial solution exists if

$$\text{determinant } |H^{e}_{ij} - S_{ij}\epsilon_i| = 0 \qquad (11)$$

Knowing the X_i's molecular orbitals, ϕ_i, can be determined by guessing the C_{ij}'s, computing the integrals in Eq. (9); solving Eq. (1); determining the C_{ij}'s from Eq. (8); comparing the original C_{ij}'s with the final C_{ij}'s, and repeating the cycle until the C_{ij}'s do not change from cycle to cycle. This procedure defines the LCAO-MO-SCF method. The energy of the MO's are ϵ_i. The total energy[9] of the molecule in a closed shell configuration, E_{total}, is not twice the sum of the orbital energies, ϵ_i, but

$$E_{total} = 2\sum_i 1/2(\epsilon_i + H^{core}_{ii}) \qquad (12)$$

In principle, the above procedure can be applied to any molecule. In practice, however, the difficulty in evaluating the J_{ij} and K_{ij} integrals and the sheer number of integrals involved has restricted the LCAO-MO-SCF method to small molecules. As a result many MO theories evolved[10-13] which attempted to semiempirically approximate the J_{ij}'s and K_{ij}'s (Eq. (9)). They have to date been applied primarily to pi-electron systems in organic molecules, and as yet have no significant utility for transition metal complexes.

Hückel Theory.

An MO theory that has transcended the mathematical difficulties associated with the LCAO-MO-SCF theory is the Hückel Theory.[14,15] In this theory the n-electron Hamiltonian is not of the form in Eq. (4). A much simpler form,

$$H^{e} = \sum_{i} H^{eff(i)} \tag{13}$$

is used where $H^{eff(i)}$ is some operator that incorporates in an average way the electron-repulsion terms of Eq. (4). Invoking the LCAO approximation (Eq. (7)) and applying the variational theorem to Eq. (1) using Eq. (13) as the Hamiltonian operator we obtain, as earlier,

$$\sum_{j} C_{i}^{j} (H_{ij}^{eff} - S_{ij}\epsilon_{i}) = 0 \tag{14}$$

Thus the problem is simply to determine the matrix elements H_{ij}^{eff} in which the cases $i \neq j$ and $i = j$ are distinguished.

$$H_{ij}^{eff} = \alpha_{ii} = \int X_{i}^{*} H^{e} X_{i} d\tau \tag{15}$$

is called the coulomb integral and is an empirical property of an atom;

$$H_{ij}^{eff} = \beta_{ij} = \int X_{i}^{*} H^{e} X_{j} d\tau \tag{16}$$

is called the resonance integral and is an empirical property of the bond. S_{ij} is again the overlap integral between the ith and jth atomic orbitals.

A critical simplifying assumption in the theory is that

$$S_{ij} = 0 \tag{17}$$

when i and j orbitals are not on neighboring atoms. It has been shown[16] that this is not a bad assumption provided that

$$\beta_{ij} = 0 \tag{18}$$

when Eq. (18) is satisfied. Thus for simple homonuclear pi-systems (ethylene, benzene, naphthalene) the problem reduces to two parameters, α_{ii} and β_{ij}. Molecular orbitals for literally hundreds of molecules have been calculated using Hückel theory. The greatest advantage of the theory is its simplicity. We need not enumerate in detail the successes of the theory in organic chemistry. Streitiewer's[16] book gives a truly superb treatment of this subject. In spite of the simplicity and limited success of the theory, several major criticisms can be leveled against it. First, from a practical standpoint, the parameters, α_{ii} and β_{ij}, required to fit one property usually differ from those required to fit another. Thus it is impossible to describe simultaneously the spectra and charge distribution of a given molecule. Furthermore, there is no finite bond order between non-adjacent atoms in a molecule in the framework of Hückel theory. This is erroneous and results from the neglect of non-neighboring interactions. From a theoretical point of view, it is simply not valid to write Eq. (13).

For such a one-electron operator the total electronic energy for a closed shell configuration is given by

$$E_{total} = 2 \sum_i \epsilon_i \qquad (19)$$

and not by Eq. (12). Even if H^e (Eq. (12)) is interpreted as the Hartree-Fock operator (Eq. (4)) it invariably counts electronic repulsion twice.[17]

Synthesis of LCAO-MO-SCF and Hückel Method - Moffitt's Atoms in Molecules Method.

Moffitt's attempt[18] to calculate thr rich electronic spectrum of molecular oxygen using LCAO-MO-SCF theory failed insofar as his results contradicted experimental facts. This prompted him to formulate his atoms-in-molecules method[19] in which atomic-spectroscopic data was empirically incorporated into molecular orbital theory. The precise logic and mathematics employed in the original argument will not be presented since an excellent discussion of the method has been given by Parr.[20] Instead, we will present a descriptive formulation of the theory relying on "intuition" rather than formal mathematics.

The basic idea is qualitatively very simple - atoms in a molecular field behave similarly to free atoms, but there is an interatomic correlation effect in molecules which vanishes at infinite internuclear distance. In other words, the Hamiltonian matrix elements of the atomic orbitals on an atom in a molecule, H_{ii}^{eff}, represent the

energy of an electron in a specific atomic orbital i, moving in the field of shielded atomic nuclei. Thus, the Hamiltonian operator for the ith electron can be written as

$$H_i^e = -1/2\nabla_i^2 - Z_\alpha/r_{i\alpha} + \sum_{j>i} \phi_j\phi_j/r_{ij} - \sum_{\beta\neq\alpha} Z_\beta/r_{i\beta} + \sum_k \phi_k\phi_k/r_{ik} \tag{20}$$

and the n-electron Hamiltonian can be written as

$$H^{eff} = \sum_i H_i^e \tag{21}$$

The symbols in Eq. (20) are defined in the same fashion as in Eq. (4); however, the sum over β refers to atoms in the molecule on which i is not centered and the sum over k is to imply electrons on the β atoms. The first three terms in Eq. (20) are therefore the free atom contributions, A_i, and the last two terms are the molecular correlation terms, V_c^i. Thus the diagonal matrix elements of Eq. (21) can be expressed as:

$$H_{ii}^{eff} = A^{ii} + V_c^{ii} \tag{22}$$

The key to the solution of Schrodinger's equation for this method in the LCAO approximation then is simply the separation of the matrix elements of the molecular Hamiltonian into intra-atomic and inter-atomic elements. The former are estimated from atomic-spectroscopic data and the latter are approximated or calculated from some orbital

theory.[21,22] The methods that have evolved in the past few years to treat transition metal complexes differ only in the procedure used to obtain these elements. Before discussing these methods a word should be said about the evaulation of the off-diagonal matrix elements, H^e_{ij} $(i \neq j)$, that arise.

By similar arguments, i.e., separation of atomic and molecular contributions in the Hamiltonian, Moffit[22] proposed that the off-diagonal matrix elements, H^e_{ij}, could be reduced to diagonal elements, H^e_{ii} and H^e_{jj}, plus V_c^{ij}, the correlation energy between them, i.e.,

$$H^e_{ij} = (1/2)S_{ij}\{H^e_{ii} + H^e_{jj}\} + 1/2\{V_{ij} + V_{ji}^*\} \qquad (23)$$

where V_{ji}^* is the complex conjugate transpose of V_{ij}. In this fashion only the correlation energies need be calculated since the H^e_{ii}'s are in principle known. Unfortunately, correlation energies are extremely difficult to calculate; consequently, they must be approximated. One such approximation was suggested by Wolfsberg and Helmholz.[23,24] In effect they incorporated the correlation terms, V_c^{ij}, into the atomic terms, H^e_{ii}, by the following equation

$$H^e_{ij} = K\, S_{ij}\{H^e_{ii} + H^e_{jj}\}/2 \qquad (24)$$

where the parameter K is varied to fit some physical observable (e.g., electronic spectra) associated with the molecular orbitals.

This approximation, however, was patterned after Mulliken's[25] approximation for potential energy integrals, V_{ij}.

e.g., $$V_{ij} = S_{ij}(V_{ii} + V_{jj})/2 \qquad (25)$$

Equation (24) is therefore frequently called the Mulliken-Wolfsberg-Helmholz (MWH) approximation.[26]

Utilizing Eq. (24), the MWH approximation, the application of semiempirical molecular orbital theory to inorganic complexes reduced (1) to the evaluation of the overlap integrals, S_{ij}, and (2) the estimation of diagonal energy matrix elements, H^e_{ii}. It is the various approaches used to estimate the latter that further distinguishes the types of molecular orbital theories employed in transition metal chemistry. These will now be discussed.

LCAO-SCCC Method.

The LCAO-SCCC method, the linear combination of atomic orbitals self-consistent in charge and configuration, was suggested by Gray[27] and has been applied to many transition complexes[28] with little or no experimental confirmation of the results. The method attempts to calculate a linear relationship for the H^e_{ii}'s in Eq. (22), in terms of the configurations of the ith orbital. For instance, in a transition metal, e.g., Mn^{2+}, the d orbital may be in one of several configurations:

$$d^5,\ d^4s,\ d^3sp,\ d^2s^2p,\ d^2sp^2,\ \text{etc.},$$

each having a different energy as obtained from spectroscopic tables[29] of the ion. Moreover, in a complex the metal may not have a formal valence state of +2 in this case, but may instead be +1; thus, giving rise to a new series of configurations;

$$d^6,\ d^5s,\ d^4sp,\ d^3s^2p,\ d^3sp^2,\ \text{etc.}$$

each again having a different energy. In order to accommodate these possibilities the method initially assumes a given charge and configuration on the atoms and uses the H_{ii}^e's corresponding to these states. The molecular orbitals are then calculated. If a Mulliken population analysis[30,31] is performed on the MO's a new charge and configuration for the atoms can be determined. New H_{ii}^e's corresponding to these new states are then used in the next cycle. In cases where the charges or configurations are non-integral, extrapolated values are used. The procedure is reiterated until the charges and configurations do not change from cycle to cycle. At this point the calculation is said to be self-consistent.

The method as described is an elegant way of obtaining the A_{ii} terms in Eq. (22). However, a basic fallacy of the method is that it neglects entirely the molecular interaction (interatomic correlation) terms, V_{ii}^c (Eq. (22)). This is equivalent to saying that the interatomic electron repulsion terms are exactly equal to the negative of the interatomic nuclear attraction terms. This is certainly not the case, nor should one naively expect it to be so. Using a

point charge approximation, one can to the first order show that these terms can be as much as +5 to +15 ev.[32] The ultimate result of such an error is that the metal orbital H_{ii}^{e}'s are much too stable. That is, their dependence on charge is about -10 to -15 ev. per metal charge unit (e.g., M^{0} to M^{+1}) rather than about -1 to -3 ev. which would result from the incorporation of the molecular terms. This is illustrated in the following way. Suppose a Pt atom were in the environment of four Cl atoms (e.g., $PtCl_4^{2-}$) and the charge on the Pt in this environment was +1. The H_{ii}^{e} for the 5d orbital if it were a free ion would be about -20 ev. In the Cl environment, however, the 5d electrons see an effective minus field due to the -0.75 charge on each Cl; thus, the 5d electrons are "destabilized" by about 10 ev. by electron-charge repulsions. It is this repulsion that is neglected in the LCAO-SCCC method. As a consequence the calculated metal-to-ligand covalency is too great and the calculated metal effective charge is too low. This has been verified in several cases by Nuclear Quadrupole Resonance studies of transition metal halides.[33-35]

Extended Hückel Theory.

Extended Hückel Theory (EHT) assumes a Hamiltonian operator of the form given by Eq. (22); the V_c^{ii} term, however, is replaced by the point charge approximation given by Pople.[36]

$$V_c^{ii} = \sum_{\beta \neq \alpha} Z_\beta^{eff}/r_\beta \qquad (26)$$

The β represents atoms on which i is not centered and Z_β^{eff} is the effective nuclear charge of atom β. In order to evaluate H_{ii}^e, it becomes necessary (1) to evaluate A_{ii} using the procedure outlined in the LCAO-SCCC method, and (2) to determine Z_β^{eff}. If we assume, as does the LCAO-SCCC method, that the ith electron on the α atom is perfectly screened from the β nuclei by electrons on the β atoms, then Z_β^{eff} would be zero. This is usually not the case. What ultimately determines the value of Z_β^{eff} is the penetration of the ith orbital into the β electron core. This can be illustrated by the following two examples. Assume that we have a diatomic molecule A-B. If the radial portion of the A wavefunctions are very contracted (e.g., H) they do not penetrate very far into the positive field of the B core; consequently, it sees an effective negative charge on atom B. On the other hand, if the A wavefunctions are diffuse, they penetrate more into the positive field on B. Furthermore, if this penetration is great enough, the A wavefunction may see an "effective" positive charge on atom B. Thus, the "diffuseness" of the orbitals (a property of only the radial part of the wavefunctions) determines (1) the sign of Z_β^{eff} and (2) its magnitude.

If one defines the potential field around atom B as $v(r)$ (where v functionally defines the charge density around B), then

$$Z_\beta^{eff}/r_\beta = \langle \phi_i | v(r) | \phi_i \rangle \qquad (27)$$

Since it is difficult to compute the integrals in Eq. (27), several approximations have been suggested. Pohl, Rein, and Appel[37] obtained the penetration correction for hydrogen halides by the use of coulomb repulsion integrals. Ros[38] has devised a method for estimating these terms by assuming the electron density contributions from individual orbitals on B are localized between concentric spherical shells. In other words, the integrals are practically zero for high and low values of r in $v(r)$.

Finally, the Z_β^{eff} can in certain cases be incorporated semi-empirically into H_{ii}^e by systematically varying the H_{ii}^e's in order to calibrate them with some observed molecular property. A description of this procedure is given in Chap. II.

Modified SCF Method.

Recently, there has been an attempt to do molecular orbital calculations on transition metal complexes in the framework of a more theoretical approach. Fenske[39] formulated an approach similar to the SCF approach insofar as all diagonal matrix elements are calculated from first principles. It, however, differs from SCF theory in that the Mulliken approximations[25] are used to simplify one center coulomb and exchange integrals and the Shulman and Sugano[40] electrostatic interatomic integrals have been approximated by point charge crystal field integrals.[41] The Hamiltonian operator for this method incorporates interatomic correlation and therefore closely resembles

the SCF Hamiltonian. The method has, however, not been tested in its ability to predict molecular properties such as charge or bond covalency, but it seems to calculate reasonable 10 D_q values for the first row hexafluorides.[42] Furthermore, it is apparently consistent[42] with the nephelauxetic effect[43] which has been attributed[43,44] to the reduction of the effective metal charge resulting from electron donation via chemical bonding.

All in all the theory outwardly appears "promising". However, as yet it has not been used to predict or verify the molecular properties of charge distributions and bond orders.

Future Improvements in Molecular Orbital Theory.

There are two areas where substantial improvement in semi-empirical MO theory could be made.

First, new methods for the evaluation of the diagonal terms, H_{ii}, must be found. A theoretical method must include the inter-atomic correlation or penetration terms. For closed shell systems Ros[45] is developing a computer program to analytically compute these terms. An empirical method is developed in this thesis (Chapters II and V) in which these terms are "calibrated" by certain molecular properties. Specifically, a molecular orbital interpretation of nuclear quadrupole resonance is developed (Chapter V) and is applied to transition metal complexes (Chapters II and VI) as a means of evaluating (1) the parameters used in MO theory and (2) the results derived from MO theory.

The second area where improvement is needed is in the evaluation of the off-diagonal matrix elements, H_{ij}. Specifically, the kinetic energy contributions to H_{ij} should be calculated explicitly and the MWH approximation should be used for the potential terms only.[46-48] This has been done for some simple organic molecules[48] but has not been used for transition metal complexes.

Thesis Goals.

The goals of this thesis are:

(1) To evaluate the variable parameters in extended Hückel theory in order to obtain the best fix values for a series of molecules. (Chapter II)

(2) To apply MO theory to the metal-metal and metal-ligand bond to determine what specific interactions are important in each. (Chapters II and IV)

(3) To apply nuclear quadrupole resonance results to verify molecular orbital calculations. (Chapters V and VI)

CHAPTER I

REFERENCES

1. P. A. M. Dirac, The Principles of Quantum Mechanics, 4th ed., Oxford Univ. Press, London, 1958.
2. R. Daudel, R. Lefebvre and C. Moser, Quantum Chemistry: Methods and Applications, Interscience, N.Y., 1959.
3. A. Fröman, J.Chem. Phys., 36, 1490 (1962); D. W. Jepsen and J. O. Hirschfelder, J. Chem. Phys., 32, 1323 (1960).
4. W. Kolos and C. C. J. Roothaan, Revs. Mod. Phys., 32, 219 (1960).
5. Y. I'Haya, Advances in Quantum Chemistry, Vol. I, Per-Olov Lowdin, Ed., Academic Press, N.Y., 1964.
6. D. R. Hartree, The Calculation of Atomic Structures, Wiley, N.Y., 1957.
7. C. C. J. Roothaan, Revs. Mod. Phys., 23, 69 (1951).
8. J. H. van Vleck, J. Chem. Phys., 2, 22 (1934).
9. B. J. Ransil, Revs. Mod. Phys., 32, 245 (1960).
10. R. Pariser and R. G. Parr, J. Chem. Phys., 21, 466 (1953).
11. R. G. Parr, J. Chem. Phys., 20, 1499 (1952).
12. J. A. Pople, Trans.Faraday Soc., 43, 1375 (1953).
13. C. M. Moser, J. Chem. Soc., 3455 (1954).
14. J. D. Roberts, Notes on Molecular Orbital Calculations, Benjamin, N.Y., 1961.
15. G. Del Re, Nuovo Cimento, 17, 644 (1960).

16. A. Streitwieser, Jr., Molecular Orbital Theory for Organic Chemists, Wiley, N.Y., 1961.

17. R. G. Parr, J. Chem. Phys., 19, 799 (1951).

18. W. Moffitt, Proc. Roy. Soc.(London), A210, 224 (1951).

19. Ibid., A210, 245 (1951).

20. R. G. Parr, Quantum Theory of Molecular Electronic Structure, Benjamin, N.Y., 1964.

21. M. Kotani, K. Ohno and K. Kayama, Handbuch der Physik, 37/2, 1 (1961).

22. J. C. Slater, Quantum Theory of Molecules and Solids, Vol. 1, McGraw-Hill, N.Y., 1963.

23. M. Wolfsberg and L. Helmholz, J. Chem. Phys., 20, 837 (1952).

24. See Chapter II of this thesis for a discussion.

25. R. Mulliken, J. chim. phys., 46, 497 (1949).

26. See Chapter II and IV of this thesis.

27. H. Basch, A. Viste and H. B. Gray, J. Chem. Phys., 44, 10 (1966).

28. C. J. Ballhausen and H. B. Gray, Molecular Orbital Theory, Benjamin, N.Y., 1964.

29. C. E. Moore, Atomic Energy Levels, U. S. National Bureau of Standards Circular 467, 1949 and 1952.

30. R. S. Mulliken, J. Chem. Phys., 23, 1833 (1955).

31. Ibid., 23, 1841 (1955).

32. For specifics, see Chapter II of this thesis.

33. R. Barnes and S. Segel, Phys. Rev. Letters, 3, 462 (1959).

34. R. Barnes and R. Engardt, J. Chem. Phys., 29, 248 (1958).

35. G. K. Semin and E. I. Fedin, Zhurnal Strukturnoi Khimii, 1, 252, 464 (1960).

36. J. A. Pople, Trans. Faraday Soc., 49, 1375 (1953).

37. H. Pohl, R. Rein and K. Appel, J. Chem. Phys., 41, 3385 (1964).

38. P. Ros, Thesis, Eindhoven, Holland (1964).

39. R. Fenske, private communication.

40. R. G. Shulman and S. Sugano, Phys. Rev., 130, 517 (1963).

41. C. J. Ballhausen, Introduction to Ligand Field Theory, McGraw-Hill, N.Y., 1962, p. 57.

42. R. Fenske, private communication. To be published in Inorg. Chem., 5, July, 1966.

43. C. J. Jorgensen, Absorption Spectra and Chemical Bonding in Complexes, Pergamon Press, Oxford, 1962, p. 134.

44. Idem., Progress in Inorganic Chemistry, Vol.4, F. A. Cotton, Ed., Interscience, N.Y., 1963, p. 73.

45. P. Ros, private communication.

46. R. S. Mulliken, J. chim. phys., 46, 497 (1949); 46, 675 (1949).

47. K. Ruedenberg, J. Chem. Phys., 34, 1861 (1961).

48. M. Newton, F. Boer, W. Palke and W.Lipscomb, Proc. Natl. Acad. Sci., 53, 1089 (1965).

CHAPTER II

THE EFFECTS OF VARIOUS PARAMETERS ON SEMIEMPIRICAL MOLECULAR ORBITAL THEORY OF METAL COMPLEXES. MOLECULAR ORBITAL THEORY OF $PtCl_4^{2-}$

INTRODUCTION

Previous studies of the electronic structure of $PtCl_4^{2-}$ have led to several ambiguities concerning the splitting of the Pt 5d orbitals. Ballhausen and Gray[1] on the basis of an MO treatment using hybrid orbitals have proposed a Pt 5d orbital order of $(d_{xz};d_{yz})$, (d_{z^2}), (d_{xy}), $(d_{x^2-y^2})$. Fenske, Rudenberg and Martin[2] proposed the same order by considering the problem in terms of electrostatic crystal field theory. Chatt, Orgel and Gamben[3] and more recently Martin[4,5] proposed a (d_{z^2}), $(d_{xz};d_{yz})$, (d_{xy}), $(d_{x^2-y^2})$ orbital order. Unfortunately, the electronic spectrum of K_2PtCl_4 both in the solid state[5,6,7] and in various solvents[3] can be interpreted using either splitting scheme. In an attempt to resolve these ambiguities, Martin[5] has studied the vibrational fine structure of the polarized spectrum at low temperatures and has suggested the latter assignment to be more probable.

The results of the various semiempirical MO theories are too qualitative to accurately calculate one-electron transition energies necessary for the unambiguous assignment of the electronic spectrum. We feel, however, that the original Pt 5d orbital splitting scheme proposed by Chatt, Orgel and Gamben[3] is correct within the limitations of a semiempirical MO theory which neglects spin. We must assume, however, that the solvent does not interact appreciably with $PtCl_4^{2-}$ along the C_4 axis. The validity of such an assumption is indicated by the lack of substantial changes of the electronic spectrum in various polar solvents[3] and by the fact that the solvent is not found coordinated to the Pt in the solid state.[8]

It is not the main purpose of this section to accurately correlate the electronic spectrum but to discuss the effects of variations of the parameters in semiempirical LCAO-MO theory on the estimation of the one-electron ground state energy levels of $PtCl_4^{2-}$ and to use Mulliken population analysis[9,10] on the eigenvectors of the ground state MO's to determine the electron distribution in the Pt-Cl bond.

METHOD OF CALCULATION

The LCAO-MO theory used is a modification of the extended Hückel MO theory. The modification is a stringent but necessary restriction on the values of the "molecular" valence state ionization potentials,* H_{ii}, of the basis set orbitals. In every calculation all overlaps, S_{ij}, are evaluated. No assumption is made as to the extent of hybridization of the ligand and/or metal wavefunctions. This ensures that the variational principle,[11] $\partial E/\partial c_i = 0$, where c_i is the MO coefficient and E is the MO eigenvalue, is satisfied for all atomic orbitals in the basis set. These conditions and the LCAO assumption,[12] i.e., $\psi^i = \sum_i c_i^j \phi_i$ where ψ^i is the jth MO and ϕ_i is the ith atomic orbital, leads directly to the familar condition for the secular determinant,

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* The distinction between molecular valence state ionization potentials, H_{ii}, and atomic valence state ionization potentials, A_{ii}, is made in order to discuss the energy of the ith atomic orbital in a molecular and free ion field respectively.

$$\text{i.e.,} \quad \det|H_{ij} - ES_{ij}| = 0, \tag{1}$$

where H_{ij} are the usual Hamiltonian matrix elements between the ϕ_ith and ϕ_jth atomic orbitals.

Choice of Atomic Orbitals and the Evaluation of Overlap Integrals.

A basis set of 25 orbitals, the Pt 6s, 6p, 5d and the Cl 3s, and 3p atomic orbitals were used to construct the molecular orbitals. We assumed that the non-valence electrons do not participate in bonding and these, together with the nuclei, form a core potential that was unchanged by interactions between the valence shell electrons.

The atomic orbitals were expressed as nodeless Slater[13] (STO) orbitals of the form:

$$\psi(n,l,m) = Nr^{n-1} \exp(-\alpha_i r) Y_l^m(\theta,\varphi) \tag{2}$$

where N is the normalization coefficient, α_i is the shielding parameter, and $Y_l^m(\theta,\varphi)$ is the usual real spherical harmonic.

The shielding parameters, α_i, were chosen in the following fashion to best approximate overlaps between self-consistent wavefunctions (SCF).* First an interpolated numerical radial wavefunction for $Cl^{1/2-}$ was obtained from SCF wavefunctions of Cl^0 and Cl^{1-}.[14,15] Numerical

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* Herman-Skillman wavefunctions for the Pt^0 6s and 5d orbitals were used; the 6p wavefunction was approximated by assuming a slightly smaller α than the 6s. The Hartree-Fock wavefunctions of Watson and Freeman were used for Cl^0 and Cl^{1-}.

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overlap integrals between the SCF ψ's for "cis" Cl 3s-3s, 3p-3p, and 3s-3p orbitals were then calculated. The α's in Eq. (2) were varied so that the overlap integrals between the STO wavefunctions were nearly the same as those obtained from SCF wavefunctions. In this way the Cl 3s and 3p shielding parameters were fixed. The same procedure was followed for Pt^{o}-$Cl^{1/2-}$ overlap integrals of the type 6s-3s, 6s-3p, 5d-3s and 5d-3p; however, only the Pt^{o} α_i's[16] needed to be varied.

The ratios of overlap integrals between STO and SCF wavefunctions are given in Table I. Table II gives the final α_i's used to calculate the overlap integrals which are given in Table III using the molecular coordinate system shown in Fig. 1.

We assumed that the overlap integrals did not change with variation of the charge distribution in the course of self-consistent charge refinement. The error inherent in such an assumption can be estimated if we assume that the Pt wavefunctions have a similar dependence on charge and configuration as some other known wavefunctions. The wavefunctions of Pt are not available for configuration and charge states other than the Pt^{o} state $5d^{9}6s^{1}$. Ros[17] has already given simple diatomic overlap integrals for a limited number of charge distributions and configurations of $CuCl_4^{2-}$. Since the 3d to Cl overlaps were not listed for Cu $d^{10}s^{1}$ and $d^{10}p^{1}$ configurations, we restricted the comparison to Cu 4s and 4p to Cl overlap integrals. Table IV lists the

overlap integral ratios Cu^{0}-$Cl^{0.5-}$:Cu^{1+}-$Cl^{0.75-}$ and Cu^{0}-$Cl^{0.5-}$:-$Cu^{0.44}$-$Cl^{0.61-}$ for the orbitals and configurations listed.

Since a Pt charge of +0.439 was obtained after full charge refinement, we concluded that although an 9% error is introduced in certain cases (6p-3s; 6s-3s) by neglecting to recalculate overlap integrals as a function of charge, the average error is only 5% to 6%.

Evaluation of the Diagonal Matrix Elements, H_{ii}.

H_{ii} is the energy of an electron in the ith atomic orbital moving in the field of the nuclei and other electrons in the molecule. In terms of the Hamiltonian operator and orthogonal wavefunctions, χ_i, these matrix elements can be expressed in the Dirac notation as:

$$H_{ii} = \langle\chi_i|-1/2\,\nabla_i^2|\chi_i\rangle - \langle\chi_i|Z_\alpha/r_\alpha|\chi_i\rangle + \langle\chi_i|\sum_{j>i}\chi_j\chi_j/r_{ij}|\chi_i\rangle$$
$$- \langle\chi_i|\sum_{\beta\neq\alpha}Z_\beta/r_\beta|\chi_i\rangle + \langle\chi_i|\sum_{\substack{k>i\\k\neq j}}\chi_k\chi_k/r_{ik}|\chi_i\rangle \qquad (3)$$

where $-1/2\,\nabla_i^2$ is the kinetic energy operator, Z_α/r_α is the nuclear attraction operation of the αth nucleus on which the ith atomic orbital is centered and $\Sigma\,\chi_j\chi_j/r_{ij}$ are the electron repulsion operators where the jth atomic orbital is on the α nucleus. k designates atomic orbitals centered on the β nuclei.

If we define the free ion contributions to H_{ii}, namely the first three terms in Eq. (3), as A_{ii} and the remaining terms as M_{ii} which

are the contributions to H_{ii} from other atoms in the molecule, we can re-express H_{ii} as:

$$H_{ii} = A_{ii} + M_{ii} \qquad (4)$$

For specific free ion electron configurations the A_{ii}'s can be explicitly evaluated. They have, however, been traditionally estimated by the valence state ionization potentials ($VSIP_{ii}$).

The A_{ii}'s for the process $Cl^{0} \rightarrow Cl^{+1} + e^{-}$ were estimated as the VSIP's given by Hinze and Jaffe[18] for the 3s and 3p orbitals in the configurations $sp^2p^2p^2$ and $s^2p^2p^2p$ respectively.

The A_{ii}'s for the process $Pt^{0} \rightarrow Pt^{1+} + e^{-}$ were estimated by averaging the spectral states and multiplicities given by Moore[19] for the configurations and processes listed in Table V. Since the spectral states of Pt^{2+} have not been recorded, we have estimated the A_{ii}'s for the process $Pt^{1+} \rightarrow Pt^{2+} + e^{-}$.

Zerner and Gouterman[20] have obtained VSIP's for many of the first row transition metals, M. They found that the VSIP's for M^{1+} were about 10 ev. higher than the M^{0} for 4s and 3d electrons and about 7 ev. higher for 3p electrons. Since the ionization potentials[19] for Ni^{1+}, Pd^{1+}, and Pt^{1+} are 10.52, 11.09 and 9.56 ev. higher than the ionization potentials for Ni^{0}, Pd^{0} and Pt^{0}, we felt that it is reasonable to expect that the behavior of the VSIP's of the Pt states are similar to the metals of the first row. Therefore, the approximation was made

that the A_{ii}'s for Pt^{1+} were 10 ev. higher than the A_{ii}'s of Pt^{o} for the 6s and 5d atomic orbitals and 7 ev. higher for the 6p atomic orbitals.

In principle the multicenter integrals of M_{ii} can be calculated. This would be a formidable calculation requiring an unjustifiable amount of computer time. They can, however, in part be estimated by the point charge approximation:

$$M_{ii} \approx \sum_{\beta \neq \alpha} Z_{eff}/r_{\beta} \qquad (5)$$

where Z_{eff} is the effective point charge of the β nucleus. The sum is over all nuclei except the nucleus on which the ith atomic orbital is centered. The inner nuclear distance between the α and β nuclei in Bohr radii is r_{β}.

Table VI lists the values of A_{ii} and M_{ii} resulting from such an approximation for the Pt 6s, 6p and 5d atomic orbitals. Δ_{ii}, defined in Table VI, is significant in two respects: (1) it is larger for the more covalent Pt-Cl bonds (i.e., Pt charge closer to zero); (2) it is larger for the more diffuse 6p orbitals. These results suggest that Δ_{ii} is in some way related to the penetration of the Pt wavefunction to the Cl inner core, an effect which is neglected in the point charge approximation of M_{ii}. The potential field around the Cl atom changes from negative to positive at some point approaching the Cl nucleus; therefore, the larger the amplitude of the Pt wavefunction, the greater

will be the stabilization of the M_{ii} from the positive portion of the Cl potential field. Thus, the Pt 6p atomic orbital should be stabilized more by this effect than the 6s and 5d orbitals.

Rather than neglect this penetration correction, the Δ_{ii} was assumed to be functionally related to it. The molecular terms H_{ii} corresponding to the Pt^{1+} states were therefore restricted to values one ev. higher than the corresponding Pt^{0} states. All intermediate values were obtained by interpolation. This is a stringent constraint on the H_{ii}'s. However, in a later section of this paper it will be shown that the one-electron molecular orbitals can only be justified experimentally if one does in fact impose such a constraint. This is only an empirical test but non-the-less a fact which we feel is significant.

Evaluation of the Off-Diagonal Matrix Elements, H_{ij}.

The H_{ij}'s are the usual Hamiltonian matrix elements between the ith and jth atomic orbitals. They have been evaluated semiempirically by the Mulliken-Wolfsberg-Helmholtz (MWH)[21] approximation, Eq. 6.

$$H_{ij} \approx KS_{ij}(H_{ii} + H_{jj})/2 \qquad (6)$$

K is the Wolfsberg-Helmholtz[22] factor and S_{ij} is the overlap integral between the ith and jth atomic orbital.

This approximation was used for all calculations. In addition, however, the MWH approximation was compared to the Ballhausen-Gray[23]

(BG) approximation (Eq. 7) for various values of K and K'.

$$H_{ij} \approx K'S_{ij}(H_{ii}H_{jj})^{1/2} \qquad (7)$$

The results of this variation are listed in Table VII for several molecular properties.

Calculations.

Using the wavefunctions and H_{ii} listed earlier the secular determinant (Eq. 1) was solved* for a full basis set of orbitals. The eigenvalues and eigenvectors were obtained and a Mulliken population analysis of the eigenvectors yielded the reduced overlap populations (bond orders) and charge distributions. The calculations were cycled n times such that the differences between the Pt charge at the n-1th cycle was less than 0.001 charge unit from the nth cycle. All calculations were performed at the M.I.T. Computation Center on the I.B.M. 7094.

RESULTS

K can be considered as a parameter that artificially controls the extent of charge flow from the ligand to the metal in the bonding region. Its value directly effects the calculated covalent character

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* A modified Fortran program written by R. Hoffman was used. Orbital α_i's were calculated by a Mad program "WAVWF" written by C. B. Harris.

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of the metal ligand bond. Thus, the calculated molecular charge densities, bond orders, and electron transition energies are very sensitive to one's choice of K.

Table VII lists the metal charge, metal-ligand bond order, and the $^1b_{2g} \rightarrow {}^1b_{1g}$ transition for various values of K in the MWH approximation and K' in the BG approximation. It is unlikely that Pt has a charge less than +0.1; therefore, an upperlimit to K = 2.0 and K' = 2.2 can be assigned. The lower limits are more difficult to ascertain. If Pauling's electroneutrality principle[24] is qualitatively correct, the Pt charge should be lowered to at least +1.0. This would then place a lower limit on K and K' at 1.5 and 1.6 respectively.

Figure 2 is a partial plot of the energy level diagram as a function of K.‡

Several features are apparent from this diagram. First, there is a strong K-dependence of the energy of the first non-occupied antibonding orbital (b_{1g}^*). The observed $^1b_{2g}^* \rightarrow {}^1b_{1g}^*$ transition energy, however, falls nicely within the above limits of K at a value of about 1.7 to 1.8.

Secondly, there is no 5d orbital inversion over large ranges of K. Specifically, the a_{1g}^* ($5d_{z^2}$) orbital is lower in energy than the

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‡ The dependence on K' is the same as on K except that energies are slightly shifted down (0.5 ev.) for K' = K.

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e_g^* ($5d_\pi$) orbital at all values of K from 1.4 to 2.8. The Ballhausen and Gray calculation gave the orbital energies $e_g^* > a_{1g}^*$.

Finally, we find the first orbital above the b_{1g}^* ($5d_\sigma$) is an a_{2u}^* ($6p_\pi$) orbital. Ballhausen and Gray, however, proposed the a_{1g}^* (6s) orbital. Intuitively, one would expect the metal $6p_\pi$ orbital to be very nearly non-bonding; consequently, the energy of the a_{2u}^* would be very near that of the atomic 6p orbitals. This is in fact clearly the case. The atomic 6s orbital mixes significantly with the ligand σ orbitals resulting in a much higher energy for the molecular a_{1g}^* orbital.

Since the metal 5d orbitals transform under different irreducible representations in D_{4h} symmetry, one could choose a different value of K for each orbital ($5d_\sigma$, $5d_\pi$, $5d_\delta$). This choice should, however, be governed by the π character of the overlap integrals (Pt-Cl)[25] such that the π interactions have larger K's than the σ interactions. This would result in a lowering of the a_{1g}^* energy relative to the e_g^*. However, no inversion of the e_g^* and b_{2g}^* levels would occur. Figure 3 is a partial one-electron molecular orbital diagram in which $K(\sigma) = 1.75$ and $K(\pi) = 2.00$.

Variation of the Metal Shielding Parameters, α_i.

The Pt 5d, 6s and 6p shielding parameters were varied over the ranges listed in Table VIII. A plot of the total electronic energy of $PtCl_4^{2-}$ revealed an energy minimum extremely near the values of

the shielding parameter determined by our method. Furthermore, this energy minimum corresponded to a reduced overlap population (bond order) maximum between Pt and Cl (Fig. 4).

The dependence of the 5d orbital splittings are extremely sensitive to the radial part of the Pt wavefunctions as shown in Fig. 5. Note also that there is no inversion of any of the occupied 5d-type molecular orbitals and that the first non-occupied antibonding molecular orbital (b_{1g}^*) is especially sensitive to the choice of the values of the α_i's.

Variation of the Pt Diagonal Matrix Elements, H_{ii}'s.

The hardest parameters to estimate are the diagonal matrix elements, H_{ii}. In most first row transition metals the free ion contribution, A_{ii} (Eq. 4) to H_{ii} can be easily calculated from "Moore's Tables"[19] for integral charge distributions. Analytic calculation of the multi-center integrals, M_{ii},(Eq. 4) is a formidable problem requiring an unjustifiable amount of computer time. In lieu of any approximations, the H_{ii}'s of the Pt were systematically varied in an attempt to arrive at a simple empirical method of estimating these terms.

Figure 6 is a partial plot of the one-electron molecular orbitals versus assumed H_{ii}'s for Pt^0. If one were to assume that the Pt^{1+} H_{ii}'s were 10 ev. higher than the corresponding matrix elements for Pt^0, then region I would be where the calculation is self-consistent in charge. The molecular orbital diagram is erroneous at this point for the following reasons:

(1) The $^1b_{2g}^* \rightarrow {}^1b_{1g}^*$ transition energy is much too large.

(2) The a_{1u}^* molecular orbital has a lower energy than the b_{2g}^* orbital.

(3) The ligand b_{1g} molecular orbital is much too high in energy.

(4) The energy difference between the ~~b_{2g}^*~~ a_{1g}^* and e_g^* molecular orbitals is too large.

The above conclusions are substantiated by spectral studies.

A more reasonable interpretation of the spectra can be made in region II (Fig. 6). This is, in fact, the region where we feel the H_{ii}'s would be most nearly correct based on our earlier arguments. In region II the Pt^{1+} H_{ii}'s are only 1 to 2 ev. above the Pt^0 H_{ii}'s. This is consistent with the behavior of carbon and boron as pointed out by Lipscomb[26] and with that of copper as shown by Ros.[17]

Furthermore, the energy minimum in Fig. 4 in effect says that the final H_{ii}'s, obtained after charge refinement, are the "best" values for the wavefunctions used.

Spectra.

We wish to emphasize that it is not the purpose of this section to make accurate computations of the positions of absorption bands in $PtCl_4^{2-}$, as we feel that the present status of semiempirical molecular orbital theory does not lend itself well to this end. One can, however, obtain qualitative information from MO theory that may be of some assistance in spectral assignments. The calculated transition energies

are listed in Table IX. These are calculated from Fig. 3. The eigenvalues and eigenvectors for K = 1.80 are listed in Tables X and XIV respectively.

The relative energies of the e_g^* vs. a_{1g}^* and a_{1g}^* vs. a_{2u} are opposite to those proposed by Ballhausen and Gray.[1] This is presumably a result of their method of obtaining hybrid orbitals[27] via the minimization of the VSIP/$S_{ij}(\theta)$ of atomic orbital. The variational principle is not rigidly satisfied in their method for orbitals that mix in the same irreducible representation. As a result, the energy of the a_{1g}^* MO is higher in their MO diagram than in ours. All wavefunctions in our calculation at least rigidly satisfy the variational principle for all atomic orbitals in the basis set.

Nature of the Pt-Cl Bond.

The Pt-Cl bond is, classically, a two-centered electron pair bond. It is, however, more appropriate to discuss the ionicity or covalency of the Pt-Cl bond in the framework of MO theory. The amount of covalency or bond order, as defined by Mulliken,[9] can be calculated from the overlap integrals and the eigenvectors of the molecular orbitals. Table XI lists the various contributions to the Pt-Cl bond covalency.

Several things are apparent from Table XI:

(1) The main contributions to the Pt-Cl bond order are from the interaction of the Pt 6s, $6p_\sigma$ and $5d_\sigma$ to Cl $3p_\sigma$ atomic orbitals respectively.

(2) The interactions of $6p_\sigma$, $6p_\sigma$-$5d_\sigma$ to Cl $3s_\sigma$ are approximately equal but only contribute 1/3 that of (1) to the covalency.

(3) The interactions of Pt $5d_\pi$ and Pt $6p_\pi$ to Cl $3p_\pi$ atomic orbitals are slightly antibonding and constitute at best a weak π field.

By summing all the above contributions to the covalency, one obtains a total Pt-Cl bond order. This is 0.403 and is almost entirely σ in character. It should be emphasized, however, that the number 0.403 represents the covalency of the Pt-Cl bond. One minus this covalency is, then, the ionicity.

The covalency of the Pt-Cl bond in $PtCl_4^{2-}$ has been measured by nuclear quadrupole resonance (NQR).[28] Marrom, McNiff, and Ragle[29] found a covalency of 0.39 and a Pt charge of +0.44. We calculated* at a Pt charge of +0.439.

The close agreement between MO results and NQR results suggests that a MO treatment of NQR would be far more useful since it would tie in with the general picture of the electronic structure of complexes. Such a theory has been derived and will be presented in a later section of this thesis.[30]

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* Both the Pt charge and Pt-Cl covalency were calculated from the parameter listed in Tables II and V with a K = 1.8.

Table XII gives the occupation of the atomic orbital after final refinement. From the occupation of the p orbitals of the Cl, we can predict a NQR asymmetry parameter of about 0.025 for K_2PtCl_4. (To be discussed later in detail.)

The complete bond order matrix is given in Table XV calculated from the Mulliken population analysis given in Table XVI. The MO charge matrix is given in Table XVII.

TABLE I

Ratio of STO:SCF Overlap Integrals

ϕ_i	Cl 3s	3p	Pt 5d	6s
Cl 3s	"cis" 0.99	"cis" 0.97	0.98	0.96
Cl 3p		"cis" 0.98	1.00	1.01

TABLE II

Orbital Shielding Parameters, α_i

ϕ_i	Cl 3s	Cl 3p	Pt 5d	Pt 6s	Pt 6p*
α_i	2.245	1.850	2.150	2.600	2.450

* Pt 6p - approximated as described in the text.

TABLE III

$PtCl_4^{2-}$ Overlap Integral Matrix: Atomic Orbitals Correspond to the Order Listed in Table XIII

OVERLAP MATRIX $PtCl_4^{2-}$

1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1673	-0.	-0.2659	-0.	0.1673	-0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1236	-0.	0.	0.	0.1236
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.2785	-0.	-0.3583	-0.	-0.2785	0.
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.1236	-0.	-0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.0461	0.	0.0778	0.	-0.0461	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.0673	-0.	0.	-0.	-0.0673
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.0798	-0.	-0.1347	-0.	0.0798	-0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	-0.	0.	-0.	-0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	0.0673	0.	0.
10	0.1673	0.	0.2785	0.	-0.0461	0.	0.0798	0.	0.	1.0000	0.	0.	0.	0.0001	-0.
11	-0.	0.1236	-0.	0.	0.	0.0673	-0.	0.	0.	0.	1.0000	0.	0.	0.	0.0004
12	-0.2659	-0.	-0.3583	-0.	0.0778	-0.	-0.1347	-0.	-0.	0.	0.	1.0000	0.	-0.0010	0.
13	-0.	0.	-0.	0.1236	0.	0.	-0.	0.	0.0673	0.	0.	0.	1.0000	-0.	-0.
14	0.1673	0.	-0.2785	-0.	-0.0461	-0.	0.0798	-0.	0.	0.0001	0.	-0.0010	-0.	1.0000	0.
15	-0.	0.1236	0.	-0.	0.	-0.0673	-0.	-0.	0.	-0.	0.0004	0.	-0.	0.	1.0000
16	0.2659	0.	-0.3583	-0.	-0.0778	-0.	0.1347	-0.	0.	0.0010	0.	-0.0039	-0.	0.	0.
17	0.	-0.	-0.	0.1236	-0.	0.	0.	0.	-0.0673	0.	-0.	-0.	0.0004	0.	0.
18	0.1673	0.	0.	0.2785	-0.0461	0.	-0.0798	0.	0.	0.0073	0.	-0.0182	0.0182	0.0073	0.
19	-0.	0.1236	-0.	-0.	0.	0.	0.	0.0673	-0.	-0.	0.0098	-0.	-0.	-0.	0.0098
20	-0.	-0.	0.1236	0.	-0.	-0.	-0.	-0.	0.0673	0.0182	-0.	-0.0269	0.0367	-0.0182	-0.
21	-0.2659	-0.	0.	-0.3583	0.0778	-0.	0.1347	-0.	0.	-0.0182	-0.	0.0367	-0.0269	-0.0182	0.
22	0.1673	0.	0.	-0.2785	-0.0461	0.	-0.0798	-0.	-0.	0.0073	0.	-0.0182	-0.0182	0.0073	0.
23	-0.	0.1236	0.	0.	0.	0.	0.	-0.0673	-0.	-0.	0.0098	0.	-0.	-0.	0.0098
24	-0.	0.	0.1236	0.	0.	0.	0.	-0.	-0.0673	0.0182	0.	-0.0269	-0.0367	-0.0182	0.
25	0.2659	0.	0.	-0.3583	-0.0778	0.	-0.1347	-0.	-0.	0.0182	-0.	-0.0367	-0.0269	0.0182	0.

	16	17	18	19	20	21	22	23	24	25
1	0.2659	0.	0.1673	-0.	-0.	-0.2659	0.1673	-0.	-0.	0.2659
2	0.	-0.	0.	0.1236	-0.	-0.	0.	0.1236	0.	0.
3	-0.3583	-0.	0.	-0.	0.1236	0.	0.	0.	0.1236	0.
4	-0.	0.1236	0.2785	-0.	0.	-0.3583	-0.2785	0.	0.	-0.3583
5	-0.0778	-0.	-0.0461	0.	-0.	0.0778	-0.0461	0.	0.	-0.0778
6	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.
7	0.1347	0.	-0.0798	0.	-0.	0.1347	-0.0798	0.	0.	-0.1347
8	-0.	0.	0.	0.0673	-0.	-0.	-0.	-0.0673	-0.	-0.
9	0.	-0.0673	0.	-0.	0.0673	0.	-0.	-0.	-0.0673	-0.
10	0.0010	0.	0.0073	-0.	0.0182	-0.0182	0.0073	-0.	0.0182	0.0182
11	0.	-0.	0.	0.0098	-0.	-0.	0.	0.0098	0.	-0.
12	-0.0039	-0.	-0.0182	-0.	-0.0269	0.0367	-0.0182	0.	-0.0269	-0.0367
13	-0.	0.0004	0.0182	-0.	0.0367	-0.0269	-0.0182	-0.	-0.0367	-0.0269
14	0.	0.	0.0073	-0.	-0.0182	-0.0182	0.0073	-0.	-0.0182	0.0182
15	0.	0.	0.	0.0098	-0.	0.	0.	0.0098	0.	0.
16	1.0000	0.	0.0182	-0.	-0.0269	-0.0367	0.0182	0.	-0.0269	0.0367
17	0.	1.0000	0.0182	0.	-0.0367	-0.0269	-0.0182	0.	0.0367	-0.0269
18	0.0182	0.0182	1.0000	0.	0.	0.	0.0001	-0.	-0.	0.0010
19	-0.	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.
20	-0.0269	-0.0367	0.	0.	1.0000	0.	0.	0.	0.0004	0.
21	-0.0367	-0.0269	0.	0.	0.	1.0000	-0.0010	0.	0.	-0.0039
22	0.0182	-0.0182	0.0001	0.	0.	-0.0010	1.0000	0.	0.	0.
23	0.	0.	-0.	0.0004	0.	0.	0.	1.0000	0.	0.
24	-0.0269	0.0367	-0.	0.	0.0004	0.	0.	0.	1.0000	0.
25	0.0367	-0.0269	0.0010	0.	0.	-0.0039	0.	0.	0.	1.0000

TABLE IV

Cu-Cl Overlap‡ Integral Ratios Over

Charge and Configuration

Configuration		$Cu^{0}-Cl^{0.50-}/Cu^{1+}-Cl^{0.75-}$	$Cu^{0}-Cl^{0.50-}/Cu^{0.44}-Cl^{0.61-}$	$\lvert\Delta\rvert$*
	$\phi_i-\phi_j$			
$3d^{9}4s^{2}$	$4s-3s$	1.16	1.09	9%
	$4s-3p_{\sigma}$	0.96	0.98	2%
$3d^{9}4p^{2}$	$4p-3s$	1.07	1.04	4%
	$4p-3p_{\sigma}$	0.83	0.91	9%
	$4p_{\pi}-3p_{\pi}$	0.93	0.96	4%

---

* $|\Delta| = |(R_2 - 1) \times 100|$

‡ All values calculated from Ref. 17.

TABLE V

Pt States and Processes Averaged* to Obtain A_{ii} for $Pt^0 \rightarrow Pt^{1+} + e^-$

i	Initial State		Final State + Orbital			Pt^0 $\langle A_{ii} \rangle$
6s	$5d^96s^1$	→	$5d^9$	+	6s	
	$5d^86s^2$	→	$5d^86s$	+	6s	-9.80
	$5d^86s6p$	→	$5d^86p$	+	6s	ev
6p	$5d^86s6p$	→	$5d^86s$	+	6p	-5.35
	$5d^96p$	→	$5d^9$	+	6p	ev
5d	$5d^{10}$	→	$5d^9$	+	5d	
	$5d^96s$	→	$5d^86s$	+	5d	-10.61
	$5d^86s^2$	→	$5d^76s^2$	+	5d	ev
	$5d^96p$	→	$5d^860$	+	5d	

* All states were averaged over multiplicities and were obtained from Ref. 19.

TABLE VI

Pt H_{ii}'s (in ev) as a Function of Charge

Pt Charge ≡ q	0	0.5	1.0	1.5	2.0
Cl Charge	-0.500	-0.625	-0.750	-0.875	-1.0
Point Charge Approximation for M_{ii}	12.3	15.4	18.5	21.7	24.7
A_{ii}					
5d	-10.61	-15.61	-20.61	-25.61	-30.61
6p	-5.35	-10.35	-15.35	-20.35	-25.35
Δ_{ii}*					
5d	-12.3	-10.4	-8.5	-6.7	-4.7
6p	-15.3	-13.4	-11.5	-9.7	-7.7

---

* $\Delta_{ii} = A_{ii}\ (Pt^{o}) - A_{ii}\ (Pt^{q}) - M_{ii}$

TABLE VII

Molecular Properties vs. K and K' (Eqs. 6 and 7)

K	Pt Charge	Pt-Cl Bond Order	$^1b_{2g}^* \rightarrow {}^1b_{1g}^*$ Tran. Energy (ev)
1.6	0.813	0.293	2.70
1.8	0.439	0.403	3.74
2.0	0.138	0.476	4.80
2.2	-0.116	0.529	5.90

K'	Pt Charge	Pt-Cl Bond Order	$^1b_{2g}^* \rightarrow {}^1b_{1g}^*$ Tran. Energy (ev)
1.5	1.23	0.057	2.14
1.7	0.849	0.220	3.11
2.0	0.397	0.371	4.62
2.2	0.157	0.436	5.68

TABLE VIII

Pt Shielding Parameter for Points in Fig. 5

α_i's	L2	L1	0	S1	S2	S3
6s	3.60	3.10	2.60	2.20	1.95	1.70
6p	3.45	2.95	2.45	2.05	1.80	1.55
5d	4.15	3.65	3.15	2.75	2.50	2.25

TABLE IX

Calculated Transition Energies from Fig. 3

Transition	Energy (ev.)
$^1b_{1g}^* \rightarrow {}^1b_{2g}^*$	2.5
$^1e_g^* \rightarrow {}^1b_{1g}^*$	2.7
$^1a_{1g}^* \rightarrow b_{1g}^*$	3.6
$^1b_{2g}^* \rightarrow {}^1a_{2u}^*$	5.0
$^1e_g^* \rightarrow {}^1a_{2u}^*$	5.2
$^1a_{1g}^* \rightarrow {}^1a_{2u}^*$	6.1

TABLE X

$PtCl_4^{2-}$ One-Electron MO Eigenvalues

MO	Energy(ev.)	Occupation
1	8.51	0
2	8.51	0
3	4.24	0
4	-4.70	0
5	-6.76	0
6	-10.49	2
7	-10.68	2
8	-10.68	2
9	-10.98	2
10	-13.49	2
11	-13.83	2
12	-13.83	2
13	-14.18	2
14	-14.58	2
15	-14.58	2
16	-14.71	2
17	-14.82	2
18	-15.09	2
19	-15.09	2
20	-15.41	2
21	-16.10	2
22	-23.29	2
23	-23.50	2
24	-23.50	2
25	-24.04	2

Sum = -625.73

TABLE XI

Pt-Cl Bond Order Contributions

Pt — Cl	3s	3p(σ)	$3p_y$	$3p_z$
6s	0.023	0.112	---	---
6p(σ)	0.040	0.132	---	---
$6p_y$	---	---	-0.005	---
$6p_z$	---	---	---	0.022
$5d_{x^2y^2}$	0.011	0.094	---	---
$5d_{z^2}$	0.002	0.008	---	---
$5d_{xz}$	---	---	---	-0.018
$5d_{xy}$	---	---	-0.017	---

TABLE XII

Atomic Orbital Occupation

ϕ_i	Pt	Pπ	Pσ					
	6s	$6p_z$	$6p_x$	$6p_y$	$5d_{z^2}$	5dπ	$5d_{xy}$	$5d_{x^2-y^2}$
Number of electrons	0.581	0.061	0.215	0.215	1.893	3.97	1.99	0.50

	Cl_1			
	3s	3p(σ)	$3p_x$	$3p_z$
Number of electrons	1.94	1.68	2.00	1.98

TABLE XIII

$PtCl_4^{2-}$ MO Input Parameters: N = principle quantum number; L = angular momentun quantum number: The orbital correspondence is:

M	Sigma	Orbitals	
0	0	z	p
1	0	x	
1	1	y	
0	0	z^2	d
1	0	xz	
2	0	x^2-y^2	
1	1	yz	
2	1	xy	

TABLE XIII

Orbital	Atom	N	L	M	Sigma	Coordinates Å. X	Y	Z	Orbital Exp.	H_{ii}
1	1	6	0	0	0	0	0	0	2.600	-9.79
2	1	6	1	0	0	0	0	0	2.450	-5.35
3	1	6	1	1	0	0	0	0	2.450	-5.35
4	1	6	1	1	1	0	0	0	2.450	-5.35
5	1	5	2	0	0	0	0	0	3.150	-10.61
6	1	5	2	1	0	0	0	0	3.150	-10.61
7	1	5	2	2	0	0	0	0	3.150	-10.61
8	1	5	2	1	1	0	0	0	3.150	-10.61
9	1	5	2	2	1	0	0	0	3.150	-10.61
10	2	3	0	0	0	2.33	0	0	2.245	-24.00
11	2	3	1	0	0	2.33	0	0	1.850	-15.10
12	2	3	1	1	0	2.33	0	0	1.850	-15.10
13	2	3	1	1	1	2.33	0	0	1.850	-15.10
14	3	3	0	0	0	-2.33	0	0	2.245	-24.00
15	3	3	1	0	0	-2.33	0	0	1.850	-15.10
16	3	3	1	1	0	-2.33	0	0	1.850	-15.10
17	3	3	1	1	1	-2.33	0	0	1.850	-15.10
18	4	3	0	0	0	0	2.33	0	2.245	-24.00
19	4	3	1	0	0	0	2.33	0	1.850	-15.10
20	4	3	1	1	0	0	2.33	0	1.850	-15.10
21	4	3	1	1	1	0	2.33	0	1.850	-15.10
22	5	3	0	0	0	0	-2.33	0	2.245	-24.00
23	5	3	1	0	0	0	-2.33	0	1.850	-15.10
24	5	3	1	1	0	0	-2.33	0	1.850	-15.10
25	5	3	1	1	1	0	-2.33	0	1.850	-15.10

$$H_{ij} = 1.80(S_{ij})(H_{ii} + H_{jj})/2.$$

TABLE XIV

$PtCl_4^{2-}$ Eigenvectors for the Eigenvalues Listed in Table X: MO's Across and AO's Down

EIGENVECTORS $PtCl_4^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	-0.0000	-0.0000	1.1991	-0.	-0.0000	0.0000	-0.	-0.	0.2726	0.0000	-0.0000	0.0000	0.	-0.	-0.
2	0.	-0.	-0.	1.0272	-0.	-0.	-0.0000	-0.0000	0.	0.	-0.	0.	0.0000	0.0000	-0.0000
3	1.3167	0.0000	0.0000	0.	0.0000	0.0000	0.	0.	0.0000	0.0000	0.0084	0.0954	-0.	0.	0.
4	0.0000	-1.3167	-0.0000	0.	-0.0000	0.0000	0.	0.	0.0000	-0.0000	0.0954	-0.0084	-0.	0.	0.
5	0.0000	0.0000	-0.3343	0.	-0.0000	0.0000	0.	0.	0.9616	0.0000	0.0000	-0.0000	-0.	0.	0.
6	0.	-0.	-0.	-0.0000	-0.	-0.	0.9499	0.2470	0.	0.	-0.	0.	0.0000	-0.2143	0.0001
7	-0.0000	-0.0000	-0.0000	0.	-0.9629	0.0000	0.	0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	0.	0.
8	0.	-0.	-0.	0.0000	-0.	-0.	-0.2470	0.9499	0.	0.	-0.	0.	0.0000	0.0001	0.2143
9	-0.0000	0.0000	-0.0000	0.	-0.0000	-0.9860	0.	0.	0.0000	0.0000	0.0000	-0.0000	-0.	0.	0.
10	-0.3947	-0.0000	-0.2424	0.	0.1365	-0.0000	0.	0.	-0.0006	0.0000	0.0009	0.0101	-0.	0.	0.
11	0.	-0.	-0.	-0.1689	-0.	-0.	-0.2100	-0.0546	0.	0.	-0.	0.	0.5049	-0.6765	0.0002
12	0.5437	0.0000	0.4186	-0.	-0.3527	0.0000	-0.	-0.	-0.0177	-0.0000	-0.0370	-0.4204	0.	-0.	-0.
13	-0.0000	0.1189	0.0000	-0.	0.0000	0.1633	-0.	-0.	0.0000	-0.5195	-0.5708	0.0502	0.	-0.	-0.
14	0.3947	0.0000	-0.2424	0.	0.1365	0.0000	0.	0.	-0.0006	-0.0000	-0.0009	-0.0101	-0.	0.	0.
15	0.	-0.	-0.	-0.1689	-0.	-0.	0.2100	0.0546	0.	0.	-0.	0.	0.5049	0.6765	-0.0003
16	0.5437	0.0000	-0.4186	0.	0.3527	0.0000	0.	0.	0.0177	-0.0000	-0.0370	-0.4204	-0.	0.	0.
17	-0.0000	0.1189	0.0000	-0.	0.0000	-0.1633	-0.	-0.	0.0000	0.5195	-0.5708	0.0502	0.	-0.	-0.
18	-0.0000	0.3947	-0.2424	-0.	-0.1365	0.0000	-0.	-0.	-0.0006	-0.0000	0.0101	-0.0009	0.	-0.	-0.
19	0.	-0.	-0.	-0.1689	-0.	-0.	0.0546	-0.2100	0.	0.	-0.	0.	-0.5049	0.0002	0.6765
20	-0.1189	-0.0000	-0.0000	0.	-0.0000	0.1633	0.	0.	-0.0000	0.5195	-0.0502	-0.5708	-0.	0.	0.
21	0.0000	-0.5437	0.4186	0.	0.3527	-0.0000	0.	0.	-0.0177	0.0000	-0.4204	0.0370	-0.	0.	0.
22	0.0000	-0.3947	-0.2424	0.	-0.1365	-0.0000	0.	0.	-0.0006	0.0000	-0.0101	0.0009	-0.	0.	0.
23	0.	-0.	-0.	-0.1689	-0.	-0.	-0.0546	0.2100	0.	0.	-0.	0.	-0.5049	-0.0002	-0.6765
24	-0.1189	-0.0000	-0.0000	-0.	-0.0000	-0.1633	-0.	-0.	0.0000	-0.5195	-0.0502	-0.5708	0.	-0.	-0.
25	0.0000	-0.5437	-0.4186	0.	-0.3527	-0.0000	0.	0.	0.0177	0.0000	-0.4204	0.0370	-0.	0.	0.

	16	17	18	19	20	21	22	23	24	25
1	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.2473	-0.0000	0.0000	0.0000	0.1394
2	0.0925	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
3	0.	0.0000	0.0256	-0.1018	0.0000	0.0000	-0.0000	-0.0020	-0.0614	0.0000
4	0.	0.0000	0.1018	0.0256	-0.0000	-0.0000	0.0000	0.0614	-0.0020	0.0000
5	0.	-0.0000	-0.0000	0.0000	0.0000	0.1026	-0.0000	0.0000	-0.0000	-0.0457
6	0.0000	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
7	0.	-0.4279	0.0000	-0.0000	-0.0000	0.0000	0.0996	-0.0000	-0.0000	0.0000
8	0.0000	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
9	0.	-0.0000	0.0000	0.0000	0.2120	-0.0000	-0.0000	-0.0000	0.0000	0.0000
10	0.	0.0333	-0.0178	0.0706	0.0000	0.1202	0.4926	-0.0228	-0.6873	0.4652
11	0.4819	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
12	-0.	0.4108	-0.1224	0.4857	0.0000	0.4007	0.0213	-0.0004	-0.0133	-0.0106
13	-0.	0.0000	0.4051	0.1021	0.4586	-0.0000	0.0000	0.0244	-0.0008	0.0000
14	0.	0.0333	0.0178	-0.0706	0.0000	0.1202	0.4926	0.0228	0.6873	0.4652
15	0.4819	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
16	0.	-0.4108	-0.1224	0.4857	-0.0000	-0.4007	-0.0213	-0.0004	-0.0133	0.0106
17	-0.	0.0000	0.4051	0.1021	-0.4586	-0.0000	0.0000	0.0244	-0.0008	0.0000
18	-0.	-0.0333	-0.0706	-0.0178	0.0000	0.1202	-0.4926	0.6873	-0.0228	0.4652
19	0.4819	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
20	0.	0.0000	0.1021	-0.4051	0.4586	0.0000	-0.0000	-0.0008	-0.0244	0.0000
21	0.	-0.4108	-0.4857	-0.1224	0.0000	0.4007	-0.0213	0.0133	-0.0004	-0.0106
22	0.	-0.0333	0.0706	0.0178	-0.0000	0.1202	-0.4926	-0.6873	0.0228	0.4652
23	0.4819	0.	-0.	-0.	0.	-0.	0.	0.	-0.	0.
24	-0.	0.0000	0.1021	-0.4051	-0.4586	0.0000	-0.0000	-0.0008	-0.0244	0.0000
25	0.	0.4108	-0.4857	-0.1224	0.0000	-0.4007	0.0213	0.0133	-0.0004	0.0106

TABLE XV

Reduced Overlap Population Matrix Atom by Atom

	1	2	3	4	5
1	17.5085	0.4032	0.4032	0.4032	0.4032
2	0.4032	14.8582	-0.0018	-0.0200	-0.0200
3	0.4032	-0.0018	14.8582	-0.0200	-0.0200
4	0.4032	-0.0200	-0.0200	14.8582	-0.0018
5	0.4032	-0.0200	-0.0200	-0.0018	14.8582

TABLE XVI

$PtCl_4^{2-}$ Mulliken Overlap Populations:

AO's Across and Down

$PtCl_4^{2-}$ - MULLIKEN OVERLAP POPULATIONS FOR 40 ELECTRONS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.6196	0.	-0.	0.	0.	0.	-0.	0.	0.	0.0234	-0.	C.1121	0.	0.0234	-0.
2	0.	0.0343	0.	0.	-0.	0.	0.	-0.	0.	0.	0.0220	C.	0.	0.	0.0220
3	-0.	0.	0.0958	-0.	0.	0.	-0.	0.	-0.	0.0396	-0.	C.1321	0.	C.0396	C.
4	0.	0.	-0.	0.0958	0.	0.	-0.	0.	0.	0.	0.	C.	-0.0047	-0.	-0.
5	0.	-0.	0.	0.	3.7492	-0.	-0.	-0.	0.	0.0018	-0.	C.0077	-0.	C.0018	-0.
6	0.	0.	0.	0.	-0.	4.0366	0.	0.	0.	0.	-0.0183	C.	0.	-0.	-0.0183
7	-0.	0.	-0.	-0.	-0.	0.	0.7721	0.	-0.	0.0111	-0.	C.0936	-0.	C.0111	-0.
8	0.	-0.	0.	0.	-0.	0.	0.	4.0366	0.	0.	-0.	C.	0.	-0.	-0.
9	0.	0.	-0.	0.	0.	0.	-0.	0.	4.0687	0.	0.	C.	-0.0172	0.	0.
10	0.0234	0.	0.0396	0.	0.0018	0.	0.0111	0.	0.	3.8115	0.	C.	0.	-0.0000	-0.
11	-0.	0.0220	-0.	0.	-0.	-0.0183	-0.	-0.	0.	0.	3.9674	-C.	0.	0.	-0.0000
12	0.1121	0.	0.1321	0.	0.0077	0.	0.0936	0.	0.	0.	-0.	3.0377	-0.	-0.0001	-0.
13	0.	0.	0.	-0.0047	-0.	0.	-0.	0.	-0.0172	0.	0.	-C.	4.0416	0.	-0.
14	0.0234	0.	0.0396	-0.	0.0018	-0.	0.0111	-0.	0.	-0.0000	0.	-C.0001	0.	3.8115	0.
15	-0.	0.0220	0.	-0.	-0.	-0.0183	-0.	-0.	0.	-0.	-0.0000	-C.	-0.	0.	3.9674
16	0.1121	0.	0.1321	-0.	0.0077	-0.	0.0936	-0.	0.	-0.0001	0.	-C.0015	0.	-0.	0.
17	-0.	-0.	0.	-0.0047	0.	0.	0.	0.	-0.0172	0.	-0.	C.	-0.0000	-0.	0.
18	0.0234	0.	-0.	0.0396	0.0018	0.	0.0111	0.	0.	-0.0004	0.	-C.0014	-0.0014	-0.0004	0.
19	-0.	0.0220	-0.	-0.	-0.	-0.	0.	-0.0183	-0.	-0.	-0.0009	C.	-0.	-0.	-0.0009
20	-0.	-0.	-0.0047	0.	0.	-0.	0.	-0.	-0.0172	-0.0014	-0.	-C.0035	-0.0048	-C.0014	-0.
21	0.1121	0.	-0.	0.1321	0.0077	0.	0.0936	0.	0.	-0.0014	0.	-C.0012	-0.0035	-0.0014	-0.
22	0.0234	0.	-0.	0.0396	0.0018	0.	0.0111	-0.	-0.	-0.0004	0.	-C.0014	-0.0014	-0.0004	0.
23	-0.	0.0220	0.	0.	-0.	-0.	0.	-0.0183	-0.	-0.	-0.0009	-C.	-0.	-0.	-0.0009
24	0.	0.	-0.0047	0.	-0.	0.	-0.	-0.	-0.0172	-0.0014	0.	-C.0035	-0.0048	-C.0014	0.
25	0.1121	0.	0.	0.1321	0.0077	0.	0.0936	-0.	-0.	-0.0014	-0.	-C.0012	-0.0035	-0.0014	0.

	16	17	18	19	20	21	22	23	24	25
1	0.1121	-0.	0.0234	-0.	-0.	0.1121	0.0234	-0.	0.	0.1121
2	0.	-0.	0.	0.0220	-0.	0.	0.	0.0220	0.	0.
3	0.1321	0.	-0.	-0.	-0.0047	-0.	-0.	0.	-0.0047	0.
4	-0.	-0.0047	0.0396	-0.	0.	0.1321	0.0396	0.	0.	0.1321
5	0.0077	0.	0.0018	-0.	0.	0.0077	0.0018	-0.	-0.	0.0077
6	-0.	0.	0.	-0.	-0.	0.	0.	-0.	0.	0.
7	0.0936	0.	0.0111	0.	0.	0.0936	0.0111	0.	-0.	0.0936
8	-0.	0.	0.	-0.0183	-0.	0.	-0.	-0.0183	-0.	-0.
9	0.	-0.0172	0.	-0.	-0.0172	0.	-0.	-0.	-0.0172	-0.
10	-0.0001	0.	-0.0004	-0.	-0.0014	-0.0014	-0.0004	-0.	-0.0014	-0.0014
11	0.	-0.	0.	-0.0009	-0.	0.	0.	-0.0009	0.	-0.
12	-0.0015	0.	-0.0014	0.	-0.0035	-0.0012	-0.0014	-0.	-0.0035	-0.0012
13	0.	-0.0000	-0.0014	-0.	-0.0048	-0.0035	-0.0014	-0.	-0.0048	-0.0035
14	-0.	-0.	-0.0004	-0.	-0.0014	-0.0014	-0.0004	-0.	-0.0014	-0.0014
15	0.	0.	0.	-0.0009	-0.	-0.	0.	-0.0009	0.	0.
16	3.0377	-0.	-0.0014	-0.	-0.0035	-0.0012	-0.0014	0.	-0.0035	-0.0012
17	-0.	4.0416	-0.0014	0.	-0.0048	-0.0035	-0.0014	0.	-0.0048	-0.0035
18	-0.0014	-0.0014	3.8115	0.	-0.	0.	-0.0000	-0.	0.	-0.0001
19	-0.	0.	0.	3.9674	0.	-0.	0.	-0.0000	0.	0.
20	-0.0035	-0.0048	-0.	0.	4.0416	0.	0.	0.	-0.0000	0.
21	-0.0012	-0.0035	0.	-0.	0.	3.0377	-0.0001	-0.	0.	-0.0015
22	-0.0014	-0.0014	-0.0000	0.	0.	-0.0001	3.8115	0.	0.	-0.
23	0.	0.	-0.	-0.0000	0.	-0.	0.	3.9674	0.	0.
24	-0.0035	-0.0048	0.	0.	-0.0000	0.	0.	0.	4.0416	0.
25	-0.0012	-0.0035	-0.0001	0.	0.	-0.0015	-0.	0.	0.	3.0377

TABLE XVII

$PtCl_4^{2-}$ MO Charge Matrix: MO's Across and AO's Down

$PtCl_4^{2-}$ - CHARGE MATRIX FOR MO-S WITH TWO ELECTRONS IN EACH

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.0000	1.4193	-0.	0.0000	0.0000	-0.	-0.	0.1586	0.0000	-0.0000	0.0000	-0.	-0.	-0.
2	0.	0.	0.	1.9388	0.	0.	-0.0000	-0.0000	0.	0.	0.	0.	-0.0000	0.0000	0.0000
3	1.7851	0.0000	0.0000	0.	0.0000	-0.0000	0.	0.	0.0000	0.0000	0.0004	0.0498	0.	0.	0.
4	0.0000	1.7851	0.0000	-0.	0.0000	0.0000	-0.	-0.	0.0000	0.0000	0.0498	0.0004	-0.	-0.	-0.
5	0.0000	0.0000	0.1066	-0.	0.0000	0.0000	-0.	-0.	1.8390	0.0000	0.0000	0.0000	-0.	-0.	-0.
6	0.	0.	0.	0.0000	0.	0.	1.7507	0.1183	0.	0.	0.	0.	0.0000	0.1309	0.0000
7	0.0000	0.0000	-0.0000	-0.	1.4045	0.0000	-0.	-0.	0.0000	0.0000	0.0000	0.0000	-0.	-0.	-0.
8	-0.	-0.	-0.	0.0000	-0.	-0.	0.1183	1.7507	-0.	-0.	-0.	-0.	0.0000	0.0000	0.1309
9	0.0000	0.0000	0.0000	-0.	0.0000	1.8578	-0.	-0.	0.0000	0.0000	0.0000	0.0000	-0.	-0.	-0.
10	0.0251	0.0000	0.0221	0.	0.0123	-0.0000	0.	0.	-0.0000	0.0000	0.0000	0.0003	0.	0.	0.
11	-0.	-0.	-0.	0.0153	-0.	-0.	0.0613	0.0041	-0.	-0.	-0.	-0.	0.5000	0.9345	0.0000
12	0.0824	0.0000	0.0964	0.	0.1365	0.0000	0.	0.	0.0006	0.0000	0.0027	0.3549	0.	0.	0.
13	-0.0000	-0.0001	0.0000	0.	0.0000	0.0356	0.	0.	0.0000	0.5000	0.6122	0.0047	0.	0.	0.
14	0.0251	0.0000	0.0221	0.	0.0123	0.0000	0.	0.	-0.0000	0.0000	0.0000	0.0003	0.	0.	0.
15	0.	0.	0.	0.0153	0.	0.	0.0613	0.0041	0.	0.	0.	0.	0.5000	0.9346	0.0000
16	0.0824	0.0000	0.0964	0.	0.1365	0.0000	0.	0.	0.0006	0.0000	0.0027	0.3549	0.	0.	0.
17	-0.0000	-0.0001	0.0000	0.	0.0000	0.0356	0.	0.	0.0000	0.5000	0.6122	0.0047	0.	0.	0.
18	0.0000	0.0251	0.0221	-0.	0.0123	0.0000	-0.	-0.	-0.0000	0.0000	0.0003	0.0000	-0.	-0.	-0.
19	0.	0.	0.	0.0153	0.	0.	0.0041	0.0613	0.	0.	0.	0.	0.5000	0.0000	0.9345
20	-0.0001	-0.0000	0.0000	0.	0.0000	0.0356	0.	0.	0.0000	0.5000	0.0047	0.6122	0.	0.	0.
21	0.0000	0.0824	0.0964	-0.	0.1365	0.0000	-0.	-0.	0.0006	0.0000	0.3549	0.0027	-0.	-0.	-0.
22	0.0000	0.0251	0.0221	0.	0.0123	0.0000	0.	0.	-0.0000	0.0000	0.0003	0.0000	0.	0.	0.
23	0.	0.	0.	0.0153	0.	0.	0.0041	0.0613	0.	0.	0.	0.	0.5000	0.0000	0.9345
24	-0.0001	-0.0000	0.0000	-0.	0.0000	0.0356	-0.	-0.	0.0000	0.5000	0.0047	0.6122	-0.	-0.	-0.
25	0.0000	0.0824	0.0964	0.	0.1365	0.0000	0.	0.	0.0006	0.0000	0.3549	0.0027	0.	0.	0.

	16	17	18	19	20	21	22	23	24	25
1	-0.	0.0000	0.0000	0.0000	0.0000	-0.2933	0.0000	0.0000	0.0000	0.1288
2	0.0612	0.	0.	0.	0.	0.	0.	0.	0.	0.
3	0.	0.0000	0.0066	0.1039	-0.0000	0.0000	0.0000	0.0001	0.0541	0.0000
4	-0.	0.0000	0.1039	0.0066	0.0000	0.0000	0.0000	0.0541	0.0001	-0.0000
5	-0.	0.0000	0.0000	0.0000	0.0000	0.0421	-0.0000	0.0000	0.0000	0.0123
6	0.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	-0.	0.5466	0.0000	0.0000	0.0000	0.0000	0.0489	0.0000	0.0000	0.0000
8	0.0000	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
9	-0.	0.0000	0.0000	-0.0000	0.1422	0.0000	0.0000	0.0000	-0.0000	0.0000
10	0.	0.0009	0.0003	0.0040	0.0000	0.0146	0.4868	0.0011	0.9693	0.4632
11	0.4847	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
12	0.	0.3625	0.0335	0.5267	0.0000	0.4015	0.0010	-0.0000	-0.0003	0.0015
13	0.	0.0000	0.3577	0.0227	0.4644	0.0000	0.0000	0.0027	0.0000	0.0000
14	0.	0.0009	0.0003	0.0040	0.0000	0.0146	0.4868	0.0011	0.9693	0.4632
15	0.4847	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.	0.3625	0.0335	0.5267	0.0000	0.4015	0.0010	-0.0000	-0.0003	0.0015
17	0.	0.0000	0.3577	0.0227	0.4644	0.0000	0.0000	0.0027	0.0000	0.0000
18	-0.	0.0009	0.0040	0.0003	0.0000	0.0146	0.4868	0.9693	0.0011	0.4632
19	0.4847	0.	0.	0.	0.	0.	0.	0.	0.	0.
20	0.	0.0000	0.0227	0.3577	0.4644	0.0000	0.0000	0.0000	0.0027	0.0000
21	-0.	0.3625	0.5267	0.0335	0.0000	0.4015	0.0010	-0.0003	-0.0000	0.0015
22	0.	0.0009	0.0040	0.0003	0.0000	0.0146	0.4868	0.9693	0.0011	0.4632
23	0.4847	0.	0.	0.	0.	0.	0.	0.	0.	0.
24	-0.	0.0000	0.0227	0.3577	0.4644	0.0000	0.0000	0.0000	0.0027	0.0000
25	0.	0.3625	0.5267	0.0335	0.0000	0.4015	0.0010	-0.0003	-0.0000	0.0015

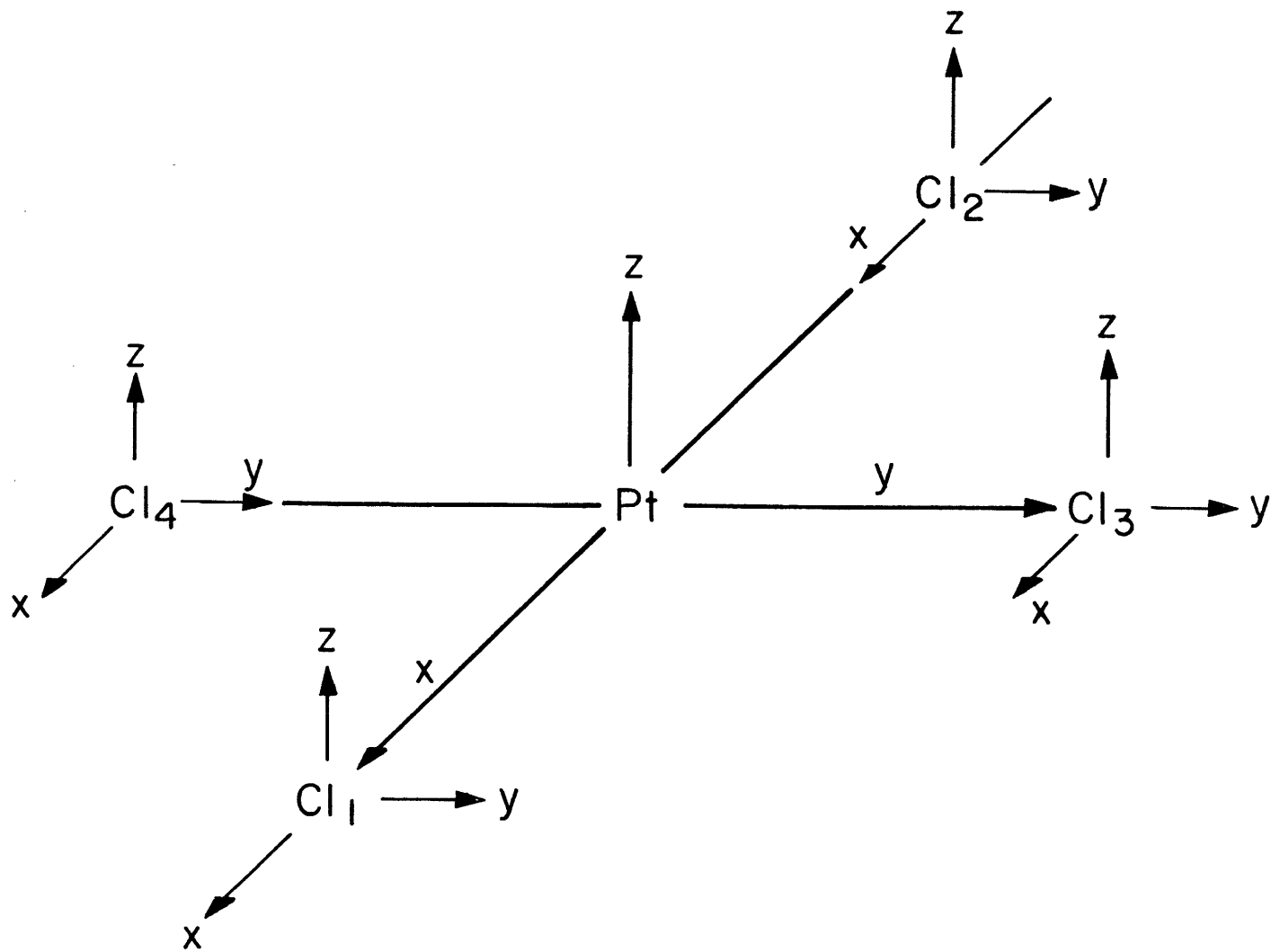
ORBITAL CHARGES

1	0.580732
2	0.061225
3	0.214888
4	0.214888
5	1.893406
6	1.999999
7	0.595485
8	1.999999
9	1.999999
10	1.940471
11	1.984692
12	1.684614
13	2.000054
14	1.940471
15	1.984693
16	1.684615
17	2.000054
18	1.940471
19	1.984693
20	2.000054
21	1.684614
22	1.940471
23	1.984692
24	2.000054
25	1.684614

NET CHARGES

1	0.439379
2	-0.609832
3	-0.609832
4	-0.609832
5	-0.609832

Fig. 1 - $PtCl_4^{2-}$ molecular coordinate system used to calculate the overlap integrals listed in Table III.



D_{4h} Symmetry

Fig. 2 - One-electron MO's vs. the Helmholz factor K.

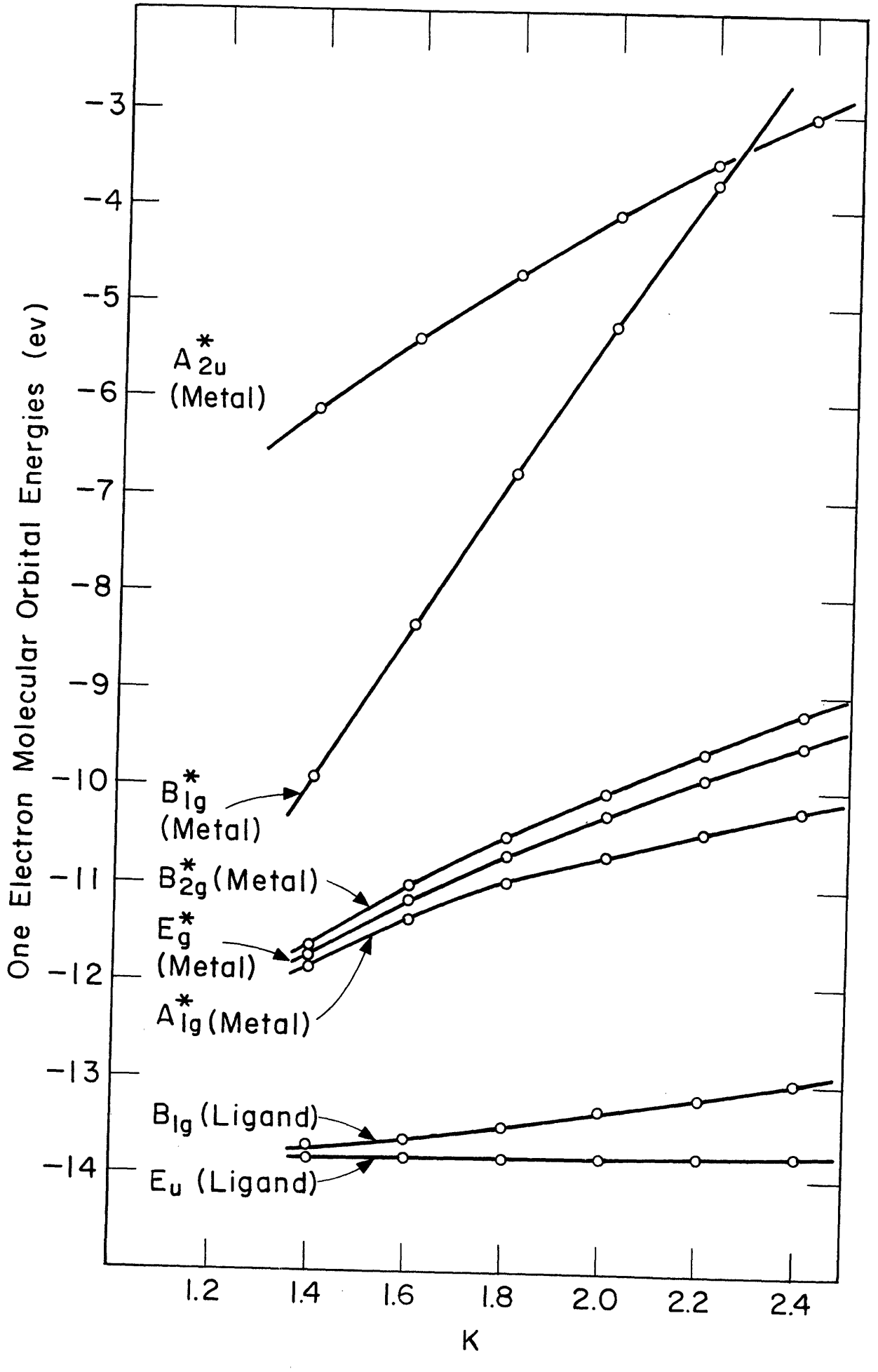

One Electron Molecular Orbital Energies (ev)
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
A^*_{2u} (Metal)
B^*_{1g} (Metal)
B^*_{2g} (Metal)
E^*_g (Metal)
A^*_{1g} (Metal)
B_{1g} (Ligand)
E_u (Ligand)
1.2
1.4
1.6
1.8
2.0
2.2
2.4
K

Fig. 3 - Partial one-electron MO diagram of $PtCl_4^{2-}$:
$K(\sigma) = 1.75$; $K(\pi) = 2.00$.

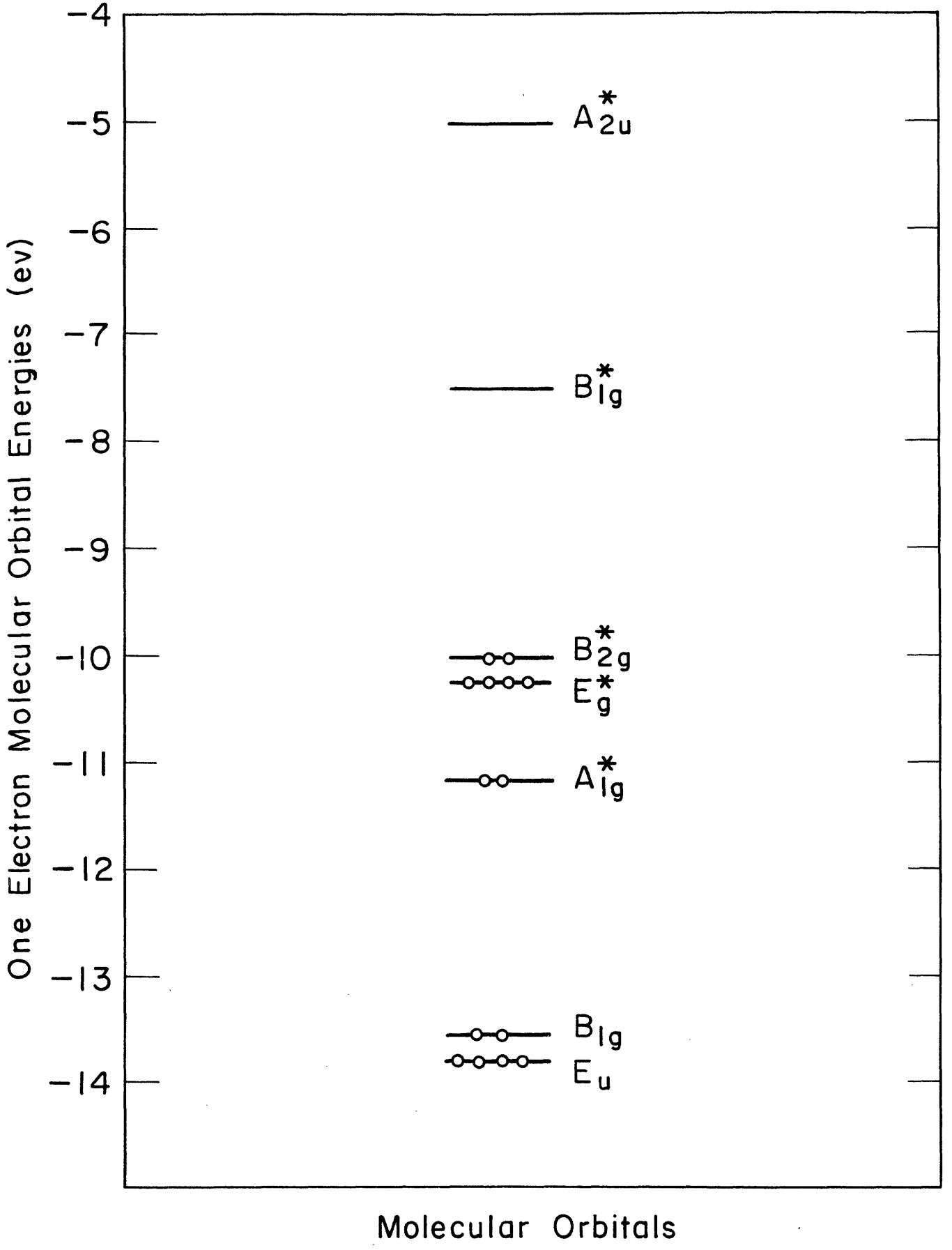

One Electron Molecular Orbital Energies (ev)
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
A^*_{2u}
B^*_{1g}
B^*_{2g}
E^*_g
A^*_{1g}
B_{1g}
E_u
Molecular Orbitals

Fig. 4 - Total electronic energy of $PtCl_4^{2-}$ vs. Pt orbital exponents.

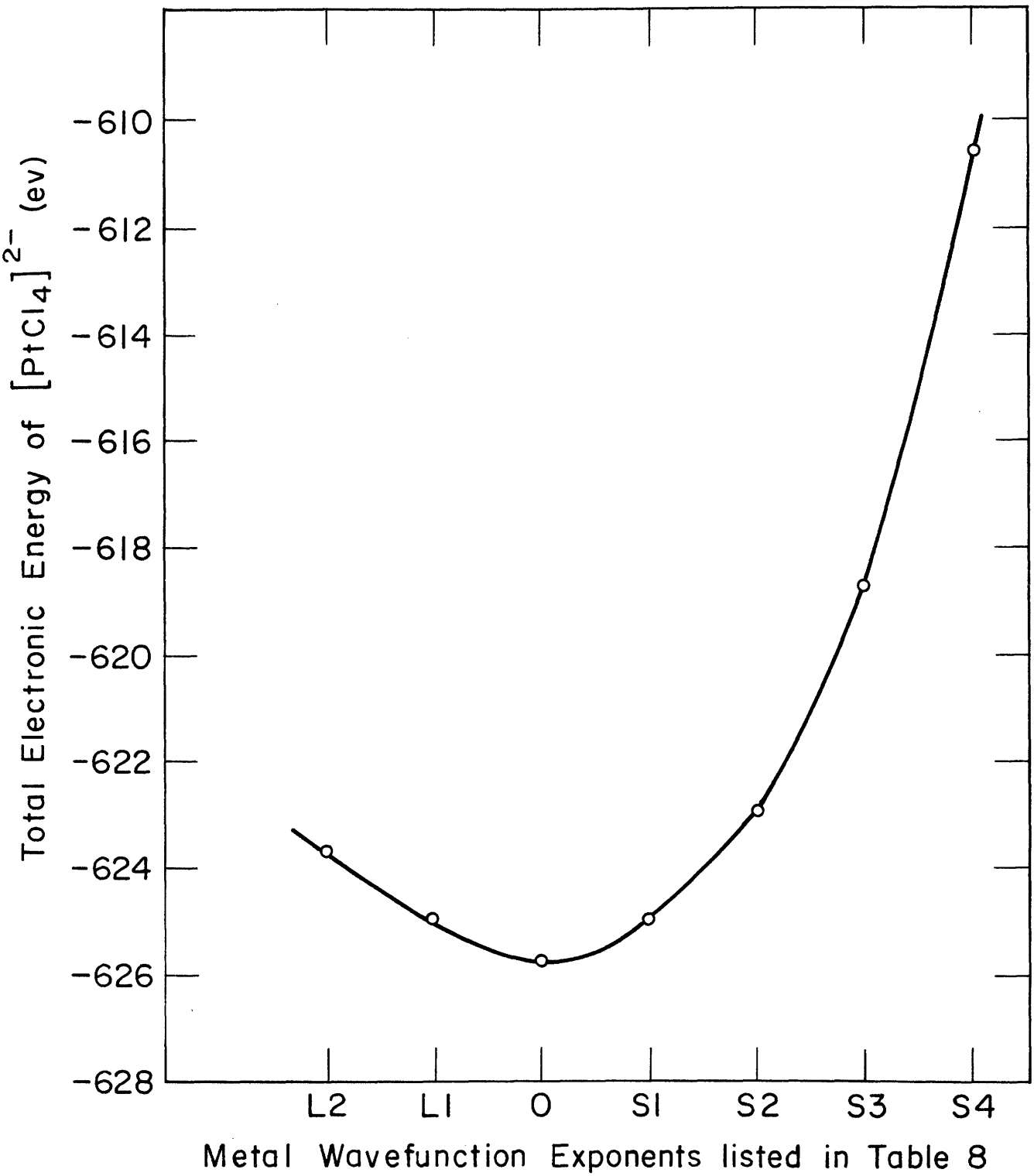

Total Electronic Energy of $[PtCl_4]^{2-}$ (ev)
-610
-612
-614
-616
-618
-620
-622
-624
-626
-628
L2
L1
0
S1
S2
S3
S4
Metal Wavefunction Exponents listed in Table 8

Fig. 5 - One-electron MO's vs. Pt orbital exponents.

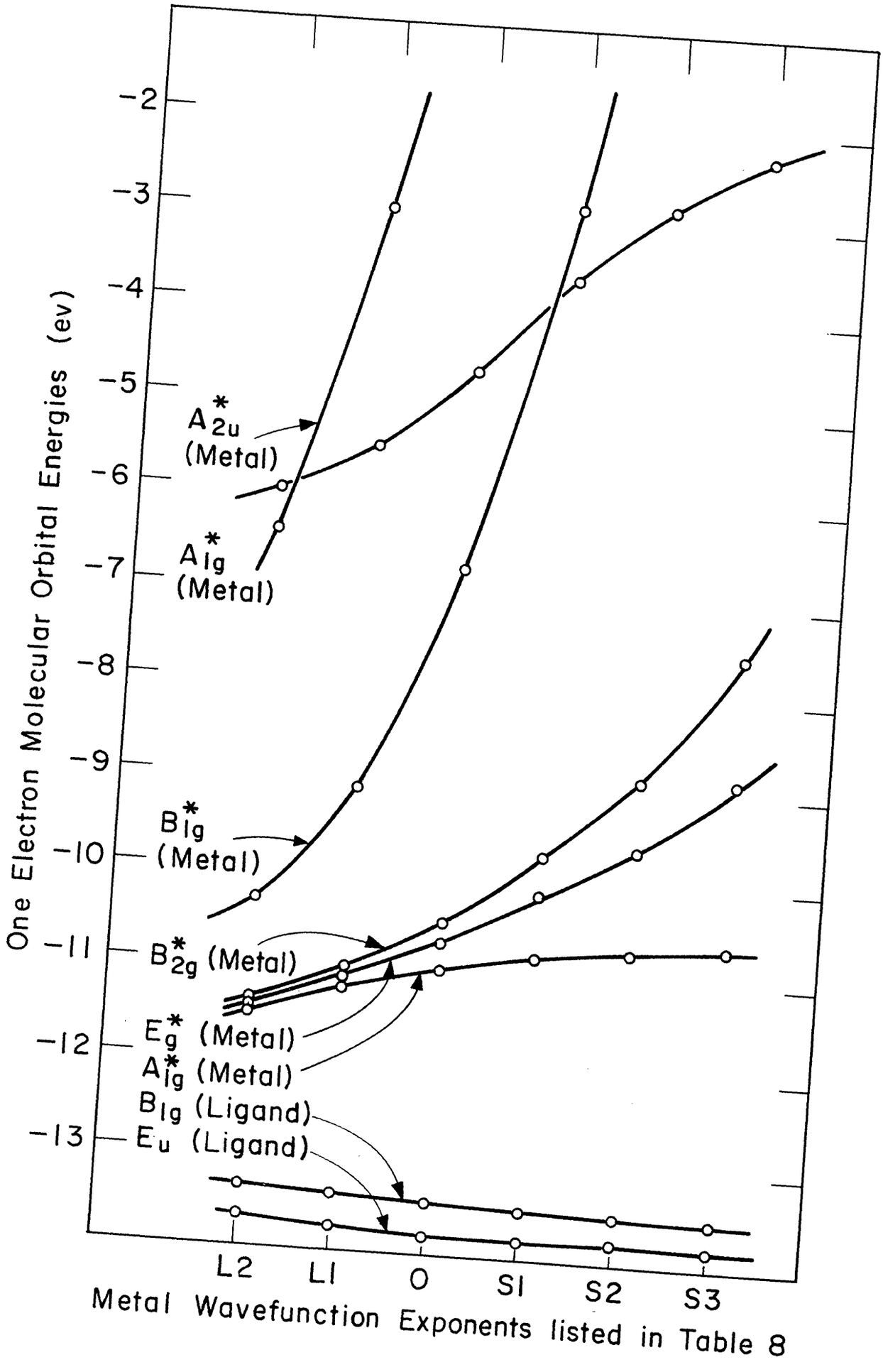
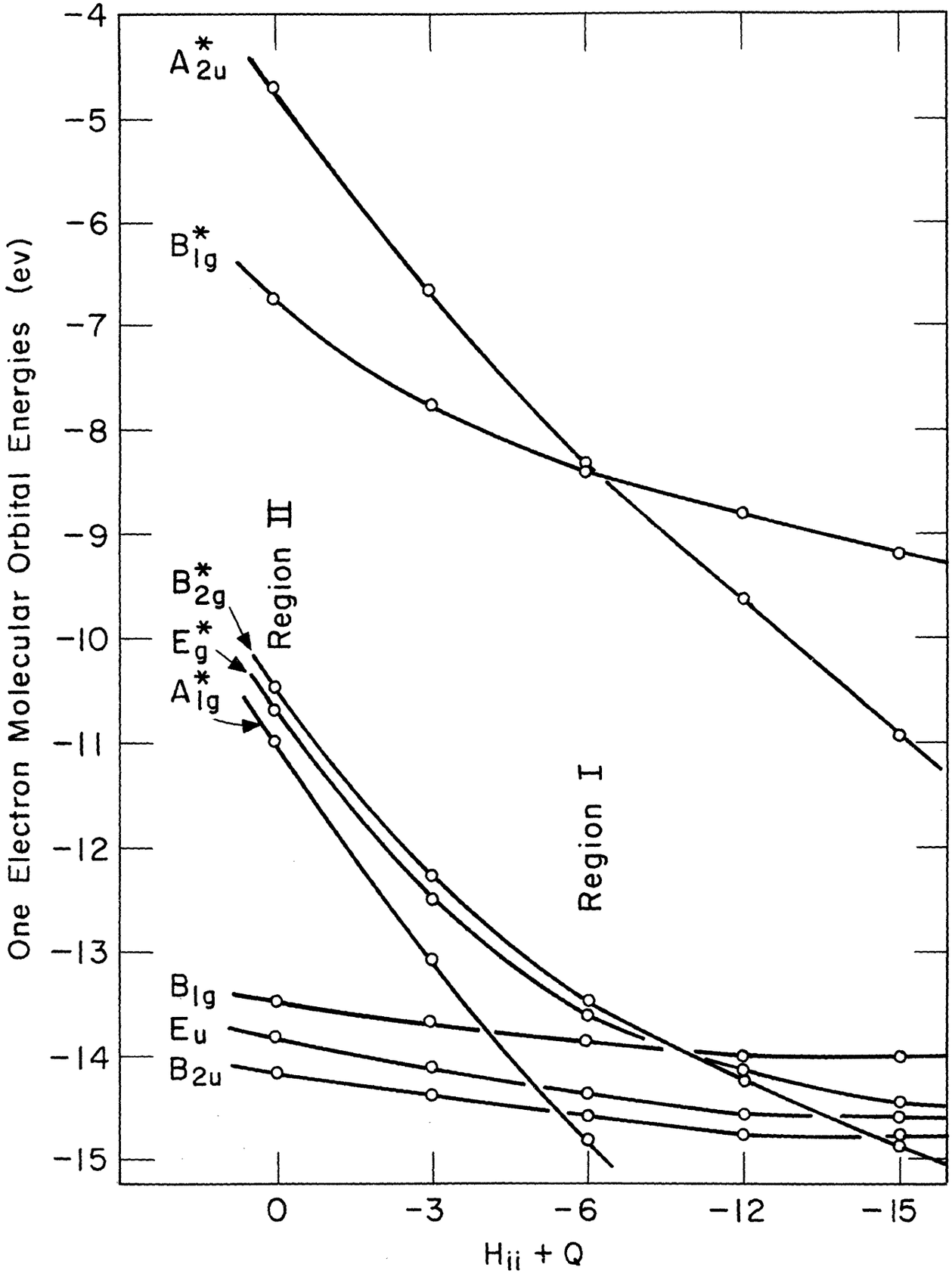

One Electron Molecular Orbital Energies (ev)
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
A^*_{2u} (Metal)
A^*_{1g} (Metal)
B^*_{1g} (Metal)
B^*_{2g} (Metal)
E^*_g (Metal)
A^*_{1g} (Metal)
B_{1g} (Ligand)
E_u (Ligand)
L2
L1
O
S1
S2
S3
Metal Wavefunction Exponents listed in Table 8

Fig. 6 - One-electron MO's vs. the diagonal matrix elements, H_{ii}.


One Electron Molecular Orbital Energies (ev)
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
A^*_{2u}
B^*_{1g}
B^*_{2g}
E^*_g
A^*_{1g}
B_{1g}
E_u
B_{2u}
Region II
Region I
0
-3
-6
-12
-15
$H_{ii} + Q$

Chapter II

REFERENCES

1. H. B. Gray and C. J. Ballhausen, J. Am. Chem. Soc., 85, 260 (1963).
2. R. F. Fenske, D. S. Martin and K. Ruedenberg, Inorg. Chem., 1, 441 (1962).
3. J. Chatt, G. A. Gamlen and L. E. Orgel, J. Chem. Soc., 486 (1958).
4. D. S. Martin, M. A. Tucker and Allen J. Kassman, Inorg. Chem., 4, 1682 (1965).
5. D. S. Martin and C. A. Lenhardt, Inorg. Chem., 3, 1368 (1964).
6. S. Yamada, J. Am. Chem. Soc., 73, 1182 (1951).

7a. P. Day, H. F. Orchard, H. F. Thompson and R. J. R. Williams, J. Chem. Phys., 42, 1973 (1965).

7b. O. S. Mortensen, Acta Chemica. Scan., 19, 1500 (1965).

8. R. G. Dickinson, J.Am. Chem. Soc., 44, 2404 (1922).
9. R. S. Mulliken, J. Chem. Phys., 23, 1833 (1955).
10. Ibid., 23, 1841 (1955).
11. R. Daudel, R. Lefebure and C. Moser, Quantum Chemistry: Methods and Applications, Interscience, N.Y., 1959.
12. J. H. Van Vleck, J. Chem. Phys., 2, 22 (1934).
13. J. C. Slater, Phys. Rev., 36, 57 (1930).
14. R. E. Watson and A. J. Freeman, Phys. Rev., 123, 521 (1961).
15. R. E. Watson and A. J. Freeman, Phys. Rev., 120, 1125 (1960).

16. F. Herman and S. Skillman, Atomic Structure Calculations, Prentice-Hall, Englewood Cliffs, N.J., 1963.

17. P. Ros, Thesis (Chemistry), Eindhoven, Holland, 1964.

18. J. Hinze and H. H. Jaffe, J. Am. Chem.Soc., 84, 540 (1962).

19a. C. E. Moore, Atomic Energy Levels, U.S. National Bureau of Standards Circular, 467, 1949 and 1952.

19b. J. A. Pople, Trans.Faraday Soc., 49, 1375 (1953).

20. M. Zerner and M. Gouterman, Theoret. Chim. Acta, 4, 44 (1966).

21. R. Mulliken, J. Chem. Phys., 46, 497 (1949).

22. M. Wolfsberg and L. Helmholz, J. Chem. Phys., 20, 837 (1952).

23. C. J. Ballhausen and H. B. Gray, Inorg. Chem., 1, 111 (1962).

24. L. Pauling, Nature of the Chemical Bond, Cornell University Press, N.Y., 1960.

25. L. C. Cusachs, Sur L'Approximation de Wolfsberg-Helmholz, Battelle Memorial Institute, Geneva (1964).

26a. M.D. Newton, F. P. Boer, W. E. Palke, and W. N. Lipscomb, P.N.A.S., 53, 1089 (1965).

26b. W. N. Lipscomb, private communication.

27. C. J. Ballhausen and H. B. Gray, Inorg. Chem., 1, 111 (1962).

28. T. P. Das and E. L. Hann, Nuclear Quadrupole Resonance Spectroscopy, Academic Press, N.Y., 1958.

29. E. P. Marrom, E. J. McNiff and J. L. Ragle, J. Phys. Chem., 67, 1719 (1963).

30. Chapter V (Thesis, C. B. Harris, 1966).

CHAPTER III

THE CRYSTAL AND MOLECULAR STRUCTURE OF DIPOTASSIUM OCTACHLORODIRHENATE(III) DIHYDRATE, $K_2[Re_2Cl_8]\cdot 2H_2O$

INTRODUCTION

The preparation and characterization of compounds containing the octachlorodirhenate(III) and octabromodirhenate(III) ions, $[Re_2Cl_8]^{2-}$ and $[Re_2Br_8]^{2-}$ has been reported.[1-3] The full characterization of these species requires both chemical and X-ray evidence. The chemistry and certain physical properties[2] of various compounds have been described. This section reports an X-ray diffraction study of the crystal and molecular structure of one such compound, namely, $K_2[Re_2Cl_8]\cdot 2H_2O$, of sufficient accuracy to show unambiguously the structure of the $[Re_2Cl_8]^{2-}$ ion.

EXPERIMENTAL

The crystals of $K_2[Re_2Cl_8]\cdot 2H_2O$ were obtained from a sample of the compound prepared in a manner described elsewhere.[3]

The crystal class and unit cell dimensions were established from zero layer Weissenberg photographs. The crystals are triclinic with the dimensions: $a = 6.75_2$ Å.; $b = 7.85_5$ Å.; $c = 7.61_0$ Å.; $\alpha = 102.0^\circ$; $\beta = 108.9^\circ$; $\gamma = 104.8^\circ$. The calculated density assuming one formula weight per unit cell is 3.66 g. cm.$^{-3}$; the approximate density, estimated by flotation in CH_2I_2, is 3.5 g. cm.$^{-3}$, thus establishing that Z = 1.

Intensity data were collected by the equi-inclination Weissenberg method with Cu Kα radiation using a crystal with approximate dimensions 0.02 × 0.02 × 0.05 mm. The levels 0kl-4kl were recorded; 579 reflections within half a sphere ($h \geq 0$) with $\sin\theta/\lambda \leq 45^\circ$ were recorded.

Intensities were estimated visually using an intensity wedge prepared by timed exposures of one reflection from the same crystal. On upper layers the elongated spots that were read were corrected for elongation. Lorentz and polarization corrections were made, but in view of the small size of the crystal, absorption corrections were omitted (μ = 480 cm.$^{-1}$; μt_{max} = 2.5).

DETERMINATION OF STRUCTURE

Using the corrected intensities, a Patterson synthesis was computed.[4] The Re-Re vector was immediately obvious. Placing one Re atom at the origin, coordinates for the other were derived. A Fourier synthesis was then computed[4] using phases determined by Re atoms alone and assuming the acentric space group P1. The eight chlorine atoms and two potassium atoms were found in this Fourier map. The positional parameters for these atoms as well as five scale factors (one for each level) were subjected to one cycle of full matrix least squares refinement.[5] The atomic scattering factors used here and subsequently were taken from the International Tables.[6] Those of Table 3.3.1A were used for K^+, Cl^- and O^o, while those for Re^o were taken from Table 3.3.1B. No corrections were made for anomalous dispersion. The set of calculated structure factors now at hand were used to compute a three-dimensional difference Fourier function from which all Re, K, and Cl atoms were removed. Only two significant peaks appeared; these were assigned to the oxygen atoms.

The positional parameters of all 14 atoms as well as a scale factor for each level were now subjected to two cycles of full matrix least squares refinement. In these cycles, temperature parameters of 1.0 for Re, 2.0 for K, and Cl and 4.0 for O were assigned and kept fixed. The calculated structure factors obtained from the second of these cycles were used to compute a three-dimensional Fourier map, which showed no significant unexplained peaks and which also showed an essentially centric distribution of atoms about the mid-point of the Re-Re line. It was therefore concluded that the correct space group is $P\bar{1}$.

Using $P\bar{1}$ and assigning the above-mentioned initial temperature factors and using the average values of the pairs of atomic coordinates for the 21 coordinates now required, eight cycles of full-matrix least squares refinement were now executed. The scale factors were not varied. Following this, one cycle was run in which the 21 positional parameters and the five scale factors were varied, but not the temperature factors. Finally, one cycle was run varying positional parameters and temperature parameters, but not the scale factors. The residual[7] was now 0.168 and the changes in positional parameters were less than the estimated standard deviations. As a final check on the correctness of the structure a three-dimensional difference Fourier map was computed. It showed no peaks of significant magnitude. The final set of calculated structure factors (F_c's) together with the observed absolute values of

the structure factors are listed in Table I. The atom coordinates and isotropic temperature factors are listed in Table II. The standard deviations, σ, were obtained from the least squares formula

$$\sigma^2(j) = a_{jj}(\Sigma w\Delta^2)/(m-n)$$

where a_{jj} is a diagonal element in the matrix inverse to the normal equation matrix.

DISCUSSION

The $(Re_2Cl_8)^{2-}$ Ion.

The two $ReCl_4$ halves of the ion are related by a crystallographic center of symmetry. This fact requires that the rotomeric configuration of the $[Re_2Cl_8]^{2-}$ ion be the eclipsed one. The principal dimensions of the ion are listed in Table III. From these, it can be seen that the symmetry of the ion is D_{4h} (4/mmm) within the significance of the individual dimensions. Thus all Re-Cl bonds have lengths in the range 2.29 ± 0.03 Å., all Cl-Re-Cl angles are in the range $87 \pm 2^{\circ}$, and all Re-Re-Cl angles are in the range $103.7 \pm 2.1^{\circ}$. Figure 1 is a sketch of the $[Re_2Cl_8]^{2-}$ ion showing the numbering system for the atoms and giving the mean values for each type of principal dimension together with the mean deviation of the individual dimensions of each type from their mean value. The eight chlorine atoms lie approximately at the corners of a cube with edges ca. 3.2 Å. in length.

The dimensions of the $[Re_2Cl_8]^{2-}$ ion may be compared with those of the Re_3Cl_9 group which has been found in Re(III) compounds derived directly from Re(III) chloride,[8-11] and in Re(III) chloride itself.[12] The average Re-Re distance in the triangular Re_3 cluster which occurs in these compounds is 2.48 Å. Since the order of the Re-Re bond is found to be 2.0 by a molecular orbital treatment,[13,14] it is evident that the Re-Re bond order in $[Re_2Cl_8]^{2-}$ must be quite high indeed, since the bond is some 0.24 Å. shorter. It was shown[14] that it is, in fact, a quadruple bond. The Re-Cl distance in $[Re_2Cl_8]^{2-}$, 2.29 ± 0.02 Å., is approximately the same as those for Re to non-bridging Cl atoms in the Re_3Cl_9 derivatives. Thus, for $[Re_3Cl_{12}]^{3-}$ we have[8] 2.36 ± 0.03, and for $Re_3Cl_9[(C_2H_5)_2C_6H_5P]_3$, the crystallographically independent distances[11] of this kind are 2.32 ± 0.02 and 2.31 ± 0.02 Å.

Crystal Packing.

The crystal of $K_2[Re_2Cl_8]\cdot 2H_2O$ is an array of K^+ and $[Re_2Cl_8]^{2-}$ ions and H_2O molecules. The arrangement of nearest neighbors around the potassium ions (both of which are crystallographically equivalent) is quite irregular. The K^+ ion lies approximately above the center of the square set of four Cl atoms, Cl_1, Cl_4, Cl_{22}, Cl_{33} of one $[Re_2Cl_8]^{2-}$ ion. These four chlorine atoms lie at distances of 3.52, 3.21, 3.41, and 3.63 Å. respectively from K^+, each distance having a standard deviation of 0.03 - 0.04 Å. In other directions about the K^+

ion there are Cl atoms of other $[Re_2Cl_8]^{2-}$ ions at distances of 3.31, 3.38, 3.40, 3.50, 4.52, 4.98 Å.; at least the first four of these are to be considered coordinated. Finally, the oxygen atom is 2.66 ± 0.08 Å. from K^+. The O atom has six Cl atoms at distances of 3.3 - 3.7 Å. from it, in directions such that O-H···Cl bonds might exist; however, these distances are all somewhat greater than those considered typical of HOH···Cl^- bonds.[15] The eight K^+-Cl distances in the range 3.21 - 3.63 Å. and the K^+-O distance of 2.66 Å are all reasonable.

The closest Re···Cl non-bonded contacts are 3.58, 4.66, and 4.84 Å., all with standard deviations of 0.03 Å. None of these closest non-bonded Cl atoms lie at all close to the extended Re-Re line. Thus, each Re atom can be considered to be coordinated by only the four Cl atoms to which it is bound in its own $[Re_2Cl_8]^{2-}$ ion.

Comparison with Previous Work.

As was shown in preceding work,[3] $K_2[Re_2Cl_8]\cdot 2H_2O$ is the correct formula for a compound previously reported[16] as $KH[ReCl_4]\cdot H_2O$, that is, as a compound of Re(II). An X-ray study has recently been carried out on the corresponding pyridinium compound, written by the Russian workers[16] as $(C_5H_6N)H[ReCl_4]$, by Kuznetsov and Kos'min.[17] They found it to contain a dimeric group, but the formula they assigned to it was $[Re_2Cl_8]^{4-}$. Some of the dimensions they report disagree rather markedly with those we found in $K_2[Re_2Cl_8]\cdot 2H_2O$; thus they give the Re-Re

distance as 2.22 ± 0.02 Å. and the Re-Cl distance as 2.43 ± 0.03 Å. Their method of refinement was described simply as "trial and error," however, and on subjecting their intensity data to full-matrix least squares refinement, we[18] have effected marked changes in atom coordinates such as to bring the dimensions of the $[Re_2Cl_8]^{2-}$ ion in their compound into good agreement with those of Fig. 1. Our reinvestigation of the structure of $(C_5H_8N)_2[Re_2Cl_8]$ as well as an investigation[18] of the corresponding collidinium compound, $(C_8H_{12}N)_2[Re_2Cl_8]$, which has the advantage over the pyridinium salt that it does not form twinned crystals, will be reported in detail elsewhere.

TABLE I

H	K	L	FOB	FCAL
0	0	-1	102	143
0	0	1	99	143
0	0	-2	99	104
0	0	2	118	104
0	0	3	122	94
0	0	-3	116	94
0	0	4	19	18
0	0	4	19	18
0	0	-5	5	4
0	0	5	17	4
0	0	-6	47	-33
0	0	6	46	-33
0	0	-7	69	-52
0	0	7	65	-52
0	0	-8	37	-39
0	0	8	38	-39
0	-1	0	81	147
0	1	0	83	147
0	1	-1	130	131
0	-1	1	130	131
0	1	1	100	113
0	1	-2	120	104
0	-1	2	120	104
0	1	2	59	50
0	1	3	60	48
0	-1	3	116	80
0	1	-4	26	24
0	1	4	65	51
0	-1	4	32	24
0	-1	5	48	31
0	1	5	37	27
0	1	-5	41	31
0	1	-6	45	-34
0	1	6	42	-33
0	-1	6	51	-34
0	-1	7	90	-76
0	1	-7	92	-76
0	1	7	31	-25
0	-2	0	92	121
0	2	0	96	121
0	-2	1	129	131
0	2	1	27	27
0	2	-2	37	28
0	-2	2	38	28
0	2	2	116	102
0	2	-3	106	57
0	-2	3	76	57
0	2	3	41	29
0	2	-4	90	63
0	-2	4	90	63
0	2	4	26	19
0	2	5	5	5
0	-2	5	59	41
0	2	-5	62	41
0	-2	6	5	3
0	2	-6	5	3
0	2	6	66	-57
0	2	7	54	-50
0	-2	7	35	-25
0	-3	0	197	174
0	3	0	179	174
0	-3	1	134	177
0	3	1	104	91
0	3	2	61	53
0	-3	2	118	88
0	3	3	130	36
0	-3	3	143	107
0	3	-3	79	107
0	3	-4	14	52
0	3	4	18	0
0	-3	4	78	52
0	-3	5	21	19
0	3	-5	34	19
0	3	5	46	-38
0	3	-6	58	29
0	-3	6	38	29
0	3	6	76	-58
0	-3	7	61	-40
0	-4	0	105	91
0	4	0	105	91
0	4	1	89	74
0	-4	1	149	151
0	-4	2	138	123
0	4	2	64	50
0	4	3	9	8
0	-4	3	102	83
0	4	4	42	33
0	-4	4	78	59
0	-4	5	56	44
0	4	5	29	-19
0	-4	6	5	1
0	-4	7	64	-48
0	-5	0	50	45
0	5	0	52	45
0	5	1	56	40
0	5	2	61	44
0	5	3	27	23
0	-6	0	62	71
0	-7	0	37	45
0	-8	0	39	30
0	-9	0	47	36
1	0	1	19	12
1	0	-2	121	117
1	0	2	42	-39
1	0	-3	195	221
1	0	3	92	-99
1	0	-4	140	125
1	0	4	69	-62
1	0	-5	89	88
1	0	5	65	-75
1	0	-6	77	79
1	0	6	59	-62
1	0	-7	21	25
1	0	7	46	-56
1	1	0	14	15
1	-1	-1	99	119
1	1	1	67	80
1	-1	1	4	-0
1	1	-2	115	85
1	-1	2	14	10
1	-1	-2	84	64
1	1	2	26	19
1	-1	3	100	-89
1	1	-3	111	90
1	-1	-3	135	136
1	1	3	70	-69
1	-1	4	138	-124
1	-1	-4	126	100
1	1	-4	164	138
1	1	4	34	-29
1	1	-5	70	78
1	-1	-5	90	34
1	1	5	44	-48
1	-1	5	65	-69
1	-1	-6	54	51
1	1	-6	67	69
1	-1	6	73	-76
1	1	6	71	-74
1	1	-7	37	40
1	1	7	40	-56
1	-1	7	51	-63
1	2	0	29	32
1	-2	-1	42	44
1	2	1	10	6
1	2	-1	64	64
1	-2	1	69	59
1	-2	2	107	80
1	-2	-2	93	91
1	2	2	30	-32
1	-2	-3	114	101
1	2	-3	119	94
1	2	3	77	-88
1	-2	3	54	-44
1	2	-4	154	119
1	-2	-4	55	58
1	2	4	71	-73
1	-2	4	53	-44
1	-2	-5	63	68
1	2	-5	36	39
1	-2	5	31	-39
1	2	5	66	-70
1	2	-6	41	47
1	2	6	31	34
1	-2	6	72	-75
1	2	-6	49	-52
1	2	7	39	-53
1	-2	7	53	-59
1	3	0	16	12
1	-3	1	78	69
1	3	-1	21	18
1	-3	1	61	52
1	3	1	15	-8
1	-3	2	6	3
1	-3	-2	128	136
1	3	2	91	-98
1	-3	3	4	6
1	3	-3	159	161
1	-3	-3	84	-84
1	-3	-4	61	74
1	-3	4	73	-66
1	3	4	54	-59
1	-3	-5	52	62
1	3	-5	118	94
1	-3	5	51	-50
1	3	5	66	-70
1	3	-6	84	76
1	3	6	40	-48
1	-3	6	47	-47
1	-3	7	51	-59
1	4	0	4	-2
1	-4	1	21	23
1	4	1	33	21
1	-4	-1	104	99
1	-4	-2	115	117
1	-4	2	35	38
1	4	2	43	-44
1	-4	-3	97	102
1	4	3	57	-58
1	-4	3	29	-25
1	-4	4	111	-106
1	4	-4	54	63
1	4	4	35	-40
1	-4	-5	36	42
1	-4	5	77	-66
1	4	5	44	-54
1	-4	6	57	-63
1	4	-7	62	-73
1	5	0	38	34
1	-5	-1	50	48
1	-5	1	65	72
1	5	1	16	-14
1	-5	-2	83	93
1	-5	2	50	32
1	5	2	53	-52
1	-5	3	14	13
1	-5	-3	52	51
1	5	3	55	-44
1	-5	4	31	-36
1	-5	6	44	-54
1	-5	7	44	-62
1	-6	0	67	67
1	-6	1	50	51
1	-6	-1	64	57
1	-6	2	22	23
1	-6	-2	96	102
1	6	2	31	-24
1	-6	3	23	39
1	-6	4	4	-14
1	-6	5	37	-42
1	-6	6	15	-18
1	-7	0	64	60
1	-7	-1	87	97
1	-7	1	58	59
1	-7	2	33	38
1	-7	3	4	15
1	-7	4	33	-33
1	-7	5	47	-45
1	-8	0	26	33
2	0	0	107	-156
2	0	1	53	-58
2	0	2	122	-116
2	0	-2	28	7
2	0	-3	36	16
2	0	3	89	-91
2	0	-4	57	39
2	0	4	69	-73
2	0	-5	101	78
2	0	5	80	-93
2	0	-6	117	106
2	0	6	25	-33
2	-1	0	102	-129
2	1	0	61	-87
2	-1	1	147	-151
2	1	1	52	-60
2	-1	2	114	-106
2	1	2	68	-71
2	-1	-2	8	-4
2	-1	-3	49	37
2	1	-3	12	0
2	1	3	87	-98
2	-1	3	92	-86
2	-1	-4	88	71
2	1	-4	90	64
2	-1	4	89	-83
2	1	4	88	-93
2	-1	-5	50	36
2	1	-5	68	50
2	1	5	57	-63
2	-1	5	73	-68
2	-1	-6	93	90
2	1	-6	59	51
2	1	6	15	-22
2	-1	6	5	-14
2	1	-7	115	101
2	-2	0	126	-92
2	2	0	99	-96
2	-2	-1	79	75
2	-2	1	56	-61
2	2	1	96	-93
2	2	-1	73	-86
2	2	2	111	-102
2	-2	-2	46	37
2	-2	2	43	-45
2	-2	3	119	-116
2	2	-3	42	33
2	2	3	56	-53
2	-2	-4	62	53
2	2	-4	60	39
2	-2	4	80	-81
2	2	4	65	-72
2	2	-5	48	31
2	-2	-5	53	48
2	2	5	27	-33
2	-2	5	73	-81
2	2	-6	80	56
2	-2	-6	70	68
2	-2	6	52	-50
2	2	-7	96	75
2	3	0	91	-98
2	-3	0	65	-55
2	3	-1	158	-145
2	-3	1	70	-68
2	3	1	77	-76
2	-3	-1	5	-9
2	-3	-2	43	36
2	3	2	85	-86
2	-3	2	73	-73
2	-3	-3	60	51
2	3	3	92	-84
2	-3	3	66	-65
2	-3	-4	53	51
2	3	4	55	-59
2	-3	4	79	-76
2	-3	-5	59	80
2	3	5	88	-100
2	-3	5	30	-34
2	-3	6	79	-79
2	-4	0	73	-58
2	4	0	73	-88
2	-4	1	141	-148
2	4	-1	5	8
2	4	-1	57	-58
2	4	1	73	-68
2	-4	2	97	-83
2	4	2	72	-66
2	-4	-2	5	-2
2	-4	-3	77	71
2	-4	3	89	-89
2	4	3	72	-74
2	-4	-4	62	58
2	-4	4	91	-91
2	4	4	77	-76
2	-4	-5	70	69
2	-4	5	67	-74
2	-4	6	77	-53
2	-5	0	16	-18
2	5	0	58	-46
2	-5	-1	49	38
2	5	1	88	-79
2	-5	1	60	-67
2	-5	-2	48	40
2	-5	2	45	-52
2	5	2	65	-59
2	-5	-3	39	33
2	5	3	48	-50
2	-5	3	73	-81
2	-5	-4	41	38
2	-5	4	78	-86
2	-5	5	44	-59
2	-5	6	61	-73
2	-6	0	22	19
2	-6	-1	20	12
2	-6	1	34	-37
2	-6	-2	48	39
2	-6	2	38	-46
2	-6	3	33	-41
2	-6	4	49	-46
2	-6	5	63	-78
2	-7	0	21	2
2	-7	-1	19	17
2	-7	1	84	-65
2	-7	2	70	-70
2	-7	3	44	-43
2	-7	4	63	-79
2	-7	5	41	-58
3	0	0	90	-113
3	0	-1	59	-119
3	0	1	73	-90
3	0	2	96	-95
3	0	-2	58	-63
3	0	-3	177	-132
3	0	3	29	-27
3	0	-4	135	-96
3	0	4	19	-15
3	0	5	6	5
3	0	-5	15	-9
3	0	6	6	-11
3	-1	0	56	-68
3	1	0	83	-103
3	1	1	109	-133
3	1	-1	63	-88
3	-1	1	80	-93
3	1	2	53	-69
3	-1	-2	68	-70
3	-1	2	87	-112
3	-1	-3	143	-111
3	-1	3	91	14
3	1	-3	89	-69
3	1	3	6	-13
3	-1	-4	119	-81
3	1	4	6	6
3	1	-4	67	-50
3	1	4	6	-12
3	-1	5	6	0
3	1	-5	28	6
3	-1	-5	6	-7
3	1	-6	17	3
3	-1	-6	22	12
3	1	-7	44	29
3	-2	0	129	-125
3	2	0	56	-54
3	-2	-1	47	-60
3	-2	1	95	-107
3	2	1	68	-70
3	2	-1	87	-107
3	2	-2	97	-96
3	-2	2	96	-94
3	2	2	19	-18
3	-2	-2	85	-72
3	-2	3	108	-82
3	2	3	37	27
3	-2	-3	30	-27
3	2	4	6	7
3	-2	-4	29	13
3	2	-4	45	-101
3	-2	4	6	-9
3	-2	5	6	9
3	-2	-5	35	17
3	2	-5	35	-32
3	2	-6	6	21
3	-2	6	23	15
3	2	-7	6	6
3	-3	0	89	-109
3	3	0	87	-81
3	-3	-1	122	-87
3	-3	1	93	-90
3	3	1	76	-60
3	-3	-1	87	-76
3	-3	2	118	-126
3	3	2	54	-50
3	-3	-2	21	-12
3	-3	3	95	-85
3	3	-3	99	-89
3	3	3	22	-11
3	-3	4	22	-21
3	3	-4	6	-16
3	-3	-5	26	14
3	3	5	30	-28
3	-4	0	104	-89
3	4	0	82	-97
3	-4	-1	120	-91
3	-4	1	87	-85
3	4	1	88	-82
3	-4	-2	138	-122
3	-4	2	105	-98
3	4	2	18	-11
3	-4	3	97	-39
3	-4	-3	81	-74
3	4	3	6	-7
3	-4	4	19	-21
3	-4	4	6	-6
3	-5	0	80	-93
3	5	0	83	-57
3	-5	1	90	-96
3	5	1	28	-29
3	-5	2	15	5
3	5	2	66	-67
3	-5	-2	78	-72
3	-5	3	66	-67
3	-5	-3	42	-41
3	-5	4	6	-6
3	-5	5	6	9
3	-6	0	71	-68
3	-6	1	62	-67
3	-6	-1	42	-40
3	-6	-2	48	-45
3	-6	2	85	-92
3	-6	3	96	-99
3	-6	-3	28	-31
3	-6	5	21	-26
3	-7	0	58	-52
3	-7	-1	80	-67
3	-7	1	84	-82
3	-7	2	64	-71
3	-7	3	48	-66
3	-7	4	32	-43
4	0	0	25	-22
4	0	-1	47	-54
4	0	1	6	-8
4	0	2	34	-36
4	0	-2	56	-62
4	0	-3	116	-102
4	0	3	39	-38
4	0	-4	106	-81
4	0	4	62	-75
4	0	-5	84	-68
4	0	5	46	-54
4	0	-6	100	-84
4	0	-7	84	-78
4	1	0	6	-1
4	-1	1	25	17
4	1	-1	20	-22
4	-1	-1	33	-43
4	1	1	6	-3
4	-1	2	20	18
4	1	2	39	42
4	1	-2	74	-129
4	-1	-2	7	-76
4	-1	3	47	43
4	1	3	46	47
4	-1	-3	52	-51
4	-1	-4	144	-111
4	1	4	50	58
4	-1	4	50	58
4	1	-4	97	-83
4	1	-5	104	-84
4	-1	5	44	64
4	-1	-5	87	-72
4	1	-6	58	-49
4	-1	-6	94	-76
4	-2	0	13	6
4	2	0	36	29
4	2	-1	17	3
4	2	1	29	27
4	-2	-1	61	-76
4	-2	1	17	-11
4	-2	2	26	25
4	2	2	35	30
4	-2	-2	80	-112
4	2	-2	36	-40
4	-2	3	56	48
4	2	3	34	36
4	-2	-3	97	-90
4	-2	4	29	33
4	2	-4	78	-71
4	-2	5	57	67
4	-2	-5	74	-65
4	-2	-4	71	-56
4	2	-7	66	-80
4	-3	0	61	-62
4	3	0	24	-11
4	-3	-1	114	-109
4	3	-1	6	14
4	3	1	27	27
4	-3	1	25	-19
4	3	2	43	41
4	-3	2	50	-42
4	-3	-2	97	-97
4	-3	3	6	-4
4	3	-3	111	-97
4	-3	3	20	21
4	3	3	49	48
4	-3	4	47	55
4	-3	-4	82	-76
4	-3	5	59	-79
4	-3	-5	43	-42
4	4	0	6	5
4	-4	0	6	-12
4	-4	-1	107	-91
4	-4	1	20	12
4	4	1	24	21
4	4	2	45	41
4	-4	2	23	-20
4	4	-2	85	-84
4	4	3	39	36
4	-4	-3	84	-77
4	-4	4	42	40
4	4	-4	85	-82
4	-4	5	41	60
4	-5	0	28	-31
4	-5	1	6	1
4	5	-1	80	-70
4	-5	-2	100	-82
4	5	2	20	14
4	-5	3	40	27
4	5	-3	80	-78
4	-5	-4	85	-82
4	5	4	28	-31
4	-6	0	58	-52
4	-6	1	84	-82
4	-6	-1	64	-71
4	-6	2	48	-66
4	-6	-2	32	-43
4	-6	3	25	-22
4	-6	-3	41	60
4	6	3	20	-22
4	-6	4	28	44
4	6	-4	47	-56
4	-7	1	20	-22
4	-7	2	22	-22

TABLE II

FINAL POSITIONAL AND ISOTROPIC TEMPERATURE PARAMETERS[a]

Atom	x/a	y/b	z/c	B
Re	0.8193(8)	0.9854(5)	0.9504(5)	0.91(7)
Cl_1	0.754(5)	0.046(3)	0.226(3)	1.3(4)
Cl_2	0.826(6)	0.279(4)	0.957(3)	2.1(5)
Cl_3	0.709(5)	0.909(3)	0.615(3)	1.5(5)
Cl_4	0.639(5)	0.675(4)	0.892(3)	1.7(5)
K	0.878(5)	0.659(4)	0.326(3)	2.7(5)
O	0.78(2)	0.46(1)	0.56(1)	3(2)

(a) Numbers in parentheses are standard deviations occurring in the last significant figure for each parameter.

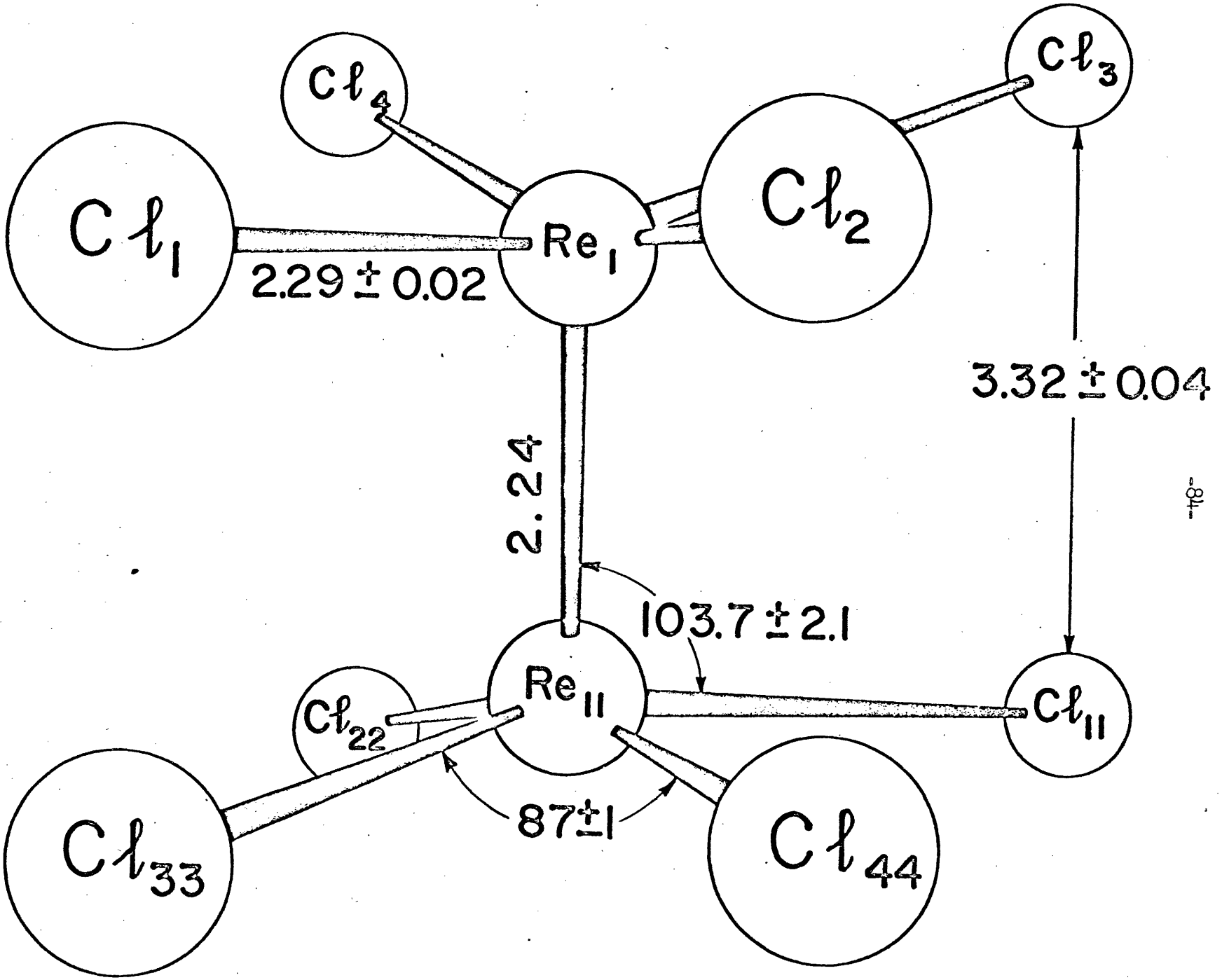
TABLE III

CRYSTALLOGRAPHICALLY INDEPENDENT[a] DISTANCES AND ANGLES IN $[Re_2Cl_8]^{2-}$

Distances, A	
Re_1-Re_{11}	2.241(7)
Re_1-Cl_1	2.26(2)
Re_1-Cl_2	2.29(3)
Re_1-Cl_3	2.31(2)
Re_1-Cl_4	2.31(3)
Cl_2-Cl_{44}	3.31(5)
Cl_3-Cl_{11}	3.33(4)
Angles, Degrees	
Cl_1-Re_1-Cl_2	85.4(8)
Cl_2-Re_1-Cl_3	88 (1)
Cl_3-Re_1-Cl_4	86.0(9)
Cl_4-Re_1-Cl_1	87.9(8)
Re_{11}-Re_1-Cl_1	105.8(6)
Re_{11}-Re_1-Cl_2	103.4(7)
Re_{11}-Re_1-Cl_3	101.7(6)
R_{11}-Re_1-Cl_4	103.6(6)

(a) The numbers in parentheses are standard deviations occurring in the last significant figure of each dimension. They were calculated from the standard deviations in Table II by the method of D.W.J. Cruickshank and A. P. Robertson, Acta Cryst., 6, 698 (1949), using a molecular geometry program for the IBM 709/7090/7094 computer, written by Dr. J. S. Wood.

Figure 1. A sketch of the $[Re_2Cl_8]^{2-}$ ion in $K_2[Re_2Cl_8]\cdot 2H_2O$. The numbering of atoms with single subscripts corresponds with that in Tables II and III. An atom with a double subscript is related to the atom with the corresponding single subscript by the center of inversion. The distances and angles are the averages of those in Table II, with the intervals representing mean derivations of the individual dimensions from these averages.


Cl4
Cl3
Cl1
Re1
Cl2
2.29 ± 0.02
3.32 ± 0.04
2.24
103.7 ± 2.1
Re11
Cl11
Cl22
87±1
Cl33
Cl44

Chapter III

REFERENCES

1. Thesis, S. J. Lippard, M.I.T. (1965).
2. Thesis, W. R. Robinson, M.I.T. (1966).
3. F. A. Cotton, N. F. Curtis, B. F. G. Johnson, and W. R. Robinson, Inorg. Chem., 4, 326 (1965).
4. Using ERFE-2, a two- and three-dimensional Fourier program for the I.B.M. 709/7090, 1962, by W. G. Sly, D. P. Shoemaker, and J. H. Van den Hende.
5. Using a full matrix least squares refinement program for the I.B.M. 709/7090, 1962, by C. T. Prewitt.
6. International Tables for X-ray Crystallography, Vol. III, Kynock Press, Birmingham, England, 1962.
7. Residual is $\Sigma||F_o| - |F_c||/\Sigma|F_o|$; the refinement program, however, minimizes $\Sigma||F_o| - |F_c||^2/\Sigma|F_o|^2$.
8. J. A. Bertrand, F. A. Cotton, and W. A. Dollase, J. Am. Chem. Soc., 85, 1349 (1963); Inorg. Chem., 2, 1166 (1963).
9. W. T. Robinson, J. E. Fergusson, and B. R. Penfold, Proc. Chem. Soc., 116 (1963).
10. J. E. Fergusson, B. R. Penfold, and W. T. Robinson, Nature, 201, 181 (1964).
11. F. A. Cotton and J. T. Mague, Inorg. Chem., 3, 1094 (1964).
12. Idem., ibid., 3, 1402 (1964).

13. F. A. Cotton and T. E. Haas, ibid., 3, 10 (1964).

14. F. A. Cotton, ibid., 4, 334 (1965).

15. See for example data summarized by G. C. Pimentel and A. L. McClellan, The Hydrogen Bond., Freeman, San Francisco, 1960, Table 9-XXV, p. 290.

16. A. S. Kotel'nikov and V. G. Tronev, Zhur. Neorg. Khim., 3, 1008 (1958).

17. B. G. Kuznetozov and P. A. Koz'min, Zhur. Struk. Khim., 4, 55 (1963).

18. F. A. Cotton and W. R. Robinson, to be published.

CHAPTER IV

MOLECULAR ORBITAL THEORY OF $Re_2Cl_8^{2-}$

INTRODUCTION

The preparation[1] and structure[2] of the $[Re_2Cl_8]^{2-}$ anion has been discussed. Its chemistry[3,4] appears to be consistent with the proposed quadrupole metal-metal bond. As such, it provides an excellent example of a molecule in which to study the effects of the various factors contributing to the metal-metal bonding. This approach, however, requires a detailed knowledge of the individual orbital contributions to the metal-metal bond; therefore, an extensive molecular orbital calculation for $[Re_2Cl_8]^{2-}$ has been undertaken. All Re-Re, Re-Cl, and Cl-Cl interactions have been considered in a semiempirical approach.

Choice of the Basis Set.

A basis set of fifty atomic orbitals, χ_i (i = 1,50), was used to construct the molecular orbitals ψ^j (j = 1,50), in the LCAO-MO approximation[5] (Eq. 1).

$$\psi^j = \sum_i C_i{}^j \chi_i \qquad (1)$$

This basis set included the Re 6s, 5d, and the Cl 3s and 3p atomic orbitals. It was assumed that the non-valence atomic orbitals on both Re atoms and the eight Cl atoms did not participate in bonding, but formed a core potential that was unaltered by interactions of the valence electrons. The atomic orbitals, χ_i's, were expressed as single term Slater Orbitals[6] (STO) as given in Eq. 2 where α_i is the shielding parameter, N_i is the normalization coefficient, n_i is the principle

quantum number, and $Y_l(\theta,\varphi)$ is the usual real spherical harmonic.

$$\chi_i = N_i r^{n_i-1} \exp(-\alpha_i r) Y_l^m(\theta,\varphi) \qquad (2)$$

All atomic orbitals were expressed in a right-handed coordinate system as shown in Fig. 1.

Evaluation of the Overlap Integrals.

The shielding parameters, α_i's, for the Re orbitals were determined by adjusting α_i to fit the overlap integrals between STO orbitals centered on Re and Re' (Fig. 1) to a numerical overlap integral between Self-Consistent Field (SCF)[7] Re wavefunctions. This method has been discussed more fully earlier.[8] The α_i's for the Re 5d and 6s orbitals were obtained in this fashion from the overlap integrals of the type Re-Re' 5d-5d and 6s-6s respectively. Since the SCF Re 6p wavefunction was not available, the Re 6p radial wavefunction distribution was assumed to be equal to that of an Re 6s.

The Cl α_i's were determined by numerically integrating the SCF Re orbital with an SCF[9-10] Cl orbital and fitting the resultant overlap with an overlap integral between STO Re and Cl wavefunctions. The Re α_i's had already been fixed by the Re-Re' overlaps; thus, only the Cl α_i's needed to be varied. The Cl 3s and 3p α_i's listed with the Re α_i's in Table 1 were obtained by averaging the α_i's from Re-Cl 5d-3s, 6s-3s, 5d-3p and 6s-3p overlaps. In this fashion all Re-Re'

and Re-Cl overlap integrals are essentially the same as overlap integrals between SCF wavefunctions. Only the very small Cl-Cl overlaps are in error. We assumed that the shielding parameters did not change with charge configuration changes. The error in such an assumption has been discussed earlier.[8]

Evaluation of the Diagonal Matrix Elements, H_{ii}.

As noted earlier,[8] H_{ii}, the energy of an electron of the ith atomic orbital moving in the field of the nuclei and other electrons of the molecule can be expressed in terms of the one-center atomic energy integrals, A_{ii}, and the multicentered molecular energy integrals, M_{ii}. This is expressed in Eq. 3.

$$H_{ii} = A_{ii} + M_{ii} \tag{3}$$

The A_{ii}'s are estimated by the Valence State Ionization Potentials ($VSIP_{ii}$) of the ith atomic orbital. The M_{ii}'s can be approximated by a point charge expression and an additional penetration correction. The same dependence on charge was assumed here for M_{ii} as was assumed in the $PtCl_4^{2-}$ molecular orbital calculation.[8] Table 2 lists the spectral states and processes[11] averaged to obtain the A_{ii}'s listed for the Re 6s, 6p and 5d orbitals. The Cl 3s and 3p A_{ii}'s used were those calculated by Hinze and Jaffe[12] for $s^2p^2p^2p$ and $sp^2p^2p^2$ states respectively.

Contrary to expectation the Re 6s atomic orbital appears to be more stable than the Re 5d in Table 2. Rather than average the 6s states (Table 2) for lower energy configurations to invert the 6s and 5d H_{ii}'s, we used the values as shown. The rational for this being that the radial portion of the 6s orbital is much more diffuse than the 5d, thus, it is stabilized more by the nuclear attraction to adjacent Re positive core in this molecule. Intuitively, one might expect this type of behavior.

Evaluation of the Off-Diagonal Matrix Elements, H_{ij}.

The H_{ij}'s, the Hamiltonian matrix elements between the ith and jth atomic orbitals, were evaluated by the Mulliken-Wolfsberg approximation[13,14] (Eq. 4).

$$H_{ij} \approx KS_{ij})H_{ii} + H_{jj})/2 \qquad (4)$$

K is the Wolfsberg-Helmholtz factor and S_{ij} is the overlap integral between the ith and jth atomic orbitals.

A K equal to 1.80 was used for all H_{ij}'s. This value is the same as the optimum value determined from previous calculations[8] and is close to the "best fit" value for small molecules.[15,16]

Method of Calculation.

The extended Huckel molecular orbital theory was employed in which all overlap integrals were evaluated. No assumption was made to the extent of hybridization of the ligand and/or metal wavefunctions.

These conditions and the LCAO-MO assumption lead directly to the familiar constraint on the secular determinant:

$$\det |H_{ij} - ES_{ij}| = 0 \qquad (5)$$

The calculation was refined on charge to a self-consistency[17] of 1/100th of a charge unit on Re.

RESULTS

Interpretation of Spectra.

A partial one electron molecular orbital diagram is given in Fig. 2. The calculated energies for the allowed electric-dipole transitions are listed in Table 3A. The calculated energies for the forbidden transitions are listed in Table 3B. Vibrational modes can contribute intensity to these transitions via a vibronic coupling mechanism. The experimental transition energies[18,19] and corresponding approximate oscillator strengths are listed in Table 3C. The eigenvalues and vectors for Fig. 2 are listed in Table IV and Table IX.

The two low energy electric-dipole forbidden transitions 20,600 $cm.^{-1}$ and 19,500 $cm.^{-1}$ are assigned to the $^1b_{2g} \rightarrow {}^1a_{2u}$ and $^1b_{2g} \rightarrow {}^1a_{1g}$ transitions respectively. Further evidence for the correctness of such an assignment is provided by the $[Re_2(RCOO)_4X_2]$ systems. Presumably the halide ions (X) are coordinated on the axial positions of the four fold axis. In order to bond the halides the Re $6p_\sigma$ orbitals must be utilized. Thus, the $^1b_{2g} \rightarrow {}^1a_{2u}$ and $^1b_{2g} \rightarrow {}^1a_{1g}$ transitions should

be absent in these molecules. Such is the case experimentally. The differences in the experimental minus the calculated transition energies are in part due to the fact that the Re 6p shielding parameter, α, was chosen equal to the Re 6s where as in reality it would be somewhat smaller.

The assignment of the $^1b_{2g} \rightarrow {}^1a_{2u}$ transition is consistent with the previous assignment.[20] The transition at 20,600 cm.$^{-1}$ ($^1b_{2g} \rightarrow {}^1a_{2g}$) was undetected in the earlier study but has since been confirmed.

The two transitions at 32,800 cm.$^{-1}$ and 39,200 cm.$^{-1}$ have oscillator strengths[20] approaching unity. As such, they should be electric-dipole allowed transitions. The 32,800 cm.$^{-1}$ transition was assigned as a $^1b_{2g} \rightarrow {}^1b_{1u}$ ($\delta \rightarrow \delta^*$). Although the agreement between the calculated and observed transition energy for this assignment is poor, no other reasonable assignment is possible. Both the $^1b_{2g} \rightarrow {}^1e_u$ and the $^1e_g \rightarrow {}^1b_{1u}$ assignments can be ruled out as possibilities. Such assignments would require an inversion of the b_{2g} and e_g (δ and π) molecular orbitals. In other words, the interaction of the Re δ orbitals would be greater than that of the Re π orbitals. Clearly this is unreasonable.

Assigning this transition as a $^1a_{1g} \rightarrow {}^1a_{2u}$ would mean that the σ to non-bonding σ separation would be less than the $\delta \rightarrow \delta^*$ separation. This is possible but highly unlikely in view of the very large overlap difference between σ and δ orbitals.

The only other possible assignment for this transition would be a $^1e_g \rightarrow {}^1a_{2u}$. If this were, in fact, the case one would expect this transition to be absent, which it is not, in the $Re_2(RCOO)_4X_2$ molecules, since the σ_n's (Fig. 2) would be greatly shifted by the interaction with the X's in such molecules. In any case polarized spectra will certainly distinguish between the $^1b_{2g} \rightarrow {}^1b_{1u}$ and $^1e_g \rightarrow {}^1a_{2u}$ possible assignments insofar as the former is z polarized while the latter is x, y polarized.

Nature of the Re-Re Bond.

The Re 5d molecular orbitals have an occupation of $(a_{1g})^2(e_g)^4(b_{2g})^2$. This $^1a_{1g}$ ground state is in agreement with the observed diamagnetism of $[Re_2Cl_8]^{2-}$.

Within the framework of the electron pair definition of a single bond, the Re-Re bond is a quadrupole bond. It is perhaps more appropriate to describe the Re-Re bond in terms of the molecular orbital description.

Bond order, as defined by Mulliken,[21] is given in Eq. 6.

$$BO_{\alpha\beta} = \sum_{ij}\sum N(i)C_i^{\alpha}C_j^{\beta}S_{ij}^{\alpha\beta} \qquad (6)$$

N(i) is the number of electrons in the ith molecular orbital, C_i^{α} and C_j^{β} are the eigenvectors of the ith and jth atomic orbital in the ith molecular orbital, $S_{ij}^{\alpha\beta}$ is the overlap between the ith and

jth atomic orbital, and the sum over i and j is restricted to orbitals on the α and β atoms. Thus the Re-Re bond order can be expressed as:

$$BO_{Re,Re} = \sigma + \pi + \delta \qquad (7)$$

σ, π, and δ are the designations for sigma, pi, and delta contributions.

Table 5 lists the various contributions to the Re-Re bond.

In an analogous way the Re-Cl bond is also described in Table 5.

It is apparent that the major portion of the Re-Re' bond is the π bond. Furthermore, it is about four times as strong as the δ bond and twice that of the σ bond. The $BO_{Re,Re}$; BO_{Re-Cl} ratio of 4.7 is the Re-Re electron pair bond order assuming a Re-Cl single bond. It is interesting to note that this ratio is consistent with the chemical conversion of $[Re_2Cl_8]^{2-}$ to $Re_2(RCOO)_4Cl_2$. This ratio suggests a simple ligand displacement reaction mechanism in which the Re-Re bond remains intact throughout the reaction despite the severe reaction conditions.

Because the Re-Re' π and σ bonds are symmetric about the four fold rotation axis in $[Re_2Cl_8]^{2-}$ they should not preferentially stabilize*

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* Since the Cl-Cl' overlap integrals would change under a C_4 rotation, there could be a very slight stabilization in one or the other symmetry. However, these effects would be energetically small compared to the energy differences between the δ bond in the two symmetries.

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the molecule in D_{4h} as opposed to D_{4d} symmetry. Only the δ bond has the proper symmetry characteristics to stabilize the molecule in an eclipised D_{4h} symmetry. However, the Cl-Cl' repulsions would be higher for a D_{4h} (as opposed to D_{4d}) configuration. Therefore, the ultimate stabilization of the molecule in D_{4h} requires that the δ bonding stabilization energy be greater than the Cl-Cl' repulsion energy.

In order to calculate the δ bond stabilization energy, either the energy of the δ molecular orbital in a staggered D_{4d} $[Re_2Cl_8]^{2-}$ configuration must be known or the energy of the δ molecular orbital in a hypothetical $[ReCl_4]^{1-}$ molecule must be known. The latter approach was preferred because it not only gives the δ bond stabilization energy but, in fact, gives the <u>total</u> Re-Re' bond energy.

The one electron molecular orbitals were calculated* for a hypothetical $[ReCl_4]^{1-}$ (1/2 of $[Re_2Cl_8]^{2-}$) molecule. The correlation between the $[ReCl_4]^{1-}$ and $[Re_2Cl_4]^{2-}$ molecular orbitals is given in Table VI for the δ, π and σ orbitals. Assuming a high spin d^4 system for $[ReCl_4]^{1-}$, Eq. 8 is the Re-Re' bond stabilization energy for individual orbital interactions (i = σ, π and δ).

$$\text{Stabilization energy}_i = [2N(i)\epsilon_i(ReCl_4)^{1-} - \epsilon_i N(i)(Re_2Cl_8)^{2-}] \quad (8)$$

---

* The same parameters were used in this calculation as were used in the $[Re_2Cl_8]^{2-}$ calculation.

+ $ReCl_4^{1-}$ has C_{4v} symmetry.

N(i) is the number of electrons in the ith molecular orbital and the ϵi's are the molecular orbital energies of the ith orbital for the species indicated. The sum of these stabilization energies is the total Re-Re' bond energy. These results are listed in Table VII.

If we assume that the four-fold rotation barrier arising from the Cl-Cl' repulsions in $[Re_2Cl_8]^{2-}$ is of the same order of magnitude as the three-fold rotation barrier in C_2Cl_6 ($\geq$ 7 kcal./mole), then the δ bond stabilization is seven times the energy of the four-fold rotational barrier. Thus, the δ bond provides a potential well far in excess of the Cl-Cl' barrier to rotation and the molecule is stabilized in an eclipsed D_{4h} rather than a staggered D_{4d} configuration.

The difference between twice the total electronic energy of $[ReCl_4]^{1-}$ and that of $[Re_2Cl_8]^{2-}$ is only 255 kcal./mole yet the Re-Re' bond energy is 366 kcal./mole. The difference, 111 kcal./mole, can be attributed to the Cl-Cl' repulsion energy that occurs when: $2[ReCl_4]^{1-} \rightarrow [Re_2Cl_8]^{2-}$.

Nature of the Re-Cl Bond.

It is apparent from Table V that the σ contribution to the Re-Cl bond order is about four times that of the π. Since the Re_1 (Fig. 1) is not in the plane of the 4Cl (Cl_1, Cl_2, Cl_3, Cl_4), the σ and π contributions to the Re-Cl bonds are not rigorously separable by molecular symmetry. Thus, the values of σ and π Re-Cl bonds in Table V are accurate only insofar as they represent an

upper limit of π bonding and lower limit of σ bonding within the framework of rigorous σ-π separability. The total Re-Cl bond order, 0.47, is, of course, not subject to the separability of σ and π systems.

All input parameters are summarized in Table VIII. The eigenvectors for the energies listed in Table IV are tabulated in Table IX. The Mulliken overlap populations are given in Table X; the orbital charges and bond order or reduced overlap population matrix are given in Tables XI and XII respectively. The overlap integrals are listed in Table XIII and the MO charge matrix is listed in Table XIV.

TABLE I

Atomic Orbital Shielding Parameters, α_i

	ϕ_i	α_i
Re	6s	1.56
	6p	1.56
	5d	2.11
Cl	3s	3.37
	3p	2.46

TABLE II

States Averaged* to Obtain Re A_{ii}'s

Re Orbital	Process	Average A_{ii}
6s	$5d^5 6s^2 \rightarrow 5d^5 6s + 6s$	
	$5d^6 6s \rightarrow 5d^6 + 6s$	-9.88 ev.
	$5d^5 6s 6p \rightarrow 5d^5 6p + 6s$	
	$5d^4 6s^2 6p \rightarrow 5d^4 6s 6p + 6s$	
6p	$5d^5 6s 6p \rightarrow 5d^5 6s + 6p$	-5.45 ev.
	$5d^4 6s^2 6p \rightarrow 5d^4 6s^2 + 6p$	
5d	$5d^5 6s^2 \rightarrow 5d^4 6s^2 + 5d$	
	$5d^6 6s \rightarrow 5d^5 6s + 5d$	-6.98 ev.
	$5d^5 6s 6p \rightarrow 5d^4 6s 6p + 5d$	
	$5d^4 6s^2 6p \rightarrow 5d^3 6s^2 6p + 5d$	

* All configurations obtained from Ref. 11.

TABLE III

A. Possible Allowed Transitions in $Re_2Cl_8^{2-}$

Transition	Polarization	Calculated Transition Energies
$^1b_{2g} \rightarrow {}^1b_{1u}$	z	18,600 cm.$^{-1}$
$^1e_g \rightarrow {}^1a_{2u}$	x,y	29,700 cm.$^{-1}$
$^1e_g \rightarrow {}^1b_{1u}$	x,y	35,860 cm.$^{-1}$
$^1a_{1g} \rightarrow {}^1a_{2u}$	z	53,270 cm.$^{-1}$
$^1b_{2g} \rightarrow {}^1e_u$	x,y	54,530 cm.$^{-1}$

B. Forbidden Transitions

Transition	Energy (calculated)
$^1b_{2g} \rightarrow {}^1a_{1g}$	10,800 cm.$^{-1}$
$^1b_{2g} \rightarrow {}^1a_{2u}$	12,400 cm.$^{-1}$
$^1e_g \rightarrow {}^1a_{1g}$	28,000 cm.$^{-1}$
$^1a_{1g} \rightarrow {}^1a_{1g}$	37,700 cm.$^{-1}$

C. Spectra of $Re_2Cl_8^{2-}$

Energy	Oscillator Strength
14,500 cm.$^{-1}$	0.023
20,600 cm.$^{-1}$	$\ll$ 0.01
32,800 cm.$^{-1}$	0.31
39,200 cm.$^{-1}$	0.65

TABLE IV

$ReCl_8^{2-}$ One-Electron MO Energies

MO	Energy(ev.)	Occupation	MO	Energy(ev.)	Occupation
1	77.39	0	26	-13.82	2
2	23.47	0	27	-13.82	2
3	23.47	0	28	-13.84	2
4	2.17	0	29	-14.16	2
5	-0.76	0	30	-14.25	2
6	-0.76	0	31	-14.25	2
7	-1.33	0	32	-14.26	2
8	-1.33	0	33	-14.32	2
9	-1.86	0	34	-14.32	2
10	-1.86	0	35	-14.46	2
11	-2.03	0	36	-14.46	2
12	-6.31	0	37	-14.46	2
13	-7.08	0	38	-14.47	2
14	-7.28	0	39	-14.53	2
15	-8.62	2	40	-14.62	2
16	-10.76	2	41	-14.70	2
17	-10.76	2	42	-15.31	2
18	-11.95	2	43	-23.27	2
19	-13.68	2	44	-23.27	2
20	-13.69	2	45	-23.27	2
21	-13.72	2	46	-23.27	2
22	-13.73	2	47	-23.31	2
23	-13.73	2	48	-23.31	2
24	-13.74	2	49	-23.62	2
25	-13.74	2	50	-24.20	2

Sum = -1139.40 ev.

TABLE V

Orbital Contributions to the Re-Re and Re-Cl Bond

Re-Re Bond

Re, Re	σ	π	δ
σ	0.684	---	---
π	---	1.345	---
δ	---	---	0.235

$BO_{Re-Re'} = 2.264$

Re-Cl Bond

Re, Cl	σ_x	π_z	π_y
σ_x	0.387	---	---
π_z	---	0.062	---
π_y	---	---	0.029

$BO_{Re-Cl} = 0.478$

z = out of the plane π bonding

y = in plane π bonding

TABLE VI

Molecular Orbital Energies (ev.)

	$ReCl_4^-$	$Re_2Cl_8^{2-}$
δ	-7.52	-8.61
π	-8.24	-10.75
σ	-10.07	-11.95
Total Electronic Energy	-13,015(kcal/mole)	-26,286(kcal/mole)

TABLE VII

Re-Re Bond Energies in $Re_2Cl_8^{2-}$

	Energy (kcal/mole)
δ	-51
π	-230
σ	-85

TABLE VIII

$Re_2Cl_8^{2-}$ MO Input Parameters: N = principle quantum number; L = angular momentum quantum number: The orbital correspondence is:

M	Sigma	Orbital	
0	0	z	p
1	0	x	
1	1	y	
0	0	z^2	d
1	0	xz	
2	0	x^2-y^2	
1	1	xz	
2	1	xy	

TABLE VIII

Orbital	Atom	N	L	M	Sigma	X	Y	Z	Orbital Exp.	H_{ii} *
1	1	6	0	0	0	0	0	1.12	1.56	-9.88
2	1	6	1	0	0	0	0	1.12	1.56	-5.45
3	1	6	1	1	0	0	0	1.12	1.56	-5.45
4	1	6	1	1	1	0	0	1.12	1.56	-5.45
5	1	5	2	0	0	0	0	1.12	2.11	-6.98
6	1	5	2	1	0	0	0	1.12	2.11	-6.98
7	1	5	2	2	0	0	0	1.12	2.11	-6.98
8	1	5	2	1	1	0	0	1.12	2.11	-6.98
9	1	5	2	2	1	0	0	1.12	2.11	-6.98
10	2	6	0	0	0	0	0	-1.12	1.56	-9.88
11	2	6	1	0	0	0	0	-1.12	1.56	-5.45
12	2	6	1	1	0	0	0	-1.12	1.56	-5.45
13	2	6	1	1	1	0	0	-1.12	1.56	-5.45
14	2	5	2	0	0	0	0	-1.12	2.11	-6.98
15	2	5	2	1	0	0	0	-1.12	2.11	-6.98
16	2	5	2	2	0	0	0	-1.12	2.11	-6.98
17	2	5	2	1	1	0	0	-1.12	2.11	-6.98
18	2	5	2	2	1	0	0	-1.12	2.11	-6.98
19	3	3	0	0	0	0	2.22	1.66	3.37	-23.45
20	3	3	1	0	0	0	2.22	1.66	2.46	-14.38
21	3	3	1	1	0	0	2.22	1.66	2.46	-14.38
22	3	3	1	1	1	0	2.22	1.66	2.46	-14.38
23	4	3	0	0	0	0	2.22	-1.66	3.37	-23.48
24	4	3	1	0	0	0	2.22	-1.66	2.46	-14.38
25	4	3	1	1	0	0	2.22	-1.66	2.46	-14.38
26	4	3	1	1	1	0	2.22	-1.66	2.46	-14.38
27	5	3	0	0	0	0	-2.22	1.66	3.37	-23.45
28	5	3	1	0	0	0	-2.22	1.66	2.46	-14.38
29	5	3	1	1	0	0	-2.22	1.66	2.46	-14.38
30	5	3	1	1	1	0	-2.22	1.66	2.46	-14.38
31	6	3	0	0	0	0	-2.22	-1.66	3.37	-23.45
32	6	3	1	0	0	0	-2.22	-1.66	2.46	-14.38
33	6	3	1	1	0	0	-2.22	-1.66	2.46	-14.38
34	6	3	1	1	1	0	-2.22	-1.66	2.46	-14.38
35	7	3	0	0	0	2.22	0	1.66	3.37	-23.45
36	7	3	1	0	0	2.22	0	1.66	2.46	-14.38
37	7	3	1	1	0	2.22	0	1.66	2.46	-14.38
38	7	3	1	1	1	2.22	0	1.66	2.46	-14.38
39	8	3	0	0	0	2.22	0	-1.66	3.37	-23.45

TABLE VIII (continued)

Orbital	Atom	N	L	M	Sigma	X	Y	Z	Orbital Exp.	H_{ii}
40	8	3	1	0	0	2.22	0	-1.66	2.46	-14.38
41	8	3	1	1	0	2.22	0	-1.66	2.46	-14.38
42	8	3	1	1	1	2.22	0	-1.66	2.46	-14.38
43	9	3	0	0	0	-2.22	0	1.66	3.37	-23.45
44	9	3	1	0	0	-2.22	0	1.66	2.46	-14.38
45	9	3	1	1	0	-2.22	0	1.66	2.46	-14.38
46	9	3	1	1	1	-2.22	0	1.66	2.46	-14.38
47	10	3	0	0	0	-2.22	0	-1.66	3.37	-23.45
48	10	3	1	0	0	-2.22	0	-1.66	2.46	-14.38
49	10	3	1	1	0	-2.22	0	-1.66	2.46	-14.38
50	10	3	1	1	1	-2.22	0	-1.66	2.46	-14.38

$$H_{ij} = 1.80\ (S_{ij})(H_{ii} + H_{jj})/2$$

TABLE IX

$Re_2Cl_8^{2-}$ MO Eigenvectors: MO's Across and AO's Down

$Re_c Cl_B^2$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1.9879	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.1453	-0.5048	-0.0000	0.0000	-0.0000	0.0000	0.1445	0.2502	-0.0000
2	-1.0561	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.5878	-0.5940	-0.0000	0.0000	-0.0000	0.0000	-0.4212	0.3456	-0.0000
3	-0.0000	-0.0000	1.4106	0.0000	-0.0039	0.6517	-0.0000	0.0000	0.0021	-0.1377	0.0000	-0.0000	0.0000	-0.0000	0.0000
4	-0.0000	-1.4106	-0.0000	-0.0000	0.6517	0.0039	0.0000	-0.0000	-0.1377	-0.0021	-0.0000	0.0000	0.0000	-0.0000	-0.0000
5	-0.2417	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.4855	0.2653	0.0000	-0.0000	0.0000	0.0000	-0.4186	0.6005	-0.0000
6	0.0000	0.0000	-0.5170	0.0000	-0.0017	0.2893	-0.0000	0.0000	0.0134	-0.8794	0.0000	-0.0000	0.0000	0.0000	0.0000
7	-0.0000	-0.0000	-0.0000	0.8751	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.7355	0.0000	0.0000	-0.0000	0.0000
8	0.0000	0.5170	0.0000	0.0000	0.2893	0.0017	0.0000	0.0000	-0.0000	-0.8794	-0.0134	-0.0000	0.0000	0.0000	-0.0000
9	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.7640	0.0000	-0.0000	-0.6481
10	-1.9879	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1452	-0.5049	-0.0000	-0.0000	-0.0000	-0.0000	0.1445	-0.2502	0.0000
11	-1.0561	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.5877	0.5941	0.0000	0.0000	0.0000	-0.0000	0.4212	0.3456	0.0000
12	0.0000	0.0000	-1.4106	0.0000	-0.0039	0.6517	-0.0000	0.0000	-0.0021	0.1377	-0.0000	-0.0000	-0.0000	-0.0000	0.0000
13	0.0000	1.4106	0.0000	-0.0000	0.6517	0.0039	0.0000	-0.0000	0.1377	0.0021	0.0000	0.0000	-0.0000	-0.0000	-0.0000
14	0.2417	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.4855	0.2654	0.0000	0.0000	0.0000	0.0000	-0.4186	-0.6005	0.0000
15	-0.0000	0.0000	-0.5170	0.0000	0.0017	-0.2893	-0.0000	-0.0000	0.0134	-0.8794	0.0000	0.0000	0.0000	-0.0000	0.0000
16	-0.0000	0.0000	0.0000	-0.8751	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.7355	0.0000	0.0000	-0.0000	0.0000
17	0.0000	0.5170	0.0000	0.0000	-0.2893	-0.0017	0.0000	0.0000	-0.8794	-0.0134	-0.0000	-0.0000	0.0000	-0.0000	0.0000
18	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.7640	0.0000	-0.0000	-0.6481
19	-0.1668	0.3396	0.0000	0.1744	-0.3127	-0.0019	0.1869	0.2041	0.1460	0.0022	-0.1611	-0.0000	-0.0960	-0.0453	0.0000
20	0.0165	-0.0355	-0.0000	-0.0841	0.0668	0.0004	-0.0127	0.0490	0.0972	0.0015	0.1052	-0.0000	0.2146	-0.1604	-0.0000
21	-0.0000	0.0000	-0.1385	-0.0000	0.0009	-0.1479	0.0000	-0.0000	-0.0011	0.0695	-0.0000	0.1838	0.0000	0.0000	0.2027
22	0.0057	-0.0789	-0.0000	-0.2373	0.1946	0.0012	-0.1983	-0.1490	-0.2192	-0.0034	0.2336	-0.0000	0.1104	-0.0077	-0.0000
23	0.1668	-0.3396	-0.0000	-0.1744	-0.3127	-0.0019	-0.1869	0.2041	-0.1460	-0.0022	-0.1611	-0.0000	-0.0960	0.0453	0.0000
24	0.0165	-0.0355	-0.0000	-0.0841	-0.0668	-0.0004	-0.0127	-0.0490	0.0972	0.0015	-0.1052	-0.0000	-0.2146	-0.1604	-0.0000
25	-0.0000	-0.0000	0.1385	-0.0000	0.0009	-0.1479	-0.0000	-0.0000	0.0011	-0.0695	0.0000	-0.1838	0.0000	-0.0000	0.2027
26	-0.0057	0.0789	0.0000	0.2373	0.1946	0.0012	0.1983	-0.1490	0.2192	0.0034	0.2336	-0.0000	0.1104	0.0077	-0.0000
27	-0.1668	-0.3396	-0.0000	0.1744	0.3127	0.0019	0.1869	0.2041	-0.1460	-0.0022	-0.1611	0.0000	-0.0960	-0.0453	-0.0000
28	0.0165	0.0355	0.0000	-0.0841	-0.0668	-0.0004	-0.0127	0.0490	-0.0972	-0.0015	0.1052	0.0000	0.2146	-0.1604	0.0000
29	-0.0000	0.0000	-0.1385	-0.0000	0.0009	-0.1479	0.0000	-0.0000	-0.0011	0.0695	-0.0000	-0.1838	0.0000	-0.0000	-0.2027
30	-0.0057	-0.0789	-0.0000	0.2373	0.1946	0.0012	0.1983	0.1490	-0.2192	-0.0034	-0.2336	0.0000	-0.1104	0.0077	-0.0000
31	0.1668	0.3396	0.0000	-0.1744	0.3127	0.0019	-0.1869	0.2041	0.1460	0.0022	-0.1611	0.0000	-0.0960	0.0453	-0.0000
32	0.0165	0.0355	0.0000	-0.0841	0.0668	0.0004	-0.0127	-0.0490	-0.0972	-0.0015	-0.1052	0.0000	-0.2146	-0.1604	0.0000
33	-0.0000	-0.0000	0.1385	-0.0000	0.0009	-0.1479	-0.0000	-0.0000	0.0011	-0.0695	0.0000	0.1838	0.0000	-0.0000	-0.2027
34	0.0057	0.0789	0.0000	-0.2373	0.1946	0.0012	-0.1983	0.1490	0.2192	0.0034	-0.2336	-0.0000	-0.1104	-0.0077	0.0000
35	-0.1668	0.0000	-0.3396	-0.1744	0.0019	-0.3127	0.1869	0.2041	-0.0022	0.1460	0.1611	0.0000	-0.0960	-0.0453	-0.0000
36	0.0165	-0.0000	0.0355	0.0841	-0.0004	0.0668	-0.0127	0.0490	-0.0015	0.0972	-0.1052	0.0000	0.2146	-0.1604	0.0000
37	0.0057	-0.0000	0.0789	0.2373	-0.0012	0.1946	-0.1983	-0.1490	0.0034	-0.2192	-0.2336	0.0000	0.1104	-0.0077	0.0000
38	-0.0000	0.1385	0.0000	0.0000	-0.1479	-0.0009	-0.0000	0.0000	0.0695	0.0011	0.0000	0.1838	-0.0000	-0.0000	0.2027
39	0.1668	-0.0000	0.3396	0.1744	0.0019	-0.3127	-0.1869	0.2041	0.0022	-0.1460	0.1611	0.0000	-0.0960	0.0453	-0.0000
40	0.0165	-0.0000	0.0355	0.0841	0.0004	-0.0668	-0.0127	-0.0490	-0.0015	0.0972	0.1052	0.0000	-0.2146	-0.1604	0.0000
41	-0.0057	0.0000	-0.0789	-0.2373	-0.0012	0.1946	0.1983	-0.1490	-0.0034	0.2192	-0.2336	-0.0000	0.1104	0.0077	-0.0000
42	-0.0000	-0.1385	-0.0000	0.0000	-0.1479	-0.0009	-0.0000	0.0000	-0.0695	-0.0011	-0.0000	-0.1838	0.0000	-0.0000	0.2027
43	-0.1668	-0.0000	0.3396	-0.1744	-0.0019	0.3127	0.1869	0.2041	0.0022	-0.1460	0.1611	0.0000	-0.0960	0.0453	-0.0000
44	0.0165	0.0000	-0.0355	0.0841	0.0004	-0.0668	-0.0127	0.0490	0.0015	-0.0972	-0.1052	-0.0000	0.2146	-0.1604	0.0000
45	-0.0057	-0.0000	0.0789	-0.2373	-0.0012	0.1946	0.1983	0.1490	0.0034	-0.2192	0.2336	0.0000	-0.1104	0.0077	0.0000
46	0.0000	0.1385	0.0000	0.0000	-0.1479	-0.0009	-0.0000	0.0000	0.0695	0.0011	0.0000	-0.1838	-0.0000	-0.0000	-0.2027
47	0.1668	0.0000	-0.3396	0.1744	-0.0019	0.3127	-0.1869	0.2041	-0.0022	0.1460	0.1611	-0.0000	-0.0960	0.0453	0.0000
48	0.0165	0.0000	-0.0355	0.0841	-0.0004	0.0668	-0.0127	-0.0490	0.0015	-0.0972	0.1052	-0.0000	-0.2146	-0.1604	-0.0000
49	0.0057	0.0000	-0.0789	0.2373	-0.0012	0.1946	-0.1983	0.1490	-0.0034	0.2192	0.2336	-0.0000	-0.1104	-0.0077	0.0000
50	0.0000	-0.1385	-0.0000	0.0000	-0.1479	-0.0009	-0.0000	0.0000	-0.0695	-0.0011	-0.0000	0.1838	0.0000	-0.0000	-0.2027

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.0000	-0.0000	-0.3122	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0735	-0.0000
2	-0.0000	0.0000	0.1220	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0904	-0.0000
3	-0.1444	0.0087	-0.0000	0.0000	0.0000	0.0000	-0.0065	-0.0030	0.0007	0.0001	-0.0354	0.0017	0.0000	-0.0000	0.1050
4	0.0087	0.1444	-0.0000	-0.0000	-0.0000	-0.0000	0.0030	-0.0065	-0.0001	0.0007	0.0017	0.0354	-0.0000	-0.0000	0.0272
5	-0.0000	-0.0000	-0.4743	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.1250	-0.0000
6	0.5187	-0.0311	-0.0000	-0.0000	-0.0000	-0.0000	0.0141	0.0064	0.0231	0.0019	0.0548	-0.0026	-0.0000	-0.0000	0.0006
7	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0037	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0165	0.0000	-0.0000
8	-0.0311	-0.5187	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0141	-0.0019	0.0231	-0.0026	-0.0548	0.0000	-0.0000	0.0001
9	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000
10	0.0000	-0.0000	-0.3122	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0735	-0.0000
11	-0.0000	-0.0000	-0.1220	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0904	0.0000
12	-0.1444	0.0087	0.0000	-0.0000	-0.0000	-0.0000	-0.0065	0.0030	0.0007	0.0001	0.0354	-0.0017	-0.0000	-0.0000	0.1050
13	0.0087	0.1444	-0.0000	0.0000	0.0000	0.0000	-0.0030	0.0065	-0.0001	0.0007	-0.0017	-0.0354	0.0000	0.0000	0.0272
14	-0.0000	-0.0000	-0.4743	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.1250	-0.0000
15	-0.5187	0.0311	-0.0000	-0.0000	0.0000	-0.0000	0.0141	0.0064	-0.0231	-0.0019	0.0548	-0.0026	0.0000	0.0000	-0.0006
16	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0165	-0.0000	-0.0000
17	0.0311	0.5187	-0.0000	-0.0000	0.0000	0.0000	-0.0064	0.0141	0.0019	-0.0231	-0.0026	-0.0548	0.0000	-0.0000	-0.0001
18	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000
19	-0.0012	-0.0195	0.0784	0.0000	0.0000	-0.0010	-0.0012	0.0027	0.0001	-0.0009	-0.0003	-0.0064	0.0030	-0.0232	-0.0160
20	0.0153	0.2547	-0.0741	-0.0000	-0.0000	0.3329	0.1203	-0.2625	0.0104	-0.1245	-0.0179	-0.3847	-0.3129	0.3163	-0.0533
21	0.0239	-0.0014	-0.0000	0.3560	0.3556	0.0000	-0.2870	-0.1315	-0.3922	-0.0327	-0.3095	0.0144	0.0000	0.0000	0.2742
22	-0.0069	-0.1154	-0.1048	-0.0000	-0.0000	-0.1240	0.1094	-0.2388	0.0236	-0.2835	0.0022	0.0474	0.1637	-0.0833	-0.0748
23	-0.0012	-0.0195	0.0784	-0.0000	-0.0000	0.0010	0.0012	-0.0027	0.0001	-0.0009	0.0003	0.0064	0.0030	0.0232	-0.0160
24	-0.0153	-0.2547	0.0741	-0.0000	-0.0000	0.3329	0.1203	-0.2625	-0.0103	0.1244	-0.0179	-0.3847	0.3129	0.3163	0.0533
25	0.0239	-0.0014	-0.0000	0.3558	0.3558	-0.0000	0.2870	0.1314	-0.3922	-0.0327	0.3095	-0.0144	0.0000	0.0000	0.2742
26	-0.0069	-0.1154	-0.1048	-0.0000	0.0000	0.1239	-0.1094	0.2388	0.0236	-0.2835	-0.0022	-0.0474	0.1637	0.0833	-0.0748
27	0.0012	0.0195	0.0784	-0.0000	-0.0000	-0.0010	0.0012	-0.0027	-0.0001	0.0009	0.0003	0.0064	0.0030	-0.0232	0.0160
28	-0.0153	-0.2547	-0.0741	0.0000	0.0000	0.3330	-0.1202	0.2625	-0.0104	0.1245	0.0179	0.3847	-0.3129	0.3163	0.0532
29	0.0239	-0.0014	-0.0000	-0.3560	-0.3556	0.0000	-0.2871	-0.1315	-0.3922	-0.0327	-0.3095	0.0144	0.0000	-0.0000	0.2742
30	-0.0069	-0.1154	0.1048	-0.0000	-0.0000	0.1239	0.1094	-0.2388	0.0236	-0.2835	0.0022	0.0474	-0.1637	0.0833	-0.0749
31	0.0012	0.0195	0.0784	-0.0000	0.0000	0.0010	-0.0012	0.0027	-0.0001	0.0009	-0.0003	-0.0064	0.0030	0.0232	0.0160
32	0.0153	0.2547	0.0741	0.0000	0.0000	0.3330	-0.1202	0.2625	0.0104	-0.1244	0.0179	0.3847	0.3129	0.3163	-0.0532
33	0.0239	-0.0014	-0.0000	0.3558	-0.3558	-0.0000	0.2870	0.1314	-0.3923	-0.0327	0.3095	-0.0144	0.0000	0.0000	0.2742
34	-0.0069	-0.1154	0.1048	-0.0000	0.0000	-0.1239	-0.1094	0.2389	0.0236	-0.2835	-0.0022	-0.0474	-0.1637	-0.0833	-0.0749
35	0.0195	-0.0012	0.0784	-0.0000	-0.0000	0.0010	0.0027	0.0012	-0.0009	-0.0001	0.0064	-0.0003	-0.0030	-0.0232	-0.0618
36	-0.2547	0.0153	-0.0741	0.0000	0.0000	-0.3329	-0.2625	-0.1202	-0.1244	-0.0104	0.3847	-0.0179	0.3129	0.3163	-0.2056
37	0.1154	-0.0069	-0.1048	0.0000	0.0000	0.1239	-0.2388	-0.1094	-0.2835	-0.0236	-0.0474	0.0022	-0.1637	-0.0833	-0.2888
38	-0.0014	-0.0239	0.0000	-0.3560	-0.3556	-0.0000	0.1314	-0.2870	0.0327	-0.3922	0.0144	0.3095	-0.0000	-0.0000	0.0711
39	0.0195	-0.0012	0.0784	0.0000	-0.0000	-0.0010	-0.0027	-0.0012	-0.0009	-0.0001	-0.0064	0.0003	-0.0030	0.0232	-0.0618
40	0.2547	-0.0153	0.0741	0.0000	-0.0000	-0.3329	-0.2625	-0.1202	0.1245	0.0104	-0.3847	-0.0179	-0.3129	0.3163	0.2056
41	0.1154	-0.0069	-0.1048	-0.0000	0.0000	-0.1239	0.2388	-0.1094	-0.2835	-0.0236	0.0474	-0.0022	-0.1637	0.0833	-0.2888
42	-0.0014	-0.0239	-0.0000	0.3558	-0.3558	0.0001	-0.1314	0.2870	0.0327	-0.3922	-0.0144	-0.3095	0.0000	0.0000	0.0711
43	-0.0195	0.0012	0.0784	0.0000	0.0000	0.0010	-0.0027	-0.0012	0.0009	0.0001	-0.0064	0.0003	-0.0030	-0.0232	0.0618
44	0.2547	-0.0153	-0.0741	-0.0000	-0.0000	-0.3330	0.2625	0.1203	0.1244	0.0104	-0.3847	0.0180	0.3129	0.3163	0.2055
45	0.1154	-0.0069	0.1048	0.0000	0.0000	-0.1239	-0.2389	-0.1094	-0.2835	-0.0236	-0.0474	0.0022	0.1637	0.0833	-0.2889
46	-0.0014	-0.0239	0.0000	0.3560	0.3556	-0.0001	0.1315	-0.2870	0.0327	-0.3922	0.0144	0.3096	-0.0000	-0.0000	0.0711
47	-0.0195	0.0012	0.0784	-0.0000	0.0000	-0.0010	0.0027	0.0012	0.0009	0.0001	0.0064	-0.0003	-0.0030	0.0232	0.0618
48	-0.2547	0.0153	0.0741	-0.0000	-0.0000	-0.3329	0.2624	0.1202	-0.1245	-0.0104	-0.3847	0.0179	-0.3129	0.3163	-0.2055
49	0.1154	-0.0069	0.1048	-0.0000	0.0000	0.1239	-0.2388	0.1094	-0.2835	-0.0236	0.0474	-0.0022	0.1637	-0.0833	-0.2888
50	-0.0014	-0.0239	-0.0000	-0.3558	0.3558	0.0000	-0.1315	0.2870	0.0327	-0.3922	-0.0144	-0.3095	0.0000	0.0000	0.0711

	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
1	-0.0000	0.0641	0.0000	-0.0000	-0.0306	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.2186	-0.0000	0.0000	0.0000
2	-0.0000	0.1184	0.0000	0.0000	-0.0709	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.1207	-0.0000	0.0000	-0.0000
3	0.0272	0.0000	0.0616	-0.0011	-0.0000	-0.0284	-0.0114	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0387
4	-0.1050	-0.0000	-0.0011	-0.0616	-0.0000	0.0114	-0.0284	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0932
5	-0.0000	0.0342	0.0000	-0.0000	0.1418	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0184	0.0000	-0.0000	-0.0000
6	0.0001	-0.0000	0.1455	-0.0025	-0.0000	0.2122	0.0847	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0111
7	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.1988	0.0000	-0.2091	-0.0000	0.1339	0.0312	0.0000
8	-0.0006	0.0000	-0.0025	-0.1455	0.0000	-0.0847	0.2122	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0268
9	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1989	0.0000	0.2257	0.0000	0.0000	-0.0000	-0.0000
10	-0.0000	0.0641	0.0000	0.0000	0.0306	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.2186	0.0000	-0.0000	-0.0000
11	0.0000	-0.1184	-0.0000	-0.0000	-0.0708	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.1207	-0.0000	0.0000	0.0000
12	0.0272	0.0000	-0.0616	0.0011	0.0000	-0.0284	-0.0114	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0387
13	-0.1050	-0.0000	0.0011	0.0615	-0.0000	0.0114	-0.0284	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0932
14	-0.0000	0.0342	-0.0000	0.0000	-0.1418	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0184	0.0000	-0.0000	-0.0000
15	-0.0001	-0.0000	0.1455	-0.0025	-0.0000	-0.2122	-0.0847	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0111
16	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.1988	0.0000	-0.2091	-0.0000	-0.0397	0.1316	0.0000
17	0.0006	0.0000	-0.0025	-0.1455	-0.0000	0.0847	-0.2122	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0268
18	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.1989	-0.0000	0.2257	0.0000	-0.0000	-0.0000	0.0000
19	0.0618	-0.0290	0.0008	0.0488	0.0484	0.0033	-0.0083	-0.0000	0.0530	-0.0000	-0.0604	-0.1185	-0.4578	-0.1218	-0.4337
20	0.2055	0.2383	-0.0020	-0.1180	0.0765	-0.1328	0.3324	0.0000	0.1083	0.0000	-0.1422	-0.1706	-0.0024	-0.0004	0.0001
21	0.0711	0.0001	0.2178	-0.0038	-0.0000	0.0544	0.0217	0.3154	0.0000	0.3013	-0.0000	0.0000	0.0000	-0.0000	0.0010
22	0.2888	-0.2271	0.0067	0.3868	0.3087	0.0815	-0.2040	-0.0000	0.2877	0.0000	-0.2597	-0.1959	-0.0071	-0.0019	-0.0045
23	0.0618	-0.0290	-0.0008	-0.0488	-0.0484	0.0033	-0.0083	0.0000	-0.0530	-0.0000	-0.0604	-0.1185	0.1225	-0.4580	0.4334
24	-0.2055	-0.2383	-0.0021	-0.1180	0.0765	0.1328	-0.3324	-0.0000	0.1083	0.0000	0.1422	0.1706	-0.0008	0.0023	0.0001
25	0.0711	0.0001	-0.2178	0.0038	0.0000	0.0544	0.0217	-0.3154	-0.0000	0.3013	-0.0000	0.0000	-0.0000	-0.0000	-0.0010
26	0.2888	-0.2271	-0.0067	-0.3867	-0.3087	0.0815	-0.2040	-0.0000	-0.2877	-0.0000	-0.2598	-0.1959	0.0019	-0.0071	0.0045
27	-0.0618	-0.0290	-0.0008	-0.0488	0.0484	-0.0033	0.0083	-0.0000	0.0530	0.0000	-0.0604	-0.1185	-0.4580	-0.1222	0.4335
28	-0.2056	0.2383	0.0021	0.1180	0.0765	0.1328	-0.3324	-0.0000	0.1083	0.0000	-0.1422	-0.1706	-0.0024	-0.0004	-0.0001
29	0.0711	0.0001	0.2178	-0.0038	-0.0000	0.0544	0.0217	-0.3154	0.0000	-0.3013	-0.0000	0.0000	0.0000	-0.0000	0.0010
30	0.2888	0.2271	0.0067	0.3868	-0.3087	0.0815	-0.2040	-0.0000	-0.2877	0.0000	0.2598	0.1959	0.0071	0.0019	-0.0045
31	-0.0618	-0.0290	0.0008	0.0488	-0.0484	-0.0033	0.0083	0.0000	-0.0530	0.0000	-0.0604	-0.1185	0.1225	-0.4575	-0.4338
32	0.2056	-0.2383	0.0020	0.1180	0.0765	-0.1328	0.3324	0.0000	0.1083	-0.0000	0.1422	0.1706	-0.0008	0.0023	-0.0001
33	0.0711	0.0001	-0.2178	0.0038	0.0000	0.0544	0.0217	0.3154	-0.0000	-0.3013	-0.0000	0.0000	-0.0000	-0.0000	-0.0010
34	0.2888	0.2271	-0.0067	-0.3867	0.3087	0.0815	-0.2040	-0.0000	0.2876	-0.0000	0.2598	0.1959	-0.0019	0.0071	0.0045
35	-0.0160	-0.0291	-0.0488	0.0008	0.0484	-0.0083	-0.0033	0.0000	-0.0530	0.0000	0.0604	-0.1185	0.4579	0.1220	-0.1802
36	-0.0533	0.2383	0.1180	-0.0021	0.0765	0.3324	0.1328	0.0000	-0.1083	0.0000	0.1422	-0.1706	0.0024	0.0004	0.0000
37	-0.0749	-0.2272	-0.3867	0.0067	0.3087	-0.2040	-0.0815	-0.0000	-0.2876	0.0000	0.2597	-0.1959	0.0071	0.0019	-0.0019
38	-0.2742	-0.0000	-0.0038	-0.2178	0.0000	-0.0217	0.0544	0.3154	0.0000	0.3013	0.0000	-0.0000	-0.0000	-0.0000	0.0025
39	-0.0160	-0.0291	0.0488	-0.0008	-0.0484	-0.0083	-0.0033	-0.0000	0.0530	0.0000	0.0604	-0.1185	-0.1225	0.4578	0.1804
40	0.0533	-0.2382	0.1180	-0.0021	0.0765	-0.3324	-0.1328	-0.0000	-0.1083	-0.0000	-0.1422	0.1706	0.0008	-0.0023	0.0000
41	-0.0748	0.2272	0.3868	-0.0067	-0.3087	-0.2040	-0.0815	-0.0000	0.2876	-0.0000	0.2598	-0.1959	-0.0019	0.0071	0.0019
42	-0.2742	-0.0000	0.0038	0.2178

TABLE X

$Re_2Cl_8^{2-}$ Mulliken Overlap Populations:

AO's Across and Down

MULLIKEN OVERLAP POPULATIONS FOR 72 ELECTRONS

$Re_2Cl_8^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.8280	-0.	-0.	0.	0.	0.	0.	-0.	0.	0.3843	0.1183	0.	-0.	-0.0116	0.
2	-0.	0.2342	0.	0.	-0.	-0.	-0.	-0.	0.	0.1183	0.0143	0.	-0.	-0.0147	0.
3	-0.	0.	0.2225	-0.	0.	-0.	-0.	-0.	-0.	-0.	-0.	0.0538	0.	-0.	0.0887
4	0.	0.	-0.	0.2225	0.	-0.	0.	-0.	0.	0.	-0.	0.	0.0538	-0.	-0.
5	0.	-0.	0.	0.	1.0617	-0.	0.	-0.	0.	-0.0116	-0.0147	0.	-0.	0.1014	0.
6	0.	-0.	-0.	-0.	-0.	1.3965	0.	0.	-0.	0.	0.	0.0887	0.	0.	0.4414
7	0.	-0.	-0.	0.	0.	0.	0.4098	0.	0.	0.	-0.	-0.	0.	-0.	-0.
8	-0.	-0.	-0.	-0.	-0.	0.	0.	1.3965	0.	0.	0.	0.	0.0887	0.	-0.
9	0.	0.	-0.	0.	-0.	0.	0.	0.	2.0421	0.	-0.	-0.	0.	-0.	0.
10	0.3843	0.1183	-0.	0.	-0.0116	0.	0.	0.	0.	0.8280	0.	-0.	0.	0.	-0.
11	0.1183	0.0143	-0.	-0.	-0.0147	0.	-0.	-0.	-0.	0.	0.2342	-0.	0.	0.	-0.
12	0.	0.	0.0538	0.	0.	0.0887	-0.	0.	-0.	-0.	-0.	0.2225	-0.	-0.	0.
13	-0.	0.	0.	0.0538	-0.	0.	0.	0.0887	0.	0.	0.	-0.	0.2225	0.	0.
14	-0.0116	-0.0147	-0.	-0.	0.1014	0.	-0.	0.	-0.	0.	0.	-0.	0.	1.0617	0.
15	0.	0.	0.0887	-0.	0.	0.4414	-0.	-0.	0.	-0.	0.	0.	0.	0.	1.3965
16	-0.	0.	0.	-0.	0.	0.	0.0018	0.	-0.	-0.	0.	0.	-0.	-0.	-0.
17	-0.	-0.	-0.	0.0887	0.	-0.	0.	0.4414	0.	0.	-0.	0.	-0.	-0.	-0.
18	0.	-0.	-0.	0.	0.	-0.	-0.	0.	0.2330	-0.	-0.	0.	-0.	-0.	-0.
19	0.0317	-0.0101	0.	0.0891	0.0187	0.	0.0273	0.0096	-0.	-0.0084	-0.0067	-0.	-0.0034	-0.0007	0.
20	-0.0021	0.0278	0.	0.0003	0.0295	0.	0.0138	-0.0075	0.	0.0043	0.0039	0.	-0.0020	0.0001	-0.
21	0.	0.	0.0258	-0.	-0.	0.0034	0.	-0.	-0.0003	0.	0.	-0.0001	-0.	-0.	-0.0002
22	0.0158	0.0113	0.	0.0324	0.0271	0.	0.0848	0.0292	-0.	0.0016	0.0036	0.	0.0025	-0.0007	-0.
23	-0.0084	-0.0067	0.	-0.0034	-0.0007	0.	-0.0001	-0.0008	-0.	0.0317	0.0101	0.	0.0891	0.0187	0.
24	0.0043	0.0039	-0.	-0.0020	0.0001	0.	0.0002	-0.0091	0.	-0.0021	0.0278	-0.	0.0003	0.0295	-0.
25	-0.	-0.	-0.0001	-0.	0.	-0.0002	-0.	-0.	-0.0026	0.	0.	0.0258	-0.	0.	0.0034
26	0.0016	0.0036	-0.	0.0025	-0.0007	0.	-0.0000	0.0049	-0.	0.0158	0.0113	-0.	0.0324	0.0271	0.
27	0.0317	0.0101	0.	0.0891	0.0187	0.	0.0273	0.0096	-0.	-0.0084	-0.0067	-0.	-0.0034	-0.0007	0.
28	-0.0021	0.0278	-0.	0.0003	0.0295	0.	0.0138	-0.0075	-0.	0.0043	0.0039	-0.	-0.0020	0.0001	-0.
29	0.	-0.	0.0258	0.	0.	0.0034	-0.	-0.	-0.0003	0.	-0.	-0.0001	0.	-0.	-0.0002
30	0.0158	0.0113	0.	0.0324	0.0271	0.	0.0848	0.0292	-0.	0.0016	0.0036	0.	0.0025	-0.0007	-0.
31	-0.0084	-0.0067	0.	-0.0034	-0.0007	0.	-0.0001	-0.0008	-0.	0.0317	0.0101	-0.	0.0891	0.0187	-0.
32	0.0043	0.0039	0.	-0.0020	0.0001	0.	0.0002	-0.0091	-0.	-0.0021	0.0278	0.	0.0003	0.0295	-0.
33	-0.	0.	-0.0001	0.	-0.	-0.0002	0.	-0.	-0.0026	0.	-0.	0.0258	-0.	-0.	0.0034
34	0.0016	0.0036	-0.	0.0025	-0.0007	0.	-0.0000	0.0049	-0.	0.0158	0.0113	-0.	0.0324	0.0271	-0.
35	0.0317	0.0101	0.0891	-0.	0.0187	0.0096	0.0273	0.	-0.	-0.0084	-0.0067	-0.0034	0.	-0.0007	-0.0008
36	-0.0021	0.0278	0.0003	0.	0.0295	-0.0075	0.0138	0.	-0.	0.0043	0.0039	-0.0020	0.	0.0001	-0.0091
37	0.0158	0.0113	0.0324	0.	0.0271	0.0292	0.0848	0.	-0.	0.0016	0.0036	0.0025	0.	-0.0007	0.0049
38	0.	-0.	-0.	0.0258	-0.	0.	-0.	0.0034	-0.0003	-0.	0.	-0.	-0.0001	-0.	-0.
39	-0.0084	-0.0067	-0.0034	0.	-0.0007	-0.0008	-0.0001	-0.	0.	0.0317	0.0101	0.0891	-0.	0.0187	0.0096
40	0.0043	0.0039	-0.0020	-0.	0.0001	-0.0091	0.0002	0.	0.	-0.0021	0.0278	0.0003	-0.	0.0295	-0.0075
41	0.0016	0.0036	0.0025	0.	-0.0007	0.0049	-0.0000	0.	0.	0.0158	0.0113	0.0324	-0.	0.0271	0.0292
42	0.	0.	-0.	-0.0001	-0.	-0.	-0.	0.	-0.0002	-0.0026	0.	-0.	0.0258	-0.	-0.
43	0.0317	0.0101	0.0891	0.	0.0187	0.0096	0.0273	-0.	0.	-0.0084	-0.0067	-0.0034	0.	-0.0007	-0.0008
44	-0.0021	0.0278	0.0003	-0.	0.0295	-0.0075	0.0138	-0.	-0.	0.0043	0.0039	-0.0020	0.	0.0001	-0.0091
45	0.0158	0.0113	0.0324	-0.	0.0271	0.0292	0.0848	-0.	0.	0.0016	0.0036	0.0025	0.	-0.0007	0.0049
46	-0.	0.	-0.	0.0258	-0.	0.	0.	0.0034	-0.0003	-0.	-0.	0.	-0.0001	0.	-0.
47	-0.0084	-0.0067	-0.0034	0.	-0.0007	-0.0008	-0.0001	0.	0.	0.0317	0.0101	0.0891	-0.	0.0187	0.0096
48	0.0043	0.0039	-0.0020	0.	0.0001	-0.0091	0.0002	0.	0.	-0.0021	0.0278	0.0003	-0.	0.0295	-0.0075
49	0.0016	0.0036	0.0025	-0.	-0.0007	0.0049	-0.0000	0.	0.	0.0158	0.0113	0.0324	-0.	0.0271	0.0292
50	-0.	-0.	0.	-0.0001	0.	-0.	-0.	-0.0002	-0.0026	-0.	-0.	0.	0.0258	-0.	-0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.	-0.	0.	0.0317	-0.0021	0.	0.0158	-0.0084	0.0043	-0.	0.0016	0.0317	-0.0021	0.	0.0158
2	0.	-0.	-0.	0.0101	0.0278	0.	0.0113	-0.0067	0.0039	-0.	0.0036	0.0101	0.0278	-0.	0.0113
3	0.	-0.	-0.	0.	0.	0.0258	0.	0.	-0.	-0.0001	-0.	0.	-0.	0.0258	0.
4	-0.	0.0887	0.	0.0891	0.0003	-0.	-0.0324	-0.0034	-0.0020	-0.	0.0025	0.0891	0.0003	0.	0.0324
5	0.	0.	0.	0.0187	0.0295	-0.	0.0271	-0.0007	0.0001	-0.	-0.0007	0.0187	0.0295	0.	0.0271
6	0.	-0.	-0.	0.	0.	0.0034	0.	0.	0.	-0.0002	0.	-0.	0.	0.0034	0.
7	0.0018	0.	-0.	0.0273	0.0138	0.	0.0848	-0.0001	0.0002	-0.	-0.0000	0.0273	0.0138	-0.	0.0848
8	0.	0.4414	0.	0.0096	-0.0075	0.	0.0292	-0.0008	-0.0091	-0.	0.0049	0.0096	-0.0075	-0.	0.0292
9	-0.	0.	0.2330	-0.	0.	-0.0003	-0.	-0.	0.	-0.0026	0.	-0.	-0.	-0.0003	0.
10	-0.	0.	-0.	-0.0084	0.0043	0.	0.0016	0.0317	-0.0021	0.	0.0158	-0.0084	0.0043	0.	0.0016
11	0.	-0.	-0.	-0.0067	0.0039	0.	0.0036	0.0101	0.0278	0.	0.0113	-0.0067	0.0039	-0.	0.0036
12	0.	-0.	0.	-0.	0.	-0.0001	0.	0.	-0.	0.0258	0.	-0.	-0.	-0.0001	0.
13	-0.	0.	-0.	-0.0034	-0.0020	-0.	0.0025	0.0891	0.0003	-0.	0.0324	-0.0034	-0.0020	0.	0.0025
14	-0.	-0.	-0.	-0.0007	0.0001	-0.	-0.0007	0.0187	0.0295	0.	0.0271	-0.0007	0.0001	-0.	-0.0007
15	-0.	-0.	-0.	0.	-0.	-0.0002	-0.	-0.	0.	0.0034	0.	0.	-0.	-0.0002	-0.
16	0.4098	-0.	-0.	-0.0001	0.0002	-0.	-0.0000	0.0273	0.0138	-0.	0.0848	-0.0001	0.0002	-0.	-0.0000
17	-0.	1.3965	0.	-0.0008	-0.0091	0.	0.0049	0.0096	-0.0075	-0.	0.0292	-0.0008	-0.0091	0.	0.0049
18	-0.	0.	2.0421	0.	0.	-0.0026	0.	0.	-0.	-0.0003	-0.	0.	0.	-0.0026	-0.
19	-0.0001	-0.0008	0.	3.5474	0.	0.	0.	-0.0000	-0.0001	-0.	-0.	0.	-0.	-0.	-0.0000
20	0.0002	-0.0091	0.	0.	3.7500	-0.	-0.	-0.0001	-0.0003	0.	-0.	0.	-0.0000	-0.	0.
21	-0.	0.	-0.0026	0.	-0.	3.8673	0.	0.	0.	0.0001	0.	-0.	-0.	-0.0000	0.
22	-0.0000	0.0049	0.	0.	-0.	0.	3.3925	0.	0.	-0.	0.0000	-0.0000	-0.	-0.	-0.0000
23	0.0273	0.0096	0.	-0.0000	-0.0001	0.	0.	3.5474	-0.	0.	0.	-0.	-0.	0.	0.
24	0.0138	-0.0075	-0.	-0.0001	-0.0003	0.	0.	-0.	3.7500	0.	0.	-0.	-0.0000	-0.	0.0000
25	-0.	-0.	-0.0003	-0.	0.	0.0001	-0.	0.	0.	3.8673	0.	-0.	-0.	-0.	0.
26	0.0848	0.0292	-0.	0.	-0.	0.	0.0000	0.	0.	0.	3.3925	0.	0.0000	0.	-0.0000
27	-0.0001	-0.0008	0.	0.	-0.	-0.	-0.0000	-0.	-0.	-0.	0.	3.5474	0.	0.	-0.
28	0.0002	-0.0091	0.	-0.	-0.0000	-0.	-0.	-0.0000	-0.	-0.0000	-0.	0.0000	3.7500	-0.	-0.
29	-0.	0.	-0.0026	-0.	-0.	-0.0000	-0.	0.	-0.	-0.	0.	0.	-0.	3.8673	-0.
30	-0.0000	0.0049	-0.	-0.0000	0.	0.	-0.0000	0.	0.0000	0.	-0.0000	0.	-0.	-0.	3.3925
31	0.0273	0.0096	0.	0.	-0.	-0.	0.	0.	0.	-0.	-0.0000	-0.0000	-0.0001	-0.	-0.
32	0.0138	-0.0075	-0.	-0.	-0.0000	-0.	0.0000	-0.	-0.0000	-0.	-0.	-0.0001	-0.0003	0.	-0.
33	0.	0.	-0.0003	-0.	0.	-0.	-0.	0.	0.	-0.0000	-0.	0.	-0.	0.0001	0.
34	0.0848	0.0292	0.	0.	0.0000	0.	-0.0000	-0.0000	0.	0.	-0.0000	0.	0.	-0.	0.0000
35	-0.0001	0.	-0.	-0.0000	-0.	-0.0002	-0.0000	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	-0.0000
36	0.0002	-0.	0.	-0.	-0.0002	0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	0.	-0.0002	-0.	-0.
37	-0.0000	-0.	-0.	-0.0000	0.	-0.0006	0.0003	-0.0000	-0.0000	0.0000	-0.0000	-0.	-0.	-0.0006	0.0003
38	-0.	-0.0002	-0.0026	-0.0002	0.	-0.0005	-0.0006	-0.0000	-0.0000	0.0000	-0.0000	-0.0002	-0.	-0.0005	-0.0006
39	0.0273	-0.	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0001	-0.0000	-0.0002	-0.0000	-0.	-0.0000	-0.0000	-0.0000
40	0.0138	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	0.	-0.0002	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000
41	0.0848	0.	-0.	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.	-0.0006	0.0003	-0.0000	-0.0000	-0.0000	0.0000
42	-0.	0.0034	-0.0003	-0.0000	-0.0000	0.0000	-0.0000	-0.0002	-0.	-0.0005	-0.0006	-0.0000	-0.0000	0.0000	-0.0000
43	-0.0001	-0.	0.	-0.0000	-0.	-0.0002	-0.0000	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	-0.0000
44	0.0002	-0.	0.	0.	-0.0002	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	0.	-0.0002	0.	0.
45	-0.0000	-0.	-0.	-0.0000	-0.	-0.0006	0.0003	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.	-0.0006	0.0003
46	0.	-0.0002	-0.0026	-0.0002	-0.	-0.0005	-0.0006	-0.0000	-0.0000	0.0000	-0.0000	-0.0002	0.	-0.0005	-0.0006
47	0.0273	-0.	0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	-0.0000	-0.	-0.0000	-0.0000	-0.0000
48	0.0138	-0.	0.	-0.0000	-0.0000	-0.0000	-0.0000	0.	-0.0002	0.	0.	-0.0000	-0.0000	-0.0000	-0.0000
49	0.0848	0.	0.	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.	-0.0006	0.0003	-0.0000	-0.0000	-0.0000	0.0000
50	0.	0.0034	-0.0003	-0.0000	-0.0000	0.0000	-0.0000	-0.0002	0.	-0.0005	-0.0006	-0.0000	-0.0000	0.0000	-0.0000

	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
1	-0.0084	0.0043	-0.	0.0016	0.0317	-0.0021	0.0158	0.	-0.0084	0.0043	0.0016	0.	0.0317	-0.0021	0.0158
2	-0.0067	0.0039	0.	0.0036	0.0101	0.0278	0.0113	-0.	-0.0067	0.0039	0.0036	0.	0.0101	0.0278	0.0113
3	0.	0.	-0.0001	-0.	0.0891	0.0003	0.0324	-0.	-0.0034	-0.0020	0.0025	-0.	0.0891	0.0003	0.0324
4	-0.0034	-0.0020	0.	0.0025	-0.	0.	0.	0.0258	0.	-0.	0.	-0.0001	0.	-0.	-0.
5	-0.0007	0.0001	-0.	-0.0007	0.0187	0.0295	0.0271	-0.	-0.0007	0.0001	-0.0007	-0.	0.0187	0.0295	0.0271
6	0.	0.	-0.0002	0.	0.0096	-0.0075	0.0292	0.	-0.0008	-0.0091	0.0049	-0.	0.0096	-0.0075	0.0292
7	-0.0001	0.0002	0.	-0.0000	0.0273	0.0138	0.0848	-0.	-0.0001	0.0002	-0.0000	0.	0.0273	0.0138	0.0848
8	-0.0008	-0.0091	-0.	0.0049	0.	0.	0.	0.0034	-0.	0.	0.	-0.0002	-0.	-0.	-0.
9	-0.	-0.	-0.0026	-0.	-0.	-0.	-0.	-0.	-0.0003	0.	-0.	-0.0026	0.	-0.	0.
10	0.0317	-0.0021	0.	0.0158	-0.0084	0.0043	0.0016	-0.	0.0317	-0.0021	0.0158	0.	-0.0084	0.0043	0.0016
11	0.0101	0.0278	-0.	0.0113	-0.0067	0.0039	0.0036	0.	0.0101	0.0278	0.0113	0.	-0.0067	0.0039	0.0036
12	-0.	0.	0.0258	-0.	-0.0034	-0.0020	0.0025	-0.	0.0891	0.0003	0.0324	-0.	-0.0034	-0.0020	0.0025
13	0.0891	0.0003	-0.	0.0324	0.	0.	0.	-0.0001	-0.	-0.	-0.	0.0258	0.	0.	0.
14	0.0187	0.0295	-0.	0.0271	-0.0007	0.0001	-0.0007	-0.	0.0187	0.0295	0.0271	0.	-0.0007	0.0001	-0.0007
15	-0.	-0.	0.0034	-0.	-0.0008	-0.0091	0.0049	-0.	0.0096	-0.0075	0.0292	-0.	-0.0008	-0.0091	0.0049
16	0.0273	0.0138	0.	0.0848	-0.0001	0.0002	-0.0000	-0.	0.0273	0.0138	0.0848	-0.	-0.0001	0.0002	-0.0000
17	0.0096	-0.0075	0.	0.0292	0.	-0.	-0.	-0.0002	-0.	-0.	0.	0.0034	-0.	-0.	-0.
18	0.	-0.	-0.0003	0.	-0.	-0.	-0.	-0.0026	-0.	-0.	-0.	-0.0003	0.	-0.	-0.
19	0.	-0.	-0.	0.	-0.0000	0.	-0.0000	-0.0002	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
20	-0.	-0.0000	0.	0.0000	-0.	-0.0002	0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	-0.
21	-0.	-0.	-0.	-0.	-0.0002	0.	-0.0006	-0.0005	-0.0000	-0.0000	-0.0000	0.0000	-0.0002	-0.	-0.0006
22	0.	0.0000	-0.	-0.0000	-0.0000	0.	0.0003	-0.0006	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.	0.0003
23	0.	-0.	0.	-0.0000	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0000	-0.0002	-0.	-0.0000	-0.0000
24	0.	-0.0000	0.	0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	-0.	-0.	-0.0000	-0.0000	-0.0000
25	-0.	-0.	-0.0000	0.	-0.0000	-0.0000	-0.0000	0.0000	-0.0002	-0.	-0.0006	-0.0005	-0.0000	-0.0000	-0.0000
26	-0.0000	-0.	-0.	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.	0.0003	-0.0006	-0.0000	-0.0000	0.0000
27	-0.0000	-0.0001	0.	0.	-0.0000	0.	-0.0000	-0.0002	-0.	-0.0000	-0.0000	-0.0000	-0.0000	0.	-0.0000
28	-0.0001	-0.0003	-0.	0.	-0.	-0.0002	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0002	0.
29	-0.	0.	0.0001	-0.	-0.0002	-0.	-0.0006	-0.0005	-0.0000	-0.0000	-0.0000	-0.0000	-0.0002	0.	-0.0006
30	-0.	-0.	0.	0.0000	-0.0000	-0.	0.0003	-0.0006	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.	0.0003
31	3.5474	-0.	0.	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0000	-0.0002	-0.	-0.0000	-0.0000
32	-0.	3.7500	-0.	-0.	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0000	-0.0000	-0.0002	0.	-0.0000	-0.0000
33	0.	0.	3.8673	0.	-0.	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0002	0.	-0.0006	-0.0005	-0.0000
34	-0.	-0.	0.	3.3925	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.	0.0003	-0.0006	-0.0000	-0.0000
35	-0.	-0.0000	-0.0000	-0.0000	3.5474	0.	0.	0.	-0.0000	-0.0001	-0.	0.	0.	-0.	-0.0000
36	-0.0000	-0.0000	-0.0000	-0.0000	0.	3.7500	-0.	0.	-0.0001	-0.0003	-0.	-0.	0.	-0.0000	0.
37	-0.0000	-0.0000	-0.0000	0.0000	0.	-0.	3.3925	0.	0.	0.	0.0000	0.	-0.0000	-0.	-0.0000
38	-0.0000	-0.0000	0.0000	-0.0000	0.	0.	0.	3.8673	-0.	0.	-0.	0.0001	0.	0.	0.
39	-0.0000	-0.	-0.0002	-0.0000	-0.0000	-0.0001	0.	-0.	3.5474	-0.	0.	-0.	0.	-0.	0.
40	0.	-0.0002	0.	0.	-0.0001	-0.0003	0.	-0.	0.	3.7500	0.	-0.	-0.	-0.0000	0.0000
41	-0.0000	0.	-0.0006	0.0003	-0.	-0.	0.0000	-0.	0.	0.	3.3925	0.	0.	-0.0000	-0.0000
42	-0.0002	0.	-0.0005	-0.0006	0.	-0.	0.	0.0001	0.	-0.	0.	3.8673	-0.	-0.	0.
43	-0.	-0.0000	-0.0000	-0.0000	-0.	-0.0000	-0.	0.	-0.	-0.	-0.	0.	3.5474	0.	-0.
44	-0.0000	-0.0000	-0.0000	-0.0000	-0.	-0.0000	-0.	0.	-0.	-0.0000	0.0000	-0.	0.	3.7500	0.
45	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.	-0.0000	0.	0.	0.0000	-0.0000	0.	-0.	0.	3.3925
46	-0.0000	-0.0000	0.0000	-0.0000	0.	-0.	-0.	-0.0000	-0.	-0.	-0.	-0.	0.	-0.	-0.
47	-0.0000	-0.	-0.0002	-0.0000	0.	-0.	0.	-0.	0.	0.	-0.	-0.0000	-0.	-0.0000	-0.0001
48	0.	-0.0002	-0.	-0.	-0.	-0.0000	0.0000	0.	-0.	-0.0000	-0.	-0.	-0.0001	-0.0003	-0.
49	-0.0000	-0.	-0.0006	0.0003	0.	0.0000	-0.0000	0.	-0.0000	0.	-0.0000	0.	0.	0.	0.0000
50	-0.0002	-0.	-0.0005	-0.0006	0.	0.	0.	-0.	0.	0.	0.	-0.0000	-0.	0.	-0.

	46	47	48	49	50
1	-0.	-0.0084	0.0043	0.0016	-0.
2	-0.	-0.0067	0.0039	0.0036	-0.
3	-0.	-0.0034	-0.0020	0.0025	0.
4	0.0258	0.	-0.	-0.	-0.0001
5	-0.	-0.0007	0.0001	-0.0007	0.
6	0.	-0.0008	-0.0091	0.0049	-0.
7	0.	-0.0001	0.0002	-0.0000	-0.
8	0.0034	0.	0.	0.	-0.0002
9	-0.0003	0.	-0.	-0.	-0.0026
10	-0.	0.0317	-0.0021	0.0158	-0.
11	-0.	0.0101	0.0278	0.0113	-0.
12	-0.	0.0891	0.0003	0.0324	0.
13	-0.0001	-0.	0.	-0.	0.0258
14	0.	0.0187	0.0295	0.0271	-0.
15	-0.	0.0096	-0.0075	0.0292	-0.
16	0.	0.0273	0.0138	0.0848	0.
17	-0.0002	-0.	0.	0.	0.0034
18	-0.0026	0.	-0.	0.	-0.0003
19	-0.0002	-0.	-0.0000	-0.0000	-0.0000
20	-0.	-0.0000	-0.0000	-0.0000	-0.0000
21	-0.0005	-0.0000	-0.0000	-0.0000	0.0000
22	-0.0006	-0.0000	-0.0000	0.0000	-0.0000
23	-0.0000	-0.0000	0.	-0.0000	-0.0002
24	-0.0000	-0.	-0.0002	0.	0.
25	0.0000	-0.0002	0.	-0.0006	-0.0005
26	-0.0000	-0.0000	0.	0.0003	-0.0006
27	-0.0002	-0.	-0.0000	-0.0000	-0.0000
28	0.	-0.0000	-0.0000	-0.0000	-0.0000
29	-0.0005	-0.0000	-0.0000	-0.0000	0.0000
30	-0.0006	-0.0000	-0.0000	0.0000	-0.0000
31	-0.0000	-0.0000	0.	-0.0000	-0.0002
32	-0.0000	-0.	-0.0002	-0.	-0.
33	0.0000	-0.0002	-0.	-0.0006	-0.0005
34	-0.0000	-0.0000	-0.	0.0003	-0.0006
35	0.	0.	-0.	0.	0.
36	-0.	-0.	-0.0000	0.0000	0.
37	-0.	0.	0.0000	-0.0000	0.
38	-0.0000	-0.	0.	0.	-0.
39	0.	0.	-0.	-0.0000	0.
40	-0.	0.	-0.0000	0.	-0.
41	-0.	-0.0000	-0.	-0.0000	0.
42	-0.	-0.	-0.	0.	-0.0000
43	0.	-0.0000	-0.0001	0.	-0.
44	-0.	-0.0001	-0.0003	0.	0.
45	-0.	-0.	-0.	0.0000	-0.
46	3.8673	0.	-0.	0.	0.0001
47	0.	3.5474	-0.	-0.	0.
48	-0.	-0.	3.7500	-0.	0.
49	0.	-0.	-0.	3.3925	0.
50	0.0001	0.	0.	0.	3.8673

TABLE XI

$Re_2Cl_8^{2-}$ Orbital and Atomic Charges

Orbitals	Orbital Charges	Orbitals	Orbital Charges
1	0.745	41	1.802
2	0.276	42	1.945
3	0.327	43	1.857
4	0.327	44	1.904
5	0.716	45	1.802
6	0.993	46	1.945
7	0.458	47	1.857
8	0.993	48	1.904
9	1.132	49	1.802
10	0.745	50	1.945
11	0.276		
12	0.327		
13	0.327		
14	0.716		
15	0.993		
16	0.458		
17	0.993		
18	1.132		
19	1.857		
20	1.904		
21	1.945		
22	1.802		
23	1.857		
24	1.904		
25	1.945		
26	1.802		
27	1.857		
28	1.904		
29	1.945		
30	1.802		
31	1.857		
32	1.904		
33	1.945		
34	1.802		
35	1.857		
36	1.904		
37	1.802		
38	1.945		
39	1.857		
40	1.904		

Atom	Net Charges
1	1.03
2	1.03
3	-0.51
4	-0.51
5	-0.51
6	-0.51
7	-0.51
8	-0.51
9	-0.51
10	-0.51

TABLE XII

Reduced Overlap Population Matrix Atom by Atom

	1	2	3	4	5	6	7	8	9	10
1	7.81	2.26	0.48	-0.01	0.48	-0.01	0.48	-0.01	0.48	-0.01
2	2.26	7.81	-0.01	0.48	-0.01	0.48	-0.01	0.48	-0.01	0.48
3	0.48	-0.01	14.56	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
4	-0.01	0.48	-0.00	14.56	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
5	0.48	-0.01	-0.00	-0.00	14.56	-0.00	-0.00	-0.00	-0.00	-0.00
6	-0.01	0.48	-0.00	-0.00	-0.00	14.56	-0.00	-0.00	-0.00	-0.00
7	0.48	-0.01	-0.00	-0.00	-0.00	-0.00	14.56	-0.00	-0.00	-0.00
8	-0.01	0.48	-0.00	-0.00	-0.00	-0.00	-0.00	14.56	-0.00	-0.00
9	0.48	-0.01	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	14.56	-0.00
10	-0.01	0.48	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	14.56

TABLE XIII

$Re_2Cl_8^{2-}$ Overlap Integral Matrix:

AO's Correspond to the Order

Listed in Table VIII

TOTAL OVERLAP MATRIX

$Re_2Cl_8^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.6131	0.4571	-0.	-0.	-0.0203	0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.4571	-0.1186	0.	0.	0.0706	0.
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.5362	0.	0.	0.2487
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.5362	0.	0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.0203	-0.0706	-0.	-0.	0.1339	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.	-0.2487	-0.	0.	-0.3696
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	0.	0.	-0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	-0.	-0.2487	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	-0.	0.	0.	0.	0.	0.
10	0.6131	-0.4571	0.	0.	-0.0203	0.	-0.	0.	-0.	1.0000	0.	0.	0.	0.	0.
11	0.4571	-0.1186	0.	0.	-0.0706	-0.	0.	-0.	0.	0.	1.0000	0.	0.	0.	0.
12	-0.	0.	0.5362	0.	-0.	-0.2487	0.	-0.	0.	0.	0.	1.0000	0.	0.	0.
13	-0.	0.	0.	0.5362	-0.	-0.	0.	-0.2487	0.	0.	0.	0.	1.0000	0.	0.
14	-0.0203	0.0706	0.	0.	0.1339	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.
15	0.	0.	0.2487	0.	0.	-0.3696	0.	0.	0.	0.	0.	0.	0.	0.	1.0000
16	-0.	-0.	-0.	-0.	0.	0.	0.1350	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	0.	0.	0.2487	0.	0.	0.	-0.3696	0.	0.	0.	0.	0.	0.	0.
18	-0.	-0.	-0.	-0.	0.	0.	0.	0.	0.1350	0.	0.	0.	0.	0.	0.
19	0.1917	0.0746	0.	0.3067	-0.0829	0.	-0.1628	0.0792	0.	0.0518	0.0686	0.	0.0548	0.0056	0.
20	-0.0242	0.1106	-0.	-0.0625	0.0762	-0.	0.0773	0.0936	-0.	-0.0533	-0.0587	-0.	-0.0668	-0.0079	-0.
21	-0.	-0.	0.1257	0.	-0.	0.0319	-0.	-0.	0.1312	-0.	-0.	0.0250	0.	-0.	0.0064
22	-0.0994	-0.0625	0.	-0.1310	0.0860	0.	0.1866	-0.1227	0.	-0.0425	-0.0668	0.	-0.0283	-0.0152	0.
23	0.0518	-0.0686	0.	0.0548	0.0056	-0.	-0.0046	-0.0115	0.	0.1917	-0.0746	0.	-0.3067	-0.0829	-0.
24	0.0533	-0.0587	0.	0.0668	0.0079	0.	-0.0124	-0.0260	-0.	0.0242	0.1106	-0.	0.0625	-0.0762	0.
25	-0.	-0.	0.0250	-0.	0.	-0.0064	0.	0.	0.0051	-0.	-0.	0.1257	-0.	0.	-0.0319
26	-0.0425	0.0668	-0.	-0.0283	-0.0152	0.	0.0048	0.0184	-0.	-0.0994	0.0625	-0.	-0.1310	0.0860	0.
27	0.1917	0.0746	0.	-0.3067	-0.0829	0.	-0.1628	-0.0792	-0.	0.0518	0.0686	0.	-0.0548	0.0056	0.
28	-0.0242	0.1106	0.	0.0625	0.0762	0.	0.0773	-0.0936	-0.	-0.0533	-0.0587	0.	0.0668	-0.0079	0.
29	-0.	0.	0.1257	0.	0.	0.0319	0.	-0.	-0.1312	-0.	0.	0.0250	0.	0.	0.0064
30	0.0994	0.0625	0.	-0.1310	-0.0860	0.	-0.1866	-0.1227	-0.	0.0425	0.0668	0.	-0.0283	0.0152	0.
31	0.0518	-0.0686	0.	-0.0548	0.0056	-0.	-0.0046	0.0115	-0.	0.1917	-0.0746	0.	-0.3067	-0.0829	-0.
32	0.0533	-0.0587	0.	-0.0668	0.0079	-0.	-0.0124	0.0260	-0.	0.0242	0.1106	0.	-0.0625	-0.0762	-0.
33	-0.	0.	0.0250	-0.	-0.	-0.0064	-0.	0.	-0.0051	-0.	0.	0.1257	-0.	-0.	-0.0319
34	0.0425	-0.0668	-0.	-0.0283	0.0152	0.	-0.0048	0.0184	-0.	0.0994	-0.0625	-0.	-0.1310	-0.0860	0.
35	0.1917	0.0746	0.	0.3067	-0.0829	0.0792	0.1628	0.	0.	0.0518	0.0686	0.0548	0.	0.0056	0.0115
36	-0.0242	0.1106	-0.0625	0.	0.0762	0.0936	-0.0773	0.	0.	-0.0533	-0.0587	-0.0668	0.	-0.0079	-0.0260
37	-0.0994	-0.0625	-0.1310	-0.	0.0860	-0.1227	-0.1866	-0.	-0.	-0.0425	-0.0668	-0.0283	-0.	-0.0152	-0.0184
38	-0.	0.	-0.	0.1257	0.	0.	-0.	0.0319	0.1312	-0.	0.	-0.	0.0250	0.	-0.
39	0.0518	-0.0686	0.0548	0.	0.0056	-0.0115	0.0046	-0.	0.	0.1917	-0.0746	0.3067	0.	-0.0829	-0.0792
40	0.0533	-0.0587	0.0668	0.	0.0079	-0.0260	0.0124	-0.	0.	0.0242	0.1106	0.0625	0.	-0.0762	0.0936
41	-0.0425	0.0668	-0.0283	0.	-0.0152	0.0184	-0.0048	-0.	0.	-0.0994	0.0625	-0.1310	0.	0.0860	0.1227
42	-0.	0.	0.	0.0250	-0.	-0.	0.	-0.0064	0.0051	-0.	0.	0.	0.1257	-0.	0.
43	0.1917	0.0746	-0.3067	-0.	-0.0829	-0.0792	0.1628	0.	0.	0.0518	0.0686	-0.0548	-0.	0.0056	-0.0115
44	-0.0242	0.1106	0.0625	-0.	0.0762	-0.0936	-0.0773	-0.	0.	-0.0533	-0.0587	0.0668	-0.	-0.0079	0.0260
45	0.0994	0.0625	-0.1310	-0.	-0.0860	-0.1227	0.1866	-0.	-0.	0.0425	0.0668	-0.0283	-0.	0.0152	-0.0184
46	0.	-0.	-0.	0.1257	-0.	0.	0.	0.0319	-0.1312	0.	-0.	-0.	0.0250	-0.	-0.
47	0.0518	-0.0686	-0.0548	-0.	0.0056	0.0115	0.0046	0.	0.	0.1917	-0.0746	-0.3067	-0.	-0.0829	0.0792
48	0.0533	-0.0587	-0.0668	-0.	0.0079	0.0260	0.0124	0.	0.	0.0242	0.1106	-0.0625	-0.	-0.0762	-0.0936
49	0.0425	-0.0668	-0.0283	0.	0.0152	0.0184	0.0048	-0.	-0.	0.0994	-0.0625	-0.1310	0.	-0.0860	0.1227

	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
1	0.0518	0.0533	-0.	0.0425	0.1917	-0.0242	-0.0994	-0.	0.0518	0.0533	-0.0425	-0.	0.1917	-0.0242	0.0994
2	-0.0686	-0.0587	0.	-0.0668	0.0746	0.1106	-0.0625	0.	-0.0686	-0.0587	0.0668	0.	0.0746	0.1106	0.0625
3	0.	0.	0.0250	-0.	0.3067	-0.0625	-0.1310	-0.	0.0548	0.0668	-0.0283	0.	-0.3067	0.0625	-0.1310
4	-0.0548	-0.0668	-0.	-0.0283	0.	0.	-0.	0.1257	0.	0.	0.	0.0250	-0.	-0.	-0.
5	0.0056	0.0079	-0.	0.0152	-0.0829	0.0762	0.0860	0.	0.0056	0.0079	-0.0152	-0.	-0.0829	0.0762	-0.0860
6	-0.	-0.	-0.0064	0.	0.0792	0.0936	-0.1227	0.	-0.0115	-0.0260	0.0184	-0.	-0.0792	-0.0936	-0.1227
7	-0.0046	-0.0124	-0.	-0.0048	0.1628	-0.0773	-0.1866	-0.	0.0046	0.0124	-0.0048	0.	0.1628	-0.0773	0.1866
8	0.0115	0.0260	0.	0.0184	0.	0.	-0.	0.0319	-0.	-0.	-0.	-0.0064	-0.	-0.	-0.
9	-0.	-0.	-0.0051	0.	0.	0.	-0.	0.1312	0.	0.	0.	0.0051	0.	0.	0.
10	0.1917	0.0242	-0.	0.0994	0.0518	-0.0533	-0.0425	-0.	0.1917	0.0242	-0.0994	-0.	0.0518	-0.0533	0.0425
11	-0.0746	0.1106	0.	-0.0625	0.0686	-0.0587	-0.0668	0.	-0.0746	0.1106	0.0625	0.	0.0686	-0.0587	0.0668
12	0.	0.	0.1257	-0.	0.0548	-0.0668	-0.0283	-0.	0.3067	0.0625	-0.1310	0.	-0.0548	0.0668	-0.0283
13	-0.3067	-0.0625	-0.	-0.1310	0.	0.	-0.	0.0250	0.	0.	0.	0.1257	-0.	-0.	-0.
14	-0.0829	-0.0762	-0.	-0.0860	0.0056	-0.0079	-0.0152	0.	-0.0829	-0.0762	0.0860	-0.	0.0056	-0.0079	0.0152
15	-0.	-0.	-0.0319	0.	0.0115	-0.0260	-0.0184	-0.	-0.0792	0.0936	0.1227	0.	-0.0115	0.0260	-0.0184
16	-0.1628	-0.0773	-0.	-0.1866	0.0046	-0.0124	-0.0048	-0.	0.1628	0.0773	-0.1866	0.	0.0046	-0.0124	0.0048
17	0.0792	-0.0936	-0.	0.1227	0.	0.	-0.	0.0064	-0.	-0.	-0.	-0.0319	-0.	-0.	-0.
18	-0.	-0.	-0.1312	0.	0.	0.	-0.	0.0051	0.	0.	0.	0.1312	0.	0.	0.
19	0.	0.	-0.	0.	0.0001	-0.	-0.0014	0.0014	0.	0.0000	-0.0000	0.0000	0.0001	-0.	0.0014
20	-0.	-0.0000	0.	-0.0000	0.	0.0012	0.	0.	-0.0000	-0.0001	0.0000	-0.0000	0.	0.0012	0.
21	-0.	0.	-0.	0.	-0.	0.0014	0.	-0.0051	0.0063	0.0000	-0.0000	0.0000	-0.0014	0.	-0.0051
22	-0.	-0.0000	-0.	-0.0000	-0.0014	0.	0.0063	-0.0051	-0.0000	-0.0000	0.0000	-0.0000	-0.0014	-0.	-0.0063
23	0.	0.	-0.	0.0000	0.	-0.0000	-0.0000	0.0000	0.0001	0.	-0.0014	0.0014	0.	-0.0000	0.0000
24	-0.	0.0000	0.	-0.	0.0000	-0.0001	-0.0000	0.0000	-0.	0.0012	0.	-0.	0.0000	-0.0001	0.0000
25	0.	0.	0.0000	-0.	0.0000	-0.0000	-0.0000	0.0000	0.0014	0.	-0.0051	0.0063	-0.0000	0.0000	-0.0000
26	-0.0000	-0.	-0.	-0.0002	-0.0000	0.0000	0.0000	-0.0000	-0.0014	0.	0.0063	-0.0051	-0.0000	0.0000	-0.0000
27	0.0001	0.0011	-0.	-0.	0.0001	-0.	-0.0014	-0.0014	0.	0.0000	-0.0000	-0.0000	0.0001	-0.	0.0014
28	-0.0011	-0.0067	0.	0.	0.	0.0012	-0.	0.	-0.0000	-0.0001	0.0000	0.0000	0.	0.0012	-0.
29	0.	0.	0.0007	0.	0.0014	-0.	-0.0051	-0.0063	0.0000	0.0000	-0.0000	-0.0000	-0.0014	-0.	-0.0051
30	0.	0.	0.	0.0007	0.0014	0.	-0.0063	-0.0051	0.0000	0.0000	-0.0000	-0.0000	0.0014	-0.	0.0063
31	1.0000	0.	0.	0.	0.	-0.0000	-0.0000	-0.0000	0.0001	0.	-0.0014	-0.0014	0.	-0.0000	0.0000
32	0.	1.0000	0.	0.	0.0000	-0.0001	-0.0000	-0.0000	-0.	0.0012	-0.	0.	0.0000	-0.0001	0.0000
33	0.	0.	1.0000	0.	0.0000	-0.0000	-0.0000	-0.0000	0.0014	-0.	-0.0051	-0.0063	-0.0000	0.0000	-0.0000
34	0.	0.	0.	1.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0014	0.	-0.0063	-0.0051	0.0000	-0.0000	0.0000
35	0.	0.0000	0.0000	0.0000	1.0000	0.	0.	0.	0.0001	0.0011	-0.	-0.	0.	-0.	0.0000
36	-0.0000	-0.0001	-0.0000	-0.0000	0.	1.0000	0.	0.	-0.0011	-0.0067	0.	0.	0.	0.0000	0.
37	-0.0000	-0.0000	-0.0000	-0.0000	0.	0.	1.0000	0.	0.	0.	0.0007	0.	-0.0000	0.	-0.0002
38	-0.0000	-0.0000	-0.0000	-0.0000	0.	0.	0.	1.0000	0.	0.	0.	0.0007	-0.	-0.	-0.
39	0.0001	-0.	0.0014	0.0014	0.0001	-0.0011	0.	0.	1.0000	0.	0.	0.	0.	-0.	0.
40	0.	0.0012	-0.	0.	0.0011	-0.0067	0.	0.	0.	1.0000	0.	0.	-0.	0.0000	0.0000
41	-0.0014	-0.	-0.0051	-0.0063	-0.	0.	0.0007	0.	0.	0.	1.0000	0.	-0.	0.0000	-0.0000
42	-0.0014	0.	-0.0063	-0.0051	-0.	0.	0.	0.0007	0.	0.	0.	1.0000	-0.	-0.	-0.
43	0.	0.0000	-0.0000	0.0000	0.	0.	-0.0000	-0.	0.	-0.	-0.	-0.	1.0000	0.	0.
44	-0.0000	-0.0001	0.0000	-0.0000	-0.	0.	0.0000	0.	-0.	-0.0000	0.0000	-0.	0.	1.0000	0.
45	0.0000	0.0000	-0.0000	0.0000	0.0000	0.	-0.0002	-0.	0.	0.0000	-0.0000	-0.	0.	0.	1.0000
46	-0.0000	-0.0000	0.0000	-0.0000	0.	-0.	-0.	0.0000	0.	-0.	-0.	0.	0.	0.	0.
47	0.0001	-0.	-0.0014	0.0014	0.	-0.	-0.	-0.	0.	-0.	-0.0000	-0.	0.0001	-0.0011	0.
48	0.	0.0012	-0.	-0.	0.	-0.0000	-0.0000	-0.	0.	0.0000	-0.	-0.	0.0011	-0.0067	0.
49	0.0014	-0.	-0.0051	0.0063	0.	-0.0000	-0.0000	0.	0.0000	-0.	-0.0002	0.	-0.	0.	0.0007
50	-0.0014	-0.	0.0063	-0.0051	0.	-0.	0.	0.	0.	-0.	0.	0.0000	-0.	0.	0.

	46	47	48	49	50
1	0.	0.0518	0.0533	0.0425	0.
2	-0.	-0.0686	-0.0587	-0.0668	-0.
3	-0.	-0.0548	-0.0668	-0.0283	0.
4	0.1257	-0.	-0.	0.	0.0250
5	-0.	0.0056	0.0079	0.0152	0.
6	0.	0.0115	0.0260	0.0184	-0.
7	0.	0.0046	0.0124	0.0048	-0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.	0.	-0.	0.1917	-0.0242	-0.	-0.0994	0.0518	0.0533	-0.	-0.0425	0.1917	-0.0242	-0.	0.0994
2	-0.	0.	-0.	0.0746	0.1106	-0.	-0.0625	-0.0686	-0.0587	-0.	0.0668	0.0746	0.1106	0.	0.0625
3	-0.	0.	-0.	0.	-0.	0.1257	0.	-0.	-0.	0.0250	-0.	0.	-0.	0.1257	0.
4	-0.	0.2487	-0.	0.3067	-0.0625	0.	-0.1310	0.0548	0.0668	-0.	-0.0283	-0.3067	0.0625	0.	-0.1310
5	0.	0.	0.	-0.0829	0.0762	-0.	0.0860	0.0056	0.0079	0.	-0.0152	-0.0829	0.0762	0.	-0.0860
6	0.	0.	0.	0.	-0.	0.0319	-0.	-0.	-0.	0.0064	0.	0.	0.	0.0319	-0.
7	0.1350	0.	-0.	-0.1628	0.0773	-0.	-0.1866	-0.0046	-0.0124	0.	0.0048	-0.1628	0.0773	0.	-0.1866
8	0.	-0.3696	0.	0.0792	0.0936	-0.	-0.1227	-0.0115	-0.0260	0.	0.0184	-0.0792	-0.0936	-0.	-0.1227
9	0.	0.	0.1350	0.	-0.	0.1312	0.	0.	-0.	0.0051	-0.	-0.	-0.	-0.1312	-0.
10	0.	0.	0.	0.0518	-0.0533	-0.	-0.0425	0.1917	0.0242	-0.	-0.0994	0.0518	-0.0533	-0.	0.0425
11	0.	0.	0.	0.0686	-0.0587	-0.	-0.0668	-0.0746	0.1106	-0.	0.0625	0.0686	-0.0587	0.	0.0668
12	0.	0.	0.	0.	-0.	0.0250	0.	0.	-0.	0.1257	-0.	0.	0.	0.0250	0.
13	0.	0.	0.	0.0548	-0.0668	0.	-0.0283	0.3067	0.0625	-0.	-0.1310	-0.0548	0.0668	0.	-0.0283
14	0.	0.	0.	0.0056	-0.0079	-0.	-0.0152	-0.0829	-0.0762	0.	0.0860	0.0056	-0.0079	0.	0.0152
15	0.	0.	0.	0.	-0.	0.0064	0.	-0.	0.	-0.0319	0.	0.	0.	0.0064	0.
16	1.0000	0.	-0.	-0.0046	0.0124	-0.	0.0048	-0.1628	-0.0773	0.	0.1866	-0.0046	0.0124	0.	-0.0048
17	0.	1.0000	0.	0.0115	-0.0260	0.	-0.0184	-0.0792	0.0936	-0.	0.1227	-0.0115	0.0260	0.	-0.0184
18	0.	0.	1.0000	0.	-0.	0.0051	0.	0.	-0.	0.1312	-0.	-0.	-0.	-0.0051	-0.
19	-0.0046	0.0115	0.	1.0000	0.	0.	0.0001	0.0011	-0.	-0.	0.	-0.	-0.	0.	0.0000
20	0.0124	-0.0260	-0.	0.	1.0000	0.	0.	-0.0011	-0.0067	0.	0.	0.	0.0000	0.	0.
21	-0.	0.	0.0051	0.	0.	1.0000	0.	0.	0.	0.0007	0.	0.	0.	0.0000	0.
22	0.0048	-0.0184	0.	0.	0.	0.	1.0000	0.	0.	0.	0.0007	-0.0000	0.	0.	-0.0002
23	-0.1628	-0.0792	0.	0.0001	-0.0011	0.	0.	1.0000	0.	0.	0.	0.	-0.	-0.	0.
24	-0.0773	0.0936	-0.	0.0011	-0.0067	0.	0.	0.	1.0000	0.	0.	0.	-0.0000	0.	0.0000
25	0.	-0.	0.1312	-0.	0.	0.0007	0.	0.	0.	1.0000	0.	0.	0.	0.	0.
26	0.1866	0.1227	-0.	-0.	0.	0.	0.0007	0.	0.	0.	1.0000	-0.	0.0000	0.	-0.0000
27	-0.0046	-0.0115	-0.	0.	0.	0.	-0.0000	0.	0.	0.	-0.	1.0000	0.	0.	0.
28	0.0124	0.0260	-0.	-0.	0.0000	0.	0.	-0.	-0.0000	0.	0.0000	0.	1.0000	0.	0.
29	0.	0.	-0.0051	-0.	0.	0.0000	0.	-0.	0.	0.	-0.0000	0.	0.	1.0000	0.
30	-0.0048	-0.0184	-0.	0.0000	0.	0.	-0.0002	0.	0.0000	0.	-0.0000	0.	0.	0.	1.0000
31	-0.1628	0.0792	-0.	0.	-0.	0.	-0.	0.	-0.	0.	-0.0000	0.0001	-0.0011	0.	0.
32	-0.0773	-0.0936	-0.	0.	-0.0000	0.	-0.0000	0.	0.0000	0.	-0.	0.0011	-0.0067	0.	0.
33	-0.	-0.	-0.1312	-0.	0.	0.	-0.	-0.	0.	0.0000	-0.	-0.	0.	0.0007	0.
34	-0.1866	0.1227	0.	0.	-0.0000	-0.	-0.0000	0.0000	-0.	-0.	-0.0002	-0.	0.	0.	0.0007
35	0.0046	0.	0.	0.0001	0.	0.0014	-0.0014	0.	0.0000	0.0000	-0.0000	0.0001	0.	0.0014	0.0014
36	-0.0124	0.	-0.	0.0012	0.	0.	-0.0000	-0.0001	-0.0000	0.0000	-0.	0.0012	-0.	0.	0.
37	-0.0048	-0.	-0.	-0.0014	0.	-0.0051	0.0063	-0.0000	-0.0000	-0.0000	0.0000	-0.0014	-0.	-0.0051	-0.0063
38	-0.	0.0064	0.0051	0.0014	0.	0.0063	-0.0051	0.0000	0.0000	0.0000	-0.0000	-0.0014	0.	-0.0063	-0.0051
39	0.1628	-0.	0.	0.	-0.0000	0.0000	-0.0000	0.0001	-0.	0.0014	-0.0014	0.	-0.0000	0.0000	0.0000
40	0.0773	-0.	0.	0.0000	-0.0001	0.0000	-0.0000	0.	0.0012	0.	0.	0.0000	-0.0001	0.0000	0.0000
41	-0.1866	-0.	0.	-0.0000	0.0000	-0.0000	0.0000	-0.0014	0.	-0.0051	0.0063	-0.0000	0.0000	-0.0000	-0.0000
42	0.	-0.0319	0.1312	0.0000	-0.0000	0.0000	-0.0000	0.0014	0.	0.0063	-0.0051	-0.0000	0.0000	-0.0000	-0.0000
43	0.0046	-0.	0.	0.0001	0.	-0.0014	-0.0014	0.	0.0000	-0.0000	-0.0000	0.0001	0.	-0.0014	0.0014
44	-0.0124	-0.	0.	-0.	0.0012	0.	-0.	-0.0000	-0.0001	0.0000	0.0000	-0.	0.0012	-0.	-0.
45	0.0048	-0.	0.	0.0014	0.	-0.0051	-0.0063	0.0000	0.0000	-0.0000	-0.0000	0.0014	-0.	-0.0051	0.0063
46	0.	0.0064	-0.0051	0.0014	-0.	-0.0063	-0.0051	0.0000	0.0000	-0.0000	-0.0000	-0.0014	-0.	0.0063	-0.0051
47	0.1628	0.	0.	0.	-0.0000	-0.0000	-0.0000	0.0001	-0.	-0.0014	-0.0014	0.	-0.0000	-0.0000	0.0000
48	0.0773	0.	0.	0.0000	-0.0001	-0.0000	-0.0000	0.	0.0012	0.	-0.	0.0000	-0.0001	-0.0000	0.0000
49	0.1866	-0.	-0.	0.0000	-0.0000	-0.0000	-0.0000	0.0014	0.	-0.0051	-0.0063	0.0000	-0.0000	-0.0000	0.0000
50	-0.	-0.0319	-0.1312	0.0000	-0.0000	-0.0000	-0.0000	0.0014	-0.	-0.0063	-0.0051	-0.0000	0.0000	0.0000	-0.0000

	46	47	48	49	50
8	0.0319	0.	0.	-0.	-0.0064
9	-0.1312	0.	0.	-0.	-0.0051
10	0.	0.1917	0.0242	0.0994	0.
11	-0.	-0.0746	0.1106	-0.0625	-0.
12	-0.	-0.3067	-0.0625	-0.1310	0.
13	0.0250	-0.	-0.	0.	0.1257
14	-0.	-0.0829	-0.0762	-0.0860	0.
15	-0.	0.0792	-0.0936	0.1227	0.
16	0.	0.1628	0.0773	0.1866	-0.
17	0.0064	0.	0.	-0.	-0.0319
18	-0.0051	0.	0.	-0.	-0.1312
19	0.0014	-0.	0.0000	0.0000	0.0000
20	-0.	-0.0000	-0.0001	-0.0000	-0.0000
21	-0.0063	-0.0000	-0.0000	-0.0000	-0.0000
22	-0.0051	-0.0000	-0.0000	-0.0000	-0.0000
23	0.0000	0.0001	0.	0.0014	0.0014
24	0.0000	-0.	0.0012	0.	-0.
25	-0.0000	-0.0014	0.	-0.0051	-0.0063
26	-0.0000	-0.0014	-0.	-0.0063	-0.0051
27	-0.0014	0.	0.0000	0.0000	-0.0000
28	-0.	-0.0000	-0.0001	-0.0000	0.0000
29	0.0063	-0.0000	-0.0000	-0.0000	0.0000
30	-0.0051	0.0000	0.0000	0.0000	-0.0000
31	-0.0000	0.0001	0.	0.0014	-0.0014
32	-0.0000	-0.	0.0012	-0.	-0.
33	0.0000	-0.0014	-0.	-0.0051	0.0063
34	-0.0000	0.0014	-0.	0.0063	-0.0051
35	0.	0.	0.	0.	0.
36	-0.	-0.	-0.0000	-0.0000	-0.
37	-0.	-0.	-0.0000	-0.0000	0.
38	0.0000	-0.	-0.	0.	0.
39	0.	0.	0.	0.0000	0.
40	-0.	0.	0.0000	-0.	-0.
41	-0.	-0.0000	-0.	-0.0002	0.
42	0.	-0.	-0.	0.	0.0000
43	0.	0.0001	0.0011	-0.	-0.
44	0.	-0.0011	-0.0067	0.	0.
45	0.	0.	0.	0.0007	0.
46	1.0000	0.	0.	0.	0.0007
47	0.	1.0000	0.	0.	0.
48	0.	0.	1.0000	0.	0.
49	0.	0.	0.	1.0000	0.
50	0.0007	0.	0.	0.	1.0000

TABLE XIV

$Re_2Cl_8^{2-}$ MO Charge Matrix: MO's Across and AO's Down

CHARGE MATRIX FOR MO-S WITH TWO ELECTRONS IN EACH

$Re_2Cl_8^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.7501	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0485	0.2826	0.0000	0.0000	0.0000	0.0000	0.0611	0.1124	-0.0000
2	0.2116	0.0000	0.0000	0.0000	0.0000	0.0000	0.4841	0.4509	0.0000	0.0000	0.0000	0.0000	0.3554	0.2220	0.0000
3	-0.0000	0.0000	0.8767	0.0000	0.0000	0.0000	0.7550	0.0000	0.0000	0.0411	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.8767	0.0000	0.0000	0.7550	0.0000	0.0000	0.0000	0.0000	0.0411	0.0000	-0.0000	0.0000	0.0000	-0.0000
5	0.0133	-0.0000	0.0000	0.0000	0.0000	0.0000	0.2994	0.0941	0.0000	0.0000	0.0000	0.0000	0.3247	0.5523	0.0000
6	0.0000	0.0000	0.0670	0.0000	0.0000	0.0924	0.0000	0.0000	0.0000	0.0002	0.8475	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.7915	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7507	0.0000	0.0000	0.0000
8	0.0000	0.0670	0.0000	-0.0000	0.0924	0.0000	0.0000	0.0000	0.8475	0.0002	0.0000	-0.0000	0.0000	-0.0000	-0.0000
9	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.8683	0.0000	0.8101
10	0.7501	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0484	0.2827	0.0000	0.0000	0.0000	0.0000	0.0611	0.1124	0.0000
11	0.2116	0.0000	0.0000	0.0000	0.0000	0.0000	0.4839	0.4511	0.0000	0.0000	0.0000	0.0000	0.3554	0.2220	0.0000
12	0.0000	0.0000	0.8767	0.0000	0.0000	0.7550	-0.0000	0.0000	0.0000	0.0411	0.0000	0.0000	0.0000	0.0000	0.0000
13	-0.0000	0.8767	0.0000	0.0000	0.7550	0.0000	0.0000	0.0000	0.0000	0.0411	0.0000	0.0000	-0.0000	-0.0000	0.0000
14	0.0133	0.0000	-0.0000	0.0000	0.0000	0.0000	0.2993	0.0942	0.0000	0.0000	0.0000	0.0000	0.3247	0.5523	-0.0000
15	0.0000	0.0000	0.0670	0.0000	0.0000	0.0924	0.0000	0.0000	0.0000	0.0002	0.8475	0.0000	0.0000	0.0000	0.0000
16	-0.0000	-0.0000	-0.0000	0.7915	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7507	0.0000	0.0000	0.0000
17	0.0000	0.0670	0.0000	0.0000	0.0924	0.0000	0.0000	0.0000	0.8475	0.0002	0.0000	-0.0000	0.0000	0.0000	0.0000
18	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8683	0.0000	0.8101
19	0.0062	0.0215	0.0000	0.0122	0.0363	0.0000	0.0150	0.0235	0.0093	0.0000	0.0121	0.0000	0.0061	0.0013	0.0000
20	-0.0000	0.0004	0.0000	0.0044	0.0024	0.0000	0.0002	0.0006	0.0071	0.0000	0.0084	0.0000	0.0453	0.0269	0.0000
21	0.0000	0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	0.0329	0.0000	0.0000	0.0475
22	0.0001	0.0013	0.0000	0.0354	0.0242	0.0000	0.0269	0.0190	0.0357	0.0000	0.0419	0.0000	0.0133	0.0001	0.0000
23	0.0062	0.0215	0.0000	0.0122	0.0363	0.0000	0.0149	0.0235	0.0093	0.0000	0.0121	-0.0000	0.0061	0.0013	0.0000
24	-0.0000	0.0004	0.0000	0.0044	0.0024	0.0000	0.0002	0.0006	0.0071	0.0000	0.0084	0.0000	0.0453	0.0269	0.0000
25	0.0000	0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	-0.0000	0.0329	0.0000	0.0000	0.0475
26	0.0001	0.0013	0.0000	0.0354	0.0242	0.0000	0.0269	0.0190	0.0357	0.0000	0.0419	0.0000	0.0133	0.0001	0.0000
27	0.0062	0.0215	0.0000	0.0122	0.0363	0.0000	0.0150	0.0235	0.0093	0.0000	0.0121	0.0000	0.0061	0.0013	0.0000
28	-0.0000	0.0004	0.0000	0.0044	0.0024	0.0000	0.0002	0.0006	0.0071	0.0000	0.0084	0.0000	0.0453	0.0269	0.0000
29	0.0000	0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	0.0329	0.0000	0.0000	0.0475
30	0.0001	0.0013	0.0000	0.0354	0.0242	0.0000	0.0269	0.0190	0.0357	0.0000	0.0419	-0.0000	0.0133	0.0001	0.0000
31	0.0062	0.0215	0.0000	0.0122	0.0363	0.0000	0.0149	0.0235	0.0093	0.0000	0.0121	-0.0000	0.0061	0.0013	0.0000
32	-0.0000	0.0004	0.0000	0.0044	0.0024	0.0000	0.0002	0.0006	0.0071	0.0000	0.0084	0.0000	0.0453	0.0269	0.0000
33	0.0000	0.0000	0.0050	-0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	-0.0000	0.0329	0.0000	0.0000	0.0475
34	0.0001	0.0013	0.0000	0.0354	0.0242	0.0000	0.0269	0.0190	0.0357	0.0000	0.0419	0.0000	0.0133	0.0001	0.0000
35	0.0062	0.0000	0.0215	0.0122	0.0000	0.0363	0.0150	0.0235	0.0000	0.0093	0.0121	-0.0000	0.0061	0.0013	0.0000
36	-0.0000	0.0000	0.0004	0.0044	0.0000	0.0024	0.0002	0.0006	0.0000	0.0071	0.0084	0.0000	0.0453	0.0269	-0.0000
37	0.0001	0.0000	0.0013	0.0354	0.0000	0.0242	0.0269	0.0190	0.0000	0.0357	0.0419	0.0000	0.0133	0.0001	-0.0000
38	0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	0.0000	0.0329	0.0000	0.0000	0.0475
39	0.0062	0.0000	0.0215	0.0122	0.0000	0.0363	0.0149	0.0235	0.0000	0.0093	0.0121	0.0000	0.0061	0.0013	0.0000
40	-0.0000	0.0000	0.0004	0.0044	0.0000	0.0024	0.0002	0.0006	0.0000	0.0071	0.0084	0.0000	0.0453	0.0269	0.0000
41	0.0001	0.0000	0.0013	0.0354	0.0000	0.0242	0.0269	0.0190	0.0000	0.0357	0.0419	-0.0000	0.0133	0.0001	0.0000
42	-0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	-0.0000	0.0329	0.0000	0.0000	0.0475
43	0.0062	0.0000	0.0215	0.0122	0.0000	0.0363	0.0150	0.0235	0.0000	0.0093	0.0121	-0.0000	0.0061	0.0013	0.0000
44	-0.0000	0.0000	0.0004	0.0044	0.0000	0.0024	0.0002	0.0006	0.0000	0.0071	0.0084	0.0000	0.0453	0.0269	0.0000
45	0.0001	0.0000	0.0013	0.0354	0.0000	0.0242	0.0269	0.0190	0.0000	0.0357	0.0419	0.0000	0.0133	0.0001	-0.0000
46	-0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	0.0000	0.0329	0.0000	0.0000	0.0475
47	0.0062	0.0000	0.0215	0.0122	0.0000	0.0363	0.0149	0.0235	0.0000	0.0093	0.0121	0.0000	0.0061	0.0013	0.0000
48	-0.0000	0.0000	0.0004	0.0044	0.0000	0.0024	0.0002	0.0006	0.0000	0.0071	0.0084	0.0000	0.0453	0.0269	0.0000
49	0.0001	0.0000	0.0013	0.0354	0.0000	0.0242	0.0269	0.0190	0.0000	0.0357	0.0419	-0.0000	0.0133	0.0001	0.0000
50	0.0000	0.0050	0.0000	0.0000	0.0134	0.0000	0.0000	0.0000	0.0034	0.0000	0.0000	0.0329	0.0000	0.0000	0.0475

	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
1	0.0000	0.0097	0.0000	0.0000	0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1998	0.0000	0.0000	0.0000
2	0.0000	0.0621	0.0000	0.0000	0.0287	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0864	0.0000	0.0000	-0.0000
3	0.0049	0.0000	0.0202	0.0000	0.0000	0.0061	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086
4	0.0723	0.0000	0.0000	0.0202	0.0000	0.0010	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0497
5	0.0000	0.0038	0.0000	0.0000	0.0739	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	0.0000
6	-0.0000	0.0000	0.0698	0.0000	-0.0000	0.1788	0.0285	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1494	0.0000	0.1869	0.0000	0.1121	0.0084	0.0000
8	-0.0000	0.0000	0.0000	0.0698	0.0000	0.0285	0.1788	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1317	0.0000	0.0000	0.1899	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0097	0.0000	0.0000	0.0046	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1998	0.0000	0.0000	0.0000
11	0.0000	0.0621	0.0000	0.0000	0.0287	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0864	0.0000	0.0000	0.0000
12	0.0049	0.0000	0.0202	0.0000	0.0000	0.0061	0.0010	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0086
13	0.0724	0.0000	0.0000	0.0202	0.0000	0.0010	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0497
14	0.0000	0.0038	0.0000	0.0000	0.0739	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	0.0000
15	-0.0000	-0.0000	0.0698	0.0000	0.0000	0.1788	0.0285	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1494	0.0000	0.1869	0.0000	0.0073	0.1132	0.0000
17	-0.0000	-0.0000	0.0000	0.0698	0.0000	0.0285	0.1788	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0063
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1317	0.0000	0.0000	0.1899	0.0000	0.0000	0.0000	0.0000	0.0000
19	0.0028	0.0009	0.0000	0.0019	0.0020	0.0000	0.0001	0.0000	0.0024	0.0000	0.0031	0.0151	0.4388	0.0310	0.3986	
20	0.0906	0.1229	0.0000	0.0300	0.0128	0.0386	0.2418	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
21	0.0108	0.0000	0.1015	0.0000	0.0000	0.0063	0.0010	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	0.0000	-0.0000	
22	0.1782	0.1073	0.0001	0.3214	0.2084	0.0145	0.0907	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0002	-0.0000	-0.0001	
23	0.0028	0.0009	0.0000	0.0019	0.0020	0.0000	0.0001	0.0000	0.0024	0.0000	0.0031	0.0151	0.0314	0.4391	0.3981	
24	0.0906	0.1229	0.0000	0.0300	0.0128	0.0386	0.2418	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
25	0.0108	0.0000	0.1016	0.0000	0.0000	0.0063	0.0010	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
26	0.1783	0.1073	0.0001	0.3213	0.2084	0.0145	0.0907	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0000	-0.0002	-0.0001	
27	0.0028	0.0009	0.0000	0.0019	0.0020	0.0000	0.0001	0.0000	0.0024	0.0000	0.0031	0.0151	0.4392	0.0313	0.3983	
28	0.0906	0.1229	0.0000	0.0300	0.0128	0.0386	0.2418	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
29	0.0108	0.0000	0.1015	0.0000	0.0000	0.0063	0.0010	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
30	0.1782	0.1073	0.0001	0.3214	0.2084	0.0145	0.0907	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0002	-0.0000	-0.0001	
31	0.0028	0.0009	0.0000	0.0019	0.0020	0.0000	0.0001	0.0000	0.0024	0.0000	0.0031	0.0151	0.0315	0.4383	0.3988	
32	0.0906	0.1229	0.0000	0.0300	0.0128	0.0386	0.2418	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
33	0.0108	0.0000	0.1016	0.0000	0.0000	0.0063	0.0010	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
34	0.1782	0.1073	0.0001	0.3213	0.2084	0.0145	0.0907	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0000	-0.0002	-0.0001	
35	0.0002	0.0009	0.0019	0.0000	0.0020	0.0001	0.0000	-0.0000	0.0024	0.0000	0.0031	0.0151	0.4390	0.0311	0.0688	
36	0.0061	0.1229	0.0300	0.0000	0.0128	0.2418	0.0386	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
37	0.0120	0.1074	0.3213	0.0001	0.2084	0.0907	0.0145	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0002	-0.0000	-0.0000	
38	0.1607	0.0000	0.0000	0.1016	0.0000	0.0010	0.0063	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
39	0.0002	0.0009	0.0019	0.0000	0.0020	0.0001	0.0000	0.0000	0.0024	-0.0000	0.0031	0.0151	0.0314	0.4388	0.0690	
40	0.0061	0.1229	0.0300	0.0000	0.0128	0.2418	0.0386	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
41	0.0120	0.1074	0.3214	0.0001	0.2084	0.0907	0.0145	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0000	-0.0002	-0.0000	
42	0.1607	0.0000	0.0000	0.1015	0.0000	0.0010	0.0063	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
43	0.0002	0.0009	0.0019	0.0000	0.0020	0.0001	0.0000	0.0000	0.0024	0.0000	0.0031	0.0151	0.4391	0.0311	0.0689	
44	0.0061	0.1230	0.0300	0.0000	0.0128	0.2418	0.0386	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
45	0.0120	0.1073	0.3213	0.0001	0.2084	0.0907	0.0145	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0002	-0.0000	-0.0000	
46	0.1607	0.0000	0.0000	0.1016	0.0000	0.0010	0.0063	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	
47	0.0002	0.0009	0.0019	0.0000	0.0020	0.0001	0.0000	0.0000	0.0024	-0.0000	0.0031	0.0151	0.0314	0.4387	0.0687	
48	0.0061	0.1230	0.0300	0.0000	0.0128	0.2418	0.0386	0.0000	0.0261	0.0000	0.0459	0.0719	-0.0000	-0.0000	-0.0000	
49	0.0120	0.1073	0.3214	0.0001	0.2084	0.0907	0.0145	0.0000	0.1842	0.0000	0.1542	0.0905	-0.0000	-0.0002	-0.0000	
50	0.1607	0.0000	0.0000	0.1015	0.0000	0.0010	0.0063	0.2171	0.0000	0.2025	0.0000	0.0000	-0.0000	-0.0000	-0.0000	

	46	47	48	49	50
1	0.0000	0.0000	0.0000	0.0675	0.2027
2	-0.0000	0.0000	0.0000	0.0175	-0.0027
3	0.0497	0.0704	0.0032	0.0000	0.0000
4	0.0086	0.0032	0.0704	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0151	0.0075
6	0.0063	0.0055	0.0003	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0011	0.0003	0.0055	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	-0.0000
10	0.0000	0.0000	0.0000	0.0675	0.2027
11	0.0000	0.0000	0.0000	0.0175	-0.0027

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0000	0.0000	0.2440	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0169	0.0000
2	0.0000	0.0000	0.0477	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0361	0.0000
3	0.0868	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0000	-0.0000	0.0035	0.0000	0.0000	0.0000	0.0724
4	0.0003	0.0868	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	-0.0000	-0.0000	0.0000	0.0035	0.0000	0.0000	0.0049
5	0.0000	0.0000	0.5662	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0461	0.0000
6	0.6901	0.0025	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.0019	0.0000	0.0075	0.0000	0.0000	0.0000	-0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000
8	0.0025	0.6901	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0019	0.0000	0.0075	0.0000	0.0000	-0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.2440	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0169	0.0000
11	0.0000	0.0000	0.0477	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0361	0.0000
12	0.0868	0.0003	0.0000	0.0000	-0.0000	0.0000	0.0001	0.0000	-0.0000	-0.0000	0.0035	0.0000	-0.0000	0.0000	0.0724
13	0.0003	0.0868	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0001	-0.0000	-0.0000	0.0000	0.0035	0.0000	0.0000	0.0049
14	0.0000	0.0000	0.5662	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0461	0.0000
15	0.6901	0.0025	-0.0000	0.0000	0.0000	-0.0000	0.0005	0.0001	0.0019	0.0000	0.0075	0.0000	0.0000	0.0000	-0.0000
16	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000
17	0.0025	0.6901	0.0000	0.0000	0.0000	0.0000	0.0001	0.0005	0.0000	0.0019	0.0000	0.0075	0.0000	0.0000	-0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000
19	0.0000	0.0001	0.0063	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0002
20	0.0003	0.0896	0.0092	0.0000	0.0000	0.2194	0.0286	0.1365	0.0002	0.0305	0.0006	0.2967	0.1957	0.2101	0.0061
21	0.0007	0.0000	0.0000	0.2502	0.2499	0.0000	0.1633	0.0343	0.3051	0.0021	0.1921	0.0004	0.0000	0.0000	0.1607
22	0.0001	0.0194	0.0199	0.0000	0.0000	0.0305	0.0237	0.1132	0.0011	0.1600	0.0000	0.0046	0.0540	0.0146	0.0120
23	0.0000	0.0001	0.0063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0002
24	0.0003	0.0896	0.0092	0.0000	0.0000	0.2194	0.0286	0.1365	0.0002	0.0305	0.0006	0.2967	0.1957	0.2101	0.0061
25	0.0007	0.0000	0.0000	0.2499	0.2501	0.0000	0.1633	0.0342	0.3051	0.0021	0.1921	0.0004	0.0000	0.0000	0.1607
26	0.0001	0.0194	0.0199	0.0000	0.0000	0.0305	0.0237	0.1132	0.0011	0.1600	0.0000	0.0046	0.0540	0.0146	0.0120
27	0.0000	0.0001	0.0063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0002
28	0.0003	0.0896	0.0092	0.0000	0.0000	0.2196	0.0286	0.1364	0.0002	0.0305	0.0006	0.2967	0.1957	0.2101	0.0061
29	0.0007	0.0000	0.0000	0.2501	0.2499	0.0000	0.1634	0.0343	0.3051	0.0021	0.1921	0.0004	0.0000	0.0000	0.1607
30	0.0001	0.0194	0.0199	0.0000	0.0000	0.0304	0.0238	0.1132	0.0011	0.1600	0.0000	0.0046	0.0540	0.0146	0.0120
31	0.0000	0.0001	0.0063	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0002
32	0.0003	0.0896	0.0092	0.0000	0.0000	0.2196	0.0286	0.1364	0.0002	0.0305	0.0006	0.2967	0.1957	0.2101	0.0061
33	0.0007	0.0000	0.0000	0.2499	0.2501	0.0000	0.1633	0.0343	0.3051	0.0021	0.1921	0.0004	0.0000	0.0000	0.1607
34	0.0001	0.0194	0.0199	0.0000	0.0000	0.0304	0.0238	0.1133	0.0011	0.1600	0.0000	0.0046	0.0540	0.0146	0.0120
35	0.0001	0.0000	0.0063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0028
36	0.0896

Fig. 1 - Molecular coordinate system used to calculate the overlap integrals listed in Table XIII.

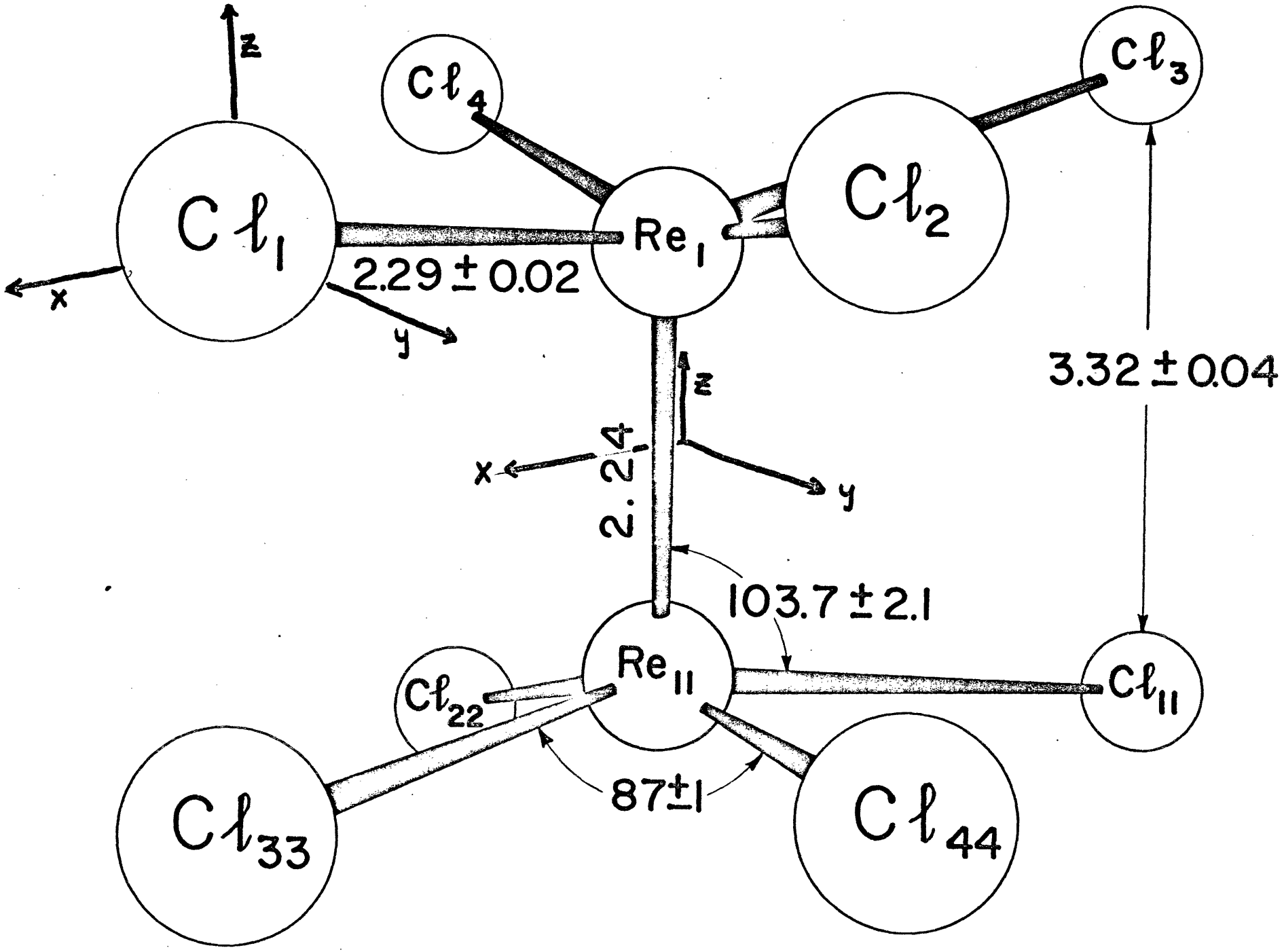
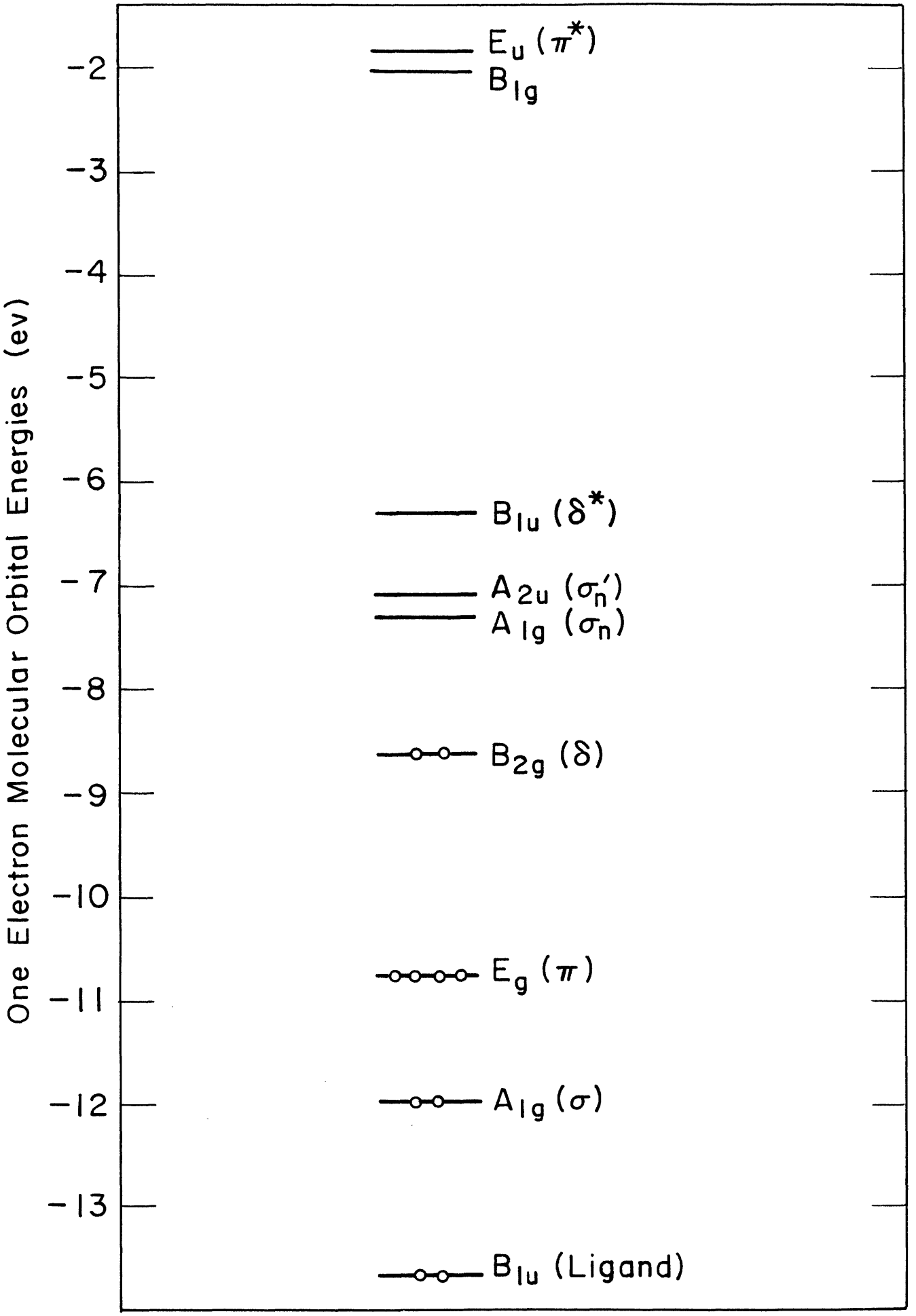

z
Cl4
Cl3
Cl1
Re1
Cl2
2.29 ± 0.02
x
y
z
3.32 ± 0.04
x
2.24
y
103.7 ± 2.1
Re11
Cl11
Cl22
87±1
Cl33
Cl44

Fig. 2 - Partial one-electron MO diagram for $Re_2Cl_8^{2-}$.


One Electron Molecular Orbital Energies (ev)
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
E_u (π^*)
B_{1g}
B_{1u} (δ^*)
A_{2u} (σ_n')
A_{1g} (σ_n)
B_{2g} (δ)
E_g (π)
A_{1g} (σ)
B_{1u} (Ligand)

CHAPTER IV

REFERENCES

1. F. A. Cotton, N. F. Curtis, B. F. G. Johnson and W. R. Robinson, Inorg. Chem., 4, 326 (1965).
2. Chapter III of this thesis.
3. F. A. Cotton, N. F. Curtis and W. R. Robinson, Inorg. Chem., 4, 1696 (1965).
4. F. A. Cotton and W. R. Robinson, unpublished work.
5. J. H. van Vleck, J. Chem. Phys., 2, 22 (1934).
6. J. C. Slater, Phys. Rev., 36, 57 (1930).
7. F. Herman and S. Skillman, Atomic Structure Calculations, Prentice-Hall, Englewood Cliffs, N.J., 1963.
8. Chapter II of this thesis.
9. R. E. Watson and A. J. Freeman, Phys. Rev., 123, 521 (1961).
10. R. E. Watson and A. J. Freeman, Phys. Rev., 120, 1125 (1960).
11. C. E. Moore, Atomic Energy Levels, U. S. National Bureau of Standards Circular, 467, 1949 and 1952.
12. J. Hinze and H. H. Jaffe, J. Am. Chem. Soc., 84, 540 (1962).
13. R. Mulliken, J. Chem. Phys., 46, 497 (1949).
14. M. Wolfsberg and L. Helmholz, J. Chem. Phys., 20, 837 (1952).
15. M. D. Newton, F. P. Boer, W. E. Palke and W. N. Lipscomb, Proc. Natl. Acad. Sci., 53, 1089 (1965).
16. W. N. Lipscomb, private communication.
17. Same method utilized in Chapter II.

18. W. R. Robinson, Ph.D. thesis, M.I.T. (1966).

19. F. A. Cotton, C. B. Harris and W. R. Robinson, unpublished work.

20. F. A. Cotton, Inorg. Chem., 4, 334 (1965).

21. R. W. Mulliken, J. Chem. Phys., 23, 1833 (1955).

CHAPTER V

CORRELATION OF NUCLEAR QUADRUPOLE COUPLING CONSTANTS WITH MOLECULAR ELECTRONIC STRUCTURE USING MOLECULAR ORBITAL THEORY

Derivation of eqQ.

Direct quadrupole spectroscopy is potentially a more useful tool for the chemist than the relatively limited literature to date might suggest.[1] Although experimental problems have been troublesome in the past, recent work[2] has considerably advanced the "state of the art". From the theoretical or interpretative side, chemists have depended almost exclusively upon the basic considerations and relationships concerning the connection between chemical bonding and quadrupole resonance frequencies put forward by Townes and Dailey.[3]

It is the purpose of this chapter to derive, in a very general way, an expression for the nuclear quadrupole coupling constant, $eq_\alpha Q_\alpha$, for a given atom, α, possessing a nuclear quadrupole moment, Q_α, in a molecular field gradient of magnitude q_α at nucleus α. The chief features of the derivation of $eq_\alpha Q_\alpha$, which leads to a result which is more general than the Townes and Dailey relationship,[3] are the following. First, no hybridization of s and p orbitals is assumed. Secondly, a basis set of orthogonal molecular orbitals, ψ^K, that span all atoms in the molecule is used. The expression derived does, however, reduce to the Townes and Dailey relationship under appropriate limiting conditions.

The desirability of an expression giving $eq_\alpha Q_\alpha$ in terms of the LCAO-MO expressions for occupation numbers of a set of molecular

orbitals for the entire molecule is, in general terms, selfevident. Such an expression should be of particular utility in the case of many transition metal complexes, for which LCAO-MO treatments of the electronic structure are becoming increasingly of interest, since a means of evaluating such treatments in terms of their ability to predict physical observables other than electronic energy differences is conspicuously needed.

Let $\phi_i (i = 1 \cdots n)$ be the atomic orbitals used to construct the molecular orbitals, ψ^K $(K = 1 \cdots n)$ in the LCAO-MO approximation, Eq. (1), in which

$$\psi^K = \sum_{i=1}^{n} C_i{}^K \phi_i \qquad (1)$$

$C_i{}^K$ is the coefficient of the ith atomic orbital in the Kth molecular orbital and the i's span all atomic orbitals of the atoms in the molecule. It is convenient to require that all atomic orbitals on the same atom be orthogonal. q_α, the field gradient existing at the location of a nucleus α (or at any other point in the molecule), is now a property of only (1) the distribution of electrons in the molecule and (2) the distribution of the other nuclei in the molecule. It can, therefore, be expressed as a sum of components, $q_\alpha{}^K$, due to the electrons in each of the molecular orbitals, ψ^K, plus a resultant of the charges of the nuclei, $q_\alpha{}^{\text{nucl.}}$, viz.,

$$q_\alpha = \sum_K N^K q_\alpha{}^K + q_\alpha{}^{\text{nucl.}} \qquad (2)$$

in which N^K is the number of electrons in ψ^K. The term $q_\alpha{}^K$ must have the form[1] (3).

$$q_\alpha^K = e \int \psi^{K*} \left(\frac{3\cos^2\theta - 1}{r_\alpha^3}\right) \psi^K d\tau \qquad (3)$$

where r_α represents a distance measured from nucleus α and the angle θ is measured relative to a fixed direction, usually along a bond or along the bisector of a bond angle, but, in general along the Z axis of a molecular coordinate system.

By combining (1) and (2) we obtain (4):

$$q_\alpha = \sum_K \sum_i \sum_j N^K C_i^K C_j^K q_\alpha^{ij} + q_\alpha^{\text{nucl.}} \qquad (4)$$

where

$$q_\alpha^{ij} = e \int \phi_i^* \left(\frac{3\cos^2\theta - 1}{r_\alpha^3}\right) \phi_j d\tau \qquad (5)$$

The terms in the summation (4) are of four types, as shown explicitly in (6). The q_α^{ii}, in which i refers to orbitals on atom α, are one-center integrals. The q_α^{ij} and q_α^{jj}, where j denotes an orbital not on atom α, are two-center integrals. The q_α^{jk} in which j and k denote orbitals on different atoms, neither of which is atom α, are three-center integrals.

$$q_\alpha = \sum_K N^K \Big\{ \sum_i |C_i^K|^2 q_\alpha^{ii} + \sum_j |C_j^K|^2 q_\alpha^{jj} + \sum_{i,j} C_i^K C_j^K q_\alpha^{ij} + \sum_{j,k} C_j^K C_k^K q_\alpha^{jk} \Big\} + q_\alpha^{\text{nucl.}} \qquad (6)$$

Up to this point no approximations (other than the LCAO-MO approximation itself) have been made. However, the evaluation of all ($\sim N^3$, for N atomic orbitals in the basis set) integrals in (4) and (6) would be impractical for all but the simplest molecules. Moreover, these expressions would be applicable only to those few small molecules in which MO calculations have been carried out using as a basis set the core orbitals[4] as well as the valence shell orbitals of all atoms. It is therefore virtually a necessity to simplify (4) and (6), without, however, sacrificing too much in generality or accuracy.

The following simplifications appear suitable:

(1) The sum over all core orbitals on atom α will be designated P. For unperturbed core orbitals there would be spherical symmetry and hence no contribution to q_α, but because the core suffers polarization, an effect well known as the Sternheimer correction,[5] P has a finite value, the disposition of which will be considered later.

(2) The sum over all the two-center integrals, q_α^{jj} in (6), for which j refers to a <u>core</u> orbital, plus $q_\alpha^{\text{nucl.}}$ will be approximated by q_α^{core}, a resultant of the contributions of the cores of all atoms in the molecule except atom α, the charge on each core being taken as the charge on that atom when its valence-shell electrons are removed. Due to the compactness of cores, nucleus α can be taken to lie entirely outside the electron density of all of them to a high degree of accuracy; thus we are essentially invoking Gauss' theorem.

(3) The sum over all non-core two-center terms, q_α^{jj}, plus $1/2 \sum_{i,j} C_i^K C_j^K q_{ij}$ is assumed to be equal to the negative of q_α^{core}, defined above. This is equivalent to assuming that the non-core electrons of all atoms but atom α together with half the overlap populations of all bonds formed by atom α exactly screen the nucleus of α from the potential due to the cores of all other atoms in the molecule. This will not, of course, be precisely true, but the error arising from this assumption can be shown to be of the order of only a few percent. This error was estimated by computing the field gradient at one Cl atom due to the net effective charges on all other atoms of $PtCl_4^{2-}$, the effective charges being those provided by a population analysis and charge distribution computation using the eigenvectors provided by an LCAO-MO calculation for this complex. The result in this particular case was about 2.5% of the total field gradient.

(4) All three-center integrals are neglected entirely, since they are inherently small and decrease as a function of r_α^3.

With these four simplifications, we now write (4) and (6) in the following way:

$$q_\alpha = \sum_K N^K \{\sum_i |C_i^K|^2 \bar{q}_\alpha^{ii} + \sum_{\substack{i,j \\ i \neq j}} C_i^K C_j^K \bar{q}_\alpha^{ij}\} + P \qquad (7)$$

where the bar indicates that i and j are summed only over non-core orbitals.

We now introduce a Mulliken-type[6] relationship, namely,

$$\bar{q}_\alpha^{ij} = S_{ij} \bar{q}_\alpha^{ii} \qquad (8)$$

which permits (7) to be written as:

$$q_\alpha = \sum_i f_i \bar{q}_\alpha^{ii} + P \tag{9}$$

where

$$f_i = \sum_K N^K \{|c_i^K|^2 + c_i^K \sum_{j(>i)} c_j^K S_{ij}\}$$

and f_i is simply a molecular orbital expression for the occupation of ϕ_i.

When (9) is multiplied by eQ_α and terms rearranged slightly, (10) is obtained.

$$eq_\alpha Q_\alpha = \sum_i f_i \{e\bar{q}_\alpha^{ii} Q_\alpha + (eQ_\alpha P/\Sigma f_i)\}. \tag{10}$$

If we assume, following Townes and Dailey,[3] that the polarization term, $P/\Sigma f_i$, though inherently large, varies negligibly from molecule to molecule, and is incorporated in the experimental value for the free atom, then the term in the {} brackets in (10) may be replaced by the known quantity for the free atom. For Cl^{35}, for example, the value 109.7 mc/sec is used for p electrons, N^K being simultaneously replaced by $2-N^K$ since the atom has one hole in a p shell. Thus, for Cl^{35} we finally arrive at (11).

$$eqQ = 109.7 \sum_i \sum_K (2-N^K)\{|c_i^K|^2 + \sum_{j(>i)} c_i^K c_j^K S_{ij}\} \tag{11}$$

The expression (11) is the molecular orbital analog to the valence bond theory expression of Townes and Dailey, and incorporates the same

basic approximations, except, of course, for those which stem directly from the valence bond formalism itself. There are some important advantages to Eq. (11), however. First, no assumption is, or need be, made as to s-p hybridization. Second, no assumption is, or need be, made concerning the extent of π-bonding. Third, the asymmetry parameter, η, can be predicted along with eqQ. Of course, more computation than in the Townes and Dailey treatment is required in order to realize these potential advantages.

In order to illustrate the applicability of the expressions derived here in utilizing measured nuclear quadrupole coupling constants to evaluate or monitor the results of LCAO-MO calculations for transition metal complexes, some relevant figures are presented in Table 1. The molecular orbital calculations themselves will be fully described in Chap. VI. Some results not directly connected with the problem of the quadrupole coupling constants are presented to indicate the general nature of the results.

It may be seen that in these cases, the observed and calculated values of eqQ for Cl^{35} as a ligand agree fairly well. The trend through the series of hexachlorometallate(IV) complexes is particularly well represented.

TABLE I

Comparison with Experiment[a]

		$ReCl_6^{2-}$	$OsCl_6^{2-}$	$IrCl_6^{2-}$	$PtCl_6^{2-}$	$PtCl_4^{2-}$
1.	M-Cl bond order, calcd.	0.438	0.454	0.475	0.475	0.403
2.	M charge, calcd.	1.3	1.2	0.90	0.69	0.44
3.	% M d orbital in T_{2g} MO's, calcd.	89	90	85	81	--
	obs.	--	--	~70-85[b]	--	--
4.	d-orbital splitting, in ev. calcd.	4.9	3.4	4.1	4.3	--
	obs.	4.2[c]	--	--	~ 3.6[c]	--
5.	eqQ for Cl^{35}, in mc/sec calcd.	32	38	44	51	34
	obs.	27.8[d]	33.8[e]	41.6[e]	52.0[f]	36.1[g]
6.	Asymmetry parameter, calcd.	--	--	--	--	0.025

a. Calculated values of parameters 1-4 are obtained from LCAO-MO calculations to be fully described in Chap. VI. They are given here to show that reasonable values for these as well as eqQ are simultaneously obtained.

b. ~ 70% from hyperfine splitting; ~ 85 from g value. Cf., B. N. Figgis, Introduction to Ligand Fields, John Wiley, N.Y., 1966.

c. C. J. Ballhausen, Introduction to Ligand Field Theory, McGraw-Hill, N.Y., 1962.

d. R. Ikeda, D. Nakamura, and M. Kubo, J. Phys. Chem., 69, 2101 (1965).

e. Idem., Bull. Chem. Soc. Japan, 36, 1056 (1963).

f. D. Nakamura, Y. Kurita, K. Ito, and M. Kubo, J. Amer. Chem. Soc., 82, 5783 (1960).

g. E. P. Marram, E. J. McNiff, and J. L. Ragle, J. Phys. Chem., 67, 1719 (1963).

REFERENCES

1. For general background see Das, T. P., and E. L. Hahn, Nuclear Quadrupole Resonance Spectroscopy, Academic Press, N.Y., 1958, and Semin, G. K., and E. I. Fedin, Zhurnal Strukturnoi Khimii, 1, 252, 464 (1960).

2. Peterson, G. E., and P. M. Bridenbaugh, Rev. Sci, Instr., 35, 698 (1964).

3. Townes, C. H., and B. P. Dailey, J. Chem. Phys., 17, 782 (1949).

4. The core is defined to include the nucleus plus all filled orbitals of lower energy than those of the valence shell. Thus, the core of Pt includes the orbitals 1s, 2s, 2p, ... 5s, 5p, and 5d, 6s, and 6p being considered as valence orbitals.

5. Sternheimer, R. M., Phys. Rev., 84, 244 (1951); 86, 316 (1952); 95, 736 (1954).

6. Mulliken, R. S., J. Chim. Phys., 46, 497, 675 (1949).

CHAPTER VI

MOLECULAR ORBITAL CALCULATION ON MCl_6^{2-}

(M =Re(IV), Os(IV), Ir(IV) and Pt(IV))

INTRODUCTION

In the preceding chapters (II and IV) a molecular orbital method was developed and applied to the calculation of molecular properties. An interpretation of nuclear quadrupole resonance, based on the principles of molecular orbital theory, was derived in Chapter V and applied to the series MCl_6^{2-} (M = Re(IV), Os(IV), Ir(IV) and Pt(IV)). This chapter will deal with the specifics of the MO calculations of this series and with the application of these MO's to the verification and prediction of molecular properties associated with these molecules.

ORBITAL BASIS SET

The metal 6s, 6p and 5d atomic orbitals and the Cl 3s and 3p atomic orbitals, a total of 33 wavefunctions, were used to construct molecular orbitals in the LCAO-MO approximation.[1] All wavefunctions were expressed as Slater Nodeless Orbitals (STO).[2] The functional form of STO orbitals is given by Eq. (2) in Chapter II. The shielding parameters, α_i (Eq. (2), Chapter II), for the basis set in this calculation were determined in precisely the same fashion as in the $PtCl_4^{2-}$ calculation (Chapter II).

Herman-Skillman radial wavefunctions[3] were used for the metal 6s and 5d atomic orbitals. The radial portion of the 6p atomic orbitals were approximated as a 6s atomic orbital. Watson-Freeman[4] wavefunctions were used for the Cl 3s and 3p radial wavefunctions.

The metal-to-chloride inter-nuclear distance[5] was 2.36Å. in all cases.*

DIAGONAL MATRIX ELEMENTS, H_{ii}

The diagonal Hamiltonian matrix elements,** H_{ii}, for the metal orbitals were approximated by Valence State Ionization Potentials (VSIP) listed in Table I. Since the spectral assignment of the states listed in Moore's Tables[6] are incomplete, we assumed that there was a linear decrease in the VSIP's of 2.5 ev. going from Re to Pt.‡

CALCULATIONS

All overlap integrals, S_{ij}, were calculated and all off-diagonal matrix elements, H_{ij}, were approximated by the MWH‡‡ approximation with a Helmholz factor, K, equal to 1.80. The secular equations

---

* Although there is a slight variation in this value depending on the cation of the respective complex, we feel the variation is too small to appreciably effect the final results.

** See Chapter II for a complete discussion of these matrix results.

‡ This somewhat parallels the behavior of the first ionization potentials of the neutral metals.[6]

‡‡ See Chapter II for details.

(Chapter II, Eq. (1)) were solved and the MO energies and eigenvectors were determined in each case ($ReCl_6^{2-}$, $OsCl_6^{2-}$, $IrCl_6^{2-}$, $PtCl_6^{2-}$). The same dependence of H_{ij} with charge was assumed in these calculations as in the $PtCl_4^{2-}$ and $Re_2Cl_8^{2-}$ MO calculations (Chapter II and IV).

For each molecule, the calculation was recycled to a self-consistency of a 0.01 charge unit on the metal.

All overlap integrals are tabulated in Tables II-V for the Re, Os, Ir and Pt cases respectively; all eigenvectors for the final cycle are listed in Tables VI-IX; all molecular orbital energies and orbital occupations are listed in Table X; all Mulliken overlap populations[7,8] and reduced overlap populations or bond orders are listed in Tables XI-XIV; all MO charge matrix elements are listed in Tables XV-XVIII; and all orbital occupations and atomic charges are listed in Table XIX.

ELECTRONIC SPECTRA

The semiempirical MO theory utilized in these calculations is not well suited for quantitatively describing electronic spectra because it does not explicitly include electron repulsion integrals in the Hamiltonian. However, it can provide useful information about trends in a given series of related molecules.

Among other things, Table XX lists the energies of the last occupied MO's, $\epsilon_{t_{2g}}$; delta (Δ), the separation between the t_{2g} and

e_g MO's, and the charge transfer energies, $t_{2u} \rightarrow t_{2g}$.

The experimental Δ for all members of the series is about 4.1 ev.[9] In view of the sensitivity[10] of the calculated Δ to the values of the variable parameters in the theory, it is gratifying to calculate an average* Δ equal to 4.2 ev.

Although no apparent trend is evident in either the experimental or calculated Δ, there is definitely a trend in the charge transfer spectra, $t_{2u} \rightarrow t_{2g}$, across the series. Jorgensen[9] has pointed out that the $t_{2u} \rightarrow t_{2g}$ transition decreases about 0.75 ev. for each new electron in the partly filled t_{2g} molecular orbital with metals of a constant oxidation number. For the series treated in this chapter the experimental differences[9] in the $t_{2u} \rightarrow t_{2g}$ transition for Re(IV) to Os(IV) and Os(IV) to Ir(IV) are about 0.9 ev. and 0.6 ev. respectively. The calculated differences are in close agreement being 0.87 ev. and 0.39 ev. respectively.

It is interesting to note that the general decrease in the charge transfer energies parallels the general decrease in the calculated t_{2g} MO energies, $\epsilon_{t_{2g}}$. In the framework of Extended Hückel Theory, $\epsilon_{t_{2g}}$ represents the calculated first ionization potentials of the molecules. There are no experimental ionization

---

* Obtained by averaging Δ's of the four members of the series in Table XX.

---

potentials available for this series. However, it would not be surprising if future experiments paralleled the calculated $\epsilon_{t_{2g}}$ behavior since it is known[11,12] that the effective charge of the metal decreases from $ReCl_6^{2-}$ to $PtCl_6^{2-}$ resulting in a decrease of the electron-nuclear attraction energies.

CHARGE DISTRIBUTIONS AND METAL-CHLORIDE BOND ORDERS

An important aspect of the results in Table XX is the uniform decrease of the effective metal charge in these complexes going from $ReCl_6^{2-}$ to $PtCl_6^{2-}$. A general decrease in charge is exactly what one would expect. Nuclear quadrupole resonance (nqr) data[11,12] provides direct evidence for the validity of this trend.

The similarity of the metal-chloride (M-Cl) bond orders or covalencies (Table XX) is intriguing when juxtaposed with the effective metal charge decrease. The lack of an appreciable increase in the M-Cl bond order with a substantial metal charge decrease results from the increased occupation of the antibonding t_{2g} MO going across the series. When bond order is reduced to its sigma (σ) and pi (π) contributions, one notes (Table XX) a general increase in σ covalency across the series resulting from an electron flow from the Cl $3p_\sigma$ orbitals. This results in decreasing the effective metal charge across the series. However, the antibonding character of the t_{2g} electron added to each member in the series, causes a decrease in the M-Cl π-bond order. The inherent symmetry

of the π orbitals do not provide as effective a mechanism for Cl to metal charge flow as the σ orbitals. Consequently, the effective metal charge decreases across the series via electron flow from the Cl p_σ orbital. This results in a net increase in σ bond covalency. Since, however, the t_{2g} MO is a antibonding π-type orbital, there is an increased negative π-bond order across the series. This, to a large extent, cancels out the increased σ bond order increase resulting in a more uniform total metal-chloride bond order for the compounds listed.

Finally, it is interesting to note that the decrease in the effective metal charge across the series is consistent with the nephalauxetic effect.[13,14]

SPIN DENSITIES

With the exception of $PtCl_6^{2-}$ which has filled t_{2g} MO's, all other complexes in Table XX have one or more unpaired electrons. As such, they are subject to esr studies. The only esr study available in the series is that for $IrCl_6^{2-}$.[15,16] The Cl^{35} hyperfine has been interpreted as arising from a spin density of only 70% on the Ir. The g value indicates that about 85% of the spin density is on the Ir.

One can calculate the spin density on the metals by squaring the t_{2g} MO's and obtaining the Mulliken overlap population[7,8] (Tables XI-XIV). The ability to calculate reasonable spin densities

(Table XX) from the t_{2g} Mo coefficients indicates that this MO method properly estimates the percent of Cl p_π bonding in the $IrCl_6^{2-}$ case. The general trend of increased ligand participation in the t_{2g} MO across the series (Table XX) could be verified in the future with esr studies on the $ReCl_6^{2-}$ and $OsCl_6^{2-}$ complexes.

The verification of Cl p_σ bonding to the metals is provided by nuclear quadrupole resonance studies.

NUCLEAR QUADRUPOLE RESONANCE (nqr) COUPLING CONSTANTS (eqQ)

In nuclear quadrupole resonance one measures transitions between nuclear spin states which are split by the interaction of the nucleus with the electric field produced by the electrons. Consequently, the electron distribution in well-defined atomic and molecular systems containing quadrupolar nuclei can be measured. Because the resonance frequency is dependent upon the local electronic environment of the nucleus, nqr, like esr, sometimes affords the only feasible physical method for the elucidation of electronic structure.

The interpretation of nqr spectra of halide ions has always been done in terms of a valence bond approach[17] (the well-known Townes-Dailey treatment), but for complexes in particular, and other compounds as well, a molecular orbital treatment would be far more useful since it would tie in with the general picture of electronic structures of complexes and with the results of other kinds of

measurements (e.g., esr, nmr), and would be more flexible. Such a theory was developed in Chapter V. It will now be applied to the molecules treated in this chapter.

Using Eq. (11) of Chapter V, the nqr relationships[18] between Cl p_σ and p_π electrons, the eigenfunctions or MO coefficients listed in Tables VI-IX, and the overlap integrals listed in Tables II-V, we calculated the nqr coupling constants, eqQ, tabulated in Table XX.

The excellent agreement between calculated and observed eqQ's substantiates our belief that the MO method employed gives reasonable predictions and explanations of the bonding properties in these complexes. Furthermore, the increase in eqQ across the series verifies the contention that the effective metal charge decreases across the series via electron donation through the Cl $3p_\sigma$ orbitals.

The occupation of the Cl orbitals is given in Table XX. Note the decrease in the number of Cl $3p_\sigma$ electrons across the series. The Cl 3s occupation stays constant, presumably because (1) the Cl 3s orbital energy is very stable with respect to the 3p, and (2) the Cl 3p radial wavefunctions is more diffuse than the 3s wavefunction.

TABLE I

MCl_6^{2-} MO Input Parameters:

N = principle quantum number; L = angular momentum quantum number: The orbital correspondence is:

M	Sigma	Orbitals	
0	0	z	p
1	0	x	
1	1	y	
0	0	z^2	d
1	0	xz	
2	0	x^2-y^2	
1	1	yz	
2	1	xy	

Input Parameters

ORBITAL	ATOM	N	L	M	SIGMA	Coordinates in Å X	Y	Z	$ReCl_6^{2-}$ Orb. EXP	$ReCl_6^{2-}$ (Hii) ALPHA	$OsCl_6^{2-}$ Orb. EXP	$OsCl_6^{2-}$ (Hii) ALPHA	$IrCl_6^{2-}$ Orb. EXP	$IrCl_6^{2-}$ (Hii) ALPHA	$PtCl_6^{2-}$ Orb. EXP	$PtCl_6^{2-}$ (Hii) ALPHA
1	1	6	0	0	0	0.	0.	0.	2.500	-8.67	2.540	-9.50	2.500	-10.33	2.580	-11.16
2	1	6	1	0	0	0.	0.	0.	2.200	-4.22	2.240	-5.05	2.200	-5.88	2.280	-6.71
3	1	6	1	1	0	0.	0.	0.	2.200	-4.22	2.240	-5.05	2.200	-5.88	2.280	-6.71
4	1	6	1	1	1	0.	0.	0.	2.200	-4.22	2.240	-5.05	2.200	-5.88	2.280	-6.71
5	1	5	2	0	0	0.	0.	0.	2.920	-9.48	3.220	-10.31	3.125	-11.14	3.135	-11.97
6	1	5	2	1	0	0.	0.	0.	2.920	-9.48	3.220	-10.31	3.125	-11.14	3.135	-11.97
7	1	5	2	2	0	0.	0.	0.	2.920	-9.48	3.220	-10.31	3.125	-11.14	3.135	-11.97
8	1	5	2	1	1	0.	0.	0.	2.920	-9.48	3.220	-10.31	3.125	-11.14	3.135	-11.97
9	1	5	2	2	1	0.	0.	0.	2.920	-9.48	3.220	-10.31	3.125	-11.14	3.135	-11.97
10	2	3	0	0	0	2.360000	0.	0.	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
11	2	3	1	0	0	2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
12	2	3	1	1	0	2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
13	2	3	1	1	1	2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
14	3	3	0	0	0	-2.360000	0.	0.	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
15	3	3	1	0	0	-2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
16	3	3	1	1	0	-2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
17	3	3	1	1	1	-2.360000	0.	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
18	4	3	0	0	0	0.	2.360000	0.	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
19	4	3	1	0	0	0.	2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
20	4	3	1	1	0	0.	2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
21	4	3	1	1	1	0.	2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
22	5	3	0	0	0	0.	-2.360000	0.	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
23	5	3	1	0	0	0.	-2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
24	5	3	1	1	0	0.	-2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
25	5	3	1	1	1	0.	-2.360000	0.	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
26	6	3	0	0	0	0.	0.	2.360000	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
27	6	3	1	0	0	0.	0.	2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
28	6	3	1	1	0	0.	0.	2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
29	6	3	1	1	1	0.	0.	2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
30	7	3	0	0	0	0.	0.	-2.360000	2.200	-23.45	2.200	-23.45	2.200	-23.45	2.200	-23.45
31	7	3	1	0	0	0.	0.	-2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
32	7	3	1	1	0	0.	0.	-2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38
33	7	3	1	1	1	0.	0.	-2.360000	1.820	-14.38	1.820	-14.38	1.820	-14.38	1.820	-14.38

TABLE II

$ReCl_6^{2-}$ Overlap Integral Matrix

TOTAL OVERLAP MATRIX

$ReCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1784	-0.	-0.2716	-0.	0.1784	-0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1475	-0.	0.	0.	0.1475
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.3334	-0.	-0.3661	-0.	0.3334	0.
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.1475	-0.	-0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.0568	0.	0.0896	0.	-0.0568	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.0826	-0.	0.	-0.	-0.0826
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.0984	-0.	-0.1552	-0.	0.0984	-0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	-0.	0.	-0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	0.	-0.	0.
10	0.1784	0.	0.3334	0.	-0.0568	0.	0.0984	0.	0.	1.0000	0.	0.	0.	0.0826	0.
11	-0.	0.1475	-0.	0.	0.	0.0826	-0.	0.	0.	0.	1.0000	0.	0.	0.	0.0004
12	-0.2716	-0.	-0.3661	-0.	0.0896	-0.	-0.1552	-0.	-0.	0.	0.	1.0000	0.	-0.0010	0.
13	-0.	0.	-0.	0.1475	0.	0.	-0.	0.	0.0826	0.	0.	0.	1.0000	-0.	-0.
14	0.1784	0.	-0.3334	-0.	-0.0568	-0.	0.0984	-0.	0.	0.0002	0.	-0.0010	-0.	1.0000	0.
15	-0.	0.1475	0.	-0.	0.	-0.0826	-0.	-0.	0.	-0.	0.0004	0.	-0.	0.	1.0000
16	0.2716	0.	-0.3661	-0.	-0.0896	-0.	0.1552	-0.	0.	0.0010	0.	-0.0040	-0.	0.	0.
17	0.	-0.	-0.	0.1475	-0.	0.	0.	-0.	-0.0826	0.	-0.	-0.	0.0004	0.	0.
18	0.1784	0.	0.	0.3334	-0.0568	0.	-0.0984	0.	0.	0.0078	0.	-0.0189	0.0189	0.0078	0.
19	-0.	0.1475	-0.	-0.	0.	0.	0.	0.0826	-0.	0.0101	-0.	-0.	-0.	0.	0.0101
20	-0.	-0.	0.1475	0.	-0.	-0.	-0.	-0.	0.0826	0.0189	-0.	0.0274	0.0375	-0.0189	-0.
21	-0.2716	-0.	0.	-0.3661	0.0896	-0.	0.1552	-0.	0.	-0.0189	-0.	0.0375	-0.0274	0.0189	0.
22	0.1784	0.	0.	-0.3334	-0.0568	0.	-0.0984	-0.	-0.	0.0078	0.	-0.0189	-0.0189	0.0078	0.
23	-0.	0.1475	0.	0.	0.	0.	0.	-0.0826	-0.	-0.	0.0101	0.	-0.	-0.	0.0101
24	-0.	0.	0.1475	0.	0.	0.	0.	-0.	-0.0826	0.0189	0.	-0.0274	-0.0375	0.0189	0.
25	0.2716	0.	0.	-0.3661	-0.0896	0.	-0.1552	-0.	-0.	0.0189	-0.	-0.0375	-0.0274	0.0189	0.
26	0.1784	0.3334	0.	0.	0.1136	0.	0.	0.	0.	0.0078	0.0189	-0.0189	-0.	0.0078	0.0189
27	-0.2716	-0.3661	-0.	0.	-0.1793	-0.	-0.	0.	-0.	-0.0189	-0.0274	0.0375	-0.	-0.0189	-0.0274
28	-0.	-0.	0.1475	-0.	-0.	0.0826	0.	-0.	0.	0.0189	0.0375	-0.0274	-0.	-0.0189	-0.0375
29	-0.	0.	-0.	0.1475	0.	-0.	-0.	0.0826	-0.	0.	-0.	-0.	0.0161	-0.	0.
30	0.1784	-0.3334	0.	0.	0.1136	-0.	0.	-0.	0.	0.0078	-0.0189	-0.0189	-0.	0.0078	-0.0189
31	0.2716	-0.3661	0.	0.	0.1793	-0.	0.	-0.	0.	0.0189	-0.0274	-0.0375	-0.	0.0189	-0.0274
32	-0.	0.	0.1475	0.	-0.	-0.0826	0.	-0.	0.	0.0189	-0.0375	-0.0274	0.	-0.0189	0.0375
33	-0.	0.	0.	0.1475	-0.	-0.	0.	-0.0826	0.	0.	-0.	0.	0.0161	-0.	0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.2716	0.	0.1784	-0.	-0.	-0.2716	0.1784	-0.	-0.	0.2716	0.1784	-0.2716	-0.	-0.	0.1784
2	0.	-0.	0.	0.1475	-0.	-0.	0.	0.1475	0.	0.	0.3334	-0.3661	-0.	0.	-0.3334
3	-0.3661	-0.	0.	-0.	0.1475	0.	0.	0.	0.1475	0.	0.	-0.	0.1475	-0.	0.
4	-0.	0.1475	0.3334	-0.	0.	-0.3661	-0.3334	0.	0.	-0.3661	0.	0.	-0.	0.1475	0.
5	-0.0896	-0.	-0.0568	0.	-0.	0.0896	-0.0568	0.	0.	-0.0896	0.1136	-0.1793	-0.	0.	0.1136
6	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.	0.	-0.	0.0826	-0.	-0.
7	0.1552	0.	-0.0984	0.	0.	0.1552	-0.0984	0.	0.	-0.1552	0.	-0.	0.	-0.	0.
8	-0.	0.	0.	0.0826	-0.	-0.	-0.	-0.0826	-0.	-0.	0.	0.	-0.	0.0826	-0.
9	0.	-0.0826	0.	-0.	0.0826	0.	-0.	-0.	-0.0826	-0.	0.	-0.	0.	-0.	0.
10	0.0010	0.	0.0078	-0.	0.0189	-0.0189	0.0078	-0.	0.0189	0.0189	0.0078	-0.0189	0.0189	0.	0.0078
11	0.	-0.	0.	0.0101	-0.	-0.	0.	0.0101	0.	-0.	0.0189	-0.0274	0.0375	-0.	-0.0189
12	-0.0040	-0.	-0.0189	-0.	-0.0274	0.0375	-0.0189	0.	-0.0274	-0.0375	-0.0189	0.0375	-0.0274	-0.	-0.0189
13	-0.	0.0004	0.0189	-0.	0.0375	-0.0274	-0.0189	-0.	-0.0375	-0.0274	-0.	-0.	-0.	0.0161	-0.
14	0.	0.	0.0078	-0.	-0.0189	-0.0189	0.0078	-0.	-0.0189	0.0189	0.0078	-0.0189	-0.0189	-0.	0.0078
15	0.	0.	0.	0.0101	-0.	0.	0.	0.0101	0.	0.	0.0189	-0.0274	-0.0375	0.	-0.0189
16	1.0000	0.	0.0189	-0.	-0.0274	-0.0375	0.0189	0.	-0.0274	0.0375	0.0189	-0.0375	-0.0274	-0.	0.0189
17	0.	1.0000	0.0189	0.	-0.0375	-0.0274	-0.0189	0.	0.0375	-0.0274	0.	0.	-0.	0.0161	0.
18	0.0189	0.0189	1.0000	0.	0.	0.	0.0002	-0.	-0.	0.0010	0.0078	-0.0189	-0.	0.0189	0.0078
19	-0.	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.0189	-0.0274	0.	0.0375	-0.0189
20	-0.0274	-0.0375	0.	0.	1.0000	0.	0.	0.0004	0.	0.	0.	0.	0.0161	0.	0.
21	-0.0375	-0.0274	0.	0.	0.	1.0000	-0.0010	0.	0.	-0.0040	-0.0189	0.0375	0.	-0.0274	-0.0189
22	0.0189	-0.0189	0.0002	0.	0.	-0.0010	1.0000	0.	0.	0.	0.0078	-0.0189	-0.	-0.0189	0.0078
23	0.	0.	-0.	0.0004	0.	0.	0.	1.0000	0.	0.	0.0189	-0.0274	-0.	-0.0375	-0.0189
24	-0.0274	0.0375	-0.	0.	0.0004	0.	0.	0.	1.0000	0.	0.	-0.	0.0161	0.	0.
25	0.0375	-0.0274	0.0010	0.	0.	-0.0040	0.	0.	0.	1.0000	0.0189	-0.0375	0.	-0.0274	0.0189
26	0.0189	0.	0.0078	0.0189	0.	-0.0189	0.0078	0.0189	0.	0.0189	1.0000	0.	0.	0.	0.0002
27	-0.0375	0.	-0.0189	-0.0274	0.	0.0375	-0.0189	-0.0274	-0.	-0.0375	0.	1.0000	0.	0.	-0.0010
28	-0.0274	-0.	-0.	0.	0.0101	0.	-0.	-0.	0.0101	0.	0.	0.	1.0000	0.	0.
29	-0.	0.0101	0.0189	0.0375	0.	-0.0274	-0.0189	-0.0375	0.	-0.0274	0.	0.	0.	1.0000	0.
30	0.0189	0.	0.0078	-0.0189	0.	-0.0189	0.0078	-0.0189	0.	0.0189	0.0002	-0.0010	0.	0.	1.0000
31	0.0375	0.	0.0189	-0.0274	0.	-0.0375	0.0189	-0.0274	-0.	0.0375	0.0010	-0.0040	0.	0.	0.
32	-0.0274	0.	-0.	0.	0.0101	-0.	-0.	-0.	0.0101	-0.	-0.	0.	0.0004	0.	0.
33	0.	0.0101	0.0189	-0.0375	-0.	-0.0274	-0.0189	0.0375	-0.	-0.0274	-0.	0.	0.	0.0004	0.

	31	32	33
1	0.2716	-0.	-0.
2	-0.3661	0.	0.
3	0.	0.1475	0.
4	0.	0.	0.1475
5	0.1793	-0.	-0.
6	-0.	-0.0826	-0.
7	0.	0.	0.
8	-0.	-0.	-0.0826
9	0.	0.	0.
10	0.0189	0.0189	0.
11	-0.0274	-0.0375	-0.
12	-0.0375	-0.0274	0.
13	-0.	0.	0.0161
14	0.0189	-0.0189	-0.
15	-0.0274	0.0375	0.
16	0.0375	-0.0274	0.
17	0.	0.	0.0101
18	0.0189	-0.	0.0189
19	-0.0274	0.	-0.0375
20	0.	0.0101	-0.
21	-0.0375	-0.	-0.0274
22	0.0189	-0.	-0.0189
23	-0.0274	-0.	0.0375
24	-0.	0.0101	-0.
25	0.0375	-0.	-0.0274
26	0.0010	-0.	-0.
27	-0.0040	0.	0.
28	0.	0.0004	0.
29	0.	0.	0.0004
30	0.	0.	0.
31	1.0000	0.	0.
32	0.	1.0000	0.
33	0.	0.	1.0000

TABLE III

$OsCl_6^{2-}$ Overlap Integral Matrix

$OsCl_4^{2-}$ OVERLAP MATRIX

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1729	-0.	-0.2692	-0.	0.1729	-0.	0.2692	0.	0.1729	-0.	-0.	-0.2692	0.1729	-0.	-0.	0.2692	0.1729	-0.2692	-0.	-0.	0.1729	-0.	-0.	-0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1431	-0.	0.	0.	0.	0.	-0.	0.	0.1431	-0.	-0.	0.	0.1431	-0.	0.	0.	-0.	0.	0.	-0.3235	0.	0.	0.
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.	0.	0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	-0.	-0.	0.	-0.	0.	0.
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.	0.	0.	0.	0.	-0.	0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
10	0.1729	0.	0.3235	0.	-0.0414	0.	0.	0.0718	0.	1.0000	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
11	-0.	0.1431	-0.	0.	0.	0.0605	-0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
12	-0.2692	-0.	-0.3663	-0.	0.0717	-0.	-0.1242	-0.	-0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
13	-0.	0.	-0.	0.1431	0.	0.	-0.	0.	0.	0.0605	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
14	0.1729	0.	-0.3235	-0.	-0.0414	-0.	0.0718	-0.	0.	0.0002	0.	-0.0010	-0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
15	-0.	0.1431	0.	-0.	0.	-0.0605	-0.	-0.	0.	-0.	0.0004	0.	-0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
16	0.2692	0.	-0.3663	-0.	0.0717	-0.	0.1242	-0.	0.	0.0010	0.	-0.0048	-0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
17	0.	-0.	-0.	0.1431	-0.	0.	0.	0.	-0.0605	0.	-0.	-0.	0.	0.0004	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
18	0.1729	0.	0.	0.3235	-0.0414	0.	-0.0718	0.	0.	0.0078	0.	-0.0189	0.	0.0078	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
19	-0.	0.1431	-0.	-0.	0.	0.	0.	0.0605	-0.	-0.	0.0101	0.	-0.	-0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
20	-0.	-0.	0.1431	0.	-0.	-0.	-0.	-0.	0.0605	0.	-0.	-0.	0.	-0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
21	-0.2692	-0.	0.	-0.3663	0.0717	-0.	0.1242	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
22	0.1729	0.	0.	-0.3235	-0.0414	0.	-0.0718	-0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
23	-0.	0.1431	0.	0.	0.	0.	0.	-0.0605	-0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
24	-0.	0.	0.1431	0.	0.	0.	0.	-0.	-0.0605	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.
25	0.2692	0.	0.	-0.3663	-0.0717	0.	-0.1242	-0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.
26	0.1729	0.3235	0.	0.	0.0829	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.
27	-0.2692	-0.3663	-0.	0.	-0.1434	-0.	-0.	0.	-0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.
28	-0.	-0.	0.1431	-0.	0.	0.0605	-0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.
29	-0.	0.	-0.	0.1431	0.	-0.	-0.	0.0605	-0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.
30	0.1729	-0.3235	0.	0.	0.0829	-0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.
31	0.2692	-0.3663	0.	0.	0.1434	-0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.
32	-0.	0.	0.1431	0.	-0.	-0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.
33	-0.	0.	0.	0.1431	-0.	-0.	0.	-0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	1.0000

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.2692	0.	0.1729	-0.	-0.	-0.2692	0.1729	-0.	-0.	0.2692	0.1729	-0.2692	-0.	-0.	0.1729
2	0.	-0.	0.	0.1431	-0.	-0.	0.	0.1431	0.	0.	0.3235	-0.3663	-0.	0.	-0.3235
3	-0.3663	-0.	0.	-0.	0.1431	0.	0.	0.	0.1431	0.	0.	-0.	0.1431	-0.	0.
4	-0.	0.1431	0.3235	-0.	0.	-0.3663	-0.3235	0.	0.	-0.3663	0.	0.	-0.	0.1431	0.
5	-0.0717	-0.	-0.0414	0.	-0.	0.0717	-0.0414	0.	0.	-0.0717	0.0829	-0.1434	-0.	0.	0.0829
6	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.	0.	-0.	0.0605	-0.	-0.
7	0.1242	0.	-0.0718	0.	-0.	0.1242	-0.0718	0.	0.	-0.1242	0.	-0.	0.	-0.	0.
8	-0.	0.	0.	0.0605	-0.	-0.	-0.	-0.0605	-0.	-0.	0.	0.	-0.	0.0605	-0.
9	0.	-0.0605	0.	-0.	0.0605	0.	-0.	-0.	-0.0605	-0.	0.	-0.	0.	-0.	0.
10	0.0010	0.	0.0078	-0.	0.0189	-0.0189	0.0078	-0.	0.0189	0.0189	0.0078	-0.0189	0.0189	0.	0.0078
11	0.	-0.	0.	0.0101	-0.	-0.	0.	0.0101	0.	-0.	0.0189	-0.0274	0.0375	-0.	-0.0189
12	-0.0040	-0.	-0.0189	-0.	-0.0274	0.0375	-0.0189	0.	-0.0274	-0.0375	-0.0189	0.0375	-0.0274	-0.	-0.0189
13	-0.	0.0004	0.0189	-0.	0.0375	-0.0274	-0.0189	-0.	-0.0375	-0.0274	-0.	-0.	-0.	0.0101	-0.
14	0.	0.	0.0078	-0.	-0.0189	-0.0189	0.0078	-0.	-0.0189	0.0189	0.0078	-0.0189	-0.0189	-0.	0.0078
15	0.	0.	0.	0.0101	-0.	0.	0.	0.0101	0.	0.	0.0189	-0.0274	0.0375	0.	-0.0189
16	1.0000	0.	0.0189	-0.	-0.0274	-0.0375	0.0189	0.	-0.0274	0.0375	0.0189	-0.0375	0.0274	-0.	0.0189
17	0.	1.0000	0.0189	0.	-0.0375	-0.0274	-0.0189	0.	0.0375	-0.0274	0.	0.	-0.	0.0101	0.
18	0.0189	0.0189	1.0000	0.	0.	0.	0.0002	-0.	-0.	0.0010	0.0078	-0.0189	-0.	0.0189	0.0078
19	-0.	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.0189	-0.0274	0.	0.0375	-0.0189
20	-0.0274	-0.0375	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.	0.0161	0.	0.
21	-0.0375	-0.0274	0.	0.	0.	1.0000	-0.0010	0.	0.	-0.0040	-0.0189	0.0375	0.	-0.0274	-0.0189
22	0.0189	-0.0189	0.0002	0.	0.	-0.0010	1.0000	0.	0.	0.	0.0078	-0.0189	-0.	0.0189	0.0078

	23	24	25	26	27	28	29	30
23	0.	0.	-0.	0.0004	0.	0.	0.	1.0000	0.	0.	0.0189	-0.0274	-0.	0.0375	-0.0189
24	-0.0274	0.0375	-0.	0.	0.0004	0.	0.	0.	1.0000	0.	0.	-0.	0.0101	0.	0.
25	0.0375	-0.0274	0.0010	0.	-0.	-0.0040	0.	0.	0.	1.0000	0.0189	-0.0375	0.	0.0274	0.0189
26	0.0189	0.	0.0078	0.0189	0.	-0.0189	0.0078	0.0189	0.	0.0189	1.0000	0.	0.	0.	0.0002
27	-0.0375	0.	-0.0189	-0.0274	0.	0.0375	-0.0189	-0.0274	-0.	-0.0375	0.	1.0000	0.	0.	-0.0010
28	-0.0274	-0.	-0.	0.	0.0101	0.	-0.	-0.	0.0101	0.	0.	0.	1.0000	0.	0.
29	-0.	0.0101	0.0189	0.0375	0.	-0.0274	-0.0189	-0.0375	0.	-0.0274	0.	0.	0.	1.0000	0.
30	0.0189	0.	0.0078	-0.0189	0.	-0.0189	0.0078	-0.0189	0.	0.0189	0.0002	-0.0010	0.	0.	1.0000
31	0.0375	0.	0.0189	-0.0274	0.	0.0375	-0.0189	-0.0274	-0.	0.0375	0.0010	-0.0040	0.	0.	0.
32	-0.0274	0.	-0.	0.	0.0101	-0.	-0.	-0.	0.0101	-0.	-0.	0.	0.0004	0.	0.
33	0.	0.0101	0.0189	-0.0375	-0.	-0.0274	-0.0189	0.0375	-0.	-0.0274	-0.	0.	0.	0.0004	0.

	31	32	33
1	0.2692	-0.	-0.
2	-0.3663	0.	0.
3	0.	0.1431	0.
4	0.	0.	0.1431
5	0.1434	-0.	-0.
6	-0.	-0.0605	-0.
7	0.	0.	0.
8	-0.	-0.	-0.0605
9	0.	0.	0.
10	0.0189	0.0189	0.
11	-0.0274	-0.0375	-0.
12	-0.0375	-0.0274	0.
13	-0.	0.	0.0101
14	0.0189	-0.0189	-0.
15	-0.0274	0.0375	0.
16	0.0375	-0.0274	0.
17	0.	0.	0.0101
18	0.0189	-0.	0.0189
19	-0.0274	0.	-0.0375
20	0.	0.0101	-0.
21	-0.0375	-0.	-0.0274
22	0.0189	-0.	-0.0189
23	-0.0274	-0.	0.0375
24	-0.	0.0101	-0.
25	0.0375	-0.	-0.0274
26	0.0010	-0.	-0.
27	-0.0040	0.	0.
28	0.	0.0004	0.
29	0.	0.	0.0004
30	0.	0.	0.
31	1.0000	0.	0.
32	0.	1.0000	0.
33	0.	0.	1.0000

TABLE IV

$IrCl_6^{2-}$ Overlap Integral Matrix

$IrCl_4^{2-}$ OVERLAP MATRIX

1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1784	-0.	-0.2716	-0.	0.1784	-0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1475	-0.	0.	0.	0.1475
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.3334	-0.	-0.3661	-0.	-0.3334	0.
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.1475	-0.	-0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.0457	0.	0.0770	0.	-0.0457	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.0667	-0.	0.	-0.	-0.0667
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.0792	-0.	-0.1334	-0.	0.0792	-0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	-0.	0.	-0.	-0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	0.0667	0.	0.
10	0. 784	0.	0.3334	0.	-0.0457	0.	0.0792	0.	0.	1.0000	0.	0.	0.	0.0002	-0.
10	0.1784	0.	0.3334	0.	-0.0457	0.	0.0792	0.	0.	1.0000	0.	0.	0.	0.0002	-0.
11	-0.	0.1475	-0.	0.	0.	0.0667	-0.	0.	0.	0.	1.0000	0.	0.	0.	0.0004
12	-0.2716	-0.	-0.3661	-0.	0.0770	-0.	-0.1334	-0.	-0.	0.	0.	1.0000	0.	-0.0010	0.
13	-0.	0.	-0.	0.1475	0.	0.	-0.	0.	0.0667	0.	0.	0.	1.0000	-0.	-0.
14	0.1784	0.	-0.3334	-0.	-0.0457	-0.	0.0792	-0.	0.	0.0002	0.	-0.0010	-0.	1.0000	0.
15	-0.	0.1475	0.	-0.	0.	-0.0667	-0.	-0.	0.	-0.	0.0004	0.	-0.	0.	1.0000
16	0.2716	0.	-0.3661	-0.	-0.0770	-0.	0.1334	-0.	0.	0.0010	0.	-0.0040	-0.	0.	0.
17	0.	-0.	-0.	0.1475	-0.	0.	0.	0.	-0.0667	0.	-0.	-0.	0.0004	0.	0.
18	0.1784	0.	0.	0.3334	-0.0457	0.	-0.0792	0.	0.	0.0078	0.	-0.0189	0.0189	0.0078	0.
19	-0.	0.1475	-0.	-0.	0.	0.	0.	0.0667	-0.	-0.	0.0101	-0.	-0.	-0.	0.0101
20	-0.	-0.	0.1475	0.	-0.	-0.	-0.	-0.	0.0667	0.0189	-0.	-0.0274	0.0375	-0.0189	-0.
21	-0.2716	-0.	0.	-0.3661	0.0770	-0.	0.1334	-0.	0.	-0.0189	-0.	0.0375	-0.0274	-0.0189	0.
22	0.1784	0.	0.	-0.3334	-0.0457	0.	-0.0792	-0.	-0.	0.0078	0.	-0.0189	-0.0189	0.0078	0.
23	-0.	0.1475	0.	0.	0.	0.	0.	-0.0667	-0.	-0.	0.0101	0.	-0.	-0.	0.0101
24	-0.	0.	0.1475	0.	0.	0.	0.	-0.	-0.0667	0.0189	0.	-0.0274	-0.0375	-0.0189	0.
25	0.2716	0.	0.	-0.3661	-0.0770	0.	-0.1334	-0.	-0.	0.0189	-0.	-0.0375	-0.0274	0.0189	0.
26	0.1784	0.3334	0.	0.	0.0915	0.	0.	0.	0.	0.0078	0.0189	-0.0189	-0.	0.0078	0.0189
27	-0.2716	-0.3661	-0.	0.	-0.1541	-0.	-0.	0.	-0.	-0.0189	-0.0274	0.0375	-0.	-0.0189	-0.0274
28	-0.	-0.	0.1475	-0.	-0.	0.0667	0.	-0.	0.	0.0189	0.0375	-0.0274	-0.	-0.0189	-0.0375
29	-0.	0.	-0.	0.1475	0.	-0.	-0.	0.0667	-0.	0.	-0.	-0.	0.0101	-0.	0.
30	0.1784	-0.3334	0.	0.	0.0915	-0.	0.	-0.	0.	0.0078	-0.0189	-0.0189	-0.	0.0078	-0.0189
31	0.2716	-0.3661	0.	0.	0.1541	-0.	0.	-0.	0.	0.0189	-0.0274	-0.0375	-0.	0.0189	-0.0274
32	-0.	0.	0.1475	0.	-0.	-0.0667	0.	-0.	0.	0.0189	-0.0375	-0.0274	0.	-0.0189	0.0375
33	-0.	0.	0.	0.1475	-0.	-0.	0.	-0.0667	0.	0.	-0.	0.	0.0101	-0.	0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.2716	0.	0. 784	-0.	-0.	-0.2716	0.1784	-0.	-0.	0.2716	0. 784	-0.2716	-0.	-0.	0. 784
1	0.2716	0.	0.1784	-0.	-0.	-0.2716	0.1784	-0.	-0.	0.2716	0.1784	-0.2716	-0.	-0.	0.1784
2	0.	-0.	0.	0.1475	-0.	-0.	0.	0.1475	0.	0.	0.3334	-0.3661	-0.	0.	-0.3334
3	-0.3661	-0.	0.	-0.	0.1475	0.	0.	0.	0.1475	0.	0.	-0.	0.1475	-0.	0.
4	-0.	0.1475	0.3334	-0.	0.	-0.3661	-0.3334	0.	0.	-0.3661	0.	0.	-0.	0.1475	0.
5	-0.0770	-0.	-0.0457	0.	-0.	0.0770	-0.0457	0.	0.	-0.0770	0.0915	-0.1541	-0.	0.	0.0915
6	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.	0.	-0.	0.0667	-0.	-0.
7	0.1334	0.	-0.0792	0.	-0.	0.1334	-0.0792	0.	0.	-0.1334	0.	-0.	0.	-0.	0.
8	-0.	0.	0.	0.0667	-0.	-0.	-0.	-0.0667	-0.	-0.	0.	0.	-0.	0.0667	-0.
9	0.	-0.0667	0.	-0.	0.0667	0.	-0.	-0.	-0.0667	-0.	0.	-0.	0.	-0.	0.
10	0.0010	0.	0.0078	-0.	0.0189	-0.0189	0.0078	-0.	0.0189	0.0189	0.0078	-0.0189	0.0189	0.	0.0078
11	0.	-0.	0.	0.0101	-0.	-0.	0.	0.0101	0.	-0.	0.0189	-0.0274	0.0375	-0.	-0.0189
12	-0.0040	-0.	-0.0189	-0.	-0.0274	0.0375	-0.0189	0.	-0.0274	-0.0375	-0.0189	0.0375	-0.0274	-0.	-0.0189
13	-0.	0.0004	0.0189	-0.	0.0375	-0.0274	-0.0189	-0.	-0.0375	-0.0274	-0.	-0.	-0.	0.0101	-0.
14	0.	0.	0.0078	-0.	-0.0189	-0.0189	0.0078	-0.	-0.0189	0.0189	0.0078	-0.0189	-0.0189	-0.	0.0078
15	0.	0.	0.	0.0101	-0.	0.	0.	0.0101	0.	0.	0.0189	-0.0274	-0.0375	0.	-0.0189
16	1.0000	0.	0.0189	-0.	-0.0274	-0.0375	0.0189	0.	-0.0274	0.0375	0.0189	-0.0375	-0.0274	-0.	0.0189
17	0.	1.0000	0.0189	0.	-0.0375	-0.0274	-0.0189	0.	0.0375	-0.0274	0.	-0.	-0.	0.0101	0.
18	0.0189	0.0189	1.0000	0.	0.	0.	0.0002	-0.	-0.	0.0010	0.0078	-0.0189	-0.	0.0189	0.0078
19	-0.	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.0189	-0.0274	0.	0.0375	-0.0189
20	-0.0274	-0.0375	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.	0.0101	0.	0.

	21	22	23	24	25	26	27	28	29	30
21	-0.0375	-0.0274	0.	0.	0.	1.0000	-0.0010	0.	0.	-0.0040	-0.0189	0.0375	0.	-0.0274	-0.0189
22	0.0189	-0.0189	0.0002	0.	0.	-0.0010	1.0000	0.	0.	0.	0.0078	-0.0189	-0.	-0.0189	0.0078
23	0.	0.	-0.	0.0004	0.	0.	0.	1.0000	0.	0.	0.0189	-0.0274	-0.	-0.0375	-0.0189
24	-0.0274	0.0375	-0.	0.	0.0004	0.	0.	0.	1.0000	0.	0.	-0.	0.0101	0.	0.
25	0.0375	-0.0274	0.0010	0.	0.	-0.0040	0.	0.	0.	1.0000	0.0189	-0.0375	0.	-0.0274	0.0189
26	0.0189	0.	0.0078	0.0189	0.	-0.0189	0.0078	0.0189	0.	0.0189	1.0000	0.	0.	0.	0.0002
27	-0.0375	0.	-0.0189	-0.0274	0.	0.0375	-0.0189	-0.0274	-0.	-0.0375	0.	1.0000	0.	0.	-0.0010
28	-0.0274	-0.	-0.	0.	0.0101	0.	-0.	-0.	0.	0.0101	0.	0.	1.0000	0.	0.
29	-0.	0.0101	0.0189	0.0375	0.	-0.0274	-0.0189	-0.0375	0.	-0.0274	0.	0.	0.	1.0000	0.
30	0.0189	0.	0.0078	-0.0189	0.	-0.0189	0.0078	-0.0189	0.	0.0189	0.0002	-0.0010	0.	0.	1.0000
31	0.0375	0.	0.0189	-0.0274	0.	-0.0375	0.0189	-0.0274	-0.	0.0375	0.0010	-0.0040	0.	0.	0.
32	-0.0274	0.	-0.	0.	0.0101	-0.	-0.	-0.	0.0101	-0.	-0.	0.	0.0004	0.	0.
33	0.	0.0101	0.0189	-0.0375	-0.	-0.0274	-0.0189	0.0375	-0.	-0.0274	-0.	0.	0.	0.0004	0.

	31	32	33
1	0.2716	-0.	-0.
2	-0.3661	0.	0.
3	0.	0.1475	0.
4	0.	0.	0.1475
5	0.1541	-0.	-0.
6	-0.	-0.0667	-0.
7	0.	0.	0.
8	-0.	-0.	-0.0667
9	0.	0.	0.
10	0.0189	0.0189	0.
11	-0.0274	-0.0375	-0.
12	-0.0375	-0.0274	0.
13	-0.	0.	0.0101
14	0.0189	-0.0189	-0.
15	-0.0274	0.0375	0.
16	0.0375	-0.0274	0.
17	0.	0.	0.0101
18	0.0189	-0.	0.0189
19	-0.0274	0.	-0.0375
20	0.	0.0101	-0.
21	-0.0375	-0.	-0.0274
22	0.0189	-0.	-0.0189
23	-0.0274	-0.	0.0375
24	-0.	0.0101	-0.
25	0.0375	-0.	-0.0274
26	0.0010	-0.	-0.
27	-0.0040	0.	0.
28	0.	0.0004	0.
29	0.	0.	0.0004
30	0.	0.	0.
31	1.0000	0.	0.
32	0.	1.0000	0.
33	0.	0.	1.0000

TABLE V

$PtCl_6^{2-}$ Overlap Integral Matrix

$PtCl_4^{2-}$ OVERLAP MATRIX

1	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1675	-0.	-0.2666	-0.	0.1675	-0.
2	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	0.	0.1388	-0.	0.	0.	0.1388
3	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.3137	-0.	-0.3658	-0.	-0.3137	0.
4	0.	0.	0.	1.0000	0.	0.	0.	0.	0.	0.	0.	-0.	0.1388	-0.	-0.
5	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	-0.0453	0.	0.0765	0.	-0.0453	0.
6	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	0.	0.0660	-0.	0.	-0.	-0.0660
7	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.0784	-0.	-0.1324	-0.	0.0784	-0.
8	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	0.	-0.	0.	-0.	-0.
9	0.	0.	0.	0.	0.	0.	0.	0.	1.0000	0.	0.	-0.	0.0660	0.	0.
10	0.1675	0.	0.3137	0.	-0.0453	0.	0.0784	0.	0.	1.0000	0.	0.	0.	0.0002	-0.
11	-0.	0.1388	-0.	0.	0.	0.0660	-0.	0.	0.	0.	1.0000	0.	0.	0.	0.0004
12	-0.2666	-0.	-0.3658	-0.	0.0765	-0.	-0.1324	-0.	-0.	0.	0.	1.0000	0.	-0.0010	0.
13	-0.	0.	-0.	0.1388	0.	0.	-0.	0.	0.0660	0.	0.	0.	1.0000	-0.	-0.
14	0.1675	0.	-0.3137	-0.	-0.0453	-0.	0.0784	-0.	0.	0.0002	0.	-0.0010	-0.	1.0000	0.
15	-0.	0.1388	0.	-0.	0.	-0.0660	-0.	-0.	0.	-0.	0.0004	0.	-0.	0.	1.0000
16	0.2666	0.	-0.3658	-0.	-0.0765	-0.	0.1324	-0.	0.	0.0010	0.	-0.0040	-0.	0.	0.
17	0.	-0.	-0.	0.1388	-0.	0.	0.	0.	-0.0660	0.	-0.	-0.	0.0004	0.	0.
18	0.1675	0.	0.	0.3137	-0.0453	0.	-0.0784	0.	0.	0.0078	0.	-0.0189	0.0189	0.0078	0.
19	-0.	0.1388	-0.	-0.	0.	0.	0.	0.0660	-0.	-0.	0.0101	-0.	-0.	-0.	0.0101
20	-0.	-0.	0.1388	0.	-0.	-0.	-0.	-0.	0.0660	0.0189	-0.	-0.0274	0.0375	-0.0189	-0.
21	-0.2666	-0.	0.	-0.3658	0.0765	-0.	0.1324	-0.	0.	-0.0189	-0.	0.0375	-0.0274	-0.0189	0.
22	0.1675	0.	0.	-0.3137	-0.0453	0.	-0.0784	-0.	-0.	0.0078	0.	-0.0189	-0.0189	0.0078	0.
23	-0.	0.1388	0.	0.	0.	0.	0.	-0.0660	-0.	-0.	0.0101	0.	-0.	-0.	0.0101
24	-0.	0.	0.1388	0.	0.	0.	0.	-0.	-0.0660	0.0189	0.	-0.0274	-0.0375	-0.0189	0.
25	0.2666	0.	0.	-0.3658	-0.0765	0.	-0.1324	-0.	-0.	0.0189	-0.	-0.0375	-0.0274	0.0189	0.
26	0.1675	0.3137	0.	0.	0.0905	0.	0.	0.	0.	0.0078	0.0189	-0.0189	-0.	0.0078	0.0189
27	-0.2666	-0.3658	-0.	0.	-0.1529	-0.	-0.	0.	-0.	-0.0189	-0.0274	0.0375	-0.	-0.0189	-0.0274
28	-0.	-0.	0.1388	-0.	-0.	0.0660	0.	-0.	0.	0.0189	0.0375	-0.0274	-0.	-0.0189	-0.0375
29	-0.	0.	-0.	0.1388	0.	-0.	-0.	0.0660	-0.	0.	-0.	-0.	0.0101	-0.	0.
30	0.1675	-0.3137	0.	0.	0.0905	-0.	0.	-0.	0.	0.0078	-0.0189	-0.0189	-0.	0.0078	-0.0189
31	0.2666	-0.3658	0.	0.	0.1529	-0.	0.	-0.	0.	0.0189	-0.0274	-0.0375	-0.	0.0189	-0.0274
32	-0.	0.	0.1388	0.	-0.	-0.0660	0.	-0.	0.	0.0189	-0.0375	-0.0274	0.	-0.0189	0.0375
33	-0.	0.	0.	0.1388	-0.	-0.	0.	-0.0660	0.	0.	-0.	0.	0.0101	-0.	0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.2666	0.	0.1675	-0.	-0.	-0.2666	0.1675	-0.	-0.	0.2666	0.1675	-0.2666	-0.	-0.	0.1675
2	0.	-0.	0.	0.1388	-0.	-0.	0.	0.1388	0.	0.	0.3137	-0.3658	-0.	0.	-0.3137
3	-0.3658	-0.	0.	-0.	0.1388	0.	0.	0.	0.1388	0.	0.	-0.	0.1388	-0.	0.
4	-0.	0.1388	0.3137	-0.	0.	-0.3658	-0.3137	0.	0.	-0.3658	0.	0.	-0.	0.1388	0.
5	-0.0765	-0.	-0.0453	0.	-0.	0.0765	-0.0453	0.	0.	-0.0765	0.0905	-0.1529	-0.	0.	0.0905
6	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.	0.	-0.	0.0660	-0.	-0.
7	0.1324	0.	-0.0784	0.	-0.	0.1324	-0.0784	0.	0.	-0.1324	0.	-0.	0.	-0.	0.
8	-0.	0.	0.	0.0660	-0.	-0.	-0.	-0.0660	-0.	-0.	0.	0.	-0.	0.0660	-0.
9	0.	-0.0660	0.	-0.	0.0660	0.	-0.	-0.	-0.0660	-0.	0.	-0.	0.	-0.	0.
10	0.0010	0.	0.0078	-0.	0.0189	-0.0189	0.0078	-0.	0.0189	0.0189	0.0078	-0.0189	0.0189	0.	0.0078
11	0.	-0.	0.	0.0101	-0.	-0.	0.	0.0101	0.	-0.	0.0189	-0.0274	0.0375	-0.	-0.0189
12	-0.0040	-0.	-0.0189	-0.	-0.0274	0.0375	-0.0189	0.	-0.0274	-0.0375	-0.0189	0.0375	-0.0274	-0.	-0.0189
13	-0.	0.0004	0.0189	-0.	0.0375	-0.0274	-0.0189	-0.	-0.0375	-0.0274	-0.	-0.	-0.	0.0101	-0.
14	0.	0.	0.0078	-0.	-0.0189	-0.0189	0.0078	-0.	-0.0189	0.0189	0.0078	-0.0189	-0.0189	-0.	0.0078
15	0.	0.	0.	0.0101	-0.	0.	0.	0.0101	0.	0.	0.0189	-0.0274	-0.0375	0.	-0.0189
16	1.0000	0.	0.0189	-0.	-0.0274	-0.0375	0.0189	0.	-0.0274	0.0375	0.0189	-0.0375	-0.0274	-0.	0.0189
17	0.	1.0000	0.0189	0.	-0.0375	-0.0274	-0.0189	0.	0.0375	-0.0274	0.	0.	-0.	0.0101	0.
18	0.0189	0.0189	1.0000	0.	0.	0.	0.0002	-0.	-0.	0.0010	0.0078	-0.0189	-0.	0.0189	0.0078
19	-0.	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.0189	-0.0274	0.	0.0375	-0.0189
20	-0.0274	-0.0375	0.	0.	1.0000	0.	0.	0.	0.0004	0.	0.	0.	0.0101	0.	0.
21	-0.0375	-0.0274	0.	0.	0.	1.0000	-0.0010	0.	0.	-0.0040	-0.0189	0.0375	0.	-0.0274	-0.0189

22	0.0189	-0.0189	0.0002	0.	0.	-0.0010	1.0000	0.	0.	0.	0.0078	-0.0189	-0.	-0.0189	0.0078
23	0.	0.	-0.	0.0004	0.	0.	0.	1.0000	0.	0.	0.0189	-0.0274	-0.	-0.0375	-0.0189
24	-0.0274	0.0375	-0.	0.	0.0004	0.	0.	0.	1.0000	0.	0.	-0.	0.0101	0.	0.
25	0.0375	-0.0274	0.0010	0.	0.	-0.0040	0.	0.	0.	1.0000	0.0189	-0.0375	0.	-0.0274	0.0189
26	0.0189	0.	0.0078	0.0189	0.	-0.0189	0.0078	0.0189	0.	0.0189	1.0000	0.	0.	0.	0.0002
27	-0.0375	0.	-0.0189	-0.0274	0.	0.0375	-0.0189	-0.0274	-0.	-0.0375	0.	1.0000	0.	0.	-0.0010
28	-0.0274	-0.	-0.	0.	0.0101	0.	-0.	-0.	0.0101	0.	0.	0.	1.0000	0.	0.
29	-0.	0.0101	0.0189	0.0375	0.	-0.0274	-0.0189	-0.0375	0.	-0.0274	0.	0.	0.	1.0000	0.
30	0.0189	0.	0.0078	-0.0189	0.	-0.0189	0.0078	-0.0189	0.	0.0189	0.0002	-0.0010	0.	0.	1.0000
31	0.0375	0.	0.0189	-0.0274	0.	-0.0375	0.0189	-0.0274	-0.	0.0375	0.0010	-0.0040	0.	0.	0.
32	-0.0274	0.	-0.	0.	0.0101	-0.	-0.	-0.	0.0101	-0.	-0.	0.	0.0004	0.	0.
33	0.	0.0101	0.0189	-0.0375	-0.	-0.0274	-0.0189	0.0375	-0.	-0.0274	-0.	0.	0.	0.0004	0.

	31	32	33
1	0.2666	-0.	-0.
2	-0.3658	0.	0.
3	0.	0.1388	0.
4	0.	0.	0.1388
5	0.1529	-0.	-0.
6	-0.	-0.0660	-0.
7	0.	0.	0.
8	-0.	-0.	-0.0660
9	0.	0.	0.
10	0.0189	0.0189	0.
11	-0.0274	-0.0375	-0.
12	-0.0375	-0.0274	0.
13	-0.	0.	0.0101
14	0.0189	-0.0189	-0.
15	-0.0274	0.0375	0.
16	0.0375	-0.0274	0.
17	0.	0.	0.0101
18	0.0189	-0.	0.0189
19	-0.0274	0.	-0.0375
20	0.	0.0101	-0.
21	-0.0375	-0.	-0.0274
22	0.0189	-0.	-0.0189
23	-0.0274	-0.	0.0375
24	-0.	0.0101	-0.
25	0.0375	-0.	-0.0274
26	0.0010	-0.	-0.
27	-0.0040	0.	0.
28	0.	0.0004	0.
29	0.	0.	0.0004
30	0.	0.	0.
31	1.0000	0.	0.
32	0.	1.0000	0.
33	0.	0.	1.0000

TABLE VI

$ReCl_6^{2-}$

Eigenvectors: MO's Across and AO's Down

EIGENVECTORS

$ReCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	-0.0000	-0.0000	-1.4407	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
2	0.0093	0.0186	-1.4740	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0366	0.0832	-0.0248
3	-1.0424	1.0423	0.0066	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0321	-0.0386	-0.0800
4	-1.0422	-1.0423	-0.0198	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0867	-0.0226	0.0431
5	-0.0000	0.0000	-0.0000	-0.0000	0.9533	0.2462	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.9788	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
7	-0.0000	-0.0000	-0.0000	0.0000	0.2462	-0.9533	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.9788	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
9	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.9788	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000
10	0.3612	-0.3612	-0.0023	0.2549	0.0507	0.1824	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0065	-0.0077	-0.0163
11	-0.0010	-0.0021	0.1634	0.0000	0.0000	-0.0000	-0.1994	-0.0000	-0.0000	0.0000	-0.5199	-0.0235	-0.1479	-0.3384	0.1004
12	-0.4134	0.4133	0.0026	-0.3847	-0.1171	-0.4215	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.1628	0.1926	0.4054
13	0.1155	0.1155	0.0022	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.1994	-0.0000	-0.0235	0.5199	-0.3282	0.0914	-0.1744
14	-0.3612	0.3612	0.0023	0.2549	0.0507	0.1824	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0085	0.0077	0.0163
15	-0.0010	-0.0021	0.1634	-0.0000	0.0000	0.0000	0.1994	0.0000	0.0000	-0.0000	0.5199	0.0235	-0.1479	-0.3384	0.1004
16	-0.4134	0.4133	0.0026	0.3847	0.1171	0.4215	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.1628	0.1926	0.4054
17	0.1155	0.1155	0.0022	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1994	0.0000	0.0000	-0.0235	-0.5199	-0.3281	0.0914	-0.1744
18	0.3611	0.3612	0.0068	0.2549	0.1326	-0.1351	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0164	-0.0046	0.0088
19	-0.0010	-0.0021	0.1634	0.0000	0.0000	0.0000	0.0000	-0.1994	0.0000	0.5200	0.0000	0.0000	-0.1479	-0.3384	0.1004
20	0.1156	-0.1155	-0.0007	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.1994	0.0000	0.0235	-0.5199	-0.1259	0.1537	0.3235
21	-0.4133	-0.4133	-0.0078	-0.3847	-0.3065	0.3121	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.4087	0.1145	-0.2186
22	-0.3611	-0.3612	-0.0068	0.2549	0.1326	-0.1351	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0164	0.0046	-0.0088
23	-0.0010	-0.0021	0.1634	0.0000	0.0000	0.0000	-0.0000	0.1994	-0.0000	-0.5200	-0.0000	-0.0000	-0.1479	-0.3384	0.1004
24	0.1156	-0.1155	-0.0007	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.1994	-0.0000	-0.0235	0.5199	-0.1299	0.1537	0.3235
25	-0.4133	-0.4133	-0.0078	0.3847	0.3065	-0.3121	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.4087	0.1145	-0.2186
26	-0.0032	-0.0064	0.5107	0.2549	-0.1833	-0.0473	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0074	0.0169	-0.0050
27	0.0037	0.0074	-0.5845	-0.3847	0.4235	0.1094	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.1854	-0.4216	0.1259
28	0.1156	-0.1155	-0.0007	0.0000	-0.0000	0.0000	-0.1994	-0.0000	-0.0000	-0.0000	0.5199	0.0235	-0.1299	0.1537	0.3235
29	0.1155	0.1155	0.0022	0.0000	0.0000	-0.0000	0.0000	-0.1994	0.0000	-0.5200	-0.0000	-0.0000	-0.3282	0.0914	-0.1744
30	0.0032	0.0064	-0.5107	0.2549	-0.1833	-0.0473	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0074	-0.0169	0.0050
31	0.0037	0.0074	-0.5845	0.3847	-0.4235	-0.1094	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.1854	-0.4216	0.1259
32	0.1156	-0.1155	-0.0007	0.0000	-0.0000	-0.0000	0.1994	0.0000	0.0000	0.0000	-0.5199	-0.0235	-0.1299	0.1537	0.3235
33	0.1155	0.1155	0.0022	0.0000	0.0000	-0.0000	-0.0000	0.1994	-0.0000	0.5200	0.0000	-0.0000	-0.3281	0.0914	-0.1744

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.2133	0.0000	0.0000	-0.0000
2	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0797	-0.0194	0.0129	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0225
3	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0143	0.0768	0.0280	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0358
4	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0181	0.0247	-0.0771	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0511
5	0.0000	-0.0000	0.0000	0.3128	0.3039	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0578	0.0563	0.0000
6	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.2588	0.9324	-0.0000	-0.0000	0.0000	0.0000
7	0.0000	0.0000	-0.0000	0.3039	-0.3128	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0563	0.0578	0.0000
8	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.2608	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
9	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0324	-0.2588	-0.0000	0.0000	0.0000	-0.0000
10	-0.0000	0.0000	-0.0000	-0.0143	0.0567	-0.0154	-0.0830	-0.0302	0.0000	-0.0000	0.0000	0.1196	0.5633	-0.0122	-0.3681
11	0.1900	0.4212	0.2039	-0.0000	-0.0000	0.3083	-0.0750	0.0489	-0.0000	-0.4426	0.0553	-0.0000	-0.0000	0.0000	-0.0074
12	-0.0000	0.0000	-0.0000	-0.1131	0.4478	-0.0793	-0.4263	-0.1554	0.0000	-0.0000	0.0000	0.3248	0.0246	-0.0005	-0.0082
13	-0.2564	-0.0903	0.4256	0.0000	-0.0000	0.0701	0.0956	-0.2982	0.0000	-0.0553	-0.4426	0.0000	0.0000	0.0000	-0.0167
14	0.0000	-0.0000	0.0000	-0.0143	0.0567	0.0154	0.0830	0.0302	-0.0000	0.0000	-0.0000	0.1196	0.5633	-0.0122	0.3681
15	0.1900	0.4212	0.2039	-0.0000	-0.0000	0.3083	-0.0750	0.0489	0.0000	0.4426	0.0553	-0.0000	-0.0000	0.0000	-0.0074
16	-0.0000	0.0000	-0.0000	0.1131	-0.4478	-0.0793	-0.4263	-0.1554	0.0000	-0.0000	0.0000	-0.3248	-0.0246	0.0005	-0.0082
17	-0.2564	-0.0903	0.4256	0.0000	-0.0000	0.0701	0.0956	-0.2982	-0.0000	0.0553	0.4426	0.0000	0.0000	0.0000	-0.0167
18	0.0000	0.0000	-0.0000	0.0562	-0.0159	-0.0196	-0.0267	0.0833	-0.0000	-0.0000	-0.0000	0.1196	-0.2922	-0.4818	-0.5246
19	-0.1900	-0.4212	-0.2039	-0.0000	-0.0000	0.3083	-0.0750	0.0489	0.4460	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0074
20	-0.3914	0.2637	-0.1799	-0.0000	0.0000	0.0552	0.2970	0.1083	0.0000	-0.0553	-0.4426	0.0000	-0.0000	0.0000	-0.0117
21	0.0000	0.0000	-0.0000	0.4444	-0.1260	-0.1007	-0.1373	0.4280	-0.0000	-0.0000	-0.0000	0.3248	-0.0128	-0.0211	-0.0116
22	-0.0000	-0.0000	0.0000	0.0562	-0.0159	0.0196	0.0267	-0.0833	0.0000	0.0000	0.0000	0.1196	-0.2922	-0.4818	0.5246
23	-0.1900	-0.4212	-0.2039	-0.0000	-0.0000	0.3083	-0.0750	0.0489	-0.4460	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0074
24	-0.3914	0.2637	-0.1799	-0.0000	0.0000	0.0552	0.2970	0.1083	-0.0000	0.0553	0.4426	0.0000	-0.0000	0.0000	-0.0117
25	0.0000	0.0000	-0.0000	-0.4444	0.1260	-0.1007	-0.1373	0.4280	-0.0000	-0.0000	-0.0000	-0.3248	0.0128	0.0211	-0.0116
26	-0.0000	0.0000	-0.0000	-0.0419	-0.0407	-0.0861	0.0209	-0.0139	0.0000	0.0000	-0.0000	0.1196	-0.2711	0.4940	-0.2314
27	0.0000	0.0000	0.0000	-0.3313	-0.3218	-0.4425	0.1076	-0.0696	0.0000	0.0000	-0.0000	0.3248	-0.0119	0.0216	-0.0051
28	0.3914	-0.2637	0.1799	-0.0000	0.0000	0.0552	0.2970	0.1083	-0.0000	-0.4426	0.0553	0.0000	-0.0000	0.0000	-0.0117
29	0.2564	0.0903	-0.4256	0.0000	-0.0000	0.0701	0.0956	-0.2982	0.4460	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0167
30	-0.0000	0.0000	0.0000	-0.0419	-0.0407	0.0861	-0.0209	0.0139	-0.0000	-0.0000	0.0000	0.1196	-0.2711	0.4939	0.2314
31	0.0000	0.0000	0.0000	0.3313	0.3219	-0.4425	0.1076	-0.0696	0.0000	0.0000	-0.0000	0.3248	-0.0119	-0.0216	-0.0051
32	0.3914	-0.2637	0.1799	-0.0000	0.0000	0.0552	0.2970	0.1083	0.0000	0.4426	-0.0553	0.0000	-0.0000	0.0000	-0.0117
33	0.2564	0.0903	-0.4256	0.0000	-0.0000	0.0701	0.0956	-0.2982	-0.4460	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0167

	31	32	33
1	0.0000	-0.0000	-0.1560
2	-0.0210	-0.0587	0.0000
3	0.0555	-0.0061	0.0000
4	-0.0297	0.0302	0.0000
5	0.0000	0.0000	-0.0000
6	-0.0000	0.0000	-0.0000
7	-0.0000	-0.0000	0.0000
8	0.0000	0.0000	-0.0000
9	0.0000	-0.0000	-0.0000
10	0.5699	-0.0625	-0.3682
11	-0.0069	-0.0193	0.0000
12	0.0127	-0.0014	0.0148
13	-0.0097	0.0099	0.0000
14	-0.5699	0.0625	-0.3682
15	-0.0069	-0.0193	0.0000
16	0.0127	-0.0014	-0.0148
17	-0.0097	0.0099	0.0000
18	-0.3048	0.3101	-0.3682
19	-0.0069	-0.0193	0.0000
20	0.0182	-0.0020	0.0000
21	-0.0068	0.0069	0.0148
22	0.3048	-0.3101	-0.3682
23	-0.0069	-0.0193	0.0000
24	0.0182	-0.0020	0.0000
25	-0.0068	0.0069	-0.0148
26	-0.2157	-0.6035	-0.3682
27	-0.0048	-0.0134	0.0148
28	0.0182	-0.0020	0.0000
29	-0.0097	0.0099	0.0000
30	0.2157	0.6035	-0.3682
31	-0.0048	-0.0134	-0.0148
32	0.0182	-0.0020	0.0000
33	-0.0097	0.0099	0.0000

TABLE VII

$OsCl_6^{2-}$

Eigenvectors: MO's Across and AO's Down

EIGENVECTORS

$OsCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	-0.0000	0.0000	-0.0000	-1.4090	0.0000	-0.0001	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
2	1.4452	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.1020
3	-0.0000	0.0000	1.4451	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.1034	-0.0001	0.0000
4	-0.0000	-1.4451	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.1033	-0.0000
5	-0.0000	-0.0000	0.0000	-0.0001	0.0299	-0.9254	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.9754	0.0000	0.0000	-0.0032	0.0000	-0.0000	0.0000	-0.0000
7	0.0000	-0.0000	-0.0000	0.0000	-0.9249	-0.0299	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.9754	0.0000	0.0000	0.0030	0.0000	-0.0000	-0.0000
9	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.9752	-0.0000	0.0000	-0.0002	0.0000	0.0000	-0.0000	-0.0000	-0.0000
10	0.0000	-0.0000	-0.4947	0.2453	0.1293	-0.0691	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0158	-0.0000	0.0000
11	-0.1570	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.1754	-0.0000	0.0000	-0.5227	0.0000	0.0000	0.0000	0.3933
12	-0.0000	0.0000	0.5887	-0.3838	-0.3726	0.1994	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.4618	0.0005	-0.0000
13	0.0000	0.1570	-0.0000	0.0000	-0.0000	-0.0000	-0.1750	0.0000	-0.0000	-0.5202	-0.0000	-0.0000	0.0004	-0.3985	0.0000
14	-0.0000	0.0000	0.4947	0.2453	0.1293	-0.0691	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0158	0.0000	-0.0000
15	-0.1570	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1754	0.0000	-0.0000	0.5227	-0.0000	0.0000	0.0000	0.3933

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.0000	-0.0000	-0.0000	-0.0002	-0.0018	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.2377	-0.0001	-0.0015	0.0000
2	0.0002	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.1097	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
3	-0.0000	0.0000	0.0025	-0.0000	-0.0000	-0.1088	0.0001	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0825
4	0.0000	0.0027	-0.0000	-0.0000	0.0000	0.0001	0.1088	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000
5	-0.0000	0.0000	-0.0000	0.0156	0.4814	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0025	0.0033	0.1003	0.0000
6	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.2498	-0.0000	-0.0000	0.0000	-0.0000	0.0000
7	-0.0000	-0.0000	-0.0000	-0.4823	0.0156	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0002	-0.1004	0.0033	-0.0000
8	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.2497	-0.0000	0.0000	-0.0000	-0.0000
9	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.2506	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000
10	0.0000	-0.0000	-0.0004	0.0376	0.0208	0.1008	-0.0000	0.0000	0.0000	0.0000	0.0000	0.1284	-0.5027	-0.2715	-0.6763
11	0.5047	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.3050	-0.0000	0.4498	-0.0000	0.0000	-0.0000	0.0000	0.0000
12	0.0000	-0.0000	-0.0108	0.4019	0.2172	0.4619	-0.0002	0.0000	0.0000	0.0000	0.0000	0.3157	-0.0209	-0.0110	-0.0168
13	0.0000	0.5003	-0.0004	-0.0000	0.0000	0.0001	0.3055	-0.0000	-0.4528	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000
14	-0.0000	0.0000	0.0004	0.0376	0.0208	-0.1008	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.1284	-0.5027	-0.2715	0.6763
15	0.5047	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.3051	0.0000	-0.4497	0.0000	0.0000	-0.0000	0.0000	0.0000
16	0.0000	-0.0000	-0.0108	-0.4019	-0.2172	0.4619	-0.0002	0.0000	0.0000	0.0000	0.0000	-0.3157	0.0209	0.0110	-0.0168
17	0.0000	0.5003	-0.0004	-0.0000	0.0000	0.0001	0.3055	-0.0000	0.4528	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000
18	-0.0000	-0.0004	0.0000	-0.0361	0.0232	-0.0000	-0.1008	0.0000	0.0000	0.0000	0.0000	0.1284	0.4836	-0.3036	-0.0000
19	-0.5054	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.3056	0.0000	0.0000	0.4500	0.0000	-0.0000	0.0000	0.0000
20	-0.0000	0.0004	0.5007	-0.0000	-0.0000	-0.3061	0.0001	-0.0000	-0.4533	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0209
21	-0.0000	-0.0117	0.0000	-0.3868	0.2427	-0.0002	-0.4623	0.0000	0.0000	0.0000	0.0000	0.3161	0.0202	-0.0123	-0.0000
22	0.0000	0.0004	-0.0000	-0.0361	0.0232	0.0000	0.1008	-0.0000	-0.0000	-0.0000	-0.0000	0.1284	0.4836	-0.3036	0.0000
23	-0.5054	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.3056	-0.0000	0.0000	-0.4500	0.0000	-0.0000	0.0000	0.0000
24	-0.0000	0.0004	0.5007	-0.0000	-0.0000	-0.3061	0.0001	-0.0000	0.4533	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0209
25	-0.0000	-0.0117	0.0000	0.3868	-0.2427	-0.0002	-0.4623	0.0000	0.0000	0.0000	0.0000	-0.3161	-0.0202	0.0123	-0.0000
26	-0.0000	0.0000	0.0000	-0.0013	-0.0415	0.0000	-0.0000	-0.1004	0.0000	-0.0000	0.0000	0.1283	0.0183	0.5667	0.0000
27	-0.0008	-0.0000	-0.0000	-0.0145	-0.4538	0.0000	-0.0000	-0.4671	0.0000	-0.0000	0.0000	0.3209	0.0008	0.0240	0.0000
28	0.0000	-0.0005	-0.5092	-0.0000	-0.0000	-0.3131	0.0001	-0.0000	-0.0000	0.4566	-0.0000	0.0000	-0.0000	0.0000	-0.0210
29	-0.0000	-0.5095	0.0005	-0.0000	0.0000	0.0001	0.3131	-0.0000	-0.0000	0.0000	0.4564	0.0000	0.0000	-0.0000	-0.0000
30	0.0000	-0.0000	0.0000	-0.0013	-0.0415	-0.0000	0.0000	0.1004	-0.0000	0.0000	-0.0000	0.1283	0.0183	0.5667	-0.0000
31	-0.0008	0.0000	-0.0000	0.0145	0.4538	0.0000	-0.0000	-0.4671	0.0000	-0.0000	0.0000	-0.3209	-0.0008	-0.0240	0.0000
32	0.0000	-0.0005	-0.5092	-0.0000	-0.0000	-0.3131	0.0001	0.0000	-0.0000	-0.4566	0.0000	0.0000	-0.0000	0.0000	-0.0210
33	-0.0000	-0.5095	0.0005	-0.0000	0.0000	0.0001	0.3131	-0.0000	-0.0000	-0.0000	-0.4564	0.0000	0.0000	-0.0000	-0.0000

	31	32	33
1	-0.0000	-0.0000	0.1729
2	-0.0000	-0.0823	-0.0000
3	0.0000	-0.0000	0.0000
4	-0.0825	0.0000	-0.0000
5	-0.0000	0.0000	0.0007
6	-0.0000	-0.0000	0.0000
7	-0.0000	0.0000	-0.0000
8	0.0000	0.0000	0.0000
9	-0.0000	-0.0000	0.0000
10	0.0000	-0.0000	0.3623
11	-0.0000	-0.0208	-0.0000
12	0.0000	-0.0000	-0.0158
13	-0.0209	0.0000	-0.0000
14	-0.0000	0.0000	0.3623
15	-0.0000	-0.0208	-0.0000
16	0.0000	-0.0000	0.0158
17	-0.0209	0.0000	-0.0000
18	-0.6763	0.0000	0.3628
19	-0.0000	-0.0208	-0.0000
20	0.0000	-0.0000	0.0000
21	-0.0168	0.0000	-0.0158
22	0.6763	-0.0000	0.3628
23	-0.0000	-0.0208	-0.0000
24	0.0000	-0.0000	0.0000
25	-0.0168	0.0000	0.0158
26	-0.0000	-0.6764	0.3692
27	-0.0000	-0.0167	-0.0157
28	0.0000	-0.0000	-0.0000
29	-0.0210	0.0000	-0.0000
30	0.0000	0.6764	0.3692
31	-0.0000	-0.0167	0.0157
32	0.0000	-0.0000	0.0000
33	-0.0210	0.0000	-0.0000

TABLE VIII

$IrCl_6^{2-}$

Eigenvectors: MO's across and AO's down

EIGENVECTORS

$IrCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	-0.0000	-0.0000	-1.4312	-0.0002	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
2	0.0000	-0.0000	1.4688	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.1046	-0.0000	-0.0000
3	0.0000	1.4688	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.1023	0.0001
4	-1.4688	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0001	-0.1021
5	-0.0000	-0.0000	0.0000	0.0002	0.9148	0.0383	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000
6	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.9553	-0.0001	-0.0000	0.0063	-0.0000	0.0000	0.0000	-0.0000	-0.0000
7	-0.0000	0.0000	0.0000	0.0000	-0.0383	0.9156	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000
8	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0001	0.9553	0.0000	0.0000	0.0069	-0.0000	-0.0000	-0.0000	0.0000
9	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.9559	-0.0000	0.0000	-0.0006	-0.0000	-0.0000	-0.0000
10	-0.0000	-0.5219	-0.0000	0.2590	0.0865	-0.1363	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0146	0.0000
11	-0.0000	0.0000	-0.1683	0.0000	0.0000	-0.0000	0.2118	0.0000	0.0000	-0.5170	0.0000	-0.0000	0.3942	0.0000	0.0000
12	0.0000	0.6007	0.0000	-0.3932	-0.2401	0.3786	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.4495	-0.0002
13	0.1683	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2131	0.0000	-0.0000	-0.5203	-0.0000	0.0002	0.3840
14	0.0000	0.5219	0.0000	0.2590	0.0865	-0.1363	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0146	-0.0000
15	-0.0000	0.0000	-0.1683	0.0000	0.0000	-0.0000	-0.2118	-0.0000	-0.0000	0.5170	-0.0000	0.0000	0.3942	0.0000	0.0000
16	0.0000	0.6007	0.0000	0.3932	0.2402	-0.3786	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.4495	-0.0002
17	0.1683	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.2131	-0.0000	-0.0000	0.5203	-0.0000	0.0002	0.3840
18	0.5219	-0.0000	-0.0000	0.2590	0.0748	0.1430	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0148
19	-0.0000	0.0000	-0.1683	0.0000	0.0000	-0.0000	0.0000	-0.2115	-0.0000	-0.0000	-0.5167	0.0000	0.3915	0.0000	0.0000
20	-0.0000	-0.1683	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.2127	0.0000	0.0000	0.5197	-0.0000	0.3822	-0.0002
21	-0.6006	0.0000	0.0000	-0.3932	-0.2077	-0.3973	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0002	0.4488
22	-0.5219	0.0000	0.0000	0.2590	0.0748	0.1430	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0148
23	-0.0000	0.0000	-0.1683	0.0000	0.0000	-0.0000	-0.0000	0.2115	0.0000	0.0000	0.5167	-0.0000	0.3915	0.0000	0.0000
24	-0.0000	-0.1683	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.2127	0.0000	-0.0000	-0.5197	-0.0000	0.3822	-0.0002
25	-0.6006	0.0000	0.0000	0.3932	0.2077	0.3973	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0002	0.4488
26	-0.0000	0.0000	-0.5220	0.2590	-0.1612	-0.0067	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	-0.0130	-0.0000	-0.0000
27	0.0000	-0.0000	0.6009	-0.3932	0.4490	0.0188	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.4568	0.0000	0.0000
28	-0.0000	-0.1683	-0.0000	0.0000	0.0000	-0.0000	0.2156	0.0000	0.0000	0.5230	-0.0000	-0.0000	-0.0000	0.4125	-0.0002
29	0.1683	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.2157	-0.0000	0.0000	0.5232	-0.0000	-0.0000	0.0002	0.4117
30	0.0000	-0.0000	0.5220	0.2590	-0.1612	-0.0067	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0130	0.0000	0.0000
31	0.0000	-0.0000	0.6009	0.3932	-0.4490	-0.0188	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.4568	0.0000	0.0000
32	-0.0000	-0.1683	-0.0000	0.0000	0.0000	-0.0000	-0.2156	-0.0000	-0.0000	-0.5229	0.0000	-0.0000	-0.0000	0.4125	-0.0002
33	0.1683	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.2157	0.0000	-0.0000	-0.5233	-0.0000	-0.0000	0.0002	0.4117

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0000	-0.0000	-0.0000	0.0032	0.0004	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.2452	0.0024	0.0003	0.0000
2	-0.0000	-0.0000	-0.0004	-0.0000	-0.0000	-0.1239	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0981
3	0.0000	-0.0045	-0.0000	0.0000	0.0000	0.0000	-0.1252	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000
4	-0.0041	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.1253	-0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000
5	0.0000	0.0000	0.0000	0.5142	0.0210	-0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0051	0.1224	0.0051	0.0000
6	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.3228	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
7	0.0000	-0.0000	-0.0000	-0.0210	0.5129	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0004	-0.0051	0.1222	0.0000
8	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.3226	0.0000	-0.0000	-0.0000	-0.0000	-0.0000
9	-0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.3210	-0.0000	0.0000	-0.0000	-0.0000
10	-0.0000	0.0006	0.0000	0.0322	-0.0533	-0.0000	0.1108	-0.0000	0.0000	0.0000	-0.0000	0.1364	-0.2988	0.4784	0.0000
11	0.0000	0.0000	-0.5043	-0.0000	-0.0000	-0.3032	-0.0000	-0.0000	0.4414	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0199
12	-0.0000	0.0186	0.0000	0.2292	-0.3688	-0.0000	0.4675	-0.0001	0.0000	0.0000	-0.0000	0.3168	-0.0123	0.0189	0.0000
13	0.5128	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.3021	0.0000	-0.0000	-0.4368	0.0000	0.0000	-0.0000	0.0000
14	0.0000	-0.0006	0.0000	0.0322	-0.0533	0.0000	-0.1108	0.0000	-0.0000	0.0000	0.0000	0.1364	-0.2988	0.4784	-0.0000
15	0.0000	0.0000	-0.5043	-0.0000	-0.0000	-0.3032	-0.0000	-0.0000	-0.4414	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0199
16	-0.0000	0.0186	0.0000	-0.2292	0.3688	-0.0000	0.4675	-0.0001	0.0000	-0.0000	-0.0000	-0.3168	0.0123	-0.0189	0.0000
17	0.5128	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.3021	-0.0000	-0.0000	0.4368	0.0000	0.0000	-0.0000	0.0000
18	0.0006	0.0000	0.0000	0.0278	0.0555	0.0000	-0.0000	-0.1107	-0.0000	0.0000	0.0000	0.1365	-0.2584	-0.5007	0.0000
19	-0.0000	-0.0000	0.5057	-0.0000	-0.0000	-0.3043	-0.0000	-0.0000	0.0000	-0.4419	0.0000	0.0000	0.0000	0.0000	-0.0199
20	-0.0000	0.5134	0.0000	0.0000	0.0000	0.0000	-0.3033	0.0000	-0.0000	-0.0000	-0.4378	0.0000	-0.0000	0.0000	0.0000
21	0.0169	0.0000	0.0000	0.1984	0.3856	0.0000	-0.0001	-0.4682	-0.0000	0.0000	0.0000	0.3177	-0.0107	-0.0199	0.0000
22	-0.0006	-0.0000	-0.0000	0.0278	0.0555	-0.0000	0.0000	0.1107	-0.0000	-0.0000	-0.0000	0.1365	-0.2584	-0.5007	-0.0000
23	-0.0000	-0.0000	0.5057	-0.0000	-0.0000	-0.3043	-0.0000	-0.0000	-0.0000	0.4419	-0.0000	0.0000	0.0000	-0.0000	-0.0199
24	-0.0000	0.5134	0.0000	0.0000	0.0000	0.0000	-0.3033	0.0001	-0.0000	0.0000	0.4378	0.0000	-0.0000	0.0000	0.0000
25	0.0169	0.0000	0.0000	-0.1984	-0.3857	0.0000	-0.0001	-0.4682	0.0000	0.0000	0.0000	-0.3177	0.0107	0.0199	0.0000
26	-0.0000	-0.0000	0.0001	-0.0648	-0.0028	0.1114	0.0000	0.0000	-0.0000	0.0000	0.0000	0.1361	0.5692	0.0239	-0.6697
27	0.0000	0.0000	0.0017	-0.4385	-0.0183	0.4604	0.0000	0.0000	-0.0000	0.0000	0.0000	0.3087	0.0221	0.0009	-0.0182
28	0.0000	-0.4961	-0.0000	0.0000	0.0000	0.0000	-0.2922	0.0000	0.4324	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000
29	-0.4969	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.2921	0.0000	-0.4320	-0.0000	0.0000	0.0000	-0.0000	0.0000
30	-0.0000	-0.0000	-0.0001	-0.0648	-0.0028	-0.1114	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.1361	0.5692	0.0239	0.6697
31	0.0000	0.0000	0.0017	0.4385	0.0183	0.4604	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.3087	-0.0221	-0.0009	-0.0182
32	0.0000	-0.4961	-0.0000	0.0000	0.0000	0.0000	-0.2922	0.0000	-0.4324	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000
33	-0.4969	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.2921	-0.0000	0.4320	-0.0000	0.0000	0.0000	-0.0000	0.0000

	31	32	33
1	-0.0000	-0.0000	-0.1917
2	-0.0000	-0.0000	-0.0000
3	-0.0978	0.0000	0.0000
4	-0.0000	-0.0978	0.0000
5	-0.0000	0.0000	0.0012
6	0.0000	-0.0000	-0.0000
7	0.0000	-0.0000	0.0001
8	-0.0000	0.0000	-0.0000
9	-0.0000	-0.0000	-0.0000
10	-0.6698	0.0001	-0.3621
11	-0.0000	-0.0000	0.0000
12	-0.0181	0.0000	0.0158
13	-0.0000	-0.0198	0.0000
14	0.6698	-0.0001	-0.3621
15	-0.0000	-0.0000	-0.0000
16	-0.0181	0.0000	-0.0158
17	-0.0000	-0.0198	0.0000
18	-0.0001	-0.6699	-0.3631
19	-0.0000	-0.0000	0.0000
20	-0.0198	0.0000	0.0000
21	-0.0000	-0.0181	0.0158
22	0.0001	0.6699	-0.3631
23	-0.0000	-0.0000	0.0000
24	-0.0198	0.0000	0.0000
25	-0.0000	-0.0181	-0.0158
26	-0.0000	-0.0000	-0.3528
27	-0.0000	-0.0000	0.0158
28	-0.0195	0.0000	0.0000
29	-0.0000	-0.0195	0.0000
30	0.0000	0.0000	-0.3528
31	-0.0000	-0.0000	-0.0158
32	-0.0195	0.0000	0.0000
33	-0.0000	-0.0195	0.0000

TABLE IX

$PtCl_6^{2-}$

Eigenvectors: MO's Across and AO's Down

EIGENVECTORS

$PtCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	-0.0000	0.0000	-1.3741	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000
2	0.0186	-0.0228	-1.4135	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0108	-0.0087	0.1114
3	0.0006	1.4137	-0.0228	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.1112	-0.0103	-0.0116
4	-1.4137	0.0003	-0.0186	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0111	0.1114	0.0076
5	-0.0000	-0.0000	-0.0000	-0.0000	0.6305	-0.6312	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000
6	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.9311	0.0010	0.0009	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000
7	-0.0000	-0.0000	0.0000	0.0000	-0.6312	-0.6305	-0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
8	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0009	0.0092	-0.9311	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000
9	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0010	0.9311	0.0092	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000
10	-0.0002	-0.4827	0.0078	0.2374	0.1563	0.0418	0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0124	-0.0012	-0.0013
11	-0.3020	0.0025	0.1524	0.0000	0.0000	-0.0000	-0.2422	-0.0003	-0.0002	-0.0074	0.5199	0.0030	0.0390	0.0315	-0.4026
12	0.0003	0.5978	-0.0096	-0.3858	-0.4491	-0.1201	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.4277	0.0397	0.0445
13	0.1525	-0.0000	0.0020	0.0000	-0.0000	-0.0000	0.0003	-0.2422	-0.0024	-0.5199	-0.0074	-0.0002	0.0402	-0.4028	-0.0276
14	0.0002	0.4827	-0.0078	0.2374	0.1563	0.0418	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0124	0.0012	0.0013
15	-0.0020	0.0025	0.1524	0.0000	0.0000	-0.0000	0.2422	0.0003	0.0002	0.0074	-0.5199	-0.0030	0.0390	0.0315	-0.4026
16	0.0003	0.5978	-0.0096	0.3858	0.4491	0.1201	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.4277	0.0397	0.0445
17	0.1525	-0.0000	0.0020	0.0000	-0.0000	-0.0000	0.0003	0.2422	0.0024	0.5199	0.0074	0.0002	0.0402	-0.4028	-0.0276
18	0.4827	-0.0001	0.0063	0.2374	-0.0420	-0.1562	0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0012	0.0124	0.0009
19	-0.0020	0.0025	0.1524	0.0000	0.0000	-0.0000	-0.0002	-0.0024	0.2422	-0.0001	-0.0030	0.5200	0.0390	0.0315	-0.4026
20	-0.0001	-0.1524	0.0025	0.0000	0.0000	-0.0000	0.0003	-0.2422	-0.0024	0.5199	0.0074	0.0002	0.4018	0.0373	0.0418
21	-0.5979	0.0001	-0.0079	-0.3858	0.1206	0.4490	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0428	-0.4287	-0.0294
22	-0.4827	0.0001	-0.0063	0.2374	-0.0420	-0.1562	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0012	-0.0124	-0.0009
23	-0.0020	0.0025	0.1524	0.0000	0.0000	-0.0000	0.0002	0.0024	-0.2422	0.0001	0.0030	-0.5200	0.0390	0.0315	-0.4026
24	-0.0001	-0.1524	0.0025	0.0000	0.0000	-0.0000	-0.0003	0.2422	0.0024	-0.5199	-0.0074	-0.0002	0.4018	0.0373	0.0418
25	-0.5979	0.0001	-0.0079	0.3858	-0.1206	-0.4490	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0428	-0.4287	-0.0294
26	-0.0063	0.0078	0.4826	0.2374	-0.1143	0.1145	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	-0.0012	-0.0010	0.0124
27	0.0078	-0.0096	-0.5978	-0.3858	0.3285	-0.3289	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0415	0.0336	-0.4285
28	-0.0001	-0.1524	0.0025	0.0000	0.0000	-0.0000	-0.2422	-0.0003	-0.0002	0.0074	-0.5199	-0.0030	0.4018	0.0373	0.0418
29	0.1525	-0.0000	0.0020	0.0000	-0.0000	-0.0000	-0.0002	-0.0024	0.2422	0.0001	0.0030	-0.5200	0.0402	-0.4028	-0.0276
30	0.0063	-0.0078	-0.4826	0.2374	-0.1143	0.1145	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0012	0.0010	-0.0124
31	0.0078	-0.0096	-0.5978	0.3858	-0.3285	0.3289	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0415	0.0336	-0.4285
32	-0.0001	-0.1524	0.0025	0.0000	0.0000	-0.0000	0.2422	0.0003	0.0002	-0.0074	0.5199	0.0030	0.4018	0.0373	0.0418
33	0.1525	-0.0000	0.0020	0.0000	0.0000	0.0000	0.0002	0.0024	-0.2422	-0.0001	-0.0030	0.5200	0.0402	-0.4028	-0.0276

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.2713	-0.0000	-0.0000	0.0000
2	-0.0000	-0.0000	0.0000	-0.0568	-0.1389	0.0010	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0140
3	-0.0000	-0.0000	-0.0000	-0.1374	0.0560	-0.0226	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.1029
4	-0.0000	0.0000	0.0000	-0.0205	0.0095	0.1484	-0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	-0.0333
5	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.5116	0.2005	0.0000	0.0000	-0.0000	0.0000	0.0744	-0.1126	0.0000
6	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0015	0.3863	0.0170	-0.0000	0.0000	-0.0000	-0.0000
7	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.2005	-0.5116	0.0000	-0.0000	-0.0000	-0.0000	-0.1126	-0.0744	-0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.3867	0.0014	0.0030	-0.0000	-0.0000	-0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	-0.0000	0.0030	0.0170	-0.3863	-0.0000	-0.0000	-0.0000	0.0000
10	0.0000	0.0000	0.0000	0.1104	-0.0450	0.0182	0.0113	0.0745	-0.0000	0.0000	0.0000	0.1436	-0.5629	-0.0339	0.6298
11	-0.0492	-0.4659	0.1885	-0.1082	-0.2645	0.0020	0.0000	-0.0000	-0.0016	0.4213	0.0185	0.0000	0.0000	-0.0000	0.0026
12	0.0000	0.0000	0.0000	0.4294	-0.1752	0.0707	0.0625	0.4130	-0.0000	0.0000	0.0000	0.3067	-0.0210	-0.0013	0.0168
13	0.0390	-0.1923	-0.4653	-0.0391	0.0181	0.2825	-0.0000	0.0000	0.0032	0.0185	-0.4213	0.0000	0.0000	-0.0000	-0.0061
14	-0.0000	-0.0000	-0.0000	-0.1104	0.0450	-0.0182	0.0113	0.0745	-0.0000	-0.0000	-0.0000	0.1436	-0.5629	-0.0339	-0.6298
15	-0.0492	-0.4659	0.1885	-0.1082	-0.2645	0.0020	0.0000	-0.0000	0.0016	-0.4213	-0.0185	0.0000	0.0000	-0.0000	0.0026
16	0.0000	0.0000	0.0000	0.4294	-0.1752	0.0707	-0.0624	-0.4130	0.0000	0.0000	0.0000	-0.3067	0.0210	0.0013	0.0168
17	0.0390	-0.1923	-0.4653	-0.0391	0.0181	0.2825	-0.0000	0.0000	-0.0032	-0.0185	0.4213	0.0000	0.0000	-0.0000	-0.0061
18	-0.0000	-0.0000	-0.0000	0.0165	-0.0076	-0.1192	0.0589	-0.0470	0.0000	0.0000	-0.0000	0.1436	0.2521	0.5044	-0.2037
19	0.0492	0.4659	-0.1885	-0.1082	-0.2645	0.0020	0.0000	-0.0000	0.4217	0.0015	0.0033	0.0000	0.0000	-0.0000	0.0026
20	0.5011	-0.0308	0.0547	-0.2616	0.1067	-0.0431	-0.0000	-0.0000	0.0032	0.0185	-0.4213	0.0000	-0.0000	0.0000	0.0189
21	0.0000	-0.0000	-0.0000	0.0642	-0.0297	-0.4637	0.3264	-0.2606	0.0000	0.0000	-0.0000	0.3067	0.0094	0.0188	-0.0054
22	-0.0000	0.0000	0.0000	-0.0165	0.0076	0.1192	0.0589	-0.0470	-0.0000	-0.0000	0.0000	0.1436	0.2521	0.5044	0.2037
23	0.0492	0.4659	-0.1885	-0.1082	-0.2645	0.0020	0.0000	-0.0000	-0.4217	-0.0015	-0.0033	0.0000	0.0000	-0.0000	0.0026
24	0.5011	-0.0308	0.0547	-0.2616	0.1067	-0.0431	-0.0000	-0.0000	-0.0032	-0.0185	0.4213	0.0000	-0.0000	0.0000	0.0189
25	0.0000	-0.0000	-0.0000	0.0642	-0.0297	-0.4638	-0.3264	0.2606	0.0000	0.0000	-0.0000	-0.3067	-0.0094	-0.0188	-0.0054
26	0.0000	0.0000	-0.0000	0.0457	0.1116	-0.0008	-0.0702	-0.0275	-0.0000	-0.0000	0.0000	0.1436	0.3108	-0.4705	0.0858
27	0.0000	0.0000	-0.0000	0.1777	0.4342	-0.0032	-0.3889	-0.1524	-0.0000	-0.0000	0.0000	0.3067	0.0116	-0.0175	0.0023
28	-0.5011	0.0308	-0.0547	-0.2616	0.1067	-0.0431	-0.0000	-0.0000	-0.0016	0.4213	0.0185	0.0000	-0.0000	0.0000	0.0189
29	-0.0390	0.1923	0.4653	-0.0391	0.0181	0.2825	-0.0000	0.0000	0.4217	0.0015	0.0033	0.0000	0.0000	-0.0000	-0.0061
30	0.0000	-0.0000	0.0000	-0.0457	-0.1116	0.0008	-0.0702	-0.0275	0.0000	-0.0000	0.0000	0.1436	0.3108	-0.4705	-0.0858
31	0.0000	0.0000	-0.0000	0.1776	0.4342	-0.0032	0.3889	0.1524	-0.0000	0.0000	-0.0000	-0.3067	-0.0116	0.0175	0.0023
32	-0.5011	0.0308	-0.0547	-0.2616	0.1067	-0.0431	-0.0000	-0.0000	0.0016	-0.4213	-0.0185	0.0000	-0.0000	0.0000	0.0189
33	-0.0390	0.1923	0.4653	-0.0391	0.0181	0.2825	-0.0000	0.0000	-0.4217	-0.0015	-0.0033	0.0000	0.0000	-0.0000	-0.0061

	31	32	33
1	-0.0000	0.0000	-0.2028
2	-0.0661	-0.0856	0.0000
3	-0.0184	0.0311	0.0000
4	-0.0848	0.0600	0.0000
5	0.0000	0.0000	-0.0000
6	0.0000	-0.0000	-0.0000
7	0.0000	0.0000	0.0000
8	0.0000	-0.0000	-0.0000
9	-0.0000	0.0000	-0.0000
10	-0.1127	0.1901	-0.3580
11	-0.0122	-0.0158	0.0000
12	-0.0030	0.0051	0.0180
13	-0.0156	0.0110	0.0000
14	0.1127	-0.1901	-0.3580
15	-0.0122	-0.0158	0.0000
16	-0.0030	0.0051	-0.0180
17	-0.0156	0.0110	0.0000
18	-0.5188	0.3672	-0.3580
19	-0.0122	-0.0158	0.0000
20	-0.0034	0.0057	0.0000
21	-0.0138	0.0098	0.0180
22	0.5188	-0.3672	-0.3580
23	-0.0122	-0.0158	0.0000
24	-0.0034	0.0057	0.0000
25	-0.0138	0.0098	-0.0180
26	-0.4045	-0.5239	-0.3580
27	-0.0108	-0.0140	0.0180
28	-0.0034	0.0057	0.0000
29	-0.0156	0.0110	0.0000
30	0.4045	0.5240	-0.3580
31	-0.0108	-0.0140	-0.0180
32	-0.0034	0.0057	0.0000
33	-0.0156	0.0110	0.0000

TABLE X

MCl_6^{2-}

MO Energies and Occupations

One-Electron MO's, Energies (evs), and Occupations

$ReCl_6^{2-}$

E(1) =	15.922978	-0
E(2) =	15.922977	-0
E(3) =	15.922973	-0
E(4) =	13.158327	-0
E(5) =	-5.055788	-0
E(6) =	-5.055789	-0
E(7) =	-9.975790	1
E(8) =	-9.975791	1
E(9) =	-9.975791	1
E(10) =	-12.893078	2
E(11) =	-12.893082	2
E(12) =	-12.893085	2
E(13) =	-13.026818	2
E(14) =	-13.026818	2
E(15) =	-13.026819	2
E(16) =	-13.569983	2
E(17) =	-13.569983	2
E(18) =	-13.569984	2
E(19) =	-14.443088	2
E(20) =	-14.443092	2
E(21) =	-14.443093	2
E(22) =	-14.708545	2
E(23) =	-14.708547	2
E(24) =	-14.885012	2
E(25) =	-14.885014	2
E(26) =	-14.885014	2
E(27) =	-15.272014	2
E(28) =	-22.889675	2
E(29) =	-22.889681	2
E(30) =	-23.060750	2
E(31) =	-23.060752	2
E(32) =	-23.060753	2
E(33) =	-23.957092	2

SUM= -811.38617706 EV

$OsCl_6^{2-}$

E(1) =	14.588212	-0
E(2) =	14.572948	-0
E(3) =	14.571782	-0
E(4) =	11.809145	-0
E(5) =	-7.474939	-0
E(6) =	-7.477324	-0
E(7) =	-10.870753	1
E(8) =	-10.871520	1
E(9) =	-10.871582	2
E(10) =	-12.905411	2
E(11) =	-12.916589	2
E(12) =	-12.917463	2
E(13) =	-13.074122	2
E(14) =	-13.074391	2
E(15) =	-13.078174	2
E(16) =	-13.582958	2
E(17) =	-13.594901	2
E(18) =	-13.595798	2
E(19) =	-14.385522	2
E(20) =	-14.397450	2
E(21) =	-14.789720	2
E(22) =	-14.790298	2
E(23) =	-14.797803	2
E(24) =	-14.817941	2
E(25) =	-14.829841	2
E(26) =	-14.830734	2
E(27) =	-15.903396	2
E(28) =	-22.815436	2
E(29) =	-22.829128	2
E(30) =	-23.111908	2
E(31) =	-23.113436	2
E(32) =	-23.133256	2
E(33) =	-24.056898	2

SUM= -826.17053223 EV

$IrCl_6^{2-}$

E(1) =	16.184533	-0
E(2) =	16.181977	-0
E(3) =	16.157160	-0
E(4) =	13.555161	-0
E(5) =	-7.196794	-0
E(6) =	-7.201034	-0
E(7) =	-11.306806	1
E(8) =	-11.307014	2
E(9) =	-11.309068	2
E(10) =	-12.957402	2
E(11) =	-12.959175	2
E(12) =	-12.976795	2
E(13) =	-13.133170	2
E(14) =	-13.137708	2
E(15) =	-13.138251	2
E(16) =	-13.638061	2
E(17) =	-13.640000	2
E(18) =	-13.658090	2
E(19) =	-14.783201	2
E(20) =	-14.801493	2
E(21) =	-14.894679	2
E(22) =	-14.907079	2
E(23) =	-14.908359	2
E(24) =	-15.012228	2
E(25) =	-15.014055	2
E(26) =	-15.031329	2
E(27) =	-16.054650	2
E(28) =	-22.909454	2
E(29) =	-22.931126	2
E(30) =	-23.193068	2
E(31) =	-23.223679	2
E(32) =	-23.226826	2
E(33) =	-24.216744	2

SUM= -845.23217010 EV

$PtCl_6^{2-}$

E(1) =	13.339157	-0
E(2) =	13.339157	-0
E(3) =	13.339149	-0
E(4) =	10.637692	-0
E(5) =	-7.527399	-0
E(6) =	-7.527399	-0
E(7) =	-11.825438	2
E(8) =	-11.825442	2
E(9) =	-11.825443	2
E(10) =	-12.997242	2
E(11) =	-12.997244	2
E(12) =	-12.997246	2
E(13) =	-13.204478	2
E(14) =	-13.204479	2
E(15) =	-13.204482	2
E(16) =	-13.679607	2
E(17) =	-13.679613	2
E(18) =	-13.679613	2
E(19) =	-15.022671	2
E(20) =	-15.022673	2
E(21) =	-15.022674	2
E(22) =	-15.092400	2
E(23) =	-15.092402	2
E(24) =	-15.169003	2
E(25) =	-15.169006	2
E(26) =	-15.169007	2
E(27) =	-16.272351	2
E(28) =	-22.976844	2
E(29) =	-22.976854	2
E(30) =	-23.280633	2
E(31) =	-23.280634	2
E(32) =	-23.280637	2
E(33) =	-24.296836	2

SUM= -864.48986053 EV

TABLE XI

$ReCl_6^{2-}$

Mulliken Overlap Populations:

AO's Down and Across; $ReCl_6^{2-}$ Bond Order Matrix

MULLIKEN OVERLAP POPULATIONS FOR 32 ELECTRONS

$ReCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.2793	0.	-0.	-0.	-0.	0.	0.	0.	0.	0.0228	0.	0.0778	0.	0.0228	-0.
2	0.	0.0807	-0.	-0.	0.	0.	0.	0.	0.	-0.	-0.0046	-0.	-0.	0.	-0.0046
3	-0.	-0.	0.0807	-0.	-0.	0.	-0.	0.	-0.	0.0527	0.	0.1204	-0.	0.0527	-0.
4	-0.	-0.	-0.	0.0807	-0.	0.	-0.	-0.	-0.	0.	-0.	-0.	-0.0046	0.	0.
5	-0.	0.	-0.	-0.	0.8184	-0.	-0.	-0.	-0.	0.0048	-0.	0.0356	-0.	0.0048	-0.
6	0.	0.	0.	0.	-0.	2.1882	0.	0.	0.	0.	0.0062	0.	0.	0.	0.0062
7	0.	0.	-0.	-0.	-0.	0.	0.8184	0.	0.	0.0144	0.	0.1067	0.	0.0144	0.
8	0.	0.	0.	-0.	-0.	0.	0.	2.1882	-0.	0.	-0.	0.	-0.	-0.	0.
9	0.	0.	-0.	-0.	-0.	0.	0.	-0.	2.1882	-0.	0.	-0.	0.	0.0062	0.
10	0.0228	-0.	0.0527	0.	0.0048	0.	0.0144	0.	-0.	3.7736	-0.	0.	-0.	-0.0066	-0.
11	0.	-0.0046	0.	-0.	-0.	0.0062	0.	-0.	0.	-0.	3.9715	0.	-0.	-0.	0.0066
12	0.0778	-0.	0.1204	-0.	0.0356	0.	0.1067	0.	-0.	0.	0.	3.0400	0.	-0.0001	-0.
13	0.	-0.	-0.	-0.0046	-0.	0.	0.	-0.	0.0062	-0.	-0.	0.	3.9725	-0.	0.
14	0.0228	0.	0.0527	0.	0.0048	0.	0.0144	-0.	0.	-0.0066	-0.	-0.0001	-0.	3.7736	-0.

	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.	0.0778	-0.	0.0228	0.	0.	0.0778	0.0228	0.	-0.	0.0778	0.0228	0.0778	0.	0.	0.0228
2	-0.0046	-0.	0.	-0.	-0.0046	-0.	-0.	0.	-0.0046	0.	0.	0.0527	0.1204	-0.	-0.	0.0527
3	-0.	0.1204	-0.	-0.	0.	-0.0046	0.	-0.	-0.	-0.0046	-0.	-0.	-0.	-0.0046	-0.	0.
4	0.	-0.	-0.0046	0.0527	-0.	-0.	0.1204	0.0527	-0.	-0.	0.1204	-0.	0.	0.	-0.0048	0.
5	-0.	0.0356	0.	0.0048	-0.	-0.	0.0356	0.0048	-0.	-0.	0.0356	0.0192	0.1423	-0.	0.	0.0192
6	0.	0.	-0.	0.	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.0062	-0.	-0.
7	0.	0.1067	-0.	0.0144	-0.	0.	0.1067	0.0144	-0.	-0.	0.1067	0.	0.	0.	0.	0.
8	0.	-0.	-0.	0.	0.0062	0.	0.	-0.	0.0062	-0.	0.	0.	-0.	-0.	0.0062	0.
9	0.	0.	0.0062	-0.	0.	0.0062	0.	-0.	0.	0.0062	-0.	0.	0.	0.	0.	-0.
10	-0.0066	-0.0001	-0.	-0.0003	-0.	-0.0016	-0.0010	-0.0003	-0.	-0.0016	-0.0010	-0.0003	-0.0010	-0.0016	-0.	-0.0003
11	-0.	0.	-0.	-0.0003	-0.	-0.	-0.	-0.0003	0.	0.	-0.0016	-0.0038	-0.0077	0.	-0.	-0.0018
12	-0.0020	-0.	-0.0010	0.	-0.0038	-0.0002	-0.0010	-0.	-0.0038	-0.0002	-0.0010	-0.0002	-0.0038	-0.	-0.	-0.0010
13	-0.	0.0000	-0.0016	-0.	-0.0077	-0.0038	-0.0016	-0.	-0.0077	-0.0038	-0.	-0.	-0.	-0.0069	0.	0.
14	-0.	0.	-0.0003	0.	-0.0016	-0.0010	-0.0003	0.	-0.0016	-0.0010	-0.0003	-0.0010	-0.0016	-0.	-0.	-0.0003
15	-0.	-0.	0.	-0.0003	0.	0.	-0.	-0.0003	0.	-0.	-0.0016	-0.0038	-0.0077	0.	-0.	-0.0018
16	3.0400	0.	-0.0010	0.	-0.0038	-0.0002	-0.0010	-0.	-0.0038	-0.0002	-0.0010	-0.0002	-0.0038	-0.	-0.	-0.0010
17	0.	3.9715	-0.0016	0.	-0.0077	-0.0038	-0.0016	-0.	-0.0077	-0.0038	0.	-0.	-0.	-0.0069	-0.	0.
18	-0.0010	-0.0016	3.7737	-0.	0.	0.	-0.0000	-0.	0.	-0.0001	-0.0003	-0.0010	0.	-0.0016	-0.0003	-0.0003
19	0.	0.	-0.	3.9715	0.	0.	-0.	0.0000	-0.	0.	-0.0016	-0.0038	0.	-0.0077	-0.0018	-0.0018
20	-0.0038	-0.0077	0.	0.	3.9715	-0.	-0.	0.	0.0000	-0.	-0.	0.	-0.0003	0.	-0.	0.
21	-0.0002	-0.0038	0.	0.	-0.	3.0400	-0.0001	0.	-0.	-0.0020	-0.0010	-0.0002	-0.	-0.0038	-0.0010	-0.0010
22	-0.0010	-0.0016	-0.0000	-0.	-0.	-0.0001	3.7737	-0.	-0.	-0.	-0.0003	-0.0010	0.	-0.0016	-0.0003	-0.0003
23	-0.	-0.	-0.	0.0000	0.	0.	-0.	3.9715	0.	-0.	-0.0016	-0.0038	-0.	-0.0077	-0.0018	-0.0018
24	-0.0038	-0.0077	0.	-0.	0.0000	-0.	-0.	0.	3.9715	-0.	-0.	-0.	-0.0003	0.	-0.	0.
25	-0.0002	-0.0038	-0.0001	0.	-0.	-0.0020	-0.	-0.	-0.	3.0400	-0.0010	-0.0002	-0.	-0.0038	-0.0010	-0.0010
26	-0.0010	0.	-0.0003	-0.0016	-0.	-0.0010	-0.0003	-0.0016	-0.	-0.0010	3.7737	0.	-0.	0.	-0.0003	-0.0003
27	-0.0002	-0.	-0.0010	-0.0038	0.	-0.0002	-0.0010	-0.0038	-0.	-0.0002	0.	3.0406	0.	0.	-0.	-0.0001
28	-0.0038	-0.	0.	0.	-0.0003	-0.	0.	-0.	-0.0003	-0.	-0.	0.	3.9715	-0.	0.	0.
29	-0.	-0.0003	-0.0016	-0.0077	0.	-0.0038	-0.0016	-0.0077	0.	-0.0038	0.	0.	-0.	3.9715	-0.	-0.
30	-0.0010	-0.	-0.0003	-0.0016	0.	-0.0010	-0.0003	-0.0016	-0.	-0.0010	-0.0000	-0.0001	0.	-0.	3.7737	-0.
31	-0.0002	0.	-0.0010	-0.0038	0.	-0.0002	-0.0010	-0.0038	-0.	-0.0002	-0.0001	-0.0026	0.	0.	-0.	3.0400
32	-0.0038	0.	-0.	-0.0003	0.	-0.	-0.0003	0.	-0.	0.	-0.	0.	-0.0000	-0.	-0.	0.
33	0.	-0.0003	-0.0016	-0.0077	-0.	-0.0038	-0.0016	-0.0077	0.	-0.0038	-0.	-0.	-0.	0.0060	-0.	1.

	31	32	33
1	0.0778	0.	0.
2	0.1204	0.	0.
3	-0.	-0.0046	0.
4	-0.	-0.	-0.0046
5	0.1423	-0.	-0.
6	0.	0.0062	-0.
7	0.	-0.	-0.
8	0.	-0.	0.0062
9	0.	0.	-0.
10	-0.0010	-0.0016	-0.
11	-0.0038	-0.0077	0.
12	-0.0002	-0.0038	0.
13	-0.	0.	-0.0003
14	-0.0010	-0.0016	-0.
15	-0.0038	-0.0077	-0.
16	-0.0002	-0.0038	0.
17	0.	0.	-0.0003
18	-0.0010	0.	-0.0016
19	-0.0038	-0.	-0.0077
20	0.	-0.0003	-0.
21	-0.0002	0.	-0.0038
22	-0.0010	0.	-0.0016
23	-0.0038	-0.	-0.0077
24	-0.	-0.0003	0.
25	-0.0002	0.	-0.0038
26	-0.0001	0.	-0.
27	-0.0020	0.	-0.
28	0.	0.0000	-0.
29	0.	-0.	0.0000
30	-0.	0.	-0.
31	3.0400	0.	0.
32	0.	3.9715	-0.
33	0.	-0.	3.9715

REDUCED OVERLAP POPULATION MATRIX ATOM BY ATOM

	1	2	3	4	5	6	7
1	8.7226	0.4383	0.4383	0.4383	0.4383	0.4383	0.4383
2	0.4383	14.7566	-0.0022	-0.0212	-0.0212	-0.0212	-0.0212
3	0.4383	-0.0022	14.7566	-0.0212	-0.0212	-0.0212	-0.0212
4	0.4383	-0.0212	-0.0212	14.7566	-0.0022	-0.0212	-0.0212
5	0.4383	-0.0212	-0.0212	-0.0022	14.7566	-0.0212	-0.0212
6	0.4383	-0.0212	-0.0212	-0.0212	-0.0212	14.7566	-0.0022
7	0.4383	-0.0212	-0.0212	-0.0212	-0.0212	-0.0022	14.7566

TABLE XII

$OsCl_6^{2-}$

Mulliken Overlap Populations:

AO's Down and Across; $OsCl_6^{2-}$ Bond Order Matrix

MULLIKEN OVERLAP POPULATIONS FOR 52 ELECTRONS

$OsCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.3457	-0.	-0.	-0.	-0.	0.	0.	0.	0.	0.0225	0.	0.0842	-0.	0.0225	0.
2	-0.	0.1168	-0.	-0.	0.	0.	-0.	0.	0.	0.	-0.0028	-0.	0.	0.	-0.0028
3	-0.	-0.	0.1173	-0.	-0.	0.	-0.	0.	0.	0.0601	0.	0.1416	0.	0.0601	0.
4	-0.	-0.	-0.	0.1172	0.	0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.0028	-0.	0.
5	-0.	0.	-0.	0.	0.9681	-0.	-0.	0.	-0.	0.0030	0.	0.0312	-0.	0.0030	0.
6	0.	0.	0.	-0.	-0.	2.1524	-0.	0.	0.	0.	0.0069	0.	-0.	-0.	0.0069
7	0.	-0.	-0.	-0.	-0.	-0.	0.9717	0.	0.	0.0091	0.	0.0936	-0.	0.0091	0.
8	0.	0.	0.	-0.	0.	0.	0.	4.0552	0.	0.	-0.	0.	-0.	0.	-0.
9	0.	0.	0.	-0.	-0.	0.	0.	0.	2.1532	0.	-0.	0.	0.0068	0.	-0.
10	0.0225	0.	0.0601	-0.	0.0030	0.	0.0091	0.	0.	3.7751	-0.	0.	-0.	0.0000	0.
11	0.	-0.0028	0.	-0.	0.	0.0069	0.	-0.	-0.	-0.	3.9749	-0.	-0.	-0.	0.0000
12	0.0842	-0.	0.1416	-0.	0.0312	0.	0.0936	0.	0.	0.	-0.	2.9450	-0.	-0.0001	-0.
13	-0.	0.	0.	-0.0028	-0.	-0.	-0.	-0.	0.0068	-0.	-0.	-0.	3.9752	-0.	0.
14	0.0225	0.	0.0601	-0.	0.0030	-0.	0.0091	0.	0.	0.0000	-0.	-0.0001	-0.	3.7751	0.
15	0.	-0.0028	0.	0.	0.	0.0069	0.	-0.	-0.	0.	0.0000	-0.	0.	0.	3.9749
16	0.0842	-0.	0.1416	-0.	0.0312	0.	0.0936	0.	0.	-0.0001	-0.	-0.0019	0.	-0.	-0.
17	0.	-0.	-0.	-0.0028	0.	0.	0.	0.	0.0068	0.	0.	0.	0.0000	0.	-0.
18	0.0225	-0.	-0.	0.0601	0.0030	0.	0.0091	-0.	-0.	-0.0004	-0.	-0.0014	-0.0018	-0.0004	0.
19	0.	-0.0028	0.	0.	-0.	-0.	-0.	-0.0138	0.	0.	-0.0003	0.	-0.	-0.	-0.0003
20	0.	-0.	-0.0028	-0.	-0.	0.	0.	0.	0.0068	-0.0018	0.	-0.0041	-0.0075	-0.0018	0.

21	0.0842	-0.	-0.	0.1415	0.0312	0.	0.0935	-0.	0.	-0.0014	-0.	-0.0005	-0.0041	-0.0014	0.
22	0.0225	0.	-0.	0.0601	0.0030	0.	0.0091	-0.	-0.	-0.0004	-0.	-0.0014	-0.0018	-0.0004	-0.
23	0.	-0.0028	-0.	0.	-0.	0.	-0.	-0.0138	-0.	-0.	-0.0003	-0.	0.	-0.	-0.0003
24	-0.	0.	-0.0028	0.	0.	-0.	-0.	-0.	0.0068	-0.0018	-0.	-0.0041	-0.0075	-0.0018	-0.
25	0.0842	-0.	-0.	0.1415	0.0312	0.	0.0935	-0.	-0.	-0.0014	-0.	-0.0005	-0.0041	-0.0014	0.
26	0.0225	0.0600	-0.	-0.	0.0122	0.	-0.	0.	0.	-0.0004	-0.0018	-0.0014	-0.	-0.0004	-0.0018
27	0.0842	0.1413	-0.	0.	0.1245	0.	0.	-0.	0.	-0.0014	-0.0041	-0.0005	-0.	-0.0014	-0.0041
28	0.	-0.	-0.0028	0.	-0.	0.0067	-0.	0.	-0.	-0.0018	-0.0075	-0.0041	-0.	-0.0018	-0.0075
29	-0.	0.	0.	-0.0028	-0.	0.	0.	-0.0138	0.	0.	-0.	0.	-0.0003	-0.	-0.
30	0.0225	0.0600	-0.	0.	0.0122	0.	-0.	0.	-0.	-0.0004	-0.0018	-0.0014	0.	-0.0004	-0.0018
31	0.0842	0.1413	0.	0.	0.1245	0.	0.	-0.	0.	-0.0014	-0.0041	-0.0005	-0.	-0.0014	-0.0041
32	-0.	0.	-0.0028	-0.	-0.	0.0067	-0.	-0.	-0.	-0.0018	-0.0075	-0.0041	0.	-0.0018	-0.0075
33	-0.	-0.	-0.	-0.0028	0.	-0.	-0.	-0.0138	0.	0.	0.	-0.	-0.0003	-0.	0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0842	0.	0.0225	0.	0.	0.0842	0.0225	0.	-0.	0.0842	0.0225	0.0842	0.	-0.	0.0225
2	-0.	-0.	-0.	-0.0028	-0.	-0.	0.	-0.0028	0.	-0.	0.0600	0.1413	-0.	0.	0.0600
3	0.1416	-0.	-0.	0.	-0.0028	-0.	-0.	-0.	-0.0028	-0.	-0.	-0.	-0.0028	0.	-0.
4	-0.	-0.0028	0.0601	0.	-0.	0.1415	0.0601	0.	0.	0.1415	-0.	0.	-0.	-0.0028	0.
5	0.0312	0.	0.0030	-0.	-0.	0.0312	0.0030	-0.	0.	0.0312	0.0122	0.1245	-0.	-0.	0.0122
6	0.	0.	0.	-0.	0.	0.	0.	-0.	-0.	0.	0.	0.	0.0067	0.	0.
7	0.0936	0.	0.0091	-0.	0.	0.0935	0.0091	-0.	-0.	0.0935	-0.	0.	-0.	0.	-0.
8	0.	0.	-0.	-0.0138	0.	-0.	-0.	-0.0138	-0.	-0.	0.	-0.	0.	-0.0138	0.
9	0.	0.0068	-0.	0.	0.0068	0.	-0.	-0.	0.0068	-0.	0.	0.	-0.	0.	-0.
10	-0.0001	0.	-0.0004	0.	-0.0018	-0.0014	-0.0004	-0.	-0.0018	-0.0014	-0.0004	-0.0014	-0.0018	0.	-0.0004
11	-0.	0.	-0.	-0.0003	0.	-0.	-0.	-0.0003	-0.	-0.	-0.0018	-0.0041	-0.0075	-0.	-0.0018
12	-0.0019	0.	-0.0014	0.	-0.0041	-0.0005	-0.0014	-0.	-0.0041	-0.0005	-0.0014	-0.0005	-0.0041	0.	-0.0014
13	0.	0.0000	-0.0018	-0.	-0.0075	-0.0041	-0.0018	0.	-0.0075	-0.0041	-0.	-0.	-0.	-0.0003	0.
14	-0.	0.	-0.0004	-0.	-0.0018	-0.0014	-0.0004	-0.	-0.0018	-0.0014	-0.0004	-0.0014	-0.0018	-0.	-0.0004
15	-0.	-0.	0.	-0.0003	0.	0.	-0.	-0.0003	-0.	0.	-0.0018	-0.0041	-0.0075	-0.	-0.0018
16	2.9450	-0.	-0.0014	0.	-0.0041	-0.0005	-0.0014	-0.	-0.0041	-0.0005	-0.0014	-0.0005	-0.0041	0.	-0.0014
17	-0.	3.9752	-0.0018	-0.	-0.0075	-0.0041	-0.0018	0.	-0.0075	-0.0041	0.	0.	-0.	-0.0003	-0.
18	-0.0014	-0.0018	3.7751	-0.	0.	0.	0.0000	-0.	-0.	-0.0001	-0.0004	-0.0014	0.	-0.0018	-0.0004
19	0.	-0.	-0.	4.0365	0.	0.	-0.	-0.0000	-0.	0.	-0.0018	-0.0041	0.	-0.0052	-0.0018
20	-0.0041	-0.0075	0.	0.	3.9753	-0.	-0.	-0.	0.0000	0.	0.	-0.	-0.0003	0.	0.
21	-0.0005	-0.0041	0.	0.	-0.	2.9452	-0.0001	-0.	-0.	-0.0019	-0.0014	-0.0005	-0.	-0.0041	-0.0014
22	-0.0014	-0.0018	0.0000	-0.	-0.	-0.0001	3.7751	-0.	-0.	-0.	-0.0004	-0.0014	0.	-0.0018	-0.0004
23	-0.	0.	-0.	-0.0000	-0.	-0.	-0.	4.0365	0.	-0.	-0.0018	-0.0041	0.	-0.0052	-0.0018
24	-0.0041	-0.0075	-0.	0.0000	-0.	-0.	0.	3.9753	0.	0.	0.	0.	-0.0003	-0.	-0.
25	-0.0005	-0.0041	-0.0001	0.	0.	-0.0019	-0.	-0.	0.	2.9452	-0.0014	-0.0005	0.	-0.0041	-0.0014
26	-0.0014	0.	-0.0004	-0.0018	0.	-0.0014	-0.0004	-0.0018	0.	-0.0014	3.7753	0.	-0.	0.	0.0000
27	-0.0005	0.	-0.0014	-0.0041	-0.	-0.0005	-0.0014	-0.0041	0.	-0.0005	0.	2.9483	0.	-0.	-0.0001
28	-0.0041	-0.	0.	0.	-0.0003	-0.	0.	0.	-0.0003	0.	-0.	0.	3.9761	0.	0.
29	0.	-0.0003	-0.0018	-0.0052	0.	-0.0041	-0.0018	-0.0052	-0.	-0.0041	0.	-0.	0.	4.0365	-0.
30	-0.0014	-0.	-0.0004	-0.0018	0.	-0.0014	-0.0004	-0.0018	-0.	-0.0014	0.0000	-0.0001	0.	-0.	3.7753
31	-0.0005	0.	-0.0014	-0.0041	-0.	-0.0005	-0.0014	-0.0041	0.	-0.0005	-0.0001	-0.0019	0.	-0.	-0.
32	-0.0041	0.	0.	-0.	-0.0003	0.	0.	-0.	-0.0003	0.	0.	0.	0.0000	-0.	0.
33	-0.	-0.0003	-0.0018	-0.0052	0.	-0.0041	-0.0018	-0.0052	-0.	-0.0041	-0.	0.	-0.	-0.0000	-0.

	31	32	33
1	0.0842	-0.	-0.
2	0.1413	0.	-0.
3	0.	-0.0028	-0.
4	0.	-0.	-0.0028
5	0.1245	-0.	0.
6	0.	0.0067	-0.
7	0.	-0.	-0.
8	-0.	-0.	-0.0138
9	0.	-0.	0.
10	-0.0014	-0.0018	0.
11	-0.0041	-0.0075	0.
12	-0.0005	-0.0041	-0.
13	-0.	0.	-0.0003
14	-0.0014	-0.0018	-0.
15	-0.0041	-0.0075	0.
16	-0.0005	-0.0041	-0.
17	0.	0.	-0.0003
18	-0.0014	0.	-0.0018
19	-0.0041	-0.	-0.0052
20	-0.	-0.0003	0.
21	-0.0005	0.	-0.0041
22	-0.0014	0.	-0.0018
23	-0.0041	-0.	-0.0052
24	0.	-0.0003	-0.
25	-0.0005	0.	-0.0041
26	-0.0001	0.	-0.
27	-0.0019	0.	0.
28	0.	0.0000	-0.
29	-0.	-0.	-0.0000
30	-0.	0.	-0.
31	2.9483	-0.	0.
32	-0.	3.9761	0.
33	0.	0.	4.0365

REDUCED OVERLAP POPULATION MATRIX ATOM BY ATOM

	1	2	3	4	5	6	7
1	10.9977	0.4535	0.4535	0.4328	0.4328	0.4321	0.4321
2	0.4535	14.6702	-0.0020	-0.0231	-0.0231	-0.0231	-0.0231
3	0.4535	-0.0020	14.6702	-0.0231	-0.0231	-0.0231	-0.0231
4	0.4328	-0.0231	-0.0231	14.7321	-0.0020	-0.0208	-0.0208
5	0.4328	-0.0231	-0.0231	-0.0020	14.7321	-0.0208	-0.0208
6	0.4321	-0.0231	-0.0231	-0.0208	-0.0208	14.7361	-0.0020
7	0.4321	-0.0231	-0.0231	-0.0208	-0.0208	-0.0020	14.7362

TABLE XIII

$IrCl_6^{2-}$

Mulliken Overlap Populations:

AO's Down and Across; $IrCl_6^{2-}$ Bond Order Matrix

MULLIKEN OVERLAP POPULATIONS FOR 53 ELECTRONS

$IrCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.3875	0.	-0.	-0.	0.	0.	0.	0.	0.	0.0253	0.	0.0871	0.	0.0253	0.
2	0.	0.1436	-0.	-0.	0.	-0.	-0.	-0.	0.	0.	-0.0009	0.	0.	0.	-0.0009
3	-0.	-0.	0.1429	-0.	0.	0.	-0.	0.	-0.	0.0709	0.	0.1505	0.	0.0709	0.
4	-0.	-0.	-0.	0.1428	0.	0.	0.	0.	0.	-0.	-0.	-0.	-0.0009	0.	0.
5	0.	0.	0.	0.	1.1195	0.	-0.	0.	0.	0.0034	0.	0.0340	0.	0.0034	0.
6	0.	-0.	0.	0.	0.	2.2421	0.	-0.	-0.	0.	0.0102	0.	0.	0.	0.0102
7	0.	-0.	-0.	0.	-0.	0.	1.1137	0.	-0.	0.0101	-0.	0.1022	0.	0.0101	-0.
8	0.	-0.	0.	0.	0.	-0.	0.	4.0673	0.	0.	0.	0.	0.	-0.	0.
9	0.	0.	-0.	0.	0.	-0.	-0.	0.	4.0673	0.	0.	0.	-0.0168	0.	-0.
10	0.0253	0.	0.0709	-0.	0.0034	0.	0.0101	0.	0.	3.7316	0.	0.	0.	0.0000	-0.
11	0.	-0.0009	0.	-0.	0.	0.0102	-0.	0.	0.	0.	3.9462	0.	-0.	0.	0.0000
12	0.0871	0.	0.1505	-0.	0.0340	0.	0.1022	0.	0.	0.	0.	2.8437	-0.	-0.0001	-0.
13	0.	0.	0.	-0.0009	0.	0.	0.	0.	-0.0168	0.	-0.	-0.	4.0360	-0.	-0.
14	0.0253	0.	0.0709	0.	0.0034	0.	0.0101	-0.	0.	0.0000	0.	-0.0001	-0.	3.7316	-0.
15	0.	-0.0009	0.	0.	0.	0.0102	-0.	0.	-0.	-0.	0.0000	-0.	-0.	-0.	3.9462
16	0.0871	0.	0.1505	-0.	0.0340	0.	0.1022	-0.	0.	-0.0001	-0.	-0.0021	0.	-0.	-0.
17	-0.	-0.	-0.	-0.0009	0.	-0.	-0.	0.	-0.0168	-0.	-0.	0.	-0.0000	0.	-0.
18	0.0253	-0.	-0.	0.0709	0.0034	0.	0.0101	-0.	0.	-0.0004	0.	-0.0013	-0.0019	-0.0004	0.
19	0.	-0.0009	0.	-0.	0.	0.	0.	-0.0168	0.	0.	-0.0003	-0.	-0.	-0.	-0.0003
20	0.	0.	-0.0009	0.	0.	-0.	-0.	0.	-0.0168	-0.0019	0.	-0.0044	-0.0051	-0.0019	-0.
21	0.0871	-0.	-0.	0.1505	0.0340	0.	0.1022	-0.	-0.	-0.0013	-0.	0.0006	-0.0044	-0.0013	0.
22	0.0253	0.	0.	0.0709	0.0034	-0.	0.0101	-0.	0.	-0.0004	-0.	-0.0013	-0.0019	-0.0004	-0.
23	0.	-0.0009	-0.	-0.	0.	-0.	0.	-0.0168	0.	-0.	-0.0003	0.	-0.	-0.	-0.0003
24	-0.	0.	-0.0009	0.	-0.	-0.	0.	-0.	-0.0168	-0.0019	0.	-0.0044	-0.0051	-0.0019	-0.
25	0.0871	0.	-0.	0.1505	0.0340	0.	0.1022	-0.	0.	-0.0013	0.	0.0006	-0.0044	-0.0013	0.
26	0.0253	0.0710	-0.	-0.	0.0134	-0.	-0.	0.	0.	-0.0004	-0.0019	-0.0013	0.	-0.0004	-0.0019
27	0.0870	0.1509	-0.	0.	0.1366	-0.	0.	-0.	0.	-0.0013	-0.0044	0.0006	-0.	-0.0013	-0.0044
28	0.	-0.	-0.0009	-0.	0.	0.0106	0.	-0.	0.	-0.0019	-0.0085	-0.0044	0.	-0.0019	-0.0085
29	-0.	0.	0.	-0.0009	-0.	-0.	0.	-0.0168	0.	-0.	0.	0.	-0.0003	-0.	0.
30	0.0253	0.0710	-0.	-0.	0.0134	-0.	-0.	0.	0.	-0.0004	-0.0019	-0.0013	-0.	-0.0004	-0.0019
31	0.0870	0.1509	-0.	-0.	0.1366	-0.	0.	0.	0.	-0.0013	-0.0044	0.0006	-0.	-0.0013	-0.0044
32	0.	0.	-0.0009	0.	0.	0.0106	0.	0.	-0.	-0.0019	-0.0085	-0.0044	0.	-0.0019	-0.0085
33	-0.	0.	0.	-0.0009	0.	0.	-0.	-0.0168	-0.	0.	-0.	-0.	-0.0003	-0.	-0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0871	-0.	0.0253	0.	0.	0.0871	0.0253	0.	-0.	0.0871	0.0253	0.0870	0.	-0.	0.0253
2	0.	-0.	-0.	-0.0009	0.	-0.	0.	-0.0009	0.	0.	0.0710	0.1509	-0.	0.	0.0710
3	0.1505	-0.	-0.	0.	-0.0009	-0.	0.	-0.	-0.0009	-0.	-0.	-0.	-0.0009	0.	-0.
4	-0.	-0.0009	0.0709	-0.	0.	0.1505	0.0709	-0.	0.	0.1505	-0.	0.	-0.	-0.0009	-0.
5	0.0340	0.	0.0034	0.	0.	0.0340	0.0034	0.	-0.	0.0340	0.0134	0.1366	0.	-0.	0.0134
6	0.	-0.	0.	0.	-0.	0.	-0.	-0.	-0.	0.	-0.	-0.	0.0106	-0.	-0.
7	0.1022	-0.	0.0101	0.	-0.	0.1022	0.0101	0.	0.	0.1022	-0.	0.	0.	0.	-0.
8	-0.	0.	-0.	-0.0168	0.	-0.	-0.	-0.0168	-0.	-0.	0.	-0.	-0.	-0.0168	0.
9	0.	-0.0168	0.	0.	-0.0168	-0.	0.	0.	-0.0168	0.	0.	0.	0.	0.	0.
10	-0.0001	-0.	-0.0004	0.	-0.0019	-0.0013	-0.0004	-0.	-0.0019	-0.0013	-0.0004	-0.0013	-0.0019	-0.	-0.0004
11	-0.	-0.	0.	-0.0003	0.	-0.	-0.	-0.0003	0.	0.	-0.0019	-0.0044	-0.0085	0.	-0.0019
12	-0.0021	0.	-0.0013	-0.	-0.0044	0.0006	-0.0013	0.	-0.0044	0.0006	-0.0013	0.0006	-0.0044	0.	-0.0013
13	0.	-0.0000	-0.0019	-0.	-0.0051	-0.0044	-0.0019	-0.	-0.0051	-0.0044	0.	-0.	0.	-0.0003	-0.
14	-0.	0.	-0.0004	-0.	-0.0019	-0.0013	-0.0004	-0.	-0.0019	-0.0013	-0.0004	-0.0013	-0.0019	-0.	-0.0004
15	-0.	-0.	0.	-0.0003	-0.	-0.	-0.	-0.0003	-0.	0.	-0.0019	-0.0044	-0.0085	0.	-0.0019
16	2.8437	-0.	-0.0013	-0.	-0.0044	0.0006	-0.0013	-0.	-0.0044	0.0006	-0.0013	0.0006	-0.0044	0.	-0.0013
17	-0.	4.0360	-0.0019	0.	-0.0051	-0.0044	-0.0019	0.	-0.0051	-0.0044	-0.	0.	-0.	-0.0003	0.
18	-0.0013	-0.0019	3.7316	0.	-0.	0.	0.0000	-0.	-0.	-0.0001	-0.0004	-0.0013	-0.	-0.0019	-0.0004
19	-0.	0.	0.	4.0359	0.	0.	-0.	-0.0000	0.	0.	-0.0019	-0.0044	-0.	-0.0051	-0.0019
20	-0.0044	-0.0051	-0.	0.	4.0360	0.	0.	0.	-0.0000	0.	0.	0.	-0.0003	-0.	0.
21	0.0006	-0.0044	0.	0.	0.	2.8442	-0.0001	0.	-0.	-0.0021	-0.0013	0.0006	0.	-0.0044	-0.0013
22	-0.0013	-0.0019	0.0000	-0.	0.	-0.0001	3.7316	-0.	0.	-0.	-0.0004	-0.0013	-0.	-0.0019	-0.0004
23	-0.	0.	-0.	-0.0000	0.	0.	-0.	4.0359	0.	0.	-0.0019	-0.0044	-0.	-0.0051	-0.0019
24	-0.0044	-0.0051	-0.	0.	-0.0000	-0.	0.	0.	4.0360	-0.	0.	-0.	-0.0003	-0.	0.
25	0.0006	-0.0044	-0.0001	0.	0.	-0.0021	-0.	0.	-0.	2.8442	-0.0013	0.0006	0.	-0.0044	-0.0013
26	-0.0013	-0.	-0.0004	-0.0019	0.	-0.0013	-0.0004	-0.0019	0.	-0.0013	3.7314	0.	0.	-0.	0.0000
27	0.0006	0.	-0.0013	-0.0044	0.	0.0006	-0.0013	-0.0044	-0.	0.0006	0.	2.8388	0.	0.	-0.0001
28	-0.0044	-0.	-0.	-0.	-0.0003	0.	-0.	-0.	-0.0003	0.	0.	0.	3.9429	-0.	0.
29	0.	-0.0003	-0.0019	-0.0051	-0.	-0.0044	-0.0019	-0.0051	-0.	-0.0044	-0.	0.	-0.	4.0359	0.
30	-0.0013	0.	-0.0004	-0.0019	0.	-0.0013	-0.0004	-0.0019	0.	-0.0013	0.0000	-0.0001	0.	0.	3.7314
31	0.0006	0.	-0.0013	-0.0044	0.	0.0006	-0.0013	-0.0044	-0.	0.0006	-0.0001	-0.0021	0.	0.	-0.
32	-0.0044	-0.	0.	0.	-0.0003	-0.	-0.	0.	-0.0003	-0.	-0.	0.	0.0000	0.	0.
33	-0.	-0.0003	-0.0019	-0.0051	0.	-0.0044	-0.0019	-0.0051	0.	-0.0044	0.	0.	0.	-0.0000	0.

	31	32	33
1	0.0870	0.	-0.
2	0.1509	0.	0.
3	-0.	-0.0009	0.
4	-0.	0.	-0.0009
5	0.1366	0.	0.
6	-0.	0.0106	0.
7	0.	0.	-0.
8	0.	0.	-0.0168
9	0.	-0.	-0.
10	-0.0013	-0.0019	0.
11	-0.0044	-0.0085	-0.
12	0.0006	-0.0044	-0.
13	-0.	0.	-0.0003
14	-0.0013	-0.0019	-0.
15	-0.0044	-0.0085	-0.
16	0.0006	-0.0044	-0.
17	-0.	-0.0003	0.
18	-0.0013	-0.0019	0.
19	-0.0044	-0.0051	0.
20	-0.	-0.0003	0.
21	0.0006	-0.	-0.0044
22	-0.0013	-0.	-0.0019
23	-0.0044	0.	-0.0051
24	-0.	-0.0003	0.
25	0.0006	-0.	-0.0044
26	-0.0001	-0.	0.
27	-0.0021	0.	0.
28	0.	0.0000	0.
29	0.	0.	-0.0000
30	-0.	0.	0.
31	2.8388	0.	0.
32	0.	3.9429	-0.
33	0.	-0.	4.0359

REDUCED OVERLAP POPULATION MATRIX ATOM BY ATOM

	1	2	3	4	5	6	7
1	13.4268	0.4751	0.4751	0.4480	0.4480	0.4762	0.4762
2	0.4751	14.5574	-0.0023	-0.0205	-0.0205	-0.0239	-0.0239
3	0.4751	-0.0023	14.5574	-0.0205	-0.0205	-0.0239	-0.0239
4	0.4480	-0.0205	-0.0205	14.6477	-0.0023	-0.0205	-0.0205
5	0.4480	-0.0205	-0.0205	-0.0023	14.6477	-0.0205	-0.0205
6	0.4762	-0.0239	-0.0239	-0.0205	-0.0205	14.5490	-0.0023
7	0.4762	-0.0239	-0.0239	-0.0205	-0.0205	-0.0023	14.5490

TABLE XIV

$PtCl_6^{2-}$

Mulliken Overlap Populations:

AO's Down and Across; $PtCl_6^{2-}$ Bond Order Matrix

MULLIKEN OVERLAP POPULATIONS FOR 54 ELECTRONS

$PtCl_6^{2}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.4590	-0.	-0.	-0.	-0.	0.	0.	0.	0.	0.0226	0.	0.0926	0.	0.0226	0.
2	-0.	0.1881	-0.	-0.	0.	0.	0.	-0.	0.	0.	-0.0003	-0.	0.	0.	-0.0003
3	-0.	-0.	0.1881	-0.	0.	-0.	0.	0.	0.	0.0704	-0.	0.1711	-0.	0.0704	-0.
4	-0.	-0.	-0.	0.1881	-0.	0.	0.	0.	0.	-0.	-0.	-0.	-0.0003	0.	-0.
5	-0.	0.	0.	-0.	1.2808	0.	0.	0.	0.	0.0031	-0.	0.0347	-0.	0.0031	0.
6	0.	0.	-0.	0.	0.	4.0659	-0.	-0.	-0.	-0.	-0.0165	0.	-0.	-0.	-0.0165
7	0.	0.	0.	0.	0.	-0.	1.2808	0.	0.	0.0094	0.	0.1040	0.	0.0094	0.
8	0.	-0.	0.	0.	0.	-0.	0.	4.0659	-0.	0.	-0.	0.	0.	-0.	-0.
9	0.	0.	0.	0.	0.	-0.	0.	-0.	4.0659	0.	0.	0.	-0.0165	0.	0.
10	0.0226	0.	0.0704	-0.	0.0031	-0.	0.0094	0.	0.	3.7306	-0.	0.	0.	0.0000	-0.
11	0.	-0.0003	-0.	-0.	-0.	-0.0165	0.	-0.	0.	-0.	4.0343	-0.	0.	0.	-0.0000
12	0.0926	-0.	0.1711	-0.	0.0347	0.	0.1040	0.	0.	0.	-0.	2.7046	0.	-0.0001	-0.
13	0.	0.	-0.	-0.0003	-0.	-0.	0.	0.	-0.0165	0.	0.	0.	4.0343	-0.	-0.
14	0.0226	0.	0.0704	0.	0.0031	-0.	0.0094	-0.	0.	0.0000	0.	-0.0001	-0.	3.7306	0.
15	0.	-0.0003	-0.	-0.	0.	-0.0165	0.	-0.	0.	-0.	-0.0000	-0.	-0.	0.	4.0343
16	0.0926	0.	0.1711	0.	0.0347	-0.	0.1040	-0.	-0.	-0.0001	-0.	-0.0022	0.	-0.	-0.
17	-0.	-0.	0.	-0.0003	-0.	0.	0.	0.	-0.0165	0.	-0.	0.	-0.0000	0.	0.
18	0.0226	-0.	-0.	0.0704	0.0031	-0.	0.0094	-0.	0.	-0.0004	-0.	-0.0012	-0.0020	-0.0004	-0.
19	0.	-0.0003	-0.	-0.	-0.	-0.	0.	-0.0165	0.	0.	-0.0003	0.	0.	-0.	-0.0003
20	-0.	0.	-0.0003	-0.	0.	0.	-0.	-0.	-0.0165	-0.0020	0.	-0.0046	-0.0051	-0.0020	0.
21	0.0926	-0.	0.	0.1711	0.0347	-0.	0.1040	-0.	-0.	-0.0012	-0.	0.0010	-0.0046	-0.0012	0.
22	0.0226	0.	0.	0.0704	0.0031	0.	0.0094	-0.	0.	-0.0004	-0.	-0.0012	-0.0020	-0.0004	-0.
23	0.	-0.0003	0.	-0.	-0.	-0.	-0.	-0.0165	-0.	-0.	-0.0003	-0.	0.	-0.	-0.0003
24	-0.	-0.	-0.0003	-0.	-0.	0.	-0.	-0.	-0.0165	-0.0020	-0.	-0.0046	-0.0051	-0.0020	-0.
25	0.0926	0.	0.	0.1711	0.0347	-0.	0.1040	-0.	0.	-0.0012	0.	0.0010	-0.0046	-0.0012	-0.
26	0.0226	0.0704	-0.	-0.	0.0126	0.	0.	-0.	0.	-0.0004	-0.0020	-0.0012	-0.	-0.0004	-0.0020
27	0.0926	0.1711	-0.	0.	0.1387	0.	0.	-0.	0.	-0.0012	-0.0046	0.0010	0.	-0.0012	-0.0046
28	-0.	0.	-0.0003	0.	0.	-0.0165	0.	0.	-0.	-0.0020	-0.0051	-0.0046	-0.	-0.0020	-0.0051
29	0.	0.	-0.	-0.0003	-0.	-0.	0.	-0.0165	0.	-0.	0.	0.	-0.0003	-0.	-0.
30	0.0226	0.0704	0.	0.	0.0126	-0.	0.	-0.	0.	-0.0004	-0.0020	-0.0012	-0.	-0.0004	-0.0020
31	0.0926	0.1711	0.	-0.	0.1387	-0.	0.	-0.	0.	-0.0012	-0.0046	0.0010	-0.	-0.0012	-0.0046
32	-0.	-0.	-0.0003	-0.	0.	-0.0165	0.	-0.	-0.	-0.0020	-0.0051	-0.0046	0.	-0.0020	-0.0051
33	0.	0.	0.	-0.0003	0.	0.	0.	-0.0165	-0.	-0.	0.	-0.	-0.0003	-0.	-0.

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0926	-0.	0.0226	0.	-0.	0.0926	0.0226	0.	-0.	0.0926	0.0226	0.0926	-0.	0.	0.0226
2	0.	-0.	-0.	-0.0003	0.	-0.	0.	-0.0003	-0.	0.	0.0704	0.1711	0.	0.	0.0704
3	0.1711	0.	-0.	-0.	-0.0003	0.	0.	0.	-0.0003	0.	-0.	-0.	-0.0003	-0.	0.
4	0.	-0.0003	0.0704	-0.	-0.	0.1711	0.0704	-0.	-0.	0.1711	-0.	0.	0.	-0.0003	0.
5	0.0347	-0.	0.0031	-0.	0.	0.0347	0.0031	-0.	-0.	0.0347	0.0126	0.1387	0.	-0.	0.0126
6	-0.	0.	-0.	-0.	0.	-0.	0.	-0.	0.	-0.	0.	0.	-0.0165	-0.	-0.
7	0.1040	0.	0.0094	0.	-0.	0.1040	0.0094	-0.	-0.	0.1040	0.	0.	0.	0.	0.
8	-0.	0.	-0.	-0.0165	-0.	-0.	-0.	-0.0165	-0.	-0.	-0.	-0.	0.	-0.0165	-0.
9	-0.	-0.0165	0.	0.	-0.0165	-0.	0.	-0.	-0.0165	0.	0.	0.	-0.	0.	0.
10	-0.0001	0.	-0.0004	0.	-0.0020	-0.0012	-0.0004	-0.	-0.0020	-0.0012	-0.0004	-0.0012	-0.0020	-0.	-0.0004
11	-0.	-0.	-0.	-0.0003	0.	-0.	-0.	-0.0003	-0.	0.	-0.0020	-0.0046	-0.0051	0.	-0.0020
12	-0.0022	0.	-0.0012	0.	-0.0046	0.0010	-0.0012	-0.	-0.0046	0.0010	-0.0012	0.0010	-0.0046	0.	-0.0012
13	0.	-0.0000	-0.0020	0.	-0.0051	-0.0046	-0.0020	0.	-0.0051	-0.0046	-0.	0.	-0.	-0.0003	-0.
14	-0.	0.	-0.0004	-0.	-0.0020	-0.0012	-0.0004	-0.	-0.0020	-0.0012	-0.0004	-0.0012	-0.0020	-0.	-0.0004
15	-0.	0.	-0.	-0.0003	0.	0.	-0.	-0.0003	-0.	-0.	-0.0020	-0.0046	-0.0051	-0.	-0.0020
16	2.7046	-0.	-0.0012	0.	-0.0046	0.0010	-0.0012	-0.	-0.0046	0.0010	-0.0012	0.0010	-0.0046	0.	-0.0012
17	-0.	4.0343	-0.0020	-0.	-0.0051	-0.0046	-0.0020	-0.	-0.0051	-0.0046	0.	-0.	-0.	-0.0003	0.
18	-0.0012	-0.0020	3.7306	-0.	-0.	0.	0.0000	0.	-0.	-0.0001	-0.0004	-0.0012	-0.	-0.0020	-0.0004
19	0.	-0.	-0.	4.0343	-0.	0.	-0.	-0.0000	-0.	-0.	-0.0020	-0.0046	-0.	-0.0051	-0.0020
20	-0.0046	-0.0051	-0.	-0.	4.0343	0.	-0.	-0.	-0.0000	-0.	0.	0.	-0.0003	0.	-0.
21	0.0010	-0.0046	0.	0.	0.	2.7046	-0.0001	-0.	0.	-0.0022	-0.0012	0.0010	0.	-0.0046	-0.0012
22	-0.0012	-0.0020	0.0000	-0.	-0.	-0.0001	3.7306	-0.	-0.	-0.	-0.0004	-0.0012	0.	-0.0020	-0.0004
23	-0.	-0.	0.	-0.0000	-0.	-0.	-0.	4.0344	-0.	-0.	-0.0020	-0.0046	0.	-0.0051	-0.0020
24	-0.0046	-0.0051	-0.	-0.	-0.0000	0.	-0.	-0.	4.0343	-0.	0.	-0.	-0.0003	0.	-0.
25	0.0010	-0.0046	-0.0001	-0.	-0.	-0.0022	-0.	-0.	-0.	2.7046	-0.0012	0.0010	-0.	-0.0046	-0.0012
26	-0.0012	0.	-0.0004	-0.0020	0.	-0.0012	-0.0004	-0.0020	0.	-0.0012	3.7306	0.	0.	0.	0.0000
27	0.0010	-0.	-0.0012	-0.0046	0.	0.0010	-0.0012	-0.0046	-0.	0.0010	0.	2.7046	0.	-0.	-0.0001
28	-0.0046	-0.	-0.	-0.	-0.0003	0.	0.	0.	-0.0003	-0.	0.	0.	4.0343	-0.	-0.
29	0.	-0.0003	-0.0020	-0.0051	0.	-0.0046	-0.0020	-0.0051	0.	-0.0046	0.	-0.	-0.	4.0343	0.
30	-0.0012	0.	-0.0004	-0.0020	-0.	-0.0012	-0.0004	-0.0020	-0.	-0.0012	0.0000	-0.0001	-0.	0.	3.7306
31	0.0010	-0.	-0.0012	-0.0046	0.	0.0010	-0.0012	-0.0046	-0.	0.0010	-0.0001	-0.0022	0.	-0.	-0.
32	-0.0046	0.	-0.	-0.	-0.0003	-0.	0.	0.	-0.0003	0.	-0.	0.	-0.0000	-0.	-0.
33	-0.	-0.0003	-0.0020	-0.0051	-0.	-0.0046	-0.0020	-0.0051	-0.	-0.0046	-0.	-0.	-0.	-0.0000	0.

	31	32	33
1	0.0926	-0.	0.
2	0.1711	-0.	0.
3	0.	-0.0003	0.
4	-0.	-0.	-0.0003
5	0.1387	0.	0.
6	-0.	-0.0165	0.
7	0.	0.	0.
8	-0.	-0.	-0.0165
9	0.	-0.	-0.
10	-0.0012	-0.0020	-0.
11	-0.0046	-0.0051	0.
12	0.0010	-0.0046	-0.
13	-0.	0.	-0.0003
14	-0.0012	-0.0020	-0.
15	-0.0046	-0.0051	-0.
16	0.0010	-0.0046	-0.
17	-0.	0.	-0.0003
18	-0.0012	-0.	-0.0020
19	-0.0046	-0.	-0.0051
20	0.	-0.0003	-0.
21	0.0010	-0.	-0.0046
22	-0.0012	0.	-0.0020
23	-0.0046	0.	-0.0051
24	-0.	-0.0003	-0.
25	0.0010	0.	-0.0046
26	-0.0001	-0.	-0.
27	-0.0022	0.	-0.
28	0.	-0.0000	-0.
29	-0.	-0.	-0.0000
30	-0.	-0.	0.
31	2.7046	0.	-0.
32	0.	4.0343	-0.
33	-0.	-0.	4.0343

REDUCED OVERLAP POPULATION MATRIX ATOM BY ATOM

	1	2	3	4	5	6	7
1	15.7826	0.4745	0.4745	0.4745	0.4745	0.4745	0.4745
2	0.4745	14.5039	-0.0024	-0.0203	-0.0203	-0.0203	-0.0203
3	0.4745	-0.0024	14.5039	-0.0203	-0.0203	-0.0203	-0.0203
4	0.4745	-0.0203	-0.0203	14.5039	-0.0024	-0.0203	-0.0203
5	0.4745	-0.0203	-0.0203	-0.0024	14.5039	-0.0203	-0.0203
6	0.4745	-0.0203	-0.0203	-0.0203	-0.0203	14.5039	-0.0024
7	0.4745	-0.0203	-0.0203	-0.0203	-0.0203	-0.0024	14.5039

TABLE XV

$ReCl_6^{2-}$ MO Charge Matrix:

MO's Across and AO's Down

CHARGE MATRIX FOR MS-S WITH TWO ELECTRONS IN EACH

$ReCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.0000	0.0000	1.5587	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0001	0.0003	1.7954	0.	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0351	0.0030
3	0.8980	0.8977	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0072	0.0315
4	0.8976	0.8978	0.0003	0.0000	-0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0320	0.0025	0.0092
5	-0.0000	-0.0000	0.0000	0.0000	1.2643	0.0843	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7871	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
7	0.0000	0.0000	0.0000	0.0000	0.0843	1.2643	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7871	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7871	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0158	0.0158	0.0000	0.0180	0.0016	0.0205	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0006
11	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.4990	0.0010	0.4998	0.2087	0.0184
12	0.0351	0.0350	0.0000	0.0556	0.0140	0.1811	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0520	0.0728	0.3223
13	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0010	0.4998	0.1943	0.0153
14	0.0158	0.0158	0.0000	0.0180	0.0016	0.0205	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0006
15	0.0000	0.0000	0.0002	-0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.4998	0.0010	0.4998	0.2087	0.0184
16	0.0351	0.0350	0.0000	0.0556	0.0140	0.1811	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0520	0.0728	0.3223
17	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0010	0.4998	0.1943	0.0153
18	0.0158	0.0158	0.0000	0.0180	0.0109	0.0113	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
19	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.0000	0.0000
20	0.0001	0.0001	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0010	0.4998	0.0308	0.0432
21	0.0350	0.0350	0.0000	0.0556	0.0957	0.0993	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0277	0.0257
22	0.0158	0.0158	0.0000	0.0180	0.0109	0.0113	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
23	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24	0.0001	0.0001	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0010	0.4998	0.0308	0.0432
25	0.0350	0.0350	0.0000	0.0556	0.0957	0.0993	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0277	0.0257
26	0.0000	0.0000	0.0316	0.0180	0.0207	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
27	0.0000	0.0000	0.0701	0.0556	0.1828	0.0122	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0674	0.0311
28	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.4990	0.0010	0.0000	0.0308	0.0432
29	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.0000	0.1943	0.0153	0.0556
30	0.0000	0.0000	0.0316	0.0180	0.0207	0.0014	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
31	0.0000	0.0000	0.0701	0.0556	0.1828	0.0122	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0674	0.0311	0.0311
32	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.4990	0.0010	0.0308	0.0432	0.1912
33	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0532	0.0000	0.0000	0.0000	0.0000	0.1943	0.0152	0.0556

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2622	0.0000	0.0000	0.0000
2	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0842	0.0050	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0080
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0027	0.0782	0.0104	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0202
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0081	0.0788	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0411
5	0.0000	0.0000	0.0000	0.2981	0.2814	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0186	0.0552	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2096	0.0033	-0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.2814	0.2981	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0552	0.0188	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2129	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033	0.2096	0.0000	0.0000	0.0000	0.0000
10	-0.0000	-0.0000	-0.0000	0.0002	0.0027	0.0002	0.0059	0.0008	0.0000	0.0000	0.0000	0.0000	0.0145	0.0413	0.0003	0.2804
11	0.0708	0.3477	0.0815	0.0000	0.0000	0.2142	0.0127	0.0053	0.0000	0.4399	0.0069	-0.0000	0.0000	0.0000	0.0000	0.0003
12	0.0000	0.0000	0.0000	0.0282	0.4423	0.0143	0.4139	0.0550	0.0000	0.0000	0.0000	0.0000	0.2752	0.0011	0.0000	-0.0001
13	0.1289	0.0160	0.3551	0.0000	0.0000	0.0111	0.0206	0.2004	0.0000	0.0000	0.0069	0.4399	0.0000	0.0000	0.0000	0.0015
14	-0.0000	-0.0000	-0.0000	0.0002	0.0027	0.0002	0.0059	0.0008	0.0000	0.0000	0.0000	0.0145	0.0413	0.0003	0.2804	
15	0.0708	0.3477	0.0815	0.0000	0.0000	0.2142	0.0127	0.0053	0.0000	0.4399	0.0069	0.0000	0.0000	0.0000	0.0000	0.0003
16	0.0000	0.0000	0.0000	0.0282	0.4423	0.0143	0.4139	0.0550	0.0000	0.0000	0.0000	0.2752	0.0021	0.0000	-0.0001	
17	0.1289	0.0160	0.3551	0.0000	0.0000	0.0111	0.0206	0.2004	0.0000	0.0000	0.0069	0.4399	0.0000	0.0000	0.0000	0.0015
18	0.0000	-0.0000	-0.0000	0.0027	0.0002	0.0003	0.0006	0.0059	0.0000	0.0000	0.0000	0.0145	0.1726	0.4691	0.5895	
19	0.0708	0.3477	0.0815	0.0000	0.0000	0.2142	0.0127	0.0053	0.4468	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
20	0.3003	0.1363	0.0634	0.0000	0.0000	0.0069	0.1989	0.0264	0.0000	0.0069	0.4399	0.0000	0.0000	0.0000	0.0000	0.0007
21	0.0000	0.0000	0.0000	0.4356	0.0350	0.0231	0.0429	0.4177	0.0000	-0.0000	0.0000	0.2752	0.0003	0.0000	-0.0002	
22	0.0000	-0.0000	-0.0000	0.0027	0.0002	0.0003	0.0006	0.0059	0.0000	0.0000	0.0000	0.0145	0.1726	0.4691	0.5895	
23	0.0708	0.3477	0.0815	0.0000	0.0000	0.2142	0.0127	0.0053	0.4468	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0003
24	0.3003	0.1363	0.0634	0.0000	0.0000	0.0069	0.1989	0.0264	0.0000	0.0069	0.4399	0.0000	0.0000	0.0000	0.0000	0.0007
25	0.0000	0.0000	0.0000	0.4356	0.0350	0.0231	0.0429	0.4172	0.0000	0.0000	0.0000	0.2752	0.0003	0.0000	-0.0002	
26	0.0000	-0.0000	0.0000	0.0015	0.0014	0.0063	0.0004	0.0002	0.0000	0.0000	0.0000	0.0145	0.1486	0.4931	0.1108	
27	0.0000	0.0000	0.0000	0.2421	0.2285	0.4458	0.0264	0.0110	0.0000	0.0000	0.0000	0.2752	0.0003	0.0000	-0.0000	
28	0.3003	0.1363	0.0634	0.0000	0.0000	0.0069	0.1989	0.0264	0.0000	0.4399	0.0000	0.0069	0.0000	0.0000	0.0000	0.0007
29	0.1289	0.0160	0.3551	0.0000	0.0000	0.0111	0.0206	0.2005	0.4468	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
30	-0.0000	0.0000	0.0000	0.0015	0.0014	0.0063	0.0004	0.0002	0.0000	0.0000	0.0000	0.0145	0.1486	0.4931	0.1108
31	0.0000	0.0000	0.0000	0.2421	0.2285	0.4458	0.0264	0.0110	0.0000	0.0000	0.0000	0.2752	0.0003	0.0000	-0.0000
32	0.3003	0.1363	0.0634	0.0000	0.0000	0.0069	0.1989	0.0264	0.0000	0.4399	0.0069	0.0000	0.0000	0.0000	0.0007
33	0.1289	0.0160	0.3551	0.0000	0.0000	0.0111	0.0206	0.2005	0.4468	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0015

	31	32	33
1	0.0000	0.0000	0.1791
2	0.0069	0.0544	0.0000
3	0.0485	0.0006	0.0000
4	0.0139	0.0144	0.0000
5	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000
10	0.6722	0.0081	0.3009
11	0.0002	0.0019	0.0000
12	-0.0002	-0.0000	0.0026
13	0.0005	0.0005	0.0000
14	0.6722	0.0081	0.3009
15	0.0002	0.0019	0.0000
16	-0.0002	-0.0000	0.0026
17	0.0005	0.0005	0.0000
18	0.1923	0.1990	0.3009
19	0.0002	0.0019	0.0000
20	0.0017	0.0000	0.0000
21	-0.0001	-0.0001	0.0026
22	0.1923	0.1990	0.3009
23	0.0002	0.0019	0.0000
24	0.0017	0.0000	0.0000
25	-0.0001	-0.0001	0.0026
26	0.0962	0.7537	0.3009
27	-0.0000	-0.0003	0.0026
28	0.0017	0.0000	0.0000
29	0.0005	0.0005	0.0000
30	0.0962	0.7537	0.3009
31	-0.0000	-0.0003	0.0026
32	0.0017	0.0000	0.0000
33	0.0005	0.0005	0.0000

TABLE XVI

$OsCl_6^{2-}$ MO Charge Matrix:

MO's Across and AO's Down

CHARGE MATRIX FOR MO-S WITH TWO ELECTRONS IN EACH

$OsCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.0000	0.0000	1.5069	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000
2	1.7458	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0454
3	0.0000	0.0000	1.7453	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0473	0.0000
4	0.0000	1.7453	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0472	0.0000
5	-0.0000	-0.0000	0.0000	0.0000	0.0014	1.3094	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.8204	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	-0.0000	0.0000	1.3074	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	1.8205	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	1.8194	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0380	0.0190	0.0119	0.0034	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000
11	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0454	0.0000	0.0000	0.5058	0.0000	0.0000	0.0000	0.2841
12	0.0000	0.0000	0.0867	0.0632	0.1673	0.0479	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4203	0.0000	0.0000

	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
13	0.0000	0.0014	0.0000	-0.0000	0.0000	0.0000	0.0452	0.0000	0.0000	0.5004	0.0000	0.0000	0.0000	0.2914	0.0000			
14	0.0000	0.0000	0.0380	0.0190	0.0119	0.0034	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000			
15	0.0014	0.0000	0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0454	0.0000	0.0000	0.5058	0.0000	0.0000	0.0000	0.2841			
16	0.0000	0.0000	0.0867	0.0632	0.1673	0.0479	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4203	0.0000			
17	0.0000	0.0014	0.0000	0.0000	-0.0000	0.0000	0.0452	0.0000	0.0000	0.5004	0.0000	0.0000	0.0000	0.2914	0.0000			
18	0.0000	0.0380	0.0000	0.0190	0.0110	0.0043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000			
19	0.0014	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0453	0.0000	0.0000	0.5054	0.0000	0.0000	0.2821			
20	0.0000	0.0000	0.0014	0.0000	0.0000	0.0000	0.0451	0.0000	0.0000	0.4996	0.0000	0.0000	0.2900	0.0000	0.0000			
21	0.0000	0.0866	0.0000	0.0632	0.1552	0.0599	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4196	0.0000			
22	0.0000	0.0380	0.0000	0.0190	0.0110	0.0043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000			
23	0.0014	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0453	0.0000	0.0000	0.5054	0.0000	0.0000	0.2821			
24	0.0000	0.0000	0.0014	-0.0000	0.0000	-0.0000	0.0451	0.0000	0.0000	0.4996	0.0000	0.0000	0.2900	0.0000	0.0000			
25	0.0000	0.0866	0.0000	0.0632	0.1552	0.0599	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4196	0.0000			
26	0.0379	0.0000	0.0000	0.0190	0.0000	0.0153	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007			
27	0.0865	0.0000	0.0000	0.0632	0.0002	0.2138	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4105			
28	0.0000	0.0000	0.0014	0.0000	0.0000	-0.0000	0.0000	0.0444	0.0000	0.0000	0.4942	0.0000	0.2654	0.0000	0.0000			
29	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0444	0.0000	0.0000	0.4946	0.0000	0.2648	0.0000			
30	0.0379	0.0000	0.0000	0.0190	0.0000	0.0153	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007			
31	0.0865	0.0000	0.0000	0.0632	0.0002	0.2138	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4105			
32	0.0000	0.0000	0.0014	0.0000	0.0000	-0.0000	0.0000	0.0444	0.0000	0.0000	0.4942	0.0000	0.2654	0.0000	0.0000			
33	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0444	0.0000	0.0000	0.4946	0.0000	0.2649	0.0000			

	31	32	33
1	0.0000	0.0000	0.1995
2	0.0000	0.0855	0.0000
3	0.0000	0.0000	0.0000
4	0.0857	0.0000	0.0000
5	0.0000	0.0000	0.0000
6	-0.0000	-0.0000	0.0000
7	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.2933
11	0.0000	0.0024	0.0000
12	-0.0000	-0.0000	0.0029
13	0.0024	0.0000	0.0000
14	0.0000	0.0000	0.2933
15	0.0000	0.0024	0.0000
16	-0.0000	-0.0000	0.0029
17	0.0024	0.0000	0.0000
18	0.9528	0.0000	0.2941
19	0.0000	0.0024	0.0000
20	0.0000	0.0000	0.0000
21	-0.0005	-0.0000	0.0029
22	0.9528	0.0000	0.2941
23	0.0000	0.0024	0.0000
24	0.0000	0.0000	0.0000
25	-0.0005	-0.0000	0.0029
26	0.0000	0.9529	0.3041
27	-0.0000	-0.0005	0.0029
28	0.0000	0.0000	-0.0000
29	0.0024	0.0000	0.0000
30	0.0000	0.9529	0.3041
31	-0.0000	-0.0005	0.0029
32	0.0000	0.0000	0.0000
33	0.0024	0.0000	0.0000

TABLE XVII

$IrCl_6^{2-}$ MO Charge Matrix:

MO's Across and AO's Down

CHARGE MATRIX FOR MO-S WITH TWO ELECTRONS IN EACH

$IrCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.0000	0.0000	1.4692	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	1.7081	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0452	0.0000	0.0000
3	0.0000	1.7089	0.0000	0.0000	0.0000	-0.0000	-0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0423	0.0000
4	1.7090	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0420
5	-0.0000	0.0000	0.0000	0.0000	1.2134	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7163	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7	-0.0000	0.0000	0.0000	0.0000	0.0021	1.2164	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	1.7165	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7190	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0461	0.0000	0.0217	0.0054	0.0135	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
11	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000	0.0695	0.0000	0.0000	0.4933	0.0000	0.0000	0.2848	0.0000	0.0000
12	0.0000	0.0943	0.0000	0.0667	0.0693	0.1723	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3969	0.0000
13	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0704	0.0000	0.0000	0.5007	0.0000	0.0000	0.2705
14	0.0000	0.0461	0.0000	0.0217	0.0054	0.0135	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
15	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000	0.0695	0.0000	0.0000	0.4933	0.0000	0.0000	0.2848	0.0000	0.0000
16	0.0000	0.0943	0.0000	0.0667	0.0693	0.1723	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3969	0.0000
17	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0704	0.0000	0.0000	0.5007	0.0000	0.0000	0.2706
18	0.0461	0.0000	0.0000	0.0217	0.0041	0.0149	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005
19	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000	0.0693	0.0000	0.0000	0.4926	0.0000	0.2808	0.0000	0.0000
20	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0701	0.0000	0.0000	0.4993	0.0000	0.2679	0.0000
21	0.0942	0.0000	0.0000	0.0667	0.0518	0.1896	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3956
22	0.0461	0.0000	0.0000	0.0217	0.0041	0.0149	-0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005
23	0.0000	0.0000	0.0026	0.0000	-0.0000	0.0000	0.0000	0.0693	0.0000	0.0000	0.4927	0.0000	0.2808	0.0000	0.0000
24	0.0000	0.0026	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0701	0.0000	0.0000	0.4993	0.0000	0.2679	0.0000
25	0.0942	0.0000	0.0000	0.0667	0.0518	0.1896	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3956
26	0.0000	0.0000	0.0462	0.0217	0.0189	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000
27	0.0000	0.0000	0.0945	0.0668	0.2429	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4113	0.0000	0.0000
28	0.0000	0.0026	0.0000	-0.0000	0.0000	0.0000	0.0723	0.0000	0.0000	0.5066	0.0000	0.0000	0.0000	0.3135	0.0000
29	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0724	0.0000	0.0000	0.5073	0.0000	0.0000	0.0000	0.3123
30	0.0000	0.0000	0.0462	0.0217	0.0189	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0005	0.0000	0.0000
31	0.0000	0.0000	0.0945	0.0668	0.2429	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4113	0.0000	0.0000
32	0.0000	0.0026	0.0000	-0.0000	0.0000	0.0000	0.0723	0.0000	0.0000	0.5066	0.0000	0.0000	0.0000	0.3136	0.0000
33	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0724	0.0000	0.0000	0.5073	0.0000	0.0000	0.0000	0.3123

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2999	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000	0.0000	0.1402	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.1065
3	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.1425	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1427	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.7177	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0654	0.0001	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2836	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	-0.0000	0.0000	0.0000	0.0012	0.7149	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0652	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2834	0.0000	0.0000	-0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2810	-0.0000	0.0000	0.0000	0.0000
10	-0.0000	-0.0000	-0.0000	0.0010	0.0028	0.0000	0.0104	0.0000	0.0000	0.0000	0.0000	0.0199	0.1793	0.4604	0.0000
11	0.0000	0.0000	0.4987	0.0000	0.0000	0.2115	0.0000	0.0000	0.4371	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0023
12	0.0000	0.0007	0.0000	0.1169	0.3036	0.0000	0.5088	0.0000	0.0000	0.0000	0.0000	0.2671	0.0003	0.0007	-0.0000
13	0.5142	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2103	0.0000	0.0000	0.4289	0.0000	0.0000	0.0000	0.0000
14	-0.0000	-0.0000	0.0000	0.0010	0.0028	0.0000	0.0104	0.0000	0.0000	0.0000	0.0000	0.0199	0.1793	0.4604	0.0000
15	0.0000	0.0000	0.4987	0.0000	0.0000	0.2115	0.0000	0.0000	0.4371	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023
16	0.0000	0.0007	0.0000	0.1169	0.3036	0.0000	0.5088	0.0000	0.0000	0.0000	0.0000	0.2671	0.0003	0.0007	-0.0000
17	0.5142	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2103	0.0000	0.0000	0.4289	0.0000	0.0000	0.0000	0.0000
18	-0.0000	0.0000	-0.0000	0.0008	0.0030	0.0000	0.0000	0.0104	0.0000	0.0000	0.0000	0.0199	0.1340	0.5042	0.0000
19	0.0000	0.0000	0.5013	0.0000	0.0000	0.2129	0.0000	0.0000	0.0000	0.4380	0.0000	0.0000	0.0000	0.0000	0.0023
20	0.0000	0.5154	0.0000	0.0000	0.0000	0.0000	0.2118	0.0000	0.0000	0.0000	0.4306	0.0000	0.0000	0.0000	0.0000
21	0.0006	0.0000	0.0000	0.0875	0.3318	0.0000	0.0000	0.5103	0.0000	0.0000	0.0000	0.2684	0.0003	0.0008	-0.0000
22	-0.0000	-0.0000	-0.0000	0.0008	0.0030	0.0000	0.0000	0.0104	0.0000	0.0000	0.0000	0.0199	0.1340	0.5042	0.0000
23	0.0000	0.0000	0.5013	0.0000	0.0000	0.2129	0.0000	0.0000	0.0000	0.4380	0.0000	0.0000	0.0000	0.0000	0.0023
24	0.0000	0.5154	0.0000	0.0000	0.0000	0.0000	0.2118	0.0000	0.0000	0.0000	0.4306	0.0000	0.0000	0.0000	0.0000
25	0.0006	0.0000	0.0000	0.0875	0.3318	0.0000	0.0000	0.5103	0.0000	0.0000	0.0000	0.2684	0.0003	0.0008	-0.0000
26	0.0000	0.0000	-0.0000	0.0041	0.0000	0.0106	0.0000	0.0000	0.0000	0.0000	0.0000	0.0198	0.6524	0.0012	0.9427
27	0.0000	0.0000	0.0000	0.4302	0.0007	0.4949	0.0000	0.0000	0.0000	0.0000	0.0000	0.2549	0.0009	0.0000	-0.0007
28	0.0000	0.4838	0.0000	0.0000	0.0000	0.0000	0.1977	0.0000	0.4211	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	0.4852	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1976	0.0000	0.4203	0.0000	0.0000	0.0000	0.0000	0.0000
30	-0.0000	-0.0000	-0.0000	0.0041	0.0000	0.0106	0.0000	0.0000	0.0000	0.0000	0.0000	0.0198	0.6524	0.0012	0.9427
31	0.0000	0.0000	0.0000	0.4302	0.0007	0.4949	0.0000	0.0000	0.0000	0.0000	0.0000	0.2549	0.0009	0.0000	-0.0007
32	0.0000	0.4838	0.0000	0.0000	0.0000	0.0000	0.1977	0.0000	0.4211	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	0.4852	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1976	0.0000	0.4203	0.0000	0.0000	0.0000	0.0000	0.0000

	31	32	33
1	0.0000	0.0000	0.2308
2	0.0000	0.0000	0.0000
3	0.1062	0.0000	0.0000
4	0.0000	0.1062	0.0000
5	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000
10	0.9430	0.0000	0.2960
11	0.0000	0.0000	0.0000
12	-0.0007	-0.0000	0.0031
13	0.0000	0.0023	0.0000
14	0.9430	0.0000	0.2960
15	0.0000	0.0000	0.0000
16	-0.0007	-0.0000	0.0031
17	0.0000	0.0023	0.0000
18	0.0000	0.9430	0.2975
19	0.0000	0.0000	-0.0000
20	0.0023	0.0000	0.0000
21	-0.0000	-0.0007	0.0031
22	0.0000	0.9430	0.2975
23	0.0000	0.0000	-0.0000
24	0.0023	0.0000	0.0000
25	-0.0000	-0.0007	0.0031
26	0.0000	0.0000	0.2819
27	-0.0000	-0.0000	0.0031
28	0.0023	0.0000	0.0000
29	0.0000	0.0023	0.0000
30	0.0000	0.0000	0.2819
31	-0.0000	-0.0000	0.0031
32	0.0023	0.0000	0.0000
33	0.0000	0.0023	0.0000

TABLE XVIII

$PtCl_6^{2-}$ MO Charge Matrix:

MO's Across and AO's Down

CHARGE MATRIX FOR MO-S WITH TWO ELECTRONS IN EACH

$PtCl_6^{2-}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	0.0000	0.0000	0.0000	1.4250	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000
2	0.0003	0.0004	1.6642	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0003	0.0466
3	0.0000	1.6645	0.0004	0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0464	0.0004	0.0005
4	1.6646	0.0000	0.0003	0.0000	0.0000	-0.0000	-0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0005	0.0468	0.0002
5	-0.0000	0.0000	0.0000	0.0000	0.5657	0.5670	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	1.6148	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	-0.0000	-0.0000	0.0000	0.0000	0.5670	0.5657	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	1.6147	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.6147	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0483	0.0000	0.0209	0.0186	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000
11	0.0000	0.0000	0.0031	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.0001	0.4999	0.0000	0.0028	0.0018	0.2991
12	0.0000	0.1129	0.0000	0.0749	0.2512	0.0180	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3614	0.0031	0.0039
13	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.4999	0.0001	0.0000	0.0030	0.2993	0.0014
14	0.0000	0.0483	0.0000	0.0209	0.0186	0.0013	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000
15	0.0000	0.0000	0.0031	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.0001	0.4999	0.0000	0.0028	0.0018	0.2991
16	0.0000	0.1129	0.0000	0.0749	0.2512	0.0180	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.3614	0.0031	0.0039
17	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.4999	0.0001	0.0000	0.0030	0.2993	0.0014
18	0.0483	0.0000	0.0000	0.0209	0.0013	0.0185	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
19	0.0000	0.0000	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.5000	0.0028	0.0018	0.2991
20	0.0000	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.4999	0.0001	0.0000	0.2979	0.0026	0.0032
21	0.1129	0.0000	0.0000	0.0749	0.0181	0.2511	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.3631	0.0017
22	0.0483	0.0000	0.0000	0.0209	0.0013	0.0185	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
23	0.0000	0.0000	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.5000	0.0028	0.0018	0.2991
24	0.0000	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.4999	0.0001	0.0000	0.2979	0.0026	0.0032
25	0.1129	0.0000	0.0000	0.0749	0.0181	0.2511	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.3631	0.0017
26	0.0000	0.0000	0.0483	0.0209	0.0099	0.0100	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
27	0.0000	0.0000	0.1129	0.0749	0.1344	0.1348	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034	0.0022	0.3628
28	0.0000	0.0031	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.0001	0.4999	0.0000	0.2979	0.0026	0.0032
29	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.5000	0.0030	0.2993	0.0014
30	0.0000	0.0000	0.0483	0.0209	0.0099	0.0100	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
31	0.0000	0.0000	0.1129	0.0749	0.1344	0.1348	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034	0.0022	0.3628
32	0.0000	0.0031	0.0000	0.0000	0.0000	-0.0000	0.0963	0.0000	0.0000	0.0001	0.4999	0.0000	0.2979	0.0026	0.0032
33	0.0031	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0963	0.0000	0.0000	0.5000	0.0030	0.2993	0.0014

	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3350	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0248	0.1482	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019
3	0.0000	0.0000	0.0000	0.1450	0.0241	0.0039	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1022
4	0.0000	0.0000	0.0000	0.0032	0.0007	0.1691	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0107
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6866	0.1055	0.0000	0.0000	0.0000	0.0000	0.0228	0.0524	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3844	0.0007	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1055	0.6866	0.0000	0.0000	0.0000	0.0000	0.0524	0.0228	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3851	0.0000	0.0000	-0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.3844	0.0000	0.0000	0.0000
10	-0.0000	0.0000	0.0000	0.0106	0.0018	0.0003	0.0001	0.0059	0.0000	0.0000	0.0000	0.0227	0.6385	0.0023	0.8357
11	0.0047	0.4256	0.0696	0.0273	0.1634	0.0000	0.0000	0.0000	0.0000	0.0000	0.4029	0.0008	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.4352	0.0724	0.0118	0.0089	0.3878	0.0000	0.0000	0.0000	0.2548	0.0008	0.0000	-0.0008
13	0.0030	0.0725	0.4245	0.0036	0.0008	0.1864	0.0000	0.0000	0.0000	0.0000	0.0008	0.4029	0.0000	0.0000	0.0002
14	-0.0000	0.0000	0.0000	0.0106	0.0018	0.0003	0.0001	0.0059	0.0000	0.0000	0.0000	0.0227	0.6385	0.0023	0.8357
15	0.0047	0.4256	0.0696	0.0273	0.1634	0.0000	0.0000	0.0000	0.0000	0.0000	0.4029	0.0008	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.4352	0.0724	0.0118	0.0089	0.3878	0.0000	0.0000	0.0000	0.2548	0.0008	0.0000	-0.0008
17	0.0030	0.0725	0.4245	0.0036	0.0008	0.1864	0.0000	0.0000	0.0000	0.0000	0.0008	0.4029	0.0000	0.0000	0.0002
18	0.0000	-0.0000	-0.0000	0.0002	0.0001	0.0123	0.0037	0.0023	0.0000	0.0000	0.0000	0.0227	0.1281	0.5127	0.0874
19	0.0047	0.4256	0.0696	0.0273	0.1634	0.0000	0.0000	0.0000	0.4037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20	0.4923	0.0019	0.0059	0.1598	0.0266	0.0043	0.0000	0.0000	0.0000	0.0008	0.4029	0.0000	0.0000	0.0000	0.0021
21	0.0000	0.0000	0.0000	0.0097	0.0021	0.5076	0.2423	0.1544	0.0000	0.0000	0.0000	0.2548	0.0002	0.0007	-0.0001
22	0.0000	-0.0000	-0.0000	0.0002	0.0001	0.0124	0.0037	0.0023	0.0000	0.0000	0.0000	0.0227	0.1281	0.5127	0.0874
23	0.0047	0.4256	0.0696	0.0274	0.1634	0.0000	0.0000	0.0000	0.4037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24	0.4923	0.0019	0.0059	0.1598	0.0266	0.0043	0.0000	0.0000	0.0000	0.0008	0.4029	0.0000	0.0000	0.0000	0.0021
25	0.0000	0.0000	0.0000	0.0097	0.0021	0.5076	0.2423	0.1544	0.0000	0.0000	0.0000	0.2548	0.0002	0.0007	-0.0001
26	-0.0000	-0.0000	-0.0000	0.0018	0.0108	0.0000	0.0052	0.0008	0.0000	0.0000	0.0000	0.0227	0.1946	0.4462	0.0155
27	0.0000	0.0000	0.0000	0.0745	0.4449	0.0000	0.3438	0.0528	0.0000	0.0000	0.0000	0.2548	0.0003	0.0006	-0.0000
28	0.4923	0.0019	0.0059	0.1598	0.0266	0.0043	0.0000	0.0000	0.0000	0.4029	0.0008	0.0000	0.0000	0.0000	0.0021
29	0.0030	0.0725	0.4245	0.0036	0.0008	0.1864	0.0000	0.0000	0.4037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
30	0.0000	-0.0000	-0.0000	0.0018	0.0108	0.0000	0.0052	0.0008	0.0000	0.0000	0.0000	0.0227	0.1946	0.4462	0.0155
31	0.0000	0.0000	0.0000	0.0745	0.4449	0.0000	0.3438	0.0528	0.0000	0.0000	0.0000	0.2548	0.0003	0.0006	-0.0000
32	0.4923	0.0019	0.0059	0.1598	0.0266	0.0043	0.0000	0.0000	0.0000	0.4029	0.0008	0.0000	0.0000	0.0000	0.0021
33	0.0030	0.0725	0.4245	0.0036	0.0008	0.1864	0.0000	0.0000	0.4037	0.0000	0.0000	0.0000	0.0000	-0.0000	0.0002

	31	32	33
1	0.0000	0.0000	0.2400
2	0.0422	0.0707	0.0000
3	0.0033	0.0093	0.0000
4	0.0693	0.0347	0.0000
5	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000
10	0.0268	0.0762	0.2897
11	0.0009	0.0015	0.0000
12	-0.0000	-0.0001	0.0037
13	0.0015	0.0007	0.0000
14	0.0268	0.0762	0.2897
15	0.0009	0.0015	0.0000
16	-0.0000	-0.0001	0.0037
17	0.0015	0.0007	0.0000
18	0.5671	0.2841	0.2897
19	0.0009	0.0015	0.0000
20	0.0001	0.0002	0.0000
21	-0.0005	-0.0003	0.0037
22	0.5671	0.2841	0.2897
23	0.0009	0.0015	0.0000
24	0.0001	0.0002	0.0000
25	-0.0005	-0.0003	0.0037
26	0.3448	0.5784	0.2897
27	-0.0003	-0.0005	0.0037
28	0.0001	0.0002	0.0000
29	0.0015	0.0007	0.0000
30	0.3448	0.5784	0.2897
31	-0.0003	-0.0005	0.0037
32	0.0001	0.0002	0.0000
33	0.0015	0.0007	0.0000

TABLE XIX

MCl_6^{2-} Orbital Occupations and Atomic Charges

Atomic NET CHARGES

		$ReCl_6^{2-}$	$OsCl_6^{2-}$	$IrCl_6^{2-}$	$PtCl_6^{2-}$
M	1	1.323642	1.182747	0.887297	0.685256
Cl	2	-0.553918	-0.514638	-0.470732	-0.447519
	3	-0.553917	-0.514639	-0.470733	-0.447520
	4	-0.553920	-0.537471	-0.505733	-0.447520
	5	-0.553920	-0.537472	-0.505735	-0.447522
	6	-0.553920	-0.539199	-0.467116	-0.447520
	7	-0.553920	-0.539200	-0.467116	-0.447520

Atom No.

ORBITAL CHARGES

1	0.441262	0.493131	0.530787	0.574989
2	0.204276	0.254192	0.291943	0.335091
3	0.204276	0.254733	0.291119	0.335091
4	0.204276	0.254694	0.291034	0.335091
5	0.651443	0.689237	0.784508	0.867245
6	1.106462	1.089796	1.141868	1.999997
7	0.651442	0.691196	0.781450	0.867245
8	1.106461	1.999998	1.999998	1.999998
9	1.106462	1.090277	1.999997	1.999998
10	1.928286	1.927749	1.913289	1.910892
11	1.973156	1.975943	1.962601	1.996849
12	1.679319	1.634910	1.597450	1.542930
13	1.973156	1.976037	1.997393	1.996849
14	1.928286	1.927748	1.913289	1.910893
15	1.973156	1.975943	1.962601	1.996849
16	1.679319	1.634910	1.597450	1.542930
17	1.973156	1.976038	1.997393	1.996849
18	1.928287	1.927756	1.913304	1.910893
19	1.973156	1.998634	1.997375	1.996849
20	1.973157	1.976071	1.997391	1.996848
21	1.679319	1.635010	1.597663	1.542930
22	1.928287	1.927756	1.913304	1.910893
23	1.973156	1.998634	1.997375	1.996850
24	1.973157	1.976072	1.997392	1.996849
25	1.679319	1.635010	1.597663	1.542930
26	1.928287	1.927836	1.913150	1.910893
27	1.679319	1.636313	1.595361	1.542930
28	1.973157	1.976420	1.961220	1.996848
29	1.973158	1.998629	1.997385	1.996849
30	1.928287	1.927837	1.913150	1.910893
31	1.679319	1.636313	1.595362	1.542930
32	1.973157	1.976420	1.961221	1.996848
33	1.973156	1.998629	1.997384	1.996848

orbital No.

TABLE XX

MCl_6^{2-} Molecular Properties

	$ReCl_6^{2-}$	$OsCl_6^{2-}$	$IrCl_6^{2-}$	$PtCl_6^{2-}$
$\epsilon_{t_{2g}}$ (ev.)	-9.98	-10.87	-11.31	-11.83
$t_{2g} \rightarrow e_g$ (Δ)[ev.]	4.91	3.39	4.11	4.30
$t_{2u} \rightarrow t_{2g}$ (ev.)	2.91	2.04	1.65	(1.17)
Metal Charge	1.32	1.18	0.89	0.69
Metal-Cl Bond Order	0.438	0.454	0.475	0.475
σ Bond Order	0.435	0.445	0.484	0.508
π Bond Order	0.003	0.009	-0.009	-0.033
% Metal in T_{2g} MO	89	90	85	81
eqQ: Calc.	32	38	44	51
Obs.[11,12]	27.8	33.8	41.6	52.0
Cl Occupation				
3s	1.93	1.93	1.91	1.91
$3p_\sigma$	1.68	1.63	1.60	1.54
$3p_\pi$	3.94	3.95	3.96	3.99

CHAPTER VI

REFERENCES

1. J. H. van Vleck, J. Chem. Phys., 2, 22 (1934).
2. J. C. Slater, Phys. Rev., 36, 57 (1930).
3. F. Herman and S. Skillman, Atomic Structure Calculations, Prentice-Hall, Englewood Cliffs, N.J., 1963.
4. R. E. Watson and A. J. Freeman, Phys. Rev., 123, 521 (1961); 120, 1125 (1960).
5. Tables of Interatomic Distances and Configuration in Molecules and Ions, The Chemical Society, London, 1958.
6. C. E. Moore, Atomic Energy Levels, U.S. National Bureau of Standards Circular 467, 1949 and 1952.
7. R. S. Mulliken, J. Chem. Phys., 23, 1833 (1955).
8. Ibid., 23, 1841 (1955).
9. I. Prigogine, Ed., Advances in Chemical Physics, Vol. V., pgs. 33-147, Interscience, N.Y., 1963.
10. Chapter II of this thesis.

11a. R. Ikeda, D. Nakamura and M. Kubo, J. Phys. Chem., 69, 2101 (1965).

11b. Idem., Bull Chem. Soc. Japan, 36, 1056 (1963).

12. D. Nakamura, Y. Kurita, K. Ito and M. Kubo, J. Am. Chem. Soc., 82, 5783 (1960).
13. C. J. Jorgensen, Absorption Spectra and Chemical Bonding in Complexes, Pergamon Press, Oxford, 1962, p. 134.

14. Idem., Progress in Inorganic Chemistry, Vol 4, F. A. Cotton, Ed., Interscience, N.Y., (1963); p. 73.

15. J. Owen and K. W. H. Stevens, Nature, 171, 836 (1953).

16. B. N. Figgis, Introduction to Ligand Fields, McGraw-Hill, N.Y., 1966.

17. C. H. Townes and B. P. Dailey, J. Chem. Phys., 17, 782 (1949).

18. T. P. Das and E. L. Hahn, Nuclear Quadrupole Resonance Spectroscopy, Academic Press, N.Y., 1958.

ACKNOWLEDGEMENT

My admiration and gratitude goes to Professor F. Albert Cotton for his inspiring interest and valuable quidance in the planning of this research. Thanks goes to Professor J. S. Wood who has contributed crystallorgaphic advice; Professor Roald Hoffman, Professor George Koster, and Dr. Pieter Ros for assistance and guidance in the molecular orbital calculations.

My appreciation goes to the M.I.T. Computation Center and to Miss Marilyn A. Milan for her aid in the preparation of this manuscript.

My sincere thanks goes to Professor Alan Davison and the group members for their friendship.

I would like to express my gratitude to the N.I.H. for granting me a pre-doctoral fellowship.

Finally, I would like to express my affection for my parents and particularly for my wife, Sara. Without her love, encouragement, and enduring patience, this thesis would not have been possible.

BIOGRAPHICAL SKETCH

Charles B. Harris was born on April 24, 1940, in New York City. He attended public schools in Grosse Pointe, Michigan. On September 9, 1961, he married the former Sara Ann Mikesell of Allen Park, Michigan. In June 1963, he graduated with honors from the University of Michigan with a B.S. in Chemistry. In the Summer of 1963 he was presented an N.S.F. award in Chemistry. As an undergraduate he did research in the fields of biochemistry and biophysics. In the Fall of 1963 he entered graduate school at Massachusetts Institute of Technology and was awarded an N.I.H. pre-doctoral fellowship in February 1965. He was elected to Sigma Xi in May 1966, and received an A.E.C. post-doctoral fellowship for the period June 1966, through August 1967, for work under the supervision of Professor F. A. Cotton.