NBS TECHNICAL NOTE

438

Compendium of *ab initio* Calculations of Molecular Energies and Properties

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards

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National Bureau of Standards
Washington, D.C. 20234

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COMPENDIUM OF ab initio CALCULATIONS OF MOLECULAR ENERGIES AND PROPERTIES

ABSTRACT

The number of *ab initio* molecular electronic calculations has increased dramatically in the last few years. Both the practitioners and other interested students of the results of the calculations have found it increasingly difficult to determine the present status of these calculations. This compendium references the work from 1960 to the present and abstracts from the mass of data the best values for several observable properties including the total energy, dissociation energy, electron affinity, spectroscopic constants, electric moments, field gradients, polarizabilities, and magnetic constants. In order to provide an insight into molecular electronic structure tables of orbital energies are also included.

These tables are meant to direct attention to the successes and failures of the calculations by compiling a large percentage of the best results in a reasonably compact form. Its usefulness will be limited in time by rapid advance in the field.

KEY WORDS: *ab initio* electronic calculation, molecular electronic structure, energy, dissociation energy, dipole moment, quadrupole moment, polarizability, electron affinity, field gradient, spectroscopic constants, magnetic constants, orbital energy.

A. Preface

The increasing accessibility of powerful digital computers has inspired many investigators to the calculation of accurate electronic energies and other properties for molecules. In recent years a sufficient number of *ab initio* calculations have been completed to provide the evidence of the successes and failures of the variational techniques that form the bulk of the calculations. I do not believe the range of these calculations is widely known. This compendium is an effort to provide the non-specialist with an insight into the results that have been obtained to date as well as to summarize a wide range of data for the specialist.

This compendium will reference the variational calculations and will abstract from the more accurate calculations the values of certain observables e.g. the total energies, electric moments, field gradients and orbital energies. It is not our intention to critically review this material in any way. Several recent studies already provide that service.[a] This compendium is intended to supplement the present and, perhaps, future reviews by providing a selected compilation of the raw material of the accurate calculations.

Much unpublished material has been included. Indeed without the 1967 references this report would be significantly shorter. It is hoped that the papers will soon be published so that the full content of this work will be available. In order to assist the reader to access this information, the address of the authors of unpublished material is given.

The calculations have been assigned to two broad groups: 1. Hartree-Fock (H.F.) and 2. Beyond Hartree-Fock. This division and the imputation of superiority to the second category refers only to the conceptual approach. In the latter the dynamical electron interaction is in some fashion taken into consideration. Often, though, the energy for the H.F. approximation is the lowest obtained for a given molecule; but the energy is not an absolute criterion of value. Listing the advantages and disadvantages of the H.F. approximation will suffice to show why certain information was tabulated.

The Hartree-Fock approach is important for the following reasons:

1. At the equilibrium geometry the H.F. function dominates the wave function. In near degeneracy cases electron correlation must be considered but for many systems the H.F. function describes the electronic behavior and electrons can be associated with a given spatial orbital. The orbital energies determine the spectroscopy of the molecule and the coefficients tell us much of the bonding properties of the orbital.

2. Expectation values of one-electron operators are good to second-order (often within 10% of experiment) when perturbed by the correlation potential. This holds for the perturbation by external fields. 3. Hartree-Fock energies provide a basis for determining correlation energies empirically and systematic calculations lay the basis for semi-empirical estimation of correlation energies.

The major disadvantages of the Hartree-Fock approximation are 1. Correlation error is significant for the energy of dissociation, excitation, and ionization or detachment. 2. Asymptotic behavior of the potential surface is poor except in exceptional cases involving closed shell fragments. This behavior reflects itself in appreciable, 20% - 50%, errors in the spectroscopic constants.

Each section will be preceded by a description of the tables. Table B is an annotated bibliography of ab initio calculations. Tables C, D, E, and F include selected results for, respectively, the one-electron properties such as the moments and field gradients, the static polarizabilities, the magnetic constants, and the spectroscopic constants. Dissociation energies, electron affinities, and orbital energies are found, respectively, in Tables G, H, and I. In order to illustrate the range of the data generated by the calculations the energy and properties as a function of internuclear distance are given in Tables J and K. Table L very briefly illustrates the rapidly increasing area of polyatomic calculations based upon Gaussian-type basis functions.

It is hoped that the numbers are sufficient witness to the successes or failures of the present techniques and that outside of writing a book on the subject the less commentary the better.

a. See:
Nesbet, R. K. "Approximate Hartree-Fock calculations on small molecules" which will appear in Adv. in Quantum Chemistry, ed. P. O. Lowdin, Academic Press, N. Y., 1967, Vol. 3; Wahl, A. C., Bertoncini, P. J., Das, G., and Gilbert, T. L., "Recent progress beyond the Hartree-Fock method for diatomic molecules" which will appear in the Int. J. of Quantum Chem. 1, 0000 (1967).

B. Annotated Bibliography: Introduction

This section attempts to summarize ab initio molecular energy calculations from 1960 to the present including many unpublished results. The molecules are organized in the following order: hydrides AH; homonuclear A_2; heteronuclear AB; triatomics AH_2, ABH, ABC; tetratomic AH_3, ABH_2, ABCH, ABCD; pentatomic AH_4. A, B, etc. are selected in the periodic table order with $A < B < C < D$ or in the periodic table order of the first element to appear in the usual chemical nomenclature. In addition to the reference and the state of the molecule (note that the state is often not repeated when subsequent references refer to the same state) a very brief description of the method and results are given.

The Description of Method is minimal. A single symbol will denote a wide variety of calculations which are of unequal significance. The explanatory symbols which are listed in the glossary refer to the basic technique of the calculation but there is little or none of explanatory detail. Similarly the Basis Set column is devoid of detail; the use of the word "Extend." to denote a basis set larger than the minimum of one function per atomic orbital is perhaps overused since sets of almost minimal as well as saturated character will be similarly characterized. In most cases the energy, E, is given at a distance, R, and permits some judgment. For the polyatomic molecules the angles and distances are listed in the most compact form as given in the reference. This may not be completely unambiguous but consideration of the molecular symmetry and the convention of listing the internuclear separations in the order given in the formula heading should mitigate any difficulties. Again we note that the references are pointers only and the details suffer. In this section E and R are in atomic units.

The column, P, notes the properties considered in this calculation. Since many unpublished calculations are listed, it may happen that the results when published will be in separate papers. It can also be noted that Hartree-Fock results from the Laboratory of Molecular Structure and Spectra at the University of Chicago include all one-electron properties but the references are, in some cases, to published results which do not include these values. This situation may be more prevalent as computer packages for one-electron properties are being widely disseminated. In particular note that the Quantum Chemistry Program Exchange at Indiana University is distributing such a package as QCPE 103 written by T. Janiszewski and A. C. Wahl.

The check in the column E(R) indicates that a portion of the potential curve or surface has been calculated.

In order to facilitate a rapid judgment of the accuracy of a calculation a table of ground state H.F. atomic energies that was given by E. Clementi (Tables of Atomic Functions, Supplement to IBM J. Res. Develop. 9, 2 (1965)) and experimental values recommended by Cade and Huo (1967a,b) is also included after the references.

A table of the conversion factors for the atomic units is also given.

a. See:

"Hartree-Fock Wave Functions for Diatomic Molecules AH, A_2, and AB"
Compiled by P. E. Cade to be published last quarter 1967.

Glossary

Hartree-Fock	Refers to restricted H.F. as proposed by Roothaan. Indicates close approach to the H.F. energy limit.
Nesbet	Refers to equivalence and symmetry restriction variant of the H.F. method
SCF	Self-consistent field restricted H.F.
MO	Molecular orbital (signifies calculation of the energy of a state using the unoccupied MO's of an SCF calculation)
SOC	Superposition of configurations
VB	Valence bond
NO	Natural orbital
Valence	Refers to configurations arising only from excitation of valence orbitals
IS	Ionic states
DODS	Different orbital different spin
OC	One center
STF	Slater type function
ETF	Elliptic type function
GTF	Gaussian type function
BA	Best atom basis
BI	Best ion basis
DZ	Double zeta basis
BA + P	Best atom plus polarization basis
E	Energy in atomic units
R	Internuclear distance in atomic units
T	Term values; excited state energies
ω	Spectroscopic constants
μ	Dipole moment
Q	Quadrupole moment
q	Field gradient
P	Polarizability
I_3	Octupole moment
Vib-rot	Nuclear Schrodinger equation is evaluated
I	Ionization potential
EA	Electron affinity

Reference	State	Description of Method	P	E(R)	R	E
		H_2				
Davidson (1961)	$E^1\Sigma_g^+$	VB-ETF	Vib-rot	✓	1.92	-0.7175
Fraga and Ransil (1961b)	$X^1\Sigma_g^+$	SCF-Min.STF SOC-MO	T,ω	✓	1.402	-1.15919
Davidson and Jones (1962a)	$X^1\Sigma_g^+$	Best open-shell ETF	NO	✓		
Davidson and Jones (1962b)	$X^1\Sigma_g^+$	NO Expansion of Kolos-Roothaan Function	Energy for truncated expansions			
Bishop (1963)	$X^1\Sigma_g^+$	OC-SOC			1.4	-1.16042
Harris and Taylor (1963)	$X^1\Sigma_g^+$	SOC-DODS ETF			1.4	-1.16862
Hagstrum and Shull (1963)	$X^1\Sigma_g^+$	SOC-ETF	NO		1.4	-1.173128
Taylor (1963a)	$B^1\Sigma_u^+$	SOC-ETF			2.3	-0.74371
	$b^3\Sigma_u^+$	SOC-ETF			Repulsive curve	
Kolos and Wolniewicz (1963)	$X^1\Sigma_g^+$	Non-adiabatic 4 particle calculation	$D_o = 36091\ \mathrm{cm}^{-1}$ $R_o = 1.4191^a$			
Kolos and Wolniewicz (1964a)	$X^1\Sigma_g^+$	Accurate adiabatic calculation	H_2 $D_e^{calc} = D_e^{exp} + 4.2\ \mathrm{cm}^{-1}$			
Kolos and Wolniewicz (1964b)	$X^1\Sigma_g^+$	Accurate non-adiabatic calculation	H_2 $D_o^{calc} = D_o^{exp} + 0.6\ \mathrm{cm}^{-1}$			
			D_2 $D_o^{calc} = D_o^{exp} + 1.3\ \mathrm{cm}^{-1}$			
Browne (1964a)	$c^1\Pi_u$	SOC ETF	ω,Q,q	✓	1.947	-0.714533
	$c^3\Pi_u$	SOC ETF	ω,Q,q	✓	1.96	-0.733439

Reference	State	Description of Method	P	E(R)	R	E
		H_2				
Browne (1964b)	$3d^1\Delta_g$	SOC ETF	ω,Q,q NO	✓	1.99	-0.757014
	$3d^3\Delta_g$		ω,Q,q	✓	1.99	-0.657178
	$2p^1\Pi_g$, $2p^3\Pi_g$, $3d^1\Delta_u$, $3d^3\Delta_u$		Long range repulsive curve			
Goodisman (1964)	$X^1\Sigma_g^+$	James-Coolidge trial function				-1.1738
Gerhauser and Taylor (1964)	$E^1\Sigma_g^+$	SOC ETF		✓	1.9	-0.71643
	$a^3\Sigma_g^+$	SOC ETF		✓	1.87	-0.72730
Wakefield and Davidson(1965)	$2s^3\Sigma_g^+$	SOC ETF Λ doubling	Vib-rot	✓	1.864	-0.736615
	3s			✓	1.990	-0.66048
	3d			✓	1.984	-0.659325
Wright and Davidson (1965)	$3d^3\Pi_g$	SOC ETF	Vib-rot	✓	2.0	-0.65929
Kolos and Wolniewicz (1965)	$X^1\Sigma_g^+$	Generalized James-Coolidge trial function	Powers of r	✓	1.401	-1.1744746
	$b^3\Sigma_u^+$		E for large R Repulsive curve			
	$c^1\Pi_u$			✓	1.951	-0.7183492
Das and Wahl (1966)	$X^1\Sigma_g^+$	Extend. H.F. NO	ω	✓	1.4	-1.169837
Hoyland (1966b)	$c^3\Pi_u$	OC STF	ω	✓	1.948	-0.73567
	$c^1\Pi_u$		ω	✓	1.940	-0.71609
	$^3\Pi_g$		ω	✓	1.990	-0.65817
	$^1\Pi_g$		ω	✓	1.990	-0.65803

Reference	State	Description of Method	P	E(R)	R	E
		H_2				
Rothenberg and Davidson (1966a)	$2p\,^1\Pi_u$	SOC ETF	Vib-rot	✓	1.950	-0.717961
	3p		Vib-rot	✓	1.981	-0.655055
	4f		Vib-rot	✓	2.000	-0.633939
	4p		Vib-rot	✓	1.985	-0.632404
Rothenberg and Davidson (1966b)	$2s\,^1\Sigma_g^+$	SOC ETF	ω,NO	✓	2.00	-0.717244
	3d		ω,NO	✓	2.00	-0.659817
	3s		ω,NO	✓	2.00	-0.654481
	$2s\,^3\Sigma_g^+$		ω,NO	✓	2.00	-0.735976
	3d		ω,NO	✓	2.00	-0.660093
	3s		ω,NO	✓	2.00	-0.659404
	$2p\,^1\Sigma_u^+$			✓	2.00	-0.750402
	3p		ω,NO	✓	2.00	-0.664715
	$2p\,^3\Sigma_u^+$			✓	Repulsive curve	
	3p		ω,NO	✓	2.00	-0.682866
	$2p\,^1\Pi_u$		ω,NO	✓	2.00	-0.717832
	3p		ω,NO	✓	2.00	-0.655035
	4f		ω,NO	✓	2.00	-0.633939
	4p		ω,NO	✓	2.00	-0.632391
	$2p\,^3\Pi_u$		ω,NO	✓	2.00	-0.736849

Reference	State	Description of Method	P	E(R)	R	E
		H_2				
	$3p\,^3\Pi_u$		ω,NO	✓	2.00	-0.660233
	4p		ω,NO	✓	2.00	-0.634470
	4f		ω,NO	✓	2.00	-0.633940
	$3d\,^1\Pi_g$		ω,NO	✓	2.00	-0.659284
	$3d\,^3\Pi_g$		ω,NO	✓	2.00	-0.659362
	$3d\,^1\Delta_g$		ω,NO	✓	2.00	-0.657444
	$3d\,^3\Delta_g$		ω,NO	✓	2.00	-0.657502
Wolniewicz (1966)	$X\,^1\Sigma^+$	Num. integration nuclear motion	H_2 $D_o^{calc} = D_o^{exp} + 3.9$ cm^{-1}			
			HD $D_o^{calc} = D_o^{exp} + 4.7$ cm^{-1}			
			D_2 $D_o^{calc} = D_o^{exp} + 3.6$ cm^{-1}			
Kolos and Wolniewicz (1966a)	$B\,^1\Sigma_u^+$	Generalized James-Coolidge trial Function	D_e to 1.6 cm^{-1}		2.43	-0.7566611
Kolos and Wolniewicz (1966b)	$X\,^1\Sigma_g^+$	H-D perturbation correction to vibronic function	HD $D_o^{calc} = D_o^{exp} + 1.9$ cm^{-1}			
Hayes (1967)	$X\,^1\Sigma_g^+$	OC-SOC	ω,Q	✓	1.4	-1.17258

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HeH^+					
Anex (1963)	$X^1\Sigma^+$	SOC	ETF	ω,μ	✓	1.40	-2.97424
Michels and Harris (1963)	$X^1\Sigma^+$	SOC	ETF	ω	✓	1.40	-2.94321
Conroy (1964b)	$X^1\Sigma^+$	Minimize energy variance			✓	1.40	-2.97753[b]
Preuss (1964)	$X^1\Sigma^+$	VB	STF		✓	1.442	-2.94920
Stuart and Matsen (1964)	$X^1\Sigma^+$	OC-SOC	Extend. STF		✓	1.40	-2.9691
Goodisman (1965)	$X^1\Sigma^+$		Generalized James-Coolidge	T			-2.9729
Peyerimhoff (1965)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	ω,μ	✓	1.40	-2.93259
Wolniewicz (1965)	$X^1\Sigma^+$		Generalized James-Coolidge	T	✓	1.4363	-2.978669
	$A^1\Sigma^+$				✓	Repulsive curve	
Gallup and McKnight (1966)	$X^1\Sigma^+$	SCF	Exact 1-electron diatomic			1.40	-2.903
Harris (1966)	$X^1\Sigma^+$	SOC	ETF	ω	✓	1.50	-2.9550
Hoyland (1966a)	$X^1\Sigma^+$	SOC	Non-integral ETF		✓	1.40	-2.97190
		HeH^+					
Michels (1966)	$X^1\Sigma^+$	SOC	ETF	T	✓	1.40	-2.94321
	$A^1\Sigma^+$	SOC	ETF		✓	6.0	-2.50124
	$B^1\Sigma^+$				✓	8.5	-2.18177
	$a^3\Sigma^+$				✓	4.5	-2.50300
	$b^3\Sigma^+$				✓	8.0	-2.20072
	$C^1\Pi$				✓	8.0	-2.13318
	$c^3\Pi$				✓	8.0	-2.13761
		HeH					
Michels and Harris (1963)	$X^2\Sigma^+$	SOC	DODS-ETF		✓	3.0 Repulsive curve	-3.35670
	${}^2\Pi$	SOC	DODS-ETF	ω	✓	1.5	-3.06983
	${}^2\Sigma^+$	SOC	DODS-ETF	ω	✓	1.5	-3.08304
Taylor and Harris (1964)	$X^2\Sigma^+$	SOC	DODS-ETF			3.0	-3.3618
Bender and Davidson (1966)	$X^2\Sigma^+$	SOC-NO	ETF	μ,Q		3.0 Repulsive curve	-3.38280

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiH$^+$					
Platas et al (1959)	$X^2\Sigma^+$	VB	DODS STF	I		3.01	-7.699
Browne (1964c)		VB	Extend. STF+ETF	I	✓	4.25	-7.7808
Cade and Huo (1967)		SCF Hartree Fock	Extend. STF			3.014	-7.72943
		LiH					
Karo and Olsen (1959)	$X^1\Sigma^+$	VB	Num. H.F.	μ,ω	✓	3.245	-7.9941
	$A^1\Sigma^+$				✓	4.90	-7.8963
Robinson et al (1960)	$X^1\Sigma^+$	VB	DODS STF	μ		3.01	-8.0074
Browne and Matsen (1962)	$X^1\Sigma^+$	VB	Extend. STF	μ,ω	✓	3.075	-8.04379
Ebbing (1962)		SOC	ETF	μ	✓	3.0	-8.04127
Fraga and Ransil (1962b)		SCF SOC	Min. STF	μ		3.015	-7.9836
Kahalas and Nesbet (1963)		SCF SOC	Extend. STF	μ,q	✓	3.0581	-8.0171
Browne and Matsen (1964)		VB	Extend. STF+ETF	μ,q,ω	✓	3.046	-8.0561
Csizmadia et al (1964)	$X^1\Sigma^+$	Group orbital SOC	Hartree Fock AO		✓	3.0	-7.9922
	$A^1\Sigma^+$				✓	3.0	-7.8773
	$^3\Sigma^+$				✓	Repulsive curve	
Harris and Taylor (1964)	$X^1\Sigma^+$	SOC	DODS-ETF		✓	3.2	-8.0387
Ebbing and Henderson (1965)		Geminal	ETF-NO			3.0	-8.0179
Bender and Davidson (1966)		SOC-NO	ETF	μ,q,Q		3.0147	-8.0606
Csizmadia (1966)		SCF	Extend. GTF	μ,ω	✓	3.02	-7.9842
Cade and Huo (1967a)		SCF Hartree-Fock	Extend. STF	ω,I	✓	3.015	-7.98731
Sanders and Krauss (1967)		SOC-PNO Valence	Extend. GTF		✓	3.0	-8.0188
Kapral (1967)		SOC-MO-IS	GTF lobe		✓	3.25	-7.9944
Michels (1967)	$X^1\Sigma^+$	VB	Min. STF + 2p		✓	3.25	-7.9813
	$^3\Sigma^+$	VB	Min. STF + 2p		✓	Repulsive curve	
		BeH$^+$					
Cade and Huo (1967a)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF			2.479	-14.85396
		BeH					
Cade and Huo (1967)	$X^2\Sigma^+$	SCF Hartree-Fock	Extend. STF	ω,I	✓	2.538	-15.15312
LMSS (1967)	$A^2\Pi_r$	SCF Hartree-Fock	Extend. STF			2.519	-15.05062

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BH^+					
Cade and Huo (1967a)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF			2.296	-24.82064
LMSS (1967)	$A^2\Pi_r$	SCF Hartree-Fock	Extend. STF			2.374	-24.68317
		BH					
Fraga and Ransil (1962b)	$X^1\Sigma^+$	SCF-SOC	Min. STF			2.329	-25.0903
Buenker et al (1967)		SCF	Extend. GTF lobe		✓		-25.1001
Cade and Huo (1967a)		SCF Hartree-Fock	Extend. STF	ω, I	✓	2.305	-25.13147
Kaufman and Burnelle (1967)		SCF	Extend. GTF			2.336	-25.1298
Harrison (1967)	$X^1\Sigma^+$	VB Valence	GTF lobe AO	μ, Q, q	✓	2.50	-25.1455
	$^3\Pi$			μ, Q, q	✓	2.25	-25.1134
	$^1\Pi$			μ, Q, q	✓	2.50	-25.0394
	$^3\Sigma^-$			μ, Q, q	✓	2.50	-24.9948
	$^1\Delta$			μ, Q, q	✓	2.25	-24.9207

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CH^+					
Moore et al (1965)	$X^1\Sigma^+$	VB	Extend. STF		✓	2.2356	-37.91786
Cade and Huo (1967a)		SCF Hartree-Fock	Extend. STF		✓	2.137	-37.90881
		CH					
Cade and Huo (1967a)	$X^2\Pi_r$	SCF Hartree-Fock	Extend. STF	ω, I	✓	2.086	-38.27958
		CH^-					
Cade (1967b)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF	EA		2.086	-38.29003

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NH^+					
Cade and Huo (1967a)	$X^2\Pi_r$	SCF Hartree-Fock	Extend. STF			2.048	-54.50701
		NH					
Joshi (1965)	$X^3\Sigma^-$	OC-SCF	Extend. STF	μ	✓	1.90	-54.9064
Cade and Huo (1967a)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF	ω, I	✓	1.923	-54.97838
LMSS (1967)	$^1\Delta$	SCF Hartree-Fock				1.9729	-54.91081
Harrison (1967)	$X^3\Sigma^-$	VBValence	GTF lobe AO	μ	✓	2.375	-54.9400
	$^1\Delta$			μ	✓	2.375	-54.8625
	$^1\Sigma^+$			μ	✓	2.375	-54.8312
	$^3\Pi$			μ	✓	2.375	-54.7860

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NH^-					
Cade (1967b)	$X^2\Pi_i$	SCF Hartree-Fock	Extend. STF	EA		1.923	-54.92138
		OH^+					
Cade and Huo (1967a)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF	EA		1.944	-75.00050
		OH					
Cade and Huo (1967a)	$X^2\Pi_i$	SCF Hartree-Fock	Extend. STF	ω, I	✓	1.795	-75.42127
LMSS (1967)	$A^2\Sigma^+$	SCF Hartree-Fock	Extend. STF			1.912	-75.26553

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		OH^-					
Krauss and Ransil (1960)	$X^1\Sigma^+$	SCF	Min. STF		✓	1.8342	-74.8785
Grahn (1964)		VB	Min. STF			1.8103	-74.802
Rosenfeld (1964)		SCF	Min. STF			1.8103	-74.8221
Moskowitz et al (1965)		SCF	Extend. GTF			1.8	-75.3670
Cade (1967a)		SCF Hartree-Fock	Extend. STF	μ, Q, ω, q, EA	✓	1.781	-75.41754
Fink et al (1967)		SCF	Extend.GTF lobe			1.85	-75.3413
Ritchie and King (1967b)		SCF	Extend. GTF			1.79	-75.3961
		HF^+					
Clementi (1962a)	$^2\Sigma^+$	SCF	Extend. STF		✓	2.5	-99.3988
Cade and Huo (1967a)	$X^2\Pi_i$	SCF Hartree-Fock	Extend. STF			1.7328	-99.53598
LMSS (1967)	$^2\Sigma^+$	SCF	Extend. STF			1.7328	-99.39246

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HF					
Clementi (1962)	$X^1\Sigma^+$	SCF	Extend. STF	μ, T	✓	1.7328	-100.0580
Nesbet (1962)		SCF	Extend. STF	μ, T, ω, f	✓	1.7328	-100.0571
Bishop et al (1963)		OC-VB (1)	Non-integral n STF		✓	1.7052	-99.6651
Peyerimhoff (1963)		VB (3)	Min. STF + 3d		✓	1.7328	-99.6271
Harrison (1964)		SCF	Extend. GTF			1.75	-100.0178
Moccia (1964)		OC-SCF	Extend. STF	μ		1.7328	-100.0053
Moskowitz et al (1966)		SCF	Extend. GTF	μ, Q, q		1.7328	-100.0622
Bender and Davidson (1967a)		SOC-NO	ETF	μ, Q, q		1.7328	-100.2577
Cade and Huo (1967a)		SCF Hartree-Fock	Extend. STF	μ, Q, q, I	✓	1.696	-100.07077
Erdahl et al (1967)		VB	Extend.GTF lobe	μ, Q, q			-100.1043
Whitten and Allen (1967)		SCF	Extend. GTF lobe	μ	✓		-100.0224
McLean and Yoshimine (1967)		SCF Hartree-Fock	Extend. STF	μ, Q, q, P		1.7328	-100.07046
Harris and Michels (1967)		VB - Valence	Min. and DZ STF		✓	2.0	-100.0031

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NeH$^+$					
Peyerimhoff (1965)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ, ω	✓	1.83	-128.62836
Fink et al (1967)		SCF	Extend. GTF lobe			1.93	-128.56239
		NaH$^+$					
Cade and Huo (1967b)	$X^2\Sigma^+$	SCF Hartree-Fock	Extend. STF			3.566	-162.1671
		NaH					
Cade and Huo (1967b)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	ω, I	✓	3.566	-162.3928
		MgH$^+$					
Cade and Huo (1967b)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF			3.116	-199.9082
		MgH					
Cade and Huo (1967b)	$X^2\Sigma^+$	SCF Hartree-Fock	Extend. STF	ω, I	✓	3.271	-200.1566
LMSS (1967)	$A^2\Pi_r$	SCF Hartree-Fock	Extend. STF			3.173	-200.0589
		AlH$^+$					
Cade and Huo (1967b)	$X^2\Sigma^+$	SCF Hartree-Fock	Extend. STF			3.027	-242.1930
LMSS (1967)	$A^2\Pi_r$	SCF Hartree-Fock	Extend. STF			3.007	-242.0542

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		AlH					
Cade and Huo (1967b)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	ω,I	✓	3.114	-242.4634
		SiH^+					
Cade and Huo (1967b)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF			2.874	-289.1656
		SiH					
Cade and Huo (1967b)	$X^2\Pi_r$	SCF Hartree-Fock	Extend. STF	ω,I	✓	2.874	-289.4362

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		SiH^-					
Cade (1967b)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF	EA		2.861	-289.4598
		PH^+					
Cade and Huo (1967b)	$X^2\Pi_r$	SCF Hartree-Fock	Extend. STF			2.693	-340.9386
		PH					
Cade and Huo (1967b)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF	ω,I	✓	2.708	-341.2932
LMSS (1967)	$^1\Delta$	SCF Hartree-Fock	Extend. STF			2.708	-341.2473

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		PH^-					
Cade (1967b)	$X^2\Pi_i$	SCF Hartree-Fock		EA		2.668	-341.2847
		SH^+					
Cade and Huo (1967b)	$X^3\Sigma^-$	SCF Hartree-Fock	Extend. STF			2.551	-397.7593
		SH					
LMSS (1967)	$A^2\Sigma^+$	SCF Hartree-Fock	Extend. STF			2.551	-397.9441
Cade and Huo (1967b)	$X^2\Pi_i$	SCF Hartree-Fock	Extend. STF	ω,I	✓	2.551	-398.1015

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		SH^-					
Cade (1967a)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ, Q, ω, q, EA	✓	2.551	-398.1459
		HCl^+					
Cade and Huo (1967b)	$X^2\Pi_i$	SCF Hartree-Fock	Extend. STF			2.485	-459.6752
LMSS (1967)	$A^2\Sigma^+$	SCF Hartree-Fock	Extend. STF			2.861	-459.5376

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HCl					
Moccis (1962)	$X^1\Sigma^+$	OC-SCF	Extend. STF	μ		2.404	-458.83776
Nesbet (1964b)		SCF	Extend. STF	μ,Q ω,T	✓	2.4085	-459.80374
Cade and Huo (1967b)		SCF Hartree-Fock	Extend. STF	ω,I	✓	2.4087	-460.1103
McLeen and Yoshimine (1967)		SCF Hartree-Fock	Extend. STF	μ,Q,q,P		2.4087	-460.11185

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		He_2^{++}					
Kolos and Roothsan (1960)	$^1\Sigma_g^+$	40-term James-Coolidge Junction			✓	1.3	-3.67964
Frsgs and Ransil (1962a)	$^1\Sigma_g^+$	SOC-SCF-MO	Extend. STF	ω	✓	1.3	-3.66562
McLesn et al (1962)	$^1\Sigma_g^+$	SOC	Extend. STF		✓	1.3	-3.66222
Conroy and Bruner (1966)	$^1\Sigma_g^+$	Minimize energy variance			✓	1.375	-3.6793[b]
Michels (1967)	$^1\Sigma_g^+$	VB	Extend. STF		✓	1.5	-3.6519
	(3) $^1\Sigma_g^{+*}$				✓	Repulsive curves	
	$^1\Sigma_u^+$				✓	3.0	-2.3922
	(2) $^1\Sigma_u^{+*}$				✓	Repulsive curves	
		He_2^+					
Resgsn et al (1963)	$X^2\Sigma_u$	VB	Extend. STF		✓	2.00	-4.98540
Conroy and Bruner (1966)	$X^2\Sigma_u$	Minimize energy variance			✓	2.00	-4.9846
Edmiston and Krauss (1966)	$X^2\Sigma_u$	SOC-PNO	Extend. GTF		✓	2.0626	-4.9841
Gilbert and Wshl (1967a)	$X^2\Sigma_u, {}^2\Sigma_g$	SCF Hartree-Fock	Extend. STF	ω,T	✓	Curve relative to calculated asymptote	
Browne (1966)	$^4\Sigma_u^+$	VB	STF-ETF		✓	6.0	-4.21497
	$^2\Sigma_g^+, ({}^2\Sigma_g^+)^*$				✓	Repulsive curves	
	$^4\Sigma_g^+, ({}^2\Sigma_u^+)^*$				✓		

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		He_2^+					
Michels (1967)	$X^2\Sigma_u^+$	VB	Extend STF		✓	2.05	-4.97068
	$^2\Sigma_g^{+*}$				✓	1.5	-4.0451
	$^2\Pi_g$				✓	1.5	-3.83927
	$^2\Pi_u$				✓	1.5	-4.07516
	(4) $^2\Sigma_u^{+*}$, $^2\Sigma_g^+$, (3) $^2\Sigma_g^{+*}$, $^2\Pi_g^*$, $^2\Pi_u^*$				✓	Repulsive curves	
Schwertz (1967)	$X^2\Sigma_u^+$	SCF Hartree Fock	Floating S GTF			2.06	-4.92109

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		He_2					
Moore (1960)	$X^1\Sigma_g^+$	VB	Extend. STF		✓	Repulsive curve	
Ransil (1961)		SCF	Extend. STF		✓	for the ground state	
Phillipson (1962)		SOC-MO	Extend. STF		✓		
Kim (1962)		VB	Extend. STF	E at large R			
Miller and Present (1963)		OC	Extend. STF	E at large R			
Kestner (1966)		Pair Correlations		E at large R			
Kestner and Sinanoĝlu (1966)		Pair Correlations		E at large R			
Barnett (1967)		SOC	ETF-DODS		✓		
Gilbert and Wahl (1967b)		SCF Hartree-Fock	Extend. STF		✓		
Matsumoto et al (1967)		SOC-NO	ETF	E at small R			
Morris and Present (1967)		OC-SOC	Extend. STF	E at small R			
Brigman et al (1961)	$^3\Sigma_u^+$	VB	STF-DODS	Pot. hump	✓	2.13	-5.0938
Poshusta and Matsen (1963)	$^3\Sigma_u^+$	VB	Extend. STF	Pot. hump	✓	2.13	-5.11346
				ω,Q			
Scott et al (1966)	$^1\Sigma_u^+$	VB	Extend. STF	ω	✓	2.10	-5.10509

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		Li_2^+					
LMSS (1967)	$X^2\Sigma_g^+$	SCF Hartree-Fock	Extend. STF			5.051	-14.70971
	$^2\Pi_u$	SCF Hartree-Fock	Extend. STF			5.051	-14.54197
		Li_2					
Fraga and Ransil (1962b)	$X^1\Sigma_g^+$	SOC	Min. STF			5.051	-14.8523
Das and Wahl (1966)		Extend. H.F.-Valence	Extend. STF	ω	✓	5.25	-14.8988
Das (1967)		Extend. H.F.-Valence	Extend. STF	ω	✓	5.07	-14.90260
Buenker et al (1967)		SCF	Extend. GTF lobe				-14.86501
Cade and Wahl (1967)		SCF Hartree-Fock	Extend. STF	ω	✓	5.37	-14.87179
Kapral (1967)		SOC-MO-IS	GTF lobe AO	ω	✓	5.5	-14.88715

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		Be_2					
Fraga and Ransil (1962b)	$X^1\Sigma^+$	SOC-MO	Min. STF			3.78	-29.10537
LMSS (1967)		SCF Hartree-Fock	Extend. STF	Repulsive curve		8.50	-29.14667
Bender and Davidson (1967c)	$X^1\Sigma_g^+$	SOC	NO; r_{ij}^{-1} MO	Repulsive curve		4.5	-29.21998
	$X^1\Sigma_g^+$	SOC	Extend. ETF		✓	4.5	-29.14586
	$^3\Sigma_u^+$				✓	4.0	-29.11909
	$^3\Pi_g$				✓	4.0	-29.10969
		B_2					
Padgett and Griffing (1959)	$X^5\Sigma_u^-$	SCF	Min. STF	T	✓	3.0769	-49.063
Bender and Davidson (1967b)	$X^5\Sigma_u^-$	SOC	Extend. ETF	T	✓	3.00	-49.1453
	$^3\Sigma_g^-$				✓	3.00	-49.1402
	$^3\Pi_u$				✓	3.00	-49.1144
LMSS (1967)	$^3\Sigma_g^-$	SCF Hartree-Fock	Extend. STF	Q, q		3.005	-49.09087

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		C_2					
Fraga and Ransil (1962b)	$x^1\Sigma_g^+$	SOC	Min. STF			2.3475	-75.3193
Fougere and Nesbet (1966)	$x^1\Sigma_g^+$	SOC	DZ+3d	ω, T	✓		
	$X^3\Pi_u$	SOC			✓	Curves relative to calculated asymptote.	
Buenker et al (1967)	$x^1\Sigma_g^+$	SCF	Extend. GTF lobe				-75.3500
Verhaegen et al (1967)	$x^1\Sigma_g^+$	SCF	Extend. STF	ω, T	✓	2.3716	-75.385
LMSS (1967)	$x^1\Sigma_g^+$	SCF Hartree-Fock	Extend. STF	Q, q		2.3481	-75.40620
	$A^3\Sigma_g^-$	SCF Hartree-Fock	Extend. STF	Q, q		2.5876	-75.51523

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		N_2^+					
Cade et al (1966)	$X^2\Sigma_g^+$	SCF Hartree-Fock	Extend. STF	ω	✓	2.0385	-108.4079
	$A^2\Pi_u$	SCF Hartree-Fock	Extend. STF	ω	✓	2.134	-108.4320
	$B^2\Sigma_u^+$	SCF Hartree-Fock	Extend. STF	ω	✓	1.934	-108.2702
Verhaegen et al (1967b)	$X^2\Sigma_g^+$	SCF Nesbet	Extend. STF		✓	2.068	-108.3645
	$A^2\Pi_u$	SCF Nesbet	Extend. STF		✓	2.068	-108.3877
		N_2					
Richardson (1961)	$X^1\Sigma_g^+$	SCF	DZ	T		2.067	-108.7853
Fraga and Ransil (1962)	$X^1\Sigma_g^+$	SOC	Min. STF			2.086	-108.6605
Nesbet (1964)	$X^1\Sigma_g^+$	SCF	Extend. STF	Q, ω	✓	2.068	-108.9714
Nesbet (1965)		MO-Excited states	Extend. STF	T, ω			
Cade et al (1966)	$X^1\Sigma_g^+$	SCF Hartree-Fock	Extend. STF	ω	✓	2.0132	-108.9956
Buenker et al (1967)	$X^1\Sigma_g^+$	SCF	Extend. GTF lobe				-108.9189
Kapral (1967)	$X^1\Sigma_g^+$	SOC-MO-IS	GTF lobe AO	ω	✓	2.24	-108.9441

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		O_2^+					
LMSS (1967)	$X^2\Pi_g$	SCF → Hartree-Fock	Extend. STF			2.122	-149.2257
		O_2					
Sahni and DeLorenzo (1965)	$X^3\Sigma_g^-$	SCF	Min. STF			2.28167	-149.0921
LMSS (1967)	$X^3\Sigma_g^-$	SCF → Hartree-Fock	Extend. STF	Q, q	✓	2.282	-149.6659
	$a^1\Delta_g$	SCF → Hartree-Fock	Extend. STF		✓	2.297	-149.6172
	$b^1\Sigma_g^+$	SCF → Hartree-Fock	Extend. STF		✓	2.318	-149.5683

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		O_2^-					
LMSS (1967)	$X^2\Pi_g$	SCF → Hartree-Fock	Extend. STF		✓	2.40	-149.6427
		F_2^+					
LMSS (1967)	$X^2\Pi_g$	SCF	Extend. STF			2.525	-198.1782
	$^2\Pi_u$	SCF	Extend. STF			2.525	-197.9972
	$^2\Sigma_g^+$	SCF	Extend. STF			2.525	-198.0559
	$^2\Sigma_u^+$	SCF	Extend. STF			2.525	-197.3507

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		F_2					
Hijikata (1961)	$X^1\Sigma_g^+$	VB	Min.STF	T	✓	2.664	-197.9437
Fraga and Ransil (1962b)	$X^1\Sigma_g^+$	SOC	Min. STF			2.680	-197.9558
Wahl (1964)	$X^1\Sigma_g^+$	SCF Hartree-Fock	Extend. STF	ω,Q,q T		2.680	-198.7683
Das and Wahl (1966)	$X^1\Sigma_g^+$	Extend. H.F. Valence	Extend. STF		✓	3.0	-198.8378
Buenker et al (1967)	$X^1\Sigma_g^+$	SCF	Extend. GTF lobe				-198.6929
LMSS (1967)	$X^1\Sigma_g^+$	SCF Hartree-Fock	Extend. STF	Q,q		2.525	-198.7761
Kapral (1967)	$X^1\Sigma_g^+$	SOC-MO-IS	GTF lobe AO	ω	✓	3.25	-198.7754
Das and Wahl (1967)	$X^1\Sigma_g^+$	Extend. H.F.-Valence	Extend. STF		✓	2.68	-198.8546
Horsley and Richards (1967)	$X^1\Sigma_g^+$	SCF	Extend.STF	ω,T	✓	2.68	-198.7814
	$^3\Pi_u$	SCF-Nesbet	Extend. STF	ω	✓	2.98	-198.6792
	$^3\Sigma_u^+$				✓	Repulsive curve	
	$^3\Pi_g$				✓	Repulsive curve	
Harris and Michels (1967)	$X^1\Sigma_g^+$	VB	DZ STF		✓	3.1	-198.8179
		F_2^-					
Gilbert and Wahl (1967a)	$X^2\Sigma_u^+$	SCF Hartree-Fock	Extend. STF	ω,T	✓	Curve relative to calculated asymptote	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		Ne_2^+					
Gilbert and Wahl (1967a)	$X^2\Sigma_u^+$	SCF Hartree Fock	Extend. STF		✓	Curve relative to calculated asymptote	
		Ne_2					
Gilbert and Wahl (1967b)	$X^1\Sigma_g^+$	SCF Hartree Fock	Extend. STF		✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		Na_2					
Ransil (1964)	$X^1\Sigma_g^+$	SCF	Min. STF	ω	✓	5.8178	-322.3775
LMSS (1967)	$X^1\Sigma_g^+$	SCF	Extend. STF	Q,q		5.8178	-323.7116
Bertoncini and Wahl (1967)	$X^1\Sigma_g^+$	SCF	Extend. STF	Q	✓	5.8	-323.7096
		Mg_2					
Ransil (1964)	$^1\Sigma_g^+$	SCF	Min. STF			6.1	-397.8652
		Al_2					
Ransil (1964)	$^3\Sigma_g^-$	SCF	Min. STF			4.838	-482.3287
	$^1\Delta_g$					4.838	-482.3237
	$^1\Sigma_g^+$					4.838	-482.3003
		Si_2					
Ransil (1964)	$^3\Sigma_g^-$	SCF	Min. STF	ω	✓	4.5	-576.2190
	$^1\Delta_g$				✓	4.653	-576.1893
	$^1\Sigma_g^+$				✓	4.653	-576.1645

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		P_2					
Ransil (1964)	$^1\Sigma_g^+$	SCF	Min. STF	ω	✓	3.5798	-679.8020
Boyd and Lipscomb (1967)		SCF	Min. STF+3d			3.850	-679.1664
		S_2					
Ransil (1964)	$^3\Sigma_g^-$	SCF	Min. STF	ω	✓	3.93	-793.2791
	$^1\Delta_g$				✓	3.57	-793.2393
	$^1\Sigma_g^+$				✓	3.57	-793.2055
		Cl_2^+					
LMSS (1967	$X^2\Pi_g$	SCF	Extend. STF			3.5748	-918.5171
	$^2\Pi_u$	SCF	Extend. STF			4.25	-918.4230
	$^2\Sigma_g$	SCF	Extend. STF			3.7564	-918.3938
		Cl_2					
Ransil (1964)	$X\,^1\Sigma_g^+$	SCF	Min. STF	ω	✓	4.1	-917.0723
Gilbert and Wahl (1967c)	$X\,^1\Sigma_g^+$	SCF	Extend. STF	ω	✓	3.8	-918.9871

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		Cl_2^-					
Gilbert and Wahl (1967a)	$X^2\Sigma_u^+$	SCF	Extend. STF	ω,T	✓	Curve relative to computed asymptote	
		Ar_2^+					
Gilbert and Wshl (1967a)	$X^2\Sigma_u^+$	SCF	Extend. STF	ω,T	✓	Curve relative to computed asymptote	
		Ar_2					
Gilbert and Wahl (1967b)	$X\,^1\Sigma_g^+$	SCF	Extend. STF		✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		$HeLi^+$					
Schneiderman and Michels (1965)	$X^1\Sigma^+$	SOC-DODS	ETF	ω	✓	4.0	-10.1272
		HeLi					
Scheel and Griffing (1962)	$X^2\Sigma^+$	SCF	Min. STF	T	✓	Repulsive curve	
Schneiderman and Michels (1965)	$X^2\Sigma^+$	SOC-DODS	ETF	T	✓	Repulsive curve	
	$A^2\Pi$			ω	✓	3.5	-10.2550
	$a^4\Pi$			ω	✓	6.0	- 9.617
	$^2\Sigma^{+*}$			ω	✓	6.0	- 9.6322
	$^2\Sigma^{+**}$			ω	✓	5.0	- 9.5992
	$B^2\Sigma^+$ $^2\Sigma^{***}$, $^2\Sigma^{****}$				✓	Repulsive curves	
	$b^4\Sigma^+$, $c^4\Sigma^+$				✓		
		HeO					
Allen et al (1966)	$^1\Sigma^+$	VB	Extend. GTF lobe		✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HeF					
Allen et al (1966)	$^1\Sigma^+$	VB	Extend. GTF lobe		✓	Repulsive curve	
		$HeNe^+$					
Michels (1967)	$^2\Sigma^+$, $^2\Pi$	VB	Min. STF		✓	Repulsive curves	
	$^2\Sigma^{+*}$				✓	4.0	-129.81825
		HeNe					
Matcha and Nesbet (1967)	$X^1\Sigma^+$	SCF Hartree-Fock	BA+P STF	μ	✓	Repulsive curve	
		HeAr					
Matcha and Nesbet (1967)	$X^1\Sigma^+$	SCF Hartree-Fock	BA+P STF	μ	✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiB					
LMSS (1967)	$^1\Sigma^+$	SCF → Hartree-Fock	Extend. STF	μ, Q, q	✓	4.60	-31.95508
		LiC					
LMSS (1967)	$^2\Pi_r$	SCF → Hartree-Fock	Extend. STF	μ, Q, q	✓	3.80	-45.11185
		LiN					
LMSS (1967)	$^3\Sigma^-$	SCF → Hartree-Fock	Extend. STF	μ, Q, q	✓	3.40	-61.82640

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiO^+					
LMSS (1967)	$X^1\Sigma^+$	SCF	GTF lobe AO			3.184	-81.88621
		LiO					
LMSS (1967)	$^2\Pi_i$	SCF → Hartree-Fock	Extend. STF	μ, Q, q	✓	3.184	-82.31113
	$^2\Sigma^+$	SCF → Hartree-Fock	Extend. STF			3.184	-82.29619
		LiF					
Fraga and Ransil (1962b)	$X^1\Sigma^+$	SCF-SOC	Min. STF			2.85	-106.41211
McLean (1963b)		SCF	BA+P STF	μ, Q	✓	2.8877	-106.98850
McLean (1964)		SCF-Scale optimization	Extend. STF	μ; ω	✓	2.89	-106.97690
McLean and Yoshimine (1967)		SCF→ Hartree-Fock	BA+P STF	μ, Q, q, P	✓	2.8877	-106.9916
LMSS (1967)	$X^1\Sigma^+$	SCF → Hartree-Fock	Extend. STF	μ, Q, q		2.955	-106.9904
Pfeiffer (1967)	$X^1\Sigma^+$	VB	GTF lobe AO	μ, q		3.000	-106.9534
	$^1\Sigma^{+*}$					3.000	-106.7177
Wahl et al (1967)	$X^1\Sigma^+$	SCF	BI STF	μ		2.955	-106.9788

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiF$^+$					
LMSS (1967)	$^2\Pi_i$	SCF	GTF lobe AO			2.955	-106.6364
LMSS (1967)	$^2\Sigma^+$	SCF	GTF lobe AO			2.955	-106.6175
		LiNa					
LMSS (1967)	$X^1\Sigma^+$	SCF	Extend. STF	μ, Q, q		5.30	-169.2880
Bertoncini and Wahl (1967)	$X^1\Sigma^+$	Extend. H.F.-Valence	Extend. STF	ω	✓	5.50	-169.31422
		SCF Hartree-Fock	Extend. STF	ω	✓	5.50	-169.2919
		LiCl					
Matcha (1967)	$^1\Sigma^+$	SCF Hartree-Fock	BA+STF	ω, μ, q, Q	✓	3.825	-467.05466
LMSS (1967)	$X^1\Sigma^+$	SCF	Extend. STF	μ, Q, q		3.81855	-467.0499
Wahl et al (1967)	$X^1\Sigma^+$	SCF	BI STF	μ		4.71	-467.0116

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiBr					
Matcha (1967)	$^1\Sigma^+$	SCF	Extend. STF	μ, q	✓	4.0655	-2579.8901
		BeO$^+$					
LMSS (1967)	$^2\Pi_i$	SCF	Extend. STF			2.5149	-89.15694
	$^2\Sigma^+$	SCF				2.5149	-89.11320

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BeO					
Yoshimine (1964)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ,ω,Q	✓	2.4377	-89.44787
Verhaegan and Richards (1966)	$X^1\Sigma^+$	SCF MO-SOC	Extend. STF	T	✓	2.676	-89.4282
McLean and Yoshimine (1967)	$X^1\Sigma^+$	SCF Hartree-Fock	BA+P	μ,Q,q	✓	2.4377	-89.4541
Huo et al (1967)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ,ω	✓	2.5149	-89.4499
	$a^3\Pi$	SCF Hartree-Fock	Extend. STF	μ,ω	✓	2.7647	-89.4877
	$A^1\Pi$	SCF Hartree-Fock	Extend. STF	μ,ω	✓	2.7647	-89.4835
		BeF^+					
LMSS (1967)	$^1\Sigma^+$	SCF	Extend. STF			2.572	-113.8388
		BeF					
LMSS (1967)	$X^2\Sigma^+$	SCF	Extend. STF	μ,Q,q		2.572	-114.1688
	$^2\Pi_i$	SCF				2.634	-113.8904
	$^2\Pi_r$	SCF				2.634	-113.9982
Walker and Richards (1967)	$X^2\Sigma^+$	SCF Nesbet Hartree-Fock	Extend. STF	T		2.572	-114.1859
	$^2\Pi_i$	SCF Nesbet				2.572	-113.9164
	$^2\Pi_r$	SCF Nesbet				2.572	-114.0163
		BeNe					
Bender and Davidson (1967a)	$X^1\Sigma^+$	SCF	DZ-STF			3.0	-143.038

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BeS					
Verhaegan and Richards (1967)	$X^1\Sigma^+$	SCF	Extend. STF	T	✓	3.3	-412.0971
	$^3\Pi$					3.3	-412.0835
	$A^1\Pi$					3.3	-412.0729
	$^3\Sigma^+$					3.3	-412.0287
		BN^+					
LMSS (1967)	$^2\Pi_i$	SCF	Extend. STF			2.421	-78.54305
LMSS (1967)	$^2\Sigma^+$	SCF	Extend. STF			2.421	-78.49302
		BN					
Verhaegen et al (1967)	$^1\Sigma^+$	SCF Nesbet	Extend. STF	ω, T	✓	2.30	-78.9004
LMSS (1967)	$^3\Sigma^-$	SCF	Extend. STF	μ,Q q		2.421	-78.96701

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BO^+					
LMSS (1967)	$^1\Sigma^+$	SCF	Extend. STF			2.275	-99.06898
	$^3\Sigma^-$	SCF				2.275	-98.97693
		BO					
LMSS (1967)	$X^2\Sigma^+$	SCF	Extend. STF	μ,Q q		2.275	-99.55550
	$^2\Pi_i$	SCF	Extend. STF	μ,Q, q		2.555	-99.47757
	$^2\Pi_r$	SCF	Extend. STF	μ,Q, q		2.275	-99.24030
		BO^-					
LMSS (1967)	$^1\Sigma^+$	SCF	Extend. STF			2.275	-99.59493

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BF^+					
LMSS (1967)	$X^2\Sigma^+$	SCF	Extend. STF			2.391	-123.7952
	$^2\Pi_i$	SCF	Extend. STF			2.64	-123.5769
	$^2\Pi_r$	SCF	Extend. STF			2.391	-123.5499
		BF					
Fraga and Ransil (1962)	$X^1\Sigma^+$	SOC	Min. STF	μ		2.385	-123.6756
Nesbet (1964)	$X^1\Sigma^+$	SCF	Extend. STF	μ,Q,ω		2.385	-124.14038
Huo (1965)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ,Q,ω	✓	2.354	-124.1664
Lefebvre-Brion and Moser (1965)	Excited	MO	Extend. STF	T	✓		
McLean and Yoshimine(1967)	$X^1\Sigma^+$	SCF Hartree-Fock	BA+P	μ,Q,q,P	✓	2.391	-124.1671
Kapral (1967)	$X^1\Sigma^+$	SOC-MO-IS	GTF lobe AO	ω	✓	2.5775	-124.0962

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CN^+					
LMSS (1967)	$a^1\Sigma^+$	SCF	Extend. STF			2.217	-91.6410
	$^3\Sigma^-$	SCF				2.576	-91.75452
		CN					
LMSS (1967)	$^2\Pi_r$	SCF	Extend. STF			2.214	-91.85104
		CO^+					
LMSS (1967)	$X^2\Sigma^+$	SCF	Extend. STF			2.107	-112.2915
	$^2\Pi_i$	SCF				2.350	-112.2304
	$^2\Pi_r$	SCF				2.107	-111.9131

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CO					
Lefebvre-Brion et al (1960)	Excited	MO	Min. STF	T	✓		
Merryman et al (1960)	Excited	MO	Min. STF	T	✓		
Lefebvre-Brion et al (1961)	Excited	MO	Min. STF	T	✓	2.1319	-112.5752
Fraga and Ransil (1962b)	$X^1\Sigma^+$	SOC	Min. STF			2.132	-112.3960
Lefebvre-Brion et al (1964)	Excited	MO	Extend. STF	T	✓		
Nesbet (1964)	$X^1\Sigma^+$	SCF	Extend. STF	μ, Q, ω	✓	2.132	-112.7588
Nesbet (1965)	Excited	MO	Extend. STF	T	✓		
Huo (1965)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ, Q, q, ω	✓	2.081	-112.7879
McLean and Yoshimine (1967)	$X^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ, Q, q, P	✓	2.132	-112.7891
Huo (1966)	$a^3\Pi$	SCF Hartree-Fock	Extend. STF	μ, Q, q	✓	2.2853	-112.5742
		CF^+					
LMSS (1967)	$X^1\Sigma^+$	SCF	Extend. STF			2.322	-136.8862

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CF					
LMSS(1967)	$X^2\Pi_r$	SCF	Extend. STF	μ, Q, q		2.402	-137.2169
		CS					
Richards (1967)	$X^1\Sigma^+$	SCF	Extend. STF	μ		2.89964	-435.3297
		NO^+					
Lefebvre-Brion and Moser(1966)	Excited	SCF-MO	Extend. STF	T	Excitation energies only		
LMSS (1967)	$X^1\Sigma^+$	SCF	Extend. STF			2.007	-128.9560

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NO					
Lefebvre-Brion and Moser (1965)	Excited	SCF-MO	Extend. STF	T		Excitation energies only	
Lefebvre-Brion and Moser (1966)	Excited, NO^+	SCF-MO	Extend. STF	T		Excitation energies only	
LMSS (1967)	$X^2\Pi_r$	SCF	Extend. STF	μ, Q, q		2.1747	-129.2837

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NeO					
Allen et al (1966)	$^1\Sigma^+$	VB	Extend. GTF lobe		✓	Repulsive curve	
		NeF					
Allen et al (1966)	$^1\Sigma^+$	VB	Extend. GTF lobe		✓	Repulsive curve	
		Ne Ar					
Matcha and Nesbet (1967)	$X^1\Sigma^+$	SCF	BA+P STF	μ	✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NaF					
Matcha (1967)	$^{1}\Sigma^{+}$	SCF Hartree-Fock	BA+P STF	$\omega,\mu,q,$ Q	✓	3.628	-261.37849
Wahl et al (1967)		SCF Hartree-Fock	BI+P STF	ω,μ	✓	3.5	-261.3773
Das and Wahl (1967)		Extend. Hartree-Fock		NO,ω	✓	3.65	-261.4002
		NaCl					
Matcha (1967)	$^{1}\Sigma^{+}$	SCF Hartree-Fock	BA+P STF	$\omega,\mu,q,$ Q	✓	4.485	-621.4574
Wahl and Gilbert (1967)		SCF Hartree-Fock	BI+P STF	$\omega,\mu,$ Born parameters	✓	4.461	-621.4398
		NaBr					
Matcha (1967)	$^{1}\Sigma^{+}$	SCF	Extend. STF	μ,q		4.729	-2734.2876

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		MgO					
Richards et al (1966)	$^{1}\Sigma^{+}$	SCF	Extend. STF	T,ω	✓	3.4	-274.2784
	a $^{3}\Pi$	SCF Nesbet	Extend. STF	ω	✓	3.4	-274.3331
	$^{3}\Sigma^{+}$			ω	✓	3.3	-274.4757
McLean and Yoshimine (1967)	$^{1}\Sigma^{+}$	SCF Hartree-Fock	Extend. STF	μ,Q,q	✓	3.3052	-274.3751
		MgF					
Walker and Richards (1967)	$^{2}\Sigma^{+}$	SCF Nesbet	Extend. STF	T	✓	3.25	-299.0790
	$^{2}\Pi_{i}$				✓	3.25	-298.9493
		AlF					
McLean and Yoshimine (1967)	$^{1}\Sigma^{+}$	SCF Hartree-Fock	Extend. STF	μ,Q,q,P	✓	3.126	-341.4832

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		SiO					
McLean and Yoshimine(1967)	$^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ,Q,q,P	✓	2.75	-363.8523
		PN					
McLean and Yoshimine(1967)	$^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ,Q,q,P	✓	2.67	-395.1857
		PO					
Boyd and Lipscomb(1967)	$^2\Pi$	SCF	Min. STF+P3d	μ		2.738	-414.1371

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		PO^-					
Boyd and Lipscomb(1967)	$^3\Sigma^-$	SCF	Min. STF+P3d			2.859	-414.1168
		ClF					
Stevens (1967a)	$^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ		3.0768	-558.8955
		KF					
Matcha (1967)	$^1\Sigma^+$	SCF Hartree-Fock		μ,q	✓	4.1035	-698.68501
Wahl et al (1967)		SCF		μ		4.9720	-698.6645
		KCl					
Matcha (1967)	$^1\Sigma^+$	SCF	Extend. STF	μ,q	✓	5.039	-1058.7583

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CaO					
McLean and Yoshimine(1967)	$^1\Sigma^+$	SCF Hartree-Fock	Extend. STF	μ, Q, q	✓	3.4412	-751.5591
		ScO					
Carlson et al (1965)	$X^2\Sigma^+$	SCF	Extend. STF	T,ω,μ,	✓	3.05	-888.178
		ScF					
Carlson and Moser(1967)	$X^1\Sigma^+$	SCF	Extend. STF	T,ω,μ	✓	3.31	-858.5453
Cheetham and Richards(1967)	$^3\Pi$	SCF Nesbet	Extend. STF	T	✓	3.51	-858.5107
	$^3\Sigma^+$			T	✓	3.61	-858.4564
	$^3\Sigma^-$			T	✓	3.71	-858.4230
	$^3\Phi$			T	✓	3.51	-858.4166

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		TiO					
Carlson and Moser (1963)		SCF	Min. STF+P	T			
Carlson and Nesbet (1964)	$^1\Sigma^+$	SCF	Extend. STF	T,μ,ω	✓	3.0618	-921.4959
	$X^3\Delta_r$	MO	Extend. STF	μ,ω	✓	3.0618	-921.5418
Carlson and Moser (1967)	$X^3\Delta_r$	SCF	Extend. STF	T,μ,ω	✓	2.91	-922.4976
		VO					
Carlson and Moser (1966)	$^2\Delta$	SCF	Extend. STF	T		2.91	-1015.7627
	$^4\Sigma^-$	MO	Extend. STF			2.91	-1015.8917

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		RbF					
Matcha (1967)	$^1\Sigma^+$	SCF	Extend. STF	μ, q		4.3653	-3037.7727
		SrO					
McLean and Yoshimine(1967)	$^1\Sigma^+$	SCF	DZ+P	μ, Q, q, P	✓	3.6283	-3206.2311

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		H_3^+					
						Equilateral	
Christoffersen et al (1964)	$^1A_1$	SOC-VB			✓	1.625	-1.3002
Conroy (1964a)	$^1A_1$	Minimize energy variance			✓	Energy surface	
Conroy (1964b)	$^1A_1$	Minimize energy variance			✓	1.68	-1.357
Christoffersen (1964)	$^1A_1$	SOC-MO	Extend. STF	ω	✓	1.6575	-1.3326
Hoyland (1964)	$^1A_1$	VB	Generalized ETF			1.68	-1.2726
Lester and Krauss (1966)	$^1A_1$	Correlated Closed-Shell	Extend. GTF			1.68	-1.2984
Pearson et al (1966)	$^1A_1$	VB	Generalized GTF	ω	✓	1.66	-1.3185
Joshi (1966)	$^1A_1$	OC-SCF	Extend. STF		✓	1.6229	-1.2863
Conroy and Bruner (1966)	^1E	Minimize energy variance			✓	3.0	-0.6721
Considine and Hayes (1967)	$^1A_1$	OC-SOC	Extend. STF			Linear 1.8	-1.2466
Schwartz (1967)	$^1A_1$	SCF → Hartree-Fock	Floating S GTF			1.6405	-1.2999
Schwartz (1967)	$^1A_1$	SOC-MO-"Out of-plane" Correlation included.	Floating S GTF			1.6504	-1.3376

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		H_3					
Boys and Shavitt (1959)	$^2\Sigma_u^+$	SOC-VB	Extend. STF	ω	✓	1.778	-1.6274
Hoyland (1964)		SOC-VB	Generalized ETF			1.78	-1.5889
Krauss (1964)		SCF → Hartree-Fock	Extend. GTF		✓	1.73	-1.5930
Edmiston and Krauss (1965)		SOC-PNO	Extend. GTF			1.8	-1.6493
Conroy and Bruner (1965)		Minimize energy variance			✓	Energy surface	
Conroy and Bruner (1966)		Minimize energy variance			✓	1.75	-1.6551
Considine and Hayes (1967)		OC-SOC	Extend. STF			1.8	-1.6121
Shavitt et al (1967)		SOC	Extend. STF	Surface	✓	1.8	-1.6521
Schwartz (1967)		SCF → Hartree-Fock	Floating s GTF			1.7	-1.5940
Edmiston and Krauss (1967)		SOC-PNO	Extend. GTF	Surface	✓	1.8	-1.6493
		HeH_2					
Roberts (1963)	$^1A_1$	VB	Min. STF	E at large R	✓		
Krauss and Mies (1965)	$^1A_1$	SCF → Hartree-Fock	Extend. GTF		✓	Analytic interaction potential	
		LiH_2^-					
Preuss and Diercksen (1967)	$X^1\Sigma_g^+$	SCF	Extend. GTF		✓	3.5	-8.5313

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BeH_2					
Peyerimhoff et al (1966)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe		✓	2.54	-15.7123
Harris and Michels (1967)		VB	Min. STF		✓	2.54	-15.7202
		BH_2^+					
Peyerimhoff et al (1966)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe		✓	2.45	-25.4363
		BH_2^-					
Peyerimhoff et al (1966)	$^1A_1$	SCF	Extend. GTF lobe		✓	2.35, 104°	-25.6823
Geller et al (1967)	$^1A_1$	SCF → Hartree-Fock	Extend. GTF			2.222, 131°	-25.7086

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CH_2					
Krauss (1964)	$^1A_1$	SCF	Extend. GTF		✓	2.1,105°	-38.8026
	$^3\Sigma_g^-$	SCF	Extend. GTF		✓	1.95	-38.8936
Foster and Boys (1960)	$^3B_1$	SOC	Min. STF+DZK	ω	✓	2.11,129°	-38.904
	$^1A_1$	SOC	Min. STF+DZK	ω	✓	2.21,90°	-38.865
	$^1B_1$	SOC	Min. STF+DZK	ω	✓	2.11,132°	-38.808
Harrison (1967)	$^3B_1$	VB	Extend. GTF lobe		✓	2.0,138°	-38.893
	$^1A_1$				✓	2.0,108°	-38.843
	$^1B_1$				✓	2.0,148°	-38.822
		NH_2^+					
Peyerimhoff et al (1966)	$^1A_1$	SCF	Extend. GTF lobe		✓	2.05,130°	-55.0932
		NH_2					
Krauss (1964)	$^2B_1$	SCF	Extend. GTF		✓	1.95,105°	-55.4537
		NH_2^-					
Fink et al (1967)	$^1A_1$	SCF	GTF lobe AO		✓	2.05,100°	-55.3795
Ritchie and King (1967b)		SCF Hartree-Fock	Extend. GTF		✓	1.903, 105°	-55.5077
		H_2O^+					
Krauss (1964)	$^2B_1$	SCF	Extend. GTF		✓	1.9,115°	-75.4465
Miller et al (1967)	$^2B_1$	SCF	Extend. GTF			1.81,105°	-75.6025

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		H_2O					
McWeeny and Ohno (1960)	$^1A_1$	Group Orbital	Min. STF				
Krauss (1964)	$^1A_1$	SCF	Extend. GTF		✓	1.8,105°	-75.8453
Moccia (1964c)	$^1A_1$	OC-SCF	Extend. STF	μ		1.814,106°	-75.9224
Moskowitz and Harrison (1965)	$^1A_1$	SCF	Extend. GTF	μ		1.8,105°	-76.0421
Fink et al (1967)	$^1A_1$	SCF	Extend. GTF lobe AO	μ	✓	1.83,110°	-76.0031
Ritchie and King(1967a)		SCF	Extend. GTF			1.8,105°	-76.0343
Snyder (1967)		SCF	Extend. GTF			1.81098 104°26'	-76.020
Miller et al (1967)	X^1A_1	SCF	Extend. GTF	μ, f		1.81,105°	-76.0161
	$^3B_1$	SCF	Extend. GTF		✓	1.81,105°	-75.7788
	$^1B_1$	SCF	Extend. GTF		✓	1.81,105°	-75.7642
		H_2F^+					
Fink et al (1967)	$^1A_1$	SCF	GTF lobe AO			1.9,130°	-100.1773

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		$(H_2F)^-$					
Ritchie and King (1966)	$^1\Sigma^+$	SCF	Extend. GTF		✓	1.9,2.2	-100.575
		NeH_2					
Kapral (1967)	$^1\Sigma_g^+$	VB	GTF lobe AO		✓	Repulsive curve	
		H_2S					
Moccia (1964c)	$^1A_1$	OC-SCF	Extend. STF	μ		2.509,89°	-397.5891

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		$(Li_2H)^+$					
Preuss and Diercksen (1967)	$^1\Sigma_g^+$	SCF	Extend.GTF	ω	✓	3.2	-15.2887
		$(Li_2H)^-$					
Preuss and Diercksen (1967)	$^1\Sigma_g^+$	SCF	Extend.GTF	ω	✓	3.41	-15.3874

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		LiOH					
Buenker and Peyerimhoff (1966)	$^1\Sigma^+$	SCF	Extend. GTF lobe		✓	3.0236, 1.833	-82.9092
Ritchie and King (1967b)		SCF Hartree-Fock	Extend. GTF			3.00, 1.79	-82.9285
		HCN					
McLean (1962)	$^1\Sigma^+$	SCF	Min. STF			2.0, 2.187	-92.5474
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF Hartree-Fock	BA+P	μ, Q, q, P	✓	2.014, 2.179	-92.9147
Pan and Allen (1967)	$^1\Sigma^+$	SCF	Extend. GTF lobe AO	μ, Q		2.00, 2.1775	-92.8287
		FOH					
Buenker and Peyerimhoff (1966)	^1A	SCF	Extend. GTF lobe		✓	2.65, 1.833, 100°	-174.7196

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		$(FHF)^-$					
Clementi (1961)	$^1\Sigma_g^+$	SCF	Min. STF			2.135	-198.2826
Clementi and McLean (1962b)	$^1\Sigma_g^+$	SCF	Extend. STF			2.126	-199.3791
Erdahl (1967)	$^1\Sigma_g^+$	VB-Valence	Extend. GTF lobe AO	ω	✓	2.2	-199.4924
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	DZ+P STF	Q,q,P	✓	2.1	-199.5730
		BeF_2					
Peyerimhoff et al (1967)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe			2.072	-213.6527
		Li_2O					
Buenker and Peyerimhoff (1966)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe		✓	3.313	- 89.7743
		HeF_2					
Allen et al (1965)	$^1A_1$	VB	Extend. GTF lobe		✓		
		C_3					
Clementi (1961)	$^1\Sigma_g^+$	SCF	Min. STF			2.519	-113.0875
Clementi and McLean (1962a)	$^1\Sigma_g^+$	SCF	Extend. STF			2.519	-113.1652
		NeC_2					
Ha and Allen (1967)	$^1A_1$	SCF	GTF lobe AO		✓	Repulsive curve	
		$(OCN)^-$					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF Hartree-Fock	BA+P STF	μ,Q,q,P		2.213, 2.281	-167.2698
		FCN					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF Hartree-Fock	BA+P STF	μ, Q,q,P		2.38109, 2.20156	-191.7798
		$(SCN)^-$					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	DZ+P STF	μ,Q,q,P		2.95, 2.30	-489.9107
		ClCN					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	DZ+P STF	μ,Q,q,P		3.0784, 2.1978	-551.8247

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		CO_2					
McLean (1960)	$X^1\Sigma_g^+$	SCF	Min. STF			2.1944	-186.8427
McLean (1963)	$X^1\Sigma_g^+$	SCF	Extend. STF	Q		2.1944	-186.9300
Peyerimhoff et al (1967)	$X^1\Sigma_g^+$	SCF	Extend. GTF lobe AO			2.196	-187.4929
McLean and Yoshimine (1967)	$X^1\Sigma_g^+$	SCF Hartree-Fock	BA+P STF	Q,q	✓	2.1944	-187.7228
		SCO					
McLean and Yoshimine (1967)	$X^1\Sigma^+$	SCF	DZ+P STF	μ,Q,q,P		2.9442, 2.2016	-510.3309
		N_3^-					
Clementi (1961)	$^1\Sigma_g^+$	SCF	Min. STF			2.217	-162.5422
Clementi and McLean (1963)	$^1\Sigma_g^+$	SCF	Extend. STF			2.268	-162.7048
Peyerimhoff and Buenker (1967)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe	T		2.20	-163.1123
		N_2O					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	BA+P STF	μ,Q,q,P	✓	2.1273, 2.2418	-183.7567
		NeN_2					
Ha and Allen (1967)	$^1A_1$	SCR	GTF lobe AO		✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NO_2^+					
Clementi (1961)	$^1\Sigma_g^+$	SCF	Min. STF			2.173	-202.9011
Clementi and McLean (1963)	$^1\Sigma_g^+$	SCF	Extend. STF			2.173	-203.1082
Pfeiffer(1967)	$^1\Sigma_g^+$	SCF	Extend. GTF lobe			2.1806	-203.4547
		NO_2^-					
Pfeiffer (1967)	$^1A_1$	SCF	DZ GTF lobe AO			2.3356, 115.4°	-203.9551
		NF_2^+					
Geller et al (1967)	$^1A_1$	SCF	GTF		✓	2.58, 103°	-250.0189

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		O_3					
Peyerimhoff and Buenker(1967)	$^1A_1$	SCF	GTF lobe AO	T		2.50 116.8°	-224.1618
		NeO_2					
Ha and Allen (1967)	$^1A_1$	SCF	GTF lobe AO		✓	Repulsive curve	
		F_2O					
Buenker and Peyerimhoff (1966)	$^1A_1$	SCF	Extend. GTF lobe		✓	2.64, 102°	-273.4456

Reference	State	Description of Method	Basis Set	P	E(R)	R	E B72
		NeF_2					
Allen et al (1966)	$^1A_1$	VB	Extend. GTF lobe		✓	Repulsive curve	
Ha and Allen(1967)	$^1A_1$	SCF	GTF lobe AO		✓	Repulsive curve	

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		H_4^+					
Schwartz (1967)	$^2\Sigma_u^+$	SCF	GTF		✓	$R_{out}=R_{in}$ 1.6	-1.7443
		H_4					
Schwartz (1967)	$^1\Sigma_g^+$	SCF	GTF		✓	$R_{out}=R_{in}$ 1.6	-2.1669
Stevena (1967b)	$^1B_{2g}$	SOC	DZ (s)		✓	2.437	-2.0785
	$^3A_{2g}$				✓	2.34	-2.0683
		BeH_3^-					
Peyerimhoff et al (1966)	$^1A_1$	SCF	Extend. GTF			2.54	-16.2540
Joshi (1967)	$^1A_1$	OC-SCF	Extend. STF		✓	2.500	-16.1440

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BH_3					
Kaufman and Burnelle(1966)	$^1A_1'$	SCF	Extend. GTF			2.243	-26.3734
Peyerimhoff et al (1966)	$^1A_1'$	SCF	Extend. GTF lobe			2.31	-26.3652
Palke and Lipscomb(1966)	$^1A_1'$	SCF	Min. STF			2.25	-26.3377
Palke and Lipscomb(1966)	$^1A_1'$	SCF	Optimized Min. STF			2.25	-26.3517
Joshi (1967)	$^1A_1'$	OC-SCF	Extend. STF		✓	2.191	-26.2358
		CH_3^+					
Herman et al (1966)	$^1A_1'$	OC-SCF	Extend. STF			2.013	-39.0189
Peyerimhoff et al (1966)		SCF	Extend. GTF lobe			2.10	-39.2346
Joshi (1967)		OC-SCF	Extend. STF			2.032	-39.1178
Kari and Csizmadia(1967)		SCF	Extend. GTF			1.95	-39.2173
Bünau et al (1967)		SCF	Extend. GTF	ω	✓	2.05	-39.1440
		CH_3					
Morokuma and Pedersen (1967)	$^2A_1''$	SCF	GTF		✓	2.041	-39.1933
Hackmeyer and Whitten (1967)	$^2A_1''$	SCF Hartree-Fock	Extend. GTF lobe			2.00	-39.5394
		CH_3^-					
Rutledge and Saturno (1965)	$^1A_1'$	OC-SCF	Extend. STF			1.935	-39.2361
Fink et al (1967)	$^1A_1$	SCF	GTF lobe AO			2.0 111°	-39.3801
Ritter (1967)	$^1A_1'$	OC-SCF	Extend. STF			2.013	-39.2734
Kari and Csizmadia(1967b)	$^1A_1'$	SCF Hartree-Fock	Extend. GTF	μ,T		1.95, 115°	-39.4799
Ritchie and King (1967b)	$^1A_1$	SCF	Extend. GTF			2.12, 109°23'	-39.4633
		CF_3					
Morokuma and Pedersen (1967)	$^2A_1''$	SCR	GTF			2.513, 15°	-332.5690

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NH_3^+					
Kaldor and Shavitt (1966)	$^2A_1$	SCF	Bond orbitals			120° 1.967	-55.7641
		NH_3					
Bishop et al (1963)	$^1A_1$	OC-SCF	Min. STF	ω		1.9161	-55.6052
Reeves and Harrison (1963)	$^1A_1$	SCF	GTF	μ		106°48' 1.9162	-54.1144
Moccia (1964b)	$^1A_1$	OC-SCF	Extend. STF	μ		108°54' 1.928	-55.97482
Joshi (1965)	$^1A_1$	OC-SCF	Extend. STF	μ		109°34' 1.867	-56.08419
Rajagopal (1965)	$^1A_1$	SCF → Hartree Fock	Extend. STF	μ,Q		109°30' 1.9053	-56.2268
Bishop (1966)	$^1A_1$	OC-SOC	Extend. STF		✓	104°10' 1.8592	-55.8698
Kaldor and Shavitt (1966a)	$^1A_1$	SCF	DZ STF	μ,T	✓	106°48' 1.910	-56.0992
Rutledge and Saturno(1966)	$^1A_1$	OC-SOC	Extend. STF		✓	120° 1.823	-56.0222
Fink et al (1967)	$^1A_1$	SCF	GTF lobe AO	μ		115° 1.91	-56.1464
Ritchie and King (1967b)	$^1A_1$	SCF	Extend. GTF			105° 1.903	-56.2015
Snyder (1967)	$^1A_1$	SCF	Extend. GTF	μ		106°44' 1.91638	-56.183

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		H_3O^+					
Grahn (1962)	$^1A_1$	VB	Min. STF			120° 1.80	-76.174
Bishop (1965)	$^1A_1$	OC-SOC	Extend. STF		✓	115°5' 1.80	-76.0184
Moskowitz and Harrison(1965)		SCF	Extend. GTF			120° 1.8	-76.3203
Fink et al (1967)		SCF	GTF lobe AO			120° 1.83	-76.2669
		PH_3					
Moccia (1964b)	$^1A_1$	OC-SCF	Extend. STF	μ		89°48' 2.672	-341.3960
Boyd and Lipscomb(1967)		SCF	Min. STF+3d	μ		93°22' 2.680	-341.3094
		HCCH					
McLean (1960)	$^1\Sigma_g^+$	SCF	Min. STF			2.002, 2.281	-76.5433
Moskowitz (1965)		SCF	Extend. GTF			2.002, 2.281	-76.760

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HCCH					
Buenker et al (1967a)	$^1\Sigma_g^+$	SCF	Extend. GTFlobe			2.002, 2.272	-76.7916
McLean and Yoshimine (1967)		SCF Hartree-Fock	BA+P	Q,q		2.002, 2.281	-76.3540
		HCHO					
Newton and Palke (1966)	$^1A_1$	SCF	Min. STF	μ			-113.4496
Buenker and Whitten (1967)	$^1A_1$	SCF	Extend. GTF lobe	μ			-113.8094

Reference	State	Description of Method	Basis Set	P	E(R)	R	E B79
		H_2O_2					
						dihedral angle	
Kaldor and Shavitt (1966b)	$^1A_1$	SCF	Scaled Min. STF	μ	✓	120°	-150.1565
Davidson and Allen (1967)	$^1A_1$	SCF	Extend. GTF lobe		✓	180°	-150.7004
Pedersen and Morokuma (1967)	$^1A_1$	SCF	GTF		✓	150°	-149.28845
		LiCCH					
Veillard (1967)	$^1\Sigma^+$	SCF	BA + P	μ		3.55, 2.2696, 2.0088	-83.7305
		FCCH					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	BA+P STF	μ,Q,q		2.417, 2.264, 1.990	-175.7236
		ClCCH					
McLean and Yoshimine (1967)	$^1\Sigma^+$	SCF	DZ+P STF	μ,Q,q		3.084, 2.288, 1.988	-535.7673

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		HCOF					
Csizmadia et al (1966)	$^1A_1$	SCF	Extend. GTF	μ	✓		-212.1139
		$(CN)_2$					
McLean and Yoshimine (1967)	$^1\Sigma_g^+$	SCF	BA+P	μ,Q,q		2.186, 2.608	-261.4288
		NF_3					
Burnelle and Kaufman(1967)	$^1A_1$	SCF	GTF			2.591, 102° 9'	-348.8037

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		BH_4^-					
Krauss (1964)	$^1A_1$	SCF	Extend. GTF		✓	2.35	-26.946
Hegstrom et al (1967)	$^1A_1$	SCF	Optimized Min. STF			2.372	-26.9232
Fink et al (1967)	$^1A_1$	SCF	GTF lobe AO			2.35	-26.9490
		CH_4					
Nesbet(1960)	$^1A_1$	SOC-MO	GTF			2.0665	-39.1742
Saturno and Parr(1960)		SOC-OC	STF			2.0	-39.804
Albasiny and Cooper (1961)		SCF-OC	Numerical			2.00	-39.90
Krauss (1963)		SCF	Extend. GTF		✓	2.0665	-40.1668
Woznick (1964)		SCF	Extend. STF			2.0665	-40.1810
Sinai (1964)		SCF	Min. STF	I_3		2.0	-39.863
Rutledge and Saturno(1965)		SOC-OC	Extend. STF		✓		-39.859
Klessinger and McWeeny (1965)		Group orbital	Min. STF			2.067	-40.092
Fink et al (1967)		SCF	GTF lobe AO			2.04	-40.1711
Ritchie and King(1967a)		SCF Hartree-Fock	Extend. CTF			2.12	-40.1933
Snyder (1967)		SCF	Extend. GTF			2.0665	-40.189

Reference	State	Description of Method	Basis Set	P	E(R)	R	E
		NH_4^+					
Grein (1962)	$^1A_1$	OC-SCF	Min. STF	ω,P	✓	1.835	-55.684
Krauss (1963)		SCF	Extend. GTF			1.94	-56.504
Moccia (1964b)		OC-SCF	Extend. STF			1.990	-56.2177
Rajagopal(1965)		SCF	Extend. STF			1.905	-56.5216
Fink et al (1967)		SCF	GTF lobe AO			1.98	-56.4996
		PH_4^+					
Moccia (1964b)	$^1A_1$	OC-SCF	Extend. STF			2.750	-341.5493
		SiH_4^+					
Moccia (1964a)	$^1A_1$	OC-SCF	Extend. STF			2.787	-290.1024

a. R_o is the inverse square root of the expectation value of $1/R^2$. Comparison can be made to the experimental rotational constant B_o for the zeroth vibrational level.

b. Upper bound result. Extrapolated results are significantly lower. This calculation cannot be summarized simply and reference must be made to the original article for even a minimal description of the method.

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Experimental and Hartree-Fock Atomic Energies

Atom	State	Hartree-Fock[a]	Experimental[b]
		-E	
He	^1S_o	2.86168	2.90372[c]
Li	$^2S_{1/2}$	7.43272	7.4780
Be	^1S_o	14.57302	14.6685
B	$^2P_{1/2}$	24.52905	24.6579
C	^3P_o	37.68861	37.8558
N	$^4S_{3/2}$	54.40091	54.6122
O	$^3P_2$	74.80936	75.1101
F	$^2P_{3/2}$	99.40928	99.8053

Experimental and Hartree-Fock Atomic Energies

Atom	State	Hartree-Fock [a]	Experimental [b]
		-E	
Ne	^1S_o	128.54701	129.056
Na	$^2S_{1/2}$	161.85889	162.441
Mg	^1S_o	199.61458	200.333
Al	$^2P_{1/2}$	241.87665	242.752
Si	^3P_o	288.85426	289.927
P	$^4S_{3/2}$	340.71866	342.025
S	$^3P_2$	397.50475	399.144
Cl	$^2P_{3/2}$	459.48201	461.514
Ar	^1S_o	526.8175	529.303

a. Clementi, E. (1965). Tables of Atomic Functions.
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b. Cade and Huo (1967a,b). The analysis of the recommended "experimental" values is given in detail. For the rough comparison with molecular energies for which this table is included these values are more than adequate.

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Atomic Unit Conversions

E 1a.u. (Hartree) = 27.20976 eV

R 1a.u. (Bohr) = 0.529172 Å

μ 1a.u. = 2.54158 10^{-18} esu cm (Debye)

θ 1a.u. = 1.34492 10^{-26} esu cm^2

q 1a.u. = 3.24140 10^{15} esu/cm^3

C. One electron properties : Introduction

The results of a selected set of diatomic calculations are given for the dipole moment and derivative, the quadrupole moment, and the field gradients. The results are in cgs units: μ in Debyes, 10^{-18} esu cm, μ' in 10^{-10} esu, θ in 10^{-26} esu cm^2, and q in 10^{15} $\mathrm{esu/cm}^3$. When available experimental values are included. These are not referenced and were obtained for the most part from the theoretical paper that is referenced.

The polyatomic tables do not include the derivative of the dipole moment but the Larmor susceptibility χ_L in units of 10^{-5} $\mathrm{erg/gauss}^2$ mole is included. Note that such values are usually available in diatomic studies for which the quadrupole moment is given.

The properties are defined as follows:

1. Dipole moment

$$\mu = \sum_A Z_A d_A - e < z >$$

2. Quadrupole moment

$$\theta = \sum_A Z_A d_A^2 - \frac{1}{2} e < 3z^2 - r^2 >$$

3. $\chi_L = - \dfrac{e^2}{6mc^2} < r^2 >$

4. Field gradient

Only the q_{zz} component of the field gradient is tabulated here.[a]

$$q_A = \sum_B Z_B \frac{3\cos^2\theta_{AB} - 1}{d_B^3} - e < \frac{3\cos^2\theta_A - 1}{r_A^3} >$$

For the first three properties all distances are measured from a common origin which is commonly chosen to be the center of mass or the centroid of charge. Consideration of the gauge is discussed by McLean and Yoshimine (1966) who also illustrate the interrelations which exist between properties which depend on the square of the electronic coordinates. Note that some authors have not selected the center of mass as origin in determining the quadrupole moment and those cases are noted.

Polarity of μ is defined positive for A^+B^- and H^+A^-.

The field gradient is determined in a coordinate system relative to the atom in question.

[a] The field gradient tensor has been calculated ab initio only for formaldehyde. See Lowe and Flygare (1964), J. Chem. Phys. 41, 2153; Flygare et al (1966), J. Chem. Phys. 45, 2793.

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
H_2						
$c^1\Pi_u$	Browne (1964a)			-6.697	0.209	
$c^3\Pi_u$				-3.102	0.223	
$^1\Delta_g$	Browne (1964b)			-46.32	0.259	
$^3\Delta_g$				-47.13	0.259	
$X^1\Sigma_g^+$	McLean and Yoshimine(1966)			0.477		
	Exp			0.460		
$X^1\Sigma_g^+(H^+D^-)$	Kolos and Wolniewicz(1966b)	$1.54\ 10^{-3}$				
LiH						
$X^1\Sigma^+$	Ebbing (1962)	-5.96	-2.47			
	Kahalas and Nesbet(1963)	-5.888			-0.108	
	Browne and Matsen(1964)	-5.93			-0.112	
	Bender and Davidson(1966)	-5.965			-0.113	0.149
	Csizmadia (1966)	-6.008				
	Cade and Huo (1966)	-6.002				
	Exp.	-5.88	-2.0			
BeH						
$X^2\Sigma^+$	Cade and Huo(1966)	-0.282				
BH						
$X^1\Sigma^+$	Cade and Huo(1966)	1.733				
$X^1\Sigma^+$	Harrison (1967)	1.584		-3.366[a]	-1.823	0.549
$^3\Pi$		0.295		0.061[a]	-0.332	0.927
$^1\Pi$		1.196		1.289[a]	0.067	0.566
$^3\Sigma^-$		-0.338		5.075[a]	1.853	0.989
$^1\Delta$		-0.864		4.768[a]	1.866	0.967
CH						
$X^2\Pi_r$	Cade and Huo(1966)	1.570				
	Exp	1.46				

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
		NH				
$X^3\Sigma^-$	Joshi (1965)	1.931				
$X^3\Sigma^-$	Cade and Huo(1966)	1.627				
$X^3\Sigma^-$	Harrison (1967)	1.016				
$^1\Delta$		0.989				
$^1\Sigma^+$		0.869				
$^3\Pi$		1.294				
$^1\Delta$	Huo(1966)	1.65				
$^3\Pi$		1.38				
$^1\Pi$		1.85				
		OH				
$X^2\Pi_i$	Cade and Huo(1966)	1.780				
	Exp	1.66				

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
		FH				
$X^1\Sigma^+$	Nesbet(1962)	1.827	1.029			
	Clementi(1962)	1.984				
	Moccia (1964)	2.014				
	Cade and Huo(1966)	1.942				
	Moskowitz et al(1966)	1.921		2.539^a	9.299	
	Erdahl et al(1967)	2.008		2.390^a	10.48	1.771
	Whitten and Allen(1967)	1.98				
	Bender and Davidson(1967)	1.649			8.720	1.769
	McLean and Yoshimine(1967)	1.934		2.325	9.313	1.694
	Exp	1.82				
		NaH				
$X^1\Sigma^+$	Cade and Huo(1966)	-6.962				
		MgH				
$X^2\Sigma^+$	Cade and Huo(1966)	-1.516				

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
AlH						
$X^1\Sigma^+$	Cade and Huo(1966)	0.170				
SiH						
$X^2\Pi_r$	Cade and Huo(1966)	0.302				
PH						
$X^3\Sigma^-$	Cade and Huo(1966)	0.538				
SH						
$X^2\Pi_i$	Cade and Huo(1966)	0.861				
ClH						
$X^1\Sigma^+$	Moccia(1962)	2.166				
	Nesbet(1964b)	1.488	1.788	3.957		
	Cade and Huo(1966)	1.197				
	Menna et al(1966)		3.61			
	McLean and Yoshimine(1967)	1.215		3.744	11.55	0.908
	Exp	1.08	±1.00			

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
He_2						
$^3\Sigma_u^+$	Poshusta and Matsen(1963)			7.625		
Li_2						
$X^1\Sigma_g^+$	LMSS(1967)			13.886	-0.0162	
B_2						
$^3\Sigma_g^-$	LMSS(1967)			1.582	0.365	
C_2						
$X^1\Sigma_g^+$	LMSS(1967)			3.733	2.706	
$A^3\Sigma_g^-$	LMSS(1967)			-4.960	-4.156	
N_2						
$X^1\Sigma_g^+$	Nesbet(1964a)			-1.221		
$X^1\Sigma_g^+$	LMSS(1967)			-1.264	-4.411	

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
N_2^+						
$X^2\Sigma_g^+$	LMSS(1967)			4.246	2.256	
$A^2\Pi_u$	LMSS(1967)			1.845	-5.755	
O_2						
$X^3\Sigma_g^-$	LMSS(1967)			-0.376	4.483	
F_2						
$X^1\Sigma_g^+$	Wahl(1964)			0.886	22.262	
Na_2						
$X^1\Sigma_g^+$	LMSS(1967)			13.984		

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
LiF						
$X^1\Sigma_g^+$	McLean(1964)	6.30	4.08			
	Pfeiffer(1967)	6.28	3.95		-0.089	
	McLean and Yoshimine(1967)	6.295		5.769	-0.118	-0.896
	Exp	6.28	4.35		-0.128	
LiCl						
$X^1\Sigma^+$	Matcha (1967)	7.256	2.30		-0.068	-0.399
	Exp	7.13	2.3			
LiBr						
$X^1\Sigma^+$	Matcha (1967)	6.98			-0.069	-1.433
	Exp	7.27				
BeO						
$X^1\Sigma^+$	Yoshimine (1964)	7.290				
	McLean and Yoshimine(1967)	7.353		6.354	-2.824	-0.161

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
	BF					
$X^1\Sigma^+$	Nesbet (1964a)	-0.617	4.88	-4.382		
	Huo (1965)	-1.04	5.56	-4.53[b]	-1.753	1.702
	McLean and Yoshimine (1967)	-0.883		-4.482	-1.755	1.980
	CO					
$X^1\Sigma^+$	Lefebvre-Brion et al (1963)	0.132				-2.071
	Nesbet (1964a)	0.361	3.83	-1.306	-3.32	-2.201
	Huo (1965)	0.274	4.39	-2.19[b]		
	McLean and Yoshimine (1966)	C^-O^+	Analysis of sign of μ			
	Huo (1966)	0.274		-2.14	-3.82	-2.201
	McLean and Yoshimine (1967)	0.280		-2.204	-3.808	-2.348
$X^1\Sigma^+$	Exp	-0.112	2.97	±1.63		
$a^3\Pi$	Huo (1966)	2.46		1.07	0.016	3.153
	Exp	1.38				

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
	CS					
$X^1\Sigma^+$	Richards (1967)	1.6				
	Exp	1.98				
	NaF					
$X^1\Sigma^+$	Matcha (1967)	8.35			-1.224	-0.266
	Exp	8.16				
	NaCl					
$X^1\Sigma^+$	Matcha (1967)	9.10			-0.811	-0.648
	Exp	9.00				
	NaBr					
$X^1\Sigma^+$	Matcha (1967)	8.74			-0.586	-0.162
	McLean and Yoshimine (1967)			17.5		

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
	MgO					
$^1\Sigma^+$	McLean and Yoshimine (1967)	8.842		0.221	-0.517	6.321
	AlF					
$^1\Sigma^+$	McLean and Yoshimine (1967)	1.337		-6.713	-3.867	0.456
	SiO					
$^1\Sigma^+$	McLean and Yoshimine (1967)	3.397		-5.219	-7.952	-3.006
	PN					
$^1\Sigma^+$	McLean and Yoshimine (1967)	3.241		-2.818	-7.828	-4.954
	ClF					
$^1\Sigma^+$	Stevens (1967)	1.099				
	Exp	0.88				

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
	KF					
$^1\Sigma^+$	Matcha (1967)	8.69			-1.962	-1.158
	Exp	8.60				
	KCl					
$^1\Sigma^+$	Matcha (1967)	10.46			-1.413	-0.326
	Exp	10.27				
	CaO					
$^1\Sigma^+$	McLean and Yoshimine (1967)	10.946		-7.578	-0.846	-1.432
	ScO					
$^2\Sigma^+$	Carlson et al (1965)	2.6	1.5			
$^2\Delta_r$		7.7	1.0			

Molecule and State	Reference	μ	μ'	θ	q_1	q_2
	ScF					
$^1\Sigma^+$	Carlson and Moser (1967)	4.64				
$^3\Delta_r$		5.77				
	TiO					
$^3\Delta_r$	Carlson and Moser (1967)	5.93				
$^1\Sigma^+$		4.25				
	RbF					
$^1\Sigma^+$	Matcha (1967)	8.76			-2.813	-0.704
	Exp	8.55				
	SrO					
$^1\Sigma^+$	McLean and Yoshimine (1967)	10.207		-14.24	-0.805	-1.500

Molecule and State	Reference	μ	θ	q_1	q_2	q_3	χ_L
	H_2O						
$^1A_1$	Moccia (1964)	2.08					
	Moskowitz and Harrison (1965)	1.99					
	Fink et al (1967)	2.50					
	Exp	1.85	2.				
	H_2S						
$^1A_1$	Moccia (1964)	1.72					
	Exp	0.97					
	HCN						
$^1\Sigma^+$	McLean and Yoshimine (1967)	3.292	2.710	1.027	-1.580	-3.903	-3.925
	Pan and Allen (1967)	3.37					
	Exp	2.98					

Molecule and State	Reference	μ	θ	q_1	q_2	q_3	χ_L
			$(FHF)^-$				
$^1\Sigma_g^+$	McLean and Yoshimine (1967)		-7.513	2.295	0.106	2.295	-8.934
			$(OCN)^-$				
$^1\Sigma^+$	McLean and Yoshimine (1967)	1.800	-10.87	3.078	-2.002	-0.770	-9.887
			CO_2				
$^1\Sigma_g^+$	McLean and Yoshimine (1967)		-5.281	2.446	-2.362	2.446	-9.021
	Exp		-3.				
			N_2O				
$^1\Sigma^+$	McLean and Yoshimine (1967)	0.638	-3.745	-1.284	-1.559	8.310	-8.604
	Exp	0.167	-2.5				
			FCN				
$^1\Sigma^+$	McLean and Yoshimine (1967)	2.279	-4.214	10.54	-0.476	-2.416	-9.567

Molecule and State	Reference	μ	θ	q_1	q_2	q_3	q_4	χ_L
			$(SCN)^-$					
$^1\Sigma^+$	McLean and Yoshimine (1967)	2.155	-11.47	5.500	-1.861	-1.424		-16.83
			SCO					
$^1\Sigma^+$	McLean and Yoshimine (1967)	0.985	-1.479	6.417	-2.418	0.995		-16.02
			ClCN					
$^1\Sigma^+$	McLean and Yoshimine (1967)	3.052	-3.828	15.27	-0.785	-3.145		-16.16
			NH_3					
$^1A_1$	Moccia (1964b)	1.51						
	Joshi (1965)	1.52						
	Rajagopal (1965)	1.39	-0.270^a					
	Kaldor and Shavitt (1966a)	2.29						
	Fink et al (1967)	1.49						
	Exp	1.47						
			C_2H_2					
$^1\Sigma_g^+$	McLean and Yoshimine (1967)		7.232	1.111	-1.236			-4.852

Molecule and State	Reference	μ	θ	q_1	q_2	q_3	q_4	χ_L
		LiCCH						
$^1\Sigma^+$	Veillard (1967)	6.166	21.08					
		HCCF						
$^1\Sigma^+$	McLean and Yoshimine (1967)	0.913	4.528	10.59	0.099	-0.621	1.173	-10.80
		HCCCl						
$^1\Sigma^+$	McLean and Yoshimine (1967)	0.421	7.764	14.40	-0.329	-0.963	1.170	-17.64
		NCCN						
$^1\Sigma_g^+$	McLean and Yoshimine (1967)		-9.063	-4.049	-1.084			-19.48

Molecule and State	Reference	μ	θ	q_1	q_2	q_3	q_4	q_5
		HCCCN						
	McLean and Yoshimine (1967)	4.126	4.480	-3.548	-1.196	-0.559	-1.335	1.105

a. Origin of coordinates at heavy mass.

b. Origin of coordinates at mid-point of molecule.

D. Static Polarizabilities: Introduction

Two different techniques have been used to obtain the polarizabilities. A perturbation approach has been applied to a few molecules based on both zero-order H.F. and, in the case of H_2, very accurate wave functions. These are summarized in the table on D1. The H_2 work is very extensive and results are reported for polarizabilities averaged over numerous vibration-rotation levels.

The second approach has been to solve the H.F. equations with the field included in the Hamiltonian. Previous work in this direction has been reported by Cohen and Roothaan (J. Chem. Phys. 43, S34 (1965)) for atoms and a large number of linear molecules has recently been treated by McLean and Yoshimine. Their polarizability and hyperpolarizability tensor components are listed in the table on D2. Note the γ and B columns are to be multiplied by the scale factor at the top of the respective columns. Definitions and discussion of this procedure are referred to their publication and Buckingham (1959). Note that, with the exception of HCN, all the values are reported for the molecular geometries listed in the References.

Molecular Polarizabilities[a]

Reference	Molecule	α_{xx}	α_{zz}
Kolos and Wolniewicz (1967)	H_2	0.7022	1.0021
Stevens and Lipscomb (1964a)	LiH	4.063	3.35
O'Hare and Hurst (1967)		5.080	3.35
Stevens and Lipscomb (1964b)	HF	0.623	0.859
O'Hare and Hurst (1967)		0.791	1.002
Stevens and Lipscomb (1964c)	F_2	0.77	2.15
O'Hare and Hurst (1967)		0.949	2.248
O'Hare and Hurst (1967)	N_2	1.954	4.046
Exp		1.45	2.38
McLean and Yoshimine (1967)	CO		2.11
O'Hare and Hurst (1967)		2.088	3.222
Exp		1.625	2.60
O'Hare and Hurst (1967)	Li_2	40.649	59.848
	BF	3.738	2.716

a. Units: 10^{-24} cm^2

Molecular Polarizabilities[a]

Molecule	α_{zz}	β_{zzz}	γ_{zzzz}	$A_{z\,zz}$	$B_{zz\,zz}$	$3/2\ C_{zz\,zz}$
			10^3		10^2	
HF	8.07	-74.		31.6	-1.5	34.
HCl	23.4	-288.	1.	137.	-5.7	167.
LiF	8.40	$27.\cdot 10^1$	4.	38.5	-1.0	53.
BF	23.6	57.	4.	$-33.\cdot 10^1$	-8.	513.
CO	21.1	$19.\cdot 10^1$	1.	-83.	-6.1	203.5
NaBr	45.4	$6.\cdot 10^3$	$3.\cdot 10^2$	31.	$-8.\cdot 10^1$	$39.\cdot 10^1$
KCl	39.7	$31.\cdot 10^2$	$1.\cdot 10^2$	$44.\cdot 10^1$	$1.\cdot 10^1$	$108.\cdot 10^1$
RbF	24.1	$88.\cdot 10^1$		$16.\cdot 10^1$		$57.\cdot 10^1$
AlF	45.	$-8.\cdot 10^2$	-6.	$-66.\cdot 10^1$	-7.	$106.\cdot 10^1$
SiO	39.6	$35.\cdot 10^1$	3.	-49.	-2.	$58.\cdot 10^1$
PN	49.7	$15.\cdot 10^1$		215.	-10.7	506.
SrO	62.3			$1.\cdot 10^1$		$9.\cdot 10^2$
HCN[b]	33.2	$2.\cdot 10^2$	5.	-94.	-13.	$36.\cdot 10^1$
N_2O	40.6	$3.\cdot 10^2$	8.	-85.	-4.6	$38.\cdot 10^1$
$(OCN)^-$	41.1	$-1.\cdot 10^2$		$17.\cdot 10^1$	-3.	$59.\cdot 10^1$
FCN	32.5	$-1.\cdot 10^2$		267.	-2.	515.
SCO	62.7			44.	-6.	$83.\cdot 10^1$

Molecular Polarizabilities

Molecule	α_{zz}	β_{zzz}	γ_{zzzz}	$A_{z\,zz}$	$B_{zz\,zz}$	$3/2\ C_{zz\,zz}$
			10^3		10^2	
$(SCN)^-$	73.5			$28.\cdot 10^1$	-7.	$114.\cdot 10^1$
ClCN	53.3	$-14.\cdot 10^1$		378.	-3.2	978.
FCCH	46.4	$-8.\cdot 10^2$	8.	$61.\cdot 10^1$	-17.	$107.\cdot 10^1$
ClCCH	76.1	$-17.\cdot 10^2$	15.	$102.\cdot 10^1$	-40.	$207.\cdot 10^1$
NCCCH	95.					$2.\cdot 10^3$

a. For notation see Buckingham, A.D. (1959), Quart. Rev. 13, 194

b. HCN $R_1 = 1.81287$, $R_2 = 2.38053$

Entire table is due to
McLean and Yoshimine (1967)

Units: α $10^{-25}\,cm^2$, β $10^{-33}\,cm^5/esu$, γ $10^{-40}\,cm^7/esu^2$

A $10^{-34}\,cm^4$, B $10^{-41}\,cm^6/esu$, C $10^{-42}\,cm^5$

E. Magnetic Constants: Introduction

This table slightly extends and updates a similar table in Nesbet's review on H.F. calculations (Adv. Quant. Chem. , Vol. 3, 1967). It is provided as another test of the accuracy of one-electron properties of H.F. functions. All the calculations are based on perturbation of approximate H.F. functions.

Ground State Magnetic Constants of Diatomic Molecules

Molecule (AB)		LiH	Li_2	FH	F_2	BH
χ(ppm)	calc	-7.630	-28.94	-10.27	-10.617	18.75
	obs			-8.6		
σ_A(ppm)	calc	90.15	98.58	404.65	-199.7	-261.7
	obs				-210.1	
σ_B(ppm)	calc	26.45		28.11		24.46
	obs			27.9		
C_A(kc/sec)	calc	9.45	0.240	336.0	152.0	492.9
	obs	9.92		± 305	157	
C_B(kc/sec)	calc	-9.15		-69.97		-14.92
	obs	-10.1		± 71		
μ_J/J(nm)	calc	-0.6677	0.1100	0.738	-0.101	-8.30
	obs	-0.654	0.10797	0.7392	-0.121	

LiH- Stevens and Lipscomb (1964a)

Li_2- Stevens and Lipscomb (1965b)

HF - Stevens and Lipscomb (1964b)

F_2 - Stevens and Lipscomb (1964c)

BH - Hegstrom and Lipscomb (1966)

F. Spectroscopic Constants: Introduction

The results presented were obtained by a Dunham analysis of accurate H.F. and, for the few electron diatomics, accurate beyond H.F. calculations: Details of the fits will vary and in the case of H_2 extreme care has gone into the procedure. For the most accurate calculations the spectroscopic constants are usually ignored and the vibration-rotation energy levels are calculated by numerical integration of the Schrodinger equation. Unfortunately, the accuracy of most calculations do not warrant an effort beyond the spectroscopic constants. Nontheless, these results are considered the best obtainable for their type of calculation.

In order to facilitate comparison with experimental values, ω_e, $\omega_e x_e$, B_e, α_e are given in cm^{-1} and r_e in Å. Experimental values are given when provided by the theoretical paper in question.

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Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
		H_2				
$c^1\Pi_u$	Browne (1964a)	2452	41.91		1.204	1.030
	Exp	2442.7	67.03		1.626	1.033
$c^3\Pi_u$	Browne (1964a)	2429	36.40		1.296	1.04
	Exp	2465.0	61.40		1.425	1.038
$^1\Delta_g$	Browne (1964b)	2351.0	58.56		1.57	1.05
$^3\Delta_g$		2349.0	58.78		1.57	1.05
$X^1\Sigma_g^+$	Das and Wahl (1966)	4398				0.74
	Exp	4395.2				0.7416
$2s^1\Sigma_g^+$	Rothenberg and Davidson (1966b)	2354				1.009
3d		2296				1.073
3s		2502				1.042
$3d^3\Sigma_g^+$		2271				1.064
3s		2734				1.060
$3p^1\Sigma_u^+$		2127				1.095
$3p^3\Sigma_u^+$		2230				1.096
$2p^1\Pi_u$		2468				1.031
3p		2389				1.048
4f		2413				1.058

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
H_2						
$3d\,^1\Pi_g$		2286				1.063
$3d\,^3\Pi_g$		2288				1.063
$3d\,^1\Delta_g$		2354				1.053
$3d\,^3\Delta_g$		2354				1.053
$X\,^1\Sigma_g^+$	Baran and Kolos (1962)	4401.4	119.3	60.879		0.7413
	McLean (1964)	4402.3	121.82	60.880		0.7412
	Cashion (1966)	4402.744	121.548	60.8550		0.741405
	Exp	4400.39	120.82	60.864		0.74116
HeH^+						
$X\,^1\Sigma^+$	Anex (1963)	3286				0.765
	Peyerimhoff (1965)	3233	176	35.30	2.82	0.0770
	Wolniewicz (1965)					0.774
$X\,^1\Sigma^+$	Michels (1966)	3379	313.7	35.85	3.785	0.764
$A\,^1\Sigma^+$		209.7	89.71	2.343	0.7977	2.990
$B\,^1\Sigma^+$		381.8	6.535	1.038	0.01449	4.491
$C\,^1\Pi$		220.3	10.18	1.197	0.06081	4.183
$a\,^3\Sigma^+$		373.0	99.62	3.739	0.8156	2.366
$b\,^3\Sigma^+$		395.8	5.882	1.244	0.02724	4.103
$c\,^3\Pi$		225.5	6.595	1.255	0.04136	4.085

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
HeH						
$^2\Pi$	Michels and Harris (1963)	4065	252	38.0		0.742
$^2\Sigma^+$		4195	273	39.8		0.725
LiH						
$X\,^1\Sigma^+$	Browne and Matsen (1964)	1438	86			1.612
	Cade and Huo (1967a)	1433	23.26	7.426	0.1945	1.605
	Exp.	1405.6	23.20	7.513	0.213	1.595
BeH						
$X\,^2\Sigma^+$	Cade and Huo (1967a)	2147	34.60	10.392	0.2647	1.338
	Exp.	2058.6	35.5	10.308	0.300	1.343
BH						
$X\,^1\Sigma^+$	Cade and Huo (1967a)	2499	49.04	12.273	0.3726	1.797
	Exp	2367.5	~ 49	12.016	0.408	1.611
CH						
$X\,^2\Pi_r$	Cade and Huo (1967a)	3053	55.50	14.882	0.4712	1.104
	Exp	2868.5	64.4	14.448	0.530	1.124

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	NH					
$X^3\Sigma^-$	Cade and Huo(1967a)	3556	66.78	17.319	0.575	1.017
	Exp	3125		16.668	0.646	1.038
	OH					
$X^2\Pi_i$	Cade and Huo(1967a)	4062	74.54	19.712	0.6501	0.950
	Exp	3735.2	82.81	18.871	0.714	0.0971
	OH^-					
$X^1\Sigma^+$	Cade (1967a)	4087.9	87.82	20.023	0.722	0.942
	Exp	3735		18.87		0.971
	HF					
$X^1\Sigma^+$	Cade and Huo(1967a)	4469	80.34	21.868	0.7693	0.897
	Exp	4139.0	90.44	20.949	0.797	0.917
	NaH					
$X^1\Sigma^+$	Cade and Huo(1967a)	1187	14.71	4.766	0.1151	1.914
	Exp	1172.2	19.72	4.901	0.135	1.837

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	MgH					
$X^2\Sigma^+$	Cade and Huo(1967a)	1598	21.79	5.859	0.1315	1.725
	Exp	1495.7	31.5	5.818	0.167	1.731
	AlH					
$X^1\Sigma^+$	Cade and Huo(1967a)	1741	26.86	6.394	0.1719	1.647
	Exp	1682.6	29.09	6.391	0.186	1.648
	SiH					
$X^2\Pi_r$	Cade and Huo(1967a)	2144	30.91	7.558	0.1894	1.514
	Exp	2042.5	35.67	7.498	0.214	1.521
	PH					
$X^3\Sigma^-$	Cade and Huo(1967a)	2515	36.37	8.664	0.2145	1.412
	SH					
$X^2\Pi_i$	Cade and Huo(1967a)	2860	42.32	9.756	0.2494	1.330
	HCl					
$X^1\Sigma^+$	Cade and Huo(1967a)	3181	47.76	10.767	0.2682	1.264

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	HCl					
$X^1\Sigma^+$	Exp	2989.7	52.05	10.591	0.302	1.275
	He_2^+					
$X^2\Sigma_u^+$	Gilbert and Wahl (1967b)	1790		7.42		1.1
	He_2					
$^3\Sigma_u^+$	Poshusta and Matsen (1963)	1743	91.7	6.6	0.26	1.13
$^1\Sigma_u^+$	Scott et al (1966)	1665	43.4	6.739	0.216	1.12
	Li_2					
$^1\Sigma_g^+$	Das and Wahl (1966) H.F.	326				2.78
	OVC	345				2.69
	Exp	351				2.67
	C_2					
$^1\Sigma_g^+$	Fougere and Nesbet (1966)	1503				1.356
$^3\Pi_u$		1538				1.394
$^3\Sigma_g^-$		1328				1.444
$^1\Pi_u$		1527				1.392
$^1\Sigma_g^+$	Verhaegen et al (1967)	1970				1.255
$^3\Pi_u$		1710				1.300
$^1\Pi_u$		1730				1.306

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	N_2^+					
$X^2\Sigma_g^+$	Cade et al (1966)	2570.5	9.809	2.065	0.0148	1.080
	Exp	2207.1	16.14	1.932	0.020	1.118
$A^2\Pi_u$	Cade et al (1966)	2312.5	6.082	1.887	0.0155	1.129
	Exp	1902.8	14.91	1.740	0.018	1.176
$B^2\Sigma_u^+$	Cade et al (1966)	3101.8	19.88	2.296	0.0128	1.024
	Exp	2419.8	23.19	2.073	0.020	1.075

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
N_2						
$X^1\Sigma_g^+$	Cade et al (1966)	2729.6	8.378	2.121	0.0135	1.065
	Exp	2358.1	14.188	1.999	0.0178	1.097
F_2						
$X^1\Sigma_g^+$	Wahl (1964)	1257	9.85	1.003	0.0108	1.33
	Das and Wahl (1966)	678				1.45
	Das and Wahl (1967)	704				1.44
	Harris and Michels (1967)	1072	16.44	0.9087	0.012	1.398
	Exp	923.1	16.04	0.8938	0.022	1.409
F_2^-						
$X^2\Sigma_u^+$	Gilbert and Wahl (1967b)	510		0.50		1.9
Ne_2^+						
$X^2\Sigma_u^+$	Gilbert and Wahl (1967b)	660		0.59		1.7
Cl_2						
$X^2\Sigma_u^+$	Gilbert and Wahl (1967c)	577	2.2	0.24	0.0023	2.00
$X^2\Sigma_u^+$	Exp	559.7	2.70	0.24407	0.00153	1.9878
Cl_2^-						
$X^2\Sigma_u^+$	Gilbert and Wahl(1967b)	260	2.	0.136	0.001	2.65
Ar_2^+						
$X^2\Sigma_u^+$	Gilbert and Wahl(1967b)	300		0.139		2.4

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	$HeLi^+$					
$X^1\Sigma^+$	Schneiderman and Michels (1965)	232.8	20.41	1.513	0.122	2.095
	HeLi					
$^2\Sigma^{**}$	Schneiderman and Michels (1965)	375.2	11.07	1.019	0.3043	2.553
$^2\Sigma^*$		284.2	5.32	0.724	0.0090	3.029
$a^4\Pi$		353.6	2.53	0.841	0.0086	2.810
$A^2\Pi$		285.7	39.68	1.722	0.183	1.964
	LiF					
$X^1\Sigma^+$	McLean (1964)	1134.5	9.441	1.580	0.0182	1.528
	Exp	964.1	8.895	1.509	0.0241	1.564
	LiNa					
$X^1\Sigma^+$	Bertoncini and Wahl (1967) H.F.	264				2.94
	NO	256				2.90

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	LiCl					
$X^1\Sigma^+$	Matcha (1967)	671.5	4.671	0.704	0.0076	2.024
	Exp	641.0	4.2	0.706	0.0080	2.021
	BeO					
$X^1\Sigma^+$	Yoshimine (1964)	1807.7	10.687	1.757	0.0151	1.290
	Exp	1487.3	11.830	1.651	0.0190	1.331
$B^1\Sigma^+$	Verhaegen and Richards (1966)	1554				1.356
$b^3\Sigma^+$		1409				1.403
$A^1\Pi$		1399				1.441
$a^3\Pi$		1372				1.436
	BN					
$^1\Pi$	Verhaegen et al (1967)	1790				1.306
$^1\Sigma^+$		2020				1.246
$^3\Sigma^+$		2070				1.220
$X^3\Pi$		1750				1.305

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
		BF				
$X^1\Sigma^+$	Nesbet (1964a)	1413.8	9.9	1.495		1.272
	Huo (1965)	1496	12.07	1.559	0.0185	1.246
	Exp	1402.1	11.8	1.510	0.016	1.265
		CO				
$X^1\Sigma^+$	Nesbet (1964a)	2357.2	11.1	1.965		1.119
	Huo (1965)	2431	11.69	2.027	0.0153	1.101
	Exp	2169.8	13.295	1.931	0.0175	1.128
		NaF				
$X^1\Sigma^+$	Matcha (1967)	588.3	4.387	0.439	0.00468	1.920
	Das and Wahl (1967)	590				1.93
	Wahl et al (1967)	603				1.93
	Exp	536.1	3.83	0.437	0.00457	1.926

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
		NaCl				
$X^1\Sigma^+$	Matcha (1967)	378.3	2.589	0.215	0.00179	2.373
	Wahl and Gilbert (1967)	341				2.42
	Exp	364.6	2.05	0.218	0.00162	2.360

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Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
		MgO				
$B^1\Sigma^+$	Richards et al (1966)	1055				1.666
$A^1\Pi$		887				1.812
$b^3\Sigma^+$		856				1.762
$a^3\Pi$		880				1.814
$X^1\Sigma^+$		808				1.785
		ScO				
$B^2\Sigma^+$	Carlson et al (1965)	1329				1.678
$A^2\Pi_r$		1174				1.625
$^2\Delta_r$		1318				1.654
$X^2\Sigma^+$		1373				1.615
		ScF				
$^1\Delta$	Carlson et al (1965)	970				1.801
$^3\Delta_r$		902				1.751
$^1\Sigma^+$		909				1.806

Molecule and State	Reference	ω_e	$\omega_e x_e$	B_e	α_e	r_e
	TiO					
$d^1\Sigma^+$	Carlson and Moser(1967)	1737				1.526
$X^3\Delta_r$		1731				1.542

H_3^+ Spectroscopic Constants

Reference	A_1	E
Coulson (1935)	3170	
Christoffersen (1964)	3354	2790
Pearson et al (1966)	3610	4440

Calculated Geometry and Vibrational Frequencies

	H_2O	H_2S	NH_3	PH_3	CH_4	SiH_4	NH_4^+	PH_4^+
R_e(Å)	0.960	1.328	1.018	1.414	1.104	1.475	1.053	1.455
HXH_e	106.39°	89.40°	109.16°	89.26	Tetrahedral	Tetrahedral	Tetrahedral	Tetrahedral
ω_1 (Cm^{-1})	4411	3112	3672	2839	3709	2542	3634	2462
ω_2	1364	985	645	902	1262	845		
ω_3	4211	2798	3874	2791	3830	2557		
ω_4			1035	864	1122	714		

Menna et al (1966)

G. Dissociation Energies : Introduction

Hartree-Fock dissociation energies are obtained by substracting the atomic H.F. energies from the molecular H.F. energy.

Beyond Hartree-Fock dissociation energies are obtained relative to the natural limit for the procedure at hand. In the case of the valence extended Hartree-Fock or NO procedures, the asymptotic limit is again the H.F. atom energies. For the VB calculations it is dependent on the basis set that is used.

Hydride Dissociation Energy

Molecule	State	D_e(eV)		
		Hartree-Fock[a]	Beyond H.F.	Exptl.
LiH	$^1\Sigma^+$	1.49	2.24[b], 2.36[c]	2.52
BeH	$^2\Sigma^+$	2.18		(2.6)
BH	$^1\Sigma^+$	2.78		3.58
CH	$^2\Pi_r$	2.47		3.65
NH	$^3\Sigma^-$	2.10		(3.8)
OH	$^2\Pi_i$	3.03		4.63
HF	$^1\Sigma^+$	4.38	2.77[d]	6.12
NaH	$^1\Sigma^+$	0.93		(2.3)
MgH	$^2\Sigma^+$	1.15		(2.3)
AlH	$^1\Sigma^+$	2.36		3.01
SiH	$^2\Pi_r$	2.23		(3.32)
PH	$^3\Sigma^-$	2.03		(3.34)
SH	$^2\Pi_i$	2.63		3.70
HCl	$^1\Sigma^+$	3.48		4.616

a. All Hartree-Fock results: Cade and Huo (1967a,b)

b. Bender and Davidson (1966)

c. Sanders and Krauss (1967)

d. Harris and Michels (1967)

Homonuclear Dissociation Energy

Molecule	State	D_e (eV) Hartree-Fock	 Beyond Hartree-Fock	 Exptl.
He_2^+	$X^2\Sigma_u^+$	2.7[a]		
Li_2	$X^1\Sigma_g^+$	0.17[c]	0.99[d]	1.1
B_2	$^3\Sigma_g^-$	0.89[c]		
C_2	$X^1\Sigma_g^+$	0.79[c]	5.39[e]	6.36
N_2	$X^1\Sigma_g^+$	5.18[f]		9.90
N_2^+	$X^2\Sigma_g^+$	3.13[f]		8.86
N_2^+	$A^2\Pi_u$	3.59[f]		7.73
O_2	$X^3\Sigma_g^-$	1.28[c]		5.21
O_2	$a^1\Delta_g$	-0.06[c]		4.23
O_2	$b^1\Sigma_g^+$	-1.39[c]		3.57
F_2	$X^1\Sigma_g^+$	-1.37[c]	0.95[g],0.41[h],2.01[h]	1.69
F_2^-	$X^2\Sigma_u^+$	1.66[a]		
Ne_2^+	$X^2\Sigma_u^+$	1.65[a]		
Na_2	$X^1\Sigma_g^+$	0.07[c]		0.74

Molecule	State	D_e (eV) Hartree-Fock	 Beyond Hartree-Fock	 Exptl
Cl_2	$X^1\Sigma_g^+$	0.87[i]		2.51
Cl_2^-	$X^2\Sigma_u^+$	1.28[a]		
Ar_2^+	$X^2\Sigma_u^+$	1.25[a]		

a. Gilbert and Wahl (1967a)

b. Reagan et al (1963)

c. LMSS (1967)

d. Das (1967)

e. Fougere and Nesbet (1966)

f. Cade et al (1966)

g. Das and Wahl (1967)

h. Harris and Michels (1967), the first number is for the Hartree-Fock basis while the second is obtained with a minimal Slater basis.

i. Gilbert and Wahl (1967c)

		Heteropolar Dissociation Energy		
Molecule	State	Hartree-Fock	Beyond Hartree-Fock	Exptl.
HeLi	$A^2\Pi$		0.06[a]	
	$a^4\Pi$		0.89	
	$^2\Sigma^*$		0.41	
	$^2\Sigma^{**}$		0.45	
LiO	$^2\Pi_i$	1.88[b]		
LiF	$X^1\Sigma^+$	4.07[c]		
LiNa	$X^1\Sigma^+$	0.05[d]	0.65[d]	
LiCl	$X^1\Sigma^+$	3.83[e]		4.84
BeO	$X^1\Sigma^+$	4.13[f]		4.7
BeF	$X^2\Sigma^+$	5.07[b]		
BF	$X^1\Sigma^+$	6.19[g]		8.58±0.5
BO	$X^2\Sigma^+$	5.91[b]		≤7.52
CO	$X^1\Sigma^+$	7.92[c]		11.242
	$a^3\Pi$	2.07[h]		5.206
NO	$X^2\Pi_r$	2.00[i]		
NaF	$X^1\Sigma^+$	3.05[e]	3.7[j]	4.95
NaCl	$X^1\Sigma^+$	3.18[e]		4.22

a. Schneiderman and Michels (1965)

b. LMSS (1967)

c. McLean and Yoshimine (1967)

d. Bertoncini and Wahl (1967)

e. Matcha (1967)

f. McLean and Yoshimine (1967)

g. Huo (1965)

h. Huo (1966)

i. Estimated from LMSS (1967) NO total energy and ground state atom energies of -129.21027 a.u.

j. Das and Wahl (1967)

H. Electron Affinities: Introduction

Ab initio calculation of electron affinities from beyond H.F. results is not possible today; direct calculation of the electron affinity of a molecule by the difference in the H.F. energies of the ion and neutral molecule yields poor results. Systematic study of the homologous series of molecules and analyogous atoms does permit the estimation of the correlation energy and other properties of the ion. Cade (1967a,b) has completed such a program for the hydride ions.

The use of orbital energy from singlet symmetric ions is also illustrated. Note that other ions are listed in the orbital energy tables.

Electron Affinities of Molecules(eV)

Molecule	EA(HF)	$-\varepsilon^{a}$	EA(Corr)	EA (Exptl.)
CH[b]			1.61	> 1.4
NH			0.22	> 0
OH	-0.10	2.90	1.91	1.83
SiH	0.64		~ 1.46	
PH	-0.23		~ 0.93	
SH	1.21	2.42	2.25	~ 2.3
NO_2[c]		3.45		≥ 3.82[d]

a. Orbital with smallest energy for closed-shell ions.

b. Hydride results from Cade (1967a); (1967b).

c. Pfeiffer (Princeton) (1967).

d. Curran, R. K. (1962), Phys. Rev. 125, 910

I. Orbital Energies: Introduction

A variety of orbital energies are tabulated at the geometries listed in Section B. The majority of diatomic results are for accurate H.F. calculations and are likely to be unchanged by future work. This can not be said for many of the polyatomic cases. Nonetheless, the orbital energies tabulated here will provide the qualitative insight to the molecular shell structure and are presented to that purpose.

Many molecules are missing from the following tables since the orbital energies were presented with the potential energy curves in subsequent sections.

Hartree-Fock Oribital Energies

Homonuclear Diatomic

Orbital	$-\epsilon$				
	H_2 $(^1\Sigma_g^+)$	$Li_2(^1\Sigma_g^+)$	$B_2(^3\Sigma_g^-)$	$C_2(^1\Sigma_g^+)$	$N_2(^1\Sigma_g^+)$
$1\sigma_g$	0.5946[a]	2.4523[a]	7.7039[a]	11.3598[a]	15.6819[b]
$2\sigma_g$		0.1816	0.7057	1.0613	1.4736
$3\sigma_g$					0.6349
$4\sigma_g$					
$5\sigma_g$					
$1\sigma_u$		2.4520	7.7031	11.3575	15.6783
$2\sigma_u$			0.3636	0.5172	0.7780
$3\sigma_u$					
$4\sigma_u$					
$1\Pi_u$			0.3594	0.4579	0.6154
$1\Pi_g$					

Orbital	-ε			
	$O_2(^3\Sigma_g^-)^a$	$O_2^-(^2\Pi_g)^a$	$F_2(^1\Sigma_g^+)^a$	$Na_2(^1\Sigma_g^+)^a$
$1\sigma_g$	20.7296	20.2877	26.4207	40.4763
$2\sigma_g$	1.6488	1.1865	1.8075	2.7957
$3\sigma_g$	0.7357	0.3150	0.7823	1.5179
$4\sigma_g$				0.1698
$5\sigma_g$				
$1\sigma_u$	20.7286	20.2871	26.4204	40.4763
$2\sigma_u$	1.0987	0.7260	1.4763	2.7956
$3\sigma_u$				1.5160
$4\sigma_u$				
$1\Pi_u$	0.7052	0.3062	0.8282	1.5164
$1\Pi_g$	0.5319	0.08375	0.6507	1.5162

a. LMSS (1967)

b. Cade et al (1966)

Hartree-Fock Orbital Energies
Heteropolar Diatomic

Orbital	-ε			
	$LiB\ (^1\Sigma^+)^a$	$LiC(^2\Pi_r)^a$	$LiN(^3\Sigma^-)^a$	$LiO(^2\Pi_i)^a$
1σ	7.6336	11.1940	15.4463	20.4493
2σ	2.4508	2.4435	2.4344	2.4387
3σ	0.4583	0.6218	0.8203	1.0893
4σ	0.1978	0.2462	0.3031	0.4027
5σ				
6σ				
7σ				
1Π		0.2912	0.3774	0.4100
2Π				

Hartree-Fock Orbital Energies

Heteropolar Diatomic

Orbital		$-\epsilon$		
	LiF ($^1\Sigma^+$)[b]	LiNa ($^1\Sigma^+$)[a]	LiCl ($^1\Sigma^+$)[c]	LiBr ($^1\Sigma^+$)[c]
1σ	26.1114	40.4727	104.7244	489.9253
2σ	2.4286	2.7923	10.4502	65.0563
3σ	1.3817	2.4637	7.9166	58.4110
4σ	0.5046	1.5136	2.4762	9.7284
5σ		0.1783	0.9683	7.3362
6σ			0.4037	3.0691
7σ				2.4750
8σ				0.8918
9σ				0.3656
1Π	0.4786	1.5129	7.9164	58.4095
2Π			0.3759	7.3349
3Π				3.0675
4Π				0.3373
1δ				3.0700

Hartree-Fock Orbital Energies

Heteropolar Diatomic

Orbital		$-\epsilon$		
	BeO($^1\Sigma^+$)[b]	BeF($^2\Sigma^+$)[d]	BeF($^2\Pi_r$)[d]	BO($^2\Sigma^+$)[a]
1σ	20.4514	26.2399	26.1924	20.5551
2σ	4.6994	4.7335	4.7370	7.6796
3σ	1.1580	1.5614	1.5251	1.3258
4σ	0.4649	0.6980	0.6556	0.6315
5σ				0.5177
6σ				
7σ				
1Π	0.3943	0.3397	0.6275	0.5197
2Π			0.1688	

Orbital	$-\epsilon$			
	$BO^-(^1\Sigma^+)^a$	BF $(^1\Sigma^+)^b$	CN $(^2\Pi_r)^a$	CO $(^1\Sigma^+)^b$
1σ	20.2287	26.3759	15.6173	20.6643
2σ	7.2777	7.7079	11.3236	11.3597
3σ	1.0150	1.6977	1.2199	1.5210
4σ	0.3339	0.8533	0.5828	0.8038
5σ	0.0737	0.4044		0.5544
6σ				
7σ				
1Π	0.2179	0.7444	0.5194	0.6395
2Π			0.2429	

Orbital	$-\epsilon$			
	$CF(^2\Pi_r)^a$	$CS(^1\Sigma^+)^f$	$NO(^2\Pi_r)^a$	$NaF(^1\Sigma^+)^c$
1σ	26.3744	91.9531	20.6911	40.4664
2σ	11.3405	11.3434	15.7179	26.0627
3σ	1.7081	9.0359	1.5939	2.7872
4σ	0.9086	6.7117	0.9257	1.5131
5σ	0.5480	1.1071	0.6802	1.3205
6σ		0.6921		0.4395
7σ		0.4705		
1Π	0.7449	6.6959	0.6710	1.5107
2Π		0.4634		0.4262

Orbital	$-\epsilon$			
	NaCl($^1\Sigma^+$)^c	NaBr($^1\Sigma^+$)^c	MgO($^1\Sigma^+$)^b	AlF($^1\Sigma^+$)^b
1σ	104.6965	489.9002	49.0580	58.4962
2σ	40.4996	65.0351	20.4374	26.2456
3σ	10.4216	58.3893	3.7949	4.9067
4σ	7.8881	40.4971	2.3092	3.2166
5σ	2.8191	9.7068	1.0785	1.5344
6σ	1.5418	7.3145	0.3177	0.6756
7σ	0.9354	3.0485		0.3365
8σ	0.3639	2.8165		
9σ		1.5374		
10σ		0.8643		
11σ		0.3315		
1Π	7.8879	58.3877	2.3112	3.2158
2Π	1.5419	7.3128	0.3496	0.6157
3Π	0.3474	3.0468		
4Π		1.5383		
5Π		0.3141		
1δ		0.3049		

Orbital	$-\epsilon$			
	SiO($^1\Sigma^+$)^b	PN($^1\Sigma^+$)^b	ClF($^1\Sigma^+$)^g	KF ($^1\Sigma^+$)^c
1σ	68.8027	79.9725	104.9343	133.4936
2σ	20.5239	15.5855	26.3673	26.0335
3σ	6.1539	7.5238	10.6541	14.4498
4σ	4.2559	5.4161	8.1220	11.4796
5σ	1.2787	1.1597	1.6347	1.7108
6σ	0.6103	0.6481	1.1020	1.3047
7σ	0.4345	0.4844	0.7011	0.9103
8σ				0.4090
9σ				
1Π	4.2551	5.4146	8.1174	11.4797
2Π	0.4864	0.4574	0.7237	0.9211
3Π			0.4908	0.4010

Orbital	-ε			
	KCl($^1\Sigma^+$)^c	CaO($^1\Sigma^+$)^b	RbF($^1\Sigma^+$)^c	SrO($^1\Sigma^+$)^b
1σ	133.5253	149.2651	551.4045	583.6000
2σ	104.6734	20.3183	74.9900	80.2804
3σ	14.4822	16.7186	67.8463	72.8900
4σ	11.5124	13.5279	26.0271	20.3036
5σ	10.3995	2.1479	12.0819	13.3588
6σ	7.8649	1.2834	9.4361	10.5848
7σ	1.7436	0.9525	4.6733	5.5703
8σ	0.9650	0.2653	1.4808	1.7823
9σ	0.8990		1.2962	1.1006
10σ	0.3372		0.7634	0.8648
11σ			0.3974	0.2487
1Π	11.5126	13.5270	67.8458	72.8891
2Π	7.8648	1.2556	9.4367	10.5857
3Π	0.9528	0.2617	4.6753	5.5695
4Π	0.3281		0.7737	0.9993
5Π			0.3964	0.2491
1δ			4.6759	5.5695

a. LMSS (1967)

b. McLean and Yoshimine (1967)

c. Matcha (1967)

d. Walker and Richards (1967)

e. Verhaegen and Richards (1967)

f. Richards (1967)

g. Stevens (1967)

Hartree-Fock Orbital Energies

Linear Triatomic

Orbital	-ε			
	LiOH($^1\Sigma^+$)^a	(FHF)$^-$($^1\Sigma_g^+$)^{b,c}	C_3 ($^1\Sigma_g^+$)^{c,d}	(OCN)$^-$ ($^1\Sigma^+$)^b
1σ	20.4042	25.9331	11.2504	20.3177
2σ	2.4381	25.9331	11.2502	15.2657
3σ	1.1644	1.2505	1.1630	11.0716
4σ	0.5470	1.1961	0.8673	1.1851
5σ		0.4676	1.0377	0.9063
6σ		0.2717	0.4324	0.4694
7σ			0.4777	0.2928
1Π	0.3701	0.3165	0.4016	0.3675
2Π		0.2864		0.1349

Orbital		$-\epsilon$		
	FCN($^1\Sigma^+$)^b	(SCN)$^-$ ($^1\Sigma^+$)^b	ClCN($^1\Sigma^+$)^b	CO_2($^1\Sigma_g^+$)^{b,c}
1σ	26.4410	91.7031	104.9336	20.6492
2σ	15.6113	15.3121	15.6063	20.6493
3σ	11.3988	11.0670	11.3479	11.4601
4σ	1.7701	8.7079	10.6579	14.7698
5σ	1.2536	6.3903	8.1244	1.5299
6σ	0.9331	0.9503	1.2717	0.7434
7σ	0.6020	0.7823	1.1949	0.8002
8σ		0.3903	0.7570	
9σ		0.3059	0.5884	
1Π	0.8182	6.3872	8.1218	0.7149
2Π	0.5004	0.2785	0.5983	0.5443
3Π		0.1124	0.4646	

Orbital		$-\epsilon$		
	BeF_2 ($^1\Sigma_g^+$)^{c,e}	SCO ($^1\Sigma^+$)^b	N_3^- ($^1\Sigma_g^+$)^{c,f}	Li_2O ($^1\Sigma_g^+$)^{a,g}
1σ	26.1833	91.9960	15.4687	20.3398
2σ	26.1829	20.6575	15.2198	2.3625
3σ	4.7709	11.4411	15.2200	2.3627
4σ	1.5310	8.9991	0.9674	0.3260
5σ	1.5246	6.6805	1.1950	1.0080
6σ	0.6531	1.5026	0.2810	
7σ	0.6448	1.0941	0.3505	
8σ		0.7796		
9σ		0.6386		
1Π	0.6275	6.6777	0.3991	0.2655
2Π	0.5982	0.6561		
3Π		0.4226		

a. Ritchie and King (1967b)

b. McLean and Yoshimine (1967)

c. Orbitals are alternately gerade and ungerade for σ and vice versa for Π.

d. Clementi and McLean (1962a)

e. Peyerimhoff et al (1967)

f. Peyerimhoff and Buenker (1967)

g. Buenker and Peyerimhoff (1966)

Hartree-Fock Orbital Energies

Non-linear Triatomic

Orbital	$-\epsilon$			
	$FOH(^1A\ )^a$	$NO_2^-(^1A_1)^b$	$O_3\ (^1A_1)^c$	$F_2O\ (^1A_1)^a$
1a	26.3435	20.2663	20.8896	26.3833
2a	20.6866	15.4767	20.7255	20.8043
3a	1.6751	1.2922	1.7233	1.7760
4a	1.3239	0.5764	1.1108	1.2860
5a	0.7864	0.4181	0.8168	0.8084
6a	0.6925	0.1495	0.5657	0.7268
7a	0.6039	0.1267	0.4906	0.6522
8a				
1b	0.7353	20.2666	20.7255	26.3833
2b	0.5484	1.0594	1.4263	1.6443
3b		0.3811	0.7808	0.8273
4b		0.3797	0.7602	0.7945
5b		0.1838	0.5807	0.6811
6b				0.5887

a. Buenker and Peyerimhoff (1966)

b. Pfeiffer (1967)

c. Peyerimhoff and Buenker (1967)

Hartree-Fock Orbital Energies, AH_2

Orbital	$-\epsilon$				
	$BH_2^-(^1A_1)^a$	$CH_2(^1A_1)^b$	$NH_2^-(1A_1)^c$	$H_2O\ (1A_1)^d$	$H_2S\ (1A_1)^e$
$1a_1$	7.3903	11.3120	15.1656	20.5624	92.4785
$2a_1$	0.4481	0.9095	0.7335	1.3615	9.0798
$3a_1$	0.00213	0.3859	0.0913	0.5737	6.6350
$4a_1$					0.9403
$5a_1$					0.4543
$1b_2$	0.2957	0.5712	0.2727	0.7273	6.6362
$2b_2$					0.5307
$1b_1$			0.0205	0.5046	6.6318
$2b_1$					0.3506

a. Geller et al (1967)

b. Krauss (1964)

c. Ritchie and King (1967b)

d. Ritchie and King (1967a)

e. Moccia (1964c)

Hartree-Fock Orbital Energies
Linear Tetratomics

Orbital	$-\varepsilon$		
	HCCH$(^1\Sigma_g^+)$[a]	HCCH$(^1\Sigma_g^+)$[b]	NCCN$(^1\Sigma_g^+)$[a]
$1\sigma_g$	11.2440	11.2585	15.6576
$2\sigma_g$	1.0296	1.0406	11.3554
$3\sigma_g$	0.6828	0.6835	1.3048
$4\sigma_g$			0.9868
$5\sigma_g$			0.6279
$1\sigma_u$	11.2403	11.2548	15.6576
$2\sigma_u$	0.7698	0.7658	11.3543
$3\sigma_u$			1.2797
$4\sigma_u$			0.6438
$1\Pi_u$	0.4103	0.4131	0.6035
$1\Pi_g$			0.5004

a. McLean and Yoshimine (1967)

b. Buenker et al (1967)

Hartree-Fock Orbital Energies
Linear Tetratomics

Orbital	$-\varepsilon$		
	LiCCH$(^1\Sigma^+)$	FCCH $(^1\Sigma^+)$	ClCCH $(^1\Sigma^+)$
1σ	11.1454	26.3837	104.8889
2σ	11.1250	11.3410	11.2984
3σ	2.4519	11.2470	11.2495
4σ	0.9404	1.7071	10.6136
5σ	0.6596	1.0529	8.0802
6σ	0.4207	0.8632	1.1941
7σ		0.7281	1.0198
8σ			0.7513
9σ			0.6722
1Π	0.3270	0.7617	8.0778
2Π		0.4196	0.5503
3Π			0.3919

McLean and Yoshimine (1967)

Hartree-Fock Orbital Energies, AH_3

Orbital	$-\epsilon$			
	BeH_3^- $(^1A_1')^b$	BH_3 $(^1A_1')^b$	CH_3 $(^2A_1'')^c$	CH_3^- $(^1A_1')^d$
$1a_1$	4.4740	7.6173	11.2041	10.8872
$2a_1$	0.2808	0.6943	0.9155	0.6153
$3a_1$			0.3723	-0.0077
1e	0.1530	0.4833	0.5834	0.2717

Orbital	$-\epsilon$	
	NH_3 $(^1A_1)^e$	PH_3 $(^1A_1)^f$
$1a_1$	15.4876	80.1650
$2a_1$	1.1935	7.4798
$3a_1$	0.3859	5.2572
$4a_1$		0.8380
$5a_1$		0.3671
1e	0.5967	5.2587
2e		0.4778

a. Both C_{3v} and D_{3h} symmetries are represented; for the D_{3h} orbitals the appropriate primes must be added.

b. Peyerimhoff et al (1966)

c. Hackmeyer and Whitten (1967)

d. Kari and Csizmadia (1967b)

e. Rajagopal (1965)

f. Moccia (1964b)

Hartree-Fock Orbital Energies, AH_4

Orbital	$-\epsilon$	
	BH_4^- $(^1A_1)^a$	CH_4 $(^1A_1)^b$
$1a_1$	7.2676	11.2216
$2a_1$	0.4434	0.9295
$1t_2$	0.1765	0.5348

a. Krauss (1964)

b. Ritchie and King (1967a)

J. Energy and Properties as a Function of the Internuclear Distance: Introduction

Results are presented for a series of diatomic molecules calculated to high accuracy in the H.F. approximation. These studies were carried out at the IBM laboratory at San Jose but similar results or capability exist at other laboratories (e.g. LMSS or Argonne). Since these results were available they are presented as a witness to one area of calculational capability.

Units: μ 10^{-18} esu cm, θ 10^{-26} esu cm^2, q 10^{15} esu/cm^3,

X_L 10^{-5} erg/gauss^2 mole

LiF ($1\sigma^2$ $2\sigma^2$ $3\sigma^2$ $4\sigma^2$ $1\Pi^4$, $^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.45	106.9569	5.277	4.229	-0.040	-2.879	-2.061
2.65	106.9819	5.742	4.921	-0.094	-1.894	-2.208
2.7877	106.9894	6.062	5.408	-0.112	-1.291	-2.316
2.8377[a]	106.9916	6.295	5.769	-0.118	-0.869	-2.397
2.9877	106.9916	6.529	6.138	-0.121	-0.536	-2.481
3.20	106.9869	7.033	6.950	-0.118	0.115	-2.669
3.55	106.9713	7.885	8.384	-0.102	0.337	-3.008

a. $-\epsilon$: 26.1114, 2.4286, 1.3817, 0.5046, 0.4786

McLean and Yoshimine (1967)

LiCl ($1\sigma^2 \rightarrow 6\sigma^2\ 1\Pi^4\ 2\Pi^4\ ,\ {}^1\Sigma^+$)

R	-E	μ^a	q_1	q_2
3.35	467.0387	6.167		
3.60	467.0517	6.709	-0.0574	-0.514
3.66	467.0531	6.843		
3.723	467.0541	6.984		
3.825^b	467.0547	7.218	-0.0679	0.389
3.91	467.0543	7.415	-0.0700	0.687
4.00	467.0533	7.626		
4.10	467.0515	7.864	-0.0719	1.271
4.55	467.0381	8.966		

a. $\mu_\nu = 7.218 + 0.0753\ (\nu+1/2) + 0.0002\ (\nu+1/2)^2$;

$\mu_\nu\ (\text{exp}) = 7.0853 + 0.0864\ (\nu+1/2) + 0.0006\ (\nu+1/2)^2$

b. $-\varepsilon$: 104.7244, 10.4502, 7.9166, 2.4762, 0.9683, 0.4037, 7.9164, 0.3759.

Matcha (1967)

BeO ($1\sigma^2 2\sigma^2 3\sigma^2 4\sigma^2 1\Pi^4, {}^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
1.80	89.18098	5.745	3.476	-6.395	0.489	-2.030
2.10	89.39983	6.508	4.838	-5.101	-0.001	-2.313
2.35	89.45122	7.138	5.962	-3.478	-0.140	-2.570
2.4377^a	89.4541[illegible]	7.353	6.354	-2.824	-0.161	-2.665
2.50	89.45299	7.502	6.631	-2.329	-0.170	-2.734
2.75	89.43088	8.037	7.693	0.019	-0.173	-3.020
3.10	89.37967	8.223	8.649	5.523	-0.124	-3.473
3.80	89.30961	5.380	7.110	17.81	-0.024	-4.737
5.50	89.26894	1.430	4.360	24.43	0.005	-3.489

a. $-\varepsilon$: 20.4514, 4.6994, 1.1580, 0.4649, 0.3943

McLean and Yoshimine (1967)

BF ($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4,\ {}^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.00	124.1090	-1.931	-4.312	-1.791	-1.189	-3.077
2.10	124.1413	-1.689	-4.393	-1.834	-0.285	-3.192
2.1925	124.1582	-1.448	-4.447	-1.835	0.498	-3.301
2.391[a]	124.1671	-0.883	-4.482	-1.755	1.980	-3.541
2.5775	124.1559	-0.293	-4.401	-1.624	3.108	-3.775
2.77	124.1352	0.371	-4.193	-1.463	4.005	-4.027
2.9625	124.1107	1.083	-3.855	-1.297	4.653	-4.289

a. $-\epsilon$: 26.3759, 7.7079, 1.6977, 0.8533, 0.4044, 0.7444

McLean and Yoshimine (1967)

CO ($1\sigma^2 \rightarrow 5\sigma^2 1\Pi^4, {}^1\Sigma^+$)

R	-E	μ	ϵ	q_1	q_2	X_L
1.80	112.7025	-0.546	-2.563	-3.574	-4.456	-2.740
1.898	112.7576	-0.319	-2.468	-3.721	-3.887	-2.859
2.015	112.7869	-0.029	-2.343	-3.798	-3.141	-3.007
2.132[a]	112.7891	0.280	-2.204	-3.808	-2.348	-3.159
2.249	112.7733	0.602	-2.048	-3.778	-1.522	-3.316
2.366	112.7461	0.934	-1.876	-3.729	-0.666	-3.479
2.483	112.7119	1.271	-1.690	-3.679	0.226	-3.647

a. $-\epsilon$: 20.6643, 11.3597, 1.5210, 0.8038, 0.5544, 0.6395

McLean and Yoshimine (1967)

NaF ($1\sigma^2 \rightarrow 6\sigma^2\ 1\Pi^4\ 2\Pi^4, {}^1\Sigma^+$)

R	-E	μ^a	q_1	q_2
3.10	261.3503	7.222		
3.36	261.3728	7.754		
3.50	261.3773	8.051		
3.56	261.3782	8.180	-1.334	-0.538
3.628[b]		8.35	-1.249	-0.355
3.71	261.3781	8.510	-1.158	-0.155
3.7794	261.3773	8.510	-1.088	-0.0044
3.90	261.3750	8.941		
4.35	261.3603	10.02		

a. $\mu_\nu = 8.337 + 0.610\ (\nu+1/2) + 0.002\ (\nu+1/2)^2$;

μ_ν (exp) $= 8.1235 + 0.0644\ (\nu+1/2) + 0.0004\ (\nu+1/2)^2$

b. $-\epsilon$: 40.4665, 26.0627, 2.7872, 1.5131, 1.3205,
0.4395, 1.5107, 0.4262

Matcha (1967)

NaCl ($1\sigma^2 \rightarrow 8\sigma^2\ 1\Pi^4\ 3\Pi^4, {}^1\Sigma^+$)

R	-E	μ^a	q_1	q_2
3.70	621.4167	7.603		
4.15	621.4521	8.444	-1.025	-0.263
4.30	621.4559	8.754	-0.919	0.187
4.40	621.4571	8.968		
4.4609	621.4574	9.101		
4.485[b]	621.4574	9.101	-0.805	0.680
4.60	621.4570	9.412	-0.743	0.953
4.75	621.4553	9.758		
5.00	621.4505	10.356		

a. $\mu_\nu = 9.154 + 0.0580\ (\ \nu + 1/2\ ) + 0.0003\ (\ \nu\ 1/2\ )^2$;

μ_ν (exp)$= 8.9734 + 0.0570\ (\nu+1/2) + 0.0005\ (\nu+1/2)^2$

b. $-\epsilon$: 104.6965, 40.4996, 10.4216, 7.881, 2.8191,
1.5418, 0.9354, 0.3639; 7.8879, 1.5419, 0.3474

Matcha (1967)

MgO ($1\sigma^2 \rightarrow 6\sigma^2 \; 1\Pi^4 \; 2\Pi^4$, $^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.50	274.2087	8.217	0.681	-0.746	0.379	-4.731
3.00	274.3653	9.250	0.361	-0.756	2.545	-5.808
3.20	274.3754	9.082	0.315	-0.594	4.859	-6.317
3.3052[a]	274.3751	8.842	0.221	-0.517	6.321	-6.603
3.40	274.3732	8.580	0.118	-0.458	7.666	-6.867
3.60	274.3653	7.868	-0.093	-0.359	10.50	-7.456
4.10	274.3405	6.041	-0.217	-0.209	16.04	-9.050
5.10	274.3073	3.512	-0.662	-0.072	21.50	-12.70

a. $-\epsilon$: -49.0580, -20.4374, -3.7949, -2.3092, -1.0785, -0.3177, -2.3112, -0.3496.

McLean and Yoshimine (1967)

AlF ($1\sigma^2 \rightarrow 7\sigma^2 \; 1\Pi^4 \; 2\Pi^4$, $^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.60	341.4127	-0.030	-5.944	-6.415	-2.312	-5.938
2.85	341.4687	0.568	-6.322	-4.994	-0.843	-6.535
3.05	341.4824	1.114	-6.608	-4.141	0.133	-7.045
3.126[a]	341.4832	1.337	-6.713	-3.867	0.456	-7.247
3.25	341.4811	1.717	-6.876	-3.465	0.928	-7.586
3.45	341.4718	2.369	-7.126	-2.920	1.551	-8.157
3.70	341.4544	3.240	-7.418	-2.375	2.116	-8.917

a. $-\epsilon$: -58.4962, -26.2456, -4.9067, -3.2166, -1.5344, -0.6756, -0.3365, -3.2158, -0.6156

McLean and Yoshimine (1967)

SiO ($1\sigma^2 \rightarrow 7\sigma,^2\ 1\Pi^4\ \ 2\Pi^4,\ ^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.304	363.6988	2.280	-5.123	-10.97	-5.082	-5.149
2.50	363.8085	2.745	-5.124	-9.427	-4.249	-5.574
2.604	363.8365	3.010	-5.153	-8.752	-3.748	-5.812
2.75[a]	363.8523	3.397	-5.219	-7.952	-3.006	-6.160
2.854	363.8516	3.681	-5.282	-7.473	-2.458	-6.419
3.104	363.8250	4.378	-5.484	-6.584	-1.085	-7.075
3.404	363.7693	5.204	-5.831	-5.945	0.732	-7.925

a. $-\epsilon$: -68.8027, -20.5239, -6.1539, -4.2559,
-1.2787, -0.6103, -0.4345, -4.2551, -0.4864

McLean and Yoshimine (1967)

PN ($1\sigma^2 \rightarrow\ 7\sigma^2\ \ 1\Pi^4\ \ 2\Pi\ ^4,\ ^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.268	395.0243	3.238	-3.803	-11.66	-5.376	-5.053
2.45	395.1376	3.246	-3.338	-9.758	-5.270	-5.437
2.568	395.1725	3.244	-3.055	-8.677	-5.116	-5.699
2.67[a]	395.1857	3.241	-2.818	-7.828	-4.953	-5.932
2.818	395.1848	3.232	-2.487	-6.720	-4.686	-6.283
3.068	395.1497	3.211	-1.958	-5.112	-4.204	-6.903
3.368	395.0800	3.178	-1.375	-3.477	-3.670	-7.705

a. $-\epsilon$: -79.9725, -15.5855, -7.5238, -5.4161, -1.1597,
-0.6481, -0.4844, -5.4146, -0.4574

McLean and Yoshimine (1967)

CaO ($1\sigma^2 \rightarrow 8\sigma^2 \; 1\Pi^4 \rightarrow 3\Pi^4, \; {}^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
2.9912	751.4896	9.366	-7.667	-0.452	-1.306	-7.602
3.1412	751.5243	10.022	-7.596	-0.817	-1.646	-8.050
3.2912	751.5415	10.552	-7.557	-0.909	-1.686	-8.523
3.4412[a]	751.5478	10.946	-7.578	-0.846	-1.432	-9.023
3.6412	751.5435	11.203	-7.756	-0.628	-0.530	-9.737
3.8912	751.5264	10.652	-8.384	-0.264	2.346	-10.74
4.1412	751.5065	8.241	-8.692	-0.219	2.292	-11.95

a. $-\epsilon$: -149.2651, -20.3183, -16.7186, -13.5279, -2.1479, -1.2834, -0.9525, -0.2653, -13.5270, -1.2556, -0.2617

McLean and Yoshimine (1967)

SrO ($1\sigma^2 \rightarrow 11\sigma^2 \; 1\Pi^4 \rightarrow 5\Pi^4 \; 1\delta^4, \; {}^1\Sigma^+$)

R	-E	μ	θ	q_1	q_2	X_L
3.10	3206.1729	7.643	-12.46	2.372	0.715	-9.820
3.25	3206.2059	8.439	-13.01	0.878	-0.150	-10.36
3.40	3206.2242	9.185	-13.52	-0.055	-0.840	-10.94
3.525	3206.2306	9.763	-13.93	-0.598	-1.263	-11.44
3.6283[a]	3206.2311	10.207	-14.24	-0.805	-1.500	-11.87
3.78	3206.2262	10.798	-14.68	-0.911	-1.638	-12.52
4.10	3206.2007	11.663	-15.55	-0.618	-0.727	-14.02

a. $-\epsilon$: 583.6000, 80.2804, 72.8900, 20.3036, 13.3588, 10.5848, 5.5703, 1.7823, 1.1006, 0.8649, 0.2487, 72.8891, 10.5857, 5.5695, 0.9993, 0.2491, 5.5695.

McLean and Yoshimine (1967)

K. Potential Energy Curves: Introduction

Examples of accurate H.F., extended H.F., SOC, and VB techniques are tabulated below. Both distances and energies are given in atomic units. In a number of instances figures were lifted from the original papers to illustrate the different techniques.

A very few polyatomic curves are included. The VB calculation of BeH_2 and the diatomic VB calculations show proper asymptotic dependence. Since they have also been used to obtain a number of the excited states it was felt that the VB calculations should be included even when more accurate surfaces may exist for a given state as in He_2^+.

Hartree-Fock results are included near equilibrium for stable polyatomic species including the orbital energies. One example of a reaction surface is included which also exhibits proper asymptotic dependence even though it is an approximate H.F. calculation.

In this section both R and E are in atomic units.

Potential Energy Curves of Hydrogen

R	State			
	$X^1\Sigma_g^+$	$b^3\Sigma_u^+$	$B^1\Sigma_u^+$	$C^1\Pi_u$
1.0	-1.1245385	-0.6215227	-0.5812963	-0.5724911
1.5	-1.1728537	-0.8096095	-0.7200327	-0.7004638
2.0	-1.1381312	-0.8970636	-0.7520541	-0.7182230
2.5	-1.0939273	-0.9454463		-0.7071783
3.0	-1.0573118	-0.9720104	-0.7524996	-0.6892372
4.0	-1.0163689	-0.9933781	-0.7354677	-0.6566106
5.0	-1.0037626	-0.9986849	-0.7147955	-0.6369889
6.0	-1.0008150	-0.9998125	-0.6948364	-0.6283423
∞	-1.0	-1.0	-0.625	-0.625

$X^1\Sigma_g^+$, $b^3\Sigma_u^+$, $C^1\Pi_u$: Kolos and Wolniewicz (1965c)

$B^1\Sigma_u^+$: Kolos and Wolniewicz (1966a)

Potential Energy Curves of HeH^+

R	Hartree-Fock	Correlated	ΔE
1.2	-2.917390	-2.9620088	0.044619
1.4	-2.932594	-2.9779726	0.045379
1.6	-2.930450	-2.9762475	0.045797
1.8	-2.921683	-2.9675157	0.045833
2.5	-2.888782		
3.5	-2.868619		
4.5	-2.863752		
∞	-2.8616799	-2.9037244	0.0420445

a. Peyerimhoff (1965)

b. Wolniewicz (1965)

Energy As A Function of the Internuclear Distance

HeH

R	E ($X^2\Sigma^+$)	E ($^2\Pi$)	E ($^2\Sigma^+$)
1.0	-3.00243	-3.00243	-3.02196
1.25	-3.06456	-3.06456	-3.08194
1.5	-3.06983	-3.06983	-3.08304
2.0	-3.04399	-3.04399	-3.04801
3.0	-3.01159	-3.01159	-3.01045
4.0	-3.00382	-3.00382	-3.00321
6.0	-3.00112	-3.00112	
10.0			-3.00082

Michels and Harris (1963)

	LiH ($1\sigma^2\ 2\sigma^2$, $^1\Sigma^+$)	BeH($1\sigma^2\ 2\sigma^2\ 3\sigma$, $^2\Sigma^+$)
R	-E	
2.00	7.91322	15.11955
2.20	7.94594	15.14217
2.40	7.96663	15.15170
2.528[b]		15.15313
2.60	7.97887	15.15274
2.80	7.98517	15.14832
3.015[a]	7.98731	
3.00		15.14045
3.20	7.98646	
3.30		15.12496
3.60	7.97932	
3.70		15.10139
4.00	7.96824	15.08338

a. LiH, -ε : 2.4452, 0.3017

b. BeH, -ε : 4.7064, 0.4732, 0.3126

Cade and Huo (1967a)

	BH ($1\sigma^2\ 2\sigma^2\ 3\sigma^2$, $^1\Sigma^+$)	CH($1\sigma^2\ 2\sigma^2\ 3\sigma^2\ 1\Pi$, $^2\Pi_r$)
R	-E	
1.60		38.21353
1.70	25.05938	38.24259
2.00	25.11803	38.27826
2.086[b]		38.27958
2.20	25.13016	38.27767
2.305[a]	25.13147	
2.40	25.13056	38.26755
2.60	25.12408	
2.70		38.24395
2.90	25.10763	
3.20	25.08779	
3.50	25.06724	38.17233

a. BH, -ε : 7.6842, 0.6524, 0.3479

b. CH, -ε : 11.3135, 0.8349, 0.4563, 0.4145

Cade and Huo (1967a)

Energy As A Function of the Internuclear Distance

R	NH ($1\sigma^2\ 2\sigma^2\ 3\sigma^2\ 1\Pi^2$, $^3\Sigma^-$)	OH ($1\sigma^2\ 2\sigma^2\ 3\sigma^2\ 1\Pi^3$, $^2\Pi_i$)
	-E	
1.40		75.34382
1.45	54.88846	
1.50		75.38378
1.55	54.92947	
1.70	54.96392	75.41829
1.795[b]		75.42127
1.90	54.97826	75.41837
1.923[a]	54.97838	
2.10	54.97254	75.40163
2.30	54.95667	
2.40		75.36367
2.60	54.92492	75.33582
2.80		75.30822
3.00	54.87971	

a. NH, $-\epsilon$: 15.6082, 1.0480, 0.5535, 0.5377

b. OH, $-\epsilon$: 20.6165, 1.3138, 0.6662, 0.5731

Cade and Huo (1967a)

HF ($1\sigma^2 2\sigma^2\ 3\sigma^2\ 1\Pi^4$, $^1\Sigma^+$)

R	-E
1.325	99.93645
1.37	100.01003
1.427	100.03280
1.50	100.05264
1.65	100.06996
1.696[a]	100.07077
1.80	100.06731
1.933	100.05540
2.10	100.03357
2.243	100.01183
2.40	99.98676

a. $-\epsilon$: 26.2939, 1.6079, 0.7759, 0.6521

Cade and Huo (1967a)

Energy As A Function of the Internuclear Distance

R	NaH ($1\sigma^2 \rightarrow 4\sigma^2\ 1\Pi^4$, $^1\Sigma^+$)	MgH($1\sigma^2 \rightarrow 4\sigma^2\ 5\sigma\ \ 1\Pi^4$, $^2\Sigma^+$)
	-E	
2.00	162.2012	199.9699
2.20	162.2651	200.0448
2.50	162.3285	200.1112
2.75	162.3601	
2.80		200.1433
3.00	162.3788	
3.10		200.1553
3.20	162.3872	
3.259[b]		200.1566
3.40	162.3915	200.1557
3.566[a]	162.3928	
3.70	162.3927	
3.80		200.1467
4.15		200.1344
4.25	162.3854	
4.50		200.1206
5.00	162.3675	

a. NaH, $-\epsilon$: 40.4662, 2.7869, 1.5077, 0.2752, 1.5090

b. MgH, $-\epsilon$: 49.0450, 3.7818, 2.2988, 0.3909, 0.2594, 2.3005

Cade and Huo (1967b)

Energy As A Function of the Internuclear Distance

	AlH($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4$, $^1\Sigma^+$)	SiH($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4\ 2\Pi$, $^2\Pi_r$)
R	-E	
2.00	242.2913	289.3033
2.20	242.3671	289.3715
2.40	242.4141	289.4099
2.60	242.4418	289.4290
2.80	242.4565	
2.861[b]		289.4362
3.00	242.4627	289.4347
3.113[a]	242.4634	
3.20	242.4630	289.4286
3.40	242.4597	289.4194
3.60		289.4085
3.80	242.4465	
4.00		289.3845
4.20	242.4296	
4.60	242.4119	

a. AlH, $-\epsilon$: 58.4894, 4.8999, 3.2082, 0.4966, 0.2883, 3.2090

b. SiH, $-\epsilon$: 68.8064, 6.1512, 4.2514 0.6299, 0.3776, 4.2520

Cade and Huo (1967b)

Energy As A Function of the Internuclear Distance

	PH($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4\ 2\Pi^2,\ ^3\Sigma^-$)	SH($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4\ 2\Pi^3,\ ^2\Pi_i$)
R	-E	
1.80	341.0922	397.9439
2.00	341.1970	398.0360
2.10	341.2304	398.0633
2.20	341.2546	398.0818
2.40	341.2828	398.0996
2.512		398.1017
2.60	341.2928	
2.668[a]	341.2934	
2.70		398.0972
2.80	341.2916	
3.20	341.2715	398.0604
3.40	341.2573	398.0418
3.60	341.2420	398.0229

a. PH, $-\epsilon$: 79.9631. 7.5050, 5.3961, 0.7738, 0.4583, 5.3960, 0.3785

b. SH, $-\epsilon$: 91.9840, 8.9855, 6.6657. 0.9411, 0.5444, 6.6645, 0.4122

Cade and Huo (1967b)

Energy As A Function of the Internuclear Distance

R	HCl ($1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4\ 2\Pi^4\ ,\ ^1\Sigma^+$) -E
1.80	459.9902
1.90	460.0365
2.00	460.0685
2.10	460.0896
2.20	460.1024
2.389[a]	460.1104
2.50	460.1083
2.80	460.0884
3.00	460.0689
3.20	460.0475
3.60	460.0040

a. $-\epsilon$: 104.8479, 10.5739, 8.0417, 1.1188, 0.6284. 8.0391, 0.4765

Cade and Huo (1967b)

Energy As A Function of the Internuclear Distance

$NeH^+(1\sigma^2\ 2\sigma^2\ 3\sigma^2\ 1\pi^4,\ {}^1\Sigma^+)$

R	E
1.35	-128.53942
1.5	-128.59568
1.6	-128.61469
1.7	-128.62448
1.8	-128.62812
1.83[a]	-128.62836
1.9	-128.62773
2.0	-128.62479
2.1	-128.62026
2.2	-128.61492
2.4	-128.60330
2.7	-128.58728
3.0	-128.57470
3.5	-128.56128
4.0	-128.55418
4.5	-128.55089

[a] Orbital energies: -33.3381, -2.49750, -1.45857, -1.38468.
Peyerimhoff (1965)

Potential Energy Curves of He_2^+

R	-E				
	$X^2\Sigma_u^+$	$^2\Sigma_u^{+*}$	$^2\Sigma_u^{+**}$	$^2\Sigma_u^{+***}$	$^2\Sigma_u^{+****}$
0.5	2.2926	1.8737	1.3044	0.4765	-0.6339
0.75	3.9033	3.3448	2.9825	1.9891	1.6240
1.0	4.5001	3.8088	3.4912	2.6971	2.5863
1.25	4.7736	3.9256	3.6355	3.2412	2.9834
1.5	4.9014	3.9118	3.6653	3.5470	3.5426
2.0	4.9701	3.9068	3.8281	3.6902	3.6817
2.05	4.9706	3.9089	3.8431	3.7037	3.6916
3.0	4.9356	4.0124	3.9667	3.9259	3.7568
4.0	4.9056	4.0944	4.0317	4.0201	3.8382
5.0	4.8940	4.1488	4.0730	4.0575	3.9181
6.0	4.8902	4.1768	4.0986	4.0779	3.9833
10.0	4.88849	4.1876	4.1471	4.1119	4.0964
12.0	4.88846	4.1806	4.1549	4.1198	4.1105

Michels (1967)

R	-E				
	$^2\Sigma_g^+$	$^2\Sigma_g^{+*}$	$^2\Sigma_g^{+**}$	$^2\Sigma_g^{+***}$	$^2\Sigma_g^{+****}$
0.5	2.1552	1.9677		1.0703	-0.6868
0.75	3.6223	3.3267		2.0920	1.8464
1.0	4.0108	3.6906		3.0705	2.4336
1.25	4.0779	3.7814		3.7144	3.0621
1.5	4.1818	4.0451	3.7506	3.7013	3.4179
2.0	4.5828	3.9912	3.8081	3.7496	3.6161
2.05	4.6065	3.9895	3.8149	3.7673	3.6209
3.0	4.8214	4.0447	3.8498	3.9439	3.7513
4.0	4.8713	4.1282	4.0285	4.0173	3.8283
5.0	4.8839	4.1760	4.0682	4.0546	3.9022
6.0	4.8874	4.1969	4.0914	4.0771	3.9659
8.0	4.8885	4.2042	4.1180	4.1022	4.0499
10.0	4.8886	4.1970	4.1332	4.1162	4.0895
12.0	4.8885	4.1881	4.1419	4.1249	4.1061

Michels (1967)

R	-E			
	$^2\Pi_g$	$^2\Pi_g^*$	$^2\Pi_u$	$^2\Pi_u^*$
0.5	2.0411	2.0411	2.3282	1.9999
0.75	3.3222	3.0208	3.6096	3.2905
1.0	3.7037	3.4048	3.9775	3.6660
1.2	3.8054	3.5080	4.0636	3.7546
1.5	3.8392	3.5860	4.0751	3.7743
1.75	3.8361	3.7561	4.0560	3.7725
2.0	3.8735	3.8295	4.0413	3.7782
3.0	4.0449	3.9079	4.0683	3.8933
4.0	4.0943	3.9882	4.1053	3.9798
5.0	4.1142	4.0370	4.1218	4.0289
6.0	4.1227	4.0672	4.1287	4.0595
8.0	4.1277	4.0992	4.1322	4.0928
10.0	4.1278	4.1132	4.1314	4.1080
12.0	4.1276	4.1190	4.1303	4.1152

Michels (1967)

Energy As A Function of the Internuclear Distance

Li_2, $X^1\Sigma_g^+$

R	E(SCF)	E(ODC)[a]	E(OVC)[b]
4.0	-14.852990	-14.859537	-14.884424
4.5		-14.873465	-14.895621
4.75	-14.869718	-14.877403	-14.898108
4.77			
5.0		-14.879630	-14.898849
5.25		-14.881261	-14.898876
5.37	-14.871796		
5.5	-14.871484		
6.0	-14.868655	-14.881046	-14.893667
8.0		-14.871553	-14.877459
12.0		-14.865660	-14.866116

a. ODC- Optimized Double Configurations.

b. OVC- Optimized Valence Configurations.

Energy As A Function of Internuclear Distance

$N_2(1\sigma_g{}^2 1\sigma_u{}^2 2\sigma_g{}^2 2\sigma_u{}^2 3\sigma_g{}^2 1\pi_u{}^4.\ X^1\Sigma_g^+)$

R	-E	$-\epsilon\ 2\sigma_g$	$-\epsilon\ 2\sigma_u$	$-\epsilon\ 3\sigma_g$	$-\epsilon\ 1\pi_u$
1.65	108.7887	1.6292	0.7002	0.6534	0.7355
1.82	108.9489	1.5699	0.7331	0.6459	0.6798
1.85	108.9635	1.5584	0.7387	0.6459	0.6709
1.905	108.9825	1.5372	0.7489	0.6422	0.6558
1.95	108.9914	1.5194	0.7570	0.6401	0.6438
2.0132	108.9956	1.4953	0.7687	0.6379	0.6285
2.05	108.9944	1.4803	0.7747	0.6355	0.6194
2.068	108.9928	1.4736	0.7780	0.6350	0.6154
2.0741	108.9922	1.4712	0.7790	0.6346	0.6140
2.09	108.9904	1.4651	0.7818	0.6338	0.6106
2.15	108.9799	1.4421	0.7918	0.6306	0.5974
2.20	108.9679	1.4235	0.8001	0.6280	0.5872
2.292	108.9397	1.3902	0.8149	0.6226	0.5693
2.34	108.9226	1.3736	0.8224	0.6196	0.5606
2.45	108.8792	1.3376	0.8393	0.6123	0.5418
2.90	108.6828	1.2217	0.9009	0.5759	0.4824

Cade et al (1966)

Potential Energy of F_2

R	-E		
	Hartree-Fock	Extended Hartree-Fock (OVC)	
		OVC[a]	OVC[b]
1.8	198.41814	198.44543	198.45263
2.2	198.73236	198.77720	
2.68	198.76825	198.84853	198.85464
3.0	198.73302	198.84551	
3.5	198.66024	198.83094	198.83589
6.0	198.45753	198.81799	198.81799
∞		198.81784	198.81784

a. Correlate only $3\sigma_g$

b. Additional $2\sigma_g$, $2\sigma_u$, $3\sigma_g$, $1\Pi_u$, $1\Pi_g$ excitations into $3\sigma_u^2$

Das and Wahl (1967)

Potential Energy of F_2^-

R	E^a			
	$^2\Sigma_u^+$	$^2\Pi_g$	$^2\Pi_u$	$^2\Sigma_g^+$
2.68	0.0346			
3.2	-0.0516	0.0673	0.1529	0.2027
3.6	-0.0609	0.0209	0.0751	0.1132
4.0	-0.0552	0.0037	0.0386	0.0662
4.4	-0.0457			
4.8	-0.0365			
5.2	-0.0288			
5.6	-0.0227			
6.0	-0.0179			
6.6	-0.0129			
7.2	-0.0096			
∞	0	0	0	0

a. Hartree-Fock

Gilbert and Wahl (1967c)

Potential Energy of Ne_2^+

R	E^a			
	$^2\Sigma_u^+$	$^2\Pi_g$	$^2\Pi_u$	$^2\Sigma_g^+$
2.5	0.0290			
2.8	-0.0417			
3.0	-0.0574	0.0489	0.1174	0.1961
3.2	-0.0607	0.0232	0.0736	0.1398
3.5	-0.0549	0.0049	0.0367	0.0863
4.0	-0.0378			
5.0	-0.0143			
∞	0	0	0	0

a. Hartree-Fock

Gilbert and Wahl (1967a)

Potential Energy of Ar_2^+

R	E^a			
	$^2\Sigma_u^+$	$^2\Pi_g$	$^2\Pi_u$	$^2\Sigma_g^+$
3.8	0.0015			
4.0	-0.0230			
4.2	-0.0369	0.0600	0.1188	0.1901
4.3	-0.0411			
4.5	-0.0453			
4.6	-0.0458	0.0228	0.0599	0.1154
4.7	-0.0458			
5.0	-0.0424	0.0065	0.0298	0.0712
5.5	-0.0328			
∞	0	0	0	0

a. Hartree-Fock

Gilbert and Wahl (1967a)

Potential Energy of Cl_2 , $^1\Sigma_g^+$

R	3.6	3.8	3.9	4.2
-E	918.9823	918.9871	918.9858	918.9727
		-E		
$1\sigma_g$	104.8909	104.8976	104.9006	104.9082
$2\sigma_g$	10.6172	10.6216	10.6237	10.6292
$3\sigma_g$	8.0861	8.0901	8.0921	8.0972
$4\sigma_g$	1.2506	1.2162	1.2017	1.1673
$5\sigma_g$	.6153	.5964	.5868	.5583
$1\sigma_u$	104.8909	104.8976	104.9006	104.9082
$2\sigma_u$	10.6170	10.6215	10.6236	10.6291
$3\sigma_u$	8.0858	8.0899	8.0919	8.0971
$4\sigma_u$	1.0067	1.0197	1.0256	1.0407
$1\Pi_u$	8.0810	8.0856	8.0877	8.0932
$2\Pi_u$	.5831	.5680	.5616	.5463

R	3.6	3.8	3.9	4.2
$1\ \Pi_g$	8.0810	8.0856	8.0877	8.0933
$2\ \Pi_g$	.4358	.4480	.4534	.4668

Gilbert and Wahl (1967c)

Potential Energy of Cl_2^-

R	$^2\Sigma_u^+$	$^2\Pi_g$	$^2\Pi_u$	$^2\Sigma_g^+$
3.8	0.0346	0.1955	0.3104	0.3674
4.0	0.0017	0.1402	0.2357	0.2915
4.5	-0.0387	0.0577	0.1181	0.1646
4.7	-0.0444			
5.0[a]	-0.0472	0.0213	0.0598	0.0946
5.1	-0.0471	0.0171	0.0523	0.0849
5.5	-0.0435			
6.0	-0.0361	0.0008	0.0168	0.0335
7.0	-0.0721	-0.0010	0.0057	0.0126
8.0	-0.0131	-0.0008	0.0020	0.0042
9.0	-0.0075	-0.0001	0.0011	0.0011
b	0	0	0	0

a. $-\epsilon$: 104.6033, 10.3252, 7.7930, 0.8380, 0.2542,
104.6033, 10.3252, 7.7930, 0.7904, 0.1915,
7.7913, 0.2492, 7.7913, 0.2124

b. E (Cl_2^-) = -919.0204

c. Hartree-Fock
Gilbert and Wahl (1967a,b)

Potential Energy curves of He Ne $^+$

R	-E		
	$^2\Sigma^+$	$^2\Pi$	$^2\Sigma^{+*}$
0.5		117.2660	
1.0		127.2128	
1.5	129.6685	129.1541	128.9913
2.0	130.0612	129.8814	129.4127
3.0	130.2145	130.1984	129.7877
4.0	130.2274	130.2245	129.8182
5.0	130.2273	130.2254	129.8128
6.0		130.2247	

Michels (1967)

Potential Energy of NaLi

R	-E	
	Hartree-Fock	Extended Hartree-Fock
4.0	169.26357	169.28938
5.0	169.28917	169.31231
5.5	169.29186	169.31422
6.0	169.29073	169.31286

Bertoncini and Wahl (1967)

Potential Energy of NaF

R	-E	
	Hartree-Fock	Extended Hartree-Fock (OVC)
3.1	261.3495	261.3710
3.5	261.3773	261.3991
4.0	261.3722	261.3951
4.5	261.3561	261.3797
6.0	261.3030	261.3262
12.0		261.2659
∞		261.2662

Das and Wahl (1967)

Potential Energy Curves of BeH_2

R	-E	
	$X\,^1\Sigma_g^+$	$^3\Sigma_u^+$
1.5		14.7013
2.0	15.6063	15.1374
2.5	15.7202	
3.0	15.7159	15.4626
3.5	15.6696	15.5123
4.0	15.6363	15.5701
4.5	15.5485	15.5156
∞	15.5481	

Michels (1967)

Potential and Orbital Energies of HCN

$1\sigma^2 \rightarrow 5\sigma^2\ 1\Pi^4$, $^1\Sigma^+$			
R_1	R_2	-E	$-\epsilon$
1.81287	1.96119	92.8841	15.5560,11.2393,1.2906,0.8403, 0.5753, 0.5370
1.81287	2.38053	92.8680	15.6362,11.3200,1.1903,0.8718, 0.5898, 0.4696
1.9343	2.1091	92.9160	15.5850,11.2738,1.2543,0.8244, 0.5810, 0.5089
1.9343	2.2491	92.9052	15.6118,11.3010,1.2200,0.8352, 0.5853, 0.4867
2.00899	1.76507	92.7663	15.5136,11.2113,1.3303,0.7810, 0.5597, 0.5792
2.00899	2.60325	92.8065	15.6667,11.3641,1.1405,0.8467, 0.5835, 0.4416
2.0143	2.1791[a]	92.9147	15.5978,11.2907,1.2365,0.8129, 0.5820,0.4968
2.0843	2.1091	92.9153	15.5835,11.2797,1.2534,0.7930, 0.5786, 0.5077
2.0843	2.2491	92.9048	15.6101,11.3068,1.2187,0.8043, 0.5824, 0.4855
2.23221	1.96119	92.8826	15.5520,11.2558,1.2888,0.7522, 0.5700, 0.5340

R_1	R_2	-E	-ε
2.23221	2.38053	92.8684	15.6314,11.3357,1.1861,0.7876, 0.5800, 0.4660
2.47026	2.14248	92.8846	15.5864,11.2983,1.2425,0.7277, 0.5717, 0.4992

a. Exp. R

McLean and Yoshimine (1967)

Potential and Orbital Energies of N_2O
$1\sigma^2 \rightarrow 7\sigma^2\ 1\Pi^4\ 2\Pi^4,\ {}^1\Sigma^+$

R_1	R_2	-E	-ε
1.72311	2.20908	183.6268	20.5974,15.7855,15.6358,1.7055,1.4948, 0.7881,0.6984,0.8458,0.5048
1.91457	2.01762	183.7204	20.6334,15.8097,15.6255,1.7200,1.5086, 0.8305,0.6758,0.8370,0.4971
1.91457	2.45453	183.7342	20.6163,15.8042,15.6931,1.6239,1.4010, 0.7979,0.7103,0.7704,0.5002
2.10603	2.69998	183.7169	20.6303,15.8113,15.7395,1.5369,1.3300, 0.8215,0.7005,0.7048,0.5016
2.11633	1.81586	183.6447	20.6835,15.8287,15.5998,1.8555,1.4151, 0.8867, 0.6452, 0.8887,0.4594
2.1273	2.2418	183.7567	20.6505,15.8403,15.6947,1.6105,1.4240, 0.8315, 0.6987, 0.7618,0.4914
2.34003	2.46598	183.6841	20.6610, 15.8580,15.7511,1.5139,1.3491, 0.8464, 0.6979, 0.6993, 0.4874
2.35148	2.01762	183.6958	20.6993,15.8579,15.6688, 1.7357,1.3342, 0.8810, 0.6769, 0.8071, 0.4554
2.58663	2.21938	183.6310	20.7108,15.8783,15.7217,1.6268,1.2667, 0.8824, 0.6912, 0.7399,0.4516

a. Exp. R

McLean and Yoshimine (1967)

Energy As A Function of the Internuclear Distance

$(H_2F)^-$ $(1\sigma^2 \rightarrow 4\sigma^2 \quad 1\pi^4, \quad {}^1\Sigma^+)$

R_{FH}	R_{HH}	E^a
1.74	∞	-100.517
1.85	3.00	-100.569
1.95	2.35	-100.574
1.80	2.20	-100.567*
2.20	2.10	-100.574*
2.20	1.90	-100.575
2.40	1.80	-100.577
2.70	1.60	-100.582
2.70	1.40	-100.577*
3.00	1.80	-100.577*
3.10	1.50	-100.585
3.60	1.45	-100.586
∞	1.40	-100.574

a. Potential energy along the reaction coordinate except for the points marked with an asterik

Ritchie and King (1966)

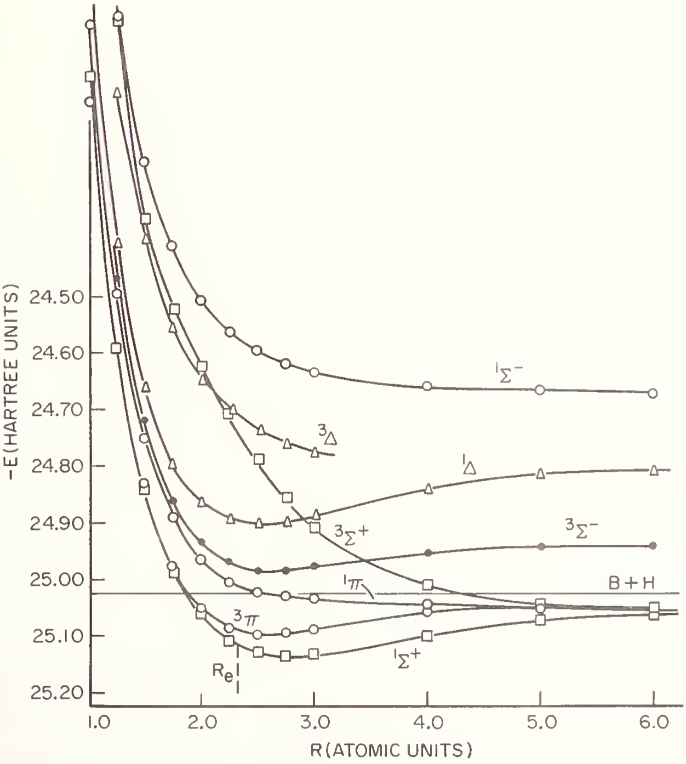


Fig. 1. Potential energy curves for ground and excited states of BH.

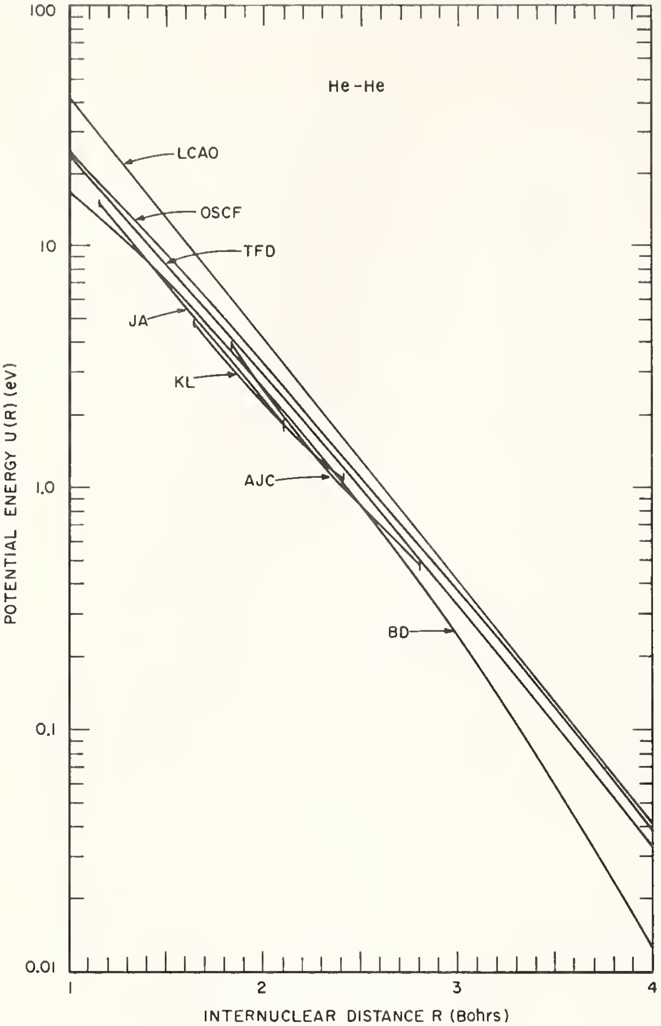


Fig. 2. He-He potential curves.
LCAO - linear combination of atomic orbitals method.
OSCF - optimized self-consistent-field (Hartree-Fock) method.
Other curves represent Thomas-Fermi-Dirac (TFD) or semi-empirical calculations. For references see original paper by Gilbert and Wahl (1967).

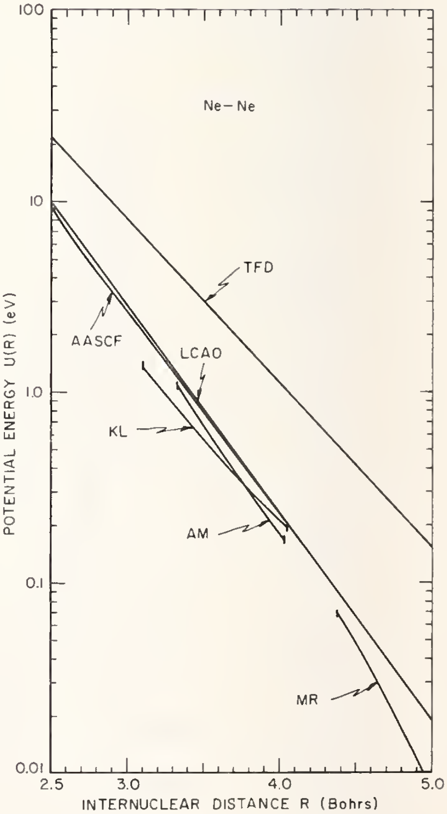


Fig. 3. Ne-Ne potential curves.
LCAO - linear combination of atomic orbitals method.
AASCF - augmented asymptotic self-consistent-field method.
Other curves represent Thomas-Fermi-Dirac (TFD) or semi-empirical calculations. For references see original paper by Gilbert and Wahl (1967).

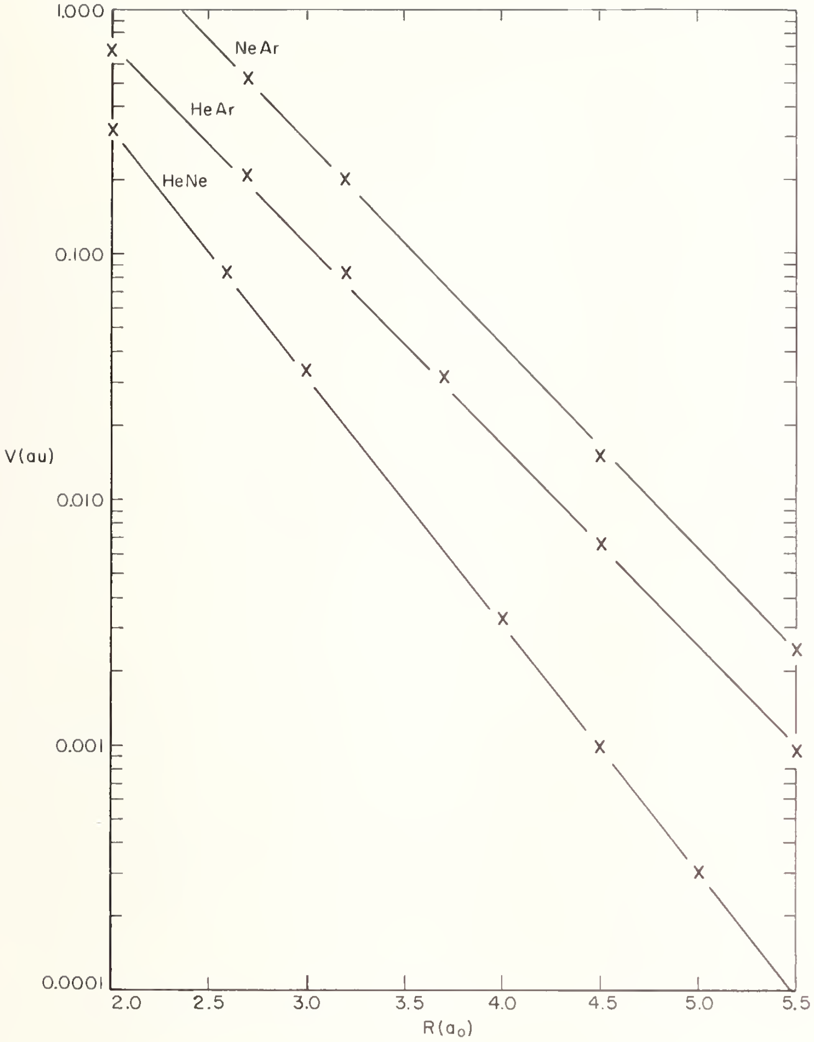


Fig. 4. Potential curves of HeNe, HeAr, NeAr. Computed interatomic potential energy V in Hartree atomic units (e^2/a_o), relative to Hartree-Fock energy of separated atoms, plotted against nuclear separation R in Bohr atomic units (a_o). Computed points are indicated. The heavy lines are simple exponential functions fitted to these points, $V = A_V \exp(-\lambda_V R)$. The parameters for HeNe, HeAr, NeAr are, respectively, A_V = 33.418, 31.395, 92.544 and λ_V = 2.322, 1.884, 1.923.

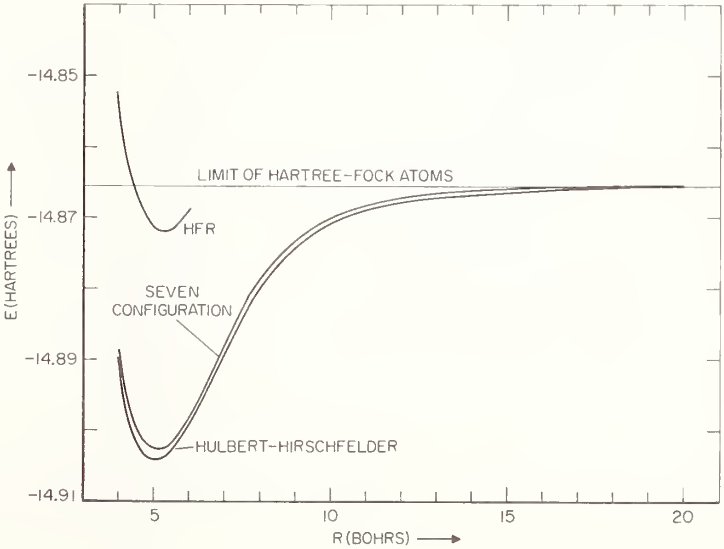


Fig. 5. Li_2 potential curve. Comparison of extended Hartree-Fock theory with experiment.

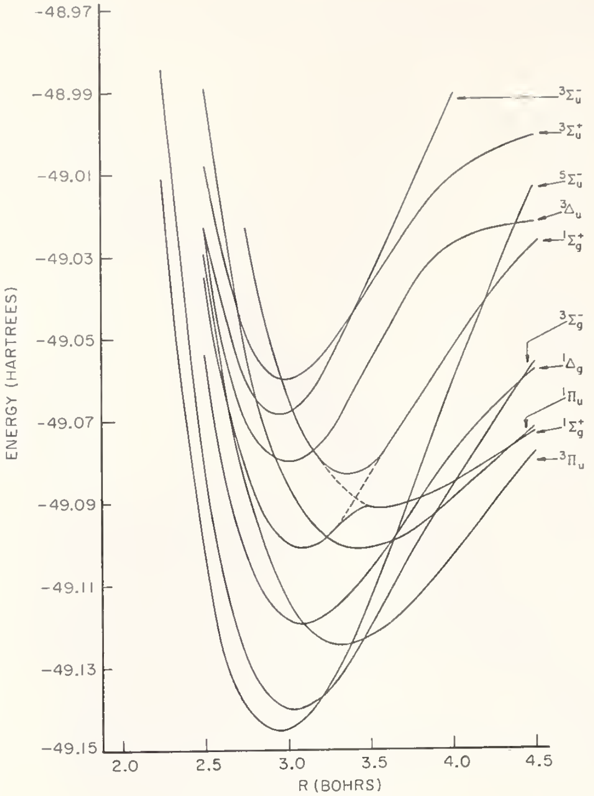


Fig. 6. Potential curves of the ten lowest electronic states of B_2 calculated using configuration interaction based on SCF molecular orbitals.

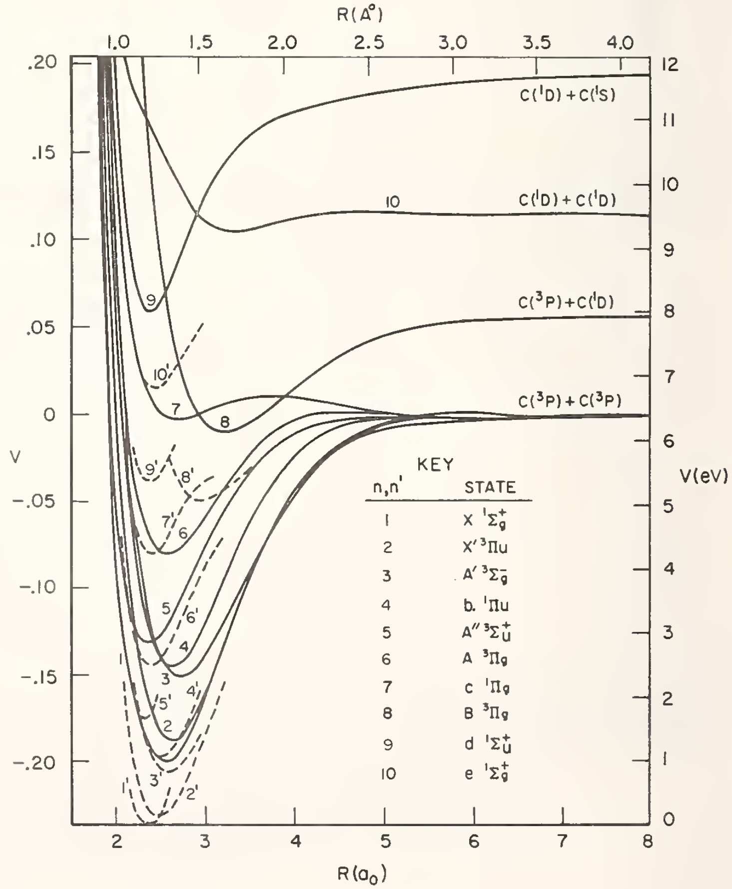


Fig. 7. Potential curves of the ten lowest electronic states of C_2 calculated using configuration interaction based on SCF molecular orbitals. The energy zero for the computed curves is chosen such that both computed and experimental curves approach the same asymptotic limits for all states which dissociate to a pair of normal (^3P) atoms. Primed numbers refer to experimental results.

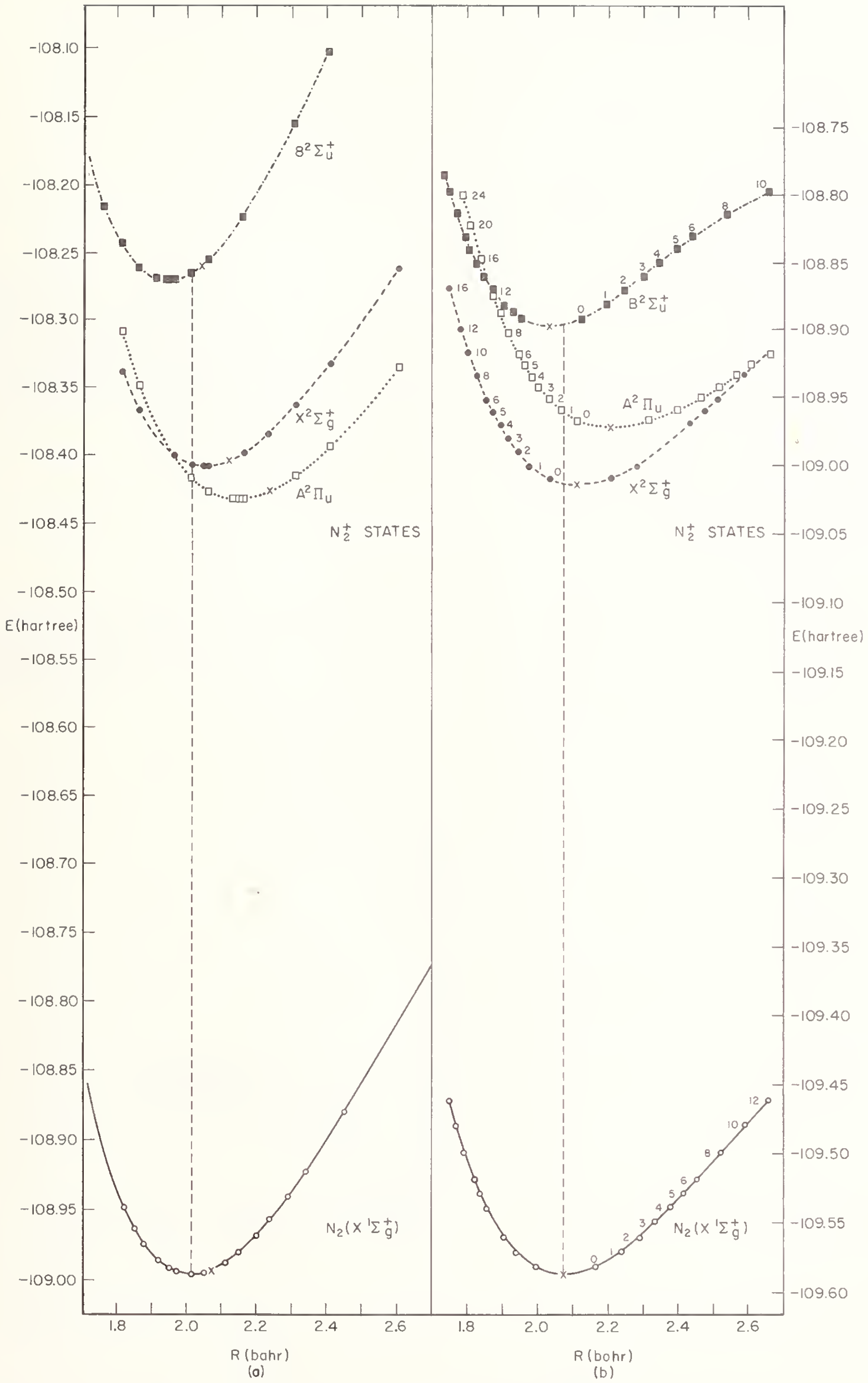


Fig. 8. Potential curves, E(R), for $N_2(X\ ^1\Sigma_g^+)$ and $N_2^+(X\ ^2\Sigma_g^+$, A $^2\Pi_u$, B $^2\Sigma_u^+)$: (a) calculated $E_{HF}(R)$ results; (b) $E_{RKR}(R)$ results of Gilmore. Note ordinate scale the same but ranges are different.

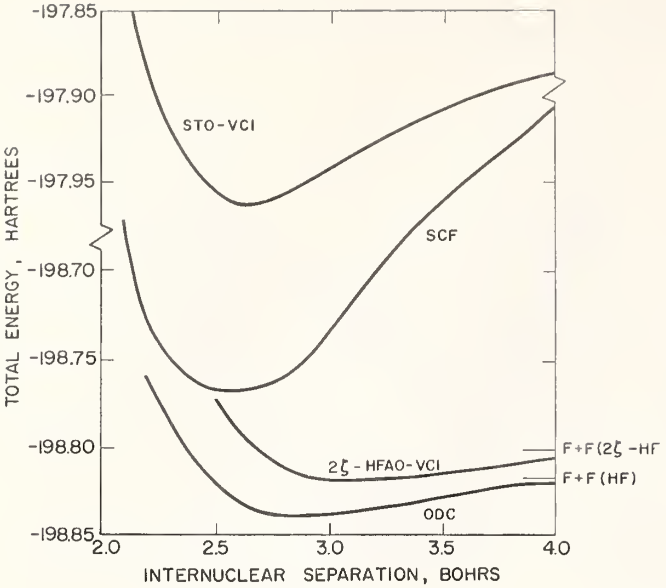


Fig. 9. Potential curves for the ground $^1\Sigma_g^+$ state of F_2. VCI - Valence configuration interaction; STO - Slater-type orbital; HFAO - Hartree-Fock atomic orbital designate Valence Bond calculations of Harris and Michels (1967). They reference the SCF and ODC (extended Hartree-Fock) calculations.

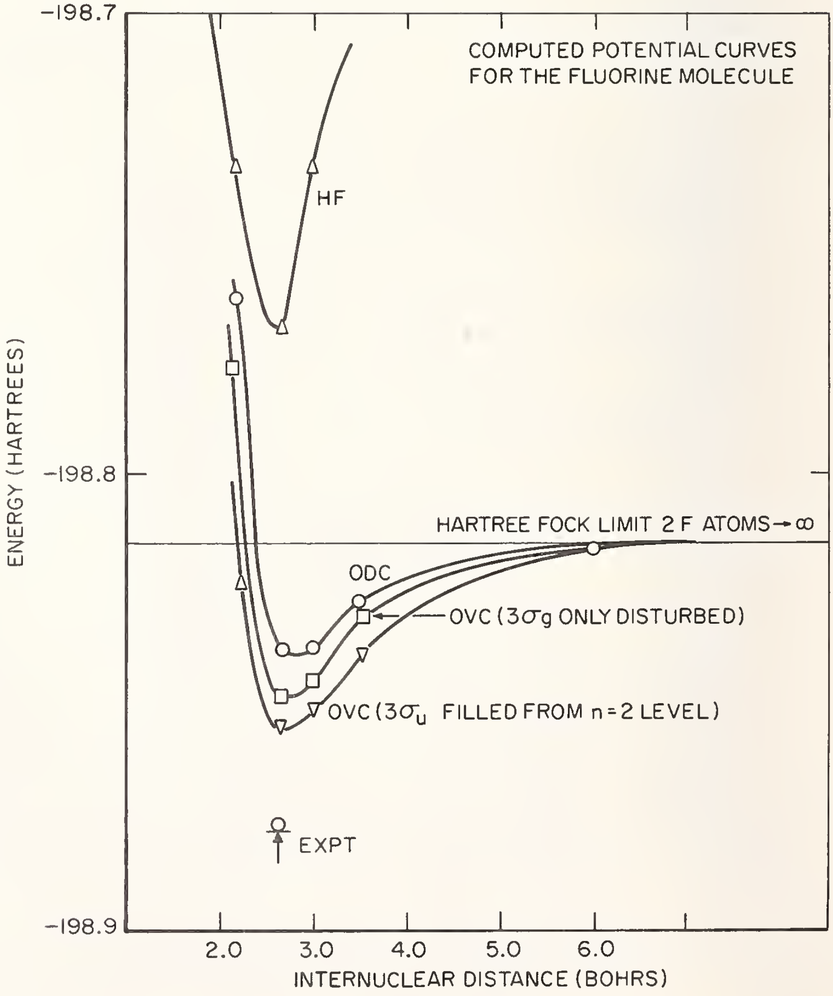


Fig. 10. Extended Hartree-Fock potential curves for F_2.

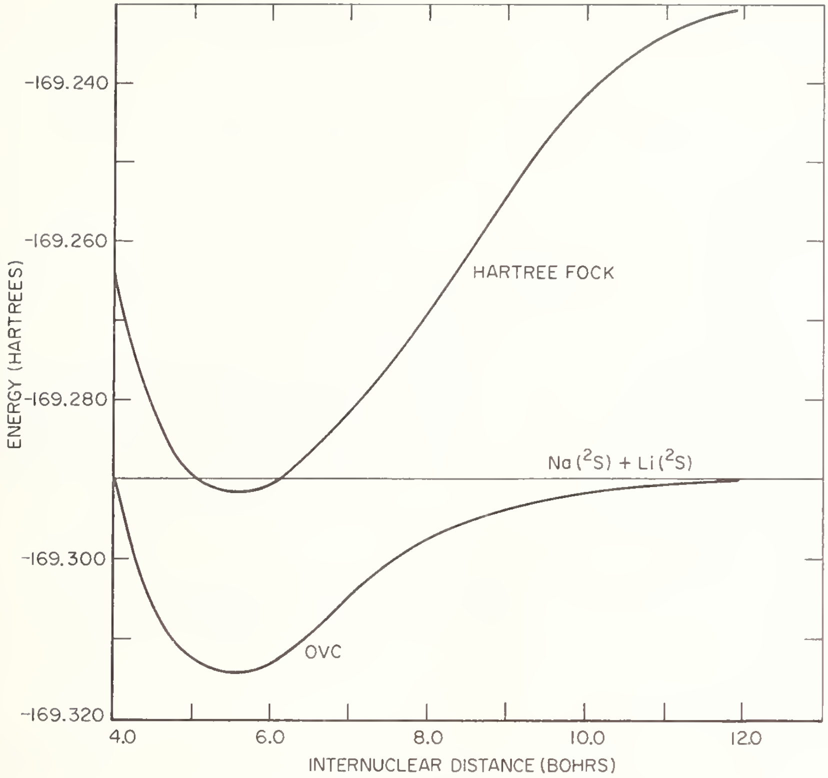


Fig. 11. Extended Hartree-Fock potential curves for LiNa.

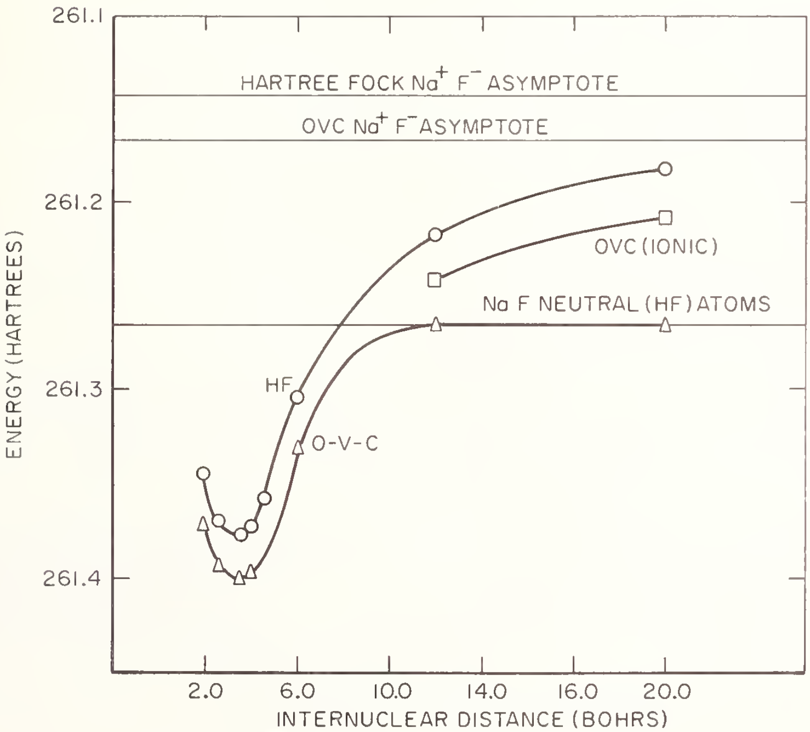


Fig. 12. Extended Hartree-Fock potential curves for NaF.

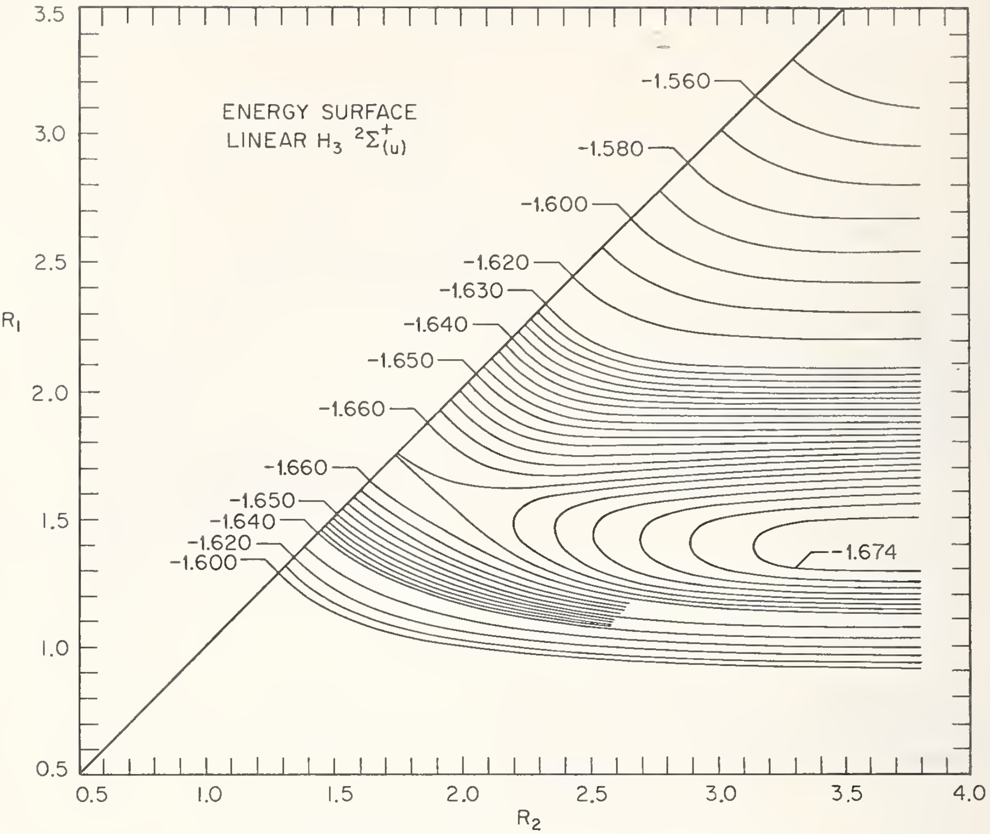


Fig. 13. Energy surface, linear H_3. Minimize energy variance.

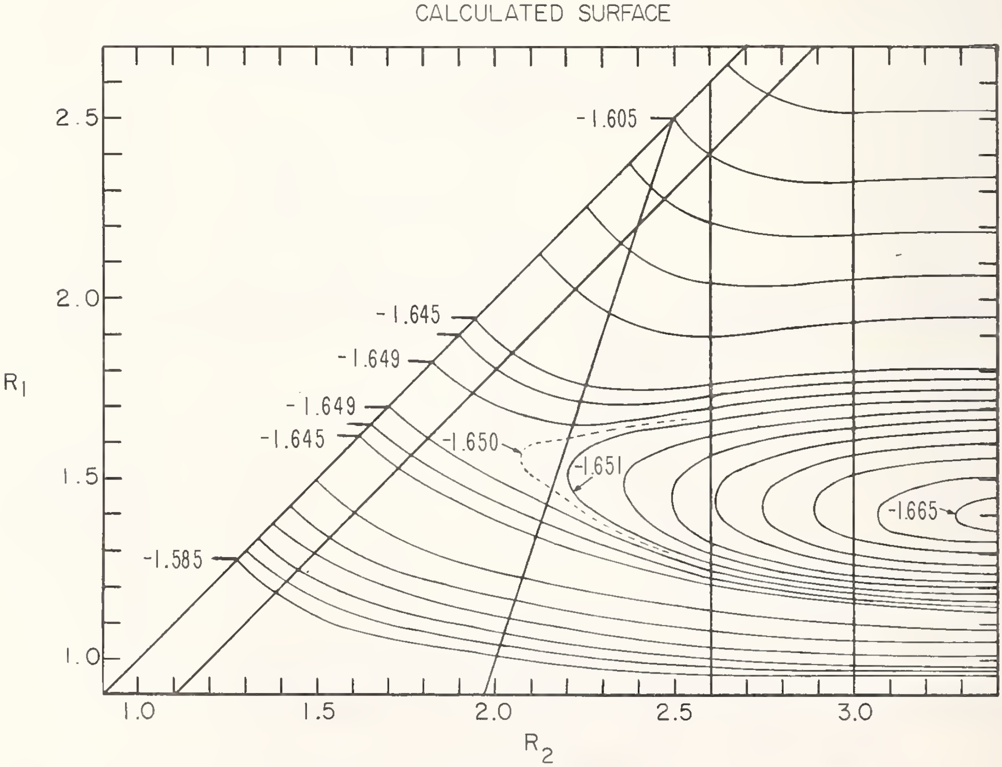


Fig. 14. Energy surface, linear H_3. Configuration interaction based on pseudo-natural orbitals.

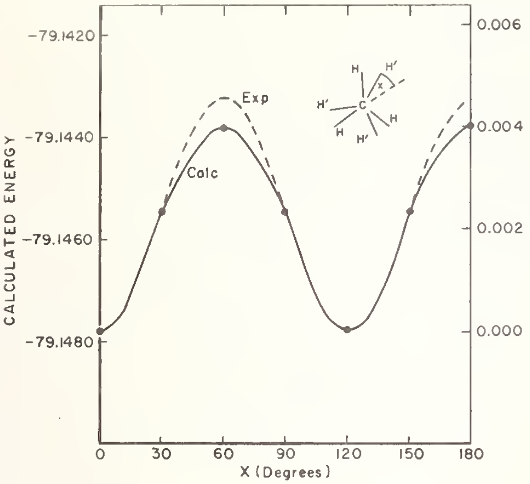


Fig. 15. Barrier to internal rotation in ethane.

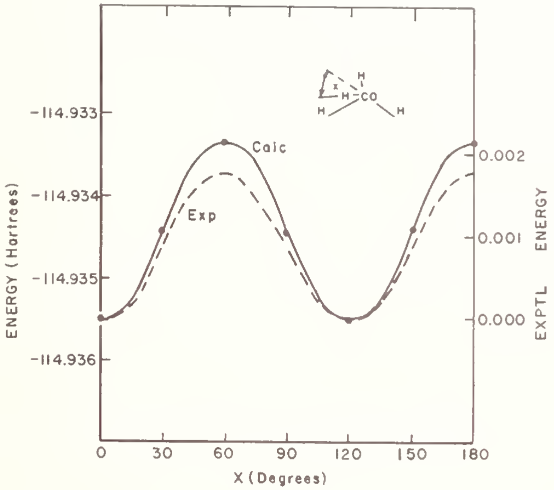


Fig. 16. Barrier to internal rotation in methyl alcohol.

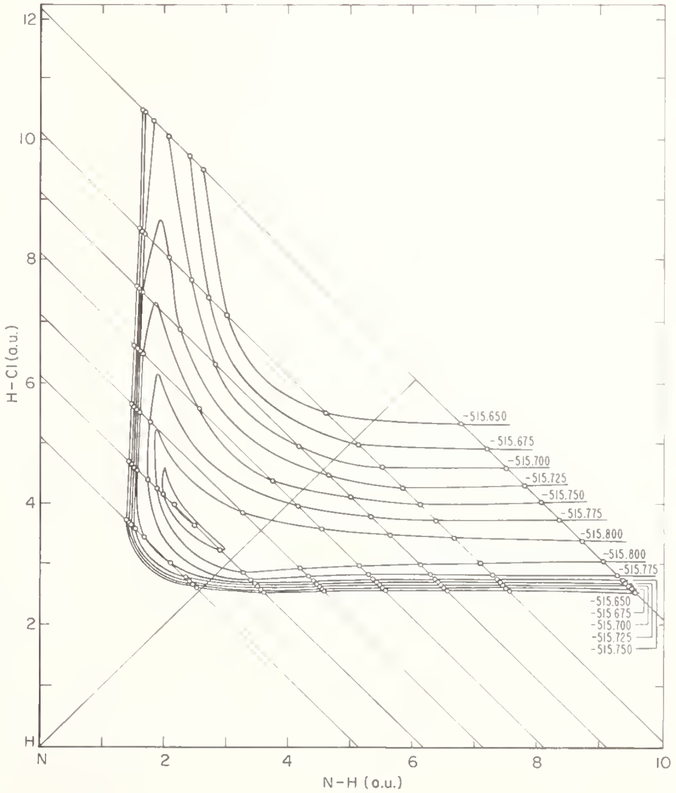


Fig. 17. Reaction surface for $NH_3 + HCl \rightarrow NH_4Cl$ (horizontal valley) or $NH_4^+ + Cl^- \rightarrow NH_4Cl$ (vertical valley). The abscissa gives the N-H(4) distances; the ordinate gives the H(4)-Cl distances. Each energy contour represents steps of 0.025 a.u. ($\cong$ 0.68 e.V.).

L. Gaussian Basis Calculations: Introduction

These results are included for the chemist; they illustrate the beginning of a capability to handle fairly large systems. The future may see the use of different basis sets or techniques and the economics of the calculations may radically alter but it is now possible to obtain H.F. approximations to large systems at more than a minimal level. They have been applied to the calculation of internal rotation barriers, the surface of a chemical reaction, and to the general understanding of the molecular shell structure and bonding characteristics. The success or lack of it at this time can be gauged by reference to the following studies. This area is moving rapidly and the conclusions obtained from these references may be very temporary but it is incontestable that large molecules can now be meaningfully treated by ab initio calculation.

C_2H_6

Basis [a] 86 GTF's contracted to 32 basis functions.

Symmetry		D_{3d}		D_{3h}
Geometry	C-C	2.915878	C-H	2.0325
Total energy		-79.1082		-79.1025
Orbital energies			$-\epsilon$	
$1a_{2u}$		11.2141	$1a_2''$	11.2127
$1a_{1g}$		11.2142	$1a_2'$	11.2126
$2a_{1g}$		1.0427	$2a_1'$	1.0423
$2a_{2g}$		0.8544	$2a_1''$	0.8537
$1e_u$		0.6191	$1e'$	0.6189
$3a_{1g}$		0.5094	$3a_1'$	0.5089
$1e_g$		0.5066	$1e''$	0.5050

Clementi and Davis (1966)

a. Best atom basis, Huzinaga (1965)

B_2H_6

Basis	See a.	54 GTF (B 9s,3p)
Symmetry	D_{2h}	
Geometry[b]	See fig. 1 Buenker et al (1966); B-B 1.70, BH, 2.55, BH_3 2.30, < BBH, 49° , β 0°	
Total energy	-52.7551	-52.753
Orbital energies	$-\epsilon$	
$1a_g$	7.6484	7.6416
$1b_{1u}$	7.6479	7.6410
$2a_g$	0.8734	0.8979
$2b_{1u}$	0.6427	0.6457
$1b_{3u}$	0.5493	0.5558
$1b_{2u}$	0.5285	0.5546
$3a_g$	0.5205	0.5174
$1b_{3g}$	0.4744	0.4737
Reference	Buenker et al (1966)	Burnelle and Kaufman (1965)

a. Linear combination of GTF, Whitten (1966); decomposed long-range p component; long-range S group.

b. β - dihedral angle between yz plane and $H_3B_2H_4$ plane.

C_2H_4

Basis Linear combination of GTF; decomposed long-range s and p components.

Symmetry D_{2d}

Geometry C-C 2.55102 , C-H 2.0236 , < HCH 117°

Total energy	-78.0012
Orbital energies	$-\epsilon$
$1a_{1g}$	11.2341
$1b_{3u}$	11.2326
$2a_{1g}$	1.0324
$2b_{3u}$	0.7987
$1b_{2u}$	0.6462
$3a_{1g}$	0.5847
$1b_{1g}$	0.5063
$1b_{1u}$	0.3676

Whitten (1966)

C_3H_6

Basis[a] Best atom linear combinations of 60s, 45p lobe functions.

Symmetry D_{3h}

Geometry C-C 2.880, C-H 2.022, < CCC 60° , < HCH 120°

Total energy -116.9164

Orbital energies -ε

$1a_1'$	11.2941
$1e'$	11.2935
$2a_1'$	1.1510
$2e'$	0.8344
$1a_2''$	0.7024
$3a_1'$	0.6257
$1e''$	0.5460
$3e'$	0.4398

[a] Whitten (1966)

Buenker et al (1967b)

C_4H_2

Basis Best atom, Huzinaga (1965) C 9s,5p;H 3s.

Symmetry $D_{\infty h}$

Geometry C-C 2.2772, C-C 2.6060, C-H 2.0107

Total energy -152.127 ± 0.004[a]

Orbital energies -ε

σ_g	σ_u	Π_u	Π_g
11.536	11.532	0.592	0.472
11.481	11.481		
1.163	1.106		
0.936	0.790		
0.776			

[a] Errors correspond to predetermined accuracy for integrals.

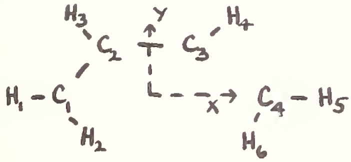
Snyder (1967)

C_4H_6; cis, trans butadiene

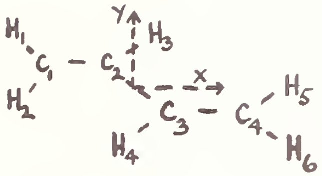
Basis Best atom linear combinations of 70s, 60p lobe functions.

Symmetry cis C_{2v} trans C_{2h}

Geometry



cis



trans

cis	x, y, z	trans	x, y, z
c_1	-2.66438,0,0	c_1	-3.2768,1.183,0
c_2	-1.40116,2.18796,0	c_2	-0.7502,1.183,0
H_1	-4.70518,0,0	H_1	-4.2916,2.9537,0
H_2	-1.64398,-1.76738,0	H_2	-4.2916,-0.5877,0
H_3	-2.42156,3.95534,0	H_3	0.264, 2.9537,0

Total energies -154.7023 -154.7103

Orbital energies -6

cis		trans	
$1a_1$	11.3463	$1a_g$	11.3466
$1b_2$	11.3457	$1b_u$	11.3459
$2b_2$	11.3045	$2b_u$	11.3098
$2a_1$	11.3045	$2a_g$	11.3098
$3a_1$	1.1155	$3a_g$	1.1089
$3b_2$	1.0109	$3b_u$	1.0214
$4a_1$	0.8570	$4a_g$	0.8331
$4b_2$	0.7442	$4b_u$	0.7751
$5a_1$	0.7073	$5a_g$	0.6638
$6a_1$	0.6292	$5b_u$	0.6603
$5b_2$	0.6022	$6a_g$	0.5742
$6b_2$	0.5370	$6b_u$	0.5693
$7a_1$	0.5261	$7a_g$	0.5140
$1b_1$	0.4768	$1a_u$	0.4765
$1a_2$	0.3541	$1b_g$	0.3579

a. Whitten (1966)

Whitten and Buenker (1967)

H_2CO

Basis Linear combination of GTF; decomposed long-range s and p components.

Symmetry C_{2v}

Geometry C-O 2.2864, C-H 2.18, < HCH 120°

Total energy -113.8094

Orbital energies	-ε
$1a_1$	20.579
$2a_1$	11.352
$3a_1$	1.422
$4a_1$	0.864
$1b_2$	0.700
$5a_1$	0.635
$1b_1$	0.527
$2b_2$	0.437

Dipole moment ($H_2C^+O^-$) 3.4

Buenker and Whitten (1967)

	Formamide (CH_3NO)	Formic Acid (CH_2O_2)
Basis:	87 GTF's grouped into 36 basis functions (Best Atom Double Zeta)	83 GTF's grouped into 34 basis functions (Best Atom Double Zeta)
Symmetry:	C_s (one reflection plane)	
Geometry:	C=O 2.3489 C-N 2.5379 C-H 2.0674 N-H 1.8803	C=0 2.2715 C-0(H)2.5379 C-H 2.0730 O-H 1.8368
Total Energies:	-168.8661	-188.6877
Orbital Energies:	-ε	
1a'	20.5325	20.6248
2a'	15.5939	20.5819
3a'	11.3867	11.4302
4a'	1.3939	1.5114
5a'	1.2388	1.4042
6a'	0.8766	0.9084
7a'	0.7669	0.7413
8a'	0.6719	0.7137
9a'	0.6012	0.6019
10a'	0.4365	0.4809
1a"	0.5774	0.6521
2a"	0.4164	0.5000
Dipole Moment	4.95 Debyes	1.49 Debyes

Comments: Also one non-planar geometry and several excited triplet states (planar geometry) in same basis.

Basch (1967)

CH_3F

Basis [a]	57 GTF's contracted to 28 basis functions.
Symmetry	C_{3v}
Geometry	C-H 2.088, C-F 2.617
	$<$ HCH 109°54°, $<$ HCF 109°02[1]
Total Energy	-138.94979
Orbital Energies	$-\varepsilon$
$1a_1$	26.23270
$2a_1$	11.31825
$3a_1$	1.55533
$4a_1$	0.94912
$5a_1$	0.65554
1e	0.69095
2e	0.52736

a. Best atom basis, Huzinaga (1965)

Krauss (1967)

Ethyl Fluoride (C_2H_5F)

Basis: 104 GTF s grouped into 23 basis functions (Hartree-Fock AO Basis).

Symmetry: C_s (one reflection plane).

Geometry: C-C 2.9102, C-F 2.5984, C-H 2.0919

	Staggered	Eclipsed
Total Energy:	-177.9409	-177.9368
Orbital Energies:	$-\varepsilon$	$-\varepsilon$
1a'	26.141	26.140
2a'	11.396	11.395
3a'	11.266	11.264
4a'	1.548	1.548
5a'	1.032	1.032
6a'	0.860	0.860
7a'	0.668	0.669
8a'	0.624	0.622
9a'	0.548	0.545
10a'	0.486	0.486
1a"	0.697	0.696
2a"	0.569	0.573
3a"	0.490	0.487
Dipole Moment:	2.56 Debyes	2.52 Debyes

Basch (1967)

C_4H_5N , Pyrrole

Basis [a] 95 GTF's contracted to 30 basis functions

Symmetry C_{2v}

Geometry See b.

Total energy -207.9313

Orbital energies -ϵ

$a_1(\sigma)$	$b_2(\sigma)$	$b_1(\Pi)$	$a_2(\Pi)$
15.7100	11.4253	0.6313	0.3879
11.4252	11.3785	0.4253	
11.3793	1.0345		
1.3239	0.7970		
1.0955	0.6243		
0.8251	0.6022		
0.7779			
0.6476			
0.5766			

a. Best atom basis, Huzinaga (1965)

b. Equilibrium value Sutton (1958)

Clementi (1967b)

C_5H_5N, Pyridine

Basis [a] 111 GTF's contracted to 35 basis functions

Symmetry C_{2v}

Geometry

	x	y		x	y
N	0.0	1.328750	C_1	-2.18521	0.0
H_1	-3.94316	1.029325	C_2	2.18521	0.0
H_2	3.94316	1.029325	C_3	-2.26896	-2.60938
H_3	4.06176	-3.58167	C_4	2.26896	-2.60938
H_4	4.06176	-3.58167	C_5	0.0	-3.97052
H_5	0.0	-6.0075			

Total energy -245.6219

Orbital energies $-\varepsilon$

$a_1(\sigma)$	$b_2(\sigma)$	$b_1(\pi)$	$a_2(\pi)$
15.6775	11.4611	0.6223	0.4472
11.4611	11.4344	0.4586	
11.4430	1.1102		
11.4343	0.9043		
1.3277	0.7260		
1.1577	0.6700		
0.9218	0.5795		
0.7791			
0.7012			
0.6394			
0.4654			

a. Best atom basis, Huzinaga (1965)

Clementi (1967c)

$C_4H_4N_2$, Pyrazine

Basis[a] 108 GTF's contracted to 34 basis functions

Symmetry C_{2v}

Geometry C-N 2.5512 C-C 2.62674 C-H 2.0598

Total energy -261.5543

Orbital energies -ε

$a_1(\sigma)$	$b_2(\sigma)$	$b_1(\Pi)$	$a_2(\Pi)$
15.6954	11.4765	0.6494	0.4618
15.6953	11.4754	0.4935	
11.4764	1.1326		
11.4754	0.9310		
1.3762	0.7552		
1.2729	0.6837		
0.9571	0.6107		
0.7797			
0.7228			
0.5327			
0.4412			

a. Best atom basis, Huzinaga (1965)

Clementi (1967d)

Li C_5H_5

Basis 72 GTF contracted to 51 basis functions

Symmetry C_5

Geometry C-C 2.69, C-H 2.02, Ring-Li 3.08

Total energy -196.2318

Ring-Li frequency is calculated as $\omega=750$ cm^{-1}.

Janoschek et al (1967b)

C_6H_6

Basis[a] Best atom linear combinations of 90 s, 90p lobe functions.

Symmetry D_{6h}

Geometry C-C 2.64, C-H 2.048

Total energy -230.312

a. Whitten (1966)

Whitten et al (1967)

Basis 78 GTF contracted to 54 basis functions.

Symmetry D_{6h}

Geometry C-C 2.63 , C-H 2.04

Total energy -227.2695

Energies determined at sufficient points to determine the following frequencies

	calc:	Exp.
ω_1	1200	1000
ω_2	4110	3062
ω_3	1376	1540
ω_4	1280	

Janoschek et al (1967a)

Acknowledgement

The bulk of this report is abstracted either from very recently published work or work that is still unpublished. Without access to this information this project would have been unthinkable. It was gratifying to find that many workers in this field were willing to take the considerable time required to summarize their unpublished work. I believe it reflects a desire to take stock in a rapidly moving field and to communicate a growing feeling of confidence in the ability to calculate meaningful molecular energies and properties.

The list of contributors is listed below in alphabetical order. I wish to thank them all for their effort and the speed of the response. The organization of their material is my responsibility alone, and I apologize beforehand to all who will find the organization is not properly responsive to the material.

I have also included addresses of the individuals since they can best answer inquiries as to their unpublished materlal.

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