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**COMPLETE HARTREE-FOCK WAVEFUNCTIONS AND
ONE-ELECTRON PROPERTIES FOR $CF(^2\Pi)$,
 $CF^+(^1\Sigma)$, AND $CF^-(^3\Sigma)$, AND CHARGE-DENSITY
DIAGRAMS FOR CF AND ITS COMPONENT ORBITALS**

P. A. G. O'Hare and Arnold C. Wahl

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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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May 1971

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT.....	5
I. INTRODUCTION.....	5
II. METHOD OF COMPUTATION, CALCULATED WAVE FUNCTIONS, AND ONE-ELECTRON PROPERTIES AND CHARGE-DENSITY DIAGRAMS.....	5
REFERENCES.....	34

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1	Charge-Density Diagrams for $CF(^2\Pi)$ at Hartree-Fock Minimum.....	32
2	Charge-Density Diagrams for $CF(^2\Pi)$ at Hartree-Fock Minimum.....	33

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
I	Wavefunction for Carbon-Fluorine at 1.95 Bohrs.....	7
II	Wavefunction for Carbon-Fluorine at 2.10 Bohrs.....	8
III	Wavefunction for Carbon-Fluorine at 2.25 Bohrs.....	9
IV	Wavefunction for Carbon-Fluorine at 2.3789 Bohrs.....	10
V	Wavefunction for Carbon-Fluorine at 2.3937 Bohrs.....	11
VI	Wavefunction for Carbon-Fluorine at 1.95 Bohrs; F ⁻ Basis Set.....	12
VII	Wavefunction for Carbon-Fluorine at 2.55 Bohrs.....	13
VIII	Wavefunction for Carbon-Fluorine at 2.70 Bohrs.....	14
IX	Wavefunction for Carbon-Fluorine at 3.00 Bohrs.....	15
X	Wavefunction for CF Positive Ion at 1.95 Bohrs.....	16

LIST OF TABLES (Continued)

<u>No.</u>	<u>Title</u>	<u>Page</u>
XI	Wavefunction for CF Positive Ion at 2.10 Bohrs.....	17
XII	Wavefunction for CF Positive Ion at 2.146 Bohrs.....	18
XIII	Wavefunction for CF Positive Ion at 2.25 Bohrs.....	19
XIV	Wavefunction for CF Positive Ion at 2.3789 Bohrs.....	20
XV	Wavefunction for CF Positive Ion at 2.55 Bohrs.....	21
XVI	Wavefunction for CF Positive Ion at 2.70 Bohrs.....	22
XVII	Wavefunction for CF Negative Ion at 2.10 Bohrs.....	23
XVIII	Wavefunction for CF Negative Ion at 2.25 Bohrs.....	24
XIX	Wavefunction for CF Negative Ion at 2.3789 Bohrs.....	25
XX	Wavefunction for CF Negative Ion at 2.55 Bohrs.....	26
XXI	Wavefunction for CF Negative Ion at 2.70 Bohrs.....	27
XXII	Wavefunction for CF Negative Ion at 3.00 Bohrs.....	28
XXIII	Expectation Values of Selected Operators for $CF(^2\Pi)$	29
XXIV	Expectation Values of Selected Operators for $CF^+(^1\Sigma)$	30
XXV	Expectation Values of Selected Operators for $CF^-(^3\Sigma)$	31

COMPLETE HARTREE-FOCK WAVEFUNCTIONS AND
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P. A. G. O'Hare and Arnold C. Wahl

ABSTRACT

Complete Hartree-Fock wavefunctions, calculated by the open-shell method of Roothaan, are given for $\text{CF}(^2\Pi)$, $\text{CF}^+(^1\Sigma)$, and $\text{CF}^-(^3\Sigma)$ at several internuclear separations. Expectation values for selected operators are tabulated. Charge-density diagrams for $\text{CF}(^2\Pi)$ and each of its component orbitals are also included in the report.

1. INTRODUCTION

The present authors have recently^{1,2} described a quantum-chemical study of the ground states of CF, CF^+ , and CF^- . Self-consistent-field wave functions, close to the Hartree-Fock limit, were computed for each species at several internuclear separations by Roothaan's³ matrix expansion method. Because of space limitations, much useful data could not be given in the original journal article.¹ Therefore, we have tabulated the complete wavefunctions and one-electron properties. These data, along with charge-density diagrams for CF and each of its component orbitals at the equilibrium internuclear separation (r_e), form the substance of this report.

II. METHOD OF COMPUTATION, CALCULATED WAVE FUNCTIONS, AND ONE-ELECTRON PROPERTIES AND CHARGE-DENSITY DIAGRAMS

Molecular self-consistent-field wavefunctions were computed for the $\text{CF}(^2\Pi)$, $\text{CF}^+(^1\Sigma)$, and $\text{CF}^-(^3\Sigma)$ species at several internuclear separations including the experimental value, 2.3937 bohrs.⁴ The calculations were based on the open-shell method of Roothaan³ and employed the BISON computer system written by Wahl, Bertoncini, Kaiser, and Land.⁵ The Slater-type accurate atomic basis sets obtained by Bagus and Gilbert⁶ were used for C(3P) and F(2P). Polarization functions corresponding to the normally unoccupied 3d-orbitals of the atoms were added to the bases. These functions (STO zetas) are 2.06 and 0.33(C),⁷ and 2.44269(F).⁸ CF has a $^2\Pi$ ground state,⁹ and the structures of the outer electron shells, in accordance with Mulliken's¹⁰ scheme, are denoted by

$$\dots(z\sigma)^2(y\sigma)^2(w\pi)^4(x\sigma)^2(v\pi)\dots\dots\dots^2\Pi \quad (1)$$

It follows that the most probable structures for the ground states of the positive and negative ions are, respectively,

$$\dots(z\sigma)^2(y\sigma)^2(w\pi)^4(x\sigma)^2\dots\dots\dots 1_{\Sigma} \quad (2)$$

and

$$\dots(z\sigma)^2(y\sigma)^2(w\pi)^4(x\sigma)^2(v\pi)^2\dots\dots\dots 3_{\Sigma} \quad (3)$$

All the computations were carried out on the IBM-360/75 machine at Argonne National Laboratory.

Wavefunctions at each internuclear separation (including the computed Hartree-Fock minimum at 2.3789 bohrs) are given in Tables I - XXII, together with the total, potential, and kinetic energies and the virial. The expansion error is believed to be no greater than 0.01 hartrees¹¹ (1 hartree = 27.20974 eV). One-electron properties are given in Tables XXIII - XXV.

In Figures 1 and 2, charge-density contours for the $CF(^2\Pi)$ molecule and for each of the component orbitals at the Hartree-Fock minimum are plotted. The inner molecular orbitals are essentially pure atomic orbitals. As the valence-shell orbitals are approached, hybridization becomes progressively more evident.

The following information is applicable to all the diagrams:

(a) The atom centers are denoted by +; the carbon atom is to the left and the fluorine atom to the right.

(b) For the initial contour, the value of the charge density is 1.0 electrons bohr⁻³.

(c) Between adjacent contours, the charge density ratio is 0.5.

(d) In the computer search, a test point is considered to be on a contour if the charge density at this point is within 1% of the contour charge density.

TABLE I. WAVEFUNCTION FOR CARBON-FLUORINE AT 1.95 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00000	-0.12602	-0.00027	0.00029	0.00313
1 0 0	5.02500	0.00000	-0.92330	0.12416	-0.13975	0.17122
3 0 0	6.08100	0.00005	0.05284	0.00865	-0.01841	0.00884
2 0 0	2.14100	-0.00028	-0.00220	-0.16126	0.24237	-0.28186
2 0 0	1.35400	-0.00050	0.00026	0.02304	0.00157	-0.74130
2 1 0	6.82700	0.00000	-0.00097	0.00015	-0.00052	0.00223
2 1 0	2.77900	0.00008	-0.00588	-0.09858	0.09968	0.14888
2 1 0	1.62500	-0.00060	0.00499	-0.07025	0.08626	0.20250
2 1 0	1.05400	-0.00015	-0.00242	0.01844	-0.02785	0.11721
3 2 0	2.06000	-0.00024	-0.00104	-0.03731	0.03000	0.03602
3 2 0	0.33000	-0.00001	0.00000	0.00123	-0.00028	0.00292
1 0 0	-14.20100	-0.08425	0.00003	-0.00382	-0.00245	0.00060
1 0 0	-7.93800	-0.95458	0.00094	0.25588	0.09920	-0.03063
3 0 0	-9.96200	0.04220	0.00020	0.03108	0.00368	-0.00056
2 0 0	-3.33200	-0.00430	-0.00157	-0.51790	-0.19163	0.05695
2 0 0	-2.05700	0.00138	0.00009	-0.40206	-0.31029	0.13443
2 1 0	-9.43500	-0.00043	0.00007	-0.00332	0.01003	0.00297
2 1 0	-4.24900	-0.00144	-0.00100	-0.04704	0.21746	0.06159
2 1 0	-2.35600	0.00095	-0.00062	-0.14994	0.46160	0.12882
2 1 0	-1.43400	-0.00008	-0.00070	-0.01604	0.18196	0.09697
3 2 0	-2.44269	-0.00002	-0.00075	-0.03691	0.04801	0.01826

ORBITAL ENERGIES, HARTREES	-26.4557	-11.3192	-1.9197	-1.0341	-0.5364
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N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00190	0.00716
2 1 1	2.77900	-0.06431	0.18177
2 1 1	1.62500	-0.17375	0.30317
2 1 1	1.03400	0.02200	0.68718
3 2 1	2.06000	-0.04761	-0.00231
3 2 1	0.33000	0.00147	-0.01908
2 1 1	-9.43500	-0.01188	-0.00212
2 1 1	-4.24900	-0.22547	-0.14257
2 1 1	-2.35600	-0.51077	-0.08780
2 1 1	-1.43400	-0.22487	-0.41052
3 2 1	-2.44269	-0.04216	0.02112

ORBITAL ENERGIES, HARTREES	-0.8846	-0.2930
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TOTAL ENERGY, HARTREES	-137.13700
KINETIC ENERGY, HARTREES	138.17845
POTENTIAL ENERGY, HARTREES	-275.31545
VIRIAL	-1.99246

In Tables I - XXII, the negative orbital exponents simply indicate that these exponents are for the fluorine atom.

TABLE II. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.10 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12591	0.00038	0.00073	0.00261
1 0 0	5.02500	-0.00001	-0.92397	0.10337	0.14289	0.17542
3 0 0	6.08100	0.00005	0.05333	0.01135	0.02399	0.00785
2 0 0	2.14100	-0.00023	-0.00200	-0.16031	-0.28364	-0.28540
2 0 0	1.35400	-0.00040	0.00059	0.01595	-0.02784	-0.71980
2 1 0	6.82700	0.00000	-0.00093	0.00019	0.00039	0.00263
2 1 0	2.77900	0.00008	-0.00523	-0.07662	-0.08289	0.13461
2 1 0	1.62500	-0.00053	0.00486	-0.08219	-0.10834	0.22416
2 1 0	1.05400	-0.00010	-0.00203	0.02387	0.04121	0.10747
3 2 0	2.06000	-0.00021	-0.00057	-0.03379	-0.02845	0.03667
3 2 0	0.33000	-0.00001	0.00000	0.00124	0.00057	0.00228
1 0 0	-14.20100	-0.08422	0.00002	-0.00400	0.00240	0.00052
1 0 0	-7.93800	-0.95474	0.00055	0.25701	-0.09526	-0.02654
3 0 0	-9.96200	0.04228	0.00010	0.02980	-0.00388	-0.00050
2 0 0	-3.33200	-0.00404	-0.00081	-0.51789	0.18640	0.04786
2 0 0	-2.05700	0.00126	-0.00064	-0.42603	0.28717	0.11312
2 1 0	-9.43500	-0.00043	0.00002	-0.00318	-0.00999	0.00352
2 1 0	-4.24900	-0.00123	-0.00052	-0.03522	-0.20803	0.07407
2 1 0	-2.35600	0.00080	-0.00069	-0.13063	-0.44457	0.14809
2 1 0	-1.43400	-0.00003	-0.00062	-0.01258	-0.18917	0.11805
3 2 0	-2.44269	0.00004	-0.00051	-0.03085	-0.04559	0.01696
ORBITAL ENERGIES, HARTREES		-26.4320	-11.3345	-1.8442	-0.9952	-0.5451

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00223	0.00788
2 1 1	2.77900	-0.04824	0.18075
2 1 1	1.62500	-0.16915	0.37063
2 1 1	1.05400	0.02074	0.59149
3 2 1	2.06000	-0.04372	0.00046
3 2 1	0.33000	0.00143	-0.01437
2 1 1	-9.43500	-0.01161	-0.00202
2 1 1	-4.24900	-0.23093	-0.13154
2 1 1	-2.35600	-0.49415	-0.08920
2 1 1	-1.43400	-0.25903	-0.35478
3 2 1	-2.44269	-0.03780	0.01820
ORBITAL ENERGIES, HARTREES		-0.8352	-0.3289

TOTAL ENERGY, HARTREES	-137.19549
KINETIC ENERGY, HARTREES	137.73292
POTENTIAL ENERGY, HARTREES	-274.92841
VIRIAL	-1.99610

TABLE III. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.25 BOHRs.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12582	0.00086	-0.00164	0.00217
1 0 0	5.02500	-0.00002	-0.92447	0.08620	-0.14865	0.17773
3 0 0	6.06100	0.00005	0.05369	0.01282	-0.02875	0.00749
2 0 0	2.14100	-0.00018	-0.00178	-0.15244	0.32091	-0.29111
2 0 0	1.35400	-0.00033	0.00071	0.00748	0.06417	-0.69293
2 1 0	6.82700	0.00000	-0.00091	-0.00002	-0.00004	0.00310
2 1 0	2.77900	0.00008	-0.00477	-0.05769	0.06607	0.12128
2 1 0	1.62500	-0.00047	0.00471	-0.08894	0.12555	0.24189
2 1 0	1.05400	-0.00007	-0.00179	0.02605	-0.05121	0.09848
3 2 0	2.06000	-0.00018	-0.00026	-0.03056	0.02690	0.03720
3 2 0	0.33000	-0.00001	-0.00001	0.00114	-0.00079	0.00171
1 0 0	-14.20100	-0.08420	0.00001	-0.00420	-0.00229	0.00044
1 0 0	-7.93800	-0.95485	0.00034	0.25900	0.09029	-0.02215
3 0 0	-9.96200	0.04233	0.00002	0.02867	0.00401	-0.00031
2 0 0	-3.33200	-0.00383	-0.00034	-0.51922	-0.17885	0.03795
2 0 0	-2.05700	0.00101	-0.00099	-0.44799	-0.26437	0.09364
2 1 0	-9.43500	-0.00043	0.00000	-0.00295	0.00977	0.00411
2 1 0	-4.24900	-0.00107	-0.00026	-0.02563	0.19875	0.08806
2 1 0	-2.35600	0.00068	-0.00063	-0.11156	0.42337	0.16991
2 1 0	-1.43400	0.00000	-0.00063	-0.01033	0.19574	0.14067
3 2 0	-2.44269	0.00008	-0.00039	-0.02546	0.04281	0.01642

ORBITAL ENERGIES, HARTREES -26.4089 -11.3531 -1.7778 -0.9576 -0.5540

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00240	0.00836
2 1 1	2.77900	-0.03635	0.18028
2 1 1	1.62500	-0.15899	0.42012
2 1 1	1.05400	0.01655	0.52035
3 2 1	2.06000	-0.03975	0.00219
3 2 1	0.33000	0.00122	-0.01136
2 1 1	-9.43500	-0.01128	-0.00185
2 1 1	-4.24900	-0.23655	-0.12047
2 1 1	-2.35600	-0.47889	-0.08638
2 1 1	-1.43400	-0.28848	-0.30796
3 2 1	-2.44269	-0.03403	0.01532

ORBITAL ENERGIES, HARTREES -0.7926 -0.3606

TOTAL ENERGY, HARTREES -137.22060
 KINETIC ENERGY, HARTREES 137.42214
 POTENTIAL ENERGY, HARTREES -274.64274
 VIRIAL -1.99853

TABLE IV. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.3789 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12576	0.00113	0.00229	0.00183
1 0 0	5.02500	-0.00002	-0.92480	0.07386	0.15585	0.17759
3 0 0	6.08100	0.00005	0.05393	0.01315	0.03206	0.00741
2 0 0	2.14100	-0.00014	-0.00160	-0.14191	-0.35089	-0.29466
2 0 0	1.35400	-0.00029	0.00072	0.00005	-0.10305	-0.66572
2 1 0	6.82700	0.00000	-0.00090	-0.00028	-0.00033	0.00351
2 1 0	2.77900	0.00009	-0.00444	-0.04413	-0.05206	0.11066
2 1 0	1.62500	-0.00043	0.00454	-0.09059	-0.13443	0.25441
2 1 0	1.05400	-0.00006	-0.00165	0.02547	0.05694	0.09159
3 2 0	2.06000	-0.00017	-0.00010	-0.02793	-0.02528	0.03752
3 2 0	0.33000	-0.00001	-0.00001	0.00098	0.00094	0.00128
1 0 0	-14.20100	-0.08419	0.00000	-0.00439	0.00217	0.00036
1 0 0	-7.93800	-0.95492	0.00024	0.26101	-0.08554	-0.01801
3 0 0	-9.96200	0.04236	-0.00002	0.02781	-0.00408	-0.00004
2 0 0	-3.33200	-0.00369	-0.00008	-0.52084	0.17109	0.02849
2 0 0	-2.05700	0.00084	-0.00109	-0.46495	0.24529	0.07762
2 1 0	-9.43500	-0.00042	-0.00001	-0.00271	-0.00944	0.00466
2 1 0	-4.24900	-0.00095	-0.00014	-0.01895	-0.19023	0.10139
2 1 0	-2.35600	0.00060	-0.00055	-0.09618	-0.40165	0.19071
2 1 0	-1.43400	0.00001	-0.00066	-0.00902	-0.19967	0.16204
3 2 0	-2.44269	0.00010	-0.00034	-0.02143	-0.04015	0.01654

ORBITAL ENERGIES, HARTREES -26.3892 -11.3700 -1.7277 -0.9272 -0.5628

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00245	-0.00865
2 1 1	2.77900	-0.02882	-0.18012
2 1 1	1.62500	-0.14736	-0.45318
2 1 1	1.05400	0.01137	-0.47282
3 2 1	2.06000	-0.03842	-0.00294
3 2 1	0.33000	0.00090	0.00961
2 1 1	-9.43500	-0.01098	0.00168
2 1 1	-4.24900	-0.24125	0.11117
2 1 1	-2.35600	-0.46693	0.08197
2 1 1	-1.43400	-0.31024	0.27357
3 2 1	-2.44269	-0.03112	-0.01304

ORBITAL ENERGIES, HARTREES -0.7603 -0.3849

TOTAL ENERGY, HARTREES -137.22595
 KINETIC ENERGY, HARTREES 137.23248
 POTENTIAL ENERGY, HARTREES -274.45842
 VIRIAL -1.99995

TABLE V. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.3937 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12575	0.00115	0.00236	0.00179
1 0 0	3.02500	-0.00002	-0.92484	0.07257	0.15681	0.17742
3 0 0	6.08100	0.00005	0.05396	0.01315	0.03240	0.00741
2 0 0	2.14100	-0.00014	-0.00158	-0.14055	-0.35426	-0.29488
2 0 0	1.35400	-0.00028	0.00072	-0.00079	-0.10794	-0.66233
2 1 0	6.82700	-0.00001	-0.00090	-0.00031	-0.00037	0.00356
2 1 0	2.77900	0.00009	-0.00441	-0.04273	-0.05050	0.10948
2 1 0	1.62500	-0.00042	0.00452	-0.09055	-0.13504	0.25571
2 1 0	1.05400	-0.00005	-0.00164	0.02551	0.05744	0.09086
3 2 0	2.06000	-0.00017	-0.00008	-0.02763	-0.02507	0.03755
3 2 0	0.33000	-0.00001	-0.00001	0.00095	0.00095	0.00123
1 0 0	-14.20100	-0.08419	0.00000	-0.00441	0.00216	0.00035
1 0 0	-7.93800	-0.95493	0.00023	0.26125	-0.08498	-0.01751
3 0 0	-9.96200	0.04236	-0.00002	0.02771	-0.00408	0.00000
2 0 0	-3.33200	-0.00367	-0.00005	-0.52104	0.17014	0.02734
2 0 0	-2.05700	0.00082	-0.00109	-0.46678	0.24314	0.07579
2 1 0	-9.43500	-0.00042	-0.00001	-0.00268	-0.00939	0.00472
2 1 0	-4.24900	-0.00094	-0.00013	-0.01827	-0.18919	0.10301
2 1 0	-2.35600	0.00059	-0.00054	-0.09450	-0.39894	0.19321
2 1 0	-1.43400	0.00001	-0.00066	-0.00890	-0.19997	0.16463
3 2 0	-2.44269	0.00010	-0.00034	-0.02101	-0.03983	0.01658

ORBITAL ENERGIES, HARTREES	-26.3869	-11.3719	-1.7223	-0.9238	-0.5637
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N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00245	-0.00867
2 1 1	2.77900	-0.02809	-0.18011
2 1 1	1.62500	-0.14591	-0.45655
2 1 1	1.05400	0.01071	-0.46799
3 2 1	2.06000	-0.03605	-0.00298
3 2 1	0.33000	0.00086	0.00944
2 1 1	-9.43500	-0.01094	0.00166
2 1 1	-4.24900	-0.24178	0.11013
2 1 1	-2.35600	-0.46562	0.08139
2 1 1	-1.43400	-0.31255	0.26993
3 2 1	-2.44269	-0.03080	-0.01279

ORBITAL ENERGIES, HARTREES	-0.7569	-0.3876
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TOTAL ENERGY, HARTREES	-137.22589
KINETIC ENERGY, HARTREES	137.21432
POTENTIAL ENERGY, HARTREES	-274.44021
VIRIAL	-2.00008

TABLE VI. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.3937 BOHRS. F - BASIS SET.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00000	-0.12575	0.00126	0.00229	0.00163
1 0 0	5.02500	0.00000	-0.92483	0.07357	0.15619	0.17755
3 0 0	6.08100	0.00001	0.05398	0.01643	0.02986	0.00592
2 0 0	2.14100	-0.00007	-0.00170	-0.15506	-0.34188	-0.28778
2 0 0	1.35400	-0.00025	0.00100	0.04445	-0.14276	-0.67198
2 1 0	6.82700	0.00000	-0.00089	-0.00001	-0.00051	0.00356
2 1 0	2.77900	0.00002	-0.00449	-0.04532	-0.05014	0.10951
2 1 0	1.62500	-0.00024	0.00468	-0.09206	-0.12845	0.25550
2 1 0	1.05400	-0.00007	-0.00168	0.04936	0.03779	0.09337
3 2 0	2.06000	-0.00010	-0.00007	-0.02487	-0.02628	0.03783
3 2 0	0.33000	0.00000	-0.00004	0.00168	0.00079	0.00342
1 0 0	-14.09000	-0.08756	0.00000	-0.00377	0.00195	0.00015
1 0 0	-7.92100	-0.95228	0.00023	0.26031	-0.08433	-0.01724
3 0 0	-9.93900	0.04295	-0.00001	0.02797	-0.00446	-0.00128
2 0 0	-3.23000	-0.00317	-0.00020	-0.61977	0.21238	0.04290
2 0 0	-1.83400	0.00051	-0.00110	-0.40428	0.22555	0.06342
2 1 0	-7.79800	-0.00073	-0.00001	-0.00349	-0.01946	0.01134
2 1 0	-3.78900	-0.00038	-0.00022	-0.03555	-0.26553	0.13464
2 1 0	-1.94600	0.00026	-0.00084	-0.09374	-0.47470	0.26934
2 1 0	-0.96800	0.00003	-0.00043	-0.00839	-0.02535	0.05599
3 2 0	-2.44269	0.00007	-0.00036	-0.02378	-0.03860	0.01634
ORBITAL ENERGIES, HARTREES		-26.3854	-11.3707	-1.7210	-0.9230	-0.5628

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00284	-0.00739
2 1 1	2.77900	-0.02389	-0.19558
2 1 1	1.62500	-0.15821	-0.40293
2 1 1	1.05400	0.02139	-0.52718
3 2 1	2.06000	-0.03670	-0.00145
3 2 1	0.33000	0.00334	-0.00279
2 1 1	-7.79800	-0.02541	0.00936
2 1 1	-3.78900	-0.32409	0.11911
2 1 1	-1.94600	-0.59961	0.20137
2 1 1	-0.96800	-0.08791	0.16502
3 2 1	-2.44269	-0.03050	-0.01310
ORBITAL ENERGIES, HARTREES		-0.7562	-0.3869

TOTAL ENERGY, HARTREES	-137.22528
KINETIC ENERGY, HARTREES	137.22466
POTENTIAL ENERGY, HARTREES	-274.44994
VIRIAL	-2.00001

TABLE VII. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.55 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12568	0.00128	0.00297	-0.00143
1 0 0	5.02500	-0.00002	-0.92516	0.06034	0.16873	-0.17341
3 0 0	6.08100	0.00005	0.05418	0.01259	0.03543	-0.00726
2 0 0	2.14100	-0.00010	-0.00139	-0.12497	-0.38964	0.29347
2 0 0	1.35400	-0.00024	0.00064	-0.00907	-0.16436	0.62265
2 1 0	6.82700	-0.00001	-0.00088	-0.00062	-0.00077	-0.00406
2 1 0	2.77900	0.00009	-0.00406	-0.02993	-0.03474	-0.09766
2 1 0	1.62500	-0.00037	0.00425	-0.08779	-0.13588	-0.26791
2 1 0	1.05400	-0.00004	-0.00150	0.02272	0.06066	-0.08396
3 2 0	2.06000	-0.00015	0.00004	-0.02463	-0.02247	-0.03778
3 2 0	0.33000	-0.00001	-0.00002	0.00068	0.00107	-0.00077
1 0 0	-14.20100	-0.08418	0.00000	-0.00462	0.00199	-0.00025
1 0 0	-7.93800	-0.95499	0.00016	0.26376	-0.07887	0.01191
3 0 0	-9.96200	0.04238	-0.00005	0.02681	-0.00408	-0.00044
2 0 0	-3.33200	-0.00353	0.00012	-0.52312	0.15941	-0.01449
2 0 0	-2.05700	0.00065	-0.00106	-0.48443	0.22108	-0.05650
2 1 0	-9.43500	-0.00041	-0.00002	-0.00237	-0.00879	-0.00543
2 1 0	-4.24900	-0.00082	-0.00005	-0.01203	-0.17713	-0.12099
2 1 0	-2.35600	0.00050	-0.00042	-0.07790	-0.36735	-0.22076
2 1 0	-1.43400	0.00001	-0.00067	-0.00784	-0.20037	-0.19372
3 2 0	-2.44269	0.00012	-0.00030	-0.01695	-0.03623	-0.01738

ORBITAL ENERGIES, HARTREES -26.3635 -11.3924 -1.6701 -0.8908 -0.5715

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00238	-0.00891
2 1 1	2.77900	-0.02181	-0.18009
2 1 1	1.62500	-0.12960	-0.48796
2 1 1	1.05400	0.00320	-0.42332
3 2 1	2.06000	-0.03221	-0.00305
3 2 1	0.33000	0.00030	0.00801
2 1 1	-9.43500	-0.01057	0.00144
2 1 1	-4.24900	-0.24705	0.09937
2 1 1	-2.35600	-0.45273	0.07467
2 1 1	-1.43400	-0.33463	0.23471
3 2 1	-2.44269	-0.02759	-0.01034

ORBITAL ENERGIES, HARTREES -0.7223 -0.4137

TOTAL ENERGY, HARTREES -137.21953
 KINETIC ENERGY, HARTREES 137.05784
 POTENTIAL ENERGY, HARTREES -274.27737
 VIRIAL -2.00118

TABLE VIII. WAVEFUNCTION FOR CARBON-FLUORINE AT 2.70 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12562	0.00128	0.00339	0.00109
1 0 0	5.02500	-0.00002	-0.92540	0.05070	0.18280	0.16523
3 0 0	6.08100	0.00004	0.05435	0.01145	0.03756	0.00683
2 0 0	2.14100	-0.00006	-0.00123	-0.10912	-0.42374	-0.28414
2 0 0	1.35400	-0.00021	0.00054	-0.01586	-0.22461	-0.57672
2 1 0	6.82700	-0.00001	-0.00086	-0.00084	-0.00100	0.00451
2 1 0	2.77900	0.00009	-0.00373	-0.02070	-0.02130	0.08721
2 1 0	1.62500	-0.00033	0.00394	-0.08190	-0.12695	0.27697
2 1 0	1.05400	-0.00003	-0.00139	0.01861	0.06079	0.07915
3 2 0	2.06000	-0.00013	0.00010	-0.02195	-0.01932	0.03779
3 2 0	0.33000	-0.00001	-0.00002	0.00038	0.00113	0.00037
1 0 0	-14.20100	-0.08418	-0.00001	-0.00481	0.00182	0.00015
1 0 0	-7.93800	-0.95503	0.00012	0.26601	-0.07279	-0.00609
3 0 0	-9.96200	0.04239	-0.00006	0.02606	-0.00398	0.00093
2 0 0	-3.33200	-0.00342	0.00020	-0.52494	0.14799	0.00121
2 0 0	-2.05700	0.00053	-0.00094	-0.49865	0.20096	0.03791
2 1 0	-9.43500	-0.00039	-0.00002	-0.00209	-0.00803	0.00611
2 1 0	-4.24900	-0.00072	-0.00002	-0.00750	-0.16315	0.13954
2 1 0	-2.35600	0.00043	-0.00032	-0.06412	-0.33189	0.24813
2 1 0	-1.43400	0.00001	-0.00065	-0.00712	-0.19488	0.22436
3 2 0	-2.44269	0.00013	-0.00028	-0.01377	-0.03244	0.01855

ORBITAL ENERGIES, HARTREES -26.3416 -11.4116 -1.6269 -0.8642 -0.5759

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00222	0.00907
2 1 1	2.77900	-0.01779	0.18017
2 1 1	1.62500	-0.11311	0.51252
2 1 1	1.05400	-0.00443	0.38899
3 2 1	2.06000	-0.02879	0.00253
3 2 1	0.33000	-0.00036	-0.00705
2 1 1	-9.43500	-0.01022	-0.00125
2 1 1	-4.24900	-0.25160	-0.08969
2 1 1	-2.35600	-0.44182	-0.06772
2 1 1	-1.43400	-0.35231	-0.20584
3 2 1	-2.44269	-0.02478	0.00831

ORBITAL ENERGIES, HARTREES -0.6928 -0.4362

TOTAL ENERGY, HARTREES -137.20677
 KINETIC ENERGY, HARTREES 136.95445
 POTENTIAL ENERGY, HARTREES -274.16122
 VIRIAL -2.00184

TABLE IX. WAVEFUNCTION FOR CARBON-FLUORINE AT 3.00 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12554	0.00106	0.00380	0.00048
1 0 0	5.02500	-0.00002	-0.92574	0.03611	0.21374	0.13650
3 0 0	6.08100	0.00003	0.05457	0.00841	0.04025	0.00519
2 0 0	2.14100	0.00000	-0.00095	-0.07894	-0.48960	-0.24128
2 0 0	1.35400	-0.00017	0.00030	-0.02537	-0.34330	-0.46049
2 1 0	6.82700	-0.00001	-0.00079	-0.00105	-0.00092	0.00526
2 1 0	2.77900	0.00009	-0.00309	-0.00932	-0.00127	0.06890
2 1 0	1.62500	-0.00025	0.00326	-0.06497	-0.08697	0.28371
2 1 0	1.05400	-0.00003	-0.00117	0.00855	0.05523	0.07747
3 2 0	2.06000	-0.00010	0.00015	-0.01725	-0.01185	0.03680
3 2 0	0.33000	-0.00001	-0.00003	-0.00030	0.00111	-0.00036
1 0 0	-14.20100	-0.08417	-0.00001	-0.00513	0.00148	-0.00005
1 0 0	-7.93800	-0.95506	0.00007	0.26972	-0.05998	0.00518
3 0 0	-9.96200	0.04238	-0.00006	0.02487	-0.00344	0.00194
2 0 0	-3.33200	-0.00326	0.00022	-0.52761	0.12184	-0.02409
2 0 0	-2.05700	0.00034	-0.00065	-0.51996	0.16281	0.00367
2 1 0	-9.43500	-0.00035	-0.00002	-0.00158	-0.00612	0.00727
2 1 0	-4.24900	-0.00056	-0.00001	-0.00174	-0.12763	0.17579
2 1 0	-2.35600	0.00032	-0.00015	-0.04264	-0.24972	0.29618
2 1 0	-1.43400	0.00001	-0.00056	-0.00613	-0.16429	0.28742
3 2 0	-2.44269	0.00014	-0.00023	-0.00910	-0.02425	0.02083

ORBITAL ENERGIES, HARTREES	-26.3007	-11.4476	-1.5572	-0.8295	-0.5725
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N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00178	-0.00929
2 1 1	2.77900	-0.01368	-0.18043
2 1 1	1.62500	-0.08095	-0.55112
2 1 1	1.05400	-0.01895	-0.33684
3 2 1	2.06000	-0.02277	-0.00049
3 2 1	0.33000	-0.00195	0.00582
2 1 1	-9.43500	-0.00960	0.00090
2 1 1	-4.24900	-0.25908	0.07247
2 1 1	-2.35600	-0.42402	0.05412
2 1 1	-1.43400	-0.37935	0.15938
3 2 1	-2.44269	-0.01985	-0.00515

ORBITAL ENERGIES, HARTREES	-0.6427	-0.4751
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TOTAL ENERGY, HARTREES	-137.17290
KINETIC ENERGY, HARTREES	-136.83030
POTENTIAL ENERGY, HARTREES	-274.00321
VIRIAL	-2.00250

TABLE X. WAVEFUNCTION FOR CF POSITIVE ION AT 1.95 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00000	-0.12581	-0.00039	0.00016	-0.00359
1 0 0	5.02500	0.00000	-0.92433	0.12987	-0.13731	-0.19162
3 0 0	6.08100	0.00006	0.05346	0.01055	-0.02028	-0.03088
2 0 0	2.14100	-0.00028	-0.00060	-0.18388	0.26936	0.44221
2 0 0	1.35400	-0.00047	0.00032	0.03741	0.01194	0.52260
2 1 0	6.82700	0.00000	-0.00110	0.00034	-0.00058	-0.00501
2 1 0	2.77900	0.00007	-0.00648	-0.16331	0.09956	-0.12642
2 1 0	1.62500	-0.00061	0.00622	-0.08059	0.09731	-0.37324
2 1 0	1.05400	-0.00015	-0.00286	0.02526	-0.01918	-0.00921
3 2 0	2.06000	-0.00025	-0.00111	-0.04010	0.03309	-0.04762
3 2 0	0.33000	-0.00002	-0.00001	0.00118	0.00027	0.00098
1 0 0	-14.20100	-0.08420	0.00003	-0.00371	-0.00264	-0.00033
1 0 0	-7.93800	-0.95480	0.00096	0.25400	0.11123	0.02936
3 0 0	-9.96200	0.04233	0.00014	0.03237	0.00530	0.00571
2 0 0	-3.33200	-0.00401	-0.00125	-0.52426	-0.22458	-0.07736
2 0 0	-2.05700	0.00144	-0.00091	-0.37869	-0.34023	-0.03807
2 1 0	-9.43500	-0.00052	0.00004	-0.00365	0.01040	-0.00266
2 1 0	-4.24900	-0.00159	-0.00086	-0.05133	0.21491	-0.06182
2 1 0	-2.35600	0.00109	-0.00084	-0.15990	0.49768	-0.14761
2 1 0	-1.43400	-0.00023	-0.00112	-0.02434	0.10847	-0.02320
3 2 0	-2.44269	-0.00008	-0.00085	-0.04059	0.04902	-0.01339

ORBITAL ENERGIES, HARTREES	-26.9052	-11.8418	-2.3503	-1.4409	-0.9563
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N L M	ZETA	1 π
2 1 1	6.82700	-0.00239
2 1 1	2.77900	-0.06614
2 1 1	1.62500	-0.21798
2 1 1	1.05400	0.03899
3 2 1	2.06000	-0.05755
3 2 1	0.33000	0.00221
2 1 1	-9.43500	-0.01266
2 1 1	-4.24900	-0.21873
2 1 1	-2.35600	-0.54897
2 1 1	-1.43400	-0.16493
3 2 1	-2.44269	-0.05188

ORBITAL ENERGIES, HARTREES	-1.2853
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TOTAL ENERGY, HARTREES	-136.87862
KINETIC ENERGY, HARTREES	137.44473
POTENTIAL ENERGY, HARTREES	-274.32335
VIRIAL	-1.99588

TABLE XI. WAVEFUNCTION FOR CF POSITIVE ION AT 2.10 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12567	0.00032	-0.00086	0.00320
1 0 0	5.02500	-0.00001	-0.92513	0.10988	-0.14385	0.19386
3 0 0	6.08100	0.00006	0.05406	0.01384	-0.02719	0.03059
2 0 0	2.14100	-0.00024	-0.00036	-0.18713	0.32291	-0.45247
2 0 0	1.35400	-0.00036	0.00056	0.03193	0.03117	-0.50519
2 1 0	6.82700	0.00000	-0.00107	0.00038	-0.00049	0.00515
2 1 0	2.77900	0.00007	-0.00585	-0.08351	0.08361	0.11871
2 1 0	1.62500	-0.00054	0.00606	-0.09486	0.11734	0.38071
2 1 0	1.05400	-0.00010	-0.00247	0.03226	-0.03027	0.00413
3 2 0	2.06000	-0.00022	-0.00066	-0.03675	0.03180	0.04645
3 2 0	0.33000	-0.00002	-0.00002	0.00121	0.00025	-0.00094
1 0 0	-14.20100	-0.08417	0.00001	-0.00386	-0.00262	0.00021
1 0 0	-7.93800	-0.95496	0.00057	0.25490	0.10868	-0.02347
3 0 0	-9.96200	0.04241	0.00003	0.03115	0.00574	-0.00455
2 0 0	-3.33200	-0.00376	-0.00051	-0.52437	-0.22245	0.06057
2 0 0	-2.05700	0.00114	-0.00147	-0.40259	-0.31693	0.03369
2 1 0	-9.43500	-0.00053	0.00000	-0.00353	0.01042	0.00353
2 1 0	-4.24900	-0.00140	-0.00039	-0.03948	0.20313	0.07287
2 1 0	-2.35600	0.00095	-0.00085	-0.14057	0.47915	0.17562
2 1 0	-1.43400	-0.00017	-0.00103	-0.02293	0.11589	0.04429
3 2 0	-2.44269	-0.00001	-0.00063	-0.03476	0.04707	0.01327

ORBITAL ENERGIES, HARTREES -26.8752 -11.8697 -2.2676 -1.4002 -0.9687

N L M	ZETA	1 π
2 1 1	6.82700	-0.00293
2 1 1	2.77900	-0.04924
2 1 1	1.62500	-0.22033
2 1 1	1.05400	0.03832
3 2 1	2.06000	-0.05430
3 2 1	0.33000	0.00256
2 1 1	-9.43500	-0.01250
2 1 1	-4.24900	-0.22303
2 1 1	-2.35600	-0.53465
2 1 1	-1.43400	-0.19671
3 2 1	-2.44269	-0.04802

ORBITAL ENERGIES, HARTREES -1.2292

TOTAL ENERGY, HARTREES -136.90399
 KINETIC ENERGY, HARTREES 136.99534
 POTENTIAL ENERGY, HARTREES -273.89933
 VIRIAL -1.99933

TABLE XII. WAVEFUNCTION FOR CF POSITIVE ION AT 2.146 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12563	0.00051	-0.00116	0.00309
1 0 0	5.02500	-0.00001	-0.92533	0.10448	-0.14660	0.19403
3 0 0	6.08100	0.00007	0.05421	0.01461	-0.02926	0.03046
2 0 0	2.14100	-0.00023	-0.00029	-0.18654	0.33943	-0.45453
2 0 0	1.35400	-0.00034	0.00058	0.02976	0.03901	-0.49897
2 1 0	6.82700	0.00000	-0.00106	0.00033	-0.00041	0.00321
2 1 0	2.77900	0.00007	-0.00569	-0.07729	0.07863	0.11642
2 1 0	1.62500	-0.00052	0.00598	-0.09829	0.12250	0.38302
2 1 0	1.05400	-0.00008	-0.00239	0.03375	-0.03305	0.00276
3 2 0	2.06000	-0.00021	-0.00056	-0.03577	0.03140	0.04619
3 2 0	0.33000	-0.00001	-0.00002	0.00121	0.00025	-0.00092
1 0 0	-14.20100	-0.08417	0.00001	-0.00392	-0.00260	0.00018
1 0 0	-7.93800	-0.95499	0.00049	0.25542	0.10761	-0.02155
3 0 0	-9.96200	0.04242	0.00001	0.03081	0.00586	-0.00418
2 0 0	-3.33200	-0.00370	-0.00035	-0.52479	-0.22121	0.05514
2 0 0	-2.05700	0.00106	-0.00155	-0.40962	-0.30972	0.03160
2 1 0	-9.43500	-0.00053	-0.00001	-0.00347	0.01037	0.00381
2 1 0	-4.24900	-0.00135	-0.00030	-0.03628	0.19947	0.07673
2 1 0	-2.35600	0.00092	-0.00082	-0.13448	0.47220	0.18462
2 1 0	-1.43400	-0.00016	-0.00102	-0.02275	0.11826	0.05117
3 2 0	-2.44269	0.00001	-0.00059	-0.03307	0.04641	0.01345

ORBITAL ENERGIES, HARTREES -26.8658 -11.8783 -2.2435 -1.3877 -0.9723

N L M	ZETA	1 π
2 1 1	6.82700	-0.00307
2 1 1	2.77900	-0.04496
2 1 1	1.62500	-0.21958
2 1 1	1.05400	0.03736
3 2 1	2.06000	-0.05321
3 2 1	0.33000	0.00263
2 1 1	-9.43500	-0.01243
2 1 1	-4.24900	-0.22450
2 1 1	-2.35600	-0.53035
2 1 1	-1.43400	-0.20579
3 2 1	-2.44269	-0.04692

ORBITAL ENERGIES, HARTREES -1.2132

TOTAL ENERGY, HARTREES -136.90513
 KINETIC ENERGY, HARTREES 136.88795
 POTENTIAL ENERGY, HARTREES -273.79308
 VIRIAL -2.00018

TABLE XIII. WAVEFUNCTION FOR CF POSITIVE ION AT 2.25 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12556	0.00088	-0.00181	0.00281
1 0 0	5.02500	-0.00002	-0.92573	0.09334	-0.15420	0.19324
3 0 0	6.08100	0.00007	0.05451	0.01589	-0.03378	0.02999
2 0 0	2.14100	-0.00021	-0.00014	-0.18290	0.37737	-0.45629
2 0 0	1.35400	-0.00029	0.00058	0.02431	0.06011	-0.48335
2 1 0	6.82700	0.00000	-0.00106	0.00014	-0.00019	0.00536
2 1 0	2.77900	0.00008	-0.00537	-0.06422	0.06731	0.11144
2 1 0	1.62500	-0.00049	0.00579	-0.10420	0.13168	0.38857
2 1 0	1.05400	-0.00006	-0.00222	0.03602	-0.03815	-0.00004
3 2 0	2.06000	-0.00019	-0.00039	-0.03359	0.03035	0.04574
3 2 0	0.33000	-0.00001	-0.00002	0.00116	0.00030	-0.00082
1 0 0	-14.20100	-0.08415	0.00000	-0.00406	-0.00254	0.00010
1 0 0	-7.93800	-0.95507	0.00036	0.25608	0.10481	-0.01693
3 0 0	-9.96200	0.04246	-0.00003	0.03008	0.00610	-0.00333
2 0 0	-3.33200	-0.00357	-0.00007	-0.52621	-0.21752	0.04218
2 0 0	-2.05700	0.00091	-0.00162	-0.42486	-0.29337	0.02548
2 1 0	-9.43500	-0.00053	-0.00002	-0.00330	0.01020	0.00444
2 1 0	-4.24900	-0.00125	-0.00016	-0.02975	0.19085	0.08630
2 1 0	-2.35600	0.00085	-0.00074	-0.12071	0.45407	0.20586
2 1 0	-1.43400	-0.00014	-0.00101	-0.02265	0.12331	0.06758
3 2 0	-2.44269	0.00005	-0.00052	-0.02943	0.04478	0.01422
ORBITAL ENERGIES, HARTREES		-26.8443	-11.8972	-2.1918	-1.3602	-0.9796

N L M	ZETA	1 π
2 1 1	6.82700	-0.00331
2 1 1	2.77900	-0.03662
2 1 1	1.62500	-0.21573
2 1 1	1.05400	0.03413
3 2 1	2.06000	-0.05066
3 2 1	0.33000	0.00275
2 1 1	-9.43500	-0.01226
2 1 1	-4.24900	-0.22797
2 1 1	-2.35600	-0.52095
2 1 1	-1.43400	-0.22511
3 2 1	-2.44269	-0.04453
ORBITAL ENERGIES, HARTREES		-1.1790

TOTAL ENERGY, HARTREES	-136.89991
KINETIC ENERGY, HARTREES	136.68649
POTENTIAL ENERGY, HARTREES	-273.58639
VIRIAL	-2.00156

TABLE XIV. WAVEFUNCTION FOR CF POSITIVE ION AT 2.3789 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00002	-0.12547	0.00121	0.00253	0.00245
1 0 0	5.02500	-0.00003	-0.92614	0.08138	0.16633	0.18940
3 0 0	6.08100	0.00007	0.05481	0.01666	0.03907	0.02892
2 0 0	2.14100	-0.00018	0.00003	-0.17475	-0.42614	-0.45110
2 0 0	1.35400	-0.00025	0.00051	0.01703	-0.09264	-0.46052
2 1 0	6.82700	0.00000	-0.00104	-0.00017	-0.00013	0.00559
2 1 0	2.77900	0.00008	-0.00500	-0.05005	-0.05331	0.10557
2 1 0	1.62500	-0.00046	0.00550	-0.10800	-0.13691	0.39660
2 1 0	1.05400	-0.00003	-0.00206	0.03691	0.04200	-0.00291
3 2 0	2.06000	-0.00018	-0.00027	-0.03096	-0.02864	0.04547
3 2 0	0.33000	-0.00001	-0.00003	0.00104	-0.00041	-0.00066
1 0 0	-14.20100	-0.08414	0.00000	-0.00424	0.00242	0.00000
1 0 0	-7.93800	-0.95513	0.00026	0.25905	-0.10065	-0.01052
3 0 0	-9.96200	0.04248	-0.00006	0.02929	-0.00634	-0.00223
2 0 0	-3.33200	-0.00344	0.00014	-0.52862	0.21126	0.02465
2 0 0	-2.05700	0.00075	-0.00156	-0.44233	0.27304	0.01521
2 1 0	-9.43500	-0.00053	-0.00003	-0.00304	-0.00982	0.00525
2 1 0	-4.24900	-0.00114	-0.00006	-0.02286	-0.17904	0.09966
2 1 0	-2.35600	0.00077	-0.00061	-0.10410	-0.42649	0.23394
2 1 0	-1.43400	-0.00012	-0.00099	-0.02288	-0.12811	0.08975
3 2 0	-2.44269	0.00008	-0.00046	-0.02534	-0.04245	0.01585

ORBITAL ENERGIES, HARTREES -26.8177 -11.9195 -2.1331 -1.3280 -0.9867

N L M	ZETA	1 π
2 1 1	6.82700	-0.00350
2 1 1	2.77900	-0.02856
2 1 1	1.62500	-0.20747
2 1 1	1.05400	0.02848
3 2 1	2.06000	-0.04734
3 2 1	0.33000	0.00280
2 1 1	-9.43500	-0.01201
2 1 1	-4.24900	-0.23246
2 1 1	-2.35600	-0.51009
2 1 1	-1.43400	-0.24666
3 2 1	-2.44269	-0.04169

ORBITAL ENERGIES, HARTREES -1.1401

TOTAL ENERGY, HARTREES -136.88209
 KINETIC ENERGY, HARTREES 136.50089
 POTENTIAL ENERGY, HARTREES -273.38387
 VIRIAL -2.00280

TABLE XV. WAVEFUNCTION FOR CF POSITIVE ION AT 2.55 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00002	-0.12538	0.00145	0.00331	-0.00191
1 0 0	5.02500	-0.00003	-0.92656	0.06809	0.18663	-0.17812
3 0 0	6.08100	0.00007	0.05512	0.01651	0.04544	-0.02628
2 0 0	2.14100	-0.00014	0.00023	-0.15969	-0.49405	0.42756
2 0 0	1.35400	-0.00020	0.00034	0.00746	-0.14493	0.42256
2 1 0	6.82700	-0.00001	-0.00102	-0.00059	-0.00048	-0.00599
2 1 0	2.77900	0.00010	-0.00454	-0.03482	-0.03534	-0.09821
2 1 0	1.62500	-0.00043	0.00503	-0.10766	-0.13119	-0.40986
2 1 0	1.05400	-0.00001	-0.00187	0.03539	0.04284	0.00524
3 2 0	2.06000	-0.00016	-0.00018	-0.02756	-0.02545	-0.04549
3 2 0	0.33000	-0.00001	-0.00003	0.00083	-0.00060	0.00034
1 0 0	-14.20100	-0.08413	-0.00001	-0.00448	0.00223	0.00015
1 0 0	-7.93800	-0.95520	0.00018	0.26221	-0.09397	0.00086
3 0 0	-9.96200	0.04250	-0.00008	0.02841	-0.00650	0.00069
2 0 0	-3.33200	-0.00330	0.00027	-0.53245	0.19976	0.00101
2 0 0	-2.05700	0.00059	-0.00133	-0.46263	0.24586	0.00252
2 1 0	-9.43500	-0.00052	-0.00003	-0.00265	-0.00900	-0.00635
2 1 0	-4.24900	-0.00101	-0.00001	-0.01558	-0.16038	-0.11927
2 1 0	-2.35600	0.00067	-0.00045	-0.08358	-0.38017	-0.27272
2 1 0	-1.43400	-0.00010	-0.00094	-0.02338	-0.12968	-0.12232
3 2 0	-2.44269	0.00012	-0.00041	-0.02063	-0.03871	-0.01892

ORBITAL ENERGIES, HARTREES	-26.7834	-11.9463	-2.0641	-1.2907	-0.9905
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N L M	ZETA	1 π
2 1 1	6.82700	-0.00357
2 1 1	2.77900	-0.02100
2 1 1	1.62500	-0.19181
2 1 1	1.05400	0.01922
3 2 1	2.06000	-0.04281
3 2 1	0.33000	0.00269
2 1 1	-9.43500	-0.01166
2 1 1	-4.24900	-0.23849
2 1 1	-2.35600	-0.49750
2 1 1	-1.43400	-0.27112
3 2 1	-2.44269	-0.03800

ORBITAL ENERGIES, HARTREES	-1.0942
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TOTAL ENERGY, HARTREES	-136.85052
KINETIC ENERGY, HARTREES	136.33372
POTENTIAL ENERGY, HARTREES	-273.18423
VIRIAL	-2.00379

TABLE XVI. WAVEFUNCTION FOR CF POSITIVE ION AT 2.70 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00002	0.12531	0.00150	0.00381	-0.00139
1 0 0	5.02500	-0.00003	0.92683	0.05836	0.20660	-0.16194
3 0 0	6.08100	0.00007	-0.05533	0.01556	0.05023	-0.02280
2 0 0	2.14100	-0.00011	-0.00038	-0.14418	-0.55346	0.39000
2 0 0	1.35400	-0.00018	-0.00017	-0.00008	-0.19477	0.38072
2 1 0	6.82700	-0.00001	0.00098	-0.00089	-0.00064	-0.00642
2 1 0	2.77900	0.00011	0.00414	-0.02460	-0.02102	-0.09204
2 1 0	1.62500	-0.00040	-0.00457	-0.10338	-0.11448	-0.42306
2 1 0	1.05400	0.00001	0.00171	0.03226	0.04004	0.00488
3 2 0	2.06000	-0.00014	0.00016	-0.02469	-0.02187	-0.04562
3 2 0	0.33000	-0.00001	0.00003	0.00061	-0.00078	-0.00001
1 0 0	-14.20100	-0.08413	0.00001	-0.00467	0.00203	0.00028
1 0 0	-7.93800	-0.95523	-0.00013	0.26497	-0.08690	-0.00808
3 0 0	-9.96200	0.04251	0.00008	0.02780	-0.00640	-0.00068
2 0 0	-3.33200	-0.00321	-0.00029	-0.53608	0.18617	0.02424
2 0 0	-2.05700	0.00048	0.00108	-0.47755	0.22157	0.01998
2 1 0	-9.43500	-0.00050	0.00003	-0.00231	-0.00801	-0.00725
2 1 0	-4.24900	-0.00092	0.00000	-0.01069	-0.14085	-0.13649
2 1 0	-2.35600	0.00060	0.00032	-0.06744	-0.33118	-0.30413
2 1 0	-1.43400	-0.00008	0.00086	-0.02375	-0.12478	-0.15265
3 2 0	-2.44269	0.00015	0.00037	-0.01713	-0.03478	-0.02199

ORBITAL ENERGIES, HARTREES -26.7552 -11.9666 -2.0120 -1.2652 -0.9870

N L M	ZETA	1 σ
2 1 1	6.82700	-0.00347
2 1 1	2.77900	-0.01656
2 1 1	1.62500	-0.17476
2 1 1	1.05400	0.01048
3 2 1	2.06000	-0.03878
3 2 1	0.33000	0.00248
2 1 1	-9.43500	-0.01137
2 1 1	-4.24900	-0.24367
2 1 1	-2.35600	-0.48854
2 1 1	-1.43400	-0.28874
3 2 1	-2.44269	-0.03481

ORBITAL ENERGIES, HARTREES -1.0592

TOTAL ENERGY, HARTREES -136.81783
 KINETIC ENERGY, HARTREES 136.23834
 POTENTIAL ENERGY, HARTREES -273.05617
 VIRIAL -2.00425

TABLE XVII. WAVEFUNCTION FOR CF NEGATIVE ION AT 2.10 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12600	0.00029	0.00029	0.00177
1 0 0	5.02500	-0.00001	-0.92366	0.09966	0.14223	0.16502
3 0 0	6.08100	0.00005	0.05315	0.00943	0.02081	-0.00858
2 0 0	2.14100	-0.00024	-0.00235	-0.14556	-0.25754	-0.18280
2 0 0	1.35400	-0.00041	0.00035	0.00557	-0.01848	-0.86665
2 1 0	6.82700	0.00000	-0.00086	0.00013	0.00029	-0.00059
2 1 0	2.77900	0.00007	-0.00500	-0.07363	-0.08325	0.16442
2 1 0	1.62500	-0.00051	0.00437	-0.07591	-0.10628	0.08044
2 1 0	1.05400	-0.00011	-0.00185	0.01911	0.05216	0.18794
3 2 0	2.06000	-0.00020	-0.00053	-0.03281	-0.02702	0.02894
3 2 0	0.33000	-0.00001	0.00001	0.00140	0.00262	0.00926
1 0 0	-14.20100	-0.08425	0.00002	-0.00405	0.00224	0.00077
1 0 0	-7.93800	-0.95463	0.00054	0.25813	-0.08688	-0.02865
3 0 0	-9.96200	0.04221	0.00013	0.02929	-0.00304	0.00315
2 0 0	-3.93200	-0.00418	-0.00097	-0.51551	0.16585	0.03515
2 0 0	-2.05700	0.00131	-0.00024	-0.43595	0.26371	0.18289
2 1 0	-9.43500	-0.00037	0.00003	-0.00301	-0.00946	0.00345
2 1 0	-4.24900	-0.00112	-0.00058	-0.03236	-0.21306	0.07419
2 1 0	-2.35600	0.00070	-0.00058	-0.12760	-0.41569	0.12149
2 1 0	-1.43400	0.00006	-0.00049	-0.00111	-0.24223	0.18194
3 2 0	-2.44269	0.00007	-0.00048	-0.02881	-0.04450	0.02143
ORBITAL ENERGIES, HARTREES		-26.1070	-10.9725	-1.5289	-0.6902	-0.2220

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00146	0.00085
2 1 1	2.77900	-0.04965	0.22512
2 1 1	1.62500	-0.13523	-0.03551
2 1 1	1.05400	0.01764	0.94676
3 2 1	2.06000	-0.03712	0.00463
3 2 1	0.33000	-0.00691	-0.24655
2 1 1	-9.43500	-0.01098	-0.00087
2 1 1	-4.24900	-0.23731	-0.12116
2 1 1	-2.35600	-0.46869	-0.03390
2 1 1	-1.43400	-0.29963	-0.37716
3 2 1	-2.44269	-0.03085	0.01830
ORBITAL ENERGIES, HARTREES		-0.5347	0.0218

TOTAL ENERGY, HARTREES	-137.12383
KINETIC ENERGY, HARTREES	138.03054
POTENTIAL ENERGY, HARTREES	-275.15437
VIRIAL	-1.99343

TABLE XVIII. WAVEFUNCTION FOR CF NEGATIVE ION AT 2.25 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12594	0.00074	-0.00110	0.00106
1 0 0	5.02500	-0.00001	-0.92401	0.08152	-0.14495	0.16780
3 0 0	6.08100	0.00005	0.05342	0.01034	-0.02396	-0.01179
2 0 0	2.14100	-0.00018	-0.00228	-0.13325	0.28108	-0.17019
2 0 0	1.35400	-0.00034	0.00049	-0.00477	0.05730	-0.85534
2 1 0	6.82700	0.00000	-0.00083	-0.00007	0.00010	-0.00023
2 1 0	2.77900	0.00008	-0.00446	-0.05436	0.06601	0.14869
2 1 0	1.62500	-0.00045	0.00413	-0.07983	0.12474	0.09163
2 1 0	1.05400	-0.00008	-0.00159	0.01940	-0.06504	0.18630
3 2 0	2.06000	-0.00018	-0.00020	-0.02922	0.02497	0.02961
3 2 0	0.33000	-0.00001	0.00000	0.00126	-0.00364	0.00774
1 0 0	-14.20100	-0.08423	0.00001	-0.00428	-0.00210	0.00073
1 0 0	-7.93800	-0.95473	0.00033	0.26030	0.07980	-0.02597
3 0 0	-9.96200	0.04226	0.00006	0.02802	0.00289	0.00279
2 0 0	-3.33200	-0.00397	-0.00051	-0.51620	-0.15323	0.03064
2 0 0	-2.05700	0.00106	-0.00056	-0.45946	-0.23774	0.15779
2 1 0	-9.43500	-0.00035	0.00001	-0.00276	0.00916	0.00372
2 1 0	-4.24900	-0.00093	-0.00032	-0.02225	0.20651	0.08929
2 1 0	-2.35600	0.00056	-0.00053	-0.10872	0.39326	0.13265
2 1 0	-1.43400	0.00009	-0.00047	0.00424	0.25552	0.21023
3 2 0	-2.44269	0.00010	-0.00034	-0.02299	0.04102	0.02008

ORBITAL ENERGIES, HARTREES -26.0629 -10.9502 -1.4431 -0.6299 -0.2066

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00149	0.00162
2 1 1	2.77900	-0.03761	0.22714
2 1 1	1.62500	-0.12028	0.01626
2 1 1	1.05400	0.01523	0.90310
3 2 1	2.06000	-0.03203	0.00547
3 2 1	0.33000	-0.00641	-0.14553
2 1 1	-9.43500	-0.01048	-0.00056
2 1 1	-4.24900	-0.24426	-0.11569
2 1 1	-2.35600	-0.44827	-0.02845
2 1 1	-1.43400	-0.33505	-0.34861
3 2 1	-2.44269	-0.02575	0.01596

ORBITAL ENERGIES, HARTREES -0.4741 0.0045

TOTAL ENERGY, HARTREES -137.16965
 KINETIC ENERGY, HARTREES 137.76382
 POTENTIAL ENERGY, HARTREES -274.93347
 VIRIAL -1.99569

TABLE XIX. WAVEFUNCTION FOR CF NEGATIVE ION AT 2.3789 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12589	0.00096	0.00166	0.00063
1 0 0	5.02500	-0.00002	-0.92426	0.06869	0.14856	0.16980
3 0 0	6.08100	0.00004	0.05361	0.01034	0.02575	-0.01258
2 0 0	2.14100	-0.00013	-0.00217	-0.12022	-0.29763	-0.17044
2 0 0	1.35400	-0.00029	0.00054	-0.01259	-0.09800	-0.83185
2 1 0	6.82700	0.00000	-0.00082	-0.00030	-0.00051	0.00030
2 1 0	2.77900	0.00008	-0.00412	-0.04098	-0.05179	0.13420
2 1 0	1.62500	-0.00040	0.00397	-0.07934	-0.13576	0.10612
2 1 0	1.05400	-0.00006	-0.00144	0.01775	0.07257	0.17895
3 2 0	2.06000	-0.00016	-0.00002	-0.02640	-0.02314	0.03042
3 2 0	0.33000	-0.00001	0.00000	0.00105	0.00437	0.00577
1 0 0	-14.20100	-0.08422	0.00001	-0.00447	0.00196	0.00067
1 0 0	-7.93800	-0.95480	0.00022	0.26232	-0.07390	-0.02353
3 0 0	-9.96200	0.04228	0.00002	0.02707	-0.00276	0.00234
2 0 0	-3.33200	-0.00382	-0.00025	-0.51732	0.14263	0.02758
2 0 0	-2.05700	0.00087	-0.00071	-0.47685	0.21769	0.13561
2 1 0	-9.43500	-0.00033	0.00000	-0.00252	-0.00884	0.00399
2 1 0	-4.24900	-0.00080	-0.00020	-0.01542	-0.20075	0.10278
2 1 0	-2.35600	0.00046	-0.00047	-0.09364	-0.37443	0.14633
2 1 0	-1.43400	0.00010	-0.00049	0.00733	-0.26179	0.23065
3 2 0	-2.44269	0.00012	-0.00028	-0.01882	-0.03779	0.01885

ORBITAL ENERGIES, HARTREES -26.0405 -10.9495 -1.3909 -0.5928 -0.2068

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00146	-0.00226
2 1 1	2.77900	-0.02998	-0.22486
2 1 1	1.62500	-0.10718	-0.05927
2 1 1	1.05400	0.01165	-0.85604
3 2 1	2.06000	-0.02833	-0.00550
3 2 1	0.33000	-0.00644	0.10134
2 1 1	-9.43500	-0.01009	0.00040
2 1 1	-4.24900	-0.24937	0.10803
2 1 1	-2.35600	-0.43408	0.02579
2 1 1	-1.43400	-0.35840	0.31689
3 2 1	-2.44269	-0.02226	-0.01397

ORBITAL ENERGIES, HARTREES -0.4393 -0.0128

TOTAL ENERGY, HARTREES -137.19238
 KINETIC ENERGY, HARTREES 137.58634
 POTENTIAL ENERGY, HARTREES -274.77872
 VIRIAL -1.99714

TABLE XX. WAVEFUNCTION FOR CF NEGATIVE ION AT 2.55 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12584	0.00106	0.00219	-0.00023
1 0 0	5.02500	-0.00002	-0.92454	0.05484	0.15555	-0.17039
3 0 0	6.08100	0.00004	0.05380	0.00947	0.02686	0.01218
2 0 0	2.14100	-0.00008	-0.00202	-0.10137	-0.31570	0.17623
2 0 0	1.35400	-0.00025	0.00052	-0.02128	-0.16035	0.79072
2 1 0	6.82700	-0.00001	-0.00080	-0.00058	-0.00102	-0.00103
2 1 0	2.77900	0.00008	-0.00375	-0.02738	-0.03456	-0.11584
2 1 0	1.62500	-0.00033	0.00373	-0.07414	-0.14181	-0.12285
2 1 0	1.05400	-0.00006	-0.00131	0.01348	0.07847	-0.16709
3 2 0	2.06000	-0.00014	0.00015	-0.02297	-0.02029	-0.03109
3 2 0	0.33000	-0.00001	-0.00001	0.00066	0.00523	-0.00303
1 0 0	-14.20100	-0.08421	0.00000	-0.00472	0.00177	-0.00058
1 0 0	-7.93800	-0.95486	0.00014	0.26490	-0.06635	0.02002
3 0 0	-9.96200	0.04230	-0.00002	0.02597	-0.00257	-0.00184
2 0 0	-3.33200	-0.00365	-0.00003	-0.51873	0.12878	-0.02300
2 0 0	-2.05700	0.00068	-0.00076	-0.49634	0.19352	-0.10896
2 1 0	-9.43500	-0.00031	-0.00001	-0.00222	-0.00830	-0.00442
2 1 0	-4.24900	-0.00065	-0.00010	-0.00851	-0.19233	-0.12167
2 1 0	-2.35600	0.00035	-0.00037	-0.07667	-0.34794	-0.16811
2 1 0	-1.43400	0.00011	-0.00051	0.01012	-0.26502	-0.25789
3 2 0	-2.44269	0.00012	-0.00024	-0.01433	-0.03326	-0.01748

ORBITAL ENERGIES, HARTREES -26.0175 -10.9580 -1.3371 -0.5526 -0.2131

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00134	-0.00297
2 1 1	2.77900	-0.02287	-0.22090
2 1 1	1.62500	-0.08948	-0.10831
2 1 1	1.05400	0.00536	-0.79879
3 2 1	2.06000	-0.02408	-0.00470
3 2 1	0.33000	-0.00715	0.07086
2 1 1	-9.43500	-0.00961	0.00024
2 1 1	-4.24900	-0.25510	0.09698
2 1 1	-2.35600	-0.41804	0.02298
2 1 1	-1.43400	-0.38299	0.27560
3 2 1	-2.44269	-0.01838	-0.01147

ORBITAL ENERGIES, HARTREES -0.4034 -0.0353

TOTAL ENERGY, HARTREES -137.20745
 KINETIC ENERGY, HARTREES 137.41718
 POTENTIAL ENERGY, HARTREES -274.62463
 VIRIAL -1.99847

TABLE XXI. WAVEFUNCTION FOR CF NEGATIVE ION AT 2.70 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00001	-0.12579	0.00103	0.00246	0.00000
1 0 0	5.02500	-0.00002	-0.92472	0.04515	0.16395	-0.16815
3 0 0	6.08100	0.00003	0.05392	0.00821	0.02687	0.01111
2 0 0	2.14100	-0.00003	-0.00189	-0.08491	-0.32984	0.18132
2 0 0	1.35400	-0.00022	0.00047	-0.02724	-0.22125	0.74727
2 1 0	6.82700	-0.00001	-0.00078	-0.00074	-0.00134	-0.00161
2 1 0	2.77900	0.00008	-0.00344	-0.01884	-0.02148	-0.10111
2 1 0	1.62500	-0.00028	0.00349	-0.06661	-0.13894	-0.13342
2 1 0	1.05400	-0.00006	-0.00121	0.00851	0.08070	-0.15658
3 2 0	2.06000	-0.00012	0.00023	-0.02025	-0.01731	-0.03116
3 2 0	0.33000	-0.00001	-0.00001	0.00025	0.00589	-0.00071
1 0 0	-14.20100	-0.08421	0.00000	-0.00491	0.00160	-0.00049
1 0 0	-7.93800	-0.95490	0.00010	0.26689	-0.06017	0.01666
3 0 0	-9.96200	0.04231	-0.00003	0.02512	-0.00238	-0.00154
2 0 0	-3.33200	-0.00353	0.00007	-0.51953	0.11700	-0.01818
2 0 0	-2.05700	0.00054	-0.00072	-0.51038	0.17468	-0.08806
2 1 0	-9.43500	-0.00028	-0.00001	-0.00197	-0.00772	-0.00483
2 1 0	-4.24900	-0.00054	-0.00006	-0.00411	-0.18355	-0.13929
2 1 0	-2.35600	0.00027	-0.00028	-0.06411	-0.32258	-0.18943
2 1 0	-1.43400	0.00010	-0.00051	0.01174	-0.26261	-0.28357
3 2 0	-2.44269	0.00012	-0.00022	-0.01124	-0.02918	-0.01655
ORBITAL ENERGIES, HARTREES		-25.9994	-10.9690	-1.2990	-0.5232	-0.2201

N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00119	-0.00347
2 1 1	2.77900	-0.01879	-0.21751
2 1 1	1.62500	-0.07430	-0.14444
2 1 1	1.05400	-0.00098	-0.75598
3 2 1	2.06000	-0.02090	-0.00339
3 2 1	0.33000	-0.00820	0.05595
2 1 1	-9.43500	-0.00921	0.00014
2 1 1	-4.24900	-0.25924	0.08762
2 1 1	-2.35600	-0.40578	0.02050
2 1 1	-1.43400	-0.40034	0.24324
3 2 1	-2.44269	-0.01552	-0.00943
ORBITAL ENERGIES, HARTREES		-0.3771	-0.0537

TOTAL ENERGY, HARTREES	-137.21199
KINETIC ENERGY, HARTREES	137.31693
POTENTIAL ENERGY, HARTREES	-274.52892
VIRIAL	-1.99924

TABLE XXII. WAVEFUNCTION FOR CF NEGATIVE ION AT 3.00 BOHRS.

N L M	ZETA	1 σ	2 σ	3 σ	4 σ	5 σ
1 0 0	9.05500	0.00000	-0.12572	0.00077	0.00265	-0.00022
1 0 0	5.02500	-0.00001	-0.92499	0.03095	0.18639	0.15385
3 0 0	6.08100	0.00001	0.05409	0.00519	0.02544	-0.00823
2 0 0	2.14100	0.00003	-0.00169	-0.05566	-0.35939	-0.18068
2 0 0	1.35400	-0.00018	0.00031	-0.03469	-0.35152	-0.63860
2 1 0	6.82700	-0.00001	-0.00071	-0.00085	-0.00148	0.00250
2 1 0	2.77900	0.00006	-0.00285	-0.00890	-0.00174	0.07576
2 1 0	1.62500	-0.00017	0.00291	-0.04765	-0.11430	0.14260
2 1 0	1.05400	-0.00007	-0.00101	-0.00259	0.08046	0.13771
3 2 0	2.06000	-0.00009	0.00032	-0.01564	-0.01033	0.02987
3 2 0	0.33000	-0.00001	-0.00002	-0.00067	0.00683	-0.00370
1 0 0	-14.20100	-0.08420	-0.00001	-0.00523	0.00130	0.00030
1 0 0	-7.93800	-0.95494	0.00006	0.26995	-0.04912	-0.00944
3 0 0	-9.96200	0.04230	-0.00004	0.02368	-0.00190	0.00120
2 0 0	-3.33200	-0.00336	0.00014	-0.51964	0.09479	0.00694
2 0 0	-2.05700	0.00035	-0.00053	-0.53149	0.14285	0.05129
2 1 0	-9.43500	-0.00023	-0.00001	-0.00154	-0.00629	0.00569
2 1 0	-4.24900	-0.00037	-0.00002	0.00126	-0.15934	0.17651
2 1 0	-2.35600	0.00016	-0.00014	-0.04527	-0.26486	0.23428
2 1 0	-1.43400	0.00009	-0.00045	0.01342	-0.23925	0.33972
3 2 0	-2.44269	0.00011	-0.00018	-0.00688	-0.02115	0.01510

ORBITAL ENERGIES, HARTREES	-25.9655	-10.9944	-1.2396	-0.4798	-0.2316
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N L M	ZETA	1 π	2 π
2 1 1	6.82700	-0.00080	-0.00426
2 1 1	2.77900	-0.01455	-0.21141
2 1 1	1.62500	-0.04665	-0.20397
2 1 1	1.05400	-0.01402	-0.68662
3 2 1	2.06000	-0.01582	0.00014
3 2 1	0.33000	-0.01107	0.03972
2 1 1	-9.43500	-0.00853	-0.00003
2 1 1	-4.24900	-0.26548	0.07107
2 1 1	-2.35600	-0.38491	0.01535
2 1 1	-1.43400	-0.42717	0.19029
3 2 1	-2.44269	-0.01099	-0.00596

ORBITAL ENERGIES, HARTREES	-0.3329	-0.0872
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TOTAL ENERGY, HARTREES	-137.20915
KINETIC ENERGY, HARTREES	137.20274
POTENTIAL ENERGY, HARTREES	-274.41109
VIRIAL	-2.00005

TABLE XXIII. Expectation Values of Selected Operators^a for CF(²II)

R , bohr	1.95	2.10	2.25	2.3789	2.3937	2.55	2.70	3.00
$3Z_A^2 - R_A^2$, bohr ²	68.21	79.87	92.39	103.9	105.2	120.1	135.3	168.5
R_A^{-1} , bohr ⁻¹	19.30	18.95	18.65	18.42	18.39	18.14	17.93	17.57
R_A^2 , bohr ²	57.15	62.88	69.13	74.88	75.56	83.05	90.70	107.4
Z_A^2 , bohr ²	41.79	47.58	53.84	59.58	60.26	67.72	75.34	91.95
$3Z_B^2 - R_B^2$, bohr ²	51.37	58.18	65.31	71.69	72.44	80.54	88.66	106.0
R_B^{-1} , bohr ⁻¹	29.52	29.32	29.15	29.02	29.01	28.88	28.77	28.59
R_B^2 , bohr ²	48.72	52.04	55.58	58.79	59.17	63.26	67.36	76.14
Z_B^2 , bohr ²	33.36	36.74	40.30	43.49	43.87	47.93	52.01	60.72
ζ	24.70	23.90	23.22	22.70	22.65	22.11	21.65	20.88
η	2.17	2.30	2.42	2.52	2.53	2.65	2.75	2.94
χ^2 , bohr ²	15.36	15.30	15.29	15.30	15.30	15.32	15.36	15.43
Z , bohr	2.16	2.58	3.01	3.38	3.42	3.88	4.32	5.21
Dipole moment, D ^b	1.94	1.44	0.93	0.48	0.42	-0.14	-0.69	-1.79
Quadrupole moment (x 10 ⁻²⁶ esu cm ²)	-2.30	-2.29	-2.21	-2.08	-2.06	-1.83	-1.55	-0.86

^a Center A = C, Center B = F.^b Positive dipole moment indicates negative end of dipole at the carbon atom.

TABLE XXIV. Expectation Values of Selected Operators^a for $CF^+(^1\Sigma)$

R , bohr	1.95	2.10	2.146	2.25	2.3789	2.55	2.70
$3Z_A^2 - R_A^2$, bohr ²	67.05	78.20	81.80	90.26	101.3	117.0	131.7
R_A^{-1} , bohr ⁻¹	18.80	18.44	18.34	18.13	17.89	17.61	17.40
R_A^2 , bohr ²	50.38	56.19	58.06	62.42	68.11	76.14	83.61
Z_A^2 , bohr ²	39.14	44.80	46.62	50.89	56.48	64.39	71.77
$3Z_B^2 - R_B^2$, bohr ²	44.30	50.19	52.04	56.35	61.87	69.56	76.68
R_B^{-1} , bohr ⁻¹	29.07	28.88	28.83	28.72	28.60	28.47	28.36
R_B^2 , bohr ²	39.01	42.18	43.18	45.47	48.38	52.41	56.10
Z_B^2 , bohr ²	27.77	30.79	31.74	33.94	36.75	40.66	44.26
ξ	22.00	21.39	21.22	20.85	20.45	19.97	19.61
η	2.42	2.55	2.59	2.68	2.79	2.92	3.02
X^2 , bohr ²	11.24	11.39	11.44	11.53	11.63	11.75	11.84
Z , bohr	2.92	3.34	3.47	3.77	4.15	4.65	5.09
Dipole moment, D ^b	0.02	-0.47	-0.63	-1.00	-1.47	-2.11	-2.65
Quadrupole moment							
($\times 10^{-26}$ esu cm ²)	-0.30	0.03	0.14	0.42	0.82	1.42	1.99

^a Center A = C, Center B = F.^b Positive dipole moment indicates negative end of dipole at the carbon atom.

TABLE XXV. Expectation Values of Selected Operators^a for $\text{CF}^-(^3\underline{\text{E}})$

R , bohr	2.10	2.25	2.3789	2.55	2.70	3.00
$3Z_A^2 - R_A^2$, bohr ²	84.08	94.02	105.0	121.3	136.8	170.8
R_A^{-1} , bohr ⁻¹	19.30	19.03	18.82	18.56	18.35	18.00
R_A^2 , bohr ²	86.97	83.41	86.38	93.18	100.4	116.8
Z_A^2 , bohr ²	57.02	59.14	63.80	71.50	79.06	95.88
$3Z_B^2 - R_B^2$, bohr ²	72.79	77.27	83.46	93.00	102.1	121.6
R_B^{-1} , bohr ⁻¹	29.64	29.49	29.37	29.22	29.11	28.92
R_B^2 , bohr ²	81.32	75.03	75.60	79.02	82.99	92.22
Z_B^2 , bohr ²	51.37	50.77	53.02	57.34	61.68	71.27
ζ	27.85	26.33	25.50	24.66	24.05	23.06
η	2.01	2.13	2.22	2.34	2.44	2.62
X^2 , bohr ²	29.95	24.26	22.58	21.68	21.31	20.95
Z , bohr	1.34	1.86	2.27	2.78	3.22	4.10
Dipole moment, D ^b	4.59	3.84	3.31	2.66	2.11	1.01
Quadrupole moment ($\times 10^{-26}$ esu cm ²)	-8.00	-5.94	-5.42	-5.20	-5.13	-5.01

^a Center A = C, Center B = F.^b Positive dipole moment indicates negative end of dipole at the carbon atom.

Figure 1. Charge-Density Diagrams for $\text{CF}(^2\Pi)$ at Hartree-Fock Minimum (A, total charge density; B, 1σ -orbital; C, 2σ -orbital; D, 3σ -orbital; E, 4σ -orbital).

Figure 2. Charge-Density Diagrams for $\text{CF}(^2\Pi)$ at Hartree-Fock Minimum (F, 5σ -orbital; G, 1π -orbital; H, 2π -orbital).

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