

SUPPLEMENTARY MATERIAL

Multistate Chemistry. Hiding and Unveiling *trans*-Chalcone in a Constrained Derivative of 4',7-Dihydroxyflavylium in Water.

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1 – NMR and ESI-MS spectra of compound F

2 – Concentration dependence of the absorption spectrum of Ct

3 – Photochemistry of Ct in CTAC micelles

4 – Computational details

1 – NMR and ESI.MS spectra of compound F

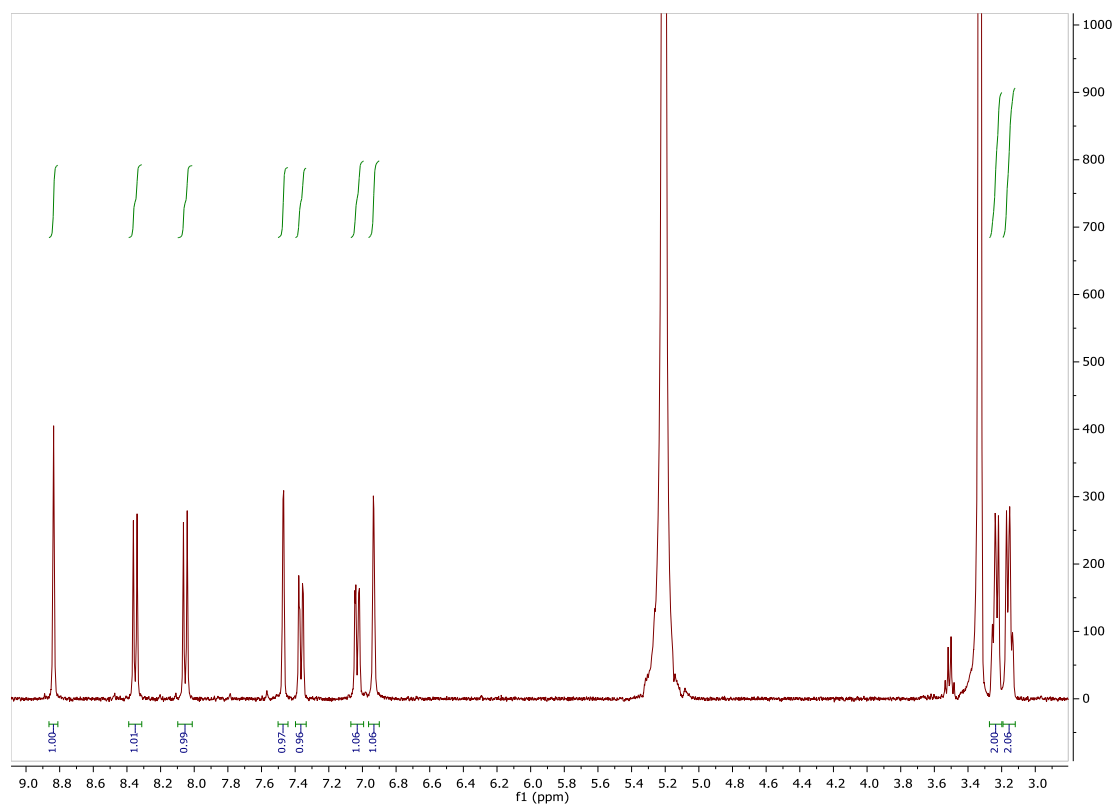


Figure S1. ¹H NMR spectrum of compound F in CD₃OD + DCl.

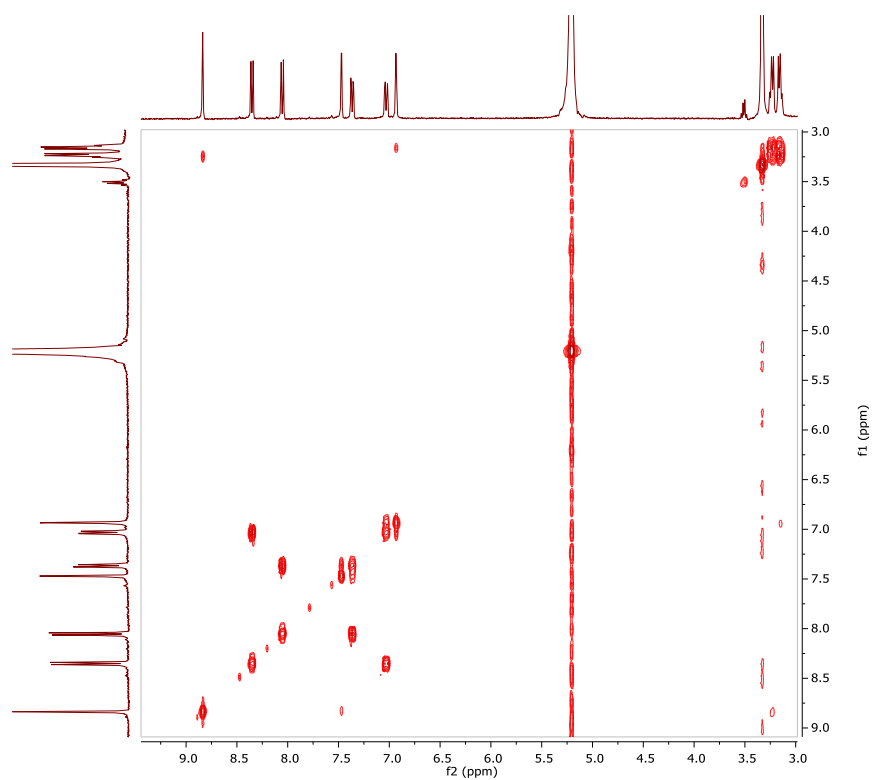


Figure S2. COSY spectrum of compound F in CD₃OD + DCl.

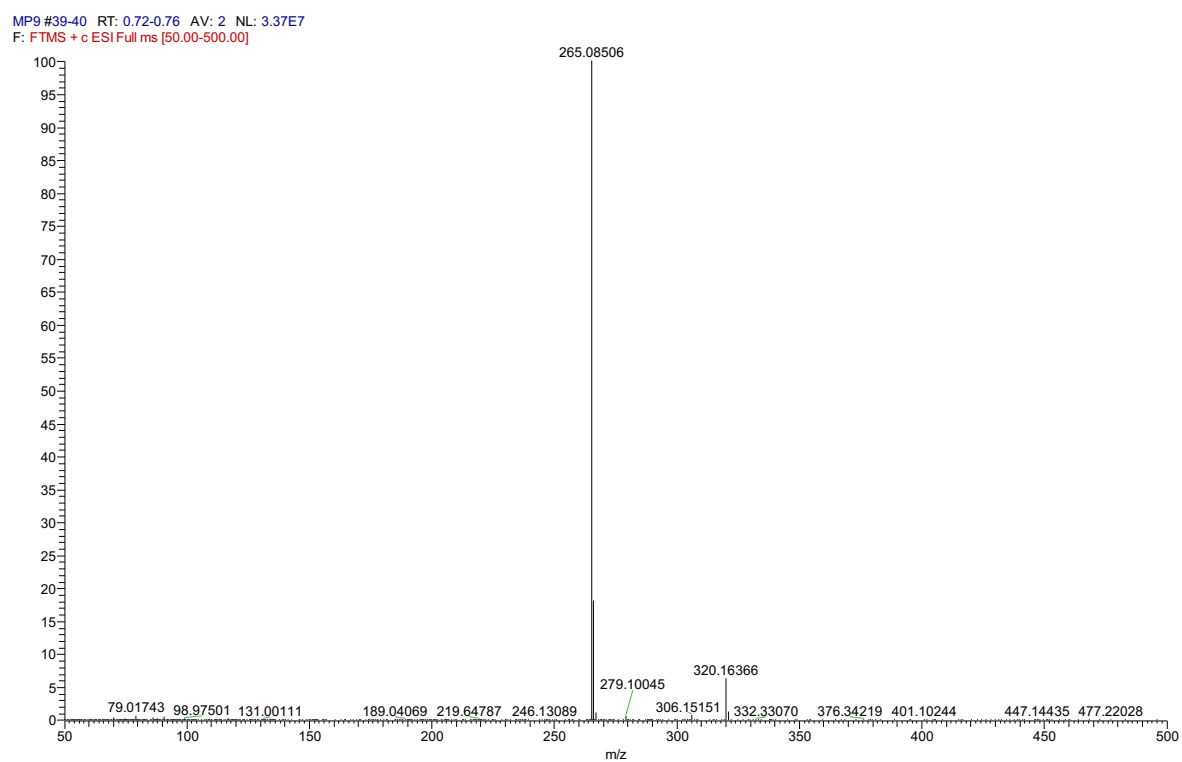
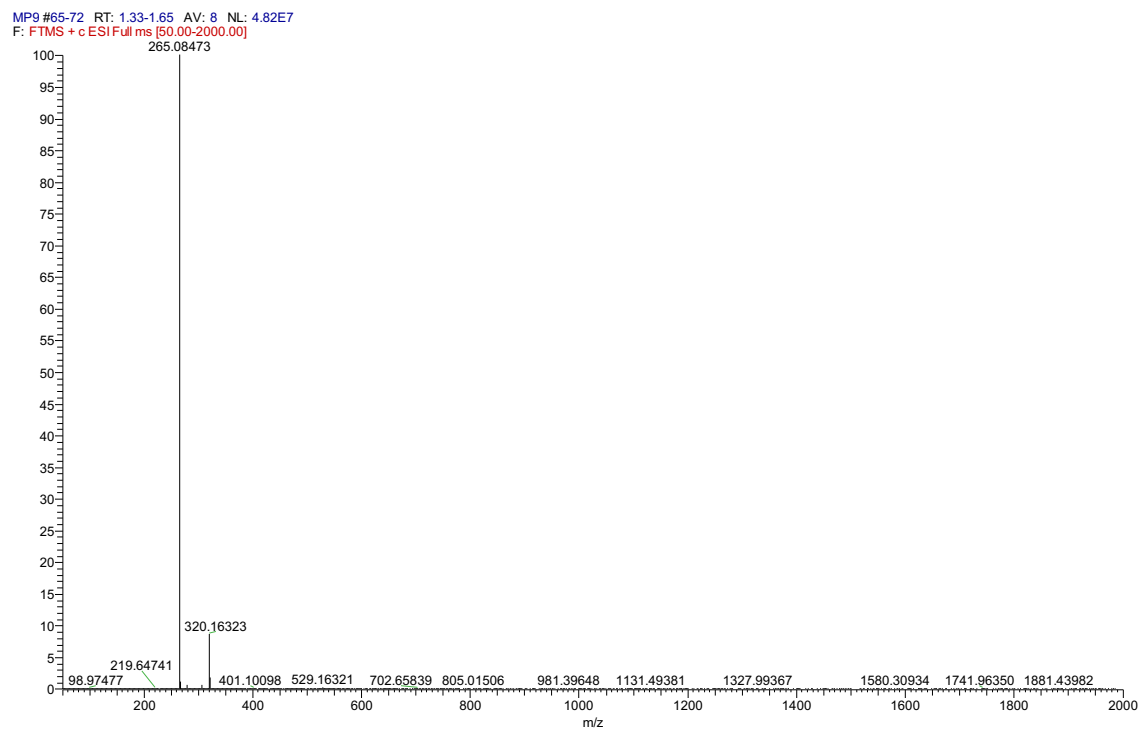


Figure S3. ESI-MS of compound F(positive mode).

2 – Concentration dependence of the absorption spectrum of Ct

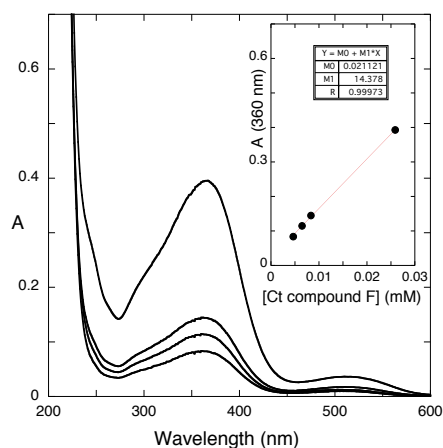


Figure S4. Absorption spectra of the *trans*-chalcone of compound **F** at different concentrations in the range 4.6 to 26 μM (covering the concentrations used in the relevant experiments in the manuscript).

The chalcone of compound **F** was obtained from a solution equilibrated at $\text{pH}=12$, where Ct^{2-} is practically the only species, followed by a reverse pH jump to $\text{pH}=6.5$, leading to almost pure **Ct**. (It should be pointed out that the kinetics of **Ct** transformation into quinoidal base is slow enough to safely run the spectrum of **Ct**.) The linearity dependence on the concentration (see inset) and the constant ratio of absorbances at the two maxima ($A_{360}/A_{510\sim 11}$) indicate that the low energy band it is not due to aggregation effects.

3 – Photochemistry of Ct in CTAC micelles

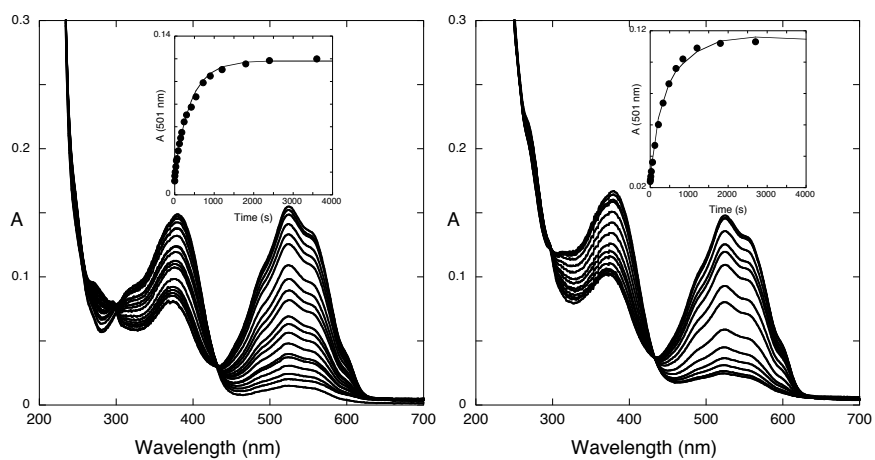


Figure S5. Spectral variations upon irradiation of compound **F**, 7.5×10^{-6} M, in the presence of 0.02 M CTABr (left, corresponding to Fig. 9b on the paper) or CTACl (right); $\lambda_{\text{irr}}=370$ nm, pH=5.6.

Inspection of Fig. S2 shows that the counter-ion of the CTA surfactant (bromide or chloride) does not have influence on the outcome of the photochemical reaction that transforms the quinoidal base **A** into the *trans*-chalcone **Ct**.

4 – Computational details

Atom Coordinates of optimized geometries

a) In vacuum

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	0.155468	-0.73120	2.33737	4.04829	12.01100
2	6	-0.037696	0.66039	2.28487	3.84903	12.01100
3	6	-0.005554	1.13079	1.77135	2.65813	12.01100
4	6	-0.004680	0.25851	1.27370	1.66522	12.01100
5	6	0.152007	-1.12609	1.29799	1.91755	12.01100
6	6	-0.059644	-1.63240	1.85233	3.10425	12.01100
7	8	-0.348178	-1.14004	2.88289	5.24206	15.99900
12	8	-0.348234	-1.98570	0.73407	1.00597	15.99900
14	8	-0.563333	2.53850	-0.65062	-1.15959	15.99900
15	6	0.327468	1.47323	-0.19832	-1.61418	12.01100
16	6	-0.013201	0.50771	0.52288	-0.75486	12.01100
17	6	0.025723	0.90744	0.68757	0.52071	12.01100
18	6	-0.020680	1.12421	-0.37953	-3.02504	12.01100
19	6	0.022078	1.90136	-1.27358	-3.77279	12.01100
20	6	-0.041214	1.63350	-1.46923	-5.12103	12.01100
21	6	0.165169	0.56419	-0.76618	-5.70548	12.01100
22	6	-0.063187	-0.22309	0.12559	-4.96266	12.01100
23	6	0.039644	0.06499	0.32626	-3.61176	12.01100
24	6	0.011153	-0.79279	0.93230	-1.34203	12.01100
25	6	0.006196	-0.70533	1.31022	-2.80847	12.01100
26	8	-0.346333	0.34308	-1.00198	-7.04145	15.99900
8	1	0.033700	1.33673	2.66260	4.62824	1.00800
13	1	0.218374	-2.88287	0.77376	1.37121	1.00800
9	1	0.031270	2.21801	1.73734	2.47591	1.00800
10	1	0.025809	-2.71461	1.88651	3.28727	1.00800
11	1	0.218409	-2.10698	2.84583	5.27872	1.00800
27	1	0.047367	2.73623	-1.80436	-3.28414	1.00800
28	1	0.032623	2.23623	-2.15344	-5.73423	1.00800
29	1	0.021790	-1.05285	0.66506	-5.44025	1.00800
30	1	0.010487	-1.20486	1.81238	-0.77747	1.00800
31	1	0.023388	-1.51954	0.08286	-1.21397	1.00800
32	1	0.018898	-0.20375	2.31253	-2.90880	1.00800
33	1	0.004115	-1.74497	1.41721	-3.21912	1.00800
34	1	0.219012	-0.41100	-0.46280	-7.32224	1.00800
35	1	0.041782	1.93279	0.31572	0.76545	1.00800

b) In water

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	0.152869	-0.76033	2.28404	4.05521	12.01100
2	6	-0.046161	0.62940	2.27236	3.85211	12.01100
3	6	-0.011347	1.10658	1.76246	2.66016	12.01100
4	6	-0.007409	0.25026	1.22279	1.67525	12.01100
5	6	0.159492	-1.13713	1.19823	1.91067	12.01100
6	6	-0.053955	-1.63860	1.72347	3.12010	12.01100
7	8	-0.357320	-1.19606	2.80895	5.24339	15.99900
12	8	-0.346036	-1.97370	0.58155	1.02058	15.99900
14	8	-0.625340	2.47510	-0.71515	-1.16441	15.99900
15	6	0.337181	1.42181	-0.22283	-1.62245	12.01100
16	6	-0.000113	0.47986	0.49601	-0.74461	12.01100
17	6	0.027744	0.89523	0.64238	0.52811	12.01100
18	6	-0.027211	1.08276	-0.39301	-3.02966	12.01100
19	6	0.023496	1.84535	-1.29599	-3.78463	12.01100
20	6	-0.046509	1.56233	-1.49655	-5.11875	12.01100
21	6	0.174819	0.49611	-0.77704	-5.70198	12.01100
22	6	-0.053985	-0.28047	0.11754	-4.95279	12.01100
23	6	0.049952	0.02768	0.32430	-3.60838	12.01100
24	6	0.016900	-0.80688	0.92584	-1.33707	12.01100
25	6	0.011634	-0.69614	1.33170	-2.79421	12.01100
26	8	-0.349410	0.30189	-0.98014	-7.04236	15.99900
8	1	0.026730	1.30027	2.66073	4.62810	1.00800
13	1	0.229359	-2.86519	0.55273	1.40187	1.00800
9	1	0.025828	2.19346	1.75876	2.47195	1.00800
10	1	0.032384	-2.71673	1.68617	3.32768	1.00800
11	1	0.229111	-2.16563	2.79186	5.25790	1.00800
27	1	0.038365	2.67687	-1.83733	-3.30302	1.00800
28	1	0.028083	2.13990	-2.20700	-5.72161	1.00800
29	1	0.032467	-1.11471	0.65759	-5.42153	1.00800
30	1	0.008530	-1.22393	1.79149	-0.75880	1.00800
31	1	0.024349	-1.53812	0.07444	-1.23801	1.00800
32	1	0.023377	-0.13838	2.30495	-2.87227	1.00800
33	1	0.005866	-1.72458	1.50050	-3.20897	1.00800
34	1	0.235524	-0.47942	-0.47971	-7.32952	1.00800
35	1	0.030735	1.91637	0.21929	0.76850	1.00800

Orbital Energies

a) In vacuum

MOLECULAR POINT GROUP

C1

EIGENVALUES OF THE REFERENCE CONFIGURATION(eV)

Symmetry: 1 A 2 A 3 A 4 A 5 A
Eigenvalue: -46.712536 -45.991310 -44.655769 -44.103970 -41.677727

Symmetry: 6 A 7 A 8 A 9 A 10 A
Eigenvalue: -40.856258 -40.071751 -36.005997 -33.315601 -31.770817

Symmetry: 11 A 12 A 13 A 14 A 15 A
Eigenvalue: -31.172829 -30.604227 -28.053801 -26.853729 -26.496115

Symmetry: 16 A 17 A 18 A 19 A 20 A
Eigenvalue: -24.770651 -23.801176 -23.191767 -22.392277 -21.932621

Symmetry: 21 A 22 A 23 A 24 A 25 A
Eigenvalue: -20.482529 -20.118685 -19.515114 -19.125792 -18.203117

Symmetry: 26 A 27 A 28 A 29 A 30 A
Eigenvalue: -17.414585 -16.926168 -16.210661 -16.102673 -15.910337

Symmetry: 31 A 32 A 33 A 34 A 35 A
Eigenvalue: -15.547507 -15.261859 -15.150486 -14.771476 -14.564418

Symmetry: 36 A 37 A 38 A 39 A 40 A
Eigenvalue: -14.471835 -14.227780 -13.795316 -13.745530 -13.236572

Symmetry: 41 A 42 A 43 A 44 A 45 A
Eigenvalue: -13.128717 -12.698458 -12.486875 -12.292969 -11.971574

Symmetry: 46 A 47 A 48 A 49 A 50 A
Eigenvalue: -11.811440 -11.668716 -9.895787 -9.362800 -9.064745

Symmetry: 51 A 52 A 53 A 54 A 55 A
Eigenvalue: -9.023972 -8.538531 -7.875340 -0.634245 0.349341

Symmetry: 56 A 57 A 58 A 59 A 60 A
Eigenvalue: 0.535268 0.675284 1.309587 2.248913 2.429736

Symmetry: 61 A 62 A 63 A 64 A 65 A
Eigenvalue: 2.575736 2.956959 3.057715 3.203868 3.437947

Symmetry: 66 A 67 A 68 A 69 A 70 A

Eigenvalue:	3.566770	3.619558	3.780236	4.016748	4.594346
Symmetry:	71 A	72 A	73 A	74 A	75 A
Eigenvalue:	5.019456	5.472884	5.630418	5.636851	5.862158
Symmetry:	76 A	77 A	78 A	79 A	80 A
Eigenvalue:	6.187963	6.431687	6.472660	6.609097	6.701492
Symmetry:	81 A	82 A	83 A	84 A	85 A
Eigenvalue:	6.773530	6.979426	7.794627	8.206978	8.751478
Symmetry:	86 A	87 A	88 A	89 A	90 A
Eigenvalue:	9.243318	9.785062	10.043938	10.261786	11.186003
Symmetry:	91 A	92 A	93 A	94 A	95 A
Eigenvalue:	11.667727	11.749449	12.213470	12.322282	12.457585
Symmetry:	96 A	97 A	98 A		
Eigenvalue:	12.981241	13.508603	14.123966		

b) In water

MOLECULAR POINT GROUP

C1

EIGENVALUES OF THE REFERENCE CONFIGURATION(eV)

Symmetry:	1 A	2 A	3 A	4 A	5 A
Eigenvalue:	-45.925503	-45.154026	-43.831482	-43.267227	-40.890285
Symmetry:	6 A	7 A	8 A	9 A	10 A
Eigenvalue:	-40.088165	-39.243481	-35.206005	-32.436214	-30.968655
Symmetry:	11 A	12 A	13 A	14 A	15 A
Eigenvalue:	-30.351149	-29.800009	-27.188547	-26.047997	-25.627550
Symmetry:	16 A	17 A	18 A	19 A	20 A
Eigenvalue:	-23.965496	-22.900894	-22.395748	-21.544361	-21.098948
Symmetry:	21 A	22 A	23 A	24 A	25 A
Eigenvalue:	-19.700127	-19.269735	-18.822847	-18.278730	-17.380905
Symmetry:	26 A	27 A	28 A	29 A	30 A
Eigenvalue:	-16.565807	-16.118954	-15.375790	-15.243039	-15.069915
Symmetry:	31 A	32 A	33 A	34 A	35 A
Eigenvalue:	-14.780364	-14.520124	-14.299602	-13.845345	-13.749308

Symmetry: 36 A 37 A 38 A 39 A 40 A
 Eigenvalue: -13.670548 -13.376549 -12.988762 -12.825703 -12.440340

Symmetry: 41 A 42 A 43 A 44 A 45 A
 Eigenvalue: -12.349964 -11.907400 -11.632830 -11.443282 -11.182432

Symmetry: 46 A 47 A 48 A 49 A 50 A
 Eigenvalue: -10.930063 -10.825171 -9.123637 -8.770055 -8.273737

Symmetry: 51 A 52 A 53 A 54 A 55 A
 Eigenvalue: -8.126726 -7.667285 -7.123973 0.061504 1.131455

Symmetry: 56 A 57 A 58 A 59 A 60 A
 Eigenvalue: 1.265982 1.625444 2.067394 3.018875 3.169535

Symmetry: 61 A 62 A 63 A 64 A 65 A
 Eigenvalue: 3.457627 3.702413 3.870119 4.073077 4.278447

Symmetry: 66 A 67 A 68 A 69 A 70 A
 Eigenvalue: 4.409700 4.446885 4.557578 4.943718 5.315961

Symmetry: 71 A 72 A 73 A 74 A 75 A
 Eigenvalue: 5.892900 6.162419 6.459784 6.513723 6.850182

Symmetry: 76 A 77 A 78 A 79 A 80 A
 Eigenvalue: 7.080290 7.314883 7.451356 7.509128 7.530534

Symmetry: 81 A 82 A 83 A 84 A 85 A
 Eigenvalue: 7.774182 7.957089 8.570798 9.149483 9.468332

Symmetry: 86 A 87 A 88 A 89 A 90 A
 Eigenvalue: 10.100410 10.668669 10.837949 11.150793 12.065989

Symmetry: 91 A 92 A 93 A 94 A 95 A
 Eigenvalue: 12.455110 12.591443 12.931208 13.212329 13.288512

Symmetry: 96 A 97 A 98 A
 Eigenvalue: 13.848492 14.187586 14.936406

Electronic Transitions (10 lowest)

a) In vacuum

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*****  
***** UV Spectrum *****  
*****
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---- Absolute Energy in eV.
---- Dipole Moments in Debye.

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*****
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0 (Reference) Absolute Energy -4169.93848

1 Spin S 0.00
State Dipole 8.7239

State Dipole Components -8.0287 3.4038 0.2478

1 (Transition) Excitation Energy 638.0 nm
15673.3 1/cm

1 -> 2 Spin S 1.00
State Dipole 9.1686
Oscillator Strength 0.0000

State Dipole Components -8.4820 3.4673 0.3104
Transition Dipole Components -0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

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53 --> 54 0.510290
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Spin Down: Occ. MO --> Unocc. MO Coefficients

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53 --> 54 0.510290
```

2 (Transition) Excitation Energy 493.9 nm
20248.2 1/cm

1 -> 3 Spin S 1.00
State Dipole 8.4632
Oscillator Strength 0.0000

State Dipole Components -7.8303 3.1948 -0.3262
Transition Dipole Components 0.0000 0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

52 --> 54 -0.379347
52 --> 55 -0.345048
51 --> 57 -0.333443

Spin Down: Occ. MO --> Unocc. MO Coefficients

52 --> 54 -0.379347
52 --> 55 -0.345048
51 --> 57 -0.333443

3 (Transition) Excitation Energy 461.4 nm
21673.7 1/cm

1 -> 4 Spin S 1.00
State Dipole 5.1072
Oscillator Strength 0.0000

State Dipole Components -4.5911 1.7988 1.3305
Transition Dipole Components 0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

49 --> 54 -0.603056

Spin Down: Occ. MO --> Unocc. MO Coefficients

49 --> 54 -0.603056

4 (Transition) Excitation Energy 453.9 nm
22033.2 1/cm

1 -> 5 Spin S 1.00
State Dipole 9.3774
Oscillator Strength 0.0000

State Dipole Components -8.6912 3.4986 0.3985
Transition Dipole Components -0.0000 0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.356532

Spin Down: Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.356532

5 (Transition) Excitation Energy 414.0 nm
 24152.8 1/cm

1 -> 6 Spin S 0.00
State Dipole 5.0734
Oscillator Strength 0.0022

State Dipole Components -4.5579 1.7826 1.3368
Transition Dipole Components -0.2239 0.1099 0.3570

Spin Up : Occ. MO --> Unocc. MO Coefficients

49 --> 54 -0.604789

Spin Down: Occ. MO --> Unocc. MO Coefficients

49 --> 54 0.604789

6 (Transition) Excitation Energy 370.3 nm
 27007.3 1/cm

1 -> 7 Spin S 1.00
State Dipole 8.2877
Oscillator Strength 0.0000

State Dipole Components -7.6953 2.8920 -1.0513
Transition Dipole Components -0.0000 -0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

53 --> 56 0.553854

Spin Down: Occ. MO --> Unocc. MO Coefficients

53 --> 56 0.553854

7 (Transition) Excitation Energy 355.0 nm
 28169.4 1/cm

1 -> 8 Spin S 1.00
State Dipole 9.1438

Oscillator Strength 0.0000

State Dipole Components -8.5218 3.2980 -0.3342
Transition Dipole Components 0.0000 0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

51 --> 57 -0.333756
50 --> 56 0.358426

Spin Down: Occ. MO --> Unocc. MO Coefficients

51 --> 57 -0.333756
50 --> 56 0.358426

8 (Transition) Excitation Energy 352.5 nm
28365.2 1/cm

1 -> 9 Spin S 1.00
State Dipole 9.1910
Oscillator Strength 0.0000

State Dipole Components -8.5382 3.3562 -0.5565
Transition Dipole Components 0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

51 --> 57 0.404924

Spin Down: Occ. MO --> Unocc. MO Coefficients

51 --> 57 0.404924

9 (Transition) Excitation Energy 349.0 nm
28651.8 1/cm

1 -> 10 Spin S 1.00
State Dipole 9.0520
Oscillator Strength 0.0000

State Dipole Components -8.3247 3.5468 -0.2433
Transition Dipole Components -0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

52 --> 57 0.412964
51 --> 54 0.345206

51 --> 55 0.323919

Spin Down: Occ. MO --> Unocc. MO Coefficients

52 --> 57 0.412964
51 --> 54 0.345206
51 --> 55 0.323919

10 (Transition) Excitation Energy 315.8 nm
31668.7 1/cm

1 -> 11 Spin S 0.00
State Dipole 14.0888
Oscillator Strength 0.9652

State Dipole Components -11.7127 6.0151 5.0126
Transition Dipole Components 1.6282 -2.4047 -7.5086

Spin Up : Occ. MO --> Unocc. MO Coefficients

53 --> 54 0.660263

Spin Down: Occ. MO --> Unocc. MO Coefficients

53 --> 54 -0.660263

b) In water

***** UV Spectrum *****

---- Absolute Energy in eV.
---- Dipole Moments in Debye.

0 (Reference) Absolute Energy -41702.59766

1 Spin S 0.00
State Dipole 10.1089

State Dipole Components -9.4073 3.6267 -0.7339

1 (Transition) Excitation Energy 633.9 nm
15774.8 1/cm

1 -> 2 Spin S 1.00
State Dipole 10.5880
Oscillator Strength 0.0000

State Dipole Components -9.9039 3.6922 -0.6207
Transition Dipole Components 0.0000 0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

53 --> 54 -0.495891

Spin Down: Occ. MO --> Unocc. MO Coefficients

53 --> 54 -0.495891

2 (Transition) Excitation Energy 488.7 nm
20462.1 1/cm

1 -> 3 Spin S 1.00
State Dipole 9.9016
Oscillator Strength 0.0000

State Dipole Components -9.1885 3.3250 -1.5989
Transition Dipole Components -0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

52 --> 54 -0.395450
52 --> 55 -0.318989
51 --> 57 -0.318695

Spin Down: Occ. MO --> Unocc. MO Coefficients

52 --> 54 -0.395450
52 --> 55 -0.318989
51 --> 57 -0.318695

3 (Transition) Excitation Energy 464.0 nm
21550.0 1/cm

1 -> 4 Spin S 1.00
State Dipole 10.7451
Oscillator Strength 0.0000

State Dipole Components -10.0986 3.6060 -0.6879
Transition Dipole Components 0.0000 0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.364296

Spin Down: Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.364296

4 (Transition) Excitation Energy 436.0 nm
22937.2 1/cm

1 -> 5 Spin S 1.00
State Dipole 6.3514
Oscillator Strength 0.0000

State Dipole Components -6.0472 1.9061 0.3718
Transition Dipole Components -0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

49 --> 54 0.608376

Spin Down: Occ. MO --> Unocc. MO Coefficients

49 --> 54 0.608376

5 (Transition) Excitation Energy 396.5 nm
25218.2 1/cm

1 -> 6 Spin S -0.00
State Dipole 6.3959
Oscillator Strength 0.0047

State Dipole Components -6.0855 1.9208 0.4305
Transition Dipole Components 0.2882 -0.1900 -0.5272

Spin Up : Occ. MO --> Unocc. MO Coefficients

49 --> 54 0.598966

Spin Down: Occ. MO --> Unocc. MO Coefficients

49 --> 54 -0.598966

6 (Transition) Excitation Energy 371.9 nm
26886.4 1/cm

1 -> 7 Spin S 1.00
State Dipole 9.9419
Oscillator Strength 0.0000

State Dipole Components -9.2502 3.1322 -1.8616
Transition Dipole Components 0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

53 --> 56 -0.510076

Spin Down: Occ. MO --> Unocc. MO Coefficients

53 --> 56 -0.510076

7 (Transition) Excitation Energy 357.2 nm
27994.1 1/cm

1 -> 8 Spin S 1.00
State Dipole 10.6921
Oscillator Strength 0.0000

State Dipole Components -10.0800 3.4123 -1.0344
Transition Dipole Components -0.0000 -0.0000 0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.408909

Spin Down: Occ. MO --> Unocc. MO Coefficients

50 --> 56 -0.408909

8 (Transition) Excitation Energy 355.0 nm
28165.8 1/cm

1 -> 9 Spin S 1.00
State Dipole 10.9953
Oscillator Strength 0.0000

State Dipole Components -10.0861 3.6519 -2.4145
Transition Dipole Components -0.0000 0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

51 --> 57 0.521808

Spin Down: Occ. MO --> Unocc. MO Coefficients

51 --> 57 0.521808

9 (Transition) Excitation Energy 351.1 nm
 28478.0 1/cm

1 -> 10 Spin S 1.00
State Dipole 10.7697
Oscillator Strength 0.0000

State Dipole Components -9.9191 3.7896 -1.7986
Transition Dipole Components 0.0000 -0.0000 -0.0000

Spin Up : Occ. MO --> Unocc. MO Coefficients

52 --> 57 0.354264
51 --> 54 0.411989
51 --> 55 0.324033

Spin Down: Occ. MO --> Unocc. MO Coefficients

52 --> 57 0.354264
51 --> 54 0.411989
51 --> 55 0.324033

10 (Transition) Excitation Energy 322.9 nm
 30971.9 1/cm

1 -> 11 Spin S -0.00
State Dipole 14.6095
Oscillator Strength 1.0007

State Dipole Components -13.0000 5.9817 2.9421
Transition Dipole Components 1.1796 -2.2982 -7.8765

Spin Up : Occ. MO --> Unocc. MO Coefficients

53 --> 54 0.662651

Spin Down: Occ. MO --> Unocc. MO Coefficients

53 --> 54 -0.662651

Molecular Orbital Coefficients

a) In vacuum

Mol. Orbital	1	2	3	4	5	6
Symmetry:	1 A	2 A	3 A	4 A	5 A	6 A
Eigenvalue	-1.71665	-1.69015	-1.64107	-1.62079	-1.53163	-1.50144
S C 1	-0.21933	-0.24150	-0.29840	0.18220	0.00206	-0.05874
Px C 1	0.00666	0.01454	0.04183	-0.03300	0.03696	-0.11978
Py C 1	0.00494	-0.00542	-0.04705	0.04574	-0.02735	0.09017
Pz C 1	0.00790	-0.01480	-0.10486	0.10011	-0.06122	0.20200
S C 2	-0.15116	-0.15016	-0.13580	0.06866	0.07248	-0.26264
Px C 2	0.05239	0.05725	0.06634	-0.03745	-0.00099	0.02076
Py C 2	0.01621	0.01136	-0.00627	0.01043	-0.01974	0.06214
Pz C 2	0.03206	0.02125	-0.01714	0.02438	-0.04296	0.13567
S C 3	-0.15518	-0.12238	-0.04109	0.00784	0.13163	-0.37693
Px C 3	0.06240	0.05451	0.02166	0.00331	-0.03332	0.12164
Py C 3	0.00653	-0.00074	-0.01228	0.00558	-0.00994	0.00708
Pz C 3	0.00577	-0.00871	-0.02844	0.01125	-0.01417	-0.00082
S C 4	-0.23648	-0.14362	0.04584	-0.05653	0.13426	-0.31868
Px C 4	0.04942	0.03960	-0.01992	0.05362	0.03218	-0.04199
Py C 4	-0.00137	-0.01331	-0.02387	0.00710	0.00489	-0.05165
Pz C 4	-0.01261	-0.03992	-0.04951	0.00404	0.01763	-0.11267
S C 5	-0.32750	-0.22796	0.10370	-0.21244	0.01470	-0.06198
Px C 5	0.02765	0.01844	-0.05548	0.08807	0.07300	-0.20934
Py C 5	0.02339	0.00561	-0.04795	0.05098	0.02417	-0.08780
Pz C 5	0.03570	-0.00112	-0.08669	0.07806	0.03953	-0.13991
S C 6	-0.22176	-0.20025	-0.08972	-0.01752	0.01418	-0.08993
Px C 6	-0.05412	-0.05211	-0.04163	0.01920	0.03603	-0.12803
Py C 6	0.01547	0.00253	-0.04721	0.05139	-0.00072	0.00059
Pz C 6	0.03271	0.00584	-0.09395	0.10143	-0.00589	0.01796
S O 7	-0.19432	-0.25281	-0.45784	0.34030	-0.11478	0.33644
Px O 7	0.01054	0.01460	0.02939	-0.02247	0.01353	-0.04435
Py O 7	0.02437	0.03103	0.05350	-0.03882	0.01096	-0.02985
Pz O 7	0.04964	0.06312	0.10855	-0.07874	0.02148	-0.05766
S O 12	-0.37551	-0.23166	0.25940	-0.39161	-0.12514	0.36037
Px O 12	-0.02607	-0.00973	0.01568	-0.00958	0.00822	-0.02208
Py O 12	-0.04645	-0.02956	0.02986	-0.04665	-0.01244	0.03448
Pz O 12	-0.08053	-0.06060	0.04985	-0.09467	-0.02143	0.07592
S O 14	-0.16020	0.14662	0.15673	0.26079	0.46619	0.21314
Px O 14	0.05644	-0.05009	-0.05472	-0.08782	-0.14744	-0.06538
Py O 14	-0.02444	0.01960	0.02476	0.03733	0.06628	0.02615
Pz O 14	0.02154	-0.02683	-0.01710	-0.03666	-0.04627	-0.03104
S C 15	-0.21842	0.19599	0.17379	0.26839	0.26247	0.12608
Px C 15	0.00096	0.00786	0.01509	0.04648	0.19036	0.08636
Py C 15	-0.00150	-0.00919	-0.00060	-0.01934	-0.07099	-0.03969
Pz C 15	-0.00296	-0.02335	0.02941	0.01765	0.13432	0.03568

S C 16	-0.21735	0.09963	0.17221	0.14160	0.08479	-0.00520
Px C 16	0.00585	0.01587	0.00317	0.04229	0.10987	0.03003
Py C 16	0.00246	-0.01793	-0.00597	-0.02810	-0.04090	-0.02543
Pz C 16	0.01009	-0.05288	-0.00592	-0.04684	0.06604	-0.01286
S C 17	-0.17964	-0.00718	0.11698	0.04651	0.16778	-0.10580
Px C 17	0.03752	0.01998	-0.02052	0.02992	0.02730	0.01597
Py C 17	-0.00789	-0.01888	-0.00605	-0.02058	-0.01598	-0.04144
Pz C 17	0.01222	-0.04951	-0.03666	-0.05301	-0.01939	-0.08042
S C 18	-0.20922	0.25857	0.05262	0.16212	-0.13348	-0.01467
Px C 18	0.01814	-0.01901	0.00196	0.00668	0.10055	0.04247
Py C 18	-0.01499	0.00714	0.01727	0.01318	-0.03680	-0.01592
Pz C 18	-0.00250	-0.02930	0.06131	0.05322	0.12236	0.05014
S C 19	-0.13051	0.19356	-0.02209	0.06426	-0.10078	-0.01309
Px C 19	0.03888	-0.05930	0.01351	-0.00878	0.06091	0.01875
Py C 19	-0.03415	0.04689	0.00183	0.02269	-0.02917	-0.00476
Pz C 19	-0.00278	-0.01245	0.04071	0.04439	0.06170	0.03063
S C 20	-0.11124	0.19827	-0.11652	-0.05638	-0.09218	-0.02995
Px C 20	0.03088	-0.05808	0.04474	0.03227	0.01659	0.00802
Py C 20	-0.03131	0.05382	-0.02738	-0.01049	-0.03514	-0.01181
Pz C 20	-0.01767	0.01714	0.03107	0.05135	-0.06900	-0.01696
S C 21	-0.15203	0.29826	-0.26303	-0.20964	0.01167	-0.00838
Px C 21	0.00174	-0.00820	0.02305	0.02902	-0.03175	-0.00782
Py C 21	-0.00434	0.00270	0.01100	0.01514	-0.03086	-0.01026
Pz C 21	-0.00846	-0.01467	0.09692	0.12518	-0.18137	-0.05300
S C 22	-0.13889	0.22932	-0.11341	-0.05164	-0.16727	-0.06169
Px C 22	-0.03408	0.05968	-0.03083	-0.01102	-0.03988	-0.01327
Py C 22	0.02052	-0.04418	0.04182	0.03161	-0.00392	-0.00025
Pz C 22	-0.02469	0.01569	0.05245	0.07068	-0.11566	-0.03481
S C 23	-0.19925	0.25138	0.01786	0.10006	-0.30658	-0.09598
Px C 23	-0.02180	0.03624	-0.00640	0.01342	-0.00931	0.00125
Py C 23	0.01451	-0.03333	0.02164	0.00454	0.01191	0.00159
Pz C 23	-0.01990	-0.00679	0.05837	0.05214	0.00603	0.00743
S C 24	-0.19083	0.08925	0.13862	0.08005	-0.13273	-0.03449
Px C 24	-0.03898	0.03194	0.02915	0.04009	-0.00244	-0.01441
Py C 24	0.01027	-0.01142	-0.00766	-0.01292	-0.00274	-0.00211
Pz C 24	0.00144	-0.04392	0.00560	-0.04010	0.06300	0.02216
S C 25	-0.15853	0.14226	0.08459	0.10266	-0.22891	-0.07127
Px C 25	-0.02903	0.03303	0.01293	0.02612	-0.03268	-0.01125
Py C 25	0.03698	-0.03974	-0.01546	-0.02704	0.05107	0.01510
Pz C 25	-0.02090	-0.00380	0.03078	0.01335	0.00975	0.00606
S O 26	-0.12987	0.30090	-0.39241	-0.38677	0.29860	0.07761
Px O 26	0.00804	-0.01942	0.02794	0.02896	-0.02653	-0.00716
Py O 26	-0.01705	0.03944	-0.05141	-0.05079	0.03866	0.00987
Pz O 26	-0.03288	0.07385	-0.08949	-0.08489	0.05286	0.01248
S H 8	-0.04231	-0.04505	-0.05216	0.03207	0.01557	-0.05973
S H 13	-0.15792	-0.10288	0.10291	-0.16753	-0.05645	0.16157
S H 9	-0.04493	-0.03029	-0.00535	0.00551	0.05017	-0.11994
S H 10	-0.07967	-0.07239	-0.03193	-0.00924	-0.01312	0.02661
S H 11	-0.08599	-0.11039	-0.19503	0.14320	-0.05063	0.14923

S H 27	-0.04199	0.05770	0.00546	0.03551	0.00340	0.01246
S H 28	-0.03040	0.05793	-0.04391	-0.02939	-0.00910	-0.00360
S H 29	-0.04468	0.07532	-0.04552	-0.02982	-0.04060	-0.01701
S H 30	-0.08911	0.01091	0.06439	0.00208	-0.04736	-0.00303
S H 31	-0.08274	0.02979	0.05988	0.02115	-0.05722	-0.00401
S H 32	-0.06168	0.05451	0.03344	0.03991	-0.08830	-0.02841
S H 33	-0.05439	0.04970	0.02553	0.03010	-0.09034	-0.02806
S H 34	-0.05722	0.13110	-0.16841	-0.16544	0.12508	0.03218
S H 35	-0.06794	0.00642	0.04563	0.03966	0.10553	-0.04019

Mol. Orbital	7	8	9	10	11	12
Symmetry:	7 A	8 A	9 A	10 A	11 A	12 A
Eigenvalue	-1.47261	-1.32320	-1.22433	-1.16756	-1.14558	-1.12468

S C 1	-0.02019	0.13436	0.07319	-0.08517	-0.09964	-0.14009
Px C 1	-0.01881	0.04549	0.01164	0.21156	-0.10669	-0.12694
Py C 1	0.02609	-0.06338	-0.02658	0.08768	0.00164	0.00549
Pz C 1	0.05593	-0.13674	-0.05761	0.16800	0.01245	0.01985
S C 2	-0.04839	0.15628	0.04975	0.33895	-0.22166	-0.27671
Px C 2	0.00891	-0.05179	-0.03540	0.11515	0.01545	0.02229
Py C 2	0.01190	-0.01751	-0.00019	-0.00192	-0.00943	-0.01816
Pz C 2	0.02489	-0.03599	0.00043	-0.01834	-0.01719	-0.03719
S C 3	-0.03937	-0.01929	-0.06640	0.34408	-0.00180	0.02729
Px C 3	0.02389	-0.05280	-0.02420	0.06591	-0.00830	-0.02702
Py C 3	-0.00743	0.06029	0.03210	0.03608	-0.06607	-0.08481
Pz C 3	-0.02136	0.13172	0.06390	0.07733	-0.13526	-0.17711
S C 4	0.01367	-0.24786	-0.11033	0.01511	0.18980	0.27072
Px C 4	0.02409	-0.09323	-0.06366	0.14730	0.01571	-0.00102
Py C 4	-0.02185	0.07862	0.02346	0.01331	-0.01930	-0.00561
Pz C 4	-0.06589	0.17110	0.02945	0.02778	-0.01296	0.00578
S C 5	-0.08560	0.06000	0.01263	-0.21605	0.09754	0.12069
Px C 5	0.03582	-0.08608	-0.01341	-0.01896	0.05450	0.11966
Py C 5	-0.00397	0.05858	0.03291	-0.10278	-0.00560	0.00079
Pz C 5	-0.03041	0.13897	0.05355	-0.19025	-0.00007	-0.02261
S C 6	-0.08062	0.21977	0.09773	-0.45697	0.03041	-0.00757
Px C 6	-0.02037	0.06216	0.03036	-0.04508	-0.01750	-0.00659
Py C 6	0.01631	-0.01195	0.00445	0.00254	-0.01384	-0.01064
Pz C 6	0.03177	-0.02701	0.00389	0.01138	-0.02405	-0.02573
S O 7	0.08548	-0.16944	-0.06891	0.10506	0.07142	0.10653
Px O 7	-0.00940	0.03146	0.01637	0.06489	-0.06690	-0.09210
Py O 7	-0.00714	0.00579	-0.00103	0.00295	0.00611	0.01072
Pz O 7	-0.01406	0.00890	-0.00409	0.00076	0.01958	0.03140
S O 12	-0.08948	0.01733	-0.04134	0.23466	-0.04763	-0.08010
Px O 12	0.01933	-0.06176	-0.00198	-0.04330	0.02997	0.06973
Py O 12	-0.01180	0.00546	-0.00065	-0.01163	0.00402	0.00795
Pz O 12	-0.05113	0.03618	-0.02096	-0.00599	0.03696	-0.01606
S O 14	-0.19049	0.17217	-0.19757	-0.00379	-0.20496	0.18347
Px O 14	0.04655	-0.03813	0.03989	0.01092	0.03400	0.00361
Py O 14	-0.00982	0.00625	-0.03199	-0.01673	-0.02895	-0.02203

Pz O 14	0.05047	-0.05674	-0.02452	-0.03884	-0.03949	-0.07165
S C 15	-0.02905	0.10809	0.07473	0.00863	0.12367	-0.13209
Px C 15	-0.15431	0.07019	-0.14458	0.01749	-0.13336	0.19778
Py C 15	0.09884	-0.05226	0.03283	-0.03815	0.01299	-0.12665
Pz C 15	0.04184	-0.07749	-0.13063	-0.11074	-0.23153	-0.08201
S C 16	0.27929	-0.23195	0.13406	-0.14327	-0.04868	-0.32288
Px C 16	-0.07786	-0.00596	-0.08878	-0.02813	0.04663	-0.10181
Py C 16	0.03473	-0.03905	0.00866	0.00313	-0.03185	0.06385
Pz C 16	-0.03244	-0.19043	-0.10456	-0.05359	-0.04416	0.00487
S C 17	0.14452	-0.45122	-0.11965	-0.07483	0.06380	-0.06497
Px C 17	-0.04074	0.06340	-0.03648	0.02385	-0.01183	-0.03625
Py C 17	0.00508	-0.03194	-0.00705	0.03378	0.03946	0.08504
Pz C 17	-0.06004	-0.01129	-0.07249	0.11142	0.12063	0.23735
S C 18	-0.18268	0.06080	0.18691	0.11453	0.39038	-0.06089
Px C 18	-0.08318	-0.01830	0.08603	0.03095	-0.01839	0.09872
Py C 18	0.09631	0.05429	-0.06488	-0.01270	0.04091	-0.07243
Pz C 18	0.12094	0.10364	0.06520	0.03098	0.07513	-0.01308
S C 19	-0.32587	-0.12910	0.30136	0.07442	0.01778	0.17049
Px C 19	0.06968	0.03071	0.00314	0.00612	-0.03735	0.05404
Py C 19	-0.05155	0.00815	-0.00704	0.01601	0.09650	-0.04057
Pz C 19	0.03420	0.10212	-0.00823	0.06221	0.20545	-0.00206
S C 20	-0.24372	-0.20958	0.23149	-0.04151	-0.32379	0.12637
Px C 20	0.02553	0.02302	0.04734	0.02824	0.02677	0.05885
Py C 20	-0.05626	-0.03245	-0.02475	-0.01758	-0.01091	-0.03936
Pz C 20	-0.10980	-0.04403	0.04931	0.01781	0.03475	0.02731
S C 21	-0.07702	-0.10096	-0.05068	-0.07822	-0.19022	-0.06389
Px C 21	-0.06472	-0.05969	0.12704	0.00071	-0.09799	0.06264
Py C 21	-0.00847	0.01876	-0.13394	-0.01891	0.05076	-0.07141
Pz C 21	-0.19581	-0.09846	-0.08517	-0.05799	-0.09903	-0.06196
S C 22	-0.09952	-0.00594	-0.43447	-0.10464	-0.07074	-0.14577
Px C 22	-0.07821	-0.05568	0.01578	-0.01917	-0.01649	-0.04955
Py C 22	0.05021	0.05413	-0.04441	0.01755	0.02788	0.04541
Pz C 22	-0.04159	0.02151	-0.08192	0.00500	0.03681	0.01051
S C 23	-0.00917	0.12628	-0.27042	0.00637	0.15790	-0.05984
Px C 23	-0.09460	-0.05300	0.12256	0.01785	0.12759	-0.09436
Py C 23	0.11330	0.07462	-0.05537	0.00888	-0.06271	0.10148
Pz C 23	0.13263	0.08459	0.19986	0.07125	0.11009	0.05226
S C 24	0.36225	-0.00406	0.20422	-0.00647	-0.23340	0.10424
Px C 24	0.06673	-0.03374	0.05931	-0.03547	0.06438	-0.12644
Py C 24	-0.00527	0.00898	-0.02542	0.00834	-0.05071	0.08989
Pz C 24	-0.03958	-0.14360	0.02628	-0.04187	-0.00528	-0.11081
S C 25	0.28483	0.22402	-0.10834	0.04997	-0.13785	0.29004
Px C 25	0.01727	0.02201	0.00821	0.00416	0.09873	-0.07421
Py C 25	-0.03239	-0.03664	0.01416	-0.00615	-0.06078	0.04564
Pz C 25	0.08754	-0.02049	0.18026	0.00801	-0.07024	0.02171
S O 26	0.25490	0.10209	0.09411	0.06843	0.15272	0.04828
Px O 26	-0.03229	-0.02747	0.02958	-0.01295	-0.07259	0.01519
Py O 26	0.03686	0.02105	-0.02017	0.00651	0.04205	-0.01296
Pz O 26	0.03219	-0.00575	0.01499	-0.01348	-0.05836	-0.00121

S H 8	-0.00931	0.04171	0.01219	0.19685	-0.11080	-0.14477
S H 13	-0.05399	0.05010	-0.01382	0.08794	-0.02555	-0.06815
S H 9	-0.00412	-0.05291	-0.05356	0.19257	0.00858	0.01431
S H 10	-0.02598	0.07135	0.03077	-0.19522	0.02284	-0.00212
S H 11	0.03541	-0.07354	-0.03113	-0.01437	0.06485	0.09064
S H 27	-0.11178	-0.02424	0.14041	0.04929	0.01324	0.12015
S H 28	-0.06063	-0.07049	0.11964	-0.01071	-0.15553	0.08525
S H 29	0.00713	0.03098	-0.21222	-0.03827	-0.02912	-0.03548
S H 30	0.14042	-0.03599	0.07710	0.00046	-0.14452	0.08942
S H 31	0.14105	-0.00213	0.08360	0.00869	-0.11248	0.04816
S H 32	0.11543	0.09039	-0.04991	0.02030	-0.06723	0.13876
S H 33	0.10530	0.09630	-0.09728	0.01827	-0.10791	0.17361
S H 34	0.11362	0.05637	-0.00096	0.03093	0.10672	0.00156
S H 35	0.03478	-0.17198	-0.09198	-0.00850	0.02253	-0.03200

Mol. Orbital	13	14	15	16	17	18
Symmetry:	13 A	14 A	15 A	16 A	17 A	18 A
Eigenvalue	-1.03096	-0.98686	-0.97371	-0.91030	-0.87468	-0.85228

S C 1	0.06395	-0.19407	0.07252	0.27292	-0.10029	0.13225
Px C 1	0.10218	-0.06980	0.19191	-0.01518	-0.01586	0.02625
Py C 1	0.01856	-0.00417	0.04908	0.01438	-0.01494	-0.02413
Pz C 1	0.02742	-0.00708	0.09061	0.03559	-0.03338	-0.05424
S C 2	0.06774	-0.11247	0.07533	-0.02799	0.05363	-0.16565
Px C 2	-0.08154	0.10134	-0.14632	-0.16160	0.10567	-0.24474
Py C 2	0.02448	-0.05333	0.04802	0.05745	-0.01420	-0.04918
Pz C 2	0.05477	-0.12528	0.11687	0.14239	-0.04239	-0.08747
S C 3	-0.15266	0.18098	-0.24612	-0.11112	0.03409	-0.01074
Px C 3	-0.08296	-0.01732	-0.13171	0.02947	0.03799	-0.21250
Py C 3	0.02652	-0.01747	0.00412	-0.06896	0.05138	-0.08116
Pz C 3	0.04888	-0.04016	0.02351	-0.14202	0.10107	-0.15648
S C 4	0.06986	0.08219	0.13443	0.04877	-0.06914	0.10850
Px C 4	-0.19294	-0.01725	-0.25832	0.18831	-0.06740	0.06105
Py C 4	-0.01029	0.06929	-0.03899	-0.06786	0.00447	0.08256
Pz C 4	-0.04953	0.14145	-0.03537	-0.13656	-0.00872	0.17691
S C 5	0.10211	0.06176	0.22456	-0.19458	0.06044	-0.17884
Px C 5	0.14881	0.05738	0.16728	-0.03468	-0.02598	0.18376
Py C 5	-0.02033	0.00950	-0.06912	-0.00439	0.00736	0.03455
Pz C 5	-0.10688	0.00437	-0.14135	-0.00231	-0.00550	0.05926
S C 6	-0.12998	-0.06160	-0.23099	0.08855	0.02979	-0.16234
Px C 6	0.08415	-0.00259	0.12625	-0.02245	-0.02948	0.20007
Py C 6	0.00976	-0.02563	-0.02896	0.07378	-0.01813	0.05629
Pz C 6	-0.00178	-0.05738	-0.07076	0.15972	-0.04246	0.10121
S O 7	-0.00182	0.12981	0.03288	-0.18468	0.04127	0.00255
Px O 7	0.07484	-0.14734	0.15478	0.21116	-0.10130	0.02077
Py O 7	-0.00740	0.03876	-0.01237	-0.08393	0.03365	-0.01285
Pz O 7	-0.02364	0.09620	-0.04026	-0.19934	0.08110	-0.03028
S O 12	-0.03825	-0.00724	-0.03095	0.06904	-0.04775	0.19838
Px O 12	0.17138	0.01043	0.22407	-0.12055	0.08727	-0.30299

Py O 12	0.01432	0.00164	0.02839	-0.03850	0.03118	-0.12979
Pz O 12	-0.08311	-0.01172	0.04805	-0.06175	0.00279	-0.16079
S O 14	0.08236	0.07456	0.01651	0.08689	0.20538	0.05118
Px O 14	0.01315	-0.01069	-0.00994	0.02623	0.02702	-0.00300
Py O 14	-0.03521	0.00610	0.01323	-0.01344	0.01957	0.01448
Pz O 14	-0.07731	-0.01342	0.01052	-0.02361	0.09649	0.05471
S C 15	-0.07157	0.11694	0.06062	-0.08376	-0.19860	0.01590
Px C 15	0.10489	-0.03388	-0.02693	0.09823	0.11288	-0.03891
Py C 15	-0.10203	0.01204	0.02939	-0.06746	-0.00145	0.04304
Pz C 15	-0.08916	-0.03778	0.00579	-0.10663	0.16754	0.10711
S C 16	-0.02152	-0.02470	-0.01055	-0.17923	-0.01543	0.03197
Px C 16	-0.21197	-0.08103	0.06623	-0.05636	-0.04402	-0.00747
Py C 16	0.07706	-0.02841	-0.03591	0.05719	0.04166	-0.05347
Pz C 16	0.04173	-0.21243	-0.00575	0.05598	0.09544	-0.11814
S C 17	-0.11275	-0.25047	-0.02291	0.15014	-0.00814	-0.10425
Px C 17	-0.17314	-0.00914	-0.08826	0.02440	-0.01397	0.04022
Py C 17	0.04222	0.02834	-0.00888	0.06164	-0.02519	-0.00570
Pz C 17	-0.00171	0.06865	-0.00613	0.19179	-0.08225	0.02052
S C 18	0.06178	0.01440	-0.00511	0.13374	0.01043	-0.08945
Px C 18	0.09422	-0.10223	-0.09072	-0.04478	-0.18580	-0.09595
Py C 18	-0.09878	0.10518	0.10415	0.03169	0.06559	0.05186
Pz C 18	-0.04754	0.09774	0.05464	-0.05582	-0.29939	-0.02190
S C 19	0.05320	-0.31678	-0.13116	-0.16454	-0.06878	0.01251
Px C 19	-0.03203	-0.07546	0.00572	-0.11605	-0.14580	0.02732
Py C 19	0.07065	0.05092	-0.02448	0.12420	0.08007	-0.07542
Pz C 19	0.13777	-0.02549	-0.06860	0.07561	-0.13602	-0.14467
S C 20	-0.24870	0.04215	0.14722	-0.06562	-0.00861	0.08091
Px C 20	-0.02355	-0.16336	-0.01604	-0.15029	-0.03922	0.09028
Py C 20	0.04640	0.07351	-0.02500	0.08744	0.06323	-0.04911
Pz C 20	0.08681	-0.19471	-0.12611	-0.12263	0.09699	0.09153
S C 21	-0.00392	0.28529	0.03278	0.12762	-0.18954	-0.13219
Px C 21	-0.16136	0.05591	0.13156	0.07597	0.11229	-0.00884
Py C 21	0.15422	-0.02996	-0.12636	-0.06695	-0.06939	0.02377
Pz C 21	0.06890	0.05790	-0.06132	-0.01246	0.07597	0.06387
S C 22	0.19760	0.01968	-0.12653	-0.13832	-0.23622	0.02261
Px C 22	0.02140	0.10412	-0.00330	0.10817	0.13536	-0.01896
Py C 22	-0.04865	-0.12180	0.03764	-0.08287	-0.02911	0.02435
Pz C 22	-0.07611	-0.08677	0.08489	0.02670	0.26272	0.05785
S C 23	-0.10082	-0.04969	0.13282	0.03650	0.22477	0.06874
Px C 23	0.04445	0.10047	-0.01211	0.11459	0.13076	-0.01516
Py C 23	-0.10694	-0.09448	0.06708	-0.07741	-0.11325	-0.02425
Pz C 23	-0.14160	0.04974	0.09515	0.06673	-0.00170	-0.01336
S C 24	0.25887	0.13483	-0.20246	0.06027	0.06376	0.04646
Px C 24	-0.05643	0.03277	0.06291	-0.08934	-0.03962	0.00518
Py C 24	0.01519	-0.04914	-0.01989	0.04700	0.01098	-0.09553
Pz C 24	0.16503	-0.00018	-0.03486	-0.03563	0.04994	0.01479
S C 25	-0.17438	-0.14626	0.06419	0.01827	-0.04450	-0.09640
Px C 25	-0.07658	0.04023	0.08943	-0.01408	0.03234	0.03252
Py C 25	0.03235	-0.04663	-0.04026	0.00975	-0.04201	-0.10046

Pz C 25	0.10927	0.14700	-0.12114	0.07717	0.01102	0.00807
S O 26	-0.02432	-0.15147	0.00915	-0.00863	0.21806	0.06277
Px O 26	-0.09220	0.12037	0.10208	0.09875	-0.08453	-0.10785
Py O 26	0.06006	-0.04933	-0.06177	-0.04917	-0.00671	0.03442
Pz O 26	-0.05185	0.16279	0.07187	0.10475	-0.24500	-0.17231
S H 8	0.03236	-0.08119	0.04506	-0.00403	0.04725	-0.23513
S H 13	-0.12866	-0.01206	-0.14250	0.08207	-0.06131	0.19297
S H 9	-0.13569	0.07823	-0.20756	-0.01635	0.02953	-0.12591
S H 10	-0.11959	-0.03096	-0.20872	0.07352	0.02978	-0.19439
S H 11	-0.05221	0.13239	-0.09727	-0.19163	0.08139	-0.02222
S H 27	0.03262	-0.20755	-0.07371	-0.14963	-0.16458	0.00201
S H 28	-0.17627	0.00360	0.12081	-0.07506	-0.07278	0.06132
S H 29	0.09481	-0.06159	-0.07644	-0.15937	-0.26779	0.01346
S H 30	0.19924	0.03148	-0.12284	0.06502	0.06271	-0.02796
S H 31	0.14937	0.07351	-0.11734	0.04399	0.04397	0.08311
S H 32	-0.09120	-0.09331	0.03986	0.00601	-0.03769	-0.10072
S H 33	-0.05813	-0.13056	0.00059	-0.00696	-0.05819	-0.07300
S H 34	0.07239	-0.15403	-0.08633	-0.09641	0.14106	0.12119
S H 35	-0.16374	-0.11494	-0.06868	0.10178	-0.00539	-0.02236

Mol. Orbital	19	20	21	22	23	24
Symmetry:	19 A	20 A	21 A	22 A	23 A	24 A
Eigenvalue	-0.82290	-0.80601	-0.75272	-0.73935	-0.71717	-0.70286

S C 1	0.05258	0.01985	-0.16124	0.09682	0.02947	-0.06029
Px C 1	-0.12558	0.01487	0.23106	-0.10925	-0.08612	0.01580
Py C 1	0.00510	0.09679	0.05096	-0.02469	0.11260	0.02930
Pz C 1	0.01706	0.21035	0.09734	-0.03280	0.21340	0.04378
S C 2	0.00879	-0.04790	0.04679	-0.05748	-0.20121	0.02298
Px C 2	0.09465	0.00410	-0.04481	-0.00931	-0.02777	0.05068
Py C 2	0.01726	0.06395	0.05598	-0.04461	-0.03440	0.03451
Pz C 2	0.02573	0.14744	0.13547	-0.07834	-0.10744	0.05540
S C 3	0.06347	0.03168	-0.09543	0.05658	0.21917	-0.01738
Px C 3	0.12730	0.11336	-0.05710	0.05140	0.06753	-0.00545
Py C 3	0.01340	-0.07380	-0.04663	-0.00512	-0.02081	0.00497
Pz C 3	0.00470	-0.14880	-0.07418	0.03425	-0.11620	-0.02258
S C 4	0.01286	0.05468	-0.00127	-0.07484	-0.03908	0.05962
Px C 4	0.04654	0.06473	0.05531	-0.05288	0.00143	-0.00445
Py C 4	-0.03800	-0.01754	0.00243	-0.02385	0.15485	0.01722
Pz C 4	-0.11371	0.01922	0.04239	0.08240	0.19286	-0.03800
S C 5	-0.06240	0.14203	0.11877	0.02594	0.07408	-0.00833
Px C 5	-0.02915	-0.12169	-0.08546	-0.00943	-0.04036	0.04785
Py C 5	-0.03346	-0.03387	0.12456	-0.10173	0.04557	0.07017
Pz C 5	-0.08870	-0.01612	0.26327	-0.14612	0.01661	0.05642
S C 6	0.11391	0.04331	0.00930	-0.02396	-0.03015	0.03513
Px C 6	-0.11489	-0.11889	-0.04075	0.07731	0.00521	-0.07942
Py C 6	0.06071	-0.06675	-0.17707	0.06702	-0.03045	-0.01884
Pz C 6	0.12923	-0.11534	-0.35925	0.15030	-0.10061	-0.06257
S O 7	-0.10589	-0.01445	0.17683	-0.07441	0.03072	0.02451

Px O 7	0.01756	0.27687	0.14679	-0.04333	0.30713	0.05039
Py O 7	-0.04684	-0.06831	0.07263	-0.04472	-0.09036	0.00928
Pz O 7	-0.10383	-0.17141	0.14572	-0.08745	-0.24379	0.00641
S O 12	-0.00014	-0.12783	-0.15152	0.08041	-0.03402	-0.02958
Px O 12	0.11687	0.14924	-0.23285	0.31602	0.01670	-0.13490
Py O 12	0.00907	0.08505	0.01677	0.01537	0.06044	-0.00067
Pz O 12	-0.05134	0.16658	0.06913	-0.04945	0.02982	-0.06851
S O 14	0.11014	0.04382	-0.00173	-0.17333	-0.03705	-0.20763
Px O 14	0.04848	0.00041	0.00323	-0.12282	-0.03286	-0.14320
Py O 14	-0.05280	0.02256	-0.01816	0.04864	0.01722	0.03980
Pz O 14	-0.06595	0.06101	0.02139	0.05874	0.01055	-0.14913
S C 15	-0.03094	0.07094	-0.06025	0.12290	-0.01561	0.22645
Px C 15	0.03536	-0.06930	0.00349	-0.08430	0.00221	0.01104
Py C 15	-0.06572	0.06732	-0.04653	-0.00576	0.02960	-0.04700
Pz C 15	-0.09793	0.07118	0.01270	0.09248	0.11902	-0.14158
S C 16	0.00553	-0.05243	-0.04895	-0.09262	0.16713	-0.00062
Px C 16	-0.22465	0.02688	-0.01766	0.18726	-0.00788	0.03635
Py C 16	0.03154	-0.05777	-0.05346	-0.22523	0.03499	-0.01257
Pz C 16	-0.02980	-0.23122	0.03963	0.00411	-0.00862	0.02197
S C 17	-0.05558	-0.09336	0.08007	-0.01053	-0.17439	-0.01883
Px C 17	-0.14273	0.09974	0.11007	0.15572	-0.00806	-0.08841
Py C 17	0.07218	0.01681	-0.04907	-0.14511	0.00327	0.05110
Pz C 17	0.09232	0.16724	0.03264	0.00027	-0.20680	0.00279
S C 18	-0.04471	-0.09278	0.02112	0.03486	-0.03101	0.06426
Px C 18	-0.07219	-0.09708	-0.01742	0.00665	0.09071	0.14095
Py C 18	0.07883	0.07425	-0.06034	-0.09522	-0.09405	-0.03775
Pz C 18	0.10828	0.04104	-0.03014	0.01289	-0.12214	0.18560
S C 19	-0.04213	-0.01412	0.03589	0.00762	0.08471	-0.19821
Px C 19	0.12174	0.01378	0.01271	-0.06249	-0.02264	-0.12472
Py C 19	-0.11220	-0.08132	-0.00664	0.02496	0.05806	0.11204
Pz C 19	-0.02176	-0.19741	0.08597	0.02945	0.09682	0.00022
S C 20	0.12444	0.08406	-0.04080	-0.01266	-0.09744	0.16639
Px C 20	0.13424	0.06789	0.00557	-0.04240	-0.06601	-0.05875
Py C 20	-0.14508	-0.01620	-0.03120	0.01334	0.06150	-0.00251
Pz C 20	-0.10261	0.13954	-0.04390	-0.00674	0.00269	-0.18032
S C 21	-0.12197	-0.03161	-0.02817	-0.01718	-0.02487	-0.09619
Px C 21	0.04855	-0.08492	0.01115	0.02943	0.06823	0.19354
Py C 21	-0.07711	0.12133	-0.06466	-0.05573	-0.07723	-0.08574
Pz C 21	-0.10560	0.17611	-0.11019	-0.00718	-0.10224	0.21968
S C 22	0.08858	0.04716	0.01746	-0.01571	-0.01701	0.04280
Px C 22	-0.14189	0.03717	-0.07078	-0.04361	0.00675	-0.04355
Py C 22	0.15532	-0.08771	0.04333	-0.00569	0.07745	0.08484
Pz C 22	0.14836	-0.14035	0.10324	0.06976	0.17608	0.11975
S C 23	0.20782	-0.08275	0.07496	-0.02485	0.03093	-0.09755
Px C 23	-0.10960	0.04283	-0.08182	-0.08772	-0.02961	-0.03936
Py C 23	0.04479	-0.04560	-0.07035	-0.09960	0.03358	-0.00609
Pz C 23	-0.03230	0.07228	-0.03013	-0.03591	-0.16815	-0.19901
S C 24	0.07286	0.05810	0.12326	0.02483	-0.00031	-0.01815
Px C 24	0.05576	0.04365	-0.15084	-0.32823	0.09045	-0.08079

Py C 24	-0.17616	-0.02204	-0.14898	-0.15621	0.06463	0.08049
Pz C 24	0.19661	-0.15626	-0.02955	-0.09289	0.15198	0.12052
S C 25	-0.21386	-0.00857	-0.09398	-0.01089	-0.01591	-0.01519
Px C 25	0.10643	0.03267	-0.13083	-0.29406	0.01564	-0.14993
Py C 25	-0.22997	-0.03909	-0.20653	-0.14435	0.11841	0.14877
Pz C 25	-0.14051	0.17565	0.01399	-0.01330	-0.09644	-0.08377
S O 26	0.03752	-0.02928	0.02987	0.03476	0.08780	0.09209
Px O 26	0.06577	-0.20769	0.10716	0.02992	0.15349	-0.08858
Py O 26	-0.05158	0.10515	-0.06349	-0.03793	-0.09499	-0.04037
Pz O 26	0.01349	-0.21007	0.10820	-0.00248	0.08757	-0.37326
S H 8	0.05678	0.06451	0.09382	-0.08776	-0.18096	0.07510
S H 13	-0.07177	-0.08973	0.12802	-0.19465	-0.01439	0.07268
S H 9	0.10980	0.11203	-0.07200	0.06808	0.17075	-0.01544
S H 10	0.14783	0.07803	-0.01068	-0.05601	-0.03908	0.07189
S H 11	-0.03867	-0.19141	-0.04421	0.00177	-0.21936	-0.02383
S H 27	0.07468	-0.03203	0.05331	-0.03668	0.03982	-0.21174
S H 28	0.21406	0.02038	0.01405	-0.02607	-0.10361	0.14091
S H 29	0.11778	0.02045	0.02695	-0.00259	-0.04241	0.05006
S H 30	-0.00539	-0.05476	-0.01221	-0.02542	0.06877	0.11240
S H 31	0.12191	-0.00121	0.21475	0.26142	-0.07461	-0.00383
S H 32	-0.20885	-0.03026	-0.23400	-0.20938	0.08756	0.05011
S H 33	-0.14470	-0.07199	0.03106	0.20055	0.01271	0.13999
S H 34	-0.03934	0.18329	-0.09454	-0.02006	-0.11643	0.14878
S H 35	-0.11193	0.04924	0.12239	0.13626	-0.11484	-0.09716

Mol. Orbital	25	26	27	28	29	30
Symmetry:	25 A	26 A	27 A	28 A	29 A	30 A
Eigenvalue	-0.66895	-0.63997	-0.62203	-0.59573	-0.59176	-0.58469

S C 1	0.07687	-0.08653	0.02038	-0.02672	-0.04563	0.02903
Px C 1	0.13283	-0.16494	-0.09335	0.09108	0.18399	-0.04043
Py C 1	-0.03626	0.06822	0.04266	0.03962	0.08912	0.04235
Pz C 1	-0.10489	0.10537	0.06399	-0.04758	0.02019	0.01539
S C 2	-0.03750	0.00772	-0.10151	-0.01411	0.04706	0.00392
Px C 2	-0.21127	0.23418	0.02026	-0.07554	-0.15417	0.01016
Py C 2	-0.03232	0.04305	-0.07341	0.04165	-0.01919	-0.01787
Pz C 2	-0.06502	0.04557	-0.19793	0.01129	-0.16536	-0.11287
S C 3	0.01946	-0.02755	0.10005	0.01629	0.07075	0.01845
Px C 3	0.00577	0.02497	0.11727	0.01357	-0.30873	-0.03866
Py C 3	-0.01698	0.04373	0.09043	0.00813	0.04541	0.07485
Pz C 3	-0.04601	0.05579	0.13818	-0.07487	-0.04146	0.07076
S C 4	-0.16935	0.07819	-0.13525	-0.03364	0.08444	0.01330
Px C 4	0.14716	-0.22862	-0.09456	0.06776	0.17800	-0.01475
Py C 4	0.04181	0.03376	0.02047	0.06434	0.14608	0.03728
Pz C 4	0.03750	0.01789	-0.02559	-0.00572	0.03809	-0.06880
S C 5	0.01824	0.04530	0.07042	-0.02461	-0.13878	0.00419
Px C 5	-0.25128	0.26581	-0.01965	-0.05971	-0.10186	-0.02001
Py C 5	0.02052	0.10297	0.05604	0.12348	0.00614	0.00324
Pz C 5	-0.01391	0.01579	0.09187	0.01324	-0.18392	-0.06561

S C 6	-0.03337	0.02575	-0.02520	0.05606	0.00889	-0.05018
Px C 6	0.15625	-0.07377	0.16065	-0.04287	-0.35811	0.01534
Py C 6	-0.01134	0.03606	-0.03077	0.02695	0.06581	0.03645
Pz C 6	-0.07249	0.00215	-0.09999	-0.08757	0.02656	0.01635
S O 7	0.05206	-0.02605	0.05839	0.08389	0.02790	-0.04781
Px O 7	-0.03140	0.06502	0.14803	0.09542	0.04559	-0.05368
Py O 7	0.06147	-0.05007	-0.02741	0.11064	0.08643	-0.01955
Pz O 7	0.12553	-0.15140	-0.10748	0.11412	0.03458	-0.11691
S O 12	-0.00060	0.03754	-0.02766	0.07209	-0.02966	-0.08990
Px O 12	0.21030	-0.16429	-0.07078	0.08933	0.08806	-0.09246
Py O 12	0.16605	-0.03912	-0.01291	0.08869	0.16599	0.09422
Pz O 12	0.04588	-0.25129	0.02136	-0.25817	0.06562	0.19918
S O 14	-0.02269	-0.06022	0.11393	-0.16162	0.02191	-0.14013
Px O 14	0.02013	-0.06712	0.13604	-0.16681	-0.01019	-0.13290
Py O 14	0.03871	0.09585	-0.08511	0.06511	0.01556	0.03558
Pz O 14	0.00099	0.07847	-0.04544	-0.12429	0.02205	-0.17429
S C 15	-0.00695	0.04517	-0.14233	0.09883	-0.00135	0.05305
Px C 15	0.05245	0.01732	0.05263	0.08401	0.00610	0.10143
Py C 15	0.03344	0.07450	-0.08190	-0.03184	0.00888	-0.03227
Pz C 15	-0.09636	0.07000	-0.18533	-0.02112	0.03628	-0.02236
S C 16	-0.10304	-0.11011	0.00550	-0.05336	0.04897	-0.01220
Px C 16	0.04909	0.21703	-0.05785	0.00115	0.05633	0.09289
Py C 16	0.10500	-0.03360	0.07050	-0.06273	0.01595	0.10962
Pz C 16	0.00500	0.05111	0.30130	0.05768	0.07860	0.07698
S C 17	0.07143	-0.02700	0.11749	-0.00207	-0.03115	0.05268
Px C 17	0.22149	0.03840	-0.07492	0.00536	-0.13993	-0.06705
Py C 17	-0.00937	-0.03862	-0.03643	-0.00250	0.09361	0.08295
Pz C 17	0.01050	-0.07274	-0.21221	-0.00619	-0.10150	-0.07233
S C 18	0.09361	0.08470	0.13301	-0.09726	0.07446	-0.10812
Px C 18	-0.01873	-0.13228	-0.03825	0.01059	-0.07892	-0.07182
Py C 18	0.11219	0.14640	0.03596	0.13427	0.00359	0.03078
Pz C 18	0.02403	-0.06465	0.04483	0.09141	-0.05659	0.09629
S C 19	-0.08106	-0.01479	-0.10439	0.00531	-0.01757	-0.01916
Px C 19	0.04124	0.04967	-0.04685	0.18240	-0.09731	0.21437
Py C 19	0.01095	-0.04057	0.04203	-0.09892	0.02420	-0.17793
Pz C 19	0.02169	-0.07371	0.02521	-0.04173	-0.08736	0.13955
S C 20	0.06224	0.00398	0.09098	-0.02601	0.02800	-0.05514
Px C 20	0.13912	0.19739	0.04347	0.00363	0.07562	-0.01569
Py C 20	-0.13052	-0.13922	-0.07831	0.06712	-0.07020	-0.07507
Pz C 20	-0.12533	0.02753	-0.11239	0.03472	0.07082	-0.11717
S C 21	-0.10319	-0.06690	0.04810	0.14390	-0.03491	0.06403
Px C 21	0.00207	-0.12824	-0.04254	-0.03415	-0.08672	-0.08593
Py C 21	0.01052	0.07317	0.03783	0.12777	-0.00498	0.01370
Pz C 21	-0.05591	-0.16546	0.06476	0.03152	-0.09169	0.10550
S C 22	0.08905	0.02411	-0.05493	-0.10205	-0.03152	0.02451
Px C 22	-0.06380	-0.01856	-0.03744	0.27025	-0.07923	0.17367
Py C 22	0.10936	0.02672	-0.06670	-0.11559	-0.01421	-0.20000
Pz C 22	0.02183	-0.04641	-0.20822	-0.00254	-0.06332	0.17896
S C 23	0.04681	0.06985	-0.01703	0.10497	-0.00612	0.11376

Px C 23	0.14222	0.19490	0.02935	-0.00492	0.04655	-0.11460
Py C 23	-0.03920	-0.10004	-0.00331	0.19287	-0.10118	-0.11274
Pz C 23	-0.07602	0.03209	0.23656	0.03528	0.09115	-0.09769
S C 24	0.08882	-0.00230	-0.05868	-0.03835	-0.05191	0.02918
Px C 24	-0.07236	-0.23167	-0.04656	-0.17568	-0.03045	0.02804
Py C 24	0.26516	0.21245	-0.10054	-0.12524	0.02776	0.19714
Pz C 24	0.07575	0.00302	-0.01178	0.22949	0.00371	-0.21263
S C 25	-0.10483	-0.05456	0.05780	0.00782	0.01360	0.00928
Px C 25	0.10478	-0.00740	-0.07849	0.14736	-0.16932	-0.08802
Py C 25	0.11880	0.08476	-0.09878	0.02563	-0.02474	-0.19725
Pz C 25	0.11184	0.08727	-0.08643	-0.27254	-0.03552	0.21717
S O 26	0.01407	-0.04419	-0.14806	-0.10192	-0.05995	0.03069
Px O 26	0.03349	0.02806	-0.20141	-0.10705	-0.06118	-0.03610
Py O 26	-0.01651	0.04610	0.14968	0.18400	0.05155	-0.07897
Pz O 26	-0.01865	0.18148	-0.01668	0.05169	0.14186	-0.06995
S H 8	-0.16492	0.15990	-0.17670	-0.02535	-0.16442	-0.06928
S H 13	-0.13550	0.06920	0.03930	-0.09087	-0.03209	0.08072
S H 9	0.03507	-0.00239	0.12739	0.03137	-0.23281	-0.04028
S H 10	-0.15325	0.07472	-0.16272	0.05042	0.32199	-0.03234
S H 11	0.03425	-0.05790	-0.11044	-0.03657	-0.00746	0.01448
S H 27	-0.01615	0.00409	-0.08530	0.13923	-0.11455	0.25374
S H 28	0.21103	0.14650	0.15320	-0.06751	0.05213	0.06192
S H 29	0.11242	0.04684	0.04895	-0.27927	0.05983	-0.26379
S H 30	0.26651	0.22053	-0.08591	0.06341	0.01457	0.04595
S H 31	-0.08578	-0.00513	0.06007	0.18263	-0.03245	-0.15927
S H 32	0.07025	0.03022	-0.07102	0.10288	-0.07796	-0.19976
S H 33	-0.15010	-0.03868	0.10873	-0.03963	0.15586	-0.01857
S H 34	-0.00839	-0.05130	0.13937	0.07425	0.00528	0.00208
S H 35	0.20159	0.01483	-0.01987	-0.00300	-0.17863	-0.07983

Mol. Orbital	31	32	33	34	35	36
Symmetry:	31 A	32 A	33 A	34 A	35 A	36 A
Eigenvalue	-0.57136	-0.56086	-0.55677	-0.54284	-0.53523	-0.53183

S C 1	0.07673	0.04201	-0.05005	-0.04420	-0.01165	-0.00415
Px C 1	-0.03150	0.01696	-0.05402	0.01482	0.04254	0.00596
Py C 1	0.16202	-0.16385	0.16107	-0.06273	-0.04612	-0.26986
Pz C 1	-0.19761	0.03927	0.04965	-0.00114	-0.12229	0.16439
S C 2	-0.02228	-0.01816	0.03463	-0.01827	-0.05041	0.00907
Px C 2	-0.02035	-0.04411	0.07993	0.00218	-0.06308	0.01868
Py C 2	0.22494	-0.09647	-0.00081	-0.05501	-0.00556	-0.11815
Pz C 2	0.10713	0.02683	-0.18175	-0.03015	-0.04107	0.12459
S C 3	-0.03522	0.01626	-0.00300	0.00788	0.02052	-0.00082
Px C 3	0.19533	0.08898	-0.18190	0.01651	0.14997	-0.03632
Py C 3	0.10869	-0.05660	0.09684	-0.00814	0.04374	-0.08056
Pz C 3	-0.18123	0.03885	0.12235	0.05721	0.03479	-0.04504
S C 4	0.00708	-0.00821	-0.00558	-0.03151	-0.01608	0.00715
Px C 4	0.01174	0.03580	-0.06362	-0.05177	-0.06468	0.02314
Py C 4	0.16609	-0.10606	0.05952	-0.02614	-0.03000	0.08189

Pz C 4	-0.17779	-0.05549	0.03589	0.01652	-0.10251	0.04888
S C 5	0.03867	0.00304	0.01091	-0.02810	-0.05399	0.00917
Px C 5	-0.06012	-0.04667	0.04136	0.06991	0.08240	-0.01831
Py C 5	0.26864	-0.14117	0.07286	0.00070	-0.03104	0.07389
Pz C 5	-0.08139	0.08503	-0.08127	0.02855	0.01845	-0.02463
S C 6	-0.00810	-0.01168	-0.02725	0.05900	0.08835	-0.01717
Px C 6	0.20230	0.08372	-0.10696	-0.05972	-0.03362	0.00606
Py C 6	0.19693	-0.12991	0.08479	-0.02306	0.01933	-0.10711
Pz C 6	-0.09715	0.04480	-0.03586	0.02703	0.06747	0.02845
S O 7	-0.03852	0.00123	-0.02869	0.12352	0.21326	-0.06375
Px O 7	-0.11895	-0.00321	-0.00805	0.20225	0.32044	-0.06816
Py O 7	0.24899	-0.17951	0.08396	0.00303	0.19355	-0.57888
Pz O 7	-0.06545	0.10680	-0.21791	0.18829	0.32626	0.16849
S O 12	-0.00570	-0.06696	-0.01256	0.10937	0.11457	0.00405
Px O 12	-0.08366	-0.02942	-0.02486	0.07491	0.08101	-0.02612
Py O 12	0.30535	-0.14358	0.12277	-0.09827	-0.22771	0.26522
Pz O 12	-0.10288	0.20990	-0.03543	-0.21637	-0.14342	-0.13645
S O 14	-0.01346	-0.27366	-0.07881	-0.04846	0.04949	0.08774
Px O 14	-0.03807	-0.40368	-0.06146	-0.08817	0.12292	0.20067
Py O 14	0.04836	0.22956	0.11266	0.00344	0.03899	0.01352
Pz O 14	-0.00361	-0.19363	-0.04987	-0.00999	-0.02622	0.02034
S C 15	0.04668	0.08707	-0.03747	-0.00167	0.02196	0.00631
Px C 15	0.01435	0.27959	0.13110	0.03026	-0.00560	-0.04600
Py C 15	0.03353	-0.05479	0.03491	-0.06469	0.11656	0.12939
Pz C 15	0.02875	0.08331	-0.03321	0.00606	-0.05714	-0.09644
S C 16	0.01746	-0.02379	-0.09242	-0.04533	0.00484	0.01271
Px C 16	0.03782	-0.04478	0.02942	0.00599	0.10770	0.10117
Py C 16	0.06637	0.06470	0.06968	0.04003	0.06698	0.09306
Pz C 16	-0.05368	0.05933	0.04246	0.01444	0.01765	-0.00442
S C 17	-0.03546	0.00074	0.07876	0.02069	0.01077	-0.01889
Px C 17	-0.04841	-0.13390	0.15364	0.05459	-0.09589	0.04604
Py C 17	0.16738	0.05451	-0.05093	-0.03249	0.08001	0.06959
Pz C 17	0.00753	0.00925	-0.03031	-0.00842	-0.03411	-0.07689
S C 18	-0.00804	-0.01211	-0.03276	-0.01979	-0.01942	-0.01056
Px C 18	-0.02089	0.03120	0.15729	-0.05452	-0.00109	0.03407
Py C 18	-0.03806	0.03433	0.01134	-0.11217	0.10675	0.05768
Pz C 18	-0.00207	-0.09164	-0.02307	0.04292	0.03909	0.07706
S C 19	0.03343	0.01239	0.04539	0.02004	0.01402	0.01739
Px C 19	-0.10985	-0.11792	0.00483	-0.10910	0.10301	0.05454
Py C 19	0.00252	0.09221	0.11062	-0.10983	-0.00401	-0.01460
Pz C 19	-0.13764	-0.20209	0.00246	0.02654	-0.08395	-0.05420
S C 20	0.01414	0.03650	0.01640	0.01084	-0.02117	0.00795
Px C 20	-0.05216	0.08819	-0.10709	-0.21314	0.03285	-0.08099
Py C 20	0.04103	0.03096	0.20190	-0.09992	0.13214	0.12458
Pz C 20	0.16947	0.18049	-0.01085	0.07339	0.04780	0.04473
S C 21	-0.01253	-0.05005	0.02555	0.02058	-0.00897	0.05398
Px C 21	-0.02550	-0.01935	0.22066	-0.16852	0.12049	0.09216
Py C 21	-0.08116	0.02828	0.00335	-0.31795	0.13042	-0.01720
Pz C 21	-0.04076	-0.14718	0.05745	0.11831	0.01002	0.02038

S C 22	-0.02759	-0.02826	0.00857	-0.00800	0.03871	-0.04383
Px C 22	-0.11968	-0.05304	-0.08713	-0.19444	0.01984	-0.02441
Py C 22	0.00072	0.07330	0.15693	-0.12578	0.05655	0.01804
Pz C 22	-0.02840	-0.03676	-0.13128	-0.00021	-0.04724	-0.02794
S C 23	-0.01227	0.03898	-0.00319	0.02089	-0.02300	0.01991
Px C 23	-0.07895	0.00908	-0.07411	-0.14292	0.02536	-0.07505
Py C 23	-0.02299	0.04870	0.22691	-0.01115	-0.02710	0.06219
Pz C 23	0.08677	0.05626	0.12525	0.11522	0.01609	0.07713
S C 24	-0.03762	0.05422	0.06779	-0.00519	-0.03687	-0.02936
Px C 24	0.05317	0.01438	-0.04502	0.03204	0.00692	-0.03528
Py C 24	0.05450	0.01007	-0.00085	0.12108	0.10748	0.15053
Pz C 24	-0.00743	-0.02957	-0.11055	-0.00684	-0.14273	0.07597
S C 25	0.00941	-0.00275	0.00179	0.01212	0.01566	-0.01439
Px C 25	-0.08079	0.05958	0.27143	0.15744	-0.11846	-0.07794
Py C 25	-0.12961	-0.09485	-0.21856	-0.08224	-0.11823	-0.17439
Pz C 25	-0.03204	0.03203	0.07944	0.02036	0.12255	-0.10080
S O 26	-0.00348	-0.04373	0.02768	-0.00288	0.11305	-0.03209
Px O 26	-0.03313	0.00842	0.12476	-0.35795	0.33000	-0.00518
Py O 26	-0.04228	0.11676	0.05995	-0.42787	0.05843	0.09411
Pz O 26	0.08994	0.16494	-0.16854	0.09391	-0.17795	-0.02188
S H 8	0.10944	-0.04706	-0.05301	-0.03961	-0.08347	0.05751
S H 13	0.01857	0.04966	0.00967	-0.07191	-0.06131	-0.01205
S H 9	0.17100	0.07490	-0.17361	0.01593	0.13634	-0.02337
S H 10	-0.19254	-0.07705	0.08131	0.08421	0.08045	-0.01150
S H 11	0.06264	0.00673	-0.01678	-0.09934	-0.15447	0.05087
S H 27	-0.10960	-0.19622	-0.02449	-0.00825	0.04778	0.03104
S H 28	-0.12287	-0.04474	-0.15130	-0.08214	-0.09026	-0.13333
S H 29	0.08070	0.06636	0.17467	0.06838	0.04964	0.01601
S H 30	0.02962	-0.00782	0.00314	0.07876	-0.00482	0.16171
S H 31	-0.09060	0.00414	0.04229	-0.09370	-0.10060	-0.09819
S H 32	-0.12795	-0.05280	-0.06245	0.00113	-0.14447	-0.17269
S H 33	0.07865	-0.07018	-0.26416	-0.13676	0.06473	0.08626
S H 34	-0.02021	-0.01287	0.01383	0.01474	-0.08865	0.03708
S H 35	-0.09369	-0.12419	0.15484	0.06425	-0.09353	-0.00395

Mol. Orbital	37	38	39	40	41	42
Symmetry:	37 A	38 A	39 A	40 A	41 A	42 A
Eigenvalue	-0.52286	-0.50697	-0.50514	-0.48643	-0.48247	-0.46666

S C 1	-0.01524	0.02500	-0.01209	0.02721	0.08203	0.01966
Px C 1	0.01497	0.01626	-0.05589	-0.02028	0.22562	0.30654
Py C 1	0.00276	-0.11519	0.02328	-0.04459	0.01201	0.07083
Pz C 1	-0.05547	-0.02708	-0.02629	-0.06541	-0.01960	0.11018
S C 2	-0.01685	-0.01733	0.01172	-0.00610	-0.01603	0.01740
Px C 2	0.00127	-0.03995	0.05116	-0.00800	-0.26074	-0.28143
Py C 2	0.12721	-0.04483	-0.09160	-0.02161	0.01562	-0.02733
Pz C 2	0.22025	-0.01538	-0.15029	-0.05892	0.04598	-0.02259
S C 3	0.00010	-0.00090	-0.02839	-0.02151	0.01525	-0.01306
Px C 3	0.00312	0.09147	-0.00597	0.06907	0.24385	0.21074

Py C 3	-0.07953	0.03751	0.01748	0.05889	-0.01821	0.00080
Pz C 3	-0.25339	0.03952	0.22317	0.08145	-0.04604	0.04201
S C 4	0.01953	0.02680	-0.01661	0.03445	0.02920	-0.06295
Px C 4	0.01169	-0.06954	-0.07065	-0.10522	-0.14590	-0.22033
Py C 4	0.13139	0.01575	-0.16996	-0.01962	-0.06064	-0.04695
Pz C 4	0.18344	-0.10646	-0.07315	-0.10307	-0.03803	-0.00035
S C 5	-0.01887	-0.01271	0.00110	0.00308	0.02643	0.06772
Px C 5	0.05566	0.04567	0.04654	0.07537	0.11631	0.17062
Py C 5	-0.04238	0.15259	-0.03177	0.01620	-0.11368	0.07036
Pz C 5	0.00203	-0.15260	-0.00608	-0.13669	-0.06007	0.01300
S C 6	0.02646	0.00654	0.00831	-0.00981	-0.06287	-0.05043
Px C 6	-0.03415	-0.01657	0.00672	-0.01544	-0.13953	-0.22749
Py C 6	0.01919	0.08203	0.01515	0.07938	-0.02723	-0.03539
Pz C 6	0.04871	0.05504	0.03323	0.10000	0.04975	-0.12261
S O 7	-0.00916	0.06956	0.08089	0.07111	-0.07216	-0.12745
Px O 7	-0.02402	0.12449	0.13366	0.12528	-0.13763	-0.22415
Py O 7	0.08227	-0.20325	0.14901	-0.00939	0.09094	-0.08327
Pz O 7	0.05627	0.26782	0.00070	0.17024	-0.01540	-0.13548
S O 12	0.12071	-0.02067	-0.03715	-0.08018	-0.15482	0.05706
Px O 12	0.13447	-0.10930	-0.07028	-0.10887	-0.13094	-0.02215
Py O 12	-0.22265	0.42446	0.05785	0.19602	-0.06597	-0.03000
Pz O 12	-0.08153	-0.13823	0.01878	0.09364	0.24787	-0.25488
S O 14	-0.03510	-0.05236	0.03364	0.02854	0.04155	-0.01677
Px O 14	-0.04943	-0.24940	0.01265	0.23245	0.02281	0.02475
Py O 14	0.06380	-0.15247	-0.13313	0.31049	-0.09293	0.07790
Pz O 14	0.01344	0.09823	0.08825	-0.02306	0.13576	-0.06163
S C 15	-0.09796	-0.04250	0.06488	0.00314	0.01749	-0.01402
Px C 15	0.07966	-0.05603	-0.14427	0.08631	-0.12440	0.06928
Py C 15	0.02884	-0.21896	-0.08182	0.33535	-0.00326	0.01318
Pz C 15	0.10977	0.20067	-0.01612	-0.01915	0.07199	-0.07869
S C 16	0.08295	-0.00632	-0.03118	0.01329	-0.03935	0.00761
Px C 16	0.02474	-0.04696	-0.07655	0.05559	0.16690	-0.12070
Py C 16	0.11088	-0.13617	-0.04400	0.03358	-0.12400	0.07370
Pz C 16	0.00678	0.00156	-0.17675	-0.12567	0.06597	-0.04482
S C 17	-0.08500	-0.00671	0.02240	-0.01551	-0.05859	0.00082
Px C 17	0.09117	-0.06966	0.07911	0.02634	-0.12562	0.13352
Py C 17	0.02360	-0.04181	-0.08093	0.04956	-0.02620	-0.08249
Pz C 17	-0.15823	0.05179	0.21456	0.07394	-0.05455	0.01710
S C 18	0.02512	0.00992	-0.03274	-0.01022	-0.00144	0.00352
Px C 18	0.09628	-0.08590	0.01761	0.25790	-0.05835	0.08464
Py C 18	-0.13557	-0.18399	-0.13863	0.11399	0.02960	-0.05167
Pz C 18	-0.17144	-0.11860	0.10686	-0.12062	-0.00919	0.03378
S C 19	0.00015	0.00455	0.00671	0.01696	0.01891	-0.00789
Px C 19	-0.03735	-0.07486	-0.10055	0.06448	0.08539	-0.08772
Py C 19	0.14035	0.00832	-0.01079	0.20076	-0.06526	0.06535
Pz C 19	0.27054	0.18126	-0.06059	0.05684	0.07845	-0.05563
S C 20	0.01204	-0.01792	0.03968	-0.00565	0.00052	0.00174
Px C 20	0.00414	0.02905	-0.02296	0.06791	-0.15516	0.11842
Py C 20	-0.04215	-0.08344	0.04114	0.01038	0.09337	-0.07538

Pz C 20	-0.27365	-0.14746	0.07062	-0.10136	-0.07223	0.05841
S C 21	0.02705	-0.02095	0.00552	-0.01830	0.04331	-0.02219
Px C 21	0.08836	0.02867	0.08497	-0.02560	0.14381	-0.12280
Py C 21	-0.00447	0.07229	-0.02883	-0.05795	-0.11482	0.09656
Pz C 21	-0.02727	0.01258	-0.14832	-0.04180	0.02806	-0.00900
S C 22	-0.04313	0.02757	-0.04889	0.01137	-0.03866	0.02863
Px C 22	-0.00793	-0.00651	0.01288	0.06971	-0.08909	0.07920
Py C 22	0.01967	0.00025	0.04102	0.06430	0.09902	-0.09504
Pz C 22	0.02559	-0.04826	0.20344	0.10880	-0.03955	0.02470
S C 23	0.03991	-0.01433	0.04118	-0.02895	0.04065	-0.02572
Px C 23	-0.08954	0.00129	-0.16763	0.05971	0.04440	-0.09115
Py C 23	0.02455	-0.05566	-0.01035	0.09919	0.05331	0.00640
Pz C 23	0.02067	0.03589	-0.14209	-0.18481	0.06916	-0.03785
S C 24	0.01540	-0.01335	0.03389	0.03228	0.01124	-0.00370
Px C 24	0.11541	0.04723	0.11854	-0.02433	-0.23873	0.17204
Py C 24	0.07232	-0.09871	0.18785	-0.17284	0.10551	-0.01861
Pz C 24	-0.08927	-0.13815	0.09159	-0.07551	0.04894	-0.01856
S C 25	0.03045	0.04512	-0.03522	-0.01188	-0.04463	0.03888
Px C 25	0.00838	0.11303	-0.05290	-0.01894	0.10181	-0.04080
Py C 25	-0.16253	0.05509	-0.05546	0.03701	-0.00078	-0.05541
Pz C 25	0.06951	0.12098	-0.04149	0.05437	-0.03523	0.00841
S O 26	-0.17441	0.01178	-0.16078	-0.06577	-0.07168	0.05478
Px O 26	-0.16325	0.14900	-0.10183	-0.30806	-0.12409	0.09631
Py O 26	0.31769	0.11646	0.42784	-0.14190	0.05433	-0.04167
Pz O 26	0.04789	-0.11009	0.19994	0.17010	-0.00080	-0.01088
S H 8	0.17843	-0.05592	-0.09149	-0.05401	-0.13439	-0.19471
S H 13	-0.09189	0.04148	0.04786	0.08318	0.13514	-0.01886
S H 9	0.04689	0.07356	-0.04842	0.04062	0.24028	0.20340
S H 10	0.05116	0.03008	0.00334	0.02919	0.11885	0.18587
S H 11	0.02886	-0.05195	-0.08450	-0.06203	0.09493	0.14041
S H 27	0.01650	0.01927	-0.08608	-0.01711	0.13053	-0.12184
S H 28	0.16756	0.13370	-0.05885	0.07995	-0.10491	0.08280
S H 29	-0.01673	0.03573	-0.09521	-0.05789	0.10976	-0.10485
S H 30	-0.02834	-0.13078	0.16019	-0.14287	0.17848	-0.07580
S H 31	-0.11219	0.02202	-0.17969	0.13607	0.07139	-0.08701
S H 32	-0.12026	0.10435	-0.08819	0.01961	0.02717	-0.05025
S H 33	-0.03321	-0.12008	0.03773	-0.00522	-0.09800	0.04532
S H 34	0.16724	-0.00092	0.12527	0.05791	0.08521	-0.06493
S H 35	0.00057	-0.03529	0.14640	0.01992	-0.11824	0.16098

Mol. Orbital	43	44	45	46	47	48
Symmetry:	43 A	44 A	45 A	46 A	47 A	48 A
Eigenvalue	-0.45888	-0.45176	-0.43995	-0.43406	-0.42882	-0.36366

S C 1	-0.01509	0.02531	-0.00747	0.00098	0.00560	0.00363
Px C 1	0.04332	-0.06380	0.01896	0.01475	-0.00528	-0.01388
Py C 1	0.06131	-0.04962	-0.09029	-0.01887	-0.04910	0.28322
Pz C 1	0.04685	-0.09993	0.07048	-0.01162	0.01430	-0.13745
S C 2	0.01395	-0.04080	-0.00603	-0.02145	0.00028	-0.01980

Px C 2	-0.02791	0.02779	-0.00200	-0.01856	0.00468	-0.00737
Py C 2	0.11531	0.07104	-0.23539	-0.01269	-0.08012	0.22997
Pz C 2	-0.10746	0.13305	0.14187	0.10208	0.03214	-0.05747
S C 3	0.00667	0.01692	0.03219	0.01395	0.00115	0.03594
Px C 3	-0.01035	-0.00476	0.00685	0.01159	0.00692	-0.01381
Py C 3	0.21587	-0.05263	-0.31303	-0.10533	-0.07176	-0.06351
Pz C 3	-0.04522	-0.15889	0.08011	-0.06745	0.03768	-0.04126
S C 4	-0.00171	0.00444	0.00869	-0.03685	0.01348	-0.00519
Px C 4	0.06742	-0.10310	0.12801	-0.08210	0.01356	0.07926
Py C 4	0.16427	0.12192	-0.24679	0.02578	-0.05110	-0.25287
Pz C 4	-0.18305	0.21743	0.09568	0.19417	-0.00200	0.16386
S C 5	0.00158	-0.00460	-0.02866	0.00953	-0.00089	-0.02983
Px C 5	-0.08080	0.10457	-0.07734	0.08142	-0.00911	-0.04842
Py C 5	0.12525	-0.09648	-0.06164	-0.00161	-0.04994	0.01503
Pz C 5	0.07124	-0.17464	0.13491	-0.07238	0.01475	0.01549
S C 6	0.01949	-0.03103	0.02383	-0.01716	-0.00223	0.01484
Px C 6	0.00729	-0.02198	0.03960	-0.04950	0.01231	0.00757
Py C 6	0.01786	0.08293	-0.17750	0.03139	-0.06231	0.28252
Pz C 6	-0.15217	0.19565	-0.00782	0.05816	0.03768	-0.15696
S O 7	-0.03678	0.04265	-0.01893	-0.00360	0.00341	-0.00517
Px O 7	-0.05938	0.09038	-0.05790	0.00098	-0.00017	0.00470
Py O 7	-0.27209	0.07395	0.30421	0.05128	0.11016	-0.26609
Pz O 7	0.01008	0.15120	-0.19525	0.01667	-0.04290	0.12464
S O 12	0.08579	-0.10592	0.06835	0.02319	-0.02766	0.00210
Px O 12	0.10669	-0.07202	0.01563	-0.01334	-0.02226	0.00768
Py O 12	-0.25962	0.07796	0.28834	0.15893	0.07627	-0.01502
Pz O 12	-0.08184	0.27141	-0.27657	-0.06900	0.01152	0.01378
S O 14	0.06758	0.04286	0.04708	-0.03539	0.01117	0.00602
Px O 14	0.11795	0.08357	0.08348	0.00690	0.22221	0.17625
Py O 14	-0.16491	-0.18501	-0.10485	-0.04767	0.38932	0.19035
Pz O 14	-0.01071	-0.04040	-0.03890	-0.29694	-0.06369	-0.18199
S C 15	0.05598	-0.00186	0.01438	-0.03289	0.01024	-0.00401
Px C 15	-0.13839	-0.06868	-0.07876	0.11306	0.09120	0.00689
Py C 15	-0.01631	-0.11069	0.01478	-0.08398	0.22935	0.05306
Pz C 15	-0.06417	-0.17394	0.00766	-0.14765	-0.04093	0.01564
S C 16	-0.03852	-0.01378	0.03947	0.02618	-0.01338	0.03081
Px C 16	0.17899	0.02526	0.12240	-0.12452	0.09754	-0.10853
Py C 16	-0.02845	0.01443	-0.09108	0.05082	0.06363	-0.33780
Pz C 16	0.07064	0.17393	0.11116	0.14981	-0.00723	0.11416
S C 17	0.06780	-0.01350	0.01017	0.03119	-0.00660	-0.00569
Px C 17	-0.09712	0.11226	-0.24723	0.09394	-0.03223	-0.23049
Py C 17	0.15359	-0.09704	-0.05110	-0.12935	0.07022	-0.42878
Pz C 17	-0.04512	-0.21316	-0.04152	-0.14586	-0.02035	0.08859
S C 18	-0.03949	0.00804	-0.02112	-0.01266	0.00055	-0.01240
Px C 18	0.06911	0.12653	0.12314	-0.15889	-0.09773	0.02044
Py C 18	-0.09466	-0.09060	-0.00913	0.15879	-0.19191	0.00574
Pz C 18	0.11521	0.17215	-0.01544	0.12013	0.04411	-0.03154
S C 19	-0.00018	-0.01980	0.00658	-0.04990	0.01573	0.00339
Px C 19	-0.09576	-0.15122	-0.01181	0.11690	-0.21065	-0.00144

Py C 19	-0.00286	0.04654	0.11845	-0.15771	-0.21538	0.02426
Pz C 19	-0.07063	-0.14829	-0.02665	-0.12854	0.10406	0.00307
S C 20	0.02985	0.02707	0.00607	0.03947	-0.00738	-0.00044
Px C 20	-0.00452	0.12322	0.08326	-0.12771	-0.18538	-0.00159
Py C 20	-0.00795	-0.07315	0.03144	0.10574	-0.25161	-0.00891
Pz C 20	0.08488	0.15572	-0.00242	0.09220	0.05136	-0.00130
S C 21	-0.04387	-0.01699	-0.01949	-0.03184	0.00337	0.00024
Px C 21	0.01864	-0.14735	-0.00653	0.14398	-0.12018	-0.02016
Py C 21	-0.04847	0.11810	0.04159	-0.16472	-0.11654	-0.01570
Pz C 21	-0.09320	-0.01402	-0.02957	-0.07373	0.04736	0.00835
S C 22	0.04304	0.03549	0.02526	0.00550	0.00636	-0.00324
Px C 22	0.01497	0.12642	0.06282	-0.13358	-0.14472	-0.02781
Py C 22	0.05385	-0.08130	0.03897	0.10795	-0.20226	-0.03366
Pz C 22	0.19064	0.02300	0.02980	0.14778	0.06000	-0.00498
S C 23	-0.00910	-0.00179	-0.00070	-0.00014	-0.00616	0.01776
Px C 23	-0.09132	-0.15605	-0.03647	0.13903	-0.16138	-0.02431
Py C 23	0.01090	0.13795	0.08705	-0.21769	-0.12552	0.00493
Pz C 23	-0.21212	-0.04899	-0.06728	-0.13175	0.04634	0.02714
S C 24	-0.00733	0.03253	-0.03293	0.00675	-0.01651	-0.00359
Px C 24	-0.15647	-0.10068	-0.08384	0.09672	-0.10085	0.00510
Py C 24	-0.04747	0.02615	0.05538	-0.12663	-0.07087	0.12967
Pz C 24	-0.23374	-0.00482	-0.17785	-0.14564	0.04070	-0.01812
S C 25	0.00839	0.01829	0.04079	-0.02664	-0.00507	0.02208
Px C 25	0.15264	0.13098	0.06880	-0.09108	0.12124	0.01830
Py C 25	0.05387	-0.08097	-0.08453	0.19153	0.08398	-0.04088
Pz C 25	0.22038	-0.02567	0.14337	0.19653	-0.04545	0.03143
S O 26	-0.04275	0.06759	0.00350	-0.05981	0.00200	0.00095
Px O 26	-0.05912	0.09416	-0.07103	-0.07302	0.27238	0.01889
Py O 26	0.12762	-0.07252	-0.08059	0.15622	0.31665	0.01490
Pz O 26	0.12742	0.00272	0.05114	0.10478	-0.11090	-0.01033
S H 8	-0.04963	0.12046	0.01380	0.04967	-0.00226	0.02803
S H 13	-0.08274	0.09504	-0.06479	-0.00475	0.01613	-0.00085
S H 9	-0.01307	0.03947	0.00419	0.04276	0.00023	0.00192
S H 10	-0.02608	0.04684	-0.03806	0.05683	-0.00947	-0.02117
S H 11	0.03418	-0.03753	0.02020	0.00683	-0.00378	0.00658
S H 27	-0.09233	-0.20324	-0.06876	0.09619	-0.00871	-0.00809
S H 28	-0.03079	0.04295	0.03196	-0.17482	0.02319	0.00639
S H 29	-0.05329	-0.14300	-0.03607	0.10543	-0.01730	0.00367
S H 30	-0.10096	0.05624	-0.02057	-0.20121	-0.00449	0.08780
S H 31	0.12002	0.04677	-0.01942	0.02783	0.11696	-0.11416
S H 32	0.10856	0.00066	-0.03282	0.10198	0.13498	-0.03061
S H 33	-0.21846	-0.12339	-0.11168	0.02221	-0.09304	-0.03160
S H 34	0.03342	-0.08254	-0.00699	0.06559	-0.00198	-0.00150
S H 35	-0.12542	0.07555	-0.21271	0.09550	-0.05363	-0.06387
Mol. Orbital	49	50	51	52	53	54
Symmetry:	49 A	50 A	51 A	52 A	53 A	54 A
Eigenvalue	-0.34408	-0.33312	-0.33162	-0.31379	-0.28941	-0.02331

S C 1	-0.00069	-0.00416	-0.00227	-0.00025	0.00150	0.00159
Px C 1	-0.00096	0.00182	0.00176	-0.00097	-0.00884	0.01066
Py C 1	0.01250	-0.05563	-0.00824	0.06824	0.32989	-0.23402
Pz C 1	-0.00677	0.02774	0.00570	-0.03119	-0.15458	0.10991
S C 2	-0.01275	-0.00643	-0.00189	-0.00111	0.00085	-0.01530
Px C 2	-0.00232	-0.01168	-0.00414	-0.00306	-0.00733	-0.00678
Py C 2	0.00379	0.40818	0.11916	0.07469	0.22597	0.05786
Pz C 2	0.02947	-0.17638	-0.05122	-0.03257	-0.10731	-0.01003
S C 3	0.02617	0.00363	0.00061	0.00056	-0.00916	0.02848
Px C 3	-0.01078	-0.01965	-0.00459	0.00195	0.01481	-0.01295
Py C 3	-0.03876	0.41842	0.11398	-0.00696	-0.16817	0.18189
Pz C 3	-0.03188	-0.19540	-0.05330	0.00260	0.08700	-0.09894
S C 4	-0.00396	0.00144	-0.00191	0.00053	-0.00740	-0.00202
Px C 4	0.03106	-0.00010	-0.00215	0.00529	-0.00216	0.02407
Py C 4	-0.00049	-0.00247	-0.00964	-0.08620	-0.38280	-0.15791
Pz C 4	0.04187	0.00734	0.00929	0.03761	0.17428	0.08451
S C 5	-0.01640	-0.00654	-0.00206	-0.00145	0.01000	-0.01470
Px C 5	-0.02143	0.02992	0.01189	0.00587	0.04055	-0.03325
Py C 5	0.01494	-0.32657	-0.09091	-0.05998	-0.27771	0.19311
Pz C 5	0.00399	0.17680	0.05242	0.03462	0.13521	-0.09891
S C 6	0.00697	0.00107	0.00096	0.00148	-0.00372	0.00979
Px C 6	0.00608	0.02127	0.00416	-0.00081	-0.01208	0.00206
Py C 6	0.02304	-0.47149	-0.12718	0.00956	0.11784	0.05926
Pz C 6	-0.02115	0.21941	0.05777	-0.00743	-0.05138	-0.03587
S O 7	-0.00248	-0.00030	-0.00030	-0.00054	-0.00108	-0.00105
Px O 7	-0.00373	-0.00263	-0.00092	0.00130	0.00898	-0.00455
Py O 7	-0.01015	0.03515	0.00435	-0.04402	-0.18455	0.06575
Pz O 7	0.00383	-0.01981	-0.00405	0.01991	0.08753	-0.02981
S O 12	0.01270	0.00345	0.01053	0.00653	-0.00307	-0.00458
Px O 12	0.00723	-0.02885	-0.00523	-0.00350	-0.02214	0.00796
Py O 12	0.01302	0.22723	0.06926	0.04400	0.14599	-0.05089
Pz O 12	-0.01411	-0.12764	-0.05100	-0.03008	-0.06969	0.03180
S O 14	0.00230	-0.00075	-0.00063	0.00200	0.00272	0.00041
Px O 14	-0.15425	0.02179	0.04907	-0.15517	-0.09462	-0.16312
Py O 14	0.36776	0.04595	0.07761	-0.26184	-0.12577	-0.31145
Pz O 14	0.74940	-0.00254	-0.06799	0.14130	0.08006	0.08212
S C 15	0.00494	-0.00161	-0.00607	-0.00060	-0.00260	-0.00300
Px C 15	0.05755	-0.00005	0.01007	0.00999	0.03012	0.20596
Py C 15	-0.07665	-0.00298	-0.00339	0.02947	0.02848	0.38226
Pz C 15	-0.22858	-0.00457	0.00335	-0.01927	-0.02310	-0.10235
S C 16	-0.07795	-0.00483	0.00979	0.01659	0.01730	0.01888
Px C 16	-0.15629	-0.04682	-0.02104	0.01017	0.18850	0.10347
Py C 16	0.02140	-0.08643	-0.01292	0.05299	0.40219	0.22286
Pz C 16	0.18559	0.02293	0.00344	-0.01317	-0.08529	-0.06203
S C 17	-0.00324	0.00562	0.00479	-0.00549	-0.00462	-0.00388
Px C 17	-0.12112	-0.03083	-0.00597	-0.01056	0.07347	-0.15805
Py C 17	-0.07501	-0.09928	-0.03221	0.00622	0.27318	-0.36241
Pz C 17	-0.07257	0.02521	0.00753	0.00142	-0.08497	0.10011
S C 18	0.08569	0.00004	-0.00047	0.00340	0.00713	-0.00082

Px C 18	0.02608	0.01491	-0.08688	0.32323	-0.08608	0.10459
Py C 18	0.02560	0.01310	-0.08926	0.37964	-0.09844	0.10981
Pz C 18	0.21846	-0.00005	0.02415	-0.11664	0.04210	-0.03867
S C 19	-0.00192	-0.00010	0.00077	0.00002	-0.00182	0.00945
Px C 19	0.05602	0.08746	-0.29864	0.04605	-0.02687	-0.14793
Py C 19	-0.07360	0.10449	-0.36181	0.05757	-0.03922	-0.16506
Pz C 19	-0.03605	-0.03399	0.11416	-0.01624	0.00834	0.05858
S C 20	0.00521	0.00047	0.00000	-0.00102	0.00031	-0.00466
Px C 20	-0.00599	0.07765	-0.22939	-0.25490	0.05514	-0.03740
Py C 20	0.03822	0.09550	-0.27892	-0.31094	0.06720	-0.04607
Pz C 20	0.01334	-0.02818	0.08477	0.09381	-0.01923	0.00908
S C 21	0.01081	0.00009	-0.00230	-0.00177	0.00180	0.00017
Px C 21	0.04086	-0.01269	0.08707	-0.26709	0.06853	0.17136
Py C 21	0.00914	-0.01693	0.10367	-0.32278	0.08460	0.20639
Pz C 21	-0.00985	0.00481	-0.03376	0.09942	-0.02539	-0.06477
S C 22	0.02963	0.00145	-0.00115	0.00539	-0.00116	0.00468
Px C 22	0.03814	-0.09875	0.35725	-0.09007	0.02366	-0.03418
Py C 22	0.03271	-0.11797	0.43074	-0.11033	0.02569	-0.04322
Pz C 22	0.05914	0.03903	-0.13633	0.04761	-0.00809	0.01849
S C 23	-0.03478	0.00200	-0.00242	-0.01162	-0.00585	-0.00940
Px C 23	-0.04400	-0.07973	0.24141	0.20465	-0.05499	-0.15434
Py C 23	0.00224	-0.08504	0.26110	0.23399	-0.07093	-0.17118
Pz C 23	-0.09178	0.02840	-0.09210	-0.09396	0.02042	0.05557
S C 24	0.02493	-0.00643	0.01820	0.01897	-0.00826	-0.01198
Px C 24	0.07509	0.01610	0.02636	0.00977	-0.04557	-0.01438
Py C 24	-0.01730	0.01923	0.01735	-0.01238	-0.07221	-0.01909
Pz C 24	-0.05449	0.00458	-0.04464	-0.03091	0.02830	0.02496
S C 25	0.01304	0.00714	0.00477	0.00020	-0.02334	-0.01829
Px C 25	-0.01270	0.02059	-0.07269	-0.05066	0.00960	0.01357
Py C 25	0.01013	0.01461	-0.06889	-0.05132	0.02931	0.01172
Pz C 25	0.07454	0.00701	0.03051	0.02564	-0.04177	-0.01896
S O 26	-0.00422	-0.00011	0.00005	-0.00020	0.00012	-0.00024
Px O 26	-0.03040	0.00907	-0.06191	0.17524	-0.03998	-0.04934
Py O 26	-0.00895	0.01156	-0.07374	0.21505	-0.04861	-0.05832
Pz O 26	0.01132	-0.00346	0.02473	-0.06378	0.01459	0.01846
S H 8	0.01773	0.00712	0.00192	0.00041	-0.00195	0.00799
S H 13	-0.00737	-0.00427	-0.00741	-0.00486	-0.00143	0.00584
S H 9	0.00357	0.00185	0.00160	0.00159	0.00519	-0.00493
S H 10	-0.00642	0.00232	0.00246	0.00035	0.00719	-0.00872
S H 11	0.00328	0.00090	0.00065	0.00084	0.00150	0.00117
S H 27	0.02460	-0.00034	0.00041	0.00094	0.00108	-0.00325
S H 28	-0.04513	-0.00138	0.00120	0.00191	-0.00142	0.00356
S H 29	-0.03741	-0.00078	0.00307	-0.00437	-0.00197	-0.00408
S H 30	-0.06536	0.01446	-0.01607	-0.03862	-0.04505	-0.01589
S H 31	-0.02834	-0.02887	-0.03712	0.00053	0.10397	0.05026
S H 32	0.00312	0.02542	-0.10754	-0.08096	0.03984	0.04244
S H 33	-0.01614	-0.02075	0.05642	0.04906	0.00687	0.00212
S H 34	0.00644	0.00015	0.00016	0.00071	-0.00031	0.00038
S H 35	-0.04386	0.00698	0.00417	-0.01290	-0.04410	-0.01715

Mol. Orbital	55	56	57	58	59	60
Symmetry:	55 A	56 A	57 A	58 A	59 A	60 A
Eigenvalue	0.01284	0.01967	0.02482	0.04813	0.08265	0.08929

S C 1	0.00203	0.01123	0.00020	0.00363	0.00154	-0.23972
Px C 1	-0.01370	-0.00182	0.00024	-0.00532	0.00029	0.02113
Py C 1	0.35411	0.00515	-0.00938	0.33340	0.21666	-0.03787
Pz C 1	-0.16666	-0.00595	0.00434	-0.15439	-0.09812	0.06320
S C 2	0.00766	-0.00837	-0.00036	-0.01471	-0.01449	0.21295
Px C 2	0.00604	-0.01216	0.00005	0.00369	0.00223	-0.04418
Py C 2	-0.08379	0.43697	-0.00304	-0.22125	-0.18818	0.04851
Pz C 2	0.03027	-0.19563	0.00171	0.11107	0.09442	-0.05360
S C 3	-0.01725	0.00882	0.00112	0.01411	0.01342	-0.24234
Px C 3	0.01508	0.01635	-0.00100	0.00445	-0.00002	0.05760
Py C 3	-0.25016	-0.42839	0.01142	-0.02576	0.11256	-0.03180
Pz C 3	0.12231	0.19078	-0.00582	0.01133	-0.04727	0.05452
S C 4	0.01730	-0.00373	-0.00129	0.02925	0.03246	0.35683
Px C 4	-0.01832	0.01122	0.00103	-0.01109	-0.00307	-0.04912
Py C 4	0.31777	-0.04489	-0.00822	0.28177	0.01666	0.02600
Pz C 4	-0.15963	0.02256	0.00401	-0.13340	-0.01169	-0.02168
S C 5	-0.00211	0.01345	0.00070	-0.03793	-0.04029	-0.33945
Px C 5	0.01102	-0.04659	-0.00053	-0.01106	-0.02252	-0.03784
Py C 5	-0.13293	0.47875	-0.00464	-0.07591	0.08861	-0.04813
Pz C 5	0.07111	-0.24757	0.00132	0.04449	-0.04314	-0.00183
S C 6	-0.00352	-0.00882	-0.00010	0.01622	0.02279	0.31914
Px C 6	0.00817	0.01865	-0.00040	0.01122	0.00972	0.04473
Py C 6	-0.20850	-0.41961	0.01132	-0.18532	-0.17143	0.02891
Pz C 6	0.09817	0.20611	-0.00532	0.07048	0.06524	-0.05614
S O 7	-0.00020	-0.00296	-0.00004	-0.00156	-0.00126	0.05149
Px O 7	0.00449	0.00030	-0.00014	0.00172	0.00018	-0.01035
Py O 7	-0.09046	-0.00099	0.00243	-0.07694	-0.04503	-0.02842
Pz O 7	0.04286	0.00798	-0.00101	0.03606	0.02103	-0.08799
S O 12	-0.00031	-0.00501	-0.00306	0.00429	0.00694	0.06488
Px O 12	-0.00245	0.01426	-0.00019	0.00532	0.00906	0.04273
Py O 12	0.03185	-0.12098	-0.00117	0.02334	-0.01154	0.05859
Pz O 12	-0.01833	0.05270	0.00102	-0.00365	0.01668	0.09908
S O 14	-0.00322	0.00057	-0.00057	-0.00079	0.00289	0.01564
Px O 14	-0.04351	0.00239	-0.00411	-0.08476	0.09291	-0.04793
Py O 14	-0.10840	0.00974	-0.00308	-0.16001	0.19935	0.01487
Pz O 14	0.02494	-0.00168	0.00631	0.02906	-0.04817	-0.02944
S C 15	0.01485	-0.00273	-0.00170	0.00252	-0.03118	-0.18971
Px C 15	0.06853	-0.00446	0.00305	0.14389	-0.19683	0.05835
Py C 15	0.15681	-0.01385	0.00750	0.26906	-0.39738	-0.02243
Pz C 15	-0.03199	0.00152	-0.00151	-0.06483	0.09334	0.00984
S C 16	-0.01639	0.00999	-0.00129	-0.01624	0.04054	0.22418
Px C 16	-0.12191	0.02540	0.00315	0.07613	0.19148	0.02456
Py C 16	-0.25726	0.05229	0.00035	0.17262	0.39508	-0.01353
Pz C 16	0.06317	-0.00644	-0.00232	-0.05071	-0.11586	0.01584

S C 17	-0.01140	-0.00993	-0.00005	-0.00682	-0.02468	-0.26100
Px C 17	0.04703	-0.01848	-0.00131	-0.14156	-0.11342	0.05659
Py C 17	0.08402	-0.02210	-0.00055	-0.36057	-0.29249	-0.04127
Pz C 17	-0.02305	0.00496	-0.00059	0.08700	0.08009	-0.02942
S C 18	-0.00922	0.00174	0.00047	0.00504	0.01029	0.19608
Px C 18	0.20790	-0.03763	-0.00291	-0.19068	0.04676	-0.00979
Py C 18	0.24000	-0.04356	-0.01184	-0.22961	0.05310	0.01359
Pz C 18	-0.08578	0.01533	0.00375	0.07376	-0.00432	0.03836
S C 19	0.00912	-0.00157	-0.00362	0.00344	-0.01749	-0.11794
Px C 19	-0.13009	0.02557	0.31490	0.03369	0.09135	0.03033
Py C 19	-0.14718	0.02939	0.37984	0.04512	0.10013	-0.03080
Pz C 19	0.05201	-0.01008	-0.11995	-0.01327	-0.03521	-0.01496
S C 20	-0.00375	0.00073	0.00159	-0.00438	0.01472	0.09811
Px C 20	-0.10390	0.01485	-0.27882	0.13627	-0.16182	-0.00958
Py C 20	-0.12490	0.01812	-0.33959	0.16508	-0.19977	0.01583
Pz C 20	0.03397	-0.00496	0.10626	-0.05312	0.06931	0.01267
S C 21	-0.00206	-0.00048	0.00436	0.00060	0.00154	-0.09308
Px C 21	0.23156	-0.04135	-0.04281	-0.21519	0.18289	0.00202
Py C 21	0.27621	-0.05004	-0.04732	-0.26111	0.23046	-0.01130
Pz C 21	-0.08748	0.01556	0.01641	0.08191	-0.07145	-0.01347
S C 22	0.00315	0.00085	-0.00629	0.00586	-0.01080	0.12559
Px C 22	-0.07528	0.02047	0.31421	0.11719	-0.13817	0.01431
Py C 22	-0.09076	0.02459	0.37753	0.14047	-0.16740	-0.00223
Pz C 22	0.02861	-0.00696	-0.12706	-0.03779	0.04693	0.01762
S C 23	-0.00000	-0.00204	0.01156	-0.01454	0.01946	-0.15346
Px C 23	-0.15792	0.02041	-0.32740	0.05454	0.05816	-0.02275
Py C 23	-0.18010	0.02183	-0.37318	0.06565	0.07471	0.01339
Pz C 23	0.06054	-0.00859	0.12983	-0.02472	-0.02033	-0.01025
S C 24	-0.01106	-0.01071	-0.02946	0.01136	-0.01191	-0.11811
Px C 24	0.01521	-0.00303	0.00609	0.00211	-0.01847	-0.07039
Py C 24	0.00505	-0.00908	-0.00453	-0.00934	0.00200	0.01501
Pz C 24	0.00937	-0.00681	0.01746	0.00474	-0.00948	-0.00088
S C 25	0.01833	0.00100	-0.00759	-0.01217	-0.04765	0.11286
Px C 25	0.00763	-0.00126	0.00609	0.00094	0.00584	0.02088
Py C 25	0.00939	-0.00230	0.02378	-0.00661	-0.00219	-0.03619
Pz C 25	0.01302	0.00213	-0.01260	-0.01049	-0.00709	-0.00647
S O 26	-0.00009	0.00015	-0.00105	0.00002	0.00002	0.02006
Px O 26	-0.05987	0.01051	0.01219	0.05033	-0.03926	-0.00503
Py O 26	-0.07150	0.01283	0.01220	0.06171	-0.04908	0.01499
Pz O 26	0.02304	-0.00370	-0.00736	-0.01882	0.01349	0.03073
S H 8	-0.00467	0.00316	0.00022	0.00691	0.00669	-0.12781
S H 13	0.00048	0.00545	0.00254	-0.00148	-0.00529	-0.04171
S H 9	0.00476	-0.00725	-0.00059	0.00052	-0.00222	0.13799
S H 10	0.00301	-0.00099	-0.00029	-0.00829	-0.01393	-0.17950
S H 11	0.00016	0.00183	-0.00000	0.00239	0.00201	-0.03354
S H 27	-0.00324	0.00076	0.00125	0.00067	0.00395	0.06020
S H 28	0.00287	-0.00047	-0.00192	0.00296	-0.01049	-0.06249
S H 29	-0.00082	-0.00019	0.00147	-0.00335	0.00280	-0.07491
S H 30	0.02604	-0.00202	0.02989	-0.02174	-0.03207	0.05092

S H 31	-0.03751	0.01358	0.01058	0.02640	0.07469	0.04378
S H 32	0.03118	-0.00342	0.08097	-0.01039	0.00767	-0.04148
S H 33	-0.03045	0.00264	-0.04115	0.02305	0.04119	-0.05900
S H 34	0.00052	-0.00011	0.00026	0.00011	-0.00108	-0.01388
S H 35	0.03206	-0.00309	0.00041	0.02018	0.00721	0.12761

Mol. Orbital	61	62	63	64	65	66
Symmetry:	61 A	62 A	63 A	64 A	65 A	66 A
Eigenvalue	0.09466	0.10867	0.11237	0.11774	0.12634	0.13108

S C 1	-0.18256	0.04460	-0.22501	0.03051	-0.25585	0.14222
Px C 1	0.02509	0.02973	0.01858	-0.02557	0.00680	0.00171
Py C 1	-0.03455	-0.26475	0.11291	0.04672	-0.01662	0.01157
Pz C 1	0.04705	0.12592	-0.03413	-0.03026	0.01323	-0.00213
S C 2	0.12423	-0.08086	0.12126	0.02701	0.14721	-0.08484
Px C 2	-0.04657	-0.01036	-0.07163	0.02448	-0.09701	0.05564
Py C 2	0.05427	0.29641	-0.09769	-0.06781	0.05210	-0.03430
Pz C 2	-0.02749	-0.12117	0.07825	0.01137	0.04852	-0.02686
S C 3	-0.11719	0.06517	-0.00848	-0.04935	0.08972	-0.05126
Px C 3	0.02587	0.01093	-0.01209	-0.00190	-0.01560	0.00350
Py C 3	-0.05179	-0.31398	0.09440	0.08185	-0.08650	0.05867
Pz C 3	0.02462	0.15540	-0.11410	-0.02990	-0.08846	0.04733
S C 4	0.14927	-0.02407	-0.09652	0.03440	-0.23959	0.15801
Px C 4	-0.06080	-0.03611	-0.05382	0.03620	0.00166	0.00148
Py C 4	0.05586	0.35765	-0.12127	-0.11617	0.07396	-0.05506
Pz C 4	0.02227	-0.16429	0.15723	0.03528	-0.00587	-0.00049
S C 5	-0.22148	-0.01623	-0.07748	0.03955	0.09942	-0.07708
Px C 5	0.01038	0.02639	0.06620	-0.02614	0.09048	-0.06568
Py C 5	-0.03875	-0.27643	0.10402	0.07137	-0.07994	0.03098
Pz C 5	-0.00717	0.15036	-0.12179	-0.02059	-0.06837	0.02735
S C 6	0.23111	-0.01225	0.20936	-0.05866	0.16752	-0.06797
Px C 6	0.03163	-0.01610	0.03278	-0.00051	0.01725	-0.01018
Py C 6	0.02814	0.23896	-0.08460	-0.04732	0.07754	-0.04478
Pz C 6	-0.03341	-0.13957	0.09280	0.02808	0.10035	-0.06689
S O 7	0.03918	-0.01080	0.04895	-0.00538	0.05427	-0.03132
Px O 7	-0.00710	-0.00411	-0.00201	0.00301	0.00160	-0.00256
Py O 7	-0.02202	0.05689	-0.05791	-0.00328	-0.03604	0.02070
Pz O 7	-0.07005	-0.01189	-0.07060	0.01743	-0.08526	0.04855
S O 12	0.05988	0.00843	0.02731	-0.01149	-0.05089	0.00016
Px O 12	0.02401	-0.00415	0.00382	-0.00161	-0.02118	0.02405
Py O 12	0.05078	0.05999	0.00072	-0.02256	-0.01154	-0.00076
Pz O 12	0.06772	-0.02152	0.05257	-0.01021	-0.01935	0.01494
S O 14	-0.02293	-0.00936	-0.02228	0.01208	-0.01049	-0.04046
Px O 14	0.06213	0.01430	0.03884	-0.09282	0.03242	0.06472
Py O 14	-0.01812	-0.02451	-0.06670	-0.10681	0.01309	-0.03338
Pz O 14	0.02818	-0.00322	0.01555	0.02013	0.01143	0.06321
S C 15	0.19406	0.07170	0.20030	-0.08721	0.11260	0.26612
Px C 15	-0.05244	-0.01398	-0.02576	0.17945	-0.03557	0.00005
Py C 15	-0.01007	0.05214	0.14736	0.25505	-0.05621	-0.01045

Pz C 15	-0.06390	0.03244	0.05427	-0.09560	-0.02318	-0.17633
S C 16	-0.14185	-0.14787	-0.36278	0.13108	-0.00777	0.05426
Px C 16	0.00155	0.05194	-0.03524	-0.08046	-0.07809	-0.12589
Py C 16	0.04535	0.11074	-0.07285	-0.18145	0.10496	0.06095
Pz C 16	0.07149	-0.02968	0.03895	0.05018	-0.05921	0.11014
S C 17	-0.00563	0.07441	0.25202	-0.08555	0.11755	-0.16959
Px C 17	-0.00461	-0.09455	0.01052	0.06473	-0.05611	0.01575
Py C 17	-0.04815	-0.19586	0.09819	0.12934	-0.03006	0.01031
Pz C 17	-0.07098	0.01962	-0.10107	-0.00983	0.07709	-0.04491
S C 18	-0.29393	0.01189	-0.01564	0.03114	-0.10415	-0.44384
Px C 18	0.04837	-0.12601	-0.11038	-0.25480	-0.06840	-0.05319
Py C 18	-0.02166	-0.13128	-0.08951	-0.30064	0.08799	-0.04131
Pz C 18	0.00522	-0.00071	-0.08250	0.15240	-0.04070	-0.04689
S C 19	0.19557	-0.03475	-0.05851	0.04921	0.18618	0.19402
Px C 19	-0.04804	0.11393	0.05736	0.21323	-0.02346	-0.02782
Py C 19	0.03105	0.14217	0.09387	0.23676	-0.01513	0.11338
Pz C 19	0.00637	-0.02817	0.02215	-0.12533	-0.04202	0.12858
S C 20	-0.19100	0.05762	0.13546	-0.13320	-0.24852	0.12370
Px C 20	0.04531	-0.12906	-0.10703	-0.13892	0.00835	-0.11482
Py C 20	-0.02887	-0.11941	-0.03402	-0.23429	0.00429	0.02593
Pz C 20	-0.00317	0.02883	-0.01780	0.09208	-0.01243	-0.11760
S C 21	0.23829	-0.09132	-0.22713	0.17173	0.12700	-0.31992
Px C 21	-0.02493	0.10825	0.06420	0.15758	0.05349	0.03387
Py C 21	0.02213	0.11461	0.03910	0.18987	-0.05194	-0.00224
Pz C 21	0.02981	-0.04396	-0.02928	-0.05144	0.01270	0.00224
S C 22	-0.30623	0.09649	0.22765	-0.13426	-0.00629	0.18283
Px C 22	-0.03017	-0.07931	-0.01229	-0.17714	-0.01141	0.02159
Py C 22	0.01888	-0.12241	-0.08282	-0.15565	0.05092	-0.09049
Pz C 22	-0.03858	0.03277	-0.00476	0.10496	0.08744	-0.13329
S C 23	0.34049	-0.07090	-0.13922	0.02151	-0.15113	0.14879
Px C 23	0.00932	0.10472	0.07247	0.18551	0.08599	0.17354
Py C 23	-0.01324	0.11601	0.05750	0.21979	-0.11377	-0.05414
Pz C 23	-0.00377	-0.01037	0.05841	-0.14088	-0.05299	0.11422
S C 24	0.17810	0.10341	0.25659	-0.06811	-0.30531	-0.23163
Px C 24	0.04066	0.03831	0.09696	-0.04404	0.03157	0.00926
Py C 24	0.00040	-0.01354	-0.04478	0.01488	-0.02852	-0.01008
Pz C 24	-0.04795	0.02913	0.06859	-0.02577	0.10634	0.01806
S C 25	-0.25643	0.00122	0.01298	0.05612	0.39323	0.11029
Px C 25	-0.05051	0.02116	0.02940	-0.00277	0.00653	-0.03893
Py C 25	0.07522	-0.01295	-0.01495	0.01000	-0.00999	0.03514
Pz C 25	0.02888	-0.04525	-0.10759	0.04176	0.04239	0.09552
S O 26	-0.05177	0.02060	0.05102	-0.03842	-0.02860	0.07099
Px O 26	0.01483	-0.02439	-0.01958	-0.02451	-0.00194	-0.00895
Py O 26	-0.03739	-0.00943	0.02397	-0.05859	-0.00591	0.04058
Pz O 26	-0.08499	0.04129	0.08710	-0.04820	-0.03044	0.12037
S H 8	-0.06812	0.04900	-0.05838	-0.02004	-0.08455	0.04808
S H 13	-0.04224	-0.00701	-0.01447	0.00754	0.05261	0.00696
S H 9	0.08319	-0.03049	0.03075	0.01970	-0.05065	0.02603
S H 10	-0.12224	0.01155	-0.11174	0.03144	-0.10966	0.03927

S H 11	-0.02319	0.00960	-0.02739	0.00016	-0.03014	0.01760
S H 27	-0.11866	0.03085	0.06001	-0.03583	-0.09386	-0.10102
S H 28	0.11128	-0.02881	-0.06610	0.07324	0.16845	-0.05246
S H 29	0.17037	-0.05338	-0.12584	0.08018	0.03675	-0.08820
S H 30	-0.08930	-0.05731	-0.09621	0.03161	0.14424	0.11229
S H 31	-0.06254	-0.02630	-0.13341	-0.00254	0.16876	0.12122
S H 32	0.10625	-0.02701	-0.02370	-0.07738	-0.20325	-0.07237
S H 33	0.10726	0.02777	0.01543	-0.01754	-0.18912	-0.03591
S H 34	0.03246	-0.01251	-0.03048	0.02460	0.02691	-0.03635
S H 35	0.01273	-0.01155	-0.14277	0.03580	-0.03220	0.13533

Mol. Orbital	67	68	69	70	71	72
Symmetry:	67 A	68 A	69 A	70 A	71 A	72 A
Eigenvalue	0.13302	0.13892	0.14761	0.16884	0.18446	0.20112

S C 1	-0.26081	0.04664	-0.00890	0.07079	-0.01141	0.25243
Px C 1	-0.09467	-0.19783	0.01535	0.02538	0.02293	-0.15902
Py C 1	-0.03369	-0.04279	0.00186	-0.00616	-0.00571	0.05556
Pz C 1	-0.02058	-0.05338	0.00352	-0.00629	-0.01120	0.13691
S C 2	0.32286	0.32551	-0.02266	-0.08551	-0.04411	0.24425
Px C 2	-0.05933	0.11517	-0.01154	0.03583	-0.01504	0.23936
Py C 2	0.04593	-0.02112	0.00367	-0.04311	-0.01443	0.08101
Pz C 2	0.02971	-0.08785	0.00532	-0.11061	-0.04258	0.15481
S C 3	-0.05791	-0.44547	0.03489	-0.20896	-0.04640	0.09129
Px C 3	-0.01802	-0.02845	0.00483	-0.08824	-0.04016	0.18286
Py C 3	-0.10409	-0.02842	-0.00223	0.00648	-0.00825	-0.04024
Pz C 3	-0.12952	-0.03963	0.00428	0.05002	0.01751	-0.10325
S C 4	-0.24019	0.15511	-0.02480	0.00298	-0.04880	0.07068
Px C 4	0.12262	0.17994	-0.01723	-0.10414	-0.03853	-0.08478
Py C 4	0.07928	0.07325	0.00148	0.10205	0.05162	0.00318
Pz C 4	-0.01453	0.10354	-0.00806	0.20770	0.04377	0.02570
S C 5	0.29239	0.17457	-0.00771	-0.19658	-0.04446	-0.06157
Px C 5	0.05369	-0.12962	0.02043	0.04227	0.04768	-0.02530
Py C 5	-0.06212	0.02978	-0.00165	0.02263	0.01166	-0.01449
Pz C 5	-0.02911	0.10017	-0.00319	0.03849	0.01340	-0.01233
S C 6	-0.01877	-0.34738	0.02437	-0.02879	-0.00343	0.04191
Px C 6	0.02965	0.05175	-0.00429	0.04560	0.02777	-0.18082
Py C 6	0.11093	0.02998	0.00079	-0.05040	-0.00822	-0.06462
Pz C 6	0.16890	0.03106	0.00205	-0.10861	-0.01769	-0.12187
S O 7	0.06170	0.00680	0.00109	0.00622	0.01820	-0.19423
Px O 7	0.01419	0.01772	-0.00093	-0.01563	-0.01189	0.12538
Py O 7	-0.03368	0.01152	-0.00189	-0.00343	-0.01136	0.10756
Pz O 7	-0.07928	0.02062	-0.00408	-0.00657	-0.02276	0.21089
S O 12	-0.06836	-0.02571	0.01320	0.08518	0.05080	-0.01812
Px O 12	-0.05361	-0.01212	-0.00499	0.02605	-0.00867	0.01382
Py O 12	-0.03982	-0.02912	0.00420	0.05309	0.02674	-0.01220
Pz O 12	-0.08712	-0.05988	0.00715	0.12534	0.05075	-0.02738
S O 14	0.01785	-0.01206	0.04256	0.02804	0.05642	0.01472
Px O 14	-0.05102	0.04015	-0.07428	-0.04807	-0.09336	-0.01657

Py O 14	0.01742	-0.00250	0.02847	0.02075	0.04692	0.00318
Pz O 14	0.02533	-0.00807	-0.04315	0.00091	-0.01833	-0.01811
S C 15	-0.11099	0.08862	-0.18975	-0.08410	-0.26378	-0.04507
Px C 15	0.05526	-0.04606	0.03057	0.00385	0.03327	-0.01683
Py C 15	-0.00650	-0.02263	-0.02857	0.02832	-0.04213	0.02495
Pz C 15	-0.07964	0.03567	-0.01583	0.03898	-0.06874	0.05604
S C 16	0.19894	-0.12561	0.09572	-0.08938	0.12486	-0.09307
Px C 16	-0.00225	0.03468	0.05163	-0.10791	0.15870	-0.00384
Py C 16	-0.02405	0.06984	-0.06620	-0.03158	-0.08101	-0.00979
Pz C 16	-0.05843	0.04365	-0.04501	-0.21124	-0.15558	-0.04044
S C 17	0.02928	-0.00608	0.02016	0.40807	0.14133	0.08847
Px C 17	-0.03629	-0.02765	0.01814	0.08973	0.05336	0.08349
Py C 17	0.00081	-0.09057	0.01566	-0.02935	-0.01670	-0.04992
Pz C 17	0.13290	-0.06596	0.02638	0.01162	0.09640	-0.07407
S C 18	-0.08670	0.00718	-0.00123	0.04439	-0.07611	0.03355
Px C 18	0.06242	-0.03530	-0.09977	0.02820	0.02299	-0.00971
Py C 18	-0.08790	0.06034	0.12443	-0.01618	0.06396	0.02887
Pz C 18	0.06574	-0.04613	0.13519	0.04352	0.20684	0.05167
S C 19	-0.06167	0.06215	0.39558	-0.01932	0.22298	0.08521
Px C 19	0.00604	-0.00796	0.05121	0.00404	0.06893	0.06039
Py C 19	0.05412	-0.02660	-0.05096	0.00147	-0.02578	-0.03071
Pz C 19	0.08371	-0.03157	-0.05837	0.01100	0.10640	0.06144
S C 20	0.23514	-0.11638	-0.28894	0.03978	0.13107	0.09440
Px C 20	-0.03273	0.00202	-0.06847	0.01434	-0.01824	0.03993
Py C 20	-0.00448	0.01280	0.02065	-0.01344	-0.02743	-0.05466
Pz C 20	-0.02843	-0.00334	-0.10549	-0.00121	-0.14581	-0.07222
S C 21	-0.16888	0.04073	-0.02633	0.01521	-0.08992	0.03142
Px C 21	-0.04360	0.03308	0.15533	-0.01779	-0.06180	-0.04736
Py C 21	0.05456	-0.04090	-0.13431	0.01718	0.04873	0.02851
Pz C 21	-0.00800	0.00368	-0.01927	-0.00738	0.00728	-0.03548
S C 22	-0.00594	0.05931	0.36415	-0.03740	-0.07599	-0.02511
Px C 22	0.00945	-0.00051	-0.05892	-0.00256	0.02793	-0.01490
Py C 22	-0.07590	0.03663	0.04983	-0.00949	-0.03775	0.01358
Pz C 22	-0.11943	0.04515	-0.00306	0.00286	-0.08184	0.00904
S C 23	0.24291	-0.12773	-0.12920	0.04300	0.14121	0.00974
Px C 23	-0.00236	0.00640	-0.00341	-0.02241	0.04436	-0.00967
Py C 23	0.07759	-0.04518	0.06146	0.04818	-0.09759	0.00340
Pz C 23	0.04665	0.01115	0.16112	-0.02752	-0.05048	-0.03001
S C 24	-0.12215	0.11879	0.04766	-0.30907	0.21301	-0.04006
Px C 24	-0.04875	0.02704	-0.04169	0.15180	-0.18440	0.09104
Py C 24	0.03968	-0.01514	0.01416	-0.02123	-0.01886	-0.01990
Pz C 24	-0.11766	0.05964	-0.11021	-0.05570	0.13558	0.01215
S C 25	-0.24861	0.09046	-0.26475	-0.06564	0.23046	0.01714
Px C 25	-0.02927	0.01998	0.05901	0.01495	-0.07917	-0.00283
Py C 25	0.01597	-0.01016	-0.08280	-0.03049	0.22509	0.02636
Pz C 25	0.11103	-0.07974	-0.02494	0.13298	-0.09793	0.02733
S O 26	0.03697	-0.00971	-0.01735	-0.00702	0.00957	-0.03871
Px O 26	0.00237	-0.00341	-0.01365	0.00384	0.01443	0.02820
Py O 26	0.00957	0.00254	0.00954	-0.00766	-0.00440	-0.03432

Pz O 26	0.04866	-0.00904	-0.00480	-0.01165	0.02174	-0.03448
S H 8	-0.20554	-0.21019	0.01632	0.12842	0.07232	-0.41960
S H 13	0.04222	-0.00103	-0.01757	-0.09640	-0.06152	0.03117
S H 9	0.02835	0.30422	-0.02437	0.24699	0.07768	-0.24034
S H 10	0.00612	0.24873	-0.01546	0.10062	0.04509	-0.20369
S H 11	-0.04503	-0.02912	0.00128	-0.02011	-0.02317	0.25200
S H 27	0.01950	-0.02876	-0.30340	0.00212	-0.24679	-0.13377
S H 28	-0.15803	0.08207	0.16301	-0.04227	-0.15973	-0.14671
S H 29	-0.01402	-0.03137	-0.30700	0.01873	0.04852	-0.01118
S H 30	0.06549	-0.07064	0.02684	0.27375	-0.19729	0.05693
S H 31	0.06524	-0.05670	-0.04079	0.24012	-0.21704	0.05630
S H 32	0.12940	-0.04782	0.18037	0.04643	-0.25167	-0.02923
S H 33	0.14554	-0.05147	0.20289	0.10140	-0.22573	0.00344
S H 34	-0.02768	0.01003	0.03480	0.00499	0.00698	0.05486
S H 35	-0.03374	-0.02851	-0.03223	-0.32812	-0.16304	-0.11161

Mol. Orbital	73	74	75	76	77	78
Symmetry:	73 A	74 A	75 A	76 A	77 A	78 A
Eigenvalue	0.20691	0.20715	0.21543	0.22740	0.23636	0.23787

S C 1	-0.06218	0.17198	0.05250	-0.06710	-0.00175	-0.02029
Px C 1	0.07001	0.12216	-0.02180	0.03011	-0.00500	-0.00666
Py C 1	-0.00888	0.06358	0.01268	-0.02618	0.00618	0.01531
Pz C 1	-0.02591	0.13261	0.03004	-0.05710	0.01143	0.02924
S C 2	-0.09018	-0.12179	0.02760	-0.02867	0.00110	-0.00525
Px C 2	-0.06732	0.11445	0.05069	-0.07125	0.00003	-0.01667
Py C 2	-0.03191	-0.07363	0.00309	0.00755	-0.00220	-0.00756
Pz C 2	-0.05842	-0.16840	-0.00125	0.02284	-0.00312	-0.00883
S C 3	-0.04855	-0.24694	-0.01525	0.04123	-0.00422	-0.01217
Px C 3	-0.06150	-0.19909	-0.02202	0.13180	-0.03145	-0.08081
Py C 3	0.02646	0.01687	-0.01884	0.03551	-0.00216	0.00193
Pz C 3	0.05016	0.05938	-0.02810	0.06372	-0.00761	-0.00770
S C 4	0.02132	-0.05943	-0.06112	0.19544	-0.03656	-0.07918
Px C 4	0.09169	0.20120	-0.03459	0.00372	0.02077	0.09214
Py C 4	-0.01799	0.06328	0.02684	-0.01887	-0.01032	-0.03374
Pz C 4	-0.01680	0.08524	0.02347	-0.00215	-0.01134	-0.04241
S C 5	0.08557	0.19342	-0.03634	0.02388	0.01624	0.07703
Px C 5	-0.04232	0.02845	0.06832	-0.21667	0.04673	0.10511
Py C 5	-0.02158	-0.09335	0.00918	-0.03820	0.01611	0.03073
Pz C 5	-0.03630	-0.16837	0.00905	-0.03775	0.00911	0.03287
S C 6	0.02572	0.24079	0.01317	-0.02544	0.00321	0.00858
Px C 6	-0.00734	-0.34243	-0.02691	0.04708	-0.00799	-0.03461
Py C 6	0.03673	0.01811	-0.02403	0.03788	-0.00184	0.01246
Pz C 6	0.07580	0.06561	-0.04549	0.06500	0.00335	0.03845
S O 7	0.04922	-0.10332	-0.03910	0.07816	-0.02033	-0.05490
Px O 7	-0.03824	0.04271	0.02993	-0.08445	0.03265	0.09631
Py O 7	-0.02537	0.05755	0.01886	-0.02955	0.00457	0.01038
Pz O 7	-0.04891	0.11485	0.03612	-0.05260	0.00604	0.01086
S O 12	-0.06687	-0.13446	0.05760	-0.19804	0.05978	0.14743

Px O 12	0.02076	0.01034	-0.03742	0.20138	-0.08462	-0.23930
Py O 12	-0.03116	-0.07165	0.02415	-0.06690	0.02242	0.03313
Pz O 12	-0.07059	-0.16105	0.05947	-0.20334	0.05858	0.14001
S O 14	-0.01312	0.00302	-0.00601	0.03012	-0.00273	0.00958
Px O 14	0.03022	-0.00692	0.00202	-0.04575	0.00147	-0.01583
Py O 14	-0.02204	0.00543	0.00971	0.01100	-0.00116	-0.01021
Pz O 14	-0.01424	0.00170	0.03714	-0.04517	-0.00332	-0.04662
S C 15	0.06676	-0.01683	0.01804	-0.12635	0.00567	-0.06313
Px C 15	-0.02466	0.00342	0.02281	-0.05185	-0.00143	-0.04836
Py C 15	0.03423	-0.00855	-0.03096	0.06781	-0.00076	0.08207
Pz C 15	0.08502	-0.01371	-0.09609	0.13845	0.00236	0.17356
S C 16	-0.10290	0.02077	0.11237	-0.18131	-0.00966	-0.17605
Px C 16	-0.01763	0.01583	-0.00603	0.04604	-0.00438	0.06599
Py C 16	0.02612	-0.00266	0.00500	-0.02683	-0.03916	-0.02199
Pz C 16	0.06138	-0.01433	-0.03348	-0.04180	0.01605	0.03677
S C 17	-0.08337	0.01367	0.05388	0.02396	-0.03366	-0.10056
Px C 17	-0.07870	-0.02883	0.04464	0.06000	-0.06756	-0.23228
Py C 17	0.01544	0.00329	-0.00305	-0.05875	0.04091	0.06799
Pz C 17	-0.07013	0.01979	0.09601	-0.17108	-0.01586	-0.08976
S C 18	0.02943	-0.00229	-0.12625	0.10341	0.00768	0.15349
Px C 18	-0.06012	0.01171	0.13691	0.14414	0.00436	0.08312
Py C 18	0.03727	-0.00663	-0.13054	-0.06043	0.01083	-0.03672
Pz C 18	-0.03839	0.00876	-0.03937	0.14881	-0.01826	0.10024
S C 19	0.09719	-0.01685	-0.22361	-0.02052	-0.01014	0.03201
Px C 19	0.10724	-0.01810	-0.15061	0.02012	-0.00879	0.09949
Py C 19	-0.03756	0.00543	0.09858	-0.04834	0.00249	-0.10009
Pz C 19	0.15680	-0.02959	-0.07137	-0.08669	-0.00000	-0.05579
S C 20	0.24558	-0.04587	-0.07327	-0.08579	-0.00050	-0.04512
Px C 20	0.19725	-0.03660	0.09465	-0.05714	0.00675	-0.05227
Py C 20	-0.19354	0.03574	-0.02023	0.05516	-0.00071	0.03343
Pz C 20	-0.10076	0.01805	0.18555	0.02117	0.00784	-0.03059
S C 21	0.23527	-0.04349	0.18154	-0.05408	0.00676	-0.05552
Px C 21	-0.11508	0.02181	0.08002	0.06588	-0.00164	0.03825
Py C 21	0.03989	-0.00817	-0.10612	-0.04724	-0.01176	-0.01556
Pz C 21	-0.18223	0.03336	-0.12823	0.02658	-0.01206	0.04224
S C 22	0.04065	-0.00641	0.21844	0.04191	0.00719	0.00419
Px C 22	-0.14500	0.02594	-0.25983	-0.07177	0.01515	-0.04825
Py C 22	0.14286	-0.02573	0.17449	-0.00251	0.02204	-0.02206
Pz C 22	0.08132	-0.01733	-0.13271	-0.19939	-0.00504	-0.15516
S C 23	-0.06317	0.01333	0.18474	0.23854	-0.00694	0.16454
Px C 23	0.01485	-0.00555	0.08971	-0.05977	-0.07064	-0.06384
Py C 23	0.00071	0.00066	-0.02423	0.05141	-0.03755	0.08249
Pz C 23	0.00332	-0.00068	0.15948	0.00380	0.00382	-0.02295
S C 24	-0.03433	0.02586	0.02512	-0.02359	0.00650	-0.01679
Px C 24	0.10106	-0.03175	-0.10798	0.19697	0.00615	0.26583
Py C 24	-0.00384	0.01200	-0.00176	-0.01147	0.23578	0.10492
Pz C 24	-0.00720	0.01120	0.00457	0.04642	0.05326	0.02541
S C 25	-0.00249	-0.00528	0.04101	0.02420	-0.00765	0.00967
Px C 25	-0.01265	0.00737	-0.13224	-0.05605	0.54809	-0.27984

Py C 25	-0.02382	-0.00077	0.16657	0.25361	0.30479	0.08750
Pz C 25	0.02085	0.00509	-0.00436	0.10626	0.10462	-0.00768
S O 26	-0.19475	0.03559	-0.13172	0.02572	-0.01607	0.04467
Px O 26	0.12257	-0.02241	0.07284	-0.01672	0.01634	-0.03772
Py O 26	-0.15747	0.02882	-0.09722	0.02043	-0.01370	0.03741
Pz O 26	-0.17625	0.03219	-0.11631	0.02051	-0.00469	0.02073
S H 8	0.13575	0.11426	-0.04320	0.03364	0.00194	0.01728
S H 13	0.09605	0.17762	-0.09700	0.40115	-0.14434	-0.38517
S H 9	0.08417	0.28962	0.02189	-0.11309	0.02365	0.06338
S H 10	-0.03114	-0.44765	-0.01657	0.01162	0.00041	-0.01613
S H 11	-0.06872	0.12188	0.05614	-0.13855	0.04752	0.13709
S H 27	-0.22503	0.03921	0.27215	0.00267	0.01152	-0.10415
S H 28	-0.41566	0.07649	0.05693	0.10183	-0.00102	0.04092
S H 29	-0.18743	0.03201	-0.40597	-0.13452	-0.01486	-0.07516
S H 30	0.04011	-0.04828	-0.05060	0.02444	-0.18503	0.00528
S H 31	0.06550	-0.03516	-0.06496	0.10650	0.19305	0.23240
S H 32	0.02308	0.00112	-0.09167	-0.18614	-0.44168	0.01672
S H 33	0.00487	0.00911	-0.13244	-0.02242	0.44466	-0.21944
S H 34	0.26279	-0.04795	0.17654	-0.03289	0.03151	-0.07495
S H 35	0.12180	-0.00549	-0.08147	-0.04722	0.08229	0.25113

Mol. Orbital	79	80	81	82	83	84
Symmetry:	79 A	80 A	81 A	82 A	83 A	84 A
Eigenvalue	0.24288	0.24628	0.24892	0.25649	0.28645	0.30160

S C 1	0.02667	0.21725	-0.00338	-0.10504	0.00958	-0.00569
Px C 1	0.00637	0.06435	-0.00165	0.05728	0.00080	-0.00783
Py C 1	-0.00656	-0.04095	0.00075	-0.00465	0.00185	-0.00003
Pz C 1	-0.01439	-0.08907	0.00180	-0.01843	0.00452	0.00023
S C 2	0.00463	0.02794	-0.00015	-0.06215	-0.00052	0.00610
Px C 2	0.02504	0.21334	-0.00331	-0.14419	0.02346	-0.02991
Py C 2	0.00437	0.03436	-0.00085	-0.02534	0.00502	-0.01588
Pz C 2	0.00449	0.05929	-0.00202	-0.04497	0.00755	-0.03161
S C 3	0.00268	0.00100	-0.00023	0.00178	0.00978	-0.02194
Px C 3	0.02779	0.02664	0.00032	0.24404	-0.09720	0.11826
Py C 3	-0.00492	-0.02279	-0.00047	0.07131	-0.01987	0.01655
Pz C 3	-0.00419	-0.05465	0.00028	0.14540	-0.02613	0.01752
S C 4	0.01975	-0.02815	0.00078	0.26566	-0.05013	0.05053
Px C 4	-0.04281	0.02419	-0.00664	0.15356	-0.02599	0.03195
Py C 4	0.01422	0.00070	0.00219	-0.01438	-0.02099	0.02693
Pz C 4	0.01894	-0.00063	0.00194	-0.04455	-0.07257	0.07886
S C 5	-0.02852	0.03669	-0.00624	0.24680	-0.02692	0.02962
Px C 5	-0.02629	0.06368	-0.00317	-0.17937	0.05417	-0.04100
Py C 5	-0.00222	0.00341	-0.00121	-0.00128	0.00417	-0.00249
Pz C 5	-0.01989	0.00333	-0.00174	0.04604	0.00164	-0.00220
S C 6	0.00033	0.01661	-0.00017	-0.00983	0.00659	-0.00722
Px C 6	-0.00470	-0.26076	0.00851	-0.13878	0.02064	-0.02254
Py C 6	-0.01255	-0.03584	-0.00066	0.11683	-0.01334	0.00961
Pz C 6	-0.02242	-0.04788	-0.00253	0.25464	-0.03024	0.02297

S O 7	0.03307	0.22154	-0.00402	0.00375	-0.00265	0.00111
Px O 7	-0.06677	-0.47081	0.00828	0.05113	-0.00009	-0.00204
Py O 7	-0.00370	-0.01505	0.00029	-0.01458	0.00113	0.00080
Pz O 7	0.00023	0.02399	-0.00037	-0.03621	0.00236	0.00192
S O 12	-0.03149	0.06362	-0.00710	0.05355	0.00690	0.01634
Px O 12	0.05749	-0.11608	0.01497	-0.30074	0.03390	-0.09118
Py O 12	0.01138	0.00460	-0.00040	-0.05147	0.01445	-0.01028
Pz O 12	-0.03373	0.04942	-0.00644	-0.00977	0.01618	0.02300
S O 14	-0.00773	-0.00001	-0.00433	-0.00038	-0.08356	-0.00325
Px O 14	0.01729	0.00026	0.00840	0.01294	0.16962	0.00544
Py O 14	-0.00679	-0.00131	-0.00243	-0.00220	-0.07701	-0.00318
Pz O 14	0.02113	-0.00337	0.00810	0.01502	0.06166	-0.00854
S C 15	0.02136	0.00098	0.02216	0.02545	0.26262	-0.01033
Px C 15	0.03167	-0.00538	0.00597	0.00831	0.05959	-0.01857
Py C 15	-0.01706	0.00663	-0.00686	-0.01143	0.00541	0.02537
Pz C 15	-0.05547	0.01524	-0.01672	-0.03626	0.14829	0.09767
S C 16	0.06832	-0.01672	0.01679	0.02034	0.12404	-0.07587
Px C 16	-0.03719	0.00692	-0.01160	-0.04182	-0.25491	-0.10581
Py C 16	-0.06404	0.00747	0.00400	0.02449	0.17077	0.02323
Pz C 16	-0.02905	0.01517	0.00354	0.04276	0.15012	-0.13937
S C 17	0.05382	-0.01204	0.00458	0.01503	-0.02817	0.05365
Px C 17	0.11068	-0.02068	0.01667	0.36604	0.21451	-0.11440
Py C 17	-0.00503	-0.00132	-0.00279	-0.18333	-0.05384	0.01420
Pz C 17	0.04658	-0.00709	0.01193	-0.07210	0.15614	-0.11826
S C 18	-0.03244	0.01258	-0.03642	-0.03497	0.24575	0.03559
Px C 18	-0.03422	0.00522	-0.01255	-0.01510	0.00306	0.05091
Py C 18	0.00213	-0.00116	0.00107	0.00837	-0.08382	-0.03077
Pz C 18	-0.02315	0.00239	-0.02938	-0.01133	-0.23281	0.07069
S C 19	0.00604	0.00210	0.00060	-0.00077	-0.02913	-0.00305
Px C 19	-0.00006	0.00870	0.00722	-0.02063	0.32795	0.01969
Py C 19	0.00873	-0.00830	0.01831	0.02009	-0.26923	-0.01862
Pz C 19	0.00881	-0.00122	0.07731	0.00927	0.00075	-0.01734
S C 20	0.00522	-0.00092	0.04099	0.00600	-0.00757	-0.00751
Px C 20	0.00161	0.00127	0.18790	0.00697	-0.07147	-0.01348
Py C 20	-0.00308	-0.00178	-0.15629	-0.00503	0.06885	0.00978
Pz C 20	-0.00003	-0.00295	-0.00377	0.00259	0.03545	-0.00332
S C 21	0.00178	0.00207	0.23317	0.00627	-0.03291	-0.01138
Px C 21	-0.00393	0.00218	0.03344	-0.00602	0.01116	0.00831
Py C 21	0.00314	-0.00025	0.00511	0.00390	-0.00779	0.00195
Pz C 21	-0.00259	0.00499	0.10343	-0.00382	0.00648	0.03273
S C 22	0.00616	-0.00053	0.02009	0.00106	-0.01022	-0.03694
Px C 22	-0.00850	-0.00416	-0.19480	0.01134	-0.03614	-0.11853
Py C 22	0.00572	0.00174	0.17133	0.00068	-0.00942	0.04544
Pz C 22	0.00404	-0.00579	0.02290	0.03095	-0.12844	-0.17637
S C 23	-0.03377	0.00854	-0.01092	-0.02806	0.07604	0.08759
Px C 23	0.03840	-0.00916	0.03750	0.02000	-0.19498	0.02409
Py C 23	-0.02149	0.00674	-0.02719	-0.01543	0.14944	-0.07007
Pz C 23	0.00236	0.00026	0.02821	0.01357	-0.03539	-0.17333
S C 24	0.00612	-0.00056	-0.00095	0.00051	-0.04771	-0.11085

Px C 24	0.04151	0.02026	-0.01622	0.02488	-0.22089	-0.27045
Py C 24	0.62637	-0.05005	0.00814	0.00329	0.01470	-0.10342
Pz C 24	0.17772	-0.02536	-0.01431	-0.04166	-0.03849	0.46362
S C 25	-0.00111	-0.00009	0.00252	0.00074	-0.03565	0.11294
Px C 25	-0.13659	0.00588	0.02584	0.01097	-0.05909	0.08637
Py C 25	-0.21334	0.03858	0.01998	0.00725	0.14298	-0.30878
Pz C 25	-0.04970	-0.00653	-0.00450	-0.05913	0.09224	0.42968
S O 26	-0.00456	0.00800	0.22426	-0.00288	0.00714	0.00750
Px O 26	0.00589	-0.01121	-0.37869	0.00176	-0.00206	0.00914
Py O 26	-0.00476	0.00856	0.26634	-0.00201	0.00309	-0.00149
Pz O 26	0.00058	-0.00240	-0.15509	-0.00170	0.00406	0.01870
S H 8	-0.01726	-0.15121	0.00295	0.11273	-0.01176	0.02718
S H 13	0.08735	-0.17898	0.02176	-0.34357	0.02838	-0.09992
S H 9	-0.02294	-0.04578	0.00054	-0.16788	0.06448	-0.07373
S H 10	-0.00169	-0.15600	0.00507	-0.13253	0.01814	-0.01382
S H 11	-0.09240	-0.64796	0.01154	0.05061	0.00250	-0.00482
S H 27	-0.00146	-0.00988	-0.04024	0.01838	-0.28076	-0.01310
S H 28	-0.00405	-0.00267	-0.17083	-0.00505	0.06179	0.00972
S H 29	-0.00685	-0.00459	-0.14740	0.01689	-0.06346	-0.11576
S H 30	-0.47816	0.05488	-0.00519	0.04235	-0.07100	-0.15061
S H 31	0.38546	-0.01029	-0.00092	0.02356	-0.08158	-0.20782
S H 32	0.17397	-0.02976	-0.02502	-0.01463	-0.05619	0.18762
S H 33	-0.10186	0.00002	0.01340	-0.00914	-0.04062	0.16071
S H 34	0.01057	-0.02028	-0.66726	0.00398	-0.00896	0.00554
S H 35	-0.11515	0.01849	-0.01663	-0.32944	-0.17613	0.09149

Mol. Orbital	85	86	87	88	89	90
Symmetry:	85 A	86 A	87 A	88 A	89 A	90 A
Eigenvalue	0.32161	0.33969	0.35959	0.36911	0.37711	0.41108

S C 1	0.03389	-0.01532	0.02033	-0.03656	0.02308	-0.00083
Px C 1	-0.11961	0.05567	-0.14035	-0.19765	-0.16360	-0.06207
Py C 1	0.04352	-0.02174	0.03885	-0.15143	0.09172	0.02177
Pz C 1	0.10122	-0.05050	0.09325	-0.30643	0.20721	0.05060
S C 2	0.10381	-0.04222	0.08468	0.06136	0.08848	0.01392
Px C 2	-0.14609	0.04909	-0.11624	-0.17498	-0.13782	-0.05771
Py C 2	-0.17135	0.05710	-0.09152	-0.02641	-0.08209	0.00096
Pz C 2	-0.37128	0.12434	-0.19764	-0.04863	-0.17505	0.00580
S C 3	-0.14908	0.03320	-0.01697	0.02206	0.01317	0.01296
Px C 3	0.47852	-0.07342	-0.00240	-0.02253	-0.08594	-0.02428
Py C 3	-0.03930	0.03347	-0.08201	-0.03436	-0.08896	0.00037
Pz C 3	-0.14090	0.08169	-0.17868	-0.07349	-0.18610	0.00298
S C 4	-0.01030	0.03584	-0.07667	-0.01193	-0.05962	0.00307
Px C 4	0.02299	-0.01233	0.00733	-0.10526	0.02840	0.03257
Py C 4	0.14411	-0.00525	-0.06420	-0.03995	-0.11613	-0.02214
Pz C 4	0.29097	-0.00153	-0.15041	-0.06877	-0.24884	-0.03899
S C 5	-0.01546	0.01228	-0.02359	-0.04336	-0.00596	0.00450
Px C 5	0.02148	-0.05621	0.13037	0.07706	0.10929	0.02662
Py C 5	-0.02367	0.00190	0.02407	0.22438	-0.01505	0.00456

Pz C 5	-0.05112	0.01343	0.03016	0.41675	-0.04230	-0.00000
S C 6	0.00784	-0.00744	-0.00151	-0.19178	0.03403	0.00179
Px C 6	-0.01611	-0.00851	-0.02067	-0.49283	0.07635	0.00506
Py C 6	-0.03215	0.01927	-0.02958	0.01701	-0.03061	-0.00585
Pz C 6	-0.06514	0.04092	-0.06104	0.07938	-0.07220	-0.01199
S O 7	-0.02596	0.01333	-0.02633	0.05950	-0.05243	-0.01401
Px O 7	-0.04928	0.02458	-0.04782	0.11769	-0.09940	-0.02738
Py O 7	0.03599	-0.01739	0.03471	-0.06403	0.06585	0.01765
Pz O 7	0.08234	-0.03971	0.07912	-0.14766	0.15039	0.04031
S O 12	-0.00627	-0.00600	0.01912	0.08945	0.00548	0.00473
Px O 12	0.00248	-0.01604	0.07191	0.24749	-0.00354	0.00520
Py O 12	-0.00460	-0.00905	0.02866	0.10372	0.00783	0.00492
Pz O 12	-0.01423	-0.01103	0.03671	0.14255	0.02359	0.00209
S O 14	-0.01843	0.03979	0.01625	0.00155	0.05371	-0.01791
Px O 14	0.02597	-0.07098	-0.02077	-0.00362	-0.08500	0.02980
Py O 14	-0.01001	0.03373	0.00759	0.00152	0.03571	-0.01642
Pz O 14	0.02175	-0.01182	-0.01447	-0.00155	-0.04373	-0.00345
S C 15	0.04207	-0.07408	-0.01913	-0.00373	-0.06564	-0.00153
Px C 15	0.04622	-0.02792	-0.05007	-0.00162	-0.11891	-0.03847
Py C 15	-0.03663	-0.02318	0.04069	-0.00071	0.05812	0.11042
Pz C 15	-0.05884	-0.17267	0.04707	-0.00451	-0.00552	0.35163
S C 16	0.04502	-0.02541	-0.00192	-0.00993	-0.05628	-0.03307
Px C 16	-0.01400	0.14021	0.10241	-0.00665	0.13283	-0.36689
Py C 16	-0.01290	-0.09419	0.01228	-0.00359	-0.00615	0.15590
Pz C 16	-0.07762	-0.08212	0.22123	-0.02664	0.17472	-0.04973
S C 17	0.07705	0.02230	-0.10465	0.00639	-0.11879	0.01648
Px C 17	-0.22414	-0.03463	0.16097	-0.02745	0.20506	-0.02837
Py C 17	0.10316	0.00269	-0.04577	0.00149	-0.09193	-0.01567
Pz C 17	0.07065	-0.06250	0.10428	-0.02175	-0.00143	-0.10934
S C 18	0.01603	-0.08889	-0.00889	-0.00171	-0.02935	-0.00030
Px C 18	-0.01345	0.04299	-0.00277	0.00684	0.06555	0.05565
Py C 18	-0.02626	-0.06562	0.03257	-0.00789	-0.04289	0.06653
Pz C 18	-0.11737	-0.08864	0.08773	-0.00502	0.04624	0.33588
S C 19	-0.03905	-0.12994	0.01413	-0.00409	-0.01875	0.07621
Px C 19	0.10651	0.24992	-0.00931	0.00347	0.01020	-0.13694
Py C 19	-0.06708	-0.09287	0.01919	-0.00245	0.00313	0.11187
Pz C 19	0.06988	0.36850	0.03600	0.00128	0.03546	-0.01019
S C 20	0.02385	0.15015	0.04105	-0.00401	-0.00260	0.07835
Px C 20	-0.03023	-0.19659	-0.11500	0.01602	0.05015	-0.22752
Py C 20	0.05215	0.28799	0.09441	-0.01059	-0.02102	0.16718
Pz C 20	0.08859	0.40812	-0.00116	0.00845	0.06542	-0.06663
S C 21	0.01257	0.04220	-0.03914	0.00713	0.03387	-0.00570
Px C 21	-0.01433	-0.14762	-0.12751	0.02064	0.07949	-0.22091
Py C 21	-0.00284	0.06304	0.16325	-0.03028	-0.14365	0.07934
Pz C 21	-0.04783	-0.19030	0.18160	-0.04145	-0.24496	-0.33198
S C 22	0.01736	-0.00525	-0.14355	0.02510	0.11699	0.00850
Px C 22	0.03088	-0.05540	-0.28128	0.04768	0.21834	0.01633
Py C 22	-0.00899	0.06998	0.17037	-0.03008	-0.14151	0.00992
Pz C 22	0.05380	0.07572	-0.19628	0.02893	0.12091	0.07300

S C 23	-0.01740	-0.02227	0.00113	0.00311	0.02393	0.00772
Px C 23	-0.03824	0.11161	0.10208	-0.00860	0.01657	0.10032
Py C 23	0.05368	-0.08515	-0.19547	0.02431	0.05919	-0.08199
Pz C 23	0.06835	0.02409	-0.31076	0.04788	0.19676	0.03697
S C 24	0.00561	0.02006	0.05892	-0.01278	-0.00653	-0.04841
Px C 24	-0.03929	0.09038	0.16938	-0.01727	0.10952	-0.23545
Py C 24	0.03572	-0.03063	-0.03154	0.00223	-0.07716	0.10495
Pz C 24	-0.10179	0.04136	-0.07717	0.04234	0.26487	-0.18607
S C 25	-0.03670	0.02670	0.05229	-0.00049	0.02699	-0.02110
Px C 25	-0.04406	0.04756	0.15994	-0.02028	-0.04872	0.01330
Py C 25	0.09259	-0.07499	-0.16961	0.01295	-0.00343	0.01709
Pz C 25	-0.06735	-0.01185	-0.15839	0.04376	0.24854	-0.15202
S O 26	-0.00938	-0.03743	0.04128	-0.00930	-0.05427	-0.06761
Px O 26	-0.01317	-0.04163	0.05882	-0.01230	-0.06870	-0.08537
Py O 26	0.00016	-0.00770	-0.00842	0.00110	0.00365	-0.00229
Pz O 26	-0.03425	-0.13489	0.12901	-0.02909	-0.17057	-0.23323
S H 8	0.24445	-0.08040	0.13958	0.10053	0.12894	0.01495
S H 13	0.00831	-0.01124	0.04676	0.11393	-0.00279	0.00338
S H 9	-0.29744	0.04873	-0.01282	0.01450	0.03081	0.01388
S H 10	-0.00878	-0.00811	-0.00719	-0.26282	0.04186	0.00199
S H 11	-0.05144	0.02352	-0.04738	0.06930	-0.08623	-0.02382
S H 27	-0.08982	-0.22973	0.00515	-0.00325	-0.01440	0.08878
S H 28	0.05771	0.30370	0.08167	-0.00835	-0.01408	0.09771
S H 29	0.02658	-0.02919	-0.20705	0.03397	0.15266	0.01022
S H 30	0.00158	0.03396	0.08029	-0.01084	-0.02620	-0.04431
S H 31	0.00869	0.01587	0.05266	-0.00004	-0.00752	-0.02756
S H 32	-0.04152	0.02429	0.03432	0.00055	0.02323	-0.01487
S H 33	-0.04849	0.03464	0.06123	-0.00168	0.03994	-0.03145
S H 34	-0.01747	-0.06901	0.05102	-0.01164	-0.06943	-0.11382
S H 35	0.13760	0.02665	-0.11165	0.02051	-0.12445	0.03118

Mol. Orbital	91	92	93	94	95	96
Symmetry:	91 A	92 A	93 A	94 A	95 A	96 A
Eigenvalue	0.42878	0.43178	0.44884	0.45284	0.45781	0.47705

S C 1	0.02261	-0.00332	0.00020	-0.00298	0.01717	-0.02540
Px C 1	0.38743	-0.06222	0.31675	0.03574	-0.17086	-0.04404
Py C 1	-0.11026	0.01297	0.08114	0.02768	-0.14501	0.09400
Pz C 1	-0.26207	0.03193	0.14908	0.05581	-0.29278	0.20121
S C 2	-0.06159	0.00608	0.01482	-0.00159	0.03536	-0.03011
Px C 2	0.37055	-0.05899	0.26838	0.02388	-0.10285	-0.08092
Py C 2	-0.03778	0.01072	-0.09363	-0.00484	-0.00967	0.05584
Pz C 2	-0.10868	0.02786	-0.22697	-0.01247	-0.01451	0.13074
S C 3	-0.11847	0.01367	0.00067	0.00131	0.02937	0.01009
Px C 3	0.24847	-0.02206	-0.07973	-0.00591	-0.09277	0.00825
Py C 3	-0.01406	0.01231	-0.16234	-0.00989	-0.03136	0.08195
Pz C 3	-0.05938	0.02929	-0.35203	-0.02105	-0.05923	0.17951
S C 4	-0.05852	0.00889	-0.00522	0.00172	-0.01343	0.01958
Px C 4	0.20411	0.00899	-0.43908	-0.02351	-0.31255	0.02478

Py C 4	0.05711	-0.00391	-0.05672	-0.00609	0.03698	0.06609
Pz C 4	0.08534	-0.00303	-0.07257	-0.00931	0.09574	0.12872
S C 5	0.00230	0.00180	-0.00642	0.00466	-0.05583	0.01548
Px C 5	0.24901	-0.00338	-0.37468	-0.01527	-0.35640	0.02654
Py C 5	0.02009	-0.00162	0.07929	0.02565	-0.18507	0.08323
Pz C 5	-0.00128	-0.00446	0.21684	0.05146	-0.29626	0.15869
S C 6	0.03424	-0.00332	-0.00403	0.00304	-0.04537	-0.00447
Px C 6	0.06584	-0.00768	0.05206	0.01782	-0.14351	0.01567
Py C 6	-0.00759	-0.00551	0.17160	0.03092	-0.12246	0.07150
Pz C 6	-0.02094	-0.01054	0.35222	0.06320	-0.24481	0.14855
S O 7	0.07670	-0.01007	-0.01848	-0.01094	0.05814	-0.04837
Px O 7	0.14591	-0.02025	-0.00408	-0.01459	0.08227	-0.07594
Py O 7	-0.09697	0.01287	0.01456	0.01130	-0.05895	0.05279
Pz O 7	-0.22096	0.02941	0.03129	0.02547	-0.13342	0.11971
S O 12	0.03289	-0.00072	-0.00602	0.00794	-0.10256	0.03437
Px O 12	0.09532	-0.00393	-0.03989	0.02040	-0.24557	0.08578
Py O 12	0.04538	-0.00164	-0.01351	0.00836	-0.11996	0.03705
Pz O 12	0.06677	-0.00585	-0.01586	0.00806	-0.17326	0.05218
S O 14	0.03860	0.09077	0.00550	-0.05862	0.00657	-0.06626
Px O 14	-0.06002	-0.15392	-0.01056	0.09998	-0.00906	0.11433
Py O 14	0.02422	0.06486	0.00431	-0.04263	0.00365	-0.04805
Pz O 14	-0.03193	-0.06257	-0.00437	0.04379	-0.00444	0.05540
S C 15	-0.01525	-0.05898	-0.00012	0.01617	0.01210	0.05180
Px C 15	-0.12521	-0.23578	-0.01749	0.11580	-0.03491	0.17742
Py C 15	0.08797	0.13723	0.01139	-0.01914	0.02749	-0.11755
Pz C 15	0.08711	0.03654	0.00906	0.14311	0.03501	-0.08807
S C 16	0.00493	-0.02673	-0.00053	0.00216	0.03493	0.05212
Px C 16	0.03944	-0.20165	-0.01683	-0.05536	0.06400	0.17303
Py C 16	0.05668	0.08335	0.00657	0.01314	0.01513	-0.08631
Pz C 16	0.25603	-0.01866	-0.00298	-0.03903	0.16539	-0.00543
S C 17	-0.07464	0.01799	0.02129	0.01121	-0.00393	0.02466
Px C 17	0.07542	-0.02480	-0.06164	-0.02378	-0.01646	-0.03622
Py C 17	0.00935	-0.00331	0.02944	0.00342	0.07638	0.04470
Pz C 17	0.18604	-0.06015	0.03463	-0.02310	0.23173	0.10370
S C 18	0.00375	-0.03747	0.00283	-0.00652	0.01705	0.03651
Px C 18	0.09788	0.37275	0.03855	-0.06918	0.06008	0.17694
Py C 18	-0.05686	-0.29909	-0.03259	0.10840	-0.04806	-0.19404
Pz C 18	0.07931	0.03074	-0.00115	0.15034	0.00851	-0.13455
S C 19	0.00374	-0.10194	0.00264	-0.04010	0.00549	-0.00418
Px C 19	0.00869	0.21525	0.00785	0.00447	0.01093	0.07578
Py C 19	-0.02256	-0.19653	-0.02191	0.08757	-0.03525	-0.16769
Pz C 19	-0.04995	-0.04978	-0.04871	0.29025	-0.08334	-0.32936
S C 20	-0.00491	-0.05863	-0.00069	-0.01595	-0.01426	-0.05169
Px C 20	-0.01820	0.15177	-0.03185	0.25289	-0.02035	-0.09142
Py C 20	0.00287	-0.11549	0.01175	-0.11178	-0.00442	-0.00745
Pz C 20	-0.03935	0.03196	-0.04715	0.31461	-0.06875	-0.26896
S C 21	-0.00382	0.01311	-0.00124	-0.00080	-0.01368	-0.03565
Px C 21	0.00305	0.14072	-0.04018	0.34842	0.00908	-0.04839
Py C 21	-0.04751	-0.04180	0.03216	-0.32087	-0.05845	-0.05482

Pz C 21	-0.14195	0.23930	-0.00399	-0.09827	-0.16090	-0.30039
S C 22	0.02712	0.04403	-0.00037	0.03336	0.01033	0.00724
Px C 22	0.05945	0.06070	-0.00996	0.15472	0.04388	0.04927
Py C 22	-0.05462	-0.00466	0.02135	-0.24117	-0.06586	-0.08629
Pz C 22	-0.01817	0.14000	0.04023	-0.34710	-0.09131	-0.14001
S C 23	0.02672	0.02786	0.00069	0.03727	0.02456	0.04616
Px C 23	0.08796	0.32342	0.02610	0.01454	0.05401	0.13541
Py C 23	-0.07747	-0.22943	-0.01088	-0.11506	-0.07406	-0.15803
Pz C 23	-0.00271	0.16686	0.03585	-0.29518	-0.08005	-0.12505
S C 24	0.01800	-0.01932	-0.00490	0.01977	0.02732	0.04482
Px C 24	0.07436	-0.12259	-0.02016	-0.01323	0.06417	0.12036
Py C 24	-0.02457	0.06213	0.00332	0.02608	-0.02174	-0.03848
Pz C 24	0.05586	-0.13418	-0.00485	-0.13011	-0.00716	-0.00946
S C 25	0.03342	0.02220	-0.00064	0.02678	0.02588	0.05073
Px C 25	0.04784	0.09704	0.00241	0.08121	0.05368	0.10821
Py C 25	-0.06575	-0.09276	-0.00013	-0.08923	-0.06158	-0.12503
Pz C 25	0.01619	-0.17007	-0.00045	-0.18131	-0.03504	-0.08434
S O 26	-0.03096	0.05011	-0.00038	-0.02545	-0.03546	-0.06607
Px O 26	-0.03522	0.05572	-0.00299	-0.00731	-0.03691	-0.07067
Py O 26	-0.00056	0.00641	0.00101	-0.00837	-0.00232	-0.00310
Pz O 26	-0.09516	0.16791	-0.00467	-0.04609	-0.10520	-0.19708
S H 8	-0.06853	0.00587	0.01141	-0.00408	0.05314	-0.03769
S H 13	0.05742	-0.00180	-0.03519	0.01029	-0.12400	0.03867
S H 9	-0.14353	0.01504	0.01070	0.00111	0.04903	0.01278
S H 10	0.05403	-0.00487	-0.00991	0.00242	-0.05439	-0.00807
S H 11	0.13069	-0.01810	0.00628	-0.00943	0.05022	-0.05628
S H 27	0.00163	-0.12993	0.00305	-0.05564	0.00503	-0.00152
S H 28	-0.01154	-0.07335	-0.00072	-0.02536	-0.02151	-0.06317
S H 29	0.03210	0.07254	-0.00036	0.04589	0.01124	0.00673
S H 30	0.00720	-0.00871	-0.00413	0.02640	0.01230	0.05185
S H 31	0.01415	-0.01110	-0.00517	0.01076	0.00406	0.02501
S H 32	0.01829	0.01442	-0.00008	0.01416	0.01349	0.02606
S H 33	0.03520	0.02385	0.00100	0.00762	0.02453	0.04550
S H 34	-0.03863	0.07898	-0.00486	0.00764	-0.04076	-0.07920
S H 35	-0.06194	0.02970	0.03849	0.00969	0.00304	0.00399

Mol. Orbital	97	98
Symmetry:	97 A	98 A
Eigenvalue	0.49643	0.51905

S C 1	-0.02029	0.02325
Px C 1	-0.04137	0.05094
Py C 1	0.05962	-0.05690
Pz C 1	0.12872	-0.12372
S C 2	-0.02622	0.03618
Px C 2	-0.06673	0.07774
Py C 2	0.04698	-0.05903
Pz C 2	0.11029	-0.13828
S C 3	0.00378	0.00426

Px C 3	0.00837	-0.02120
Py C 3	0.07037	-0.09346
Pz C 3	0.15162	-0.20044
S C 4	0.00772	0.01202
Px C 4	-0.05028	0.09583
Py C 4	0.08444	-0.13326
Pz C 4	0.17629	-0.27239
S C 5	0.00171	0.00701
Px C 5	-0.05148	0.08445
Py C 5	0.05282	-0.05100
Pz C 5	0.11166	-0.11664
S C 6	-0.01416	0.02126
Px C 6	-0.01067	0.02524
Py C 6	0.05342	-0.05574
Pz C 6	0.11282	-0.11872
S O 7	-0.03187	0.03147
Px O 7	-0.04880	0.04697
Py O 7	0.03453	-0.03353
Pz O 7	0.07814	-0.07580
S O 12	0.01717	-0.01392
Px O 12	0.03391	-0.02811
Py O 12	0.01693	-0.01323
Pz O 12	0.02470	-0.02346
S O 14	0.20552	0.07004
Px O 14	-0.34991	-0.12190
Py O 14	0.14830	0.05165
Pz O 14	-0.15165	-0.04833
S C 15	-0.04700	-0.01902
Px C 15	-0.49614	-0.10373
Py C 15	0.21969	-0.02313
Pz C 15	-0.17451	-0.30759
S C 16	0.00079	-0.04334
Px C 16	-0.12853	-0.09344
Py C 16	0.11567	-0.04627
Pz C 16	0.19073	-0.32174
S C 17	0.01372	0.02173
Px C 17	-0.03346	0.02161
Py C 17	0.06328	-0.12064
Pz C 17	0.18114	-0.40278
S C 18	-0.00156	-0.00213
Px C 18	-0.17185	-0.04420
Py C 18	0.08961	-0.05423
Pz C 18	-0.17647	-0.29026
S C 19	0.02603	-0.00422
Px C 19	-0.04754	0.03174
Py C 19	0.04738	-0.07813
Pz C 19	0.02430	-0.15946
S C 20	0.00372	-0.03175
Px C 20	-0.00520	-0.03247

Py C 20	0.00120	-0.01530
Pz C 20	-0.00966	-0.13650
S C 21	-0.01273	-0.02706
Px C 21	0.01340	-0.00333
Py C 21	-0.04137	-0.04880
Pz C 21	-0.09617	-0.16355
S C 22	-0.02889	-0.02846
Px C 22	-0.01142	-0.00071
Py C 22	-0.04141	-0.06008
Pz C 22	-0.15820	-0.18544
S C 23	-0.01940	-0.00284
Px C 23	-0.16821	-0.05856
Py C 23	0.08366	-0.01703
Pz C 23	-0.17363	-0.19895
S C 24	-0.01470	-0.01487
Px C 24	-0.07324	-0.09184
Py C 24	0.03343	0.04073
Pz C 24	-0.02668	-0.12926
S C 25	-0.01137	-0.00600
Px C 25	-0.03084	0.01915
Py C 25	0.03025	-0.01646
Pz C 25	-0.00707	-0.12725
S O 26	-0.02142	-0.03645
Px O 26	-0.01778	-0.03328
Py O 26	-0.00436	-0.00453
Pz O 26	-0.06085	-0.10246
S H 8	-0.02970	0.03648
S H 13	0.01005	-0.00514
S H 9	0.01126	-0.01016
S H 10	-0.01696	0.02365
S H 11	-0.03662	0.03514
S H 27	0.04040	0.01137
S H 28	-0.00248	-0.03690
S H 29	-0.03160	-0.02685
S H 30	-0.02516	0.00702
S H 31	-0.00795	-0.00878
S H 32	-0.00626	-0.00093
S H 33	-0.02536	-0.01951
S H 34	-0.02226	-0.03793
S H 35	0.02807	0.01853

b) In water

Mol. Orbital	1	2	3	4	5	6
Symmetry:	1 A	2 A	3 A	4 A	5 A	6 A
Eigenvalue	-1.68773	-1.65938	-1.61078	-1.59004	-1.50269	-1.47321
S C 1	0.21021	-0.26539	-0.30156	-0.15114	0.00322	0.06154
Px C 1	-0.00587	0.01697	0.04736	0.03172	0.03637	0.12457
Py C 1	-0.00573	-0.00591	-0.04926	-0.04022	-0.02570	-0.08767

Pz C 1	-0.00524	-0.02189	-0.11594	-0.09079	-0.05880	-0.20026
S C 2	0.14584	-0.16401	-0.13197	-0.05215	0.07015	0.26737
Px C 2	-0.04970	0.06226	0.06636	0.03059	-0.00099	-0.01988
Py C 2	-0.01775	0.01431	-0.00601	-0.00940	-0.01925	-0.06419
Pz C 2	-0.03021	0.02114	-0.02192	-0.02388	-0.04059	-0.13464
S C 3	0.15108	-0.13190	-0.03224	0.00099	0.12452	0.38021
Px C 3	-0.05976	0.05802	0.01718	-0.00675	-0.03180	-0.12119
Py C 3	-0.00897	0.00100	-0.01256	-0.00511	-0.01023	-0.01087
Pz C 3	-0.00582	-0.01039	-0.02918	-0.00902	-0.01172	0.00298
S C 4	0.23311	-0.15198	0.06284	0.05846	0.12584	0.31922
Px C 4	-0.04742	0.04122	-0.02667	-0.05113	0.02839	0.04078
Py C 4	-0.00177	-0.01308	-0.02510	-0.00685	0.00583	0.05479
Pz C 4	0.00872	-0.04262	-0.04682	0.00091	0.01804	0.11149
S C 5	0.31487	-0.23520	0.13988	0.20651	0.01612	0.05290
Px C 5	-0.02243	0.01582	-0.06023	-0.07830	0.06657	0.20938
Py C 5	-0.02760	0.00802	-0.05686	-0.05218	0.02570	0.09953
Pz C 5	-0.03485	-0.00404	-0.09038	-0.06699	0.03778	0.14033
S C 6	0.20999	-0.21175	-0.07482	0.02793	0.01726	0.09133
Px C 6	0.05152	-0.05521	-0.03673	-0.01208	0.03461	0.12870
Py C 6	-0.01111	-0.00308	-0.05500	-0.04765	0.00030	0.00659
Pz C 6	-0.03133	0.00319	-0.10195	-0.09080	-0.00703	-0.01781
S O 7	0.18865	-0.28559	-0.47869	-0.29542	-0.10938	-0.33280
Px O 7	-0.00871	0.01435	0.02743	0.01758	0.01221	0.04228
Py O 7	-0.02263	0.03339	0.05293	0.03177	0.00975	0.02741
Pz O 7	-0.04873	0.07202	0.11478	0.06912	0.02092	0.05849
S O 12	0.35827	-0.23398	0.30412	0.36485	-0.11401	-0.37136
Px O 12	0.02606	-0.00998	0.01736	0.00878	0.00705	0.02136
Py O 12	0.04525	-0.03001	0.03616	0.04366	-0.01103	-0.03475
Pz O 12	0.07597	-0.06144	0.06167	0.08900	-0.01811	-0.07916
S O 14	0.18111	0.16325	0.12385	-0.28294	0.46624	-0.20038
Px O 14	-0.06250	-0.05470	-0.04270	0.09323	-0.14323	0.05986
Py O 14	0.02946	0.02378	0.02162	-0.04377	0.07029	-0.02636
Pz O 14	-0.02407	-0.02891	-0.01104	0.03802	-0.04596	0.02927
S C 15	0.24167	0.21189	0.13120	-0.27998	0.24564	-0.11301
Px C 15	0.00039	0.00994	0.01196	-0.05244	0.19444	-0.08177
Py C 15	-0.00052	-0.01127	0.00025	0.02393	-0.08203	0.04146
Pz C 15	0.00497	-0.02118	0.03355	-0.02698	0.13536	-0.03371
S C 16	0.23290	0.10755	0.14928	-0.14965	0.06431	0.01175
Px C 16	-0.00325	0.01816	-0.00013	-0.04582	0.11161	-0.02750
Py C 16	-0.00475	-0.01937	-0.00290	0.02996	-0.04433	0.02536
Pz C 16	-0.01340	-0.05657	0.00468	0.04623	0.06865	0.01192
S C 17	0.18690	-0.00614	0.11465	-0.05263	0.15481	0.10786
Px C 17	-0.03867	0.02166	-0.02545	-0.02975	0.02740	-0.01573
Py C 17	0.00616	-0.02018	-0.00306	0.02185	-0.01725	0.04124
Pz C 17	-0.01653	-0.05407	-0.02724	0.05780	-0.01783	0.07774
S C 18	0.22311	0.26092	0.00586	-0.14142	-0.13954	0.01576
Px C 18	-0.01848	-0.01825	0.00492	-0.01130	0.10327	-0.04057
Py C 18	0.01585	0.00779	0.01465	-0.01307	-0.04326	0.01720
Pz C 18	0.00709	-0.02191	0.06176	-0.06797	0.11453	-0.04492

S C 19	0.13719	0.19071	-0.05265	-0.04019	-0.09566	0.01098
Px C 19	-0.03995	-0.05706	0.02206	-0.00034	0.05926	-0.01723
Py C 19	0.03600	0.04652	-0.00622	-0.01756	-0.02952	0.00471
Pz C 19	0.00528	-0.00805	0.03863	-0.05244	0.05722	-0.02749
S C 20	0.11216	0.18492	-0.13231	0.08828	-0.08011	0.02503
Px C 20	-0.02938	-0.05103	0.04579	-0.04110	0.01213	-0.00645
Py C 20	0.03208	0.05118	-0.03308	0.01977	-0.03227	0.01041
Pz C 20	0.02037	0.02114	0.02090	-0.04925	-0.06979	0.01587
S C 21	0.14707	0.26540	-0.26500	0.25594	0.03117	0.00362
Px C 21	0.00066	-0.00272	0.01613	-0.02653	-0.03051	0.00693
Py C 21	0.00529	0.00475	0.00631	-0.01221	-0.02894	0.00908
Pz C 21	0.01263	-0.00435	0.07871	-0.12687	-0.18387	0.04963
S C 22	0.13808	0.21098	-0.13097	0.08538	-0.15628	0.05512
Px C 22	0.03497	0.05646	-0.03630	0.02033	-0.03777	0.01200
Py C 22	-0.01970	-0.03913	0.04176	-0.03838	-0.00721	0.00105
Pz C 22	0.02731	0.02018	0.03947	-0.06876	-0.11744	0.03290
S C 23	0.20743	0.24668	-0.02380	-0.07099	-0.31079	0.09159
Px C 23	0.02387	0.03611	-0.01122	-0.00980	-0.00945	-0.00103
Py C 23	-0.01511	-0.03185	0.02514	-0.01036	0.00850	-0.00040
Pz C 23	0.02392	-0.00077	0.05357	-0.05959	-0.00426	-0.00389
S C 24	0.19882	0.09420	0.11656	-0.08109	-0.15205	0.03769
Px C 24	0.04334	0.03411	0.02252	-0.04039	-0.00874	0.01583
Py C 24	-0.01309	-0.01188	-0.00666	0.01261	-0.00174	0.00266
Pz C 24	-0.00331	-0.04474	0.01462	0.03593	0.06520	-0.02201
S C 25	0.16553	0.14394	0.05457	-0.09293	-0.24197	0.07119
Px C 25	0.03011	0.03261	0.00621	-0.02324	-0.03345	0.01088
Py C 25	-0.04110	-0.04170	-0.00855	0.02507	0.05602	-0.01550
Pz C 25	0.02196	-0.00179	0.02924	-0.01691	0.00525	-0.00414
S O 26	0.11784	0.25193	-0.36199	0.42676	0.31492	-0.07504
Px O 26	-0.00765	-0.01714	0.02718	-0.03371	-0.02936	0.00725
Py O 26	0.01388	0.02959	-0.04246	0.05018	0.03646	-0.00852
Pz O 26	0.03085	0.06392	-0.08573	0.09741	0.05906	-0.01291
S H 8	0.04114	-0.04993	-0.05228	-0.02604	0.01540	0.06242
S H 13	0.14821	-0.10283	0.12093	0.15481	-0.05035	-0.16442
S H 9	0.04420	-0.03290	-0.00355	-0.00324	0.04696	0.12158
S H 10	0.07516	-0.07653	-0.02722	0.01214	-0.01090	-0.02633
S H 11	0.08230	-0.12287	-0.20110	-0.12262	-0.04761	-0.14608
S H 27	0.04511	0.05849	-0.00499	-0.03067	0.00414	-0.01189
S H 28	0.03038	0.05333	-0.04674	0.03891	-0.00530	0.00246
S H 29	0.04338	0.06739	-0.04851	0.04003	-0.03689	0.01503
S H 30	0.08915	0.01257	0.05908	-0.00517	-0.05334	0.00511
S H 31	0.08577	0.03193	0.05241	-0.02217	-0.06491	0.00469
S H 32	0.06478	0.05562	0.02203	-0.03679	-0.09335	0.02845
S H 33	0.05570	0.04914	0.01530	-0.02571	-0.09348	0.02743
S H 34	0.05084	0.10746	-0.15228	0.17898	0.12960	-0.03059
S H 35	0.07076	0.00846	0.04221	-0.04320	0.10003	0.03934

Mol. Orbital	7	8	9	10	11	12
Symmetry:	7 A	8 A	9 A	10 A	11 A	12 A

Eigenvalue -1.44217 -1.29380 -1.19201 -1.13808 -1.11538 -1.09513

S C 1	0.02145	-0.13429	-0.07151	-0.07578	0.12558	0.12784
Px C 1	0.02079	-0.05250	-0.01625	0.21571	0.10951	0.09923
Py C 1	-0.02595	0.06270	0.02541	0.09920	-0.00624	-0.00757
Pz C 1	-0.05526	0.13266	0.05323	0.16473	-0.02710	-0.02566
S C 2	0.05102	-0.16487	-0.05511	0.36055	0.23636	0.22273
Px C 2	-0.00885	0.05001	0.03365	0.11735	-0.02721	-0.02654
Py C 2	-0.01268	0.02007	0.00124	0.00374	0.01119	0.01555
Pz C 2	-0.02502	0.03600	-0.00087	-0.01472	0.02455	0.03561
S C 3	0.04142	0.01173	0.06091	0.34403	-0.02796	-0.04542
Px C 3	-0.02437	0.05294	0.02346	0.07399	0.00640	0.01988
Py C 3	0.00694	-0.06057	-0.03239	0.04577	0.07707	0.07346
Pz C 3	0.02221	-0.13350	-0.06412	0.08974	0.15352	0.14888
S C 4	-0.01359	0.25100	0.11010	-0.00931	-0.23015	-0.23712
Px C 4	-0.02437	0.09078	0.06075	0.15541	-0.02480	-0.00303
Py C 4	0.02138	-0.07792	-0.02235	0.01716	0.01819	0.00053
Pz C 4	0.06709	-0.17404	-0.02905	0.02032	0.00872	-0.01026
S C 5	0.08536	-0.05474	-0.00802	-0.23181	-0.09935	-0.09426
Px C 5	-0.03663	0.09363	0.01582	-0.03210	-0.07362	-0.10830
Py C 5	0.00094	-0.05172	-0.03039	-0.10557	0.00908	-0.00284
Pz C 5	0.03124	-0.13542	-0.04813	-0.19255	0.01268	0.02786
S C 6	0.08100	-0.21442	-0.08949	-0.46100	0.00309	0.03246
Px C 6	0.02078	-0.05944	-0.02779	-0.04471	0.01938	0.00491
Py C 6	-0.01505	0.00799	-0.00662	0.00023	0.01688	0.00977
Pz C 6	-0.03156	0.02712	-0.00409	0.01845	0.02837	0.02403
S O 7	-0.08428	0.16706	0.06602	0.09572	-0.09435	-0.09974
Px O 7	0.00902	-0.03183	-0.01729	0.07116	0.07476	0.07729
Py O 7	0.00639	-0.00432	0.00175	0.00626	-0.00749	-0.00966
Pz O 7	0.01412	-0.00952	0.00395	-0.00062	-0.02263	-0.02676
S O 12	0.09285	-0.03124	0.03512	0.24114	0.04437	0.06206
Px O 12	-0.01936	0.06405	0.00316	-0.04630	-0.03577	-0.05829
Py O 12	0.01048	-0.00253	0.00029	-0.01429	-0.00481	-0.00977
Pz O 12	0.05080	-0.03846	0.02014	-0.00556	-0.03058	0.02171
S O 14	0.18191	-0.16735	0.19651	-0.00106	0.17338	-0.21616
Px O 14	-0.04221	0.03578	-0.03716	0.00857	-0.03224	-0.00136
Py O 14	0.00985	-0.00698	0.03263	-0.01336	0.03370	0.01829
Pz O 14	-0.05065	0.05733	0.02587	-0.03159	0.05617	0.06834
S C 15	0.01990	-0.10836	-0.07814	0.00613	-0.11001	0.15104
Px C 15	0.15014	-0.06445	0.14166	0.01496	0.09768	-0.21243
Py C 15	-0.10239	0.05191	-0.03703	-0.03056	0.00656	0.13208
Pz C 15	-0.04744	0.08137	0.12754	-0.08879	0.25446	0.05400
S C 16	-0.28257	0.23152	-0.13460	-0.11615	0.10916	0.31542
Px C 16	0.07285	0.00896	0.08810	-0.02458	-0.02657	0.11200
Py C 16	-0.03476	0.03694	-0.01133	0.00365	0.02100	-0.07049
Pz C 16	0.03229	0.19366	0.10423	-0.04353	0.04670	-0.00843
S C 17	-0.14722	0.45347	0.11761	-0.06021	-0.04433	0.08188
Px C 17	0.04041	-0.06723	0.03476	0.02683	0.01664	0.03226
Py C 17	-0.00537	0.03199	0.00523	0.02743	-0.05388	-0.07862

Pz C 17	0.06133	0.01170	0.07133	0.09055	-0.16368	-0.22080
S C 18	0.18674	-0.06280	-0.17944	0.08788	-0.38544	0.11492
Px C 18	0.07893	0.01814	-0.08816	0.02544	-0.00012	-0.09911
Py C 18	-0.09745	-0.05555	0.06819	-0.01094	-0.02921	0.07616
Pz C 18	-0.12395	-0.10638	-0.06676	0.02565	-0.07947	0.02012
S C 19	0.33059	0.13183	-0.30428	0.05941	-0.04262	-0.16456
Px C 19	-0.07102	-0.03143	-0.00581	0.00626	0.02601	-0.05997
Py C 19	0.05168	-0.00868	0.01142	0.01137	-0.09242	0.05674
Pz C 19	-0.03448	-0.10251	0.01072	0.04792	-0.20889	0.03019
S C 20	0.24368	0.20928	-0.23542	-0.02874	0.30130	-0.16775
Px C 20	-0.02205	-0.02089	-0.05074	0.02235	-0.03337	-0.05669
Py C 20	0.05623	0.03226	0.02719	-0.01428	0.01573	0.04039
Pz C 20	0.11457	0.04631	-0.05072	0.01324	-0.03458	-0.02156
S C 21	0.06650	0.09721	0.05402	-0.05997	0.19375	0.04056
Px C 21	0.06466	0.05832	-0.12644	0.00227	0.08409	-0.07345
Py C 21	0.00739	-0.01886	0.13518	-0.01613	-0.03807	0.07775
Pz C 21	0.20417	0.10083	0.08806	-0.04687	0.11255	0.05102
S C 22	0.10107	0.00952	0.43644	-0.08544	0.10169	0.13547
Px C 22	0.07699	0.05343	-0.01062	-0.01519	0.02231	0.04832
Py C 22	-0.04875	-0.05320	0.04367	0.01352	-0.03280	-0.04324
Pz C 22	0.04621	-0.01953	0.08340	0.00240	-0.03373	-0.00510
S C 23	0.01886	-0.12345	0.27903	0.00075	-0.13973	0.07856
Px C 23	0.08966	0.04799	-0.12026	0.01420	-0.11656	0.11048
Py C 23	-0.11377	-0.07478	0.05492	0.00786	0.04905	-0.11504
Pz C 23	-0.13235	-0.08794	-0.19778	0.05733	-0.12238	-0.04101
S C 24	-0.35378	-0.00018	-0.20077	0.00025	0.21437	-0.14502
Px C 24	-0.06848	0.03169	-0.05951	-0.03077	-0.04167	0.13355
Py C 24	0.00640	-0.01022	0.02670	0.00644	0.03735	-0.10069
Pz C 24	0.03584	0.14224	-0.02885	-0.03261	0.02444	0.10940
S C 25	-0.27125	-0.22023	0.11104	0.04035	0.09371	-0.31237
Px C 25	-0.01561	-0.02136	-0.00938	0.00200	-0.08631	0.08641
Py C 25	0.03331	0.03829	-0.01393	-0.00485	0.05417	-0.05295
Pz C 25	-0.08674	0.01827	-0.17810	0.00811	0.06279	-0.03301
S O 26	-0.27293	-0.10619	-0.09313	0.05385	-0.16243	-0.02767
Px O 26	0.03521	0.02773	-0.02845	-0.00950	0.06793	-0.02402
Py O 26	-0.03541	-0.01990	0.02115	0.00413	-0.03765	0.01851
Pz O 26	-0.03772	0.00367	-0.01512	-0.00918	0.05357	-0.00709
S H 8	0.01043	-0.04624	-0.01551	0.21160	0.11791	0.11681
S H 13	0.05479	-0.05592	0.01129	0.09207	0.02934	0.05741
S H 9	0.00481	0.04889	0.05020	0.19707	-0.02473	-0.02351
S H 10	0.02605	-0.06998	-0.02792	-0.19542	-0.00750	0.01482
S H 11	-0.03461	0.07255	0.03058	-0.02092	-0.07551	-0.07790
S H 27	0.11357	0.02593	-0.14426	0.03988	-0.03178	-0.11876
S H 28	0.06051	0.07068	-0.12336	-0.00618	0.14153	-0.10716
S H 29	-0.00627	-0.02836	0.20950	-0.03110	0.03872	0.03001
S H 30	-0.13677	0.03411	-0.07637	0.00286	0.12931	-0.11401
S H 31	-0.13714	-0.00106	-0.08191	0.01230	0.10151	-0.06719
S H 32	-0.11007	-0.08830	0.04849	0.01620	0.04393	-0.14575
S H 33	-0.09900	-0.09336	0.09846	0.01501	0.08282	-0.18982

S H 34	-0.11890	-0.05652	0.00023	0.02334	-0.10393	0.01182
S H 35	-0.03604	0.16949	0.08954	-0.00304	-0.01236	0.03916

Mol. Orbital	13	14	15	16	17	18
Symmetry:	13 A	14 A	15 A	16 A	17 A	18 A
Eigenvalue	-0.99916	-0.95725	-0.94179	-0.88072	-0.84159	-0.82303

S C 1	0.07210	-0.20754	-0.03846	0.27092	0.10778	0.12311
Px C 1	0.10898	-0.09950	-0.17649	-0.02583	0.01695	0.03054
Py C 1	0.02464	-0.01290	-0.05722	0.00503	0.01288	-0.02389
Pz C 1	0.03035	-0.02299	-0.08900	0.03342	0.03128	-0.05572
S C 2	0.07733	-0.12152	-0.05830	-0.03693	-0.07135	-0.15821
Px C 2	-0.08676	0.12880	0.12635	-0.15952	-0.12615	-0.23748
Py C 2	0.02601	-0.05801	-0.03631	0.04834	0.00434	-0.05873
Pz C 2	0.06319	-0.14679	-0.09625	0.13492	0.03133	-0.09339
S C 3	-0.16197	0.22460	0.20760	-0.09728	-0.02718	-0.00298
Px C 3	-0.08289	0.00636	0.13051	0.03384	-0.05594	-0.20906
Py C 3	0.02638	-0.01592	0.00400	-0.07210	-0.06244	-0.08307
Pz C 3	0.05124	-0.04023	-0.01458	-0.14596	-0.11578	-0.14351
S C 4	0.06622	0.05379	-0.14512	0.04814	0.08065	0.10104
Px C 4	-0.19405	0.02123	0.24799	0.20226	0.07255	0.05134
Py C 4	-0.01855	0.08143	0.03602	-0.06037	0.00844	0.08910
Pz C 4	-0.05763	0.14876	0.01103	-0.13030	0.03069	0.17735
S C 5	0.10100	0.02491	-0.22353	-0.20424	-0.07448	-0.17181
Px C 5	0.14829	0.02542	-0.17443	-0.03901	0.04174	0.17300
Py C 5	-0.01492	0.02437	0.05911	-0.00544	-0.00371	0.04043
Pz C 5	-0.11209	0.02950	0.13202	-0.00207	0.00913	0.04814
S C 6	-0.13313	-0.02391	0.23705	0.09425	-0.04732	-0.16417
Px C 6	0.08424	-0.02075	-0.12281	-0.02920	0.04657	0.19740
Py C 6	0.01386	-0.02275	0.02898	0.07510	0.02391	0.06507
Pz C 6	-0.00233	-0.04910	0.08163	0.16724	0.04831	0.09140
S O 7	-0.00686	0.12667	-0.05268	-0.18712	-0.03826	0.00831
Px O 7	0.08476	-0.17529	-0.13083	0.20818	0.10516	0.01491
Py O 7	-0.00714	0.04094	0.00149	-0.08671	-0.03463	-0.00930
Pz O 7	-0.02680	0.10144	0.02232	-0.19529	-0.08149	-0.02167
S O 12	-0.04012	-0.00181	0.03164	0.07313	0.06567	0.19415
Px O 12	0.16975	-0.02569	-0.21054	-0.12765	-0.10798	-0.27559
Py O 12	0.02582	-0.00309	-0.03768	-0.04796	-0.04914	-0.14022
Pz O 12	-0.08258	-0.02045	-0.04009	-0.05867	-0.01357	-0.14993
S O 14	0.08208	0.07164	-0.03193	0.08495	-0.20156	0.07302
Px O 14	0.01419	-0.00895	0.01103	0.02760	-0.03332	0.00161
Py O 14	-0.03643	0.00345	-0.01444	-0.01484	-0.01406	0.01493
Pz O 14	-0.08108	-0.01462	-0.00848	-0.02462	-0.09438	0.06880
S C 15	-0.07363	0.10356	-0.08096	-0.07716	0.20583	-0.00872
Px C 15	0.10304	-0.03026	0.03096	0.09098	-0.11302	-0.02936
Py C 15	-0.10538	0.00730	-0.03042	-0.06678	0.01133	0.04232
Pz C 15	-0.09387	-0.03074	0.00445	-0.11277	-0.14850	0.12903
S C 16	-0.02154	-0.01180	0.02572	-0.17472	0.02202	0.03236
Px C 16	-0.21270	-0.09761	-0.05112	-0.05806	0.04142	-0.01200

Py C 16	0.07993	-0.01719	0.04217	0.05661	-0.04655	-0.04853
Pz C 16	0.04740	-0.20777	0.04543	0.04839	-0.11357	-0.10748
S C 17	-0.10841	-0.24950	0.06579	0.14641	-0.00998	-0.10584
Px C 17	-0.17440	0.00375	0.08481	0.03031	0.01760	0.04024
Py C 17	0.04408	0.02986	0.00408	0.06104	0.02529	-0.00892
Pz C 17	0.00239	0.05840	-0.01704	0.19501	0.08212	0.00718
S C 18	0.06562	0.00622	0.00124	0.13007	-0.03165	-0.08649
Px C 18	0.09307	-0.07939	0.10829	-0.04078	0.17281	-0.11265
Py C 18	-0.10099	0.07815	-0.12570	0.03161	-0.06057	0.05466
Pz C 18	-0.04670	0.08310	-0.07344	-0.04448	0.29765	-0.05899
S C 19	0.05302	-0.27878	0.19131	-0.16561	0.06906	0.01175
Px C 19	-0.03044	-0.07486	0.01154	-0.11209	0.15310	0.00829
Py C 19	0.07249	0.05339	0.01348	0.12367	-0.09714	-0.06556
Pz C 19	0.14152	-0.01828	0.07624	0.07268	0.11129	-0.15346
S C 20	-0.24678	0.02013	-0.15878	-0.05565	0.02170	0.07073
Px C 20	-0.02354	-0.15512	0.04999	-0.15059	0.05244	0.08466
Py C 20	0.04701	0.07787	0.00983	0.08984	-0.07382	-0.04239
Pz C 20	0.08346	-0.16084	0.16357	-0.12588	-0.08256	0.10582
S C 21	-0.00316	0.27037	-0.08818	0.13662	0.17205	-0.15367
Px C 21	-0.15587	0.03060	-0.14401	0.07848	-0.11638	-0.00281
Py C 21	0.14941	-0.00435	0.13302	-0.06554	0.07748	0.01584
Pz C 21	0.06514	0.07590	0.04836	-0.00891	-0.06113	0.06839
S C 22	0.19109	0.04925	0.12760	-0.13363	0.24713	-0.00218
Px C 22	0.01921	0.09850	-0.01941	0.10484	-0.13903	-0.00364
Py C 22	-0.04707	-0.12673	-0.01206	-0.08476	0.03166	0.02058
Pz C 22	-0.07143	-0.10041	-0.06475	0.01418	-0.25235	0.08673
S C 23	-0.09648	-0.08119	-0.11894	0.02273	-0.21506	0.09119
Px C 23	0.03817	0.09507	-0.01242	0.11213	-0.13551	-0.00240
Py C 23	-0.10699	-0.10984	-0.04913	-0.07709	0.11276	-0.03837
Pz C 23	-0.13899	0.02073	-0.10773	0.06785	-0.00494	-0.01592
S C 24	0.25460	0.17536	0.17678	0.06780	-0.05780	0.05165
Px C 24	-0.05770	0.02312	-0.06444	-0.08566	0.04527	0.00078
Py C 24	0.01414	-0.04746	0.02830	0.04611	-0.02278	-0.09490
Pz C 24	0.16445	0.01659	0.04161	-0.03652	-0.04716	0.01843
S C 25	-0.16963	-0.16514	-0.04148	0.01570	0.03103	-0.10033
Px C 25	-0.07582	0.02000	-0.09416	-0.01341	-0.02630	0.02984
Py C 25	0.03257	-0.03825	0.04863	0.00915	0.03063	-0.10194
Pz C 25	0.10516	0.16495	0.08950	0.08235	-0.00905	0.00737
S O 26	-0.01897	-0.15322	0.02430	-0.02054	-0.21121	0.09019
Px O 26	-0.08761	0.09508	-0.12416	0.09972	0.06604	-0.11547
Py O 26	0.05795	-0.03476	0.07080	-0.04795	0.01179	0.03310
Pz O 26	-0.04943	0.13861	-0.10312	0.10882	0.21668	-0.19522
S H 8	0.03958	-0.08721	-0.03363	-0.01262	-0.07209	-0.23537
S H 13	-0.12803	0.01061	0.13489	0.08821	0.07634	0.17986
S H 9	-0.14041	0.11499	0.18841	-0.00708	-0.03711	-0.12310
S H 10	-0.12104	0.00146	0.20786	0.08021	-0.04824	-0.19390
S H 11	-0.05928	0.14829	0.07496	-0.18676	-0.08249	-0.01611
S H 27	0.03298	-0.18853	0.11599	-0.15072	0.16799	-0.01215
S H 28	-0.17513	-0.01762	-0.12251	-0.07046	0.08392	0.04705

S H 29	0.09072	-0.04110	0.09052	-0.15101	0.26941	-0.01529
S H 30	0.19840	0.05826	0.11815	0.06563	-0.06774	-0.02275
S H 31	0.14547	0.09704	0.10158	0.04731	-0.03550	0.08707
S H 32	-0.09004	-0.10056	-0.02644	0.00483	0.02411	-0.10089
S H 33	-0.05527	-0.13190	0.02180	-0.00958	0.04824	-0.07799
S H 34	0.06884	-0.13074	0.11480	-0.09883	-0.12312	0.13500
S H 35	-0.16187	-0.10897	0.08167	0.10204	-0.00264	-0.02187

Mol. Orbital	19	20	21	22	23	24
Symmetry:	19 A	20 A	21 A	22 A	23 A	24 A
Eigenvalue	-0.79174	-0.77537	-0.72397	-0.70815	-0.69173	-0.67173

S C 1	0.05733	-0.00514	-0.16775	-0.08555	-0.02443	-0.05568
Px C 1	-0.13015	-0.02628	0.22912	0.08749	0.08377	0.00276
Py C 1	0.00206	-0.10298	0.06350	0.02573	-0.10719	0.02453
Pz C 1	0.03152	-0.22261	0.09076	0.02420	-0.21305	0.03630
S C 2	0.00155	0.05091	0.05857	0.05682	0.19286	0.02771
Px C 2	0.09505	0.00014	-0.03537	0.01802	0.02439	0.06010
Py C 2	0.02313	-0.06451	0.06073	0.04558	0.03442	0.03801
Pz C 2	0.03479	-0.15014	0.14276	0.07465	0.10574	0.05872
S C 3	0.06483	-0.02999	-0.10372	-0.05307	-0.21397	-0.02268
Px C 3	0.13848	-0.10662	-0.06164	-0.04511	-0.06545	-0.00357
Py C 3	0.01287	0.07646	-0.04685	0.00814	0.01377	0.00751
Pz C 3	-0.00660	0.15323	-0.06850	-0.03065	0.11014	-0.01795
S C 4	0.01516	-0.05299	0.00587	0.07694	0.03896	0.06518
Px C 4	0.04821	-0.06073	0.05477	0.04485	0.00697	-0.01245
Py C 4	-0.03727	0.01012	0.00083	0.02704	-0.16067	0.01350
Pz C 4	-0.11235	-0.03852	0.03264	-0.09047	-0.18077	-0.04724
S C 5	-0.04798	-0.15713	0.10134	-0.03979	-0.07326	-0.01633
Px C 5	-0.03390	0.11921	-0.07462	0.02059	0.04001	0.05977
Py C 5	-0.03904	0.02933	0.13090	0.09467	-0.05158	0.06799
Pz C 5	-0.09600	-0.01263	0.27951	0.13195	-0.02577	0.04978
S C 6	0.11560	-0.03435	0.01751	0.02728	0.02970	0.03529
Px C 6	-0.12165	0.11008	-0.04434	-0.07515	-0.00451	-0.07666
Py C 6	0.05215	0.09087	-0.18018	-0.05847	0.03499	-0.01670
Pz C 6	0.12812	0.14438	-0.35419	-0.11800	0.10802	-0.04204
S O 7	-0.10979	-0.00125	0.17388	0.05793	-0.03187	0.01374
Px O 7	0.03766	-0.29389	0.13284	0.02760	-0.31168	0.03439
Py O 7	-0.05748	0.06229	0.08528	0.04235	0.08861	0.00709
Pz O 7	-0.11793	0.15935	0.15461	0.07596	0.22908	0.00375
S O 12	-0.00939	0.13545	-0.14116	-0.06077	0.03470	-0.01896
Px O 12	0.13365	-0.12423	-0.26644	-0.30522	0.00007	-0.14005
Py O 12	0.02649	-0.09357	-0.01162	-0.04985	-0.05701	-0.02233
Pz O 12	-0.04276	-0.16640	0.05330	0.04271	-0.02439	-0.07009
S O 14	0.11594	-0.03832	0.00271	0.18210	0.04362	-0.22049
Px O 14	0.04935	0.00211	0.00857	0.13370	0.03679	-0.16353
Py O 14	-0.05289	-0.02596	-0.02296	-0.05470	-0.01775	0.05621
Pz O 14	-0.05881	-0.07269	0.01235	-0.06052	0.00315	-0.15904
S C 15	-0.02263	-0.06570	-0.06389	-0.11818	0.01769	0.23388

Px C 15	0.02168	0.07038	0.00821	0.07732	-0.01320	0.02377
Py C 15	-0.05707	-0.07295	-0.05105	0.01470	-0.02087	-0.05077
Pz C 15	-0.08705	-0.08913	-0.00575	-0.09479	-0.10917	-0.13162
S C 16	0.00549	0.04940	-0.04576	0.10149	-0.17157	-0.00378
Px C 16	-0.21605	-0.04230	-0.03054	-0.17881	0.00815	0.04092
Py C 16	0.02481	0.05714	-0.03849	0.23244	-0.04213	-0.01436
Pz C 16	-0.04572	0.22655	0.04514	-0.00226	-0.01621	0.02502
S C 17	-0.06490	0.09158	0.08786	0.00365	0.16477	-0.01830
Px C 17	-0.13429	-0.11482	0.09850	-0.16684	0.02753	-0.09685
Py C 17	0.07362	-0.00618	-0.04168	0.15788	-0.01444	0.05696
Pz C 17	0.10252	-0.15068	0.03278	-0.00487	0.22397	0.00460
S C 18	-0.05413	0.08870	0.02567	-0.03633	0.02013	0.05674
Px C 18	-0.08569	0.08920	-0.01510	-0.00711	-0.09593	0.13113
Py C 18	0.08828	-0.06063	-0.05229	0.10251	0.09582	-0.03957
Pz C 18	0.11091	-0.01819	-0.02085	-0.00838	0.12060	0.18367
S C 19	-0.04754	0.00298	0.02695	-0.01254	-0.07676	-0.19501
Px C 19	0.11906	0.00271	0.01920	0.06125	0.02347	-0.12799
Py C 19	-0.12303	0.06914	-0.00596	-0.02769	-0.06858	0.10443
Pz C 19	-0.04545	0.18811	0.09043	-0.03895	-0.10794	-0.01585
S C 20	0.13196	-0.06250	-0.03372	0.01695	0.09249	0.16982
Px C 20	0.13705	-0.05444	0.00876	0.04335	0.06595	-0.05974
Py C 20	-0.15034	0.00454	-0.03536	-0.01480	-0.06477	-0.00950
Pz C 20	-0.08798	-0.15150	-0.05852	0.01021	0.01506	-0.16218
S C 21	-0.12804	0.02846	-0.02927	0.01717	0.02520	-0.09776
Px C 21	0.03943	0.09127	0.02081	-0.03254	-0.08417	0.17355
Py C 21	-0.06555	-0.11797	-0.06496	0.05973	0.08092	-0.09172
Pz C 21	-0.08617	-0.17681	-0.11452	0.01807	0.10779	0.22585
S C 22	0.09024	-0.03787	0.01939	0.01616	0.02385	0.03900
Px C 22	-0.13179	-0.04485	-0.07072	0.04574	-0.00600	-0.03999
Py C 22	0.14570	0.09786	0.05436	-0.00017	-0.08569	0.07166
Pz C 22	0.14104	0.13550	0.10727	-0.07644	-0.18029	0.11499
S C 23	0.20433	0.09308	0.08347	0.01827	-0.03804	-0.09464
Px C 23	-0.10424	-0.04975	-0.08063	0.09572	0.03401	-0.04597
Py C 23	0.03811	0.05490	-0.05900	0.09716	-0.03767	-0.00898
Pz C 23	-0.02569	-0.06332	-0.03102	0.03489	0.16625	-0.18807
S C 24	0.06911	-0.05626	0.12135	-0.03884	0.00946	-0.02200
Px C 24	0.05376	-0.03849	-0.13905	0.33481	-0.08385	-0.08165
Py C 24	-0.18362	0.00469	-0.13246	0.15214	-0.05917	0.07922
Pz C 24	0.17820	0.16048	-0.01368	0.10235	-0.16303	0.10884
S C 25	-0.21453	-0.00224	-0.10122	0.01685	0.01171	-0.00735
Px C 25	0.09742	-0.02108	-0.11664	0.29585	-0.00904	-0.14592
Py C 25	-0.23227	0.02124	-0.19118	0.14228	-0.11426	0.14558
Pz C 25	-0.13016	-0.18059	0.00156	0.01044	0.11080	-0.07655
S O 26	0.03725	0.01797	0.02628	-0.03479	-0.08295	0.09107
Px O 26	0.04183	0.20318	0.11020	-0.03940	-0.15666	-0.10259
Py O 26	-0.04126	-0.10067	-0.06264	0.04054	0.09020	-0.03650
Pz O 26	-0.01156	0.20656	0.10829	-0.00839	-0.08987	-0.37221
S H 8	0.05964	-0.06434	0.11032	0.09042	0.17597	0.08550
S H 13	-0.08314	0.07833	0.14676	0.18974	0.00695	0.07614

S H 9	0.12094	-0.10751	-0.08201	-0.06260	-0.16633	-0.01734
S H 10	0.14998	-0.06483	0.00019	0.06013	0.03847	0.07186
S H 11	-0.05206	0.19530	-0.03540	0.00353	0.21643	-0.01552
S H 27	0.06858	0.03558	0.05381	0.03245	-0.03460	-0.21721
S H 28	0.21660	0.00478	0.02675	0.02770	0.09579	0.13889
S H 29	0.11288	-0.00639	0.03062	0.00146	0.04167	0.04291
S H 30	-0.01416	0.04701	0.00304	0.01733	-0.06789	0.10593
S H 31	0.11966	0.00717	0.20074	-0.26990	0.07429	-0.00658
S H 32	-0.20769	0.01365	-0.22011	0.21889	-0.08087	0.04232
S H 33	-0.14970	0.06073	0.01249	-0.18849	-0.02818	0.14313
S H 34	-0.01742	-0.17828	-0.09469	0.02718	0.11497	0.15743
S H 35	-0.11190	-0.05807	0.11753	-0.15494	0.13196	-0.10762

Mol. Orbital	25	26	27	28	29	30
Symmetry:	25 A	26 A	27 A	28 A	29 A	30 A
Eigenvalue	-0.63874	-0.60878	-0.59236	-0.56505	-0.56017	-0.55381

S C 1	-0.07856	0.06396	0.02249	0.03086	-0.03956	-0.04209
Px C 1	-0.15964	0.18315	-0.06875	-0.12860	0.11666	0.06121
Py C 1	0.02329	-0.05152	0.03261	-0.07490	0.08257	-0.01946
Pz C 1	0.10816	-0.10056	0.05728	0.04482	0.04437	-0.00824
S C 2	0.03690	0.01226	-0.09208	0.00012	0.05394	0.00209
Px C 2	0.23915	-0.22239	-0.00220	0.11356	-0.08947	-0.02306
Py C 2	0.04199	-0.02960	-0.08377	-0.04355	-0.02311	0.01693
Pz C 2	0.07907	-0.01153	-0.21170	0.03476	-0.15458	0.08490
S C 3	-0.02837	0.01310	0.09663	-0.03645	0.05828	-0.00610
Px C 3	0.01084	-0.04895	0.10053	0.06363	-0.29473	-0.01391
Py C 3	0.01698	-0.05377	0.09595	-0.03240	0.04561	-0.06542
Pz C 3	0.05147	-0.07606	0.14729	0.08904	-0.01070	-0.07555
S C 4	0.16778	-0.03627	-0.13988	-0.00003	0.10601	-0.00034
Px C 4	-0.17287	0.23362	-0.07947	-0.11016	0.12973	0.03261
Py C 4	-0.05266	-0.02445	0.00674	-0.12005	0.13134	-0.00156
Pz C 4	-0.03548	-0.01954	-0.03242	0.02054	0.01583	0.08360
S C 5	-0.01401	-0.05653	0.06101	0.05831	-0.11260	-0.02641
Px C 5	0.28150	-0.23706	-0.03697	0.09240	-0.06398	0.01472
Py C 5	-0.00520	-0.11298	0.03963	-0.12611	-0.03596	0.01771
Pz C 5	0.02362	-0.02741	0.09005	0.04742	-0.17496	0.02741
S C 6	0.03423	-0.01081	-0.02456	-0.05241	-0.01462	0.05438
Px C 6	-0.13581	0.00977	0.14657	0.13879	-0.32136	-0.07653
Py C 6	0.00211	-0.02911	-0.02684	-0.04187	0.02952	-0.02235
Pz C 6	0.08175	0.00625	-0.10111	0.07146	0.06276	-0.01112
S O 7	-0.05934	0.02523	0.06243	-0.07785	-0.01300	0.05402
Px O 7	0.02763	-0.06879	0.14726	-0.09186	0.00293	0.06726
Py O 7	-0.07541	0.06421	-0.02447	-0.13698	0.03705	0.03606
Pz O 7	-0.13580	0.16162	-0.08112	-0.10811	-0.03207	0.11757
S O 12	0.01816	-0.04199	-0.03199	-0.04802	-0.06365	0.09374
Px O 12	-0.20430	0.15369	-0.05698	-0.07494	0.02126	0.10464
Py O 12	-0.19887	0.05113	-0.02159	-0.15045	0.12458	-0.03761
Pz O 12	-0.07917	0.22736	0.04539	0.20945	0.16296	-0.22780

S O 14	0.01899	0.05329	0.12887	0.17518	0.04928	0.16022
Px O 14	-0.02800	0.05106	0.15758	0.20893	0.01831	0.16603
Py O 14	-0.03170	-0.09721	-0.11368	-0.10402	0.00216	-0.06309
Pz O 14	0.01539	-0.07185	-0.05006	0.13906	0.04419	0.19577
S C 15	0.00672	-0.02601	-0.14372	-0.09707	-0.01852	-0.05210
Px C 15	-0.05907	-0.03979	0.03051	-0.12263	-0.01157	-0.12853
Py C 15	-0.02514	-0.06491	-0.08891	0.03801	0.01773	0.04009
Pz C 15	0.11605	-0.03256	-0.20315	-0.00571	0.04929	0.00581
S C 16	0.08378	0.12337	0.01619	0.03885	0.05621	0.01931
Px C 16	-0.02469	-0.20500	-0.07218	-0.02485	0.08911	-0.07675
Py C 16	-0.11867	0.01345	0.06142	0.04215	0.04024	-0.11262
Pz C 16	-0.01278	-0.08375	0.29592	-0.10205	0.06993	-0.06141
S C 17	-0.07544	0.00331	0.12762	0.00736	-0.02629	-0.05674
Px C 17	-0.20163	-0.05868	-0.08118	0.06646	-0.15567	0.05733
Py C 17	-0.00037	0.05272	-0.03604	-0.05127	0.11487	-0.07931
Pz C 17	-0.00409	0.09237	-0.19864	0.05176	-0.10705	0.04727
S C 18	-0.08891	-0.10410	0.11587	0.07268	0.08802	0.12440
Px C 18	0.00388	0.13031	-0.02530	0.02865	-0.09642	0.06150
Py C 18	-0.10151	-0.16450	0.01466	-0.14026	-0.03254	-0.02616
Pz C 18	-0.03956	0.05216	0.06979	-0.05593	-0.07396	-0.08248
S C 19	0.08934	0.03445	-0.10069	-0.00040	-0.01565	0.00894
Px C 19	-0.03419	-0.05594	-0.05081	-0.13614	-0.12302	-0.20716
Py C 19	-0.01394	0.03753	0.03255	0.09195	0.02860	0.17260
Pz C 19	-0.02553	0.06098	0.03043	0.09127	-0.05887	-0.12912
S C 20	-0.06798	-0.01490	0.08912	0.01627	0.02325	0.05936
Px C 20	-0.11660	-0.20743	0.00411	-0.03713	0.07419	0.03808
Py C 20	0.12655	0.15987	-0.06701	-0.03927	-0.09895	0.04784
Pz C 20	0.13250	0.00335	-0.10519	-0.07796	0.05334	0.09923
S C 21	0.09685	0.06519	0.05953	-0.12364	-0.06979	-0.06678
Px C 21	-0.01074	0.12825	-0.04206	0.07415	-0.08816	0.06282
Py C 21	-0.00200	-0.08643	0.01758	-0.12608	-0.03431	-0.00489
Pz C 21	0.03040	0.15452	0.10476	0.00158	-0.09813	-0.10407
S C 22	-0.08552	-0.02940	-0.04996	0.10938	0.00491	-0.01944
Px C 22	0.05950	0.02020	-0.03864	-0.22651	-0.13841	-0.16945
Py C 22	-0.09968	-0.02532	-0.08329	0.12223	-0.00164	0.18261
Pz C 22	-0.02768	0.06640	-0.20263	0.04287	-0.03791	-0.17841
S C 23	-0.03850	-0.07112	-0.03371	-0.10327	-0.02020	-0.11774
Px C 23	-0.11956	-0.20662	-0.00020	-0.02086	0.03003	0.12562
Py C 23	0.03583	0.10203	0.00738	-0.14435	-0.17600	0.09059
Pz C 23	0.08135	-0.04577	0.23236	-0.08642	0.07010	0.09156
S C 24	-0.08321	-0.00813	-0.05827	0.05075	-0.03530	-0.04606
Px C 24	0.04188	0.23194	-0.02847	0.17983	0.01233	-0.04788
Py C 24	-0.24745	-0.22819	-0.13010	0.10842	0.09692	-0.18344
Pz C 24	-0.09106	-0.00586	-0.03553	-0.18356	-0.11086	0.22285
S C 25	0.09710	0.05756	0.06621	-0.01712	0.01176	-0.00616
Px C 25	-0.09967	-0.01081	-0.08337	-0.08456	-0.22574	0.05380
Py C 25	-0.10682	-0.07798	-0.11053	0.01334	-0.05948	0.21060
Pz C 25	-0.09481	-0.09807	-0.08533	0.24557	0.08893	-0.22819
S O 26	-0.01631	0.05538	-0.12876	0.11050	-0.02349	-0.03726

Px O 26	-0.01860	-0.01168	-0.20863	0.12016	-0.02105	0.01616
Py O 26	0.01873	-0.05523	0.11174	-0.17666	-0.01394	0.07668
Pz O 26	0.04378	-0.16669	-0.05561	-0.10205	0.12231	0.07645
S H 8	0.19083	-0.12209	-0.19748	0.06691	-0.12487	0.04891
S H 13	0.13386	-0.06266	0.03612	0.08047	0.01627	-0.08944
S H 9	-0.02572	-0.02450	0.11318	0.02654	-0.23466	-0.00056
S H 10	0.13755	-0.01126	-0.14852	-0.12893	0.27912	0.08889
S H 11	-0.03346	0.06275	-0.10445	0.03136	0.00734	-0.02113
S H 27	0.02366	-0.00200	-0.07970	-0.08701	-0.12144	-0.25101
S H 28	-0.20599	-0.18066	0.12708	0.05369	0.07519	-0.02794
S H 29	-0.10193	-0.05509	0.04131	0.23749	0.11046	0.25094
S H 30	-0.24758	-0.23325	-0.12025	-0.05487	0.00080	-0.02696
S H 31	0.09506	0.00936	0.06762	-0.15752	-0.10198	0.14856
S H 32	-0.06668	-0.03016	-0.07971	-0.04991	-0.14283	0.19007
S H 33	0.13224	0.05418	0.10892	-0.00592	0.15529	0.06356
S H 34	-0.00506	0.03894	0.13955	-0.06092	-0.02407	0.00118
S H 35	-0.18425	-0.04581	-0.01722	0.09126	-0.19865	0.06740

Mol. Orbital	31	32	33	34	35	36
Symmetry:	31 A	32 A	33 A	34 A	35 A	36 A
Eigenvalue	-0.54317	-0.53360	-0.52550	-0.50881	-0.50528	-0.50238

S C 1	-0.09233	0.04122	0.04821	0.04439	0.00384	0.00635
Px C 1	0.04409	0.02306	0.07361	-0.01913	-0.03095	0.01862
Py C 1	-0.17709	-0.17025	-0.18977	0.06845	0.08222	0.24411
Pz C 1	0.20118	0.02116	-0.05910	0.04684	0.05779	-0.17519
S C 2	0.02571	-0.02490	-0.04444	0.02801	0.03053	-0.02190
Px C 2	0.02916	-0.04451	-0.09469	0.00439	0.04110	-0.06001
Py C 2	-0.24275	-0.09596	-0.00748	0.02947	0.02584	0.09364
Pz C 2	-0.12466	0.03431	0.19880	0.02458	0.02817	-0.15034
S C 3	0.03943	0.00964	0.00366	-0.00575	-0.01034	0.00860
Px C 3	-0.20806	0.12322	0.21074	-0.05279	-0.10195	0.09059
Py C 3	-0.10867	-0.05167	-0.09682	-0.02385	-0.04845	0.09183
Pz C 3	0.20208	0.04315	-0.13312	-0.03738	-0.03104	0.07825
S C 4	-0.00315	-0.02070	0.00170	0.02267	0.00323	-0.01581
Px C 4	0.00324	0.01949	0.04625	0.07553	0.05430	-0.05569
Py C 4	-0.16483	-0.11448	-0.04797	-0.00943	-0.00670	-0.11939
Pz C 4	0.16599	-0.06209	-0.03343	0.02099	0.10001	-0.08011
S C 5	-0.05788	0.00552	-0.01750	0.04199	0.03260	-0.02579
Px C 5	0.06573	-0.02720	-0.01692	-0.09513	-0.05600	0.06382
Py C 5	-0.25310	-0.13689	-0.07421	-0.05225	-0.01567	-0.09212
Pz C 5	0.06899	0.09102	0.07230	0.01632	0.02167	0.03951
S C 6	0.01806	-0.00382	0.03809	-0.07923	-0.05247	0.04340
Px C 6	-0.20357	0.11221	0.10716	0.06771	0.02188	-0.05106
Py C 6	-0.20919	-0.11446	-0.07574	-0.01783	-0.01015	0.08343
Pz C 6	0.10885	0.04392	0.05302	-0.05106	-0.05837	-0.00925
S O 7	0.06715	0.02502	0.05766	-0.17056	-0.13742	0.10894
Px O 7	0.15479	0.01988	0.04203	-0.27035	-0.20971	0.15781
Py O 7	-0.26440	-0.16389	-0.09755	-0.04423	-0.01445	0.61150

Pz O 7	0.11335	0.14268	0.28778	-0.28824	-0.27065	-0.07398
S O 12	0.01000	-0.05505	0.02673	-0.14028	-0.05881	0.02708
Px O 12	0.10658	-0.01376	0.04268	-0.07930	-0.02672	0.06673
Py O 12	-0.25926	-0.15457	-0.13212	0.05490	0.05444	-0.32646
Pz O 12	0.07127	0.18895	0.01166	0.28864	0.10398	0.07130
S O 14	-0.01648	-0.22673	0.06926	0.02215	-0.08997	-0.05180
Px O 14	-0.00094	-0.35301	0.04606	0.03879	-0.23511	-0.14311
Py O 14	-0.02937	0.23273	-0.11764	-0.01597	-0.04738	-0.02358
Pz O 14	-0.01895	-0.16221	0.04733	-0.00818	0.01429	-0.00623
S C 15	-0.02574	0.05417	0.03173	0.00427	-0.03684	-0.00014
Px C 15	0.00505	0.26485	-0.12708	-0.01530	0.03074	0.01221
Py C 15	-0.03790	-0.05617	-0.03334	0.01587	-0.19134	-0.09799
Pz C 15	-0.02940	0.08280	0.04377	-0.00837	0.10371	0.07566
S C 16	-0.02386	-0.02031	0.08859	0.04075	0.00087	-0.01302
Px C 16	-0.04413	-0.05911	0.00326	-0.05279	-0.14741	-0.07160
Py C 16	-0.05781	0.06981	-0.06296	-0.06483	-0.06653	-0.08126
Pz C 16	0.04303	0.05053	-0.01784	0.00263	-0.00728	-0.01029
S C 17	0.03454	0.00426	-0.07803	-0.01238	-0.01352	0.01770
Px C 17	0.04094	-0.11831	-0.15818	-0.04688	0.06964	-0.06938
Py C 17	-0.16022	0.05072	0.06084	-0.00518	-0.09893	-0.06086
Pz C 17	0.00672	0.01670	-0.00105	0.01938	0.03827	0.08638
S C 18	-0.00728	0.00498	0.03238	0.02957	0.02259	0.00491
Px C 18	0.01894	0.03334	-0.15946	0.04655	-0.05174	-0.04125
Py C 18	0.04150	0.01897	-0.01432	0.09664	-0.15949	-0.03113
Pz C 18	0.01652	-0.10888	0.01276	-0.03577	-0.06813	-0.05394
S C 19	-0.02932	0.02029	-0.04268	-0.03569	-0.01389	-0.01192
Px C 19	0.10783	-0.15259	0.00570	0.07899	-0.15154	-0.02083
Py C 19	-0.01908	0.11569	-0.10970	0.10063	-0.02769	0.00753
Pz C 19	0.11002	-0.21022	0.02219	-0.03029	0.11654	0.02806
S C 20	-0.01341	0.04263	-0.02333	0.00087	0.01529	-0.01403
Px C 20	0.03093	0.08358	0.09467	0.21729	-0.05887	0.08207
Py C 20	-0.03519	0.04262	-0.19127	0.03918	-0.21007	-0.07425
Pz C 20	-0.13520	0.19064	-0.00992	-0.06905	-0.04139	-0.02937
S C 21	0.01985	-0.06457	-0.01518	-0.02546	0.00236	-0.05400
Px C 21	0.01290	-0.00194	-0.19478	0.10318	-0.20365	-0.03514
Py C 21	0.06120	0.01930	0.01228	0.28362	-0.19363	0.05945
Pz C 21	0.04794	-0.15040	-0.05446	-0.10243	-0.00382	-0.02523
S C 22	0.01829	-0.01915	-0.01235	-0.00097	-0.03252	0.05013
Px C 22	0.11781	-0.10606	0.09160	0.19834	-0.06263	0.02874
Py C 22	-0.01637	0.10309	-0.14926	0.08729	-0.10391	0.00616
Pz C 22	0.03375	-0.07541	0.11772	0.00405	0.04865	0.02353
S C 23	0.02125	0.01823	0.01142	-0.01770	0.02882	-0.02473
Px C 23	0.05834	0.01470	0.06321	0.14537	-0.03480	0.07200
Py C 23	0.03107	0.05164	-0.22337	0.00951	-0.01993	-0.07698
Pz C 23	-0.07918	0.08975	-0.10569	-0.12025	0.00867	-0.07798
S C 24	0.03712	0.05428	-0.07014	0.01524	0.03182	0.01769
Px C 24	-0.04703	0.03761	0.02660	-0.04549	0.04537	0.04345
Py C 24	-0.03402	-0.00284	0.02279	-0.16070	-0.09582	-0.08545
Pz C 24	0.02709	-0.04251	0.07280	0.05845	0.11628	-0.09910

S C 25	-0.01006	-0.00165	0.00622	-0.01470	0.00073	0.01434
Px C 25	0.09577	0.06869	-0.25929	-0.12124	0.15185	0.03395
Py C 25	0.10656	-0.10647	0.18989	0.14184	0.13211	0.13348
Pz C 25	0.01543	0.04007	-0.04897	-0.06567	-0.08264	0.12628
S O 26	0.00383	-0.03205	-0.03041	-0.00923	-0.11371	0.05770
Px O 26	0.01061	0.02521	-0.09823	0.23696	-0.39259	0.11493
Py O 26	0.02403	0.09283	-0.03543	0.35912	-0.17535	-0.03495
Pz O 26	-0.07463	0.15352	0.14310	-0.03303	0.20515	-0.02819
S H 8	-0.12265	-0.04624	0.05011	0.03660	0.06258	-0.11112
S H 13	-0.02362	0.04506	-0.01616	0.08444	0.02575	-0.00219
S H 9	-0.18923	0.10251	0.20279	-0.04980	-0.09090	0.07337
S H 10	0.21099	-0.08920	-0.06709	-0.10353	-0.05185	0.06012
S H 11	-0.08246	-0.00717	-0.00084	0.13176	0.10032	-0.08509
S H 27	0.10639	-0.22889	0.04275	-0.01837	-0.05562	-0.01189
S H 28	0.09276	-0.05688	0.14904	0.11679	0.12224	0.09480
S H 29	-0.09143	0.13179	-0.16809	-0.09337	-0.03867	-0.00228
S H 30	-0.00388	-0.02740	0.00212	-0.07864	-0.02132	-0.13102
S H 31	0.07296	-0.00029	-0.05238	0.13561	0.06228	0.04507
S H 32	0.11715	-0.05137	0.02957	0.05290	0.17274	0.11841
S H 33	-0.08106	-0.08175	0.25102	0.12789	-0.09006	-0.05083
S H 34	0.01963	-0.02513	-0.00989	-0.00719	0.08111	-0.05605
S H 35	0.09418	-0.10717	-0.17082	-0.04407	0.08463	-0.00950

Mol. Orbital	37	38	39	40	41	42
Symmetry:	37 A	38 A	39 A	40 A	41 A	42 A
Eigenvalue	-0.49158	-0.47733	-0.47134	-0.45717	-0.45385	-0.43759

S C 1	0.01525	0.01481	0.01605	-0.01439	0.07919	-0.00418
Px C 1	-0.01871	0.00125	0.06158	0.04912	0.24449	-0.29227
Py C 1	-0.00887	-0.09198	-0.00664	0.02957	0.01044	-0.07710
Pz C 1	0.04188	-0.02557	0.03642	0.05788	-0.00162	-0.13706
S C 2	0.02065	-0.01171	-0.00427	-0.00095	-0.00801	-0.02794
Px C 2	0.00566	-0.01355	-0.06193	-0.03010	-0.27485	0.25695
Py C 2	-0.13617	-0.01205	0.04641	0.01649	-0.01024	0.03733
Pz C 2	-0.23489	-0.00180	0.07279	0.07596	0.02715	0.03600
S C 3	-0.01252	-0.00265	0.02445	0.02487	0.00637	0.01111
Px C 3	0.01487	0.05083	0.01495	-0.02690	0.25385	-0.17310
Py C 3	0.09181	0.05151	0.00029	-0.07000	-0.00078	-0.02179
Pz C 3	0.28534	0.00090	-0.12584	-0.09166	-0.01388	-0.04696
S C 4	-0.01633	0.03155	0.00810	-0.03387	0.03207	0.06164
Px C 4	-0.02587	-0.04756	0.05434	0.06866	-0.18453	0.17109
Py C 4	-0.16115	0.05937	0.09657	0.02378	-0.07674	0.04128
Pz C 4	-0.21499	-0.08778	0.01375	0.11098	-0.05058	0.02350
S C 5	0.02121	-0.00571	0.00619	-0.00506	0.03175	-0.05905
Px C 5	-0.04310	0.01976	-0.05292	-0.04090	0.15445	-0.12875
Py C 5	0.06579	0.16713	0.00430	-0.03990	-0.08957	-0.10987
Pz C 5	-0.01773	-0.15254	0.02660	0.11620	-0.08713	-0.04427
S C 6	-0.02330	0.00290	-0.01532	0.00360	-0.07006	0.03799
Px C 6	0.03649	-0.01347	-0.00271	-0.00438	-0.17255	0.21289

Py C 6	0.00099	0.09365	-0.03465	-0.08236	-0.03805	0.07222
Pz C 6	-0.04444	0.04115	-0.04432	-0.07207	0.06313	0.14950
S O 7	0.02855	0.05624	-0.07149	-0.07025	-0.07379	0.12983
Px O 7	0.05385	0.09542	-0.12391	-0.12259	-0.13633	0.22832
Py O 7	-0.08157	-0.20108	-0.11875	0.00695	0.04345	0.15739
Pz O 7	-0.01998	0.23121	-0.03923	-0.13839	-0.00067	0.14282
S O 12	-0.12562	-0.01262	-0.00433	0.06345	-0.15900	-0.09956
Px O 12	-0.18504	-0.12329	0.03821	0.10695	-0.15633	-0.01017
Py O 12	0.26996	0.39592	-0.05069	-0.20089	-0.00817	0.02737
Pz O 12	0.06205	-0.12711	0.02987	-0.06252	0.21988	0.33885
S O 14	0.03043	-0.04968	-0.01155	-0.00941	0.03882	0.02221
Px O 14	-0.00138	-0.25899	0.02194	-0.22538	0.03867	-0.02454
Py O 14	-0.12409	-0.15149	0.10200	-0.36381	-0.05073	-0.10659
Pz O 14	0.03079	0.09133	-0.07536	0.03757	0.15262	0.07840
S C 15	0.11556	-0.06585	-0.02966	-0.00181	0.01556	0.01446
Px C 15	-0.13301	-0.04438	0.09604	-0.12577	-0.11126	-0.08452
Py C 15	-0.08030	-0.21255	0.06641	-0.33104	0.04086	-0.02204
Pz C 15	-0.06904	0.19752	-0.01198	-0.00403	0.07585	0.06253
S C 16	-0.08013	0.00039	-0.00482	-0.01958	-0.03988	-0.01550
Px C 16	-0.05693	-0.04295	0.08317	-0.01472	0.15352	0.12164
Py C 16	-0.12912	-0.11328	-0.01360	-0.03971	-0.12019	-0.08684
Pz C 16	-0.08009	0.01335	0.16804	0.14803	0.02015	0.05530
S C 17	0.07193	-0.00597	0.00725	0.01066	-0.06387	-0.00885
Px C 17	-0.06999	-0.05506	-0.11048	-0.03150	-0.09184	-0.11187
Py C 17	-0.03683	-0.02489	0.06352	-0.05244	-0.03662	0.05758
Pz C 17	0.23025	0.02332	-0.15040	-0.10495	-0.02347	-0.03178
S C 18	-0.03678	0.01747	0.02144	0.00304	-0.00125	0.00050
Px C 18	-0.11344	-0.06626	-0.05979	-0.23643	0.01264	-0.05266
Py C 18	0.04731	-0.16670	0.16236	-0.08895	0.01828	0.05233
Pz C 18	0.17626	-0.14107	-0.04218	0.14130	-0.03606	-0.02078
S C 19	0.00643	0.00041	-0.00290	-0.01474	0.02280	0.00662
Px C 19	-0.02264	-0.05392	0.10059	-0.04408	0.07347	0.07958
Py C 19	-0.15276	0.04141	-0.05646	-0.19067	-0.00242	-0.04224
Pz C 19	-0.25042	0.20331	-0.01623	-0.07388	0.10057	0.04084
S C 20	-0.00550	-0.01794	-0.04294	0.01272	0.00387	0.00320
Px C 20	-0.01827	0.04657	-0.01648	-0.08057	-0.12158	-0.09802
Py C 20	0.02876	-0.07546	-0.02859	0.04041	0.08652	0.08010
Pz C 20	0.27400	-0.18285	0.01918	0.10645	-0.10261	-0.05087
S C 21	-0.02558	-0.02434	-0.01673	0.02186	0.04147	0.02446
Px C 21	-0.07883	0.05369	-0.10297	0.07119	0.13049	0.10973
Py C 21	-0.02849	0.10521	-0.02012	0.04807	-0.10386	-0.08115
Pz C 21	-0.02629	0.02269	0.15002	0.03686	0.01780	0.01142
S C 22	0.02190	0.03339	0.06584	-0.01453	-0.03674	-0.02748
Px C 22	-0.00356	0.00477	-0.05024	-0.07223	-0.06249	-0.06100
Py C 22	-0.02320	0.01706	-0.04244	-0.02236	0.10008	0.09356
Pz C 22	0.05100	-0.07168	-0.17870	-0.10271	-0.02310	-0.03560
S C 23	-0.02175	-0.02058	-0.05384	0.03612	0.03438	0.02553
Px C 23	0.02261	0.02079	0.18468	-0.05647	0.02598	0.07952
Py C 23	-0.05349	-0.04160	-0.01965	-0.05813	0.09115	0.03304

Pz C 23	-0.06236	0.04296	0.11392	0.17650	0.03965	0.04002
S C 24	-0.01165	-0.01016	-0.02908	-0.02630	0.01904	0.01444
Px C 24	-0.05480	0.05232	-0.17305	-0.01648	-0.21097	-0.19640
Py C 24	-0.00978	-0.11113	-0.18760	0.20713	0.08830	0.02923
Pz C 24	0.12036	-0.16303	-0.07409	0.06606	0.04570	0.04347
S C 25	-0.03576	0.05104	0.01570	0.00427	-0.04029	-0.04198
Px C 25	-0.01775	0.11591	0.07627	0.03778	0.10974	0.06566
Py C 25	0.15712	0.03828	0.12149	-0.06365	-0.02468	0.03725
Pz C 25	-0.07990	0.13883	0.04055	-0.04216	-0.03835	-0.03642
S O 26	0.10498	0.02293	0.19966	0.05639	-0.09184	-0.05215
Px O 26	0.09471	0.18316	0.14968	0.27094	-0.17045	-0.10357
Py O 26	-0.19260	0.14139	-0.51405	0.15838	0.06546	0.02346
Pz O 26	0.04023	-0.14166	-0.20390	-0.15007	0.02376	0.01007
S H 8	-0.18902	-0.01857	0.02326	0.03823	-0.16228	0.19022
S H 13	0.10504	0.02975	-0.01621	-0.06410	0.14615	0.05679
S H 9	-0.04034	0.04274	0.04010	0.00170	0.24460	-0.16596
S H 10	-0.05085	0.01796	-0.01098	-0.00373	0.15034	-0.16787
S H 11	-0.04393	-0.04292	0.07203	0.06680	0.09612	-0.13993
S H 27	-0.03943	0.02512	0.09034	0.02385	0.10320	0.09896
S H 28	-0.16550	0.15690	-0.01521	-0.11655	-0.06524	-0.07649
S H 29	-0.01594	0.04624	0.11611	0.07229	0.08196	0.09144
S H 30	0.07650	-0.15627	-0.13117	0.17772	0.16395	0.10864
S H 31	0.03607	0.03198	0.21761	-0.13674	0.06737	0.09636
S H 32	0.09974	0.09970	0.14415	-0.03539	0.01750	0.04700
S H 33	0.04858	-0.12381	-0.05296	-0.02405	-0.10406	-0.05900
S H 34	-0.11478	-0.00491	-0.16016	-0.04471	0.10167	0.06084
S H 35	0.03259	-0.03594	-0.14564	-0.02749	-0.08042	-0.14015

Mol. Orbital	43	44	45	46	47	48
Symmetry:	43 A	44 A	45 A	46 A	47 A	48 A
Eigenvalue	-0.42750	-0.42053	-0.41095	-0.40167	-0.39782	-0.33529

S C 1	0.01445	-0.02561	-0.00824	0.00266	0.00498	0.00943
Px C 1	-0.02191	0.02295	0.01856	0.01486	-0.00709	-0.02483
Py C 1	-0.06403	0.03474	-0.10116	0.00513	-0.03743	0.27171
Pz C 1	-0.03305	0.08527	0.07110	-0.02089	0.00723	-0.13695
S C 2	-0.01778	0.03854	-0.01038	-0.01739	-0.00077	-0.01789
Px C 2	0.01462	0.00946	0.00779	-0.02176	0.00775	-0.01426
Py C 2	-0.12946	-0.07271	-0.25957	0.03149	-0.05412	0.24511
Pz C 2	0.11669	-0.11591	0.15240	0.05836	0.02104	-0.06582
S C 3	-0.00116	-0.01467	0.02881	0.00869	-0.00033	0.03529
Px C 3	0.03032	-0.02107	0.02080	0.01216	0.00551	-0.01406
Py C 3	-0.22814	0.03785	-0.32941	-0.03491	-0.04251	-0.04876
Pz C 3	0.04714	0.14691	0.09516	-0.06930	0.02537	-0.04701
S C 4	0.00222	0.00190	0.00348	-0.03041	0.01120	-0.00130
Px C 4	-0.06856	0.15221	0.11221	-0.09606	0.00564	0.09078
Py C 4	-0.16034	-0.12236	-0.23310	0.05695	-0.02509	-0.24605
Pz C 4	0.18783	-0.21300	0.11233	0.14880	-0.00538	0.16060
S C 5	-0.00303	-0.00758	-0.02821	0.01393	0.00023	-0.03237

Px C 5	0.08970	-0.13964	-0.05741	0.08251	-0.00284	-0.04818
Py C 5	-0.10195	0.07151	-0.05271	0.01543	-0.04035	-0.00174
Pz C 5	-0.07448	0.18912	0.10990	-0.08828	0.00280	0.02636
S C 6	-0.02014	0.04133	0.02286	-0.02103	-0.00312	0.01258
Px C 6	-0.01654	0.06487	0.04749	-0.05799	0.01407	-0.01346
Py C 6	-0.02070	-0.08620	-0.15962	0.05430	-0.03937	0.24749
Pz C 6	0.14144	-0.18233	0.00575	0.04950	0.03403	-0.14480
S O 7	0.02517	-0.02850	-0.01700	-0.00160	0.00373	-0.00187
Px O 7	0.04521	-0.06576	-0.04417	0.00681	0.00467	0.00567
Py O 7	0.27269	-0.06219	0.30534	-0.00741	0.07615	-0.25485
Pz O 7	-0.02239	-0.13490	-0.18145	0.04333	-0.02352	0.12139
S O 12	-0.07549	0.10024	0.06506	0.00641	-0.03167	0.00189
Px O 12	-0.12693	0.08528	-0.01982	-0.02556	-0.02323	0.00428
Py O 12	0.27033	-0.08546	0.31855	0.10063	0.04214	0.00180
Pz O 12	0.05112	-0.23867	-0.27641	-0.01753	0.03798	0.00159
S O 14	-0.05917	-0.02958	0.04063	-0.03901	0.00726	0.00628
Px O 14	-0.09712	-0.08345	0.09924	-0.00971	0.21893	0.19851
Py O 14	0.17404	0.15668	-0.09828	-0.03140	0.36907	0.15438
Pz O 14	0.00160	0.08107	-0.10038	-0.27965	-0.05421	-0.24596
S C 15	-0.06066	0.00350	0.01510	-0.03514	0.01164	-0.00436
Px C 15	0.14003	0.03882	-0.05755	0.11048	0.07801	-0.01022
Py C 15	0.00673	0.09312	0.02076	-0.08065	0.17764	0.03976
Pz C 15	0.04817	0.19393	-0.01919	-0.11641	-0.03419	0.04350
S C 16	0.04652	0.01074	0.03505	0.02153	-0.02082	0.04090
Px C 16	-0.18233	0.00466	0.12061	-0.13360	0.08095	-0.09759
Py C 16	0.03731	-0.02784	-0.07346	0.04565	0.04869	-0.34796
Pz C 16	-0.04860	-0.16418	0.12450	0.11242	-0.00079	0.10067
S C 17	-0.06742	0.00873	0.02014	0.02644	-0.00367	-0.01078
Px C 17	0.07882	-0.13902	-0.21983	0.10965	-0.01552	-0.23703
Py C 17	-0.15622	0.11743	-0.04522	-0.11704	0.06142	-0.42091
Pz C 17	0.02461	0.21009	-0.06268	-0.11512	-0.02074	0.08946
S C 18	0.04298	0.00022	-0.02679	-0.01016	-0.00153	-0.01911
Px C 18	-0.08137	-0.13391	0.09080	-0.18251	-0.14074	0.00828
Py C 18	0.08979	0.08088	-0.00608	0.16965	-0.21570	-0.01022
Pz C 18	-0.09917	-0.17713	0.01275	0.09497	0.06257	-0.04667
S C 19	-0.00313	0.01959	0.00041	-0.04904	0.01260	0.00351
Px C 19	0.08384	0.15053	-0.01463	0.13942	-0.22667	-0.01332
Py C 19	-0.01359	-0.04437	0.07368	-0.15956	-0.25192	0.02548
Pz C 19	0.05832	0.16087	-0.04271	-0.10977	0.10926	0.00789
S C 20	-0.02944	-0.02411	0.01364	0.03872	-0.00500	-0.00055
Px C 20	0.00013	-0.12876	0.04715	-0.13153	-0.21044	0.00394
Py C 20	-0.00582	0.08036	0.02693	0.13579	-0.24145	-0.00809
Pz C 20	-0.06729	-0.17023	0.02058	0.06224	0.06423	-0.00330
S C 21	0.04045	0.02454	-0.02680	-0.02778	0.00539	-0.00070
Px C 21	-0.03319	0.15839	0.00811	0.17820	-0.08636	-0.01448
Py C 21	0.04778	-0.11358	0.00020	-0.17125	-0.10954	-0.00270
Pz C 21	0.10148	0.02228	-0.04499	-0.07908	0.03167	0.00529
S C 22	-0.03654	-0.04263	0.02801	-0.00404	0.00002	-0.00559
Px C 22	-0.02562	-0.13467	0.02958	-0.14826	-0.14462	-0.01739

Py C 22	-0.07126	0.08437	0.04248	0.13032	-0.17519	-0.02024
Pz C 22	-0.19311	-0.04925	0.07260	0.13805	0.06631	-0.01712
S C 23	0.00476	0.00794	-0.00082	0.00054	-0.00014	0.02219
Px C 23	0.08625	0.14836	-0.03302	0.15775	-0.16087	-0.01823
Py C 23	-0.02437	-0.12321	0.03790	-0.24118	-0.13522	0.01239
Pz C 23	0.21878	0.08192	-0.09890	-0.11876	0.04876	0.03670
S C 24	-0.00234	-0.03479	-0.02698	0.01130	-0.01451	-0.00718
Px C 24	0.16281	0.06210	-0.08210	0.10401	-0.09708	-0.00096
Py C 24	0.03901	0.00998	0.03019	-0.12846	-0.06482	0.14036
Pz C 24	0.21603	0.02997	-0.20152	-0.11659	0.04910	-0.01632
S C 25	-0.00046	-0.02065	0.03127	-0.03558	-0.00875	0.02294
Px C 25	-0.16134	-0.11733	0.07355	-0.10334	0.12664	0.02039
Py C 25	-0.05088	0.06349	-0.04119	0.21261	0.09470	-0.04901
Pz C 25	-0.20717	-0.00126	0.17770	0.17770	-0.04686	0.02842
S O 26	0.05838	-0.07374	-0.01234	-0.07693	-0.00036	0.00212
Px O 26	0.10563	-0.08742	-0.07049	-0.10800	0.27240	0.01358
Py O 26	-0.12368	0.09930	-0.02367	0.17242	0.37161	0.00402
Pz O 26	-0.14791	-0.01954	0.06956	0.11296	-0.09628	-0.00844
S H 8	0.03980	-0.08850	0.01480	0.03420	-0.00009	0.02671
S H 13	0.07656	-0.09574	-0.05946	0.00829	0.01979	-0.00006
S H 9	0.02797	-0.06374	0.00791	0.03865	-0.00067	-0.00007
S H 10	0.03780	-0.08132	-0.03117	0.05967	-0.00772	-0.01910
S H 11	-0.02220	0.02277	0.01868	0.00405	-0.00416	0.00153
S H 27	0.08590	0.20852	-0.05849	0.12581	0.00063	-0.01259
S H 28	0.02798	-0.04180	0.00328	-0.18143	0.00635	0.01113
S H 29	0.05379	0.15421	-0.02377	0.12895	-0.00792	0.00688
S H 30	0.08312	-0.00698	-0.05523	-0.19195	0.00546	0.09785
S H 31	-0.12867	-0.05012	0.00697	0.03242	0.11143	-0.11924
S H 32	-0.11679	-0.01644	0.00989	0.10347	0.14554	-0.03352
S H 33	0.22061	0.11967	-0.12956	0.05069	-0.09194	-0.03546
S H 34	-0.04660	0.08974	0.00830	0.08297	0.00031	-0.00298
S H 35	0.11500	-0.11479	-0.19406	0.11596	-0.03790	-0.06479

Mol. Orbital	49	50	51	52	53	54
Symmetry:	49 A	50 A	51 A	52 A	53 A	54 A
Eigenvalue	-0.32229	-0.30405	-0.29865	-0.28177	-0.26180	0.00226

S C 1	-0.00037	0.00689	-0.00151	0.00298	-0.00909	0.00493
Px C 1	0.00379	0.00121	0.00139	-0.00840	0.02378	-0.02155
Py C 1	-0.03403	0.08319	-0.00326	0.11735	-0.31301	0.22385
Pz C 1	0.01774	-0.04047	0.00299	-0.05691	0.15291	-0.10851
S C 2	0.01438	0.00623	-0.00062	-0.00129	-0.00201	0.01432
Px C 2	0.00336	0.01619	-0.00174	-0.00651	0.01097	0.01034
Py C 2	-0.02581	-0.40230	0.02222	0.11086	-0.21807	-0.04349
Pz C 2	-0.02316	0.17331	-0.00867	-0.04829	0.10454	0.00186
S C 3	-0.02972	-0.00266	0.00032	-0.00027	0.01210	-0.03186
Px C 3	0.01205	0.03440	-0.00121	0.00517	-0.02155	0.02011
Py C 3	0.04263	-0.42286	0.02140	-0.03491	0.16925	-0.18224
Pz C 3	0.03637	0.20286	-0.01121	0.01504	-0.09051	0.10351

S C 4	0.00381	-0.00195	-0.00182	0.00085	0.00311	0.00186
Px C 4	-0.04212	0.00012	-0.00195	0.00930	-0.00122	-0.03404
Py C 4	0.02045	0.00479	-0.00170	-0.14600	0.36553	0.14733
Pz C 4	-0.05420	-0.00669	0.00470	0.07022	-0.17546	-0.07894
S C 5	0.01990	0.01639	-0.00146	-0.00346	-0.00365	0.01077
Px C 5	0.02835	-0.04533	0.00526	0.01603	-0.05630	0.04380
Py C 5	-0.01003	0.33735	-0.01477	-0.09446	0.25883	-0.17750
Pz C 5	-0.00968	-0.18776	0.01169	0.05075	-0.12379	0.09172
S C 6	-0.00854	-0.00931	0.00125	0.00057	0.00646	-0.01093
Px C 6	-0.00489	-0.07206	0.00225	-0.00576	0.02346	0.00233
Py C 6	-0.03797	0.50295	-0.02666	0.03109	-0.10823	-0.06971
Pz C 6	0.03240	-0.23594	0.01110	-0.01702	0.04597	0.03902
S O 7	0.00250	-0.00054	-0.00018	0.00019	-0.00119	0.00143
Px O 7	0.00345	0.00464	-0.00066	0.00357	-0.01117	0.00505
Py O 7	0.02956	-0.05339	0.00184	-0.07356	0.17485	-0.06302
Pz O 7	-0.01264	0.03075	-0.00220	0.03574	-0.08746	0.03102
S O 12	-0.01177	-0.00818	0.01081	0.00575	0.00233	0.00668
Px O 12	-0.00490	0.04801	0.00009	-0.01168	0.03066	-0.01004
Py O 12	-0.01958	-0.24829	0.01987	0.06611	-0.13851	0.04964
Pz O 12	0.01649	0.13893	-0.02368	-0.03862	0.06448	-0.03015
S O 14	-0.00315	0.00068	-0.00044	0.00217	-0.00281	0.00013
Px O 14	0.13231	-0.02727	0.02851	-0.16923	0.07428	0.16837
Py O 14	-0.36857	-0.04572	0.06293	-0.26828	0.07988	0.30116
Pz O 14	-0.72862	0.01681	-0.02466	0.13409	-0.06174	-0.07457
S C 15	-0.00608	0.00249	-0.00564	0.00119	0.00374	-0.00310
Px C 15	-0.05428	0.00127	0.00763	0.03363	-0.03161	-0.23062
Py C 15	0.07975	0.00682	-0.01283	0.06334	-0.02502	-0.40456
Pz C 15	0.23395	0.00042	-0.00419	-0.03115	0.02093	0.10126
S C 16	0.06852	0.00109	0.00754	0.01973	-0.01270	-0.01721
Px C 16	0.16741	0.03980	-0.01602	0.03482	-0.18631	-0.10071
Py C 16	0.01306	0.06851	0.00921	0.10324	-0.38566	-0.21434
Pz C 16	-0.19883	-0.01557	0.00507	-0.02007	0.07728	0.05481
S C 17	0.00650	-0.00588	0.00362	-0.00606	0.00111	0.01026
Px C 17	0.15062	0.02736	-0.00149	-0.00603	-0.08424	0.17189
Py C 17	0.11152	0.08306	-0.00697	0.02929	-0.26982	0.36595
Pz C 17	0.06548	-0.02259	-0.00221	-0.00869	0.08614	-0.09749
S C 18	-0.07711	0.00074	0.00351	0.00506	-0.00667	0.00264
Px C 18	-0.03414	0.00524	-0.07543	0.31382	0.13533	-0.08468
Py C 18	-0.02933	0.00826	-0.06518	0.36529	0.15367	-0.08316
Pz C 18	-0.21515	-0.00344	0.02607	-0.10735	-0.05799	0.03466
S C 19	0.00158	-0.00020	-0.00220	0.00093	0.00235	-0.00805
Px C 19	-0.07119	-0.01970	-0.30018	0.03673	0.03511	0.15019
Py C 19	0.05400	-0.02397	-0.36886	0.04101	0.04843	0.16354
Pz C 19	0.04369	0.00800	0.11833	-0.01933	-0.01430	-0.06283
S C 20	-0.00580	-0.00053	-0.00101	-0.00305	-0.00109	0.00411
Px C 20	-0.00599	-0.02677	-0.24821	-0.25291	-0.09067	0.02541
Py C 20	-0.05408	-0.03094	-0.27845	-0.29325	-0.10564	0.02828
Pz C 20	-0.00955	0.01003	0.09411	0.10352	0.03645	-0.00294
S C 21	-0.01005	0.00028	-0.00389	0.00157	-0.00100	0.00327

Px C 21	-0.03806	-0.00506	0.09931	-0.25194	-0.10526	-0.17061
Py C 21	-0.00203	-0.00597	0.10478	-0.30494	-0.12876	-0.20207
Pz C 21	0.00883	0.00186	-0.03213	0.08080	0.03350	0.05694
S C 22	-0.02996	-0.00072	-0.00068	0.00423	0.00217	-0.00453
Px C 22	-0.02456	0.01763	0.36832	-0.09965	-0.04181	0.02687
Py C 22	-0.01426	0.02126	0.45042	-0.11556	-0.04510	0.03698
Pz C 22	-0.07044	-0.00716	-0.14629	0.06058	0.02101	-0.01357
S C 23	0.03259	-0.00203	-0.00741	-0.01204	0.00412	0.00871
Px C 23	0.05867	0.02482	0.27022	0.18126	0.07965	0.16080
Py C 23	0.01023	0.02377	0.27587	0.19478	0.09519	0.17294
Pz C 23	0.09229	-0.00957	-0.11068	-0.09532	-0.03681	-0.06303
S C 24	-0.02365	0.00246	0.02385	0.01897	0.00962	0.01369
Px C 24	-0.07732	-0.01845	0.02718	0.00249	0.04665	0.01471
Py C 24	0.00704	-0.02265	0.01087	-0.02404	0.06995	0.02196
Pz C 24	0.06193	0.00182	-0.05424	-0.02751	-0.03552	-0.02740
S C 25	-0.01568	-0.00703	0.00201	-0.00565	0.02303	0.01689
Px C 25	0.00738	-0.00439	-0.08184	-0.05050	-0.01661	-0.01457
Py C 25	-0.01109	0.00165	-0.07003	-0.03970	-0.03540	-0.01255
Pz C 25	-0.08496	-0.01025	0.03716	0.02182	0.04900	0.02079
S O 26	0.00568	0.00024	-0.00042	0.00469	0.00178	0.00116
Px O 26	0.03119	0.00438	-0.06725	0.17149	0.06437	0.05051
Py O 26	0.00507	0.00520	-0.08670	0.22414	0.08348	0.06195
Pz O 26	-0.01278	-0.00144	0.02433	-0.05269	-0.01977	-0.01848
S H 8	-0.02012	-0.01124	0.00076	0.00103	0.00224	-0.00738
S H 13	0.00661	0.00873	-0.00722	-0.00498	0.00253	-0.00778
S H 9	-0.00254	-0.00119	0.00123	0.00256	-0.00564	0.00627
S H 10	0.00920	0.00676	0.00143	0.00185	-0.01060	0.01003
S H 11	-0.00320	0.00006	0.00040	-0.00071	0.00318	-0.00338
S H 27	-0.02561	0.00082	0.00702	-0.00007	-0.00203	0.00139
S H 28	0.04700	0.00023	-0.00306	-0.00253	0.00030	-0.00484
S H 29	0.03886	0.00032	0.00819	-0.00522	0.00093	0.00304
S H 30	0.06331	-0.01075	-0.02787	-0.04723	0.03638	0.01386
S H 31	0.03694	0.03262	-0.02978	0.01771	-0.10223	-0.04970
S H 32	-0.00739	-0.00116	-0.11455	-0.06850	-0.04794	-0.04266
S H 33	0.02430	0.00694	0.05771	0.04623	-0.00381	-0.00341
S H 34	-0.00822	-0.00032	0.00098	-0.00606	-0.00226	-0.00263
S H 35	0.05280	-0.00637	0.00134	-0.02131	0.04474	0.01471

Mol. Orbital	55	56	57	58	59	60
Symmetry:	55 A	56 A	57 A	58 A	59 A	60 A
Eigenvalue	0.04158	0.04652	0.05973	0.07598	0.11094	0.11648

S C 1	-0.01477	-0.00514	0.00016	0.01788	0.03734	0.27161
Px C 1	0.03184	-0.00299	-0.00088	-0.01813	-0.01030	-0.01979
Py C 1	-0.36303	0.08304	0.01228	0.31361	0.21198	0.04516
Pz C 1	0.17622	-0.03593	-0.00581	-0.14902	-0.10276	-0.07015
S C 2	-0.00125	0.00455	0.00018	-0.02661	-0.04419	-0.24600
Px C 2	-0.01018	0.02541	0.00032	0.01198	0.01505	0.05013
Py C 2	0.03165	-0.46260	-0.00234	-0.19512	-0.18206	-0.06790

Pz C 2	-0.00633	0.20758	0.00073	0.10018	0.09288	0.06331
S C 3	0.01649	-0.00986	-0.00124	0.02085	0.03788	0.27499
Px C 3	-0.02760	-0.02610	0.00127	0.00447	-0.00892	-0.06493
Py C 3	0.30642	0.38869	-0.00829	-0.03123	0.11588	0.06290
Pz C 3	-0.15215	-0.17334	0.00469	0.01563	-0.04888	-0.06724
S C 4	-0.01714	0.01487	0.00221	0.02755	0.00617	-0.38342
Px C 4	0.02820	-0.02610	-0.00145	-0.01587	0.00758	0.05196
Py C 4	-0.32997	0.09275	0.01172	0.25778	-0.00716	-0.07461
Pz C 4	0.16961	-0.04770	-0.00620	-0.12921	-0.00855	0.03433
S C 5	0.00559	-0.03430	-0.00145	-0.04108	-0.00701	0.36709
Px C 5	-0.00795	0.07230	0.00047	-0.01310	-0.03020	0.03944
Py C 5	0.07302	-0.48954	0.00058	-0.04735	0.10892	0.06475
Pz C 5	-0.04099	0.25958	0.00086	0.03103	-0.05061	-0.00488
S C 6	0.00405	0.00940	0.00038	0.01412	-0.01165	-0.33908
Px C 6	-0.03124	-0.04513	0.00112	0.02438	0.01642	-0.05341
Py C 6	0.27873	0.36190	-0.01013	-0.19680	-0.18160	-0.05156
Pz C 6	-0.12773	-0.19033	0.00436	0.06984	0.07062	0.06588
S O 7	0.00001	0.00117	0.00006	-0.00240	-0.00740	-0.05893
Px O 7	-0.00426	0.00206	0.00013	0.00096	0.00009	0.00806
Py O 7	0.09227	-0.02047	-0.00307	-0.07163	-0.03962	0.03021
Pz O 7	-0.04826	0.00469	0.00140	0.03852	0.03301	0.10144
S O 12	0.00008	0.00910	0.00306	0.00481	-0.00083	-0.07494
Px O 12	0.00076	-0.02032	0.00010	0.00593	0.00740	-0.04548
Py O 12	-0.01830	0.13063	0.00229	0.01803	-0.02265	-0.07231
Pz O 12	0.01067	-0.05341	-0.00124	-0.00033	0.00874	-0.10573
S O 14	0.00379	-0.00120	0.00019	-0.00155	0.00466	-0.00938
Px O 14	0.04978	-0.00883	0.00230	-0.07054	0.09068	0.02316
Py O 14	0.11326	-0.02379	-0.00071	-0.12640	0.19191	-0.02471
Pz O 14	-0.02270	0.00361	-0.00401	0.01963	-0.04416	0.02574
S C 15	-0.01725	0.00443	0.00140	0.00947	-0.04355	0.13853
Px C 15	-0.08678	0.01687	0.00029	0.12875	-0.21462	-0.02528
Py C 15	-0.17944	0.03732	-0.00083	0.22803	-0.40713	0.05534
Pz C 15	0.03420	-0.00590	0.00055	-0.05254	0.09310	0.00084
S C 16	0.01716	-0.01230	0.00163	-0.01763	0.04774	-0.18898
Px C 16	0.12013	-0.03767	-0.00167	0.09308	0.20108	-0.04933
Py C 16	0.24161	-0.07458	0.00095	0.20523	0.39276	-0.04141
Pz C 16	-0.05732	0.01101	0.00156	-0.05373	-0.11855	-0.02145
S C 17	0.01260	0.00596	-0.00082	-0.01408	-0.02267	0.26492
Px C 17	-0.03575	0.02173	-0.00044	-0.15762	-0.12028	-0.02667
Py C 17	-0.05642	0.01938	-0.00410	-0.36242	-0.27188	0.08864
Pz C 17	0.01424	-0.00632	0.00210	0.08498	0.08152	0.03465
S C 18	0.00869	-0.00205	0.00280	-0.00125	0.02273	-0.11683
Px C 18	-0.18140	0.05236	0.00214	-0.21819	0.08234	-0.00660
Py C 18	-0.20318	0.05867	0.01000	-0.25624	0.09859	-0.01032
Pz C 18	0.07585	-0.02124	-0.00452	0.07989	-0.01574	-0.03939
S C 19	-0.00684	0.00162	-0.00201	0.00613	-0.02389	0.06753
Px C 19	0.12595	-0.03557	-0.31950	0.06221	0.06625	-0.02418
Py C 19	0.13913	-0.03975	-0.37770	0.07913	0.06396	0.01360
Pz C 19	-0.05272	0.01469	0.12634	-0.02480	-0.02695	0.01664

S C 20	0.00280	-0.00070	0.00345	-0.00593	0.01947	-0.04951
Px C 20	0.08401	-0.02228	0.29734	0.13059	-0.15548	0.01041
Py C 20	0.09338	-0.02501	0.34572	0.14643	-0.17589	0.00606
Pz C 20	-0.02598	0.00715	-0.11798	-0.05037	0.06633	-0.01660
S C 21	0.00748	-0.00124	-0.00848	0.00978	-0.01434	0.03223
Px C 21	-0.21143	0.05941	0.02764	-0.23564	0.18921	-0.00768
Py C 21	-0.24676	0.07016	0.02971	-0.27781	0.22851	-0.01042
Pz C 21	0.07079	-0.01981	-0.01078	0.07960	-0.06568	0.01015
S C 22	-0.00529	0.00003	0.01087	-0.00156	0.00489	-0.04450
Px C 22	0.06206	-0.02205	-0.30504	0.12288	-0.13372	0.00175
Py C 22	0.07792	-0.02737	-0.36754	0.15103	-0.16720	0.00966
Pz C 22	-0.02330	0.00738	0.13052	-0.04224	0.04966	-0.01054
S C 23	0.00171	0.00172	-0.01678	-0.00745	0.00157	0.06126
Px C 23	0.15433	-0.03901	0.32863	0.07618	0.03916	0.01572
Py C 23	0.16898	-0.04088	0.36183	0.08338	0.05159	-0.01507
Pz C 23	-0.06308	0.01683	-0.13660	-0.03451	-0.01301	0.01190
S C 24	0.01322	0.01040	0.03165	0.01370	-0.02487	0.07283
Px C 24	-0.01546	0.00466	-0.00639	0.00085	-0.02144	0.06074
Py C 24	-0.00369	0.01077	0.00489	-0.01110	-0.00065	-0.01520
Pz C 24	-0.01028	0.00973	-0.01765	0.00214	-0.00546	0.01474
S C 25	-0.01878	0.00052	0.00984	-0.01645	-0.03273	-0.04044
Px C 25	-0.00863	0.00254	-0.00749	-0.00176	0.00724	-0.00760
Py C 25	-0.00823	0.00329	-0.02740	-0.00585	-0.00643	0.01749
Pz C 25	-0.01235	-0.00194	0.01123	-0.01044	-0.00975	-0.00111
S O 26	0.00048	-0.00027	0.00022	-0.00052	0.00284	-0.00683
Px O 26	0.05573	-0.01545	-0.00929	0.05645	-0.04181	0.00398
Py O 26	0.06824	-0.01922	-0.00731	0.06958	-0.05014	-0.00138
Pz O 26	-0.02213	0.00579	0.00792	-0.02358	0.02032	-0.01027
S H 8	0.00094	-0.00141	-0.00014	0.01415	0.02465	0.14754
S H 13	-0.00074	-0.00860	-0.00254	-0.00182	-0.00019	0.04907
S H 9	-0.00456	0.00866	0.00072	-0.00263	-0.01774	-0.16098
S H 10	-0.00321	0.00131	0.00016	-0.00684	0.00472	0.18301
S H 11	0.00341	0.00010	-0.00013	0.00023	0.00379	0.03801
S H 27	0.00087	-0.00039	0.00200	-0.00197	0.00913	-0.02962
S H 28	-0.00420	0.00102	-0.00105	0.00172	-0.01046	0.03385
S H 29	0.00075	0.00004	-0.00333	-0.00074	-0.00353	0.02939
S H 30	-0.02530	0.00482	-0.03233	-0.02631	-0.02415	-0.02288
S H 31	0.03495	-0.01712	-0.01027	0.03185	0.07949	-0.03556
S H 32	-0.02974	0.00685	-0.08049	-0.01342	0.00595	0.01166
S H 33	0.02692	-0.00517	0.03721	0.02576	0.03219	0.02626
S H 34	-0.00266	0.00076	0.00244	-0.00170	-0.00113	0.00542
S H 35	-0.03612	0.01037	0.00005	0.02657	0.00730	-0.13908

Mol. Orbital	61	62	63	64	65	66
Symmetry:	61 A	62 A	63 A	64 A	65 A	66 A
Eigenvalue	0.12707	0.13606	0.14222	0.14968	0.15723	0.16205

S C 1	-0.14014	-0.11814	0.23591	-0.09535	0.32583	0.08474
Px C 1	0.02425	-0.04220	-0.01526	0.02778	0.03867	0.07925

Py C 1	-0.03675	0.28102	-0.06251	-0.01180	0.01307	0.02560
Pz C 1	0.03832	-0.13049	0.01320	0.01648	0.00804	0.02204
S C 2	0.07440	0.14118	-0.12514	0.00807	-0.25973	-0.18794
Px C 2	-0.04547	0.00385	0.07777	-0.04890	0.10921	-0.00217
Py C 2	0.06293	-0.30031	0.03150	0.03974	-0.05551	-0.01918
Pz C 2	-0.01647	0.12262	-0.05662	0.01734	-0.07256	0.00399
S C 3	-0.04472	-0.11466	-0.00910	0.07062	-0.08767	0.10379
Px C 3	0.01123	-0.01966	0.01360	-0.00075	0.01526	0.00883
Py C 3	-0.07470	0.31256	-0.00945	-0.05834	0.11976	0.06109
Pz C 3	0.01550	-0.17166	0.08906	-0.00939	0.13971	0.05568
S C 4	0.03448	0.04573	0.13091	-0.09394	0.33462	0.08991
Px C 4	-0.05845	0.03555	0.05471	-0.04287	-0.05058	-0.06989
Py C 4	0.09074	-0.36478	0.02399	0.07631	-0.09280	-0.07366
Pz C 4	0.01958	0.20741	-0.11377	-0.00889	0.03040	-0.01770
S C 5	-0.13642	-0.03069	0.05527	-0.02279	-0.23197	-0.16073
Px C 5	0.03078	-0.03351	-0.07570	0.05195	-0.11487	-0.01370
Py C 5	-0.04901	0.29737	-0.03527	-0.04605	0.10177	0.01954
Pz C 5	-0.00299	-0.17963	0.09368	-0.01635	0.06445	-0.02351
S C 6	0.16137	0.08225	-0.20247	0.10156	-0.12263	0.09421
Px C 6	0.02262	0.05029	-0.03930	0.00756	-0.02400	-0.01574
Py C 6	0.04437	-0.25266	0.01885	0.03364	-0.11703	-0.05234
Pz C 6	-0.02510	0.15663	-0.07325	0.00937	-0.16034	-0.07346
S O 7	0.03017	0.03014	-0.05279	0.01964	-0.07191	-0.02387
Px O 7	-0.00345	0.00326	0.00020	-0.00177	-0.01077	-0.01136
Py O 7	-0.01465	-0.07225	0.04883	-0.01285	0.04440	0.00831
Pz O 7	-0.05647	-0.01406	0.08023	-0.03684	0.10411	0.02493
S O 12	0.04192	0.00632	-0.01867	0.00674	0.07504	0.00951
Px O 12	0.01187	0.01361	0.00003	-0.00369	0.04746	0.03183
Py O 12	0.04226	-0.05485	-0.00979	0.01529	0.03015	0.01511
Pz O 12	0.04340	0.04425	-0.04203	0.01297	0.06156	0.04754
S O 14	-0.03150	0.00300	0.01679	-0.00504	-0.01382	-0.04478
Px O 14	0.08986	-0.01212	-0.02428	0.06989	0.02630	0.08366
Py O 14	-0.01478	-0.01181	0.05853	0.08852	-0.02314	-0.02736
Pz O 14	0.03225	0.01251	-0.01009	-0.01913	-0.00306	0.04448
S C 15	0.27644	-0.01420	-0.16061	0.04498	0.05543	0.29564
Px C 15	-0.09334	0.03169	0.01149	-0.16304	-0.01676	-0.03412
Py C 15	-0.02991	0.02548	-0.14460	-0.21625	0.03771	-0.03966
Pz C 15	-0.04442	-0.03991	-0.07086	0.10567	0.02965	-0.11550
S C 16	-0.24986	0.05953	0.34080	-0.12970	-0.13235	-0.01093
Px C 16	0.00500	-0.06915	0.02954	0.07049	0.04097	-0.13794
Py C 16	0.09455	-0.14463	0.04035	0.13741	-0.05054	0.09255
Pz C 16	0.05375	0.05464	-0.00048	-0.06751	0.09728	0.09159
S C 17	0.10121	-0.02761	-0.27743	0.13185	-0.10454	-0.11563
Px C 17	-0.04303	0.10848	0.00705	-0.05312	0.05512	0.00025
Py C 17	-0.07718	0.20953	-0.03420	-0.08853	0.01668	0.02780
Pz C 17	-0.06081	-0.05333	0.06492	0.01796	-0.14579	-0.04670
S C 18	-0.34475	-0.04290	-0.04692	0.02867	0.00942	-0.35885
Px C 18	0.03182	0.06390	0.15159	0.26022	0.04069	-0.07444
Py C 18	-0.01858	0.05632	0.12337	0.30018	-0.03820	0.05008

Pz C 18	-0.02836	0.00439	0.06876	-0.14263	-0.03345	-0.09410
S C 19	0.22243	0.04699	0.10003	-0.07161	-0.11912	0.22576
Px C 19	-0.04000	-0.07204	-0.10178	-0.21505	-0.00511	-0.04492
Py C 19	0.05593	-0.07762	-0.12902	-0.25182	0.01160	0.05107
Pz C 19	0.01503	0.02002	0.00253	0.11392	0.05177	0.07818
S C 20	-0.19706	-0.05443	-0.15406	0.12099	0.19674	-0.03514
Px C 20	0.01129	0.08815	0.14461	0.17182	-0.01710	-0.06869
Py C 20	-0.05136	0.07365	0.07293	0.23682	0.01943	0.04467
Pz C 20	-0.00684	-0.02414	-0.00629	-0.08690	-0.01378	-0.09772
S C 21	0.21139	0.07718	0.24217	-0.12448	-0.15998	-0.18801
Px C 21	0.01711	-0.07555	-0.09577	-0.18741	-0.04133	0.04121
Py C 21	0.05160	-0.07849	-0.07736	-0.21157	0.01500	-0.05685
Pz C 21	0.02099	0.03062	0.04424	0.04982	-0.00638	0.00936
S C 22	-0.27420	-0.08279	-0.25091	0.11060	0.07042	0.17502
Px C 22	-0.05590	0.05013	0.03720	0.19425	0.03071	0.02938
Py C 22	-0.01127	0.08489	0.12294	0.19176	-0.03213	-0.01948
Pz C 22	-0.03375	-0.02951	-0.02842	-0.09334	-0.07287	-0.04183
S C 23	0.32730	0.07853	0.20250	-0.04741	0.06518	-0.03544
Px C 23	0.04366	-0.06074	-0.10180	-0.21823	-0.04241	0.15624
Py C 23	-0.00825	-0.06824	-0.09479	-0.22799	0.03787	-0.12395
Pz C 23	0.00746	0.01101	-0.02707	0.12765	0.06979	0.06791
S C 24	0.21482	-0.02055	-0.20525	0.05413	0.29973	-0.28190
Px C 24	0.07340	-0.01490	-0.09294	0.04524	0.01839	0.02941
Py C 24	-0.01228	0.00546	0.04740	-0.01868	-0.00211	-0.03294
Pz C 24	-0.02515	-0.02377	-0.08031	0.03126	-0.02612	0.08488
S C 25	-0.24651	-0.03003	-0.07319	-0.03381	-0.21969	0.31673
Px C 25	-0.04304	-0.01793	-0.03913	0.00535	-0.00130	-0.01495
Py C 25	0.07879	0.02024	0.03182	-0.00883	0.01562	0.00394
Pz C 25	0.01462	0.02628	0.10692	-0.04255	-0.07327	0.06059
S O 26	-0.04543	-0.01716	-0.05398	0.02706	0.03604	0.04114
Px O 26	0.00803	0.01880	0.02947	0.03001	-0.00045	-0.00871
Py O 26	-0.03666	0.00668	-0.01430	0.05629	0.01539	0.03253
Pz O 26	-0.07189	-0.03446	-0.09721	0.02773	0.04982	0.07983
S H 8	-0.03690	-0.08000	0.06067	0.00128	0.16368	0.12171
S H 13	-0.02864	-0.00230	0.00672	-0.00255	-0.06212	0.01194
S H 9	0.04609	0.06817	-0.02100	-0.03193	0.06065	-0.06992
S H 10	-0.07884	-0.04363	0.10242	-0.05542	0.08366	-0.06508
S H 11	-0.01631	-0.02503	0.03049	-0.00815	0.04405	0.02179
S H 27	-0.12714	-0.03454	-0.08749	0.04523	0.07269	-0.11011
S H 28	0.11989	0.02754	0.07515	-0.07348	-0.12135	0.05088
S H 29	0.15430	0.04327	0.13158	-0.06968	-0.05447	-0.06719
S H 30	-0.10595	0.02303	0.07374	-0.01669	-0.14150	0.13607
S H 31	-0.06799	-0.01794	0.10240	0.00221	-0.15689	0.14756
S H 32	0.09339	0.02794	0.05883	0.06799	0.10948	-0.16600
S H 33	0.11286	-0.00705	0.00501	0.00408	0.09972	-0.14390
S H 34	0.02933	0.00999	0.03138	-0.01877	-0.02648	-0.01460
S H 35	-0.03699	-0.02119	0.16098	-0.06966	0.04646	0.13171

Mol. Orbital 67 68 69 70 71 72

Symmetry: 67 A 68 A 69 A 70 A 71 A 72 A
 Eigenvalue 0.16342 0.16749 0.18168 0.19536 0.21656 0.22646

S C 1	-0.02198	0.12248	0.00314	0.06885	0.01956	0.23458
Px C 1	-0.17680	-0.09934	-0.00930	0.03968	-0.02046	-0.17921
Py C 1	-0.04876	-0.03118	-0.00045	-0.00846	0.00380	0.03096
Pz C 1	-0.04536	-0.02310	-0.00142	0.00070	0.01016	0.11207
S C 2	0.33081	0.11225	0.01539	-0.10379	0.03376	0.26071
Px C 2	0.07621	0.10313	0.00599	0.02970	0.02052	0.22976
Py C 2	-0.00084	-0.02410	-0.00164	-0.04178	0.01030	0.10266
Pz C 2	-0.04320	-0.07858	0.00244	-0.12239	0.03059	0.19495
S C 3	-0.31089	-0.29927	-0.01110	-0.20739	0.02387	0.14855
Px C 3	-0.02646	-0.02464	-0.00240	-0.09768	0.02844	0.23233
Py C 3	-0.05268	0.00674	0.00346	0.00127	0.00771	-0.03658
Pz C 3	-0.07660	0.01690	-0.00665	0.05970	-0.01447	-0.11345
S C 4	0.02029	0.16960	0.01570	-0.00293	0.03611	0.08403
Px C 4	0.18302	0.07112	0.01696	-0.10743	0.01838	-0.14408
Py C 4	0.07590	0.05106	-0.00987	0.11278	-0.03545	-0.00915
Pz C 4	0.04152	0.09871	-0.00158	0.19809	-0.01203	0.01450
S C 5	0.25988	0.01469	0.01116	-0.18901	0.01180	-0.12764
Px C 5	-0.07605	-0.10116	-0.01668	0.04026	-0.03022	-0.02207
Py C 5	-0.01916	0.02912	-0.00208	0.02051	-0.00831	0.01517
Pz C 5	0.07148	0.07828	-0.00301	0.02646	-0.00470	0.02441
S C 6	-0.27513	-0.22335	-0.00959	-0.01601	0.00085	-0.00178
Px C 6	0.02402	0.01793	0.00049	0.03789	-0.01841	-0.11127
Py C 6	0.06192	-0.01490	0.00019	-0.04068	-0.00239	-0.08806
Pz C 6	0.08006	-0.04055	0.00169	-0.10340	-0.00033	-0.14328
S O 7	0.01505	-0.01775	-0.00120	0.00548	-0.01704	-0.17326
Px O 7	0.02009	0.00700	0.00072	-0.01515	0.00921	0.10161
Py O 7	0.00670	0.02178	0.00140	-0.00258	0.00984	0.09187
Pz O 7	0.00371	0.04114	0.00315	-0.00796	0.02126	0.19591
S O 12	-0.05867	0.00418	-0.01799	0.07797	-0.02878	0.02543
Px O 12	-0.03047	0.01284	0.00416	0.02976	0.00667	0.01258
Py O 12	-0.04526	-0.00485	-0.00605	0.05176	-0.01372	0.01139
Pz O 12	-0.09158	-0.00729	-0.00992	0.11504	-0.02394	0.02425
S O 14	-0.01842	-0.01227	-0.04724	0.03545	-0.04678	0.01575
Px O 14	0.03179	0.04867	0.08077	-0.06100	0.07415	-0.01978
Py O 14	-0.00418	-0.00429	-0.03296	0.03002	-0.04031	0.00755
Pz O 14	0.03915	-0.02639	0.04303	0.00757	0.01458	-0.01098
S C 15	0.11934	0.09986	0.20474	-0.12001	0.22164	-0.05034
Px C 15	-0.00597	-0.07108	-0.03014	0.01873	-0.02713	-0.00881
Py C 15	-0.03267	-0.02145	0.02205	0.01648	0.03836	0.01665
Pz C 15	-0.09657	0.09989	0.02559	-0.00102	0.07821	0.02873
S C 16	0.05296	-0.22228	-0.09398	-0.02181	-0.12366	-0.06197
Px C 16	-0.02433	0.02123	-0.06406	-0.09540	-0.16738	-0.00930
Py C 16	0.06349	0.07663	0.07355	-0.03180	0.06858	-0.01257
Pz C 16	0.04792	0.01929	0.05631	-0.22765	0.11334	-0.05107
S C 17	-0.06814	0.06358	-0.03585	0.40602	-0.07207	0.10296
Px C 17	-0.03807	-0.01161	-0.02602	0.11736	-0.04433	0.11355

Py C 17	-0.05601	-0.08462	-0.00667	-0.05501	0.02152	-0.05991
Pz C 17	0.01553	-0.10016	-0.02887	0.04881	-0.08776	-0.05640
S C 18	-0.24890	0.11482	0.01466	0.00193	0.08907	0.01612
Px C 18	0.02242	-0.06537	0.09711	0.03617	-0.01671	0.00233
Py C 18	-0.03559	0.12492	-0.12520	-0.02346	-0.06143	0.01609
Pz C 18	-0.02868	-0.07086	-0.14913	0.07366	-0.18202	0.05201
S C 19	0.03457	0.08943	-0.40583	0.00168	-0.20748	0.05815
Px C 19	-0.02502	-0.01251	-0.05944	0.00684	-0.06903	0.03573
Py C 19	0.06378	-0.07760	0.05484	0.01169	0.02367	-0.01792
Pz C 19	0.11718	-0.10003	0.03125	0.03105	-0.11418	0.03586
S C 20	0.21024	-0.29449	0.24183	0.07149	-0.14401	0.05448
Px C 20	-0.06319	0.04106	0.08023	0.00595	0.01475	0.01005
Py C 20	0.02876	0.01608	-0.02705	-0.01688	0.03477	-0.02608
Pz C 20	-0.07665	0.02849	0.12492	-0.01623	0.13953	-0.04642
S C 21	-0.26954	0.19512	0.07778	-0.00896	0.08055	0.00039
Px C 21	-0.02605	0.06040	-0.14352	-0.02791	0.07110	-0.02637
Py C 21	0.01058	-0.07897	0.12667	0.03133	-0.05759	0.02204
Pz C 21	-0.00259	0.01081	0.01617	-0.00413	-0.00647	-0.00921
S C 22	0.11423	0.03401	-0.37089	-0.06058	0.09502	-0.02934
Px C 22	0.03419	-0.00566	0.03848	-0.00113	-0.02957	0.00055
Py C 22	-0.07020	0.09938	-0.02981	-0.02433	0.03549	-0.00524
Pz C 22	-0.12859	0.14097	0.01625	-0.02114	0.07012	-0.00477
S C 23	0.16544	-0.30044	0.11390	0.09479	-0.12577	0.02444
Px C 23	0.06429	-0.01449	-0.00310	0.00023	-0.05218	-0.00332
Py C 23	-0.00646	-0.09244	-0.06060	0.03372	0.11719	-0.00036
Pz C 23	0.09816	-0.04287	-0.16353	-0.03462	0.06053	-0.02663
S C 24	-0.06738	0.10138	-0.07215	-0.30864	-0.24872	-0.04268
Px C 24	-0.00650	0.06225	0.04449	0.10454	0.19952	0.06422
Py C 24	0.01384	-0.04330	-0.01385	-0.01522	0.02093	-0.01932
Pz C 24	-0.03557	0.12857	0.10534	-0.03924	-0.15682	0.01411
S C 25	-0.09174	0.27253	0.26922	-0.02494	-0.27154	0.02562
Px C 25	-0.02634	0.04258	-0.05247	-0.00736	0.06832	-0.00573
Py C 25	0.02329	-0.03349	0.07120	0.00403	-0.22426	0.02990
Pz C 25	0.05700	-0.11941	0.03428	0.13261	0.11044	0.02279
S O 26	0.05895	-0.04263	0.00363	-0.00075	-0.00901	-0.00964
Px O 26	-0.00331	-0.00291	0.01549	0.00486	-0.01369	0.00902
Py O 26	0.02727	-0.00491	-0.01811	-0.00650	0.00548	-0.00978
Pz O 26	0.09260	-0.05694	-0.01421	-0.00316	-0.01902	-0.00967
S H 8	-0.22394	-0.07017	-0.01417	0.14770	-0.05684	-0.44575
S H 13	0.02798	-0.01213	0.02321	-0.08241	0.03217	-0.02291
S H 9	0.19859	0.21890	0.00532	0.25050	-0.04713	-0.30842
S H 10	0.17291	0.15998	0.00145	0.08664	-0.02747	-0.11478
S H 11	-0.02750	-0.00291	0.00016	-0.01792	0.02046	0.21866
S H 27	-0.01748	-0.03674	0.32054	-0.01838	0.23379	-0.08266
S H 28	-0.12251	0.19727	-0.13078	-0.06630	0.16831	-0.07694
S H 29	-0.06536	-0.00377	0.30064	0.03486	-0.06923	0.01243
S H 30	0.02624	-0.05349	-0.01400	0.24751	0.23691	0.05454
S H 31	0.04283	-0.04409	0.05813	0.21707	0.24504	0.04681
S H 32	0.04107	-0.13496	-0.17305	0.00605	0.26767	-0.03495

S H 33	0.06069	-0.14655	-0.20402	0.05973	0.25621	-0.00748
S H 34	-0.03488	0.03164	-0.02409	0.00055	-0.00486	0.01392
S H 35	0.03020	-0.05831	0.05231	-0.35641	0.11109	-0.14306

Mol. Orbital	73	74	75	76	77	78
Symmetry:	73 A	74 A	75 A	76 A	77 A	78 A
Eigenvalue	0.23739	0.23937	0.25174	0.26020	0.26882	0.27383

S C 1	0.19730	-0.07516	0.03222	-0.05788	0.01227	-0.00822
Px C 1	0.09685	0.01661	-0.01488	0.04221	0.03855	-0.00292
Py C 1	0.07740	-0.01635	0.00675	-0.01956	-0.01893	0.00156
Pz C 1	0.16198	-0.04488	0.02013	-0.05274	-0.04188	0.00405
S C 2	-0.07572	-0.02563	0.01569	-0.03573	-0.01790	-0.00048
Px C 2	0.15139	-0.06915	0.03406	-0.07046	-0.00132	-0.00759
Py C 2	-0.05177	-0.00423	0.00116	0.00042	0.00169	-0.00114
Pz C 2	-0.13047	0.00634	-0.00523	0.01198	-0.00194	-0.00036
S C 3	-0.20684	0.02409	-0.01178	0.02854	0.00989	-0.00116
Px C 3	-0.17167	0.02183	-0.03843	0.15823	0.13334	-0.00856
Py C 3	0.00397	0.02154	-0.01889	0.04858	0.01963	0.00108
Pz C 3	0.03347	0.02525	-0.02636	0.07934	0.04325	0.00091
S C 4	-0.05997	0.05909	-0.06797	0.21828	0.14452	-0.00478
Px C 4	0.19113	0.03844	-0.03020	0.03352	-0.03762	0.01341
Py C 4	0.05722	-0.03713	0.01772	-0.01043	0.02929	-0.00229
Pz C 4	0.07029	-0.03108	0.01120	-0.00249	0.01627	-0.00384
S C 5	0.18877	0.03571	-0.03490	0.06775	0.00644	0.00556
Px C 5	0.04304	-0.06543	0.06994	-0.22274	-0.14533	0.00305
Py C 5	-0.10119	-0.00560	0.01629	-0.05660	-0.04645	-0.00573
Pz C 5	-0.17127	0.00617	0.00987	-0.03600	-0.02991	0.00797
S C 6	0.26414	-0.03365	0.00606	-0.00974	0.00216	-0.00085
Px C 6	-0.36532	0.05265	-0.00456	-0.00739	-0.03656	0.00345
Py C 6	-0.01116	0.02995	-0.02080	0.04951	0.01629	0.00515
Pz C 6	0.05831	0.04722	-0.03945	0.09426	0.03053	0.00520
S O 7	-0.13870	0.05164	-0.02603	0.07623	0.08110	-0.00969
Px O 7	0.06673	-0.03160	0.02206	-0.08644	-0.13274	0.01956
Py O 7	0.06918	-0.02471	0.01039	-0.02373	-0.01344	0.00068
Pz O 7	0.14921	-0.05258	0.02168	-0.04787	-0.02310	0.00029
S O 12	-0.13170	-0.04316	0.05803	-0.19065	-0.14559	-0.00244
Px O 12	-0.00337	0.02050	-0.03418	0.15088	0.16113	0.00237
Py O 12	-0.07083	-0.01732	0.02247	-0.06327	-0.03914	-0.01147
Pz O 12	-0.15695	-0.04209	0.06226	-0.20732	-0.16024	-0.00316
S O 14	0.00110	-0.00698	-0.01358	0.03005	-0.01610	0.00702
Px O 14	-0.00069	0.02155	0.01770	-0.04550	0.03413	-0.01141
Py O 14	-0.00049	-0.02329	0.00022	0.01494	-0.00159	0.00210
Pz O 14	-0.00517	-0.03065	0.03731	-0.03711	0.04940	-0.01353
S C 15	-0.00412	0.04336	0.05478	-0.11955	0.09037	-0.02522
Px C 15	-0.00583	-0.03510	0.02457	-0.04817	0.04975	-0.01985
Py C 15	0.00517	0.05430	-0.03415	0.06323	-0.07922	0.02492
Pz C 15	0.01895	0.13815	-0.09281	0.11052	-0.15831	0.05288
S C 16	-0.02051	-0.16913	0.11303	-0.16274	0.18012	-0.05115

Px C 16	0.01050	-0.02294	-0.01659	0.04113	-0.07950	0.03013
Py C 16	0.00275	0.01788	0.01730	-0.02472	0.04441	0.05270
Pz C 16	-0.00005	0.05537	-0.00595	-0.04262	0.00153	0.00332
S C 17	-0.00101	-0.07074	0.02403	0.02648	0.07380	-0.01058
Px C 17	-0.04170	-0.08351	0.03061	0.09891	0.32784	-0.04270
Py C 17	0.00535	0.01713	0.00231	-0.08177	-0.12997	-0.01077
Pz C 17	-0.00806	-0.12192	0.09958	-0.17146	0.07953	-0.01725
S C 18	0.01496	0.09414	-0.13502	0.06816	-0.13420	0.03660
Px C 18	-0.00826	-0.09229	0.07819	0.15383	-0.10489	0.02761
Py C 18	0.00865	0.07185	-0.09545	-0.07829	0.04681	-0.01993
Pz C 18	0.00510	-0.00948	-0.07136	0.14403	-0.11163	0.04521
S C 19	0.02223	0.16537	-0.16236	-0.04125	-0.00946	0.01148
Px C 19	0.02161	0.16832	-0.11233	-0.00512	-0.06685	0.02852
Py C 19	-0.01143	-0.07919	0.09703	-0.02773	0.08102	-0.02830
Pz C 19	0.01846	0.17231	-0.00172	-0.08822	0.06604	-0.01710
S C 20	0.02861	0.26183	0.01686	-0.08710	0.05661	-0.01211
Px C 20	0.01546	0.15968	0.16751	-0.04083	0.05586	-0.02264
Py C 20	-0.02131	-0.20240	-0.10735	0.04995	-0.04615	0.01455
Pz C 20	-0.01966	-0.15514	0.13274	0.04070	0.00902	-0.01186
S C 21	0.01755	0.18849	0.26415	-0.03176	0.05992	-0.02487
Px C 21	-0.01335	-0.12448	0.04337	0.07252	-0.04446	0.00926
Py C 21	0.00902	0.08343	-0.07627	-0.06040	0.03005	0.00532
Pz C 21	-0.01348	-0.13364	-0.18199	0.00092	-0.02623	0.01824
S C 22	-0.00431	-0.03338	0.22712	0.07722	-0.02157	-0.00854
Px C 22	-0.00770	-0.07605	-0.28470	-0.10645	0.05003	-0.01575
Py C 22	0.00834	0.08892	0.21598	0.01790	0.01634	-0.03027
Pz C 22	0.00821	0.11362	-0.05473	-0.20702	0.16865	-0.02957
S C 23	-0.00678	-0.10406	0.10278	0.25434	-0.18711	0.05310
Px C 23	-0.00584	-0.02195	0.10733	-0.02753	0.07067	0.03918
Py C 23	0.00357	0.02152	-0.03388	0.04430	-0.06487	0.05540
Pz C 23	-0.00706	-0.05273	0.15848	0.02935	0.01100	-0.01026
S C 24	0.00980	-0.06600	0.02254	-0.02202	0.01402	-0.01263
Px C 24	0.01078	0.17008	-0.11339	0.18340	-0.22616	0.02730
Py C 24	0.00921	-0.01094	-0.00458	-0.00866	-0.06436	-0.42418
Pz C 24	0.00834	-0.01163	-0.00926	0.05240	-0.03728	-0.11333
S C 25	-0.00615	-0.01750	0.03157	0.03480	-0.01835	0.00970
Px C 25	0.00463	0.01711	-0.10208	-0.08561	0.07426	-0.51098
Py C 25	-0.00769	-0.05742	0.11231	0.24980	-0.21963	-0.15531
Pz C 25	0.01133	0.03228	-0.01598	0.09848	-0.05237	-0.07932
S O 26	-0.01419	-0.13989	-0.18119	-0.00034	-0.02337	0.01940
Px O 26	0.00871	0.08377	0.09873	0.00240	0.01192	-0.01482
Py O 26	-0.01058	-0.10267	-0.11980	-0.00060	-0.01472	0.01311
Pz O 26	-0.01498	-0.14735	-0.17857	0.00440	-0.02347	0.01328
S H 8	0.03385	0.05094	-0.02146	0.04013	0.00693	0.00416
S H 13	0.16363	0.06335	-0.09458	0.34874	0.31340	0.00591
S H 9	0.23120	-0.02512	0.03329	-0.12658	-0.10232	0.00791
S H 10	-0.49094	0.05417	0.00671	-0.04180	-0.05076	0.00047
S H 11	0.17607	-0.06886	0.04056	-0.14194	-0.19509	0.02736
S H 27	-0.04052	-0.31786	0.17654	0.03555	0.06081	-0.02933

S H 28	-0.04750	-0.43070	-0.10186	0.09858	-0.06356	0.01681
S H 29	-0.00793	-0.06773	-0.43342	-0.18965	0.09736	0.00454
S H 30	-0.02442	0.09040	-0.04208	0.02014	-0.00972	0.34257
S H 31	-0.00449	0.11744	-0.07026	0.10044	-0.19965	-0.27396
S H 32	0.00629	0.03935	-0.05036	-0.17261	0.15302	0.34384
S H 33	0.01225	0.04506	-0.10975	-0.06209	0.06253	-0.40756
S H 34	0.01756	0.17095	0.22662	0.00908	0.02455	-0.02935
S H 35	0.02108	0.12801	-0.04960	-0.08646	-0.32112	0.03283

Mol. Orbital	79	80	81	82	83	84
Symmetry:	79 A	80 A	81 A	82 A	83 A	84 A
Eigenvalue	0.27596	0.27674	0.28570	0.29242	0.31497	0.33624

S C 1	-0.21881	0.05857	-0.07523	0.00137	-0.01030	0.00153
Px C 1	-0.06532	0.01035	0.05093	-0.00085	-0.00238	-0.02653
Py C 1	0.04566	-0.01152	0.00183	0.00009	-0.00115	0.00454
Pz C 1	0.08361	-0.01847	-0.01863	0.00061	-0.00389	0.01400
S C 2	-0.02451	0.01102	-0.04832	0.00076	0.00223	0.02346
Px C 2	-0.22371	0.06310	-0.11089	0.00216	-0.02999	-0.04962
Py C 2	-0.04041	0.01275	-0.02730	0.00040	-0.01220	-0.04596
Pz C 2	-0.05875	0.02106	-0.04138	0.00041	-0.02075	-0.09357
S C 3	0.00296	-0.00093	-0.00491	0.00014	-0.01713	-0.04911
Px C 3	0.01908	-0.02760	0.19290	-0.00443	0.12026	0.19436
Py C 3	0.03136	-0.01121	0.06513	-0.00160	0.02518	0.01530
Pz C 3	0.06770	-0.02658	0.11395	-0.00237	0.02559	-0.00849
S C 4	0.06917	-0.04058	0.19498	-0.00406	0.05615	0.04271
Px C 4	-0.00003	0.00719	0.17744	-0.00462	0.02772	0.03286
Py C 4	-0.00267	-0.00411	-0.01517	0.00050	0.02925	0.05509
Pz C 4	-0.00833	0.00301	-0.06265	0.00057	0.08563	0.12884
S C 5	0.00225	-0.01091	0.25314	-0.00565	0.03165	0.02482
Px C 5	-0.09336	0.04203	-0.08657	0.00159	-0.05654	-0.03015
Py C 5	-0.01283	0.00100	0.00705	-0.00051	-0.00671	-0.00601
Pz C 5	0.00303	0.00627	0.07399	-0.00185	0.00138	-0.00664
S C 6	-0.02085	0.00359	-0.00183	0.00034	-0.00657	-0.00596
Px C 6	0.22883	-0.05013	-0.18325	0.00426	-0.02909	-0.02862
Py C 6	0.06324	-0.01942	0.09247	-0.00184	0.01330	0.00141
Pz C 6	0.07611	-0.03231	0.24081	-0.00505	0.03595	0.01092
S O 7	-0.21390	0.04897	0.00913	-0.00037	0.00233	-0.00267
Px O 7	0.45220	-0.10788	0.02705	-0.00022	0.00062	-0.00916
Py O 7	0.00520	0.00011	-0.01077	0.00022	-0.00069	0.00614
Pz O 7	-0.01064	0.00527	-0.02479	0.00051	-0.00170	0.01362
S O 12	-0.06733	0.01571	0.13217	-0.00397	-0.00414	0.01758
Px O 12	0.08247	-0.00560	-0.37998	0.01055	-0.04025	-0.08492
Py O 12	-0.01425	-0.00431	-0.05513	0.00120	-0.01801	-0.01549
Pz O 12	-0.06383	0.01956	0.07625	-0.00325	-0.01402	0.02477
S O 14	0.00120	0.00849	-0.00335	-0.00248	0.08346	-0.01152
Px O 14	-0.00167	-0.02149	0.01640	0.00469	-0.16694	0.01879
Py O 14	0.00365	0.01217	-0.00750	-0.00197	0.08237	-0.00894
Pz O 14	0.00310	-0.01433	0.00789	0.00390	-0.06063	0.00100

S C 15	0.00385	-0.01916	0.03021	0.01207	-0.25282	0.00942
Px C 15	0.00072	-0.02256	0.00015	0.00254	-0.06071	-0.00286
Py C 15	-0.01050	0.00286	0.00119	-0.00181	0.00030	0.01376
Pz C 15	-0.01941	0.01547	-0.00071	-0.00493	-0.16490	0.08961
S C 16	0.01482	-0.03628	-0.00432	0.00551	-0.11734	-0.05543
Px C 16	-0.00995	0.02350	-0.02930	-0.00451	0.23739	-0.12610
Py C 16	0.01505	0.04089	0.03161	0.00231	-0.17149	0.03050
Pz C 16	-0.00095	0.00825	0.06833	0.00349	-0.16238	-0.15235
S C 17	0.00434	-0.02456	-0.02888	0.00017	0.04265	0.07324
Px C 17	0.06061	-0.10853	0.26411	0.00126	-0.20650	-0.14584
Py C 17	-0.03035	0.02518	-0.15694	0.00158	0.05807	0.03502
Pz C 17	-0.01170	-0.02766	-0.07241	0.00615	-0.15284	-0.09649
S C 18	-0.02194	-0.00241	-0.00114	-0.02193	-0.25358	0.04403
Px C 18	-0.00601	0.01930	-0.00526	-0.00464	-0.00954	0.04490
Py C 18	0.00686	0.00660	0.00363	-0.00183	0.08487	-0.03863
Pz C 18	-0.00911	0.00548	-0.01073	-0.01727	0.21712	0.03976
S C 19	-0.00681	-0.01531	0.00289	-0.00004	0.02938	-0.01030
Px C 19	-0.02099	-0.02947	0.00511	0.00824	-0.32230	0.04408
Py C 19	0.01916	0.01960	-0.00406	0.01239	0.27340	-0.03682
Pz C 19	0.00780	0.00204	0.00312	0.05943	0.00842	-0.00911
S C 20	0.00619	0.00268	0.00209	0.02086	0.01179	-0.00493
Px C 20	0.01029	0.01135	0.00170	0.17284	0.07163	-0.01699
Py C 20	-0.00651	-0.00455	-0.00228	-0.15102	-0.07139	0.01726
Pz C 20	0.00568	0.00932	-0.00297	-0.00699	-0.03311	0.00962
S C 21	0.01094	0.01164	0.00170	0.20317	0.03657	-0.00931
Px C 21	-0.00507	-0.00288	-0.00172	0.05274	-0.01584	0.00777
Py C 21	0.00111	-0.00367	0.00255	0.00476	0.01068	-0.00115
Pz C 21	-0.00689	-0.00922	0.00348	0.13811	-0.00826	0.02350
S C 22	-0.00152	-0.00454	-0.00130	0.01472	0.00606	-0.02917
Px C 22	0.00950	0.01906	0.00554	-0.18505	0.03927	-0.11025
Py C 22	0.00523	0.00576	-0.00052	0.15554	0.01199	0.04109
Pz C 22	0.02438	0.02192	0.01048	0.00858	0.13658	-0.16193
S C 23	-0.01981	0.00253	-0.00859	0.00106	-0.08789	0.08257
Px C 23	-0.00008	-0.04011	-0.00365	0.02933	0.19381	0.00790
Py C 23	-0.01331	-0.00679	0.00105	-0.01897	-0.15523	-0.05291
Pz C 23	0.00266	0.00106	0.00746	0.02114	0.03015	-0.15097
S C 24	-0.00015	-0.00275	-0.00051	-0.00051	0.04116	-0.11355
Px C 24	-0.05484	-0.09168	0.05227	-0.00133	0.20192	-0.29957
Py C 24	-0.12095	-0.50700	-0.03727	0.00238	-0.01111	-0.09075
Pz C 24	-0.03238	-0.15047	-0.06020	-0.01549	0.05361	0.42783
S C 25	-0.00142	0.00078	0.00035	0.00141	0.03703	0.09910
Px C 25	0.11789	0.36209	0.02019	0.01081	0.04850	0.05804
Py C 25	0.03788	0.25042	0.05992	0.02325	-0.16985	-0.29571
Pz C 25	0.02823	0.09602	-0.05201	-0.00444	-0.08872	0.40927
S O 26	-0.00653	-0.00872	0.00549	0.24745	-0.00894	0.00536
Px O 26	0.00446	0.00625	-0.00747	-0.39426	0.00364	0.00658
Py O 26	-0.00435	-0.00573	0.00528	0.25656	-0.00386	-0.00178
Pz O 26	-0.00492	-0.00631	-0.00073	-0.12397	-0.00576	0.01246
S H 8	0.15064	-0.04647	0.08998	-0.00138	0.02180	0.06615

S H 13	0.15271	-0.02093	-0.51114	0.01442	-0.03860	-0.09745
S H 9	0.00776	0.01427	-0.13451	0.00307	-0.07685	-0.11868
S H 10	0.13182	-0.02526	-0.15460	0.00317	-0.02513	-0.01736
S H 11	0.62781	-0.14845	0.02006	0.00010	-0.00231	-0.01226
S H 27	0.02152	0.03236	-0.00703	-0.03395	0.27557	-0.03322
S H 28	-0.00681	-0.00345	-0.00372	-0.14739	-0.06295	0.01735
S H 29	0.01197	0.01435	0.00774	-0.13711	0.07015	-0.11133
S H 30	0.07308	0.36667	0.08605	0.00319	0.06238	-0.15918
S H 31	-0.10551	-0.33520	0.02457	0.00326	0.07486	-0.20364
S H 32	-0.06653	-0.30147	-0.05492	-0.02169	0.07508	0.17900
S H 33	0.09438	0.27699	-0.00688	0.00153	0.04223	0.14991
S H 34	0.00903	0.01271	-0.01334	-0.69058	0.01098	0.00344
S H 35	-0.05126	0.10155	-0.22395	-0.00117	0.16020	0.10299

Mol. Orbital	85	86	87	88	89	90
Symmetry:	85 A	86 A	87 A	88 A	89 A	90 A
Eigenvalue	0.34795	0.37118	0.39207	0.39829	0.40978	0.44342

S C 1	0.03975	0.01575	0.02313	-0.04099	-0.01755	-0.00129
Px C 1	-0.12021	-0.05471	-0.18393	-0.18972	0.14266	-0.08821
Py C 1	0.03705	0.01898	0.03436	-0.17061	-0.06680	0.02562
Pz C 1	0.10204	0.05059	0.10566	-0.32087	-0.16395	0.06750
S C 2	0.10824	0.04104	0.10468	0.05327	-0.07161	0.01800
Px C 2	-0.13242	-0.04262	-0.14575	-0.17452	0.11557	-0.08063
Py C 2	-0.17750	-0.05329	-0.10771	-0.01904	0.06353	0.00129
Pz C 2	-0.37626	-0.11315	-0.22156	-0.01987	0.12689	0.01288
S C 3	-0.14820	-0.02565	-0.00595	0.02863	-0.01888	0.01933
Px C 3	0.45053	0.04775	-0.03580	-0.03763	0.08094	-0.03683
Py C 3	-0.03742	-0.03537	-0.10608	-0.02759	0.07437	0.00116
Pz C 3	-0.16298	-0.08431	-0.21851	-0.05081	0.14421	0.00887
S C 4	-0.02987	-0.03849	-0.08639	-0.00579	0.03882	0.00702
Px C 4	0.01170	0.01267	0.00497	-0.13048	-0.02390	0.03276
Py C 4	0.13833	-0.00648	-0.09933	-0.03451	0.10360	-0.02728
Pz C 4	0.26566	-0.02213	-0.21462	-0.04139	0.21250	-0.04835
S C 5	-0.02261	-0.01278	-0.03061	-0.05154	0.00428	0.00474
Px C 5	0.04007	0.06008	0.15077	0.03463	-0.08122	0.02267
Py C 5	-0.01902	0.00174	0.04337	0.21981	0.00412	0.00435
Pz C 5	-0.04988	-0.01342	0.04729	0.39940	0.02548	-0.00262
S C 6	0.00968	0.00790	-0.00866	-0.19005	-0.02250	0.00142
Px C 6	-0.01499	0.01233	-0.03873	-0.49615	-0.05197	0.00415
Py C 6	-0.03663	-0.01856	-0.03799	-0.02123	0.01896	-0.00727
Pz C 6	-0.07386	-0.04231	-0.07052	0.08836	0.05452	-0.01530
S O 7	-0.02576	-0.01314	-0.03063	0.06223	0.04192	-0.01903
Px O 7	-0.05350	-0.02637	-0.05979	0.12875	0.08368	-0.03841
Py O 7	0.03637	0.01717	0.04107	-0.06507	-0.05221	0.02352
Pz O 7	0.08248	0.03922	0.09329	-0.15485	-0.12008	0.05418
S O 12	-0.00749	0.00638	0.02560	0.08125	-0.00601	0.00371
Px O 12	0.02295	0.01667	0.08481	0.23211	0.00499	0.00161
Py O 12	0.00164	0.01121	0.04302	0.11136	-0.00662	0.00401

Pz O 12	-0.01464	0.01249	0.04945	0.12333	-0.02306	0.00004
S O 14	-0.02097	-0.03796	0.03132	-0.00485	-0.05443	-0.01235
Px O 14	0.03110	0.06743	-0.04507	0.00618	0.08739	0.01924
Py O 14	-0.01383	-0.03508	0.02011	-0.00281	-0.04096	-0.01197
Pz O 14	0.02431	0.01044	-0.02722	0.00393	0.04327	-0.00437
S C 15	0.05028	0.06465	-0.03740	0.00418	0.06012	-0.01047
Px C 15	0.05110	0.02550	-0.08457	0.01412	0.11526	-0.04542
Py C 15	-0.03952	0.02346	0.06032	-0.01042	-0.05269	0.10962
Pz C 15	-0.06080	0.18586	0.04918	-0.00977	0.03734	0.34356
S C 16	0.06246	0.01854	-0.02451	-0.00256	0.05762	-0.03564
Px C 16	-0.00046	-0.13031	0.12370	-0.02322	-0.10832	-0.37328
Py C 16	-0.00805	0.09481	0.00820	-0.00439	0.01530	0.15971
Pz C 16	-0.03770	0.09419	0.24927	-0.05649	-0.11126	-0.06584
S C 17	0.06484	-0.03178	-0.13160	0.02563	0.09199	0.02168
Px C 17	-0.18538	0.05039	0.19766	-0.05583	-0.15616	-0.02938
Py C 17	0.09867	-0.01201	-0.07145	0.01561	0.08214	-0.01831
Pz C 17	0.10673	0.05740	0.08499	-0.02371	0.03733	-0.12928
S C 18	0.01920	0.08892	-0.01797	0.00198	0.02956	-0.00563
Px C 18	-0.02312	-0.04142	0.01770	-0.00007	-0.06463	0.07072
Py C 18	-0.01760	0.07141	0.01910	-0.00627	0.05756	0.05219
Pz C 18	-0.12423	0.11089	0.10246	-0.01816	-0.00401	0.33580
S C 19	-0.03318	0.14021	0.00715	-0.00345	0.02875	0.06778
Px C 19	0.09540	-0.26196	-0.00494	0.00372	-0.02604	-0.12139
Py C 19	-0.06413	0.10151	0.02060	-0.00489	0.01015	0.10476
Pz C 19	0.05374	-0.36787	0.05008	-0.00544	-0.03380	0.00470
S C 20	0.01833	-0.15104	0.04384	-0.00759	0.01294	0.07596
Px C 20	-0.01987	0.17760	-0.10563	0.02124	-0.08491	-0.20813
Py C 20	0.04017	-0.29143	0.09874	-0.01782	0.04911	0.16232
Pz C 20	0.06882	-0.41228	0.02174	0.00175	-0.07355	-0.04757
S C 21	0.01133	-0.04999	-0.02859	0.00677	-0.04509	0.00413
Px C 21	-0.00978	0.13932	-0.11347	0.02453	-0.11687	-0.20215
Py C 21	-0.00148	-0.06675	0.12653	-0.02906	0.17202	0.08203
Pz C 21	-0.03705	0.18137	0.10979	-0.02959	0.25759	-0.31523
S C 22	0.01877	0.00284	-0.11065	0.02447	-0.14455	0.01664
Px C 22	0.04399	0.05574	-0.22814	0.04892	-0.27656	0.02690
Py C 22	-0.01494	-0.07383	0.13671	-0.03002	0.17336	0.00949
Pz C 22	0.06861	-0.08430	-0.15851	0.03138	-0.16631	0.09867
S C 23	-0.02790	0.02563	0.00770	0.00061	-0.02114	0.00609
Px C 23	-0.04516	-0.10550	0.10047	-0.01718	0.00191	0.11153
Py C 23	0.06655	0.07935	-0.18479	0.03506	-0.10901	-0.08358
Pz C 23	0.08438	-0.03293	-0.25579	0.05248	-0.26775	0.06552
S C 24	0.02623	-0.01774	0.05126	-0.01547	0.02176	-0.05113
Px C 24	0.00753	-0.07874	0.18296	-0.03705	-0.06454	-0.24383
Py C 24	0.05458	0.02821	-0.05229	0.01167	0.07366	0.11637
Pz C 24	-0.18218	-0.03430	0.00199	0.02199	-0.28008	-0.18907
S C 25	-0.05450	-0.02262	0.06083	-0.00741	-0.01313	-0.02368
Px C 25	-0.04872	-0.03994	0.13951	-0.02690	0.08556	0.00937
Py C 25	0.15194	0.06912	-0.18135	0.02776	-0.03464	0.02621
Pz C 25	-0.14009	0.01527	-0.08666	0.03207	-0.28575	-0.15293

S O 26	-0.00625	0.03288	0.02439	-0.00652	0.05550	-0.06199
Px O 26	-0.01200	0.04415	0.03949	-0.00981	0.07626	-0.08425
Py O 26	0.00177	0.00329	-0.00962	0.00196	-0.01006	0.00309
Pz O 26	-0.02705	0.13451	0.07964	-0.02130	0.18348	-0.22740
S H 8	0.23983	0.07118	0.15965	0.08642	-0.09700	0.01877
S H 13	0.02932	0.01228	0.05414	0.11323	0.00616	0.00160
S H 9	-0.27820	-0.03371	0.00248	0.02626	-0.03090	0.02117
S H 10	-0.00790	0.01074	-0.01688	-0.27256	-0.02852	0.00069
S H 11	-0.05468	-0.02453	-0.05921	0.07774	0.07193	-0.03293
S H 27	-0.07913	0.23195	0.00038	-0.00262	0.02478	0.07585
S H 28	0.04322	-0.29907	0.08366	-0.01431	0.03329	0.09591
S H 29	0.03980	0.02970	-0.17173	0.03605	-0.19981	0.02148
S H 30	0.02762	-0.03253	0.06845	-0.01443	0.04458	-0.04873
S H 31	0.04140	-0.01345	0.04488	-0.00224	0.01791	-0.02891
S H 32	-0.07522	-0.02135	0.04380	-0.00465	-0.01522	-0.01663
S H 33	-0.07726	-0.03146	0.07541	-0.01049	-0.02635	-0.03493
S H 34	-0.01648	0.07814	0.03368	-0.00907	0.08060	-0.11904
S H 35	0.10531	-0.03443	-0.12533	0.03732	0.08703	0.03161

Mol. Orbital	91	92	93	94	95	96
Symmetry:	91 A	92 A	93 A	94 A	95 A	96 A
Eigenvalue	0.45772	0.46273	0.47521	0.48554	0.48834	0.50892

S C 1	-0.01900	-0.00644	-0.00226	0.00732	-0.01624	-0.02127
Px C 1	-0.37606	-0.13078	0.30779	-0.07475	0.12785	-0.04062
Py C 1	0.10099	0.02070	0.10652	-0.06806	0.13275	0.07858
Pz C 1	0.26908	0.06408	0.16442	-0.12558	0.24799	0.16547
S C 2	0.05794	0.01329	0.01388	0.01346	-0.02966	-0.02634
Px C 2	-0.35428	-0.12211	0.26062	-0.04722	0.07362	-0.06936
Py C 2	0.02938	0.01823	-0.08435	-0.00231	0.01279	0.04623
Pz C 2	0.11006	0.05591	-0.21899	0.00099	0.01886	0.11167
S C 3	0.11118	0.03091	0.00508	0.01159	-0.02423	0.00524
Px C 3	-0.23022	-0.05616	-0.08044	-0.03528	0.07843	0.01088
Py C 3	0.01197	0.02078	-0.16531	-0.00946	0.03540	0.07449
Pz C 3	0.06981	0.05482	-0.34176	-0.01418	0.06140	0.15735
S C 4	0.05802	0.01931	-0.00118	-0.00287	0.01103	0.01146
Px C 4	-0.19054	-0.02701	-0.43425	-0.12744	0.29295	0.01914
Py C 4	-0.05442	-0.00279	-0.07406	0.01613	-0.02628	0.06609
Pz C 4	-0.06916	0.00542	-0.07636	0.04857	-0.09008	0.12227
S C 5	-0.00064	0.00004	-0.00367	-0.02248	0.04675	0.01186
Px C 5	-0.24075	-0.05177	-0.37793	-0.14849	0.33129	0.02410
Py C 5	-0.03894	-0.01511	0.06861	-0.09117	0.18610	0.07271
Pz C 5	-0.01467	-0.01803	0.22874	-0.13537	0.27060	0.13538
S C 6	-0.02333	-0.00856	-0.00322	-0.01715	0.03299	-0.00486
Px C 6	-0.04911	-0.02140	0.05137	-0.05919	0.11329	0.00897
Py C 6	0.00294	-0.01096	0.18346	-0.06138	0.11504	0.06218
Pz C 6	0.01858	-0.01681	0.36495	-0.11251	0.21005	0.12650
S O 7	-0.07817	-0.02066	-0.02231	0.02479	-0.04993	-0.04015
Px O 7	-0.15261	-0.04229	-0.01302	0.03654	-0.07487	-0.06504

Py O 7	0.09608	0.02594	0.01843	-0.02437	0.04940	0.04249
Pz O 7	0.22079	0.05966	0.04145	-0.05655	0.11465	0.09810
S O 12	-0.03540	-0.00974	-0.00440	-0.04544	0.09555	0.02977
Px O 12	-0.09854	-0.02728	-0.03575	-0.11251	0.22779	0.07528
Py O 12	-0.05519	-0.01502	-0.01519	-0.06144	0.12832	0.03738
Pz O 12	-0.06833	-0.02234	-0.01438	-0.07034	0.15772	0.04415
S O 14	-0.06156	0.09379	0.00349	0.06695	0.01377	-0.09552
Px O 14	0.09875	-0.15859	-0.00723	-0.11238	-0.02531	0.16323
Py O 14	-0.04520	0.07449	0.00322	0.05248	0.01185	-0.07602
Pz O 14	0.04870	-0.06314	-0.00271	-0.05096	-0.01042	0.07632
S C 15	0.02751	-0.05162	-0.00045	-0.00855	-0.01365	0.05514
Px C 15	0.18456	-0.23315	-0.01444	-0.14508	-0.00236	0.23818
Py C 15	-0.12708	0.13100	0.01345	0.04426	-0.02624	-0.14200
Pz C 15	-0.09744	-0.01433	0.02021	-0.13271	-0.10669	-0.02563
S C 16	0.00690	-0.01986	-0.00213	0.01040	-0.02916	0.05231
Px C 16	0.01849	-0.19107	-0.03131	0.06323	-0.03883	0.19397
Py C 16	-0.07852	0.07370	0.01066	-0.00177	-0.02419	-0.09415
Pz C 16	-0.24499	-0.04305	-0.01235	0.10019	-0.16120	0.01072
S C 17	0.06975	0.03195	0.02387	-0.00772	0.00621	0.01500
Px C 17	-0.06792	-0.03732	-0.06280	0.00831	0.01486	-0.02777
Py C 17	-0.00247	0.00373	0.02733	0.02874	-0.07058	0.04501
Pz C 17	-0.15720	-0.06579	0.02410	0.11240	-0.21922	0.12164
S C 18	0.00439	-0.03634	0.00106	0.01423	-0.01189	0.03413
Px C 18	-0.14977	0.33288	0.03683	0.06029	-0.02135	0.21463
Py C 18	0.09940	-0.28843	-0.02766	-0.10299	-0.00994	-0.21046
Pz C 18	-0.08837	-0.02333	0.01101	-0.15411	-0.08765	-0.07379
S C 19	0.00843	-0.10186	-0.00131	0.04705	0.00640	-0.00611
Px C 19	-0.03382	0.21015	0.00968	-0.01424	-0.00152	0.07576
Py C 19	0.04617	-0.19729	-0.01681	-0.08710	-0.01559	-0.17012
Pz C 19	0.05323	-0.05361	-0.02574	-0.29928	-0.05014	-0.31925
S C 20	0.00922	-0.06246	-0.00196	0.00881	0.01187	-0.05075
Px C 20	0.00565	0.15804	-0.01207	-0.24984	-0.07034	-0.09150
Py C 20	0.00719	-0.12617	0.00295	0.10717	0.03878	-0.00722
Pz C 20	0.03505	0.02733	-0.02213	-0.32188	-0.06627	-0.25464
S C 21	-0.00105	0.00685	-0.00049	-0.00377	0.00935	-0.02851
Px C 21	-0.01052	0.14252	-0.01457	-0.32395	-0.13053	-0.04598
Py C 21	0.03867	-0.04242	0.01149	0.28169	0.16362	-0.04528
Pz C 21	0.10330	0.27589	-0.00304	0.02292	0.18304	-0.29063
S C 22	-0.03393	0.03159	0.00231	-0.03137	-0.02371	0.01806
Px C 22	-0.06593	0.04569	0.00081	-0.12973	-0.09403	0.05706
Py C 22	0.04570	0.00423	0.00673	0.20264	0.14532	-0.08208
Pz C 22	-0.02529	0.11933	0.02166	0.27788	0.19613	-0.09963
S C 23	-0.02693	0.02001	0.00269	-0.02868	-0.03451	0.05096
Px C 23	-0.13040	0.28444	0.03027	-0.01221	-0.04443	0.17262
Py C 23	0.10369	-0.21109	-0.02054	0.09785	0.10233	-0.18303
Pz C 23	-0.04103	0.13864	0.02030	0.22884	0.16625	-0.08080
S C 24	-0.00798	-0.01853	-0.00550	-0.01055	-0.03113	0.04841
Px C 24	-0.03291	-0.12357	-0.02894	0.02436	-0.05686	0.14163
Py C 24	0.00760	0.06766	0.00867	-0.03085	0.01369	-0.05058

Pz C 24	-0.03288	-0.14090	-0.01775	0.11488	0.03957	0.00738
S C 25	-0.03161	0.01668	0.00038	-0.01898	-0.03260	0.05589
Px C 25	-0.05006	0.08589	0.00744	-0.06027	-0.06880	0.11247
Py C 25	0.07088	-0.08274	-0.00524	0.07012	0.08572	-0.13980
Pz C 25	0.00547	-0.17254	-0.01607	0.15894	0.08233	-0.07484
S O 26	0.02208	0.05643	-0.00042	0.00910	0.04116	-0.06301
Px O 26	0.02728	0.06670	-0.00181	-0.01023	0.03627	-0.06935
Py O 26	-0.00229	0.00246	0.00065	0.00644	0.00275	0.00150
Pz O 26	0.07050	0.19759	-0.00276	-0.00341	0.11541	-0.19466
S H 8	0.06153	0.01348	0.00952	0.02043	-0.04331	-0.03153
S H 13	-0.06017	-0.01537	-0.03507	-0.06092	0.11962	0.03545
S H 9	0.13319	0.03624	0.01355	0.01956	-0.04073	0.00890
S H 10	-0.04690	-0.01488	-0.01054	-0.02265	0.04473	-0.00822
S H 11	-0.13223	-0.03744	0.00019	0.02201	-0.04595	-0.04715
S H 27	0.01387	-0.12529	-0.00242	0.06026	0.01205	-0.00895
S H 28	0.01697	-0.07878	-0.00244	0.01722	0.02121	-0.05930
S H 29	-0.04542	0.06142	0.00384	-0.04575	-0.02964	0.01889
S H 30	0.00225	-0.00843	-0.00359	-0.02320	-0.01834	0.05589
S H 31	-0.00909	-0.01193	-0.00570	-0.00969	-0.00599	0.02636
S H 32	-0.01750	0.01073	0.00043	-0.01079	-0.01716	0.02820
S H 33	-0.03480	0.01810	0.00056	-0.00269	-0.02591	0.05626
S H 34	0.03032	0.09773	-0.00238	-0.02739	0.03798	-0.08255
S H 35	0.04884	0.03750	0.03891	-0.00121	-0.00180	-0.00443

Mol. Orbital	97	98
Symmetry:	97 A	98 A
Eigenvalue	0.52138	0.54890

S C 1	0.02463	0.02075
Px C 1	0.04912	0.04480
Py C 1	-0.07839	-0.05204
Pz C 1	-0.16636	-0.11228
S C 2	0.03159	0.03282
Px C 2	0.07970	0.06831
Py C 2	-0.05433	-0.05110
Pz C 2	-0.13134	-0.12274
S C 3	-0.00263	0.00713
Px C 3	-0.01328	-0.02289
Py C 3	-0.08822	-0.08811
Pz C 3	-0.18376	-0.18130
S C 4	-0.00842	0.01471
Px C 4	0.04004	0.08199
Py C 4	-0.09948	-0.12397
Pz C 4	-0.20203	-0.25105
S C 5	-0.00556	0.00526
Px C 5	0.03871	0.06843
Py C 5	-0.07045	-0.04617
Pz C 5	-0.14555	-0.10907
S C 6	0.01447	0.01856

Px C 6	0.00863	0.02329
Py C 6	-0.06892	-0.05094
Pz C 6	-0.14481	-0.11080
S O 7	0.04102	0.02859
Px O 7	0.06511	0.04383
Py O 7	-0.04319	-0.02950
Pz O 7	-0.09952	-0.06788
S O 12	-0.02571	-0.01439
Px O 12	-0.05401	-0.02860
Py O 12	-0.02988	-0.01567
Pz O 12	-0.03719	-0.02479
S O 14	-0.17756	0.06516
Px O 14	0.29898	-0.11196
Py O 14	-0.13972	0.05183
Pz O 14	0.13188	-0.04607
S C 15	0.02805	-0.01144
Px C 15	0.43014	-0.09347
Py C 15	-0.20437	-0.02335
Pz C 15	0.15908	-0.31366
S C 16	-0.01156	-0.03344
Px C 16	0.09526	-0.08568
Py C 16	-0.10109	-0.04528
Pz C 16	-0.19695	-0.31462
S C 17	-0.01678	0.02543
Px C 17	0.03826	0.01427
Py C 17	-0.07106	-0.10756
Pz C 17	-0.20567	-0.37918
S C 18	-0.00782	0.00161
Px C 18	0.16701	-0.04185
Py C 18	-0.08942	-0.05918
Pz C 18	0.17261	-0.30322
S C 19	-0.02863	-0.00203
Px C 19	0.04815	0.03108
Py C 19	-0.04243	-0.08688
Pz C 19	-0.00587	-0.17878
S C 20	-0.00005	-0.03607
Px C 20	0.00983	-0.03954
Py C 20	-0.00005	-0.01740
Pz C 20	0.02426	-0.15286
S C 21	0.01646	-0.02944
Px C 21	-0.02103	-0.00063
Py C 21	0.06133	-0.05781
Pz C 21	0.15043	-0.20022
S C 22	0.02758	-0.02900
Px C 22	0.00285	0.00125
Py C 22	0.06587	-0.07486
Pz C 22	0.19980	-0.21303
S C 23	0.01135	0.00077
Px C 23	0.16536	-0.05981

Py C 23	-0.06876	-0.02925
Pz C 23	0.20910	-0.22450
S C 24	0.00631	-0.01127
Px C 24	0.05214	-0.08478
Py C 24	-0.02857	0.04276
Pz C 24	0.02538	-0.13602
S C 25	0.00382	-0.00175
Px C 25	0.01815	0.02739
Py C 25	-0.01475	-0.02643
Pz C 25	0.01794	-0.14065
S O 26	0.03316	-0.04429
Px O 26	0.02923	-0.04055
Py O 26	0.00375	-0.00297
Pz O 26	0.09752	-0.12793
S H 8	0.03583	0.03251
S H 13	-0.01996	-0.00609
S H 9	-0.01138	-0.00681
S H 10	0.01867	0.02144
S H 11	0.04749	0.03184
S H 27	-0.04181	0.01271
S H 28	0.00721	-0.04131
S H 29	0.03229	-0.02849
S H 30	0.01844	0.01083
S H 31	0.00317	-0.00797
S H 32	0.00192	0.00170
S H 33	0.02137	-0.01781
S H 34	0.03755	-0.04932
S H 35	-0.02666	0.01875