

Fig. S1(a). The (a) simulated and (b) measured XRPD patterns of complex **2** and the (c) simulated XRPD patterns of complex **5**. (d) The measured XRPD pattern of the product obtained by refluxing **2** in DMF.

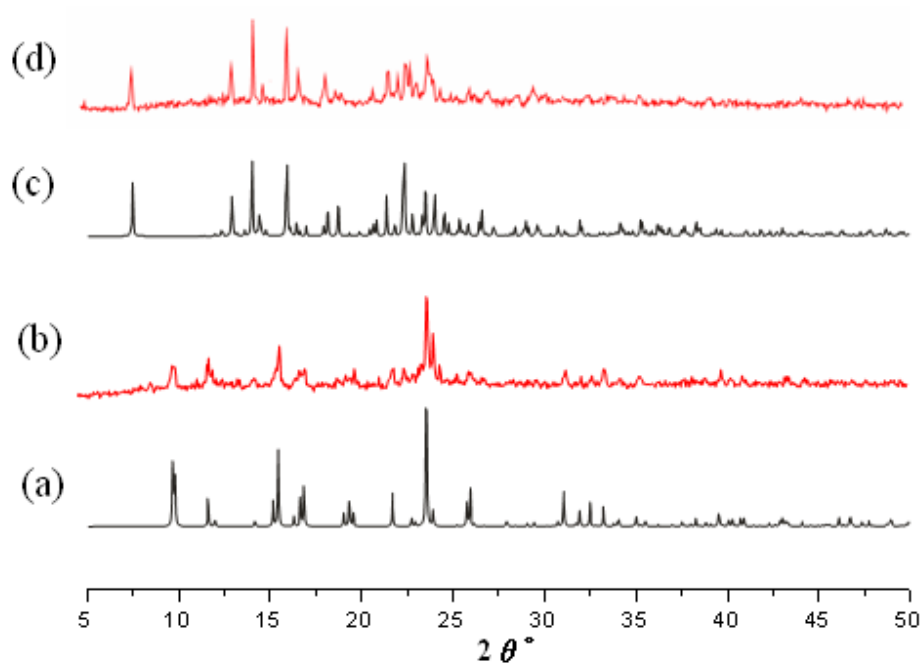


Fig. S1(b). The (a) simulated and (b) measured XRPD patterns of complex **3** and the (c) simulated XRPD patterns of complex **6**. (d) The measured XRPD pattern of the product obtained by refluxing **3** in DMF.

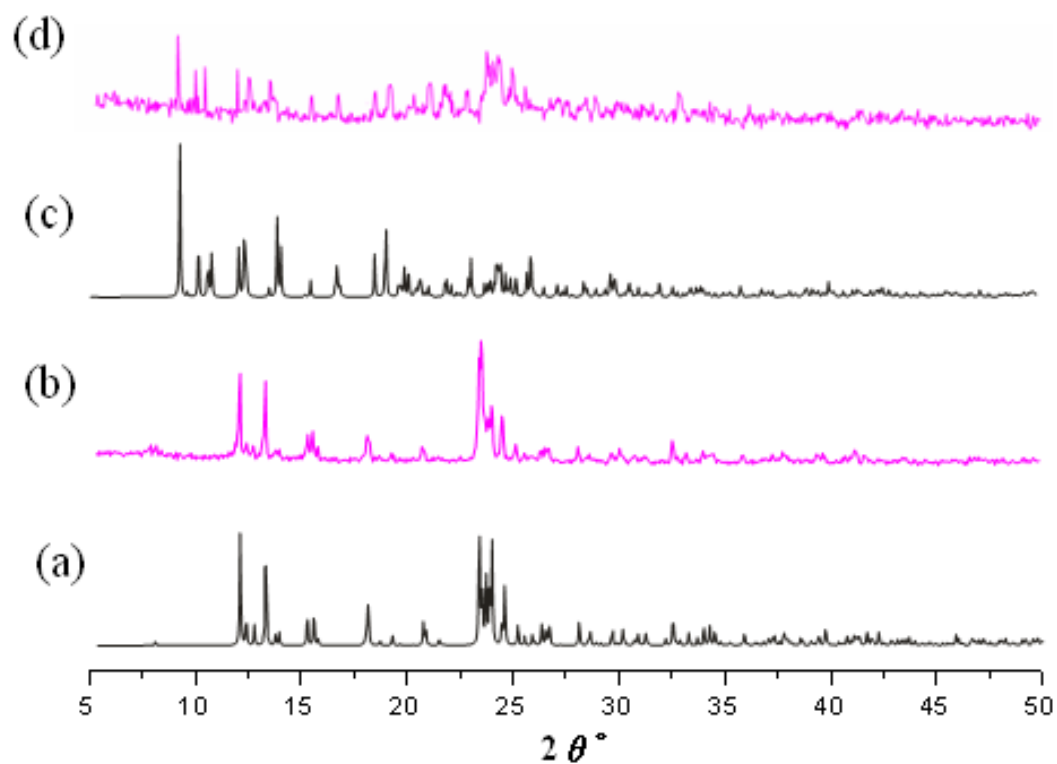


Fig. S2. The TGA curves for complexes **1 – 6**.

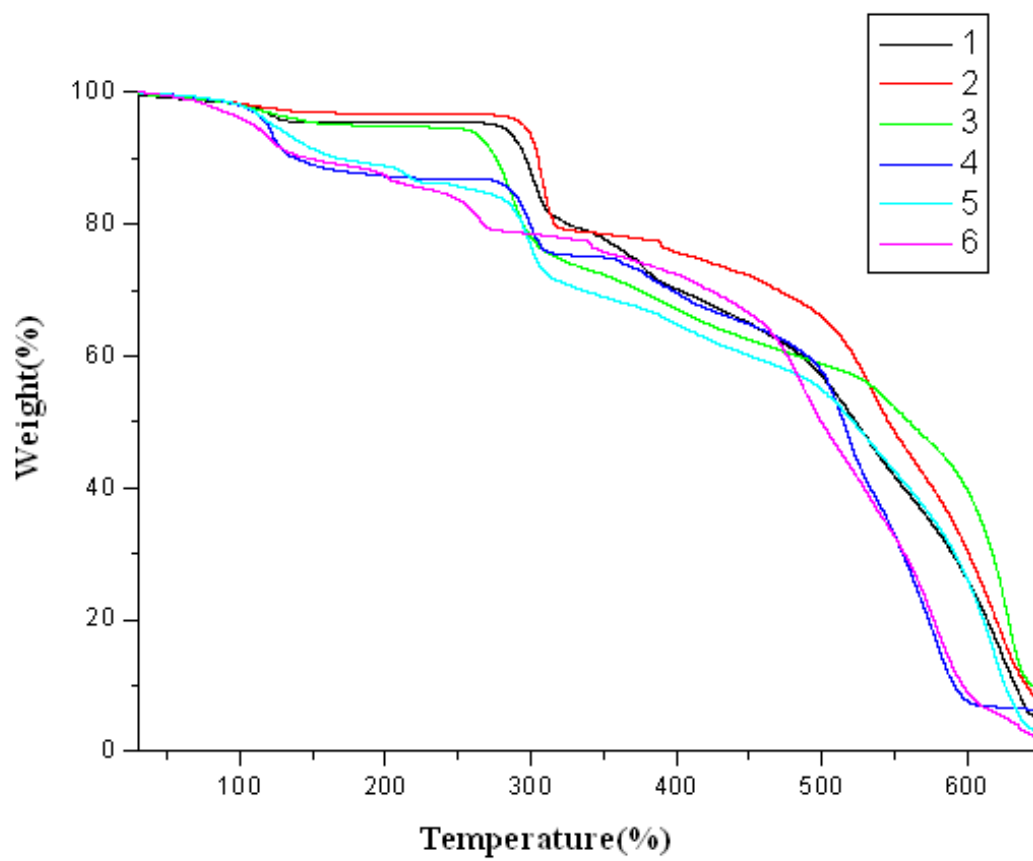


Fig. S3. Tables of Cartesian coordinates and HOMO and LUMO orbital compositions and diagrams for **1 - 6**

Cartesian coordinates

1:

ZNA	0.00000	0.00000	0.00000
ZN	-15.31040	-8.90578	5.14175
CL	-14.46088	-9.13684	7.19018
CLA	-16.15995	-10.79525	4.31764
CLB	-0.84955	1.88951	0.82408
CLC	0.84952	0.23110	-2.04845
O1	-10.61922	-8.48366	-0.25555
N1	-13.87998	-8.28436	3.85198
N2	-10.77848	-6.92863	1.38494
H2A	-10.43310	-6.25975	1.73240
C1	-13.60831	-8.90145	2.69035
H1A	-14.13367	-9.63066	2.45124
C2	-12.60265	-8.52333	1.83233
H2C	-12.45060	-8.98940	1.04203
C3	-11.81696	-7.42526	2.17538
C4	-12.09304	-6.77839	3.37395
H4A	-11.59193	-6.03818	3.63058
C5	-13.10644	-7.23468	4.17712
H5A	-13.26551	-6.79825	4.98281
C6	-10.23352	-7.45616	0.23897
C7	-9.13437	-6.60401	-0.34276
H7A	-8.60140	-6.25099	0.38677
H7B	-9.53978	-5.84991	-0.79870
C8	-8.21170	-7.30830	-1.31140
H8A	-8.73173	-7.64167	-2.05927
H8B	-7.80768	-8.07025	-0.86744
O1A	-20.00157	-4.02051	7.47479
N1A	-16.74084	-7.47812	5.24854
N2A	-19.84236	-4.66372	5.30787
H2AA	-20.18765	-4.63013	4.55491
C1A	-17.01254	-6.78069	6.36371
H1AA	-16.48713	-6.93811	7.11477

C2A	-18.01815	-5.84851	6.46518
H2CA	-18.17024	-5.39720	7.26401
C3A	-18.80381	-5.59655	5.34273
C4A	-18.52779	-6.31107	4.18326
H4AA	-19.02890	-6.16328	3.41389
C5A	-17.51435	-7.23486	4.17691
H5AA	-17.35526	-7.71443	3.39607
C6A	-20.38727	-3.93510	6.33770
C7A	-21.48645	-3.00518	5.89059
H7AA	-22.01945	-3.46049	5.22009
H7BA	-21.08100	-2.23320	5.46552
C8A	-22.40912	-2.51845	6.98487
H8AA	-21.88909	-2.03748	7.64752
H8BA	-22.81316	-3.28398	7.42272
O1B	-4.69117	-4.88525	-2.33306
N1B	-1.43044	-1.42762	-0.10682
N2B	-4.53196	-4.24203	-0.16615
H2AB	-4.87725	-4.27562	0.58681
C1B	-1.70214	-2.12506	-1.22198
H1AB	-1.17673	-1.96764	-1.97304
C2B	-2.70775	-3.05724	-1.32345
H2CB	-2.85984	-3.50855	-2.12229
C3B	-3.49341	-3.30920	-0.20101
C4B	-3.21739	-2.59467	0.95847
H4AB	-3.71850	-2.74247	1.72783
C5B	-2.20395	-1.67089	0.96482
H5AB	-2.04486	-1.19131	1.74566
C6B	-5.07687	-4.97065	-1.19597
C7B	-6.17605	-5.90058	-0.74886
H7AB	-6.70905	-5.44526	-0.07836
H7BB	-5.77060	-6.67256	-0.32380
C8B	-7.09872	-6.38731	-1.84315
H8AB	-6.57869	-6.86827	-2.50580
H8BB	-7.50276	-5.62177	-2.28100
O1C	-25.92963	-0.42215	5.39727
N1C	-29.19036	-0.62133	1.28976
N2C	-26.08884	-1.97715	3.75677
H2AC	-25.74355	-2.64603	3.40938
C1C	-28.91866	-0.00428	2.45134
H1AC	-29.44407	0.72486	2.69054

C2C	-27.91305	-0.38250	3.30937
H2CC	-27.76096	0.08366	4.09963
C3C	-27.12739	-1.48054	2.96635
C4C	-27.40341	-2.12742	1.76781
H4AC	-26.90230	-2.86760	1.51112
C5C	-28.41685	-1.67102	0.96462
H5AC	-28.57594	-2.10746	0.15887
C6C	-25.54393	-1.44961	4.90269
C7C	-24.44475	-2.30177	5.48447
H7AC	-23.91175	-2.65478	4.75491
H7BC	-24.85020	-3.05588	5.94050
C8C	-23.52208	-1.59746	6.45314
H8AC	-24.04211	-1.26407	7.20099
H8BC	-23.11803	-0.83550	6.00909
TV	-30.62080	0.00000	0.00000

2:

ZNA	0.00000	0.00000	0.00000
ZN	-15.31960	-3.19301	9.65473
BR	-16.20564	-5.26478	10.34981
BRA	-14.43354	-1.94414	11.44795
BRB	0.88606	-1.24886	-1.79324
BRC	-0.88606	2.07178	-0.69504
O1	-10.59690	-6.48941	5.43122
N1	-13.86860	-3.58477	8.29629
N2	-10.75078	-4.23933	5.58584
H2A	-10.40294	-3.51206	5.28640
C5	-13.10999	-2.58559	7.81450
H1A	-13.29090	-1.71755	8.09496
C4	-12.08249	-2.78452	6.92960
H2B	-11.58512	-2.06366	6.61676
C3	-11.79196	-4.07689	6.50465
C2	-12.55923	-5.10183	7.01261
H4A	-12.38838	-5.98231	6.76674
C1	-13.56647	-4.81490	7.87498
H5A	-14.08021	-5.52165	8.19353
C6	-10.20610	-5.40528	5.09481
C7	-9.14847	-5.16969	4.06350
H7A	-8.62229	-4.40055	4.33267
H7B	-9.58122	-4.94788	3.22421

C8	-8.21406	-6.32951	3.82784
H8A	-8.72431	-7.08806	3.50359
H8B	-7.80480	-6.58418	4.66957
O1A	-20.04234	1.97156	8.22948
N1A	-16.77054	-2.06856	8.79770
N2A	-19.88841	0.07298	7.01207
H2AA	-20.23624	-0.33237	6.33806
C5A	-17.52920	-2.58346	7.81523
H1AA	-17.34827	-3.44758	7.52287
C4A	-18.55669	-1.89613	7.22348
H2BA	-19.05413	-2.28829	6.54243
C3A	-18.84725	-0.60523	7.65274
C2A	-18.07994	-0.08533	8.67167
H4AA	-18.25082	0.76821	8.99928
C1A	-17.07279	-0.82977	9.19292
H5AA	-16.55899	-0.45233	9.87013
C6A	-20.43307	1.30182	7.31291
C7A	-21.49071	1.72755	6.34456
H7AA	-22.01690	0.94957	6.10204
H7BA	-21.05802	2.04985	5.53852
C8A	-22.42516	2.79918	6.84693
H8AA	-21.91486	3.60142	7.03885
H8BA	-22.83435	2.50174	7.67451
O1B	-4.72274	-5.16457	1.42524
N1B	-1.45094	-1.12444	0.85701
N2B	-4.56881	-3.26599	2.64265
H2AB	-4.91664	-2.86064	3.31666
C5B	-2.20960	-0.60955	1.83949
H1AB	-2.02867	0.25458	2.13185
C4B	-3.23709	-1.29688	2.43124
H2BB	-3.73453	-0.90472	3.11229
C3B	-3.52765	-2.58778	2.00198
C2B	-2.76034	-3.10768	0.98305
H4AB	-2.93122	-3.96122	0.65544
C1B	-1.75319	-2.36324	0.46179
H5AB	-1.23939	-2.74068	-0.21541
C6B	-5.11347	-4.49483	2.34181
C7B	-6.17111	-4.92057	3.31016
H7AB	-6.69730	-4.14258	3.55269
H7BB	-5.73842	-5.24287	4.11621

C8B	-7.10556	-5.99220	2.80779
H8AB	-6.59526	-6.79443	2.61587
H8BB	-7.51475	-5.69476	1.98022
O1C	-25.91646	3.29642	4.22347
N1C	-29.18826	0.39172	1.35846
N2C	-26.07039	1.04635	4.06884
H2AC	-25.72256	0.31907	4.36827
C5C	-28.42960	-0.60742	1.84021
H1AC	-28.61053	-1.47547	1.55971
C4C	-27.40211	-0.40844	2.72508
H2BC	-26.90467	-1.12933	3.03803
C3C	-27.11155	0.88386	3.15013
C2C	-27.87886	1.90876	2.64210
H4AC	-27.70798	2.78932	2.88799
C1C	-28.88601	1.62189	1.77977
H5AC	-29.39981	2.32867	1.46114
C6C	-25.52573	2.21226	4.55999
C7C	-24.46809	1.97669	5.59123
H7AC	-23.94190	1.20751	5.32208
H7BC	-24.90078	1.75486	6.43050
C8C	-23.53364	3.13654	5.82685
H8AC	-24.04394	3.89502	6.15109
H8BC	-23.12445	3.39117	4.98512
TV	-30.63920	-0.00000	0.00000

3:

ZN	0.00000	0.00000	0.00000
I1	-1.59947	-1.49130	-1.32058
I2	1.62312	1.55208	-1.19994
O1	-3.72356	1.60184	5.81868
O2	-5.60748	8.12562	6.08934
N1	-1.04284	1.11392	1.39399
N2	-2.43549	3.13634	4.78650
H2A	-2.13212	3.93860	4.84945
N3	-7.18447	6.80329	5.16372
H3A	-7.60444	6.05884	5.25868
N4	-8.34184	8.80686	1.67902
C1	-0.61280	2.31538	1.75725
H1A	0.04944	2.71312	1.23944
C2	-1.06681	2.99467	2.81828

H2B	-0.73202	3.84103	3.00929
C3	-2.05607	2.42001	3.64561
C4	-2.55557	1.17902	3.24070
H4B	-3.23799	0.77152	3.72355
C5	-2.03811	0.56392	2.13121
H5A	-2.38238	-0.26105	1.87470
C6	-3.22623	2.71306	5.80522
C7	-3.43661	3.71469	6.89351
H7A	-2.67645	4.31563	6.93742
H7B	-3.51362	3.26019	7.74698
C8	-4.72741	4.52307	6.61263
H8A	-4.64739	4.95283	5.74670
H8B	-5.47899	3.91130	6.57073
C9	-5.00523	5.55694	7.63895
H9A	-4.28572	6.20747	7.64331
H9B	-5.03804	5.14052	8.51442
C10	-6.32674	6.26644	7.36667
H10A	-7.02254	5.59747	7.27053
H10B	-6.54944	6.81142	8.13758
C11	-6.33130	7.11951	6.17484
C12	-7.47774	7.50170	4.00371
C13	-8.51372	7.01579	3.26639
H13A	-8.94300	6.23200	3.52382
C14	-8.92454	7.69188	2.13428
H14A	-9.64901	7.35201	1.66043
C15	-7.31962	9.24580	2.38271
H15A	-6.88708	10.01452	2.08797
C16	-6.83823	8.62716	3.55292
H16A	-6.10501	8.97355	4.00825
TV	-9.32233	9.97520	0.29508

4:

ZN	4.14232	-6.08754	0.51684
CL1	4.84195	-7.23141	-1.27852
CL2	4.72822	-6.87194	2.49449
O1	4.25564	0.95883	1.36267
O2	2.58862	5.88678	1.87686
N1	4.66300	-4.14504	0.25131
N2	5.08496	-0.05792	-0.49497
H2A	5.45560	0.11745	-1.25091

N3	2.07029	6.26361	-0.29245
H3A	2.42455	6.45345	-1.05275
N4	-2.10144	6.05837	-0.45036
C1	5.19346	-3.67407	-0.88847
H1A	5.45852	-4.28040	-1.54193
C2	5.35994	-2.33223	-1.12717
H2B	5.73703	-2.04908	-1.92875
C3	4.97069	-1.39877	-0.18376
C4	4.46557	-1.88107	1.02647
H4B	4.23111	-1.29615	1.71043
C5	4.32307	-3.23708	1.18355
H5A	3.96901	-3.54780	1.98541
C6	4.68975	1.02746	0.23379
C7	4.85210	2.33318	-0.51531
H7A	4.27229	2.32159	-1.29286
H7B	5.76677	2.40073	-0.83100
C8	4.53027	3.55972	0.31586
H8A	5.06953	3.55033	1.12210
H8B	3.59742	3.53131	0.58018
C9	4.79515	4.84445	-0.44882
H9A	4.29671	4.82393	-1.28071
H9B	5.73841	4.88995	-0.67039
C10	4.40614	6.10628	0.33360
H10A	4.95844	6.17333	1.12818
H10B	4.57560	6.88813	-0.21493
C11	2.95104	6.08685	0.73802
C12	0.68214	6.17967	-0.28448
C13	0.02038	6.38094	-1.48735
H13A	0.50300	6.56331	-2.26112
C14	-1.33843	6.31029	-1.52984
H14A	-1.76141	6.44303	-2.34738
C15	-1.43470	5.86710	0.69737
H15A	-1.93750	5.69679	1.46098
C16	-0.08002	5.90229	0.83412
H16A	0.32111	5.74393	1.65808
ZNA	-4.14232	6.08754	-0.51684
CL1A	-4.84193	7.23143	1.27849
CL2A	-4.72823	6.87199	-2.49456
O1A	-4.25563	-0.95878	-1.36270
O2A	-2.58863	-5.88673	-1.87691

N1A	-4.66298	4.14506	-0.25135
N2A	-5.08498	0.05797	0.49493
H2AA	-5.45558	-0.11745	1.25097
N3A	-2.07027	-6.26362	0.29248
H3AA	-2.42453	-6.45341	1.05271
N4A	2.10146	-6.05827	0.45031
C1A	-5.19347	3.67416	0.88839
H1AA	-5.45858	4.28050	1.54187
C2A	-5.35998	2.33227	1.12715
H2BA	-5.73706	2.04908	1.92879
C3A	-4.97066	1.39877	0.18378
C4A	-4.46553	1.88113	-1.02654
H4BA	-4.23112	1.29623	-1.71045
C5A	-4.32311	3.23710	-1.18358
H5AA	-3.96905	3.54784	-1.98540
C6A	-4.68974	-1.02738	-0.23385
C7A	-4.85211	-2.33318	0.51536
H7AA	-4.27230	-2.32159	1.29291
H7BA	-5.76676	-2.40068	0.83098
C8A	-4.53030	-3.55975	-0.31583
H8AA	-5.06956	-3.55034	-1.12209
H8BA	-3.59743	-3.53127	-0.58017
C9A	-4.79515	-4.84443	0.44881
H9AA	-4.29671	-4.82392	1.28073
H9BA	-5.73848	-4.88987	0.67036
C10A	-4.40610	-6.10626	-0.33360
H10C	-4.95849	-6.17334	-1.12813
H10D	-4.57565	-6.88803	0.21486
C11A	-2.95109	-6.08679	-0.73810
C12A	-0.68216	-6.17962	0.28442
C13A	-0.02043	-6.38097	1.48736
H13B	-0.50298	-6.56323	2.26107
C14A	1.33841	-6.31029	1.52989
H14B	1.76143	-6.44296	2.34734
C15A	1.43473	-5.86706	-0.69739
H15B	1.93748	-5.69673	-1.46101
C16A	0.08001	-5.90222	-0.83417
H16B	-0.32109	-5.74388	-1.65814

ZN	4.44166	3.60243	4.58922
BR1	6.75182	3.92682	4.15875
BR2	3.60625	4.39604	6.63521
O1	-0.95621	4.63150	0.14072
O2	-4.95755	3.29338	-2.87286
N1	3.41459	4.30460	2.99713
N2	1.19429	5.01736	-0.47360
H2NA	1.67093	5.25722	-1.14805
N3	-3.76132	2.56811	-4.62851
H3NA	-3.28476	2.84586	-5.28834
N4	-4.11484	-1.58304	-4.53738
C1	3.98361	4.72588	1.84754
H1A	4.90733	4.83015	1.81986
C2	3.25961	5.00542	0.72328
H2A	3.69107	5.32122	-0.03764
C3	1.88803	4.82153	0.70981
C4	1.28274	4.43786	1.89971
H4A	0.35867	4.35098	1.95828
C5	2.08359	4.19010	2.98752
H5A	1.66867	3.92285	3.77576
C6	-0.14348	4.88144	-0.71526
C7	-0.51402	5.08079	-2.17457
H7A	-0.24324	5.97061	-2.44986
H7B	-0.02322	4.44172	-2.71459
C8	-1.99192	4.91378	-2.43839
H8A	-2.48714	5.52898	-1.87519
H8B	-2.25779	4.01197	-2.19973
C9	-2.34862	5.16947	-3.88571
H9A	-1.81368	4.58887	-4.44931
H9B	-2.12417	6.08654	-4.10821
C10	-3.82880	4.93216	-4.19103
H10A	-4.36300	5.57452	-3.69822
H10B	-3.98640	5.07691	-5.13714
C11	-4.26415	3.54654	-3.82580
C12	-3.90262	1.18654	-4.54169
C13	-4.59943	0.54306	-3.53952
H13A	-5.00100	1.02173	-2.85068
C14	-4.68107	-0.82840	-3.59189
H14A	-5.16315	-1.25985	-2.92376

C15	-3.43136	-0.93850	-5.48782
H15A	-3.02792	-1.43708	-6.16128
C16	-3.30075	0.40901	-5.51283
H16A	-2.80357	0.81325	-6.18683
ZNA	-4.44166	-3.60243	-4.58922
BR1A	-6.75180	-3.92684	-4.15876
BR2A	-3.60622	-4.39609	-6.63510
O1A	0.95619	-4.63156	-0.14066
O2A	4.95757	-3.29338	2.87293
N1A	-3.41457	-4.30462	-2.99706
N2A	-1.19427	-5.01739	0.47365
H2NB	-1.67093	-5.25726	1.14810
N3A	3.76133	-2.56811	4.62864
H3NB	3.28478	-2.84586	5.28840
N4A	4.11486	1.58300	4.53744
C1A	-3.98363	-4.72587	-1.84741
H1AA	-4.90731	-4.83018	-1.81979
C2A	-3.25959	-5.00545	-0.72316
H2AA	-3.69106	-5.32124	0.03777
C3A	-1.88801	-4.82156	-0.70973
C4A	-1.28275	-4.43788	-1.89964
H4AA	-0.35865	-4.35096	-1.95814
C5A	-2.08359	-4.19014	-2.98744
H5AA	-1.66867	-3.92286	-3.77567
C6A	0.14349	-4.88145	0.71538
C7A	0.51406	-5.08082	2.17465
H7AA	0.24328	-5.97067	2.44997
H7BA	0.02322	-4.44171	2.71472
C8A	1.99191	-4.91384	2.43854
H8AA	2.48715	-5.52903	1.87526
H8BA	2.25781	-4.01203	2.19987
C9A	2.34860	-5.16944	3.88578
H9AA	1.81371	-4.58883	4.44945
H9BA	2.12421	-6.08656	4.10836
C10A	3.82878	-4.93219	4.19104
H10C	4.36302	-5.57451	3.69823
H10D	3.98644	-5.07693	5.13724
C11A	4.26418	-3.54651	3.82593
C12A	3.90261	-1.18659	4.54176
C13A	4.59944	-0.54311	3.53964

H13B	5.00103	-1.02178	2.85073
C14A	4.68107	0.82840	3.59193
H14B	5.16315	1.25988	2.92388
C15A	3.43137	0.93848	5.48792
H15B	3.02793	1.43703	6.16132
C16A	3.30074	-0.40905	5.51295
H16B	2.80360	-0.81322	6.18695

6:

ZN	4.24758	-5.67004	4.00270
I1	3.45760	-7.09049	5.96957
I2	6.62424	-5.90703	3.12837
O1	0.82928	-4.49440	-2.04283
O2	-3.85843	-1.39261	-3.18798
N1	2.96597	-5.92191	2.42244
N2	0.21633	-6.21434	-0.68932
H2A	-0.35674	-6.84850	-0.59428
N3	-2.59812	-0.27723	-4.70920
H3A	-1.98558	-0.39804	-5.30064
N4	-3.88761	3.69336	-4.41114
C1	1.75364	-6.46748	2.57343
H1A	1.51864	-6.79322	3.41222
C2	0.85373	-6.57010	1.57279
H2B	0.02884	-6.96954	1.73060
C3	1.15676	-6.07892	0.30218
C4	2.41071	-5.49760	0.13172
H4B	2.65861	-5.14483	-0.69230
C5	3.27430	-5.45247	1.19463
H5A	4.11602	-5.07931	1.06359
C6	0.09749	-5.43550	-1.82350
C7	-1.01850	-5.88494	-2.72445
H7A	-1.81879	-6.01801	-2.19272
H7B	-0.78044	-6.73818	-3.11967
C8	-1.32729	-4.87915	-3.85176
H8A	-0.49457	-4.59898	-4.26285
H8B	-1.86039	-5.31980	-4.53185
C9	-2.06949	-3.65717	-3.35778
H9A	-2.95822	-3.91936	-3.07092
H9B	-1.60437	-3.29191	-2.58891

C10	-2.18445	-2.61097	-4.39681
H10A	-2.59412	-3.00386	-5.18339
H10B	-1.29108	-2.32624	-4.64526
C11	-2.97731	-1.39771	-4.00471
C12	-3.07329	1.02124	-4.59140
C13	-4.16304	1.38780	-3.82360
H13A	-4.65152	0.74589	-3.36073
C14	-4.51340	2.71346	-3.75458
H14A	-5.23454	2.94431	-3.21462
C15	-2.86035	3.32326	-5.19861
H15A	-2.42054	3.97898	-5.69002
C16	-2.43494	2.03607	-5.30988
H16A	-1.71776	1.83081	-5.86523
ZNA	-4.24758	5.67004	-4.00270
I1A	-3.45762	7.09048	-5.96956
I2A	-6.62428	5.90710	-3.12841
O1A	-0.82927	4.49437	2.04281
O2A	3.85842	1.39263	3.18794
N1A	-2.96600	5.92196	-2.42244
N2A	-0.21636	6.21439	0.68933
H2AA	0.35671	6.84855	0.59426
N3A	2.59812	0.27718	4.70916
H3AA	1.98555	0.39800	5.30061
N4A	3.88757	-3.69331	4.41115
C1A	-1.75366	6.46747	-2.57342
H1AA	-1.51863	6.79321	-3.41224
C2A	-0.85375	6.57017	-1.57285
H2BA	-0.02883	6.96950	-1.73060
C3A	-1.15677	6.07895	-0.30216
C4A	-2.41073	5.49766	-0.13176
H4BA	-2.65864	5.14477	0.69229
C5A	-3.27435	5.45251	-1.19468
H5AA	-4.11602	5.07931	-1.06360
C6A	-0.09748	5.43556	1.82347
C7A	1.01845	5.88499	2.72441
H7AA	1.81876	6.01801	2.19270
H7BA	0.78042	6.73813	3.11965
C8A	1.32727	4.87910	3.85176
H8AA	0.49455	4.59896	4.26282
H8BA	1.86039	5.31984	4.53187

C9A	2.06947	3.65720	3.35773
H9AA	2.95824	3.91931	3.07093
H9BA	1.60434	3.29193	2.58891
C10A	2.18442	2.61097	4.39676
H10C	2.59411	3.00392	5.18340
H10D	1.29105	2.32627	4.64526
C11A	2.97732	1.39778	4.00471
C12A	3.07326	-1.02124	4.59135
C13A	4.16304	-1.38781	3.82356
H13B	4.65152	-0.74591	3.36071
C14A	4.51335	-2.71347	3.75457
H14B	5.23454	-2.94436	3.21462
C15A	2.86030	-3.32326	5.19859
H15B	2.42052	-3.97904	5.68999
C16A	2.43493	-2.03611	5.30984
H16B	1.71775	-1.83080	5.86519

HOMO and LUMO compositions

HOMO (#184) and LUMO(#185) for 1:

		181	182	183	184	185
		O	O	O	O	V
EIGENVALUES --		-0.23902	-0.23902	-0.23234	-0.23234	-0.08766
1	Zn 1S	0.00213	-0.00273	0.00000	0.00000	0.00219
2	2S	0.01198	-0.01521	0.00000	0.00000	0.00671
3	3PX	0.00000	0.00000	-0.00010	0.00388	0.00002
4	3PY	0.00039	-0.00061	0.00000	0.00000	0.02445
5	3PZ	0.00000	0.00000	0.00072	-0.02830	0.00000
6	4PX	0.00000	0.00000	0.00114	-0.04539	0.00001
7	4PY	-0.00516	0.00655	0.00000	0.00000	-0.00358
8	4PZ	0.00000	0.00000	-0.00236	0.09229	0.00000
9	5D 0	0.02794	-0.03627	0.00000	0.00000	0.00480
10	5D+1	0.03258	-0.04228	0.00000	0.00000	-0.01405
11	5D-1	0.00000	0.00000	-0.00195	0.07671	-0.00002
12	5D+2	-0.01936	0.02514	0.00000	0.00000	-0.03272
13	5D-2	0.00000	0.00000	0.00094	-0.03697	0.00000
14	6D 0	0.00466	-0.00605	0.00000	0.00000	0.00072
15	6D+1	0.00572	-0.00741	0.00000	0.00000	-0.00226
16	6D-1	0.00000	0.00000	-0.00032	0.01251	0.00000
17	6D+2	-0.00289	0.00376	0.00000	0.00000	-0.00491

18	6D-2	0.00000	0.00000	0.00014	-0.00547	0.00000
19 2	Zn 1S	-0.00276	-0.00210	0.00000	0.00000	0.00219
20	2S	-0.01546	-0.01166	0.00000	0.00000	0.00671
21	3PX	0.00001	0.00000	-0.00388	-0.00010	-0.00008
22	3PY	0.00053	0.00049	0.00000	0.00000	-0.02438
23	3PZ	0.00000	0.00000	-0.02830	-0.00072	0.00000
24	4PX	0.00001	0.00001	0.04538	0.00116	-0.00002
25	4PY	-0.00666	-0.00502	0.00000	0.00000	0.00358
26	4PZ	0.00000	0.00000	0.09228	0.00233	0.00000
27	5D 0	-0.03627	-0.02795	0.00000	0.00000	0.00479
28	5D+1	0.04229	0.03257	0.00000	0.00000	0.01402
29	5D-1	0.00000	0.00000	-0.07671	-0.00195	0.00005
30	5D+2	0.02514	0.01937	0.00000	0.00000	-0.03264
31	5D-2	0.00000	0.00000	-0.03697	-0.00094	-0.00001
32	6D 0	-0.00605	-0.00466	0.00000	0.00000	0.00072
33	6D+1	0.00742	0.00571	0.00000	0.00000	0.00226
34	6D-1	0.00000	0.00000	-0.01252	-0.00032	0.00001
35	6D+2	0.00375	0.00289	0.00000	0.00000	-0.00490
36	6D-2	0.00000	0.00000	-0.00547	-0.00014	0.00000
37 3	Cl 1S	-0.00031	-0.00023	0.00897	0.00023	-0.00259
38	2S	0.00097	0.00074	0.02439	0.00062	-0.00607
39	3PX	0.25576	0.19703	0.14530	0.00369	-0.00202
40	3PY	-0.02377	-0.01830	-0.21481	-0.00546	-0.00281
41	3PZ	-0.12359	-0.09521	0.26125	0.00664	-0.01248
42	4PX	0.29231	0.22520	0.15703	0.00399	-0.00531
43	4PY	-0.02701	-0.02080	-0.24485	-0.00622	-0.00376
44	4PZ	-0.13833	-0.10658	0.28434	0.00723	-0.01687
45 4	Cl 1S	-0.00031	-0.00023	-0.00897	-0.00023	-0.00258
46	2S	0.00096	0.00074	-0.02439	-0.00062	-0.00604
47	3PX	-0.25572	-0.19700	0.14528	0.00369	0.00204
48	3PY	-0.02378	-0.01830	0.21481	0.00546	-0.00277
49	3PZ	0.12357	0.09519	0.26124	0.00664	0.01243
50	4PX	-0.29227	-0.22517	0.15701	0.00399	0.00534
51	4PY	-0.02702	-0.02081	0.24484	0.00622	-0.00371
52	4PZ	0.13831	0.10656	0.28433	0.00723	0.01680
53 5	Cl 1S	0.00024	-0.00031	-0.00023	0.00897	-0.00259
54	2S	-0.00075	0.00096	-0.00062	0.02439	-0.00607
55	3PX	0.19701	-0.25574	0.00369	-0.14529	0.00203
56	3PY	-0.01832	0.02376	-0.00546	0.21480	0.00280
57	3PZ	0.09520	-0.12358	-0.00664	0.26125	-0.01249

58		4PX	0.22517	-0.29229	0.00399	-0.15701	0.00534
59		4PY	-0.02082	0.02702	-0.00622	0.24484	0.00375
60		4PZ	0.10655	-0.13833	-0.00723	0.28434	-0.01689
61 6	Cl	1S	0.00024	-0.00031	0.00023	-0.00897	-0.00259
62		2S	-0.00075	0.00096	0.00062	-0.02439	-0.00606
63		3PX	-0.19702	0.25575	0.00369	-0.14530	-0.00204
64		3PY	-0.01831	0.02375	0.00546	-0.21480	0.00279
65		3PZ	-0.09520	0.12358	-0.00664	0.26125	0.01248
66		4PX	-0.22518	0.29231	0.00399	-0.15703	-0.00534
67		4PY	-0.02081	0.02700	0.00622	-0.24483	0.00374
68		4PZ	-0.10656	0.13834	-0.00723	0.28434	0.01687
69 7	O	1S	-0.00008	-0.00007	0.00002	0.00000	-0.00013
70		2S	0.00035	0.00032	-0.00005	-0.00001	-0.00018
71		3S	-0.00157	-0.00146	-0.00017	0.00002	0.00369
72		4PX	0.00211	0.00158	-0.00006	0.00001	-0.07669
73		4PY	0.00023	0.00025	0.00071	0.00001	-0.08556
74		4PZ	0.00013	0.00017	0.00067	0.00001	-0.02868
75		5PX	0.00180	0.00137	0.00023	0.00000	-0.06104
76		5PY	-0.00013	-0.00027	0.00042	0.00002	-0.06592
77		5PZ	0.00134	0.00103	-0.00008	0.00002	-0.02350
78 8	N	1S	-0.00157	-0.00121	-0.00049	-0.00001	-0.00259
79		2S	0.00344	0.00265	0.00086	0.00002	0.00629
80		3S	0.00917	0.00701	0.00274	0.00007	0.01785
81		4PX	0.00046	0.00037	-0.00456	-0.00012	-0.11157
82		4PY	-0.00917	-0.00704	-0.00846	-0.00022	-0.15160
83		4PZ	-0.00559	-0.00430	-0.00052	-0.00001	-0.02410
84		5PX	0.00104	0.00079	-0.00492	-0.00013	-0.10938
85		5PY	0.00474	0.00369	-0.01051	-0.00026	-0.13715
86		5PZ	-0.02422	-0.01869	-0.01491	-0.00038	-0.02086
87 9	N	1S	-0.00032	-0.00025	-0.00008	0.00000	-0.00006
88		2S	-0.00016	-0.00011	0.00030	0.00001	-0.00046
89		3S	0.00990	0.00757	-0.00023	-0.00005	0.00257
90		4PX	-0.00053	-0.00037	-0.00021	-0.00001	0.02093
91		4PY	-0.00422	-0.00324	-0.00130	-0.00003	0.02546
92		4PZ	-0.00035	-0.00026	0.00029	0.00001	0.00579
93		5PX	0.00226	0.00098	-0.00240	-0.00001	0.04016
94		5PY	-0.00188	-0.00091	-0.00038	-0.00004	0.03548
95		5PZ	-0.01943	-0.01415	0.00310	-0.00003	0.01701
96 10	H	1S	-0.00133	-0.00105	-0.00060	-0.00001	0.00263
97		2S	-0.01106	-0.00827	-0.00242	-0.00010	0.01490

98	11	C	1S	0.00444	0.00342	0.00267	0.00007	0.00075
99			2S	-0.00637	-0.00495	-0.00484	-0.00012	-0.00267
100			3S	-0.04528	-0.03474	-0.03185	-0.00080	0.00040
101			4PX	-0.01570	-0.01209	-0.01175	-0.00030	0.09196
102			4PY	0.01387	0.01068	0.00796	0.00020	0.11344
103			4PZ	-0.00740	-0.00571	-0.00998	-0.00025	0.01772
104			5PX	0.05202	0.03981	0.00201	0.00008	0.07455
105			5PY	-0.05638	-0.04322	0.01302	0.00030	0.07953
106			5PZ	-0.02347	-0.01816	-0.04003	-0.00100	0.01565
107	12	H	1S	-0.00806	-0.00622	-0.00647	-0.00016	-0.00222
108			2S	-0.01442	-0.01091	0.02929	0.00071	-0.00892
109	13	C	1S	-0.00217	-0.00168	-0.00123	-0.00003	-0.00033
110			2S	0.00231	0.00177	0.00151	0.00004	0.00027
111			3S	0.03797	0.02924	0.02681	0.00065	0.00769
112			4PX	0.01828	0.01408	0.00558	0.00014	0.04911
113			4PY	0.00471	0.00360	-0.00237	-0.00006	0.05461
114			4PZ	-0.00233	-0.00180	-0.00116	-0.00003	0.00834
115			5PX	0.04450	0.03429	0.00525	0.00013	0.05692
116			5PY	-0.01868	-0.01436	-0.01370	-0.00035	0.06277
117			5PZ	-0.01726	-0.01354	0.01039	0.00030	0.01107
118	14	H	1S	-0.00005	-0.00004	0.00118	0.00003	-0.00099
119			2S	0.01053	0.00832	-0.00679	-0.00019	-0.00618
120	15	C	1S	0.00076	0.00058	0.00019	0.00001	-0.00026
121			2S	-0.00105	-0.00085	-0.00034	-0.00001	0.00161
122			3S	-0.01977	-0.01444	0.00257	0.00003	-0.00595
123			4PX	0.00141	0.00108	-0.00018	0.00000	-0.14890
124			4PY	0.00760	0.00587	0.00342	0.00008	-0.17520
125			4PZ	-0.00439	-0.00340	-0.00515	-0.00013	-0.02656
126			5PX	0.02412	0.01704	-0.00209	0.00011	-0.13866
127			5PY	-0.01881	-0.01350	0.00890	0.00012	-0.17778
128			5PZ	0.04011	0.03191	-0.00326	-0.00016	-0.02830
129	16	C	1S	0.00054	0.00041	0.00090	0.00002	0.00000
130			2S	-0.00022	-0.00022	-0.00009	0.00000	0.00099
131			3S	-0.01765	-0.01312	-0.02831	-0.00076	-0.01253
132			4PX	-0.00823	-0.00635	-0.00257	-0.00006	0.05525
133			4PY	-0.00668	-0.00517	0.00215	0.00006	0.06334
134			4PZ	-0.00081	-0.00061	0.00184	0.00005	0.01037
135			5PX	-0.03931	-0.02994	-0.00707	-0.00022	0.06375
136			5PY	0.00769	0.00567	-0.00352	-0.00006	0.09162
137			5PZ	0.02586	0.02023	0.01055	0.00023	0.01825

138	17	H	1S	-0.00050	-0.00040	-0.00091	-0.00002	-0.00116
139			2S	-0.00237	-0.00155	0.00302	0.00004	-0.00491
140	18	C	1S	-0.00152	-0.00118	-0.00179	-0.00005	-0.00016
141			2S	0.00198	0.00151	0.00382	0.00010	-0.00029
142			3S	0.01386	0.01043	0.01890	0.00050	0.01457
143			4PX	-0.00519	-0.00398	0.00029	0.00001	0.07936
144			4PY	-0.00908	-0.00701	-0.00180	-0.00005	0.09305
145			4PZ	-0.00734	-0.00566	-0.01372	-0.00035	0.00902
146			5PX	-0.03519	-0.02731	-0.01811	-0.00044	0.03927
147			5PY	0.04707	0.03635	0.02473	0.00062	0.07486
148			5PZ	0.02694	0.02105	-0.01378	-0.00036	0.00273
149	19	H	1S	0.00210	0.00161	0.00547	0.00014	-0.00039
150			2S	0.02672	0.02087	-0.00946	-0.00026	-0.00698
151	20	C	1S	-0.00015	-0.00013	-0.00016	0.00000	0.00136
152			2S	0.00053	0.00021	0.00040	0.00001	-0.00167
153			3S	0.01115	0.00977	-0.00213	0.00002	-0.02450
154			4PX	-0.00077	-0.00057	0.00015	0.00001	0.09740
155			4PY	-0.00115	-0.00093	-0.00047	-0.00002	0.11000
156			4PZ	-0.00136	-0.00105	-0.00078	-0.00002	0.03800
157			5PX	0.01036	0.00658	-0.00037	0.00013	0.05101
158			5PY	-0.00819	-0.00511	0.00017	-0.00008	0.04919
159			5PZ	-0.00816	-0.00434	0.00230	-0.00020	0.01784
160	21	C	1S	-0.00014	-0.00013	0.00005	0.00001	0.00034
161			2S	-0.00021	-0.00011	-0.00007	-0.00001	-0.00246
162			3S	0.00458	0.00273	-0.00001	-0.00014	0.02569
163			4PX	0.00066	0.00044	-0.00028	0.00001	-0.00400
164			4PY	-0.00003	0.00000	0.00042	0.00001	-0.01345
165			4PZ	0.00004	-0.00005	-0.00004	0.00001	-0.00474
166			5PX	0.00479	0.00115	-0.00091	0.00008	0.04981
167			5PY	-0.00233	-0.00168	-0.00071	0.00010	0.04532
168			5PZ	-0.00067	-0.00033	-0.00070	0.00001	0.00163
169	22	H	1S	-0.00038	-0.00026	0.00003	0.00000	0.01341
170			2S	0.00109	0.00068	-0.00058	-0.00001	0.03911
171	23	H	1S	0.00031	0.00020	0.00011	0.00001	-0.02281
172			2S	0.00035	0.00128	0.00088	-0.00005	-0.08757
173	24	C	1S	0.00004	-0.00002	0.00001	0.00002	-0.00331
174			2S	-0.00014	-0.00036	0.00000	-0.00002	0.00443
175			3S	-0.00053	0.00178	-0.00003	-0.00056	0.05807
176			4PX	-0.00031	-0.00033	0.00002	0.00010	0.00910
177			4PY	-0.00008	0.00001	-0.00007	-0.00007	-0.00376

178		4PZ	0.00038	0.00017	0.00000	0.00003	-0.01059
179		5PX	0.00498	0.00151	-0.00015	0.00040	-0.03555
180		5PY	-0.00276	0.00098	0.00094	-0.00021	-0.06482
181		5PZ	-0.00072	-0.00033	0.00066	-0.00039	-0.02643
182	25	H 1S	0.00005	-0.00018	0.00003	0.00004	0.00201
183		2S	-0.00113	0.00015	-0.00027	0.00013	0.02092
184	26	H 1S	0.00005	-0.00003	0.00005	0.00000	-0.00138
185		2S	0.00009	0.00154	0.00046	0.00002	-0.05612
186	27	O 1S	-0.00008	-0.00007	-0.00002	0.00000	-0.00013
187		2S	0.00035	0.00032	0.00005	0.00001	-0.00018
188		3S	-0.00157	-0.00146	0.00017	-0.00002	0.00367
189		4PX	-0.00211	-0.00158	-0.00006	0.00001	0.07622
190		4PY	0.00023	0.00024	-0.00071	-0.00001	-0.08506
191		4PZ	-0.00013	-0.00017	0.00067	0.00001	0.02851
192		5PX	-0.00180	-0.00137	0.00023	0.00000	0.06067
193		5PY	-0.00013	-0.00027	-0.00042	-0.00002	-0.06554
194		5PZ	-0.00134	-0.00103	-0.00008	0.00002	0.02337
195	28	N 1S	-0.00157	-0.00121	0.00049	0.00001	-0.00260
196		2S	0.00344	0.00265	-0.00086	-0.00002	0.00632
197		3S	0.00917	0.00701	-0.00274	-0.00007	0.01793
198		4PX	-0.00046	-0.00037	-0.00456	-0.00012	0.11085
199		4PY	-0.00916	-0.00704	0.00845	0.00022	-0.15077
200		4PZ	0.00559	0.00430	-0.00052	-0.00001	0.02401
201		5PX	-0.00104	-0.00078	-0.00492	-0.00013	0.10873
202		5PY	0.00475	0.00370	0.01051	0.00026	-0.13640
203		5PZ	0.02422	0.01869	-0.01491	-0.00037	0.02081
204	29	N 1S	-0.00032	-0.00025	0.00008	0.00000	-0.00007
205		2S	-0.00016	-0.00011	-0.00030	-0.00001	-0.00045
206		3S	0.00990	0.00757	0.00023	0.00005	0.00257
207		4PX	0.00053	0.00036	-0.00021	-0.00001	-0.02082
208		4PY	-0.00422	-0.00324	0.00130	0.00003	0.02531
209		4PZ	0.00035	0.00026	0.00029	0.00001	-0.00575
210		5PX	-0.00226	-0.00098	-0.00240	-0.00001	-0.03990
211		5PY	-0.00188	-0.00090	0.00038	0.00004	0.03530
212		5PZ	0.01943	0.01415	0.00311	-0.00003	-0.01692
213	30	H 1S	-0.00133	-0.00105	0.00060	0.00001	0.00261
214		2S	-0.01107	-0.00828	0.00242	0.00010	0.01479
215	31	C 1S	0.00444	0.00342	-0.00267	-0.00007	0.00076
216		2S	-0.00637	-0.00495	0.00484	0.00012	-0.00268
217		3S	-0.04529	-0.03475	0.03186	0.00080	0.00031

218		4PX	0.01570	0.01209	-0.01175	-0.00030	-0.09147
219		4PY	0.01387	0.01068	-0.00796	-0.00020	0.11285
220		4PZ	0.00740	0.00571	-0.00998	-0.00025	-0.01765
221		5PX	-0.05203	-0.03982	0.00200	0.00008	-0.07425
222		5PY	-0.05639	-0.04322	-0.01303	-0.00030	0.07910
223		5PZ	0.02346	0.01815	-0.04004	-0.00100	-0.01551
224	32	H 1S	-0.00806	-0.00622	0.00647	0.00016	-0.00222
225		2S	-0.01443	-0.01092	-0.02930	-0.00071	-0.00890
226	33	C 1S	-0.00217	-0.00168	0.00123	0.00003	-0.00034
227		2S	0.00231	0.00177	-0.00151	-0.00004	0.00029
228		3S	0.03798	0.02924	-0.02681	-0.00065	0.00768
229		4PX	-0.01828	-0.01408	0.00558	0.00014	-0.04881
230		4PY	0.00471	0.00360	0.00237	0.00006	0.05421
231		4PZ	0.00233	0.00180	-0.00116	-0.00003	-0.00826
232		5PX	-0.04450	-0.03429	0.00525	0.00013	-0.05665
233		5PY	-0.01868	-0.01436	0.01370	0.00035	0.06228
234		5PZ	0.01727	0.01354	0.01040	0.00030	-0.01098
235	34	H 1S	-0.00005	-0.00004	-0.00118	-0.00003	-0.00099
236		2S	0.01053	0.00832	0.00680	0.00019	-0.00614
237	35	C 1S	0.00076	0.00058	-0.00019	-0.00001	-0.00026
238		2S	-0.00105	-0.00085	0.00034	0.00001	0.00160
239		3S	-0.01978	-0.01444	-0.00258	-0.00003	-0.00588
240		4PX	-0.00140	-0.00108	-0.00018	0.00000	0.14805
241		4PY	0.00760	0.00587	-0.00342	-0.00008	-0.17421
242		4PZ	0.00440	0.00340	-0.00515	-0.00013	0.02642
243		5PX	-0.02412	-0.01704	-0.00209	0.00011	0.13791
244		5PY	-0.01882	-0.01350	-0.00890	-0.00012	-0.17679
245		5PZ	-0.04011	-0.03191	-0.00325	-0.00016	0.02800
246	36	C 1S	0.00054	0.00041	-0.00090	-0.00002	0.00000
247		2S	-0.00022	-0.00022	0.00009	0.00000	0.00100
248		3S	-0.01765	-0.01312	0.02830	0.00076	-0.01250
249		4PX	0.00823	0.00636	-0.00257	-0.00006	-0.05498
250		4PY	-0.00668	-0.00517	-0.00215	-0.00006	0.06302
251		4PZ	0.00081	0.00061	0.00184	0.00005	-0.01031
252		5PX	0.03931	0.02994	-0.00708	-0.00022	-0.06341
253		5PY	0.00770	0.00567	0.00351	0.00006	0.09123
254		5PZ	-0.02586	-0.02022	0.01056	0.00023	-0.01823
255	37	H 1S	-0.00050	-0.00040	0.00091	0.00002	-0.00116
256		2S	-0.00238	-0.00155	-0.00302	-0.00004	-0.00490
257	38	C 1S	-0.00152	-0.00118	0.00180	0.00005	-0.00016

258		2S	0.00198	0.00151	-0.00382	-0.00010	-0.00028
259		3S	0.01386	0.01043	-0.01891	-0.00050	0.01452
260		4PX	0.00519	0.00398	0.00029	0.00001	-0.07890
261		4PY	-0.00908	-0.00701	0.00181	0.00005	0.09249
262		4PZ	0.00734	0.00566	-0.01372	-0.00035	-0.00892
263		5PX	0.03520	0.02731	-0.01811	-0.00044	-0.03883
264		5PY	0.04707	0.03635	-0.02473	-0.00062	0.07448
265		5PZ	-0.02694	-0.02105	-0.01379	-0.00036	-0.00273
266	39	H 1S	0.00211	0.00162	-0.00547	-0.00014	-0.00038
267		2S	0.02672	0.02087	0.00947	0.00026	-0.00693
268	40	C 1S	-0.00015	-0.00013	0.00016	0.00000	0.00135
269		2S	0.00053	0.00021	-0.00040	-0.00001	-0.00165
270		3S	0.01115	0.00977	0.00213	-0.00002	-0.02436
271		4PX	0.00077	0.00057	0.00015	0.00001	-0.09682
272		4PY	-0.00114	-0.00093	0.00047	0.00002	0.10936
273		4PZ	0.00136	0.00105	-0.00078	-0.00002	-0.03777
274		5PX	-0.01036	-0.00658	-0.00037	0.00013	-0.05066
275		5PY	-0.00819	-0.00511	-0.00017	0.00008	0.04892
276		5PZ	0.00815	0.00434	0.00230	-0.00020	-0.01779
277	41	C 1S	-0.00014	-0.00013	-0.00005	-0.00001	0.00034
278		2S	-0.00021	-0.00011	0.00007	0.00001	-0.00245
279		3S	0.00458	0.00273	0.00002	0.00014	0.02554
280		4PX	-0.00066	-0.00044	-0.00028	0.00001	0.00396
281		4PY	-0.00003	0.00000	-0.00042	-0.00001	-0.01337
282		4PZ	-0.00004	0.00005	-0.00004	0.00001	0.00470
283		5PX	-0.00479	-0.00115	-0.00091	0.00008	-0.04951
284		5PY	-0.00233	-0.00168	0.00071	-0.00010	0.04510
285		5PZ	0.00067	0.00033	-0.00070	0.00001	-0.00165
286	42	H 1S	-0.00038	-0.00026	-0.00003	0.00000	0.01333
287		2S	0.00109	0.00068	0.00058	0.00001	0.03892
288	43	H 1S	0.00031	0.00020	-0.00011	-0.00001	-0.02268
289		2S	0.00035	0.00128	-0.00088	0.00005	-0.08708
290	44	C 1S	0.00004	-0.00002	-0.00001	-0.00002	-0.00330
291		2S	-0.00014	-0.00036	0.00000	0.00002	0.00440
292		3S	-0.00053	0.00178	0.00003	0.00056	0.05780
293		4PX	0.00031	0.00033	0.00002	0.00010	-0.00905
294		4PY	-0.00008	0.00001	0.00007	0.00007	-0.00376
295		4PZ	-0.00038	-0.00017	0.00000	0.00003	0.01052
296		5PX	-0.00498	-0.00151	-0.00015	0.00040	0.03544
297		5PY	-0.00276	0.00098	-0.00094	0.00021	-0.06449

298		5PZ	0.00072	0.00033	0.00066	-0.00039	0.02621
299	45	H 1S	0.00005	-0.00018	-0.00003	-0.00004	0.00200
300		2S	-0.00113	0.00015	0.00027	-0.00013	0.02080
301	46	H 1S	0.00005	-0.00003	-0.00005	0.00000	-0.00137
302		2S	0.00009	0.00154	-0.00046	-0.00002	-0.05585
303	47	O 1S	0.00006	-0.00009	0.00000	0.00002	-0.00013
304		2S	-0.00026	0.00040	-0.00001	-0.00005	-0.00018
305		3S	0.00114	-0.00181	0.00003	-0.00017	0.00370
306		4PX	0.00164	-0.00207	-0.00001	0.00006	0.07670
307		4PY	0.00016	-0.00029	0.00003	-0.00071	0.08558
308		4PZ	-0.00008	0.00019	-0.00002	0.00066	-0.02868
309		5PX	0.00139	-0.00178	0.00001	-0.00023	0.06106
310		5PY	-0.00006	0.00030	0.00000	-0.00042	0.06594
311		5PZ	-0.00103	0.00134	0.00002	-0.00008	-0.02350
312	48	N 1S	0.00121	-0.00157	0.00001	-0.00049	-0.00260
313		2S	-0.00265	0.00344	-0.00002	0.00086	0.00632
314		3S	-0.00708	0.00912	-0.00007	0.00274	0.01793
315		4PX	0.00035	-0.00047	-0.00011	0.00456	0.11160
316		4PY	-0.00706	0.00914	-0.00021	0.00845	0.15169
317		4PZ	0.00431	-0.00558	0.00001	-0.00052	-0.02413
318		5PX	0.00080	-0.00102	-0.00012	0.00491	0.10943
319		5PY	0.00365	-0.00479	-0.00027	0.01051	0.13723
320		5PZ	0.01865	-0.02425	0.00038	-0.01491	-0.02089
321	49	N 1S	0.00024	-0.00032	0.00000	-0.00008	-0.00007
322		2S	0.00013	-0.00015	0.00000	0.00030	-0.00045
323		3S	-0.00764	0.00984	-0.00004	-0.00023	0.00259
324		4PX	-0.00042	0.00049	0.00000	0.00021	-0.02094
325		4PY	-0.00326	0.00421	-0.00003	0.00130	-0.02547
326		4PZ	0.00028	-0.00034	0.00000	0.00029	0.00579
327		5PX	0.00193	-0.00152	-0.00011	0.00240	-0.04016
328		5PY	-0.00158	0.00135	0.00002	0.00038	-0.03550
329		5PZ	0.01517	-0.01864	-0.00019	0.00310	0.01702
330	50	H 1S	0.00102	-0.00135	0.00002	-0.00060	0.00263
331		2S	0.00859	-0.01083	0.00002	-0.00242	0.01489
332	51	C 1S	-0.00342	0.00444	-0.00007	0.00267	0.00076
333		2S	0.00490	-0.00641	0.00013	-0.00484	-0.00269
334		3S	0.03492	-0.04515	0.00082	-0.03185	0.00035
335		4PX	-0.01209	0.01570	-0.00030	0.01175	-0.09201
336		4PY	0.01069	-0.01386	0.00020	-0.00796	-0.11350
337		4PZ	0.00570	-0.00741	0.00025	-0.00998	0.01773

338		5PX	0.04014	-0.05178	0.00002	-0.00200	-0.07463
339		5PY	-0.04349	0.05618	0.00036	-0.01303	-0.07958
340		5PZ	0.01806	-0.02354	0.00103	-0.04004	0.01563
341	52	H 1S	0.00621	-0.00807	0.00017	-0.00647	-0.00222
342		2S	0.01117	-0.01424	-0.00078	0.02930	-0.00893
343	53	C 1S	0.00167	-0.00218	0.00003	-0.00123	-0.00034
344		2S	-0.00178	0.00230	-0.00004	0.00151	0.00028
345		3S	-0.02926	0.03797	-0.00072	0.02681	0.00770
346		4PX	0.01408	-0.01827	0.00014	-0.00558	-0.04914
347		4PY	0.00363	-0.00468	-0.00006	0.00237	-0.05461
348		4PZ	0.00179	-0.00234	0.00003	-0.00116	0.00833
349		5PX	0.03428	-0.04451	0.00014	-0.00525	-0.05699
350		5PY	-0.01440	0.01865	-0.00035	0.01370	-0.06276
351		5PZ	0.01325	-0.01750	-0.00023	0.01040	0.01106
352	54	H 1S	0.00003	-0.00005	-0.00003	0.00118	-0.00099
353		2S	-0.00806	0.01073	0.00015	-0.00680	-0.00617
354	55	C 1S	-0.00058	0.00075	0.00000	0.00019	-0.00026
355		2S	0.00080	-0.00109	0.00001	-0.00034	0.00161
356		3S	0.01544	-0.01900	-0.00010	0.00258	-0.00595
357		4PX	0.00108	-0.00141	-0.00001	0.00018	0.14896
358		4PY	0.00585	-0.00761	0.00009	-0.00342	0.17529
359		4PZ	0.00338	-0.00441	0.00013	-0.00515	-0.02658
360		5PX	0.01897	-0.02263	-0.00021	0.00209	0.13872
361		5PY	-0.01475	0.01786	0.00034	-0.00890	0.17788
362		5PZ	-0.03064	0.04109	0.00001	-0.00326	-0.02826
363	56	C 1S	-0.00042	0.00053	-0.00002	0.00090	0.00000
364		2S	0.00016	-0.00027	0.00001	-0.00009	0.00100
365		3S	0.01372	-0.01719	0.00068	-0.02830	-0.01254
366		4PX	-0.00634	0.00825	-0.00007	0.00257	-0.05528
367		4PY	-0.00514	0.00670	0.00005	-0.00215	-0.06337
368		4PZ	0.00062	-0.00079	-0.00005	0.00184	0.01037
369		5PX	-0.03038	0.03898	-0.00014	0.00708	-0.06378
370		5PY	0.00600	-0.00745	-0.00012	0.00351	-0.09170
371		5PZ	-0.01985	0.02615	-0.00031	0.01055	0.01829
372	57	H 1S	0.00038	-0.00051	0.00003	-0.00091	-0.00116
373		2S	0.00190	-0.00211	-0.00011	0.00302	-0.00492
374	58	C 1S	0.00117	-0.00153	0.00005	-0.00180	-0.00016
375		2S	-0.00153	0.00196	-0.00010	0.00382	-0.00029
376		3S	-0.01074	0.01362	-0.00047	0.01891	0.01459
377		4PX	-0.00400	0.00517	0.00001	-0.00029	-0.07941

378		4PY	-0.00699	0.00909	-0.00005	0.00181	-0.09310
379		4PZ	0.00565	-0.00734	0.00035	-0.01372	0.00901
380		5PX	-0.02707	0.03539	-0.00048	0.01811	-0.03923
381		5PY	0.03624	-0.04716	0.00064	-0.02473	-0.07493
382		5PZ	-0.02068	0.02723	0.00034	-0.01380	0.00272
383	59	H 1S	-0.00162	0.00210	-0.00014	0.00547	-0.00038
384		2S	-0.02052	0.02700	0.00022	-0.00947	-0.00699
385	60	C 1S	0.00012	-0.00017	0.00001	-0.00016	0.00136
386		2S	-0.00046	0.00034	-0.00001	0.00040	-0.00167
387		3S	-0.00829	0.01229	0.00013	-0.00213	-0.02453
388		4PX	-0.00060	0.00074	0.00000	-0.00015	-0.09743
389		4PY	-0.00087	0.00119	-0.00001	0.00047	-0.11003
390		4PZ	0.00105	-0.00136	0.00002	-0.00078	0.03801
391		5PX	0.00834	-0.00901	-0.00015	0.00037	-0.05102
392		5PY	-0.00661	0.00703	0.00009	-0.00017	-0.04920
393		5PZ	0.00678	-0.00628	-0.00031	0.00229	0.01785
394	61	C 1S	0.00010	-0.00016	0.00000	0.00005	0.00034
395		2S	0.00017	-0.00016	0.00000	-0.00007	-0.00246
396		3S	-0.00373	0.00381	-0.00014	-0.00002	0.02571
397		4PX	0.00052	-0.00060	-0.00002	0.00028	0.00399
398		4PY	-0.00002	0.00001	0.00001	-0.00042	0.01346
399		4PZ	-0.00005	-0.00003	0.00001	-0.00004	-0.00474
400		5PX	0.00434	-0.00233	-0.00013	0.00090	-0.04981
401		5PY	-0.00182	0.00222	-0.00013	0.00070	-0.04533
402		5PZ	0.00056	-0.00049	0.00005	-0.00070	0.00163
403	62	H 1S	0.00030	-0.00035	0.00000	0.00003	0.01342
404		2S	-0.00088	0.00093	0.00002	-0.00058	0.03910
405	63	H 1S	-0.00025	0.00027	0.00000	0.00011	-0.02282
406		2S	-0.00001	0.00132	-0.00010	0.00087	-0.08759
407	64	C 1S	-0.00004	-0.00001	0.00002	0.00001	-0.00332
408		2S	0.00004	-0.00039	-0.00002	0.00000	0.00443
409		3S	0.00097	0.00158	-0.00056	-0.00006	0.05807
410		4PX	-0.00021	0.00040	-0.00010	-0.00002	-0.00911
411		4PY	-0.00008	0.00001	0.00006	0.00007	0.00376
412		4PZ	-0.00032	0.00026	0.00003	0.00000	-0.01059
413		5PX	0.00443	-0.00273	-0.00041	0.00013	0.03555
414		5PY	-0.00292	-0.00024	0.00026	-0.00093	0.06482
415		5PZ	0.00061	-0.00050	-0.00042	0.00064	-0.02644
416	65	H 1S	-0.00010	-0.00016	0.00003	0.00003	0.00200
417		2S	0.00113	-0.00014	0.00015	-0.00026	0.02093

418	66	H	1S	-0.00006	-0.00002	0.00000	0.00005	-0.00138
419			2S	0.00031	0.00151	0.00000	0.00046	-0.05612
420	67	O	1S	0.00006	-0.00009	0.00000	-0.00002	-0.00013
421			2S	-0.00026	0.00040	0.00001	0.00005	-0.00018
422			3S	0.00114	-0.00181	-0.00003	0.00017	0.00370
423			4PX	-0.00164	0.00207	-0.00001	0.00006	-0.07656
424			4PY	0.00016	-0.00029	-0.00003	0.00071	0.08542
425			4PZ	0.00008	-0.00019	-0.00002	0.00066	0.02863
426			5PX	-0.00139	0.00178	0.00001	-0.00023	-0.06095
427			5PY	-0.00006	0.00030	0.00000	0.00042	0.06581
428			5PZ	0.00103	-0.00134	0.00002	-0.00008	0.02346
429	68	N	1S	0.00121	-0.00157	-0.00001	0.00049	-0.00260
430			2S	-0.00265	0.00344	0.00002	-0.00086	0.00633
431			3S	-0.00708	0.00912	0.00007	-0.00274	0.01795
432			4PX	-0.00035	0.00047	-0.00011	0.00456	-0.11137
433			4PY	-0.00706	0.00914	0.00021	-0.00845	0.15143
434			4PZ	-0.00431	0.00558	0.00001	-0.00052	0.02410
435			5PX	-0.00081	0.00102	-0.00012	0.00492	-0.10923
436			5PY	0.00365	-0.00479	0.00027	-0.01051	0.13700
437			5PZ	-0.01865	0.02425	0.00038	-0.01491	0.02088
438	69	N	1S	0.00024	-0.00032	0.00000	0.00008	-0.00007
439			2S	0.00013	-0.00015	0.00000	-0.00030	-0.00045
440			3S	-0.00764	0.00984	0.00004	0.00023	0.00258
441			4PX	0.00042	-0.00049	0.00000	0.00021	0.02091
442			4PY	-0.00326	0.00420	0.00003	-0.00130	-0.02543
443			4PZ	-0.00028	0.00035	0.00000	0.00029	-0.00579
444			5PX	-0.00193	0.00152	-0.00011	0.00240	0.04010
445			5PY	-0.00158	0.00135	-0.00002	-0.00038	-0.03545
446			5PZ	-0.01517	0.01864	-0.00019	0.00310	-0.01697
447	70	H	1S	0.00102	-0.00135	-0.00002	0.00060	0.00262
448			2S	0.00859	-0.01083	-0.00002	0.00242	0.01484
449	71	C	1S	-0.00342	0.00444	0.00007	-0.00267	0.00076
450			2S	0.00490	-0.00641	-0.00013	0.00484	-0.00269
451			3S	0.03492	-0.04514	-0.00082	0.03185	0.00032
452			4PX	0.01209	-0.01570	-0.00030	0.01175	0.09187
453			4PY	0.01069	-0.01386	-0.00020	0.00796	-0.11334
454			4PZ	-0.00570	0.00741	0.00025	-0.00998	-0.01772
455			5PX	-0.04014	0.05177	0.00002	-0.00200	0.07455
456			5PY	-0.04349	0.05618	-0.00036	0.01303	-0.07945
457			5PZ	-0.01806	0.02354	0.00103	-0.04004	-0.01559

458	72	H	1S	0.00621	-0.00807	-0.00017	0.00647	-0.00222
459			2S	0.01117	-0.01424	0.00078	-0.02930	-0.00893
460	73	C	1S	0.00167	-0.00218	-0.00003	0.00123	-0.00034
461			2S	-0.00178	0.00230	0.00004	-0.00151	0.00029
462			3S	-0.02926	0.03796	0.00072	-0.02681	0.00770
463			4PX	-0.01408	0.01827	0.00014	-0.00558	0.04903
464			4PY	0.00363	-0.00468	0.00006	-0.00237	-0.05447
465			4PZ	-0.00179	0.00234	0.00003	-0.00116	-0.00831
466			5PX	-0.03427	0.04451	0.00014	-0.00525	0.05689
467			5PY	-0.01440	0.01865	0.00035	-0.01370	-0.06259
468			5PZ	-0.01324	0.01750	-0.00023	0.01040	-0.01104
469	74	H	1S	0.00003	-0.00005	0.00003	-0.00118	-0.00099
470			2S	-0.00806	0.01073	-0.00015	0.00680	-0.00616
471	75	C	1S	-0.00058	0.00075	0.00000	-0.00019	-0.00026
472			2S	0.00080	-0.00109	-0.00001	0.00034	0.00161
473			3S	0.01544	-0.01900	0.00010	-0.00258	-0.00593
474			4PX	-0.00108	0.00141	-0.00001	0.00018	-0.14871
475			4PY	0.00585	-0.00761	-0.00009	0.00342	0.17499
476			4PZ	-0.00338	0.00441	0.00013	-0.00515	0.02654
477			5PX	-0.01897	0.02263	-0.00021	0.00209	-0.13846
478			5PY	-0.01475	0.01786	-0.00034	0.00889	0.17760
479			5PZ	0.03064	-0.04109	0.00001	-0.00326	0.02820
480	76	C	1S	-0.00042	0.00053	0.00002	-0.00090	0.00000
481			2S	0.00016	-0.00027	-0.00001	0.00009	0.00100
482			3S	0.01372	-0.01719	-0.00068	0.02830	-0.01255
483			4PX	0.00634	-0.00825	-0.00007	0.00257	0.05521
484			4PY	-0.00514	0.00670	-0.00005	0.00215	-0.06329
485			4PZ	-0.00062	0.00079	-0.00005	0.00184	-0.01036
486			5PX	0.03037	-0.03898	-0.00014	0.00708	0.06368
487			5PY	0.00600	-0.00745	0.00012	-0.00351	-0.09161
488			5PZ	0.01984	-0.02615	-0.00031	0.01055	-0.01827
489	77	H	1S	0.00038	-0.00051	-0.00003	0.00091	-0.00116
490			2S	0.00190	-0.00211	0.00011	-0.00302	-0.00493
491	78	C	1S	0.00117	-0.00153	-0.00005	0.00180	-0.00016
492			2S	-0.00153	0.00196	0.00010	-0.00382	-0.00029
493			3S	-0.01074	0.01362	0.00047	-0.01891	0.01458
494			4PX	0.00400	-0.00517	0.00001	-0.00029	0.07925
495			4PY	-0.00699	0.00909	0.00005	-0.00181	-0.09291
496			4PZ	-0.00565	0.00734	0.00035	-0.01372	-0.00898
497			5PX	0.02706	-0.03539	-0.00048	0.01811	0.03908

498		5PY	0.03624	-0.04716	-0.00064	0.02473	-0.07479
499		5PZ	0.02068	-0.02722	0.00034	-0.01380	-0.00273
500	79	H 1S	-0.00162	0.00210	0.00014	-0.00547	-0.00038
501		2S	-0.02052	0.02700	-0.00022	0.00947	-0.00697
502	80	C 1S	0.00012	-0.00017	-0.00001	0.00016	0.00136
503		2S	-0.00046	0.00034	0.00001	-0.00040	-0.00166
504		3S	-0.00829	0.01229	-0.00013	0.00213	-0.02451
505		4PX	0.00060	-0.00074	0.00000	-0.00015	0.09725
506		4PY	-0.00087	0.00119	0.00001	-0.00047	-0.10982
507		4PZ	-0.00105	0.00136	0.00002	-0.00078	-0.03794
508		5PX	-0.00834	0.00901	-0.00015	0.00037	0.05096
509		5PY	-0.00661	0.00703	-0.00009	0.00017	-0.04908
510		5PZ	-0.00678	0.00628	-0.00031	0.00229	-0.01778
511	81	C 1S	0.00010	-0.00016	0.00000	-0.00005	0.00034
512		2S	0.00017	-0.00016	0.00000	0.00007	-0.00245
513		3S	-0.00373	0.00381	0.00014	0.00002	0.02567
514		4PX	-0.00052	0.00060	-0.00002	0.00028	-0.00400
515		4PY	-0.00002	0.00001	-0.00001	0.00042	0.01344
516		4PZ	0.00005	0.00003	0.00001	-0.00004	0.00474
517		5PX	-0.00434	0.00233	-0.00013	0.00090	0.04974
518		5PY	-0.00182	0.00222	0.00013	-0.00070	-0.04521
519		5PZ	-0.00056	0.00049	0.00005	-0.00070	-0.00160
520	82	H 1S	0.00030	-0.00035	0.00000	-0.00003	0.01340
521		2S	-0.00088	0.00093	-0.00002	0.00058	0.03898
522	83	H 1S	-0.00025	0.00027	0.00000	-0.00011	-0.02278
523		2S	-0.00001	0.00132	0.00010	-0.00087	-0.08741
524	84	C 1S	-0.00004	-0.00001	-0.00002	-0.00001	-0.00331
525		2S	0.00004	-0.00039	0.00002	0.00000	0.00442
526		3S	0.00097	0.00158	0.00056	0.00006	0.05788
527		4PX	0.00021	-0.00040	-0.00010	-0.00002	0.00909
528		4PY	-0.00008	0.00001	-0.00006	-0.00007	0.00373
529		4PZ	0.00032	-0.00026	0.00003	0.00000	0.01058
530		5PX	-0.00443	0.00273	-0.00041	0.00013	-0.03540
531		5PY	-0.00292	-0.00024	-0.00026	0.00093	0.06465
532		5PZ	-0.00061	0.00050	-0.00042	0.00064	0.02646
533	85	H 1S	-0.00010	-0.00016	-0.00003	-0.00003	0.00200
534		2S	0.00113	-0.00014	-0.00015	0.00026	0.02090
535	86	H 1S	-0.00006	-0.00002	0.00000	-0.00005	-0.00139
536		2S	0.00031	0.00151	0.00000	-0.00046	-0.05595

HOMO (#184) and LUMO(#185) for 2:

		181	182	183	184	185
		O	O	O	O	V
EIGENVALUES --		-0.22669	-0.22669	-0.21836	-0.21836	-0.08730
1 1	Zn 1S	0.00049	-0.00295	0.00000	0.00000	0.00170
2	2S	0.00240	-0.01397	0.00000	0.00000	0.00450
3	3PX	0.00000	0.00001	-0.00013	0.01155	-0.00003
4	3PY	0.00047	-0.00321	0.00000	0.00000	0.02932
5	3PZ	0.00000	0.00000	0.00048	-0.04466	0.00000
6	4PX	0.00000	0.00001	0.00045	-0.04261	-0.00001
7	4PY	-0.00104	0.00602	0.00000	0.00000	-0.00368
8	4PZ	0.00000	0.00000	-0.00099	0.09090	0.00000
9	5D 0	0.00631	-0.03948	0.00000	0.00000	0.00564
10	5D+1	0.00740	-0.04626	0.00000	0.00000	-0.01304
11	5D-1	0.00000	0.00000	-0.00072	0.06708	0.00002
12	5D+2	-0.00424	0.02657	0.00000	0.00000	-0.03260
13	5D-2	0.00000	-0.00001	0.00035	-0.03208	0.00000
14	6D 0	0.00092	-0.00574	0.00000	0.00000	0.00082
15	6D+1	0.00113	-0.00703	0.00000	0.00000	-0.00208
16	6D-1	0.00000	0.00000	-0.00009	0.00851	0.00000
17	6D+2	-0.00053	0.00331	0.00000	0.00000	-0.00461
18	6D-2	0.00000	0.00000	0.00004	-0.00348	0.00000
19 2	Zn 1S	-0.00295	-0.00045	0.00000	0.00000	0.00169
20	2S	-0.01402	-0.00208	0.00000	0.00000	0.00449
21	3PX	0.00001	0.00000	-0.01155	-0.00012	0.00011
22	3PY	0.00320	0.00056	-0.00001	0.00000	-0.02915
23	3PZ	-0.00001	0.00000	-0.04466	-0.00048	0.00000
24	4PX	0.00001	0.00000	0.04261	0.00047	0.00001
25	4PY	-0.00604	-0.00089	-0.00001	0.00000	0.00367
26	4PZ	-0.00001	0.00000	0.09091	0.00096	0.00000
27	5D 0	-0.03948	-0.00631	0.00000	0.00000	0.00561
28	5D+1	0.04626	0.00739	0.00000	0.00000	0.01297
29	5D-1	0.00000	0.00000	-0.06708	-0.00072	-0.00006
30	5D+2	0.02657	0.00425	0.00000	0.00000	-0.03241
31	5D-2	0.00001	0.00000	-0.03208	-0.00034	0.00001
32	6D 0	-0.00574	-0.00092	0.00000	0.00000	0.00082
33	6D+1	0.00703	0.00112	0.00000	0.00000	0.00207
34	6D-1	0.00000	0.00000	-0.00851	-0.00009	-0.00001
35	6D+2	0.00331	0.00053	0.00000	0.00000	-0.00459
36	6D-2	0.00000	0.00000	-0.00348	-0.00004	0.00000

37	3	Br 1S	-0.00032	-0.00005	-0.00600	-0.00006	-0.00141
38		2S	0.00005	0.00001	-0.02908	-0.00031	-0.00711
39		3PX	-0.33012	-0.05278	0.15033	0.00162	0.00130
40		3PY	-0.02659	-0.00424	0.21898	0.00236	-0.00359
41		3PZ	0.15962	0.02552	0.27597	0.00297	0.01443
42		4PX	-0.34809	-0.05566	0.14710	0.00158	0.00509
43		4PY	-0.02822	-0.00451	0.23496	0.00253	-0.00424
44		4PZ	0.16452	0.02632	0.27211	0.00293	0.01817
45	4	Br 1S	-0.00032	-0.00005	0.00600	0.00006	-0.00140
46		2S	0.00005	0.00001	0.02908	0.00031	-0.00706
47		3PX	0.33020	0.05279	0.15034	0.00162	-0.00132
48		3PY	-0.02659	-0.00424	-0.21902	-0.00236	-0.00355
49		3PZ	-0.15967	-0.02553	0.27598	0.00297	-0.01435
50		4PX	0.34817	0.05567	0.14710	0.00158	-0.00512
51		4PY	-0.02821	-0.00451	-0.23501	-0.00253	-0.00418
52		4PZ	-0.16456	-0.02632	0.27212	0.00293	-0.01807
53	5	Br 1S	0.00005	-0.00032	0.00006	-0.00600	-0.00142
54		2S	-0.00001	0.00005	0.00031	-0.02908	-0.00713
55		3PX	-0.05279	0.33018	0.00162	-0.15034	-0.00132
56		3PY	-0.00426	0.02659	0.00236	-0.21902	0.00360
57		3PZ	-0.02553	0.15966	-0.00297	0.27597	0.01448
58		4PX	-0.05566	0.34816	0.00158	-0.14710	-0.00513
59		4PY	-0.00451	0.02821	0.00253	-0.23500	0.00424
60		4PZ	-0.02630	0.16456	-0.00293	0.27212	0.01824
61	6	Br 1S	0.00005	-0.00032	-0.00006	0.00600	-0.00141
62		2S	-0.00001	0.00005	-0.00031	0.02908	-0.00712
63		3PX	0.05278	-0.33013	0.00162	-0.15033	0.00132
64		3PY	-0.00426	0.02659	-0.00236	0.21899	0.00358
65		3PZ	0.02552	-0.15963	-0.00297	0.27596	-0.01446
66		4PX	0.05565	-0.34811	0.00158	-0.14710	0.00514
67		4PY	-0.00451	0.02821	-0.00253	0.23498	0.00422
68		4PZ	0.02629	-0.16453	-0.00293	0.27211	-0.01821
69	7	O 1S	-0.00007	-0.00002	0.00004	0.00000	-0.00017
70		2S	0.00036	0.00009	-0.00006	-0.00001	-0.00010
71		3S	-0.00181	-0.00047	-0.00042	0.00002	0.00424
72		4PX	0.00224	0.00034	-0.00041	0.00000	-0.07751
73		4PY	0.00064	0.00015	0.00045	-0.00001	-0.08209
74		4PZ	0.00038	0.00011	0.00057	0.00000	-0.02818
75		5PX	0.00201	0.00031	0.00012	-0.00001	-0.06223
76		5PY	0.00000	-0.00011	0.00014	0.00001	-0.06322

77		5PZ	0.00177	0.00028	-0.00013	0.00002	-0.02350
78	8	N 1S	-0.00208	-0.00033	-0.00053	-0.00001	-0.00284
79		2S	0.00446	0.00071	0.00092	0.00001	0.00684
80		3S	0.01349	0.00212	0.00309	0.00003	0.01945
81		4PX	0.00073	0.00013	-0.00542	-0.00006	-0.11013
82		4PY	-0.01110	-0.00176	-0.00905	-0.00010	-0.15006
83		4PZ	-0.00710	-0.00113	-0.00097	-0.00001	-0.03072
84		5PX	0.00071	0.00011	-0.00167	-0.00003	-0.10588
85		5PY	0.00433	0.00072	-0.01245	-0.00013	-0.13817
86		5PZ	-0.02094	-0.00336	-0.00654	-0.00007	-0.02844
87	9	N 1S	-0.00054	-0.00009	-0.00009	0.00000	0.00008
88		2S	0.00024	0.00005	0.00036	0.00001	-0.00102
89		3S	0.01189	0.00188	-0.00027	-0.00005	0.00409
90		4PX	-0.00064	-0.00008	0.00018	0.00000	0.02195
91		4PY	-0.00518	-0.00082	-0.00065	-0.00001	0.02436
92		4PZ	-0.00083	-0.00013	0.00035	0.00001	0.00933
93		5PX	0.00252	-0.00009	-0.00212	0.00004	0.04109
94		5PY	-0.00149	0.00010	0.00088	-0.00002	0.03367
95		5PZ	-0.02158	-0.00289	0.00223	-0.00010	0.02084
96	10	H 1S	-0.00187	-0.00031	-0.00067	0.00000	0.00347
97		2S	-0.01161	-0.00167	-0.00288	-0.00007	0.01572
98	11	C 1S	-0.00183	-0.00029	-0.00180	-0.00002	-0.00026
99		2S	0.00323	0.00050	0.00407	0.00005	-0.00006
100		3S	0.01493	0.00222	0.02276	0.00026	0.01653
101		4PX	-0.00613	-0.00097	0.00099	0.00001	0.07652
102		4PY	-0.01033	-0.00166	-0.00083	-0.00001	0.09142
103		4PZ	-0.00985	-0.00158	-0.01417	-0.00015	0.01318
104		5PX	-0.03282	-0.00538	-0.01411	-0.00014	0.03680
105		5PY	0.04429	0.00713	0.01894	0.00019	0.07369
106		5PZ	0.02652	0.00444	-0.00989	-0.00012	0.00842
107	12	H 1S	0.00310	0.00049	0.00521	0.00006	-0.00033
108		2S	0.02666	0.00445	-0.00727	-0.00010	-0.00594
109	13	C 1S	0.00059	0.00009	0.00083	0.00001	-0.00011
110		2S	-0.00097	-0.00019	-0.00042	0.00000	0.00140
111		3S	-0.01054	-0.00137	-0.02350	-0.00030	-0.01319
112		4PX	-0.01084	-0.00174	-0.00278	-0.00003	0.05381
113		4PY	-0.00962	-0.00155	0.00183	0.00002	0.06346
114		4PZ	-0.00171	-0.00026	0.00164	0.00002	0.01366
115		5PX	-0.04315	-0.00666	-0.00595	-0.00010	0.06171
116		5PY	0.00680	0.00089	-0.00213	0.00001	0.09248

117		5PZ	0.02541	0.00427	0.00863	0.00005	0.02073
118	14	H 1S	-0.00068	-0.00012	-0.00102	-0.00001	-0.00147
119		2S	-0.00409	-0.00046	0.00259	-0.00001	-0.00652
120	15	C 1S	0.00110	0.00017	0.00019	0.00000	-0.00016
121		2S	-0.00211	-0.00036	-0.00051	-0.00001	0.00165
122		3S	-0.02182	-0.00299	0.00380	0.00000	-0.00842
123		4PX	0.00238	0.00038	-0.00058	0.00000	-0.14900
124		4PY	0.01052	0.00169	0.00286	0.00003	-0.17252
125		4PZ	-0.00551	-0.00089	-0.00523	-0.00006	-0.03342
126		5PX	0.02757	0.00335	-0.00280	0.00015	-0.13779
127		5PY	-0.02278	-0.00297	0.00671	-0.00005	-0.17615
128		5PZ	0.04500	0.00786	-0.00104	-0.00010	-0.03628
129	16	C 1S	-0.00283	-0.00046	-0.00114	-0.00001	-0.00029
130		2S	0.00438	0.00069	0.00186	0.00002	0.00037
131		3S	0.03628	0.00582	0.02065	0.00019	0.00534
132		4PX	0.02302	0.00368	0.00462	0.00005	0.04743
133		4PY	0.00574	0.00090	-0.00261	-0.00003	0.05229
134		4PZ	-0.00214	-0.00035	-0.00117	-0.00001	0.01115
135		5PX	0.04805	0.00770	0.00501	0.00005	0.05500
136		5PY	-0.01781	-0.00282	-0.01313	-0.00015	0.06118
137		5PZ	-0.02100	-0.00353	0.00844	0.00013	0.01286
138	17	H 1S	0.00084	0.00013	0.00149	0.00002	-0.00126
139		2S	0.01342	0.00229	-0.00557	-0.00008	-0.00516
140	18	C 1S	0.00623	0.00099	0.00273	0.00003	0.00065
141		2S	-0.01026	-0.00167	-0.00550	-0.00006	-0.00224
142		3S	-0.05959	-0.00944	-0.03304	-0.00035	0.00178
143		4PX	-0.02344	-0.00375	-0.01147	-0.00012	0.09186
144		4PY	0.01739	0.00278	0.00892	0.00010	0.11563
145		4PZ	-0.01231	-0.00197	-0.01043	-0.00011	0.02379
146		5PX	0.05171	0.00809	0.00125	0.00005	0.07362
147		5PY	-0.05726	-0.00901	0.01415	0.00012	0.08182
148		5PZ	-0.01914	-0.00311	-0.03089	-0.00032	0.01990
149	19	H 1S	-0.01080	-0.00174	-0.00573	-0.00006	-0.00234
150		2S	-0.01505	-0.00227	0.02231	0.00021	-0.00846
151	20	C 1S	-0.00021	-0.00004	-0.00016	0.00000	0.00181
152		2S	0.00055	-0.00004	0.00046	0.00001	-0.00185
153		3S	0.01406	0.00302	-0.00139	0.00005	-0.03434
154		4PX	-0.00111	-0.00016	0.00032	0.00001	0.09826
155		4PY	-0.00168	-0.00030	-0.00031	-0.00001	0.10463
156		4PZ	-0.00167	-0.00027	-0.00074	-0.00001	0.03781

157		5PX	0.00999	0.00068	-0.00032	0.00016	0.05259
158		5PY	-0.00796	-0.00049	0.00015	-0.00009	0.04559
159		5PZ	-0.00887	-0.00003	0.00243	-0.00025	0.01829
160	21	C 1S	-0.00015	-0.00004	0.00005	0.00001	0.00010
161		2S	-0.00015	0.00000	-0.00006	-0.00001	-0.00193
162		3S	0.00373	0.00019	-0.00022	-0.00009	0.02904
163		4PX	0.00064	0.00005	-0.00035	0.00001	-0.00283
164		4PY	0.00018	0.00003	0.00040	0.00000	-0.01347
165		4PZ	-0.00006	-0.00006	-0.00008	0.00002	-0.00500
166		5PX	0.00335	-0.00121	-0.00115	0.00010	0.05396
167		5PY	-0.00230	-0.00032	-0.00056	0.00010	0.04060
168		5PZ	-0.00043	-0.00009	-0.00075	0.00000	0.00211
169	22	H 1S	-0.00038	-0.00003	0.00008	0.00000	0.01279
170		2S	0.00120	-0.00012	-0.00058	-0.00003	0.03813
171	23	H 1S	0.00048	0.00004	0.00005	0.00001	-0.02276
172		2S	0.00109	0.00087	0.00087	-0.00008	-0.08806
173	24	C 1S	0.00004	-0.00003	0.00001	0.00002	-0.00358
174		2S	-0.00031	-0.00023	0.00001	-0.00002	0.00488
175		3S	0.00016	0.00157	-0.00003	-0.00053	0.06039
176		4PX	-0.00046	-0.00014	0.00005	0.00010	0.00994
177		4PY	-0.00008	0.00005	-0.00004	-0.00007	-0.00418
178		4PZ	0.00046	-0.00002	-0.00002	0.00004	-0.01136
179		5PX	0.00463	-0.00070	-0.00012	0.00047	-0.03611
180		5PY	-0.00179	0.00207	0.00090	-0.00023	-0.06288
181		5PZ	-0.00046	0.00017	0.00067	-0.00034	-0.02896
182	25	H 1S	-0.00002	-0.00016	0.00004	0.00004	0.00199
183		2S	-0.00095	0.00044	-0.00026	0.00008	0.02160
184	26	H 1S	0.00005	-0.00004	0.00003	0.00000	-0.00131
185		2S	0.00076	0.00132	0.00040	0.00002	-0.05672
186	27	O 1S	-0.00007	-0.00002	-0.00004	0.00000	-0.00017
187		2S	0.00036	0.00009	0.00006	0.00001	-0.00010
188		3S	-0.00181	-0.00047	0.00042	-0.00002	0.00427
189		4PX	-0.00224	-0.00034	-0.00041	0.00000	0.07804
190		4PY	0.00064	0.00015	-0.00045	0.00001	-0.08263
191		4PZ	-0.00038	-0.00011	0.00057	0.00000	0.02836
192		5PX	-0.00201	-0.00031	0.00012	-0.00001	0.06266
193		5PY	0.00000	-0.00011	-0.00014	-0.00001	-0.06363
194		5PZ	-0.00178	-0.00028	-0.00013	0.00002	0.02365
195	28	N 1S	-0.00208	-0.00033	0.00052	0.00001	-0.00283
196		2S	0.00445	0.00071	-0.00091	-0.00001	0.00681

197		3S	0.01347	0.00212	-0.00308	-0.00003	0.01936
198		4PX	-0.00072	-0.00012	-0.00542	-0.00006	0.11093
199		4PY	-0.01109	-0.00176	0.00905	0.00010	-0.15099
200		4PZ	0.00709	0.00113	-0.00096	-0.00001	0.03086
201		5PX	-0.00070	-0.00011	-0.00168	-0.00003	0.10662
202		5PY	0.00434	0.00072	0.01245	0.00013	-0.13900
203		5PZ	0.02093	0.00336	-0.00654	-0.00007	0.02853
204	29	N 1S	-0.00054	-0.00009	0.00009	0.00000	0.00008
205		2S	0.00024	0.00005	-0.00036	-0.00001	-0.00103
206		3S	0.01189	0.00188	0.00027	0.00005	0.00411
207		4PX	0.00064	0.00008	0.00018	0.00000	-0.02209
208		4PY	-0.00518	-0.00082	0.00066	0.00001	0.02450
209		4PZ	0.00082	0.00013	0.00035	0.00001	-0.00937
210		5PX	-0.00253	0.00009	-0.00212	0.00004	-0.04140
211		5PY	-0.00149	0.00010	-0.00088	0.00002	0.03384
212		5PZ	0.02158	0.00289	0.00224	-0.00010	-0.02094
213	30	H 1S	-0.00187	-0.00031	0.00067	0.00000	0.00350
214		2S	-0.01161	-0.00167	0.00288	0.00007	0.01585
215	31	C 1S	-0.00183	-0.00029	0.00180	0.00002	-0.00026
216		2S	0.00323	0.00050	-0.00407	-0.00005	-0.00007
217		3S	0.01493	0.00222	-0.02276	-0.00026	0.01656
218		4PX	0.00612	0.00097	0.00099	0.00001	-0.07707
219		4PY	-0.01033	-0.00166	0.00083	0.00001	0.09208
220		4PZ	0.00985	0.00158	-0.01416	-0.00015	-0.01332
221		5PX	0.03282	0.00538	-0.01411	-0.00014	-0.03733
222		5PY	0.04430	0.00713	-0.01894	-0.00019	0.07416
223		5PZ	-0.02650	-0.00443	-0.00989	-0.00012	-0.00841
224	32	H 1S	0.00311	0.00049	-0.00521	-0.00006	-0.00034
225		2S	0.02666	0.00445	0.00727	0.00010	-0.00602
226	33	C 1S	0.00059	0.00009	-0.00083	-0.00001	-0.00011
227		2S	-0.00097	-0.00019	0.00042	0.00000	0.00140
228		3S	-0.01055	-0.00137	0.02350	0.00030	-0.01316
229		4PX	0.01084	0.00174	-0.00278	-0.00003	-0.05408
230		4PY	-0.00961	-0.00155	-0.00184	-0.00002	0.06377
231		4PZ	0.00170	0.00026	0.00164	0.00002	-0.01374
232		5PX	0.04316	0.00666	-0.00595	-0.00010	-0.06206
233		5PY	0.00680	0.00089	0.00213	-0.00001	0.09288
234		5PZ	-0.02543	-0.00427	0.00864	0.00005	-0.02080
235	34	H 1S	-0.00068	-0.00012	0.00102	0.00001	-0.00147
236		2S	-0.00408	-0.00046	-0.00259	0.00001	-0.00653

237	35	C	1S	0.00110	0.00017	-0.00019	0.00000	-0.00016
238			2S	-0.00211	-0.00036	0.00051	0.00001	0.00165
239			3S	-0.02184	-0.00299	-0.00380	0.00000	-0.00861
240			4PX	-0.00238	-0.00038	-0.00058	0.00000	0.14994
241			4PY	0.01052	0.00169	-0.00286	-0.00003	-0.17362
242			4PZ	0.00551	0.00089	-0.00523	-0.00006	0.03362
243			5PX	-0.02757	-0.00335	-0.00280	0.00015	0.13860
244			5PY	-0.02278	-0.00297	-0.00671	0.00005	-0.17727
245			5PZ	-0.04500	-0.00786	-0.00104	-0.00010	0.03663
246	36	C	1S	-0.00283	-0.00046	0.00114	0.00001	-0.00029
247			2S	0.00438	0.00069	-0.00186	-0.00002	0.00037
248			3S	0.03630	0.00582	-0.02065	-0.00019	0.00535
249			4PX	-0.02302	-0.00368	0.00462	0.00005	-0.04778
250			4PY	0.00574	0.00090	0.00261	0.00003	0.05273
251			4PZ	0.00214	0.00035	-0.00117	-0.00001	-0.01125
252			5PX	-0.04805	-0.00770	0.00501	0.00005	-0.05533
253			5PY	-0.01781	-0.00282	0.01313	0.00015	0.06173
254			5PZ	0.02100	0.00353	0.00844	0.00013	-0.01295
255	37	H	1S	0.00084	0.00013	-0.00149	-0.00002	-0.00126
256			2S	0.01343	0.00229	0.00557	0.00008	-0.00517
257	38	C	1S	0.00623	0.00099	-0.00273	-0.00003	0.00064
258			2S	-0.01026	-0.00167	0.00550	0.00006	-0.00222
259			3S	-0.05963	-0.00945	0.03305	0.00035	0.00182
260			4PX	0.02344	0.00375	-0.01147	-0.00012	-0.09239
261			4PY	0.01741	0.00278	-0.00892	-0.00010	0.11626
262			4PZ	0.01232	0.00198	-0.01043	-0.00011	-0.02388
263			5PX	-0.05171	-0.00809	0.00126	0.00005	-0.07394
264			5PY	-0.05726	-0.00901	-0.01415	-0.00012	0.08225
265			5PZ	0.01916	0.00311	-0.03089	-0.00032	-0.02006
266	39	H	1S	-0.01080	-0.00174	0.00573	0.00006	-0.00234
267			2S	-0.01503	-0.00226	-0.02231	-0.00021	-0.00848
268	40	C	1S	-0.00021	-0.00004	0.00016	0.00000	0.00182
269			2S	0.00055	-0.00004	-0.00046	-0.00001	-0.00186
270			3S	0.01406	0.00302	0.00140	-0.00005	-0.03451
271			4PX	0.00111	0.00016	0.00032	0.00001	-0.09892
272			4PY	-0.00168	-0.00030	0.00031	0.00001	0.10532
273			4PZ	0.00167	0.00027	-0.00074	-0.00001	-0.03806
274			5PX	-0.00999	-0.00068	-0.00032	0.00016	-0.05299
275			5PY	-0.00796	-0.00049	-0.00015	0.00009	0.04588
276			5PZ	0.00887	0.00003	0.00243	-0.00025	-0.01834

277	41	C	1S	-0.00015	-0.00004	-0.00005	-0.00001	0.00010
278			2S	-0.00015	0.00000	0.00006	0.00001	-0.00194
279			3S	0.00373	0.00018	0.00022	0.00009	0.02921
280			4PX	-0.00064	-0.00005	-0.00035	0.00001	0.00287
281			4PY	0.00018	0.00003	-0.00040	0.00000	-0.01355
282			4PZ	0.00006	0.00006	-0.00008	0.00002	0.00504
283			5PX	-0.00336	0.00121	-0.00115	0.00010	-0.05430
284			5PY	-0.00230	-0.00032	0.00056	-0.00010	0.04083
285			5PZ	0.00043	0.00009	-0.00075	0.00000	-0.00208
286	42	H	1S	-0.00038	-0.00003	-0.00008	0.00000	0.01288
287			2S	0.00120	-0.00012	0.00058	0.00003	0.03833
288	43	H	1S	0.00048	0.00004	-0.00005	-0.00001	-0.02292
289			2S	0.00109	0.00087	-0.00087	0.00008	-0.08861
290	44	C	1S	0.00004	-0.00003	-0.00001	-0.00002	-0.00360
291			2S	-0.00031	-0.00023	-0.00001	0.00002	0.00491
292			3S	0.00016	0.00157	0.00003	0.00053	0.06070
293			4PX	0.00046	0.00014	0.00005	0.00010	-0.01000
294			4PY	-0.00008	0.00005	0.00004	0.00007	-0.00419
295			4PZ	-0.00046	0.00002	-0.00002	0.00004	0.01144
296			5PX	-0.00463	0.00070	-0.00012	0.00047	0.03622
297			5PY	-0.00179	0.00207	-0.00090	0.00023	-0.06324
298			5PZ	0.00046	-0.00017	0.00067	-0.00034	0.02922
299	45	H	1S	-0.00002	-0.00016	-0.00004	-0.00004	0.00199
300			2S	-0.00095	0.00044	0.00026	-0.00008	0.02173
301	46	H	1S	0.00005	-0.00004	-0.00003	0.00000	-0.00132
302			2S	0.00076	0.00132	-0.00040	-0.00002	-0.05702
303	47	O	1S	0.00001	-0.00008	0.00000	0.00004	-0.00017
304			2S	-0.00003	0.00037	-0.00001	-0.00006	-0.00010
305			3S	0.00011	-0.00186	0.00003	-0.00042	0.00430
306			4PX	0.00038	-0.00224	-0.00001	0.00041	0.07814
307			4PY	0.00006	-0.00065	0.00002	-0.00045	0.08272
308			4PZ	-0.00002	0.00040	-0.00002	0.00057	-0.02839
309			5PX	0.00033	-0.00201	0.00001	-0.00012	0.06275
310			5PY	0.00010	0.00004	-0.00001	-0.00014	0.06369
311			5PZ	-0.00029	0.00177	0.00002	-0.00013	-0.02366
312	48	N	1S	0.00033	-0.00208	0.00001	-0.00052	-0.00285
313			2S	-0.00071	0.00445	-0.00001	0.00091	0.00687
314			3S	-0.00219	0.01347	-0.00003	0.00308	0.01952
315			4PX	0.00011	-0.00072	-0.00006	0.00542	0.11103
316			4PY	-0.00179	0.01109	-0.00009	0.00905	0.15124

317		4PZ	0.00114	-0.00709	0.00001	-0.00096	-0.03094
318		5PX	0.00012	-0.00070	-0.00001	0.00168	0.10673
319		5PY	0.00067	-0.00434	-0.00014	0.01245	0.13924
320		5PZ	0.00333	-0.02094	0.00007	-0.00654	-0.02863
321	49	N 1S	0.00008	-0.00054	0.00000	-0.00009	0.00008
322		2S	-0.00003	0.00025	0.00000	0.00036	-0.00102
323		3S	-0.00192	0.01188	-0.00004	-0.00027	0.00411
324		4PX	-0.00013	0.00063	0.00001	-0.00018	-0.02214
325		4PY	-0.00084	0.00517	-0.00001	0.00066	-0.02456
326		4PZ	0.00014	-0.00082	0.00000	0.00035	0.00940
327		5PX	0.00088	-0.00237	-0.00008	0.00212	-0.04149
328		5PY	-0.00056	0.00139	0.00004	-0.00088	-0.03392
329		5PZ	0.00398	-0.02141	-0.00014	0.00223	0.02093
330	50	H 1S	0.00028	-0.00188	0.00001	-0.00067	0.00350
331		2S	0.00203	-0.01155	-0.00001	-0.00288	0.01582
332	51	C 1S	0.00029	-0.00183	0.00002	-0.00180	-0.00026
333		2S	-0.00053	0.00322	-0.00004	0.00407	-0.00006
334		3S	-0.00255	0.01488	-0.00023	0.02277	0.01665
335		4PX	-0.00099	0.00612	0.00001	-0.00099	-0.07717
336		4PY	-0.00164	0.01033	-0.00001	0.00083	-0.09219
337		4PZ	0.00157	-0.00985	0.00015	-0.01417	0.01331
338		5PX	-0.00512	0.03287	-0.00017	0.01411	-0.03722
339		5PY	0.00703	-0.04431	0.00021	-0.01894	-0.07428
340		5PZ	-0.00405	0.02657	0.00009	-0.00989	0.00845
341	52	H 1S	-0.00050	0.00310	-0.00005	0.00521	-0.00033
342		2S	-0.00408	0.02672	0.00006	-0.00727	-0.00601
343	53	C 1S	-0.00010	0.00058	-0.00001	0.00083	-0.00011
344		2S	0.00012	-0.00098	0.00001	-0.00042	0.00141
345		3S	0.00199	-0.01045	0.00021	-0.02351	-0.01327
346		4PX	-0.00172	0.01084	-0.00003	0.00278	-0.05420
347		4PY	-0.00152	0.00961	0.00002	-0.00184	-0.06391
348		4PZ	0.00028	-0.00170	-0.00002	0.00164	0.01376
349		5PX	-0.00713	0.04308	-0.00002	0.00595	-0.06215
350		5PY	0.00127	-0.00674	-0.00006	0.00213	-0.09314
351		5PZ	-0.00387	0.02549	-0.00014	0.00864	0.02085
352	54	H 1S	0.00010	-0.00069	0.00001	-0.00102	-0.00148
353		2S	0.00084	-0.00402	-0.00006	0.00259	-0.00657
354	55	C 1S	-0.00018	0.00110	0.00000	0.00019	-0.00016
355		2S	0.00031	-0.00211	0.00001	-0.00051	0.00165
356		3S	0.00397	-0.02168	-0.00008	0.00380	-0.00858

357		4PX	0.00038	-0.00238	-0.00001	0.00058	0.15016
358		4PY	0.00167	-0.01053	0.00003	-0.00286	0.17388
359		4PZ	0.00087	-0.00551	0.00006	-0.00523	-0.03368
360		5PX	0.00541	-0.02724	-0.00021	0.00280	0.13876
361		5PY	-0.00428	0.02256	0.00020	-0.00671	0.17760
362		5PZ	-0.00656	0.04521	-0.00008	-0.00104	-0.03665
363 56	C	1S	0.00045	-0.00283	0.00001	-0.00114	-0.00029
364		2S	-0.00071	0.00438	-0.00002	0.00186	0.00038
365		3S	-0.00579	0.03631	-0.00026	0.02064	0.00537
366		4PX	0.00368	-0.02302	0.00005	-0.00462	-0.04782
367		4PY	0.00093	-0.00573	-0.00003	0.00261	-0.05273
368		4PZ	0.00034	-0.00214	0.00001	-0.00117	0.01125
369		5PX	0.00767	-0.04805	0.00006	-0.00501	-0.05543
370		5PY	-0.00288	0.01781	-0.00014	0.01314	-0.06171
371		5PZ	0.00319	-0.02106	-0.00005	0.00844	0.01297
372 57	H	1S	-0.00014	0.00084	-0.00002	0.00149	-0.00127
373		2S	-0.00201	0.01347	0.00004	-0.00557	-0.00520
374 58	C	1S	-0.00100	0.00623	-0.00003	0.00273	0.00065
375		2S	0.00161	-0.01027	0.00006	-0.00550	-0.00224
376		3S	0.00962	-0.05960	0.00036	-0.03305	0.00178
377		4PX	-0.00375	0.02344	-0.00012	0.01147	-0.09256
378		4PY	0.00279	-0.01740	0.00010	-0.00892	-0.11649
379		4PZ	0.00196	-0.01232	0.00011	-0.01043	0.02396
380		5PX	0.00844	-0.05165	-0.00002	-0.00126	-0.07415
381		5PY	-0.00929	0.05721	0.00018	-0.01415	-0.08240
382		5PZ	0.00302	-0.01917	0.00035	-0.03089	0.02007
383 59	H	1S	0.00172	-0.01081	0.00006	-0.00573	-0.00236
384		2S	0.00254	-0.01499	-0.00027	0.02231	-0.00853
385 60	C	1S	0.00002	-0.00021	0.00000	-0.00016	0.00183
386		2S	-0.00021	0.00051	0.00000	0.00046	-0.00187
387		3S	-0.00152	0.01430	0.00008	-0.00139	-0.03461
388		4PX	-0.00019	0.00111	0.00000	-0.00032	-0.09905
389		4PY	-0.00024	0.00169	0.00000	0.00031	-0.10544
390		4PZ	0.00027	-0.00168	0.00001	-0.00074	0.03811
391		5PX	0.00247	-0.00970	-0.00016	0.00032	-0.05313
392		5PY	-0.00202	0.00772	0.00009	-0.00015	-0.04588
393		5PZ	0.00274	-0.00843	-0.00030	0.00242	0.01828
394 61	C	1S	0.00001	-0.00016	0.00000	0.00005	0.00009
395		2S	0.00005	-0.00014	-0.00001	-0.00006	-0.00192
396		3S	-0.00099	0.00360	-0.00009	-0.00022	0.02930

397		4PX	0.00015	-0.00063	-0.00002	0.00035	0.00292
398		4PY	0.00002	-0.00018	0.00001	-0.00040	0.01358
399		4PZ	-0.00004	-0.00007	0.00002	-0.00008	-0.00506
400		5PX	0.00220	-0.00281	-0.00013	0.00114	-0.05437
401		5PY	-0.00041	0.00229	-0.00011	0.00056	-0.04083
402		5PZ	0.00005	-0.00044	0.00002	-0.00075	0.00197
403	62	H 1S	0.00009	-0.00037	0.00000	0.00008	0.01291
404		2S	-0.00049	0.00110	-0.00002	-0.00059	0.03821
405	63	H 1S	-0.00011	0.00047	0.00000	0.00005	-0.02295
406		2S	0.00049	0.00131	-0.00009	0.00087	-0.08870
407	64	C 1S	-0.00004	0.00003	0.00002	0.00001	-0.00360
408		2S	-0.00012	-0.00036	-0.00002	0.00001	0.00492
409		3S	0.00145	0.00064	-0.00053	-0.00004	0.06056
410		4PX	-0.00001	0.00048	-0.00010	-0.00005	-0.01001
411		4PY	-0.00007	0.00007	0.00007	0.00005	0.00414
412		4PZ	-0.00016	0.00044	0.00004	-0.00002	-0.01146
413		5PX	0.00211	-0.00418	-0.00047	0.00011	0.03601
414		5PY	-0.00253	0.00105	0.00024	-0.00089	0.06318
415		5PZ	0.00031	-0.00038	-0.00035	0.00067	-0.02942
416	65	H 1S	-0.00015	-0.00007	0.00004	0.00004	0.00199
417		2S	0.00072	-0.00076	0.00008	-0.00026	0.02176
418	66	H 1S	-0.00006	0.00003	-0.00001	0.00003	-0.00134
419		2S	0.00102	0.00114	0.00001	0.00040	-0.05691
420	67	O 1S	0.00001	-0.00008	0.00000	-0.00004	-0.00017
421		2S	-0.00003	0.00037	0.00001	0.00006	-0.00010
422		3S	0.00011	-0.00186	-0.00003	0.00042	0.00430
423		4PX	-0.00038	0.00224	-0.00001	0.00041	-0.07830
424		4PY	0.00006	-0.00065	-0.00002	0.00045	0.08290
425		4PZ	0.00002	-0.00040	-0.00002	0.00057	0.02846
426		5PX	-0.00033	0.00201	0.00001	-0.00012	-0.06288
427		5PY	0.00010	0.00004	0.00001	0.00014	0.06383
428		5PZ	0.00029	-0.00177	0.00002	-0.00013	0.02372
429	68	N 1S	0.00033	-0.00208	-0.00001	0.00052	-0.00285
430		2S	-0.00071	0.00446	0.00001	-0.00092	0.00686
431		3S	-0.00219	0.01348	0.00003	-0.00308	0.01950
432		4PX	-0.00011	0.00073	-0.00006	0.00542	-0.11128
433		4PY	-0.00179	0.01110	0.00009	-0.00905	0.15153
434		4PZ	-0.00114	0.00709	0.00001	-0.00097	0.03099
435		5PX	-0.00012	0.00071	-0.00001	0.00167	-0.10696
436		5PY	0.00067	-0.00434	0.00014	-0.01245	0.13951

437		5PZ	-0.00333	0.02094	0.00007	-0.00654	0.02866
438	69	N 1S	0.00008	-0.00054	0.00000	0.00009	0.00008
439		2S	-0.00003	0.00025	0.00000	-0.00036	-0.00103
440		3S	-0.00192	0.01188	0.00004	0.00027	0.00412
441		4PX	0.00013	-0.00063	0.00001	-0.00018	0.02218
442		4PY	-0.00084	0.00517	0.00001	-0.00066	-0.02460
443		4PZ	-0.00014	0.00082	0.00000	0.00035	-0.00941
444		5PX	-0.00088	0.00237	-0.00008	0.00212	0.04156
445		5PY	-0.00056	0.00139	-0.00004	0.00088	-0.03397
446		5PZ	-0.00398	0.02141	-0.00014	0.00223	-0.02099
447	70	H 1S	0.00028	-0.00188	-0.00001	0.00067	0.00351
448		2S	0.00203	-0.01155	0.00001	0.00288	0.01588
449	71	C 1S	0.00029	-0.00183	-0.00002	0.00180	-0.00026
450		2S	-0.00053	0.00322	0.00004	-0.00407	-0.00006
451		3S	-0.00255	0.01488	0.00023	-0.02277	0.01666
452		4PX	0.00099	-0.00612	0.00001	-0.00099	0.07732
453		4PY	-0.00164	0.01033	0.00001	-0.00083	-0.09238
454		4PZ	-0.00157	0.00985	0.00015	-0.01417	-0.01335
455		5PX	0.00512	-0.03287	-0.00017	0.01411	0.03737
456		5PY	0.00703	-0.04431	-0.00021	0.01894	-0.07441
457		5PZ	0.00405	-0.02657	0.00009	-0.00989	-0.00845
458	72	H 1S	-0.00050	0.00310	0.00005	-0.00521	-0.00033
459		2S	-0.00408	0.02672	-0.00006	0.00727	-0.00603
460	73	C 1S	-0.00010	0.00058	0.00001	-0.00083	-0.00011
461		2S	0.00012	-0.00098	-0.00001	0.00042	0.00141
462		3S	0.00199	-0.01044	-0.00021	0.02350	-0.01325
463		4PX	0.00172	-0.01084	-0.00003	0.00278	0.05430
464		4PY	-0.00152	0.00961	-0.00002	0.00184	-0.06403
465		4PZ	-0.00028	0.00170	-0.00002	0.00164	-0.01379
466		5PX	0.00713	-0.04308	-0.00002	0.00595	0.06228
467		5PY	0.00127	-0.00674	0.00006	-0.00213	-0.09328
468		5PZ	0.00387	-0.02549	-0.00014	0.00863	-0.02088
469	74	H 1S	0.00010	-0.00069	-0.00001	0.00102	-0.00148
470		2S	0.00084	-0.00403	0.00006	-0.00259	-0.00657
471	75	C 1S	-0.00018	0.00110	0.00000	-0.00019	-0.00016
472		2S	0.00031	-0.00211	-0.00001	0.00051	0.00165
473		3S	0.00396	-0.02167	0.00008	-0.00381	-0.00861
474		4PX	-0.00038	0.00238	-0.00001	0.00058	-0.15046
475		4PY	0.00167	-0.01053	-0.00003	0.00286	0.17423
476		4PZ	-0.00087	0.00551	0.00006	-0.00523	0.03374

477		5PX	-0.00541	0.02724	-0.00021	0.00280	-0.13906	
478		5PY	-0.00428	0.02256	-0.00020	0.00671	0.17793	
479		5PZ	0.00656	-0.04521	-0.00008	-0.00105	0.03674	
480	76	C	1S	0.00045	-0.00283	-0.00001	0.00114	-0.00029
481			2S	-0.00071	0.00438	0.00002	-0.00186	0.00038
482			3S	-0.00579	0.03630	0.00026	-0.02064	0.00537
483			4PX	-0.00368	0.02302	0.00005	-0.00462	0.04793
484			4PY	0.00093	-0.00573	0.00003	-0.00261	-0.05287
485			4PZ	-0.00034	0.00214	0.00001	-0.00117	-0.01128
486			5PX	-0.00767	0.04805	0.00006	-0.00501	0.05553
487			5PY	-0.00288	0.01781	0.00014	-0.01314	-0.06188
488			5PZ	-0.00319	0.02105	-0.00005	0.00844	-0.01300
489	77	H	1S	-0.00014	0.00084	0.00002	-0.00149	-0.00127
490			2S	-0.00201	0.01347	-0.00004	0.00557	-0.00520
491	78	C	1S	-0.00100	0.00623	0.00003	-0.00273	0.00065
492			2S	0.00161	-0.01026	-0.00006	0.00550	-0.00224
493			3S	0.00961	-0.05959	-0.00036	0.03304	0.00180
494			4PX	0.00375	-0.02344	-0.00012	0.01147	0.09273
495			4PY	0.00279	-0.01740	-0.00010	0.00892	-0.11670
496			4PZ	-0.00196	0.01232	0.00011	-0.01043	-0.02399
497			5PX	-0.00843	0.05165	-0.00002	-0.00125	0.07425
498			5PY	-0.00929	0.05721	-0.00018	0.01415	-0.08256
499			5PZ	-0.00302	0.01917	0.00035	-0.03089	-0.02012
500	79	H	1S	0.00172	-0.01081	-0.00006	0.00573	-0.00236
501			2S	0.00254	-0.01499	0.00027	-0.02231	-0.00853
502	80	C	1S	0.00002	-0.00021	0.00000	0.00016	0.00183
503			2S	-0.00021	0.00051	0.00000	-0.00046	-0.00187
504			3S	-0.00152	0.01430	-0.00008	0.00139	-0.03466
505			4PX	0.00019	-0.00111	0.00000	-0.00032	0.09926
506			4PY	-0.00024	0.00169	0.00000	-0.00031	-0.10567
507			4PZ	-0.00027	0.00168	0.00001	-0.00074	-0.03819
508			5PX	-0.00247	0.00970	-0.00016	0.00032	0.05322
509			5PY	-0.00202	0.00772	-0.00009	0.00015	-0.04601
510			5PZ	-0.00274	0.00843	-0.00030	0.00242	-0.01836
511	81	C	1S	0.00001	-0.00016	0.00000	-0.00005	0.00010
512			2S	0.00005	-0.00014	0.00001	0.00006	-0.00193
513			3S	-0.00099	0.00360	0.00009	0.00022	0.02934
514			4PX	-0.00015	0.00063	-0.00002	0.00035	-0.00290
515			4PY	0.00002	-0.00018	-0.00001	0.00040	0.01360
516			4PZ	0.00004	0.00007	0.00002	-0.00008	0.00506

517		5PX	-0.00219	0.00281	-0.00013	0.00114	0.05448
518		5PY	-0.00041	0.00229	0.00011	-0.00056	-0.04094
519		5PZ	-0.00005	0.00044	0.00002	-0.00075	-0.00202
520	82	H 1S	0.00009	-0.00037	0.00000	-0.00008	0.01293
521		2S	-0.00049	0.00110	0.00002	0.00059	0.03836
522	83	H 1S	-0.00011	0.00047	0.00000	-0.00005	-0.02300
523		2S	0.00049	0.00131	0.00009	-0.00087	-0.08890
524	84	C 1S	-0.00004	0.00003	-0.00002	-0.00001	-0.00361
525		2S	-0.00012	-0.00036	0.00002	-0.00001	0.00493
526		3S	0.00145	0.00064	0.00053	0.00004	0.06079
527		4PX	0.00001	-0.00048	-0.00010	-0.00005	0.01003
528		4PY	-0.00007	0.00007	-0.00007	-0.00005	0.00417
529		4PZ	0.00016	-0.00044	0.00004	-0.00002	0.01148
530		5PX	-0.00211	0.00418	-0.00047	0.00011	-0.03619
531		5PY	-0.00253	0.00105	-0.00024	0.00089	0.06336
532		5PZ	-0.00031	0.00038	-0.00035	0.00067	0.02941
533	85	H 1S	-0.00015	-0.00007	-0.00004	-0.00004	0.00200
534		2S	0.00072	-0.00076	-0.00008	0.00026	0.02181
535	86	H 1S	-0.00006	0.00003	0.00001	-0.00003	-0.00133
536		2S	0.00102	0.00114	-0.00001	-0.00040	-0.05710

HOMO (#92) and LUMO(#93) for **3**:

		91	92	93	94	95
		O	O	V	V	V
EIGENVALUES --		-0.21169	-0.20714	-0.09227	-0.08495	-0.07011
1	1 Zn 1S	0.00167	0.00011	-0.01379	0.00561	0.00258
2	2S	0.01282	0.00181	0.01186	-0.00813	-0.00066
3	3PX	0.01473	0.00593	0.00702	0.02770	0.00158
4	3PY	-0.00475	-0.00285	0.03812	-0.00965	-0.00489
5	3PZ	0.00336	-0.05338	0.00813	0.01116	0.02496
6	4PX	0.01435	0.00064	0.00139	0.01070	-0.00840
7	4PY	-0.00400	-0.00231	-0.00285	0.00643	0.00227
8	4PZ	-0.00326	0.09278	-0.00039	-0.00630	-0.01059
9	5D 0	-0.00566	-0.00245	0.00142	0.00058	-0.00040
10	5D+1	-0.05652	-0.00162	-0.00444	-0.00126	0.00035
11	5D-1	-0.00271	0.06235	0.00651	0.00844	0.01527
12	5D+2	0.00060	-0.00022	-0.04068	0.01168	0.00358
13	5D-2	-0.00926	-0.00326	-0.00568	-0.02171	0.00200
14	6D 0	-0.00092	-0.00041	-0.00109	0.00063	0.00008
15	6D+1	-0.00711	-0.00018	-0.00059	-0.00007	0.00007

16		6D-1	-0.00036	0.00704	0.00078	0.00111	0.00134
17		6D+2	0.00026	0.00015	-0.00532	0.00161	0.00040
18		6D-2	-0.00194	-0.00060	-0.00105	-0.00510	0.00066
19	2	I 1S	0.00070	-0.00893	-0.00245	-0.00040	-0.00110
20		2S	0.00115	-0.03017	-0.00990	0.00014	-0.00384
21		3PX	0.42876	0.02237	-0.00489	-0.00663	-0.01048
22		3PY	-0.00688	-0.26815	0.00096	0.00403	0.01456
23		3PZ	-0.00232	0.29125	0.01575	0.00331	0.00097
24		4PX	0.42464	0.02173	-0.00443	-0.01130	-0.00339
25		4PY	-0.00720	-0.27360	0.00332	0.00470	0.01799
26		4PZ	-0.00075	0.27504	0.02204	0.00435	0.00995
27	3	I 1S	0.00030	0.00879	-0.00086	0.00122	0.00138
28		2S	-0.00019	0.03068	-0.00468	0.00341	0.00475
29		3PX	-0.31537	0.00214	-0.00021	-0.00705	0.00928
30		3PY	-0.02595	0.24600	-0.00601	-0.00401	-0.01283
31		3PZ	-0.01484	0.27893	-0.00625	0.00641	0.00133
32		4PX	-0.32090	0.00097	-0.00208	-0.01131	0.00831
33		4PY	-0.02725	0.25195	-0.00709	-0.00818	-0.01753
34		4PZ	-0.01419	0.26237	-0.00982	0.01027	0.01158
35	4	O 1S	0.00006	0.00002	-0.00036	0.00004	-0.00085
36		2S	0.00003	0.00002	0.00115	0.00012	0.00206
37		3S	-0.00206	-0.00080	0.00188	-0.00079	0.00326
38		4PX	0.00324	0.00004	0.15621	0.09502	-0.05208
39		4PY	-0.00086	-0.00131	0.08882	0.05987	-0.02318
40		4PZ	0.00132	0.00001	0.06960	0.04470	-0.02166
41		5PX	0.00061	-0.00017	0.12852	0.07919	-0.04106
42		5PY	0.00146	-0.00029	0.06016	0.04573	-0.01941
43		5PZ	0.00161	0.00025	0.05533	0.03625	-0.01716
44	5	O 1S	-0.00003	-0.00001	-0.00040	0.00005	0.00160
45		2S	0.00020	-0.00007	-0.00009	-0.00046	-0.00395
46		3S	-0.00146	0.00089	0.00919	0.00009	-0.00739
47		4PX	-0.00046	-0.00008	-0.11096	0.21233	-0.05908
48		4PY	-0.00050	0.00109	0.04859	-0.08900	0.01470
49		4PZ	-0.00037	0.00017	-0.01566	0.03100	-0.00922
50		5PX	0.00088	-0.00024	-0.09192	0.17558	-0.04294
51		5PY	0.00161	-0.00007	0.03056	-0.06487	0.01519
52		5PZ	-0.00081	0.00010	-0.01320	0.02236	-0.00730
53	6	N 1S	0.00336	0.00138	-0.00498	0.00504	-0.00045
54		2S	-0.00751	-0.00305	0.01464	-0.00860	0.00183
55		3S	-0.01308	-0.00562	0.01923	-0.04303	-0.00045

56		4PX	0.00540	-0.00206	0.22922	0.15950	-0.03643
57		4PY	-0.01621	-0.00974	0.21421	0.10173	-0.02946
58		4PZ	-0.00384	-0.00005	0.07030	0.03636	-0.01934
59		5PX	0.01587	-0.00129	0.21770	0.13847	-0.04172
60		5PY	-0.00813	-0.01002	0.18680	0.08585	-0.02598
61		5PZ	-0.03031	-0.00137	0.06198	0.02472	-0.01158
62	7	N 1S	0.00022	0.00004	-0.00052	0.00089	-0.00024
63		2S	-0.00083	-0.00028	0.00125	-0.00114	0.00001
64		3S	0.00416	0.00170	0.01332	-0.00703	0.00667
65		4PX	-0.00209	0.00041	-0.03921	-0.00972	-0.00153
66		4PY	-0.00331	-0.00045	-0.03064	-0.00844	0.00223
67		4PZ	0.00030	0.00090	-0.01670	-0.00702	-0.00085
68		5PX	0.00272	0.00118	-0.07842	-0.02397	0.00232
69		5PY	0.00049	0.00042	-0.01899	-0.01410	0.00158
70		5PZ	-0.01569	-0.00106	-0.05880	-0.03790	-0.01844
71	8	H 1S	-0.00131	-0.00106	-0.00777	-0.00537	-0.00049
72		2S	-0.01376	-0.00438	-0.04291	-0.03205	-0.01669
73	9	N 1S	0.00015	-0.00015	-0.00075	-0.00056	0.00026
74		2S	-0.00060	0.00028	0.00191	0.00211	0.00063
75		3S	0.00441	0.00029	0.00829	-0.00936	-0.01616
76		4PX	-0.00033	0.00055	0.01408	0.00526	0.00315
77		4PY	-0.00071	0.00071	-0.01070	0.00433	-0.00162
78		4PZ	-0.00110	0.00066	0.00470	0.00085	-0.00264
79		5PX	-0.00325	0.00218	0.04169	-0.05110	-0.01870
80		5PY	-0.00050	0.00231	-0.00055	-0.00026	0.01211
81		5PZ	0.01574	-0.00164	0.01548	-0.02403	-0.04805
82	10	H 1S	-0.00113	0.00097	-0.00199	0.00372	0.00414
83		2S	-0.01535	0.00564	-0.01455	0.02452	0.05003
84	11	N 1S	-0.00090	-0.00073	-0.00682	-0.00057	0.00182
85		2S	0.00185	0.00126	0.01716	-0.00219	-0.00481
86		3S	0.00733	0.00623	0.03795	0.01723	-0.00982
87		4PX	-0.00038	-0.00026	-0.13676	0.27010	-0.01124
88		4PY	0.00517	0.00443	0.12549	-0.17527	0.00355
89		4PZ	0.00083	0.00242	-0.01621	0.01746	-0.01128
90		5PX	-0.00300	-0.00299	-0.13854	0.25183	-0.01436
91		5PY	0.01001	0.00314	0.11121	-0.14792	0.00235
92		5PZ	0.02890	0.00115	-0.01849	0.01757	-0.02545
93	12	C 1S	-0.00549	-0.00399	-0.00010	-0.00259	-0.00169
94		2S	0.00849	0.00838	0.00116	0.00883	0.00980
95		3S	0.05288	0.04423	0.01087	0.00129	-0.00537

96		4PX	-0.01248	-0.00752	-0.12561	-0.05519	0.11190
97		4PY	0.01649	0.01450	-0.10355	-0.04128	0.09137
98		4PZ	-0.01433	-0.01919	-0.03913	-0.00929	0.03741
99		5PX	0.04694	0.01905	-0.07779	-0.02417	0.15095
100		5PY	-0.06984	0.00056	-0.05776	-0.02292	0.07564
101		5PZ	-0.02035	-0.02520	-0.03150	-0.00053	0.05919
102	13	H 1S	0.00905	0.00830	-0.00755	0.00035	0.00360
103		2S	0.01364	-0.01744	-0.01906	0.00199	0.03024
104	14	C 1S	0.00270	0.00160	-0.00080	0.00057	0.00035
105		2S	-0.00413	-0.00269	0.00340	-0.00101	-0.00115
106		3S	-0.04294	-0.02594	-0.00189	0.01202	0.02044
107		4PX	0.01932	0.00210	-0.15060	-0.10822	-0.08744
108		4PY	-0.00289	-0.00877	-0.10016	-0.08187	-0.06375
109		4PZ	0.00252	-0.00154	-0.04866	-0.03683	-0.03024
110		5PX	0.04373	-0.00042	-0.16965	-0.11241	-0.08288
111		5PY	-0.04849	-0.01844	-0.12931	-0.09412	-0.09821
112		5PZ	0.01826	0.01022	-0.06321	-0.04116	-0.03752
113	15	H 1S	-0.00043	-0.00164	-0.00382	-0.00061	0.00087
114		2S	-0.00202	0.00444	-0.01360	-0.00481	-0.00765
115	16	C 1S	-0.00021	0.00001	0.00056	-0.00003	0.00059
116		2S	0.00089	0.00037	0.00019	0.00117	-0.00073
117		3S	-0.00215	-0.00508	-0.02560	0.00003	-0.00135
118		4PX	0.00511	0.00161	0.32040	0.18277	-0.04839
119		4PY	0.00534	0.00245	0.21627	0.11917	-0.03108
120		4PZ	-0.00699	-0.00819	0.08975	0.05025	-0.01726
121		5PX	-0.00350	0.00138	0.28133	0.17821	-0.04503
122		5PY	-0.01501	0.00040	0.24788	0.10850	-0.05123
123		5PZ	0.06145	0.00110	0.09615	0.07240	0.03767
124	17	C 1S	-0.00096	-0.00131	-0.00132	-0.00006	-0.00105
125		2S	0.00046	0.00140	0.00593	0.00184	0.00335
126		3S	0.02904	0.02911	-0.01833	-0.00701	-0.00615
127		4PX	-0.01096	-0.00042	-0.07480	-0.03819	0.13206
128		4PY	-0.00417	0.00574	-0.04580	-0.02958	0.10357
129		4PZ	-0.00153	0.00178	-0.02367	-0.01393	0.03038
130		5PX	-0.04366	-0.00737	-0.08774	-0.04933	0.12047
131		5PY	0.03879	0.01036	-0.05886	-0.00623	0.12412
132		5PZ	0.01432	0.00765	-0.03652	-0.01858	0.04936
133	18	H 1S	0.00160	0.00202	-0.00482	-0.00192	0.00045
134		2S	0.00639	-0.00085	0.00695	0.01702	0.00048
135	19	C 1S	0.00279	0.00288	0.00062	-0.00169	0.00423

136		2S	-0.00223	-0.00452	-0.00155	0.00394	-0.01111
137		3S	-0.03562	-0.04407	0.01800	0.01257	-0.04864
138		4PX	-0.00018	0.00726	-0.21325	-0.12785	-0.07207
139		4PY	-0.00806	-0.00417	-0.16818	-0.09725	-0.06692
140		4PZ	-0.01527	-0.02027	-0.05911	-0.03278	-0.03159
141		5PX	-0.04825	-0.00840	-0.17564	-0.12820	-0.09362
142		5PY	0.06824	0.01775	-0.12374	-0.05419	-0.05739
143		5PZ	0.01339	-0.01849	-0.01308	-0.02329	-0.04181
144	20	H 1S	-0.00359	-0.00633	-0.00705	0.00042	-0.00665
145		2S	-0.02985	0.01525	-0.03096	-0.01992	0.02977
146	21	C 1S	-0.00029	-0.00029	-0.00034	-0.00314	0.00040
147		2S	0.00120	0.00077	0.00478	0.01030	-0.00145
148		3S	0.00815	0.00152	-0.02577	0.00976	0.01264
149		4PX	-0.00173	-0.00041	-0.21346	-0.13057	0.05399
150		4PY	0.00154	0.00134	-0.10631	-0.07981	0.03212
151		4PZ	-0.00145	-0.00080	-0.09492	-0.06804	0.02438
152		5PX	-0.00031	-0.00176	-0.13378	-0.08286	0.04442
153		5PY	-0.00099	0.00142	0.01644	-0.01575	0.01751
154		5PZ	0.00321	0.00154	-0.05487	-0.03658	0.01835
155	22	C 1S	0.00020	0.00009	0.00140	0.00295	-0.00106
156		2S	-0.00025	-0.00037	-0.00417	-0.00931	0.00274
157		3S	-0.00338	0.00080	0.03394	0.03595	-0.00281
158		4PX	0.00113	0.00057	0.01498	0.00746	-0.00209
159		4PY	-0.00104	-0.00065	-0.00227	0.00397	0.00033
160		4PZ	-0.00046	-0.00049	0.00656	0.00389	-0.00041
161		5PX	0.00088	-0.00035	-0.09952	-0.02834	0.01247
162		5PY	0.00097	0.00112	0.01396	0.00094	0.00399
163		5PZ	-0.00338	-0.00081	0.01640	0.00812	-0.01938
164	23	H 1S	-0.00004	0.00002	-0.01714	-0.01348	0.00429
165		2S	-0.00084	-0.00023	-0.02987	-0.01601	-0.00341
166	24	H 1S	0.00003	0.00004	-0.01617	-0.01801	0.00563
167		2S	0.00202	0.00107	-0.06327	-0.05039	0.02568
168	25	C 1S	-0.00009	0.00000	-0.01578	-0.00599	0.00320
169		2S	0.00015	0.00004	0.03742	0.00949	-0.00672
170		3S	0.00195	-0.00049	0.10891	0.05989	-0.01802
171		4PX	-0.00061	-0.00015	-0.06620	-0.04491	0.01696
172		4PY	0.00008	0.00013	0.01236	-0.02395	0.00424
173		4PZ	-0.00024	-0.00002	-0.02531	-0.01277	0.00342
174		5PX	-0.00035	-0.00021	-0.07151	0.01949	0.00951
175		5PY	-0.00261	-0.00011	-0.06786	-0.03844	0.00371

176		5PZ	0.00134	0.00093	-0.01620	0.04818	0.02883
177	26	H 1S	0.00007	0.00007	0.01019	0.00019	-0.00165
178		2S	0.00160	0.00036	0.02889	0.02009	-0.00083
179	27	H 1S	0.00004	0.00003	-0.00196	0.00422	-0.00109
180		2S	-0.00096	-0.00027	0.01085	-0.02779	-0.02050
181	28	C 1S	0.00011	0.00006	-0.00388	0.01798	-0.00220
182		2S	-0.00012	-0.00014	0.00756	-0.03698	0.00598
183		3S	-0.00035	-0.00032	0.02191	-0.16821	-0.00422
184		4PX	0.00034	-0.00004	0.05777	-0.06444	0.00140
185		4PY	-0.00014	-0.00024	-0.01242	-0.03162	0.00663
186		4PZ	-0.00017	-0.00005	0.00669	-0.04008	0.00767
187		5PX	0.00173	-0.00132	0.04636	-0.09326	0.00283
188		5PY	-0.00102	0.00048	0.04103	-0.01561	0.02975
189		5PZ	-0.00165	-0.00023	-0.02589	-0.11594	-0.02436
190	29	H 1S	0.00004	-0.00009	-0.00223	-0.00018	0.00054
191		2S	-0.00095	-0.00024	-0.02094	-0.06875	-0.00882
192	30	H 1S	-0.00008	0.00012	-0.00553	0.00781	-0.00058
193		2S	-0.00038	0.00029	0.01517	0.02900	0.02350
194	31	C 1S	0.00006	-0.00012	-0.00215	-0.00386	0.00124
195		2S	0.00010	0.00030	0.00149	0.01085	-0.00290
196		3S	-0.00214	0.00003	0.07702	-0.02956	-0.01078
197		4PX	-0.00046	0.00023	-0.02032	-0.00053	0.00406
198		4PY	-0.00077	0.00072	0.00463	-0.00729	-0.00001
199		4PZ	0.00035	-0.00047	-0.00028	-0.00370	0.00109
200		5PX	-0.00075	-0.00012	0.03766	-0.13888	-0.03088
201		5PY	0.00123	-0.00121	-0.03025	-0.04257	-0.00170
202		5PZ	0.00270	-0.00132	-0.01623	0.00335	0.02000
203	32	H 1S	0.00000	0.00003	0.00069	0.00706	-0.00032
204		2S	-0.00081	0.00061	-0.00092	0.02628	-0.01226
205	33	H 1S	0.00016	-0.00008	-0.02736	0.03827	-0.00295
206		2S	0.00183	-0.00091	-0.10745	0.13275	0.00208
207	34	C 1S	-0.00025	0.00030	-0.00137	0.00071	0.00003
208		2S	0.00112	-0.00088	0.00624	-0.01098	-0.00094
209		3S	0.00643	-0.00024	0.00296	0.06171	-0.00131
210		4PX	-0.00023	-0.00057	0.14518	-0.29733	0.03223
211		4PY	0.00213	-0.00137	-0.06353	0.12281	-0.01557
212		4PZ	0.00091	-0.00096	0.02680	-0.05090	0.00325
213		5PX	-0.00003	-0.00128	0.10144	-0.17764	0.05234
214		5PY	0.00020	-0.00081	0.02185	0.00141	-0.04769
215		5PZ	-0.00343	0.00265	0.03891	-0.01385	0.00097

216	35	C	1S	-0.00040	0.00028	0.00051	-0.00115	0.00027
217			2S	0.00155	-0.00058	-0.00134	0.00159	-0.00200
218			3S	0.00218	-0.00535	-0.01703	0.03510	-0.00309
219			4PX	0.00150	0.00073	-0.19114	0.31222	0.00094
220			4PY	0.00142	-0.00214	0.11131	-0.18481	-0.00230
221			4PZ	0.00830	-0.00812	-0.01632	0.02525	-0.00440
222			5PX	-0.00018	0.00250	-0.15978	0.30737	0.02057
223			5PY	-0.01113	0.00128	0.16367	-0.21007	-0.00359
224			5PZ	-0.06535	-0.00079	0.01238	0.03338	0.07256
225	36	C	1S	0.00210	-0.00175	-0.00043	-0.00012	-0.00034
226			2S	-0.00248	0.00259	0.00191	-0.00202	0.00228
227			3S	-0.03768	0.03029	-0.02438	0.00103	-0.02657
228			4PX	-0.01742	0.00126	0.03777	-0.14706	-0.30716
229			4PY	-0.00127	0.01019	-0.01645	0.09320	0.19210
230			4PZ	-0.00089	-0.00080	0.00418	-0.01526	-0.03728
231			5PX	-0.04432	0.00069	0.06860	-0.17485	-0.34462
232			5PY	-0.05028	0.01663	-0.03400	0.11968	0.25450
233			5PZ	-0.01119	0.00609	0.01829	-0.02282	-0.04964
234	37	H	1S	-0.00120	0.00161	-0.00240	0.00168	0.00116
235			2S	-0.00726	-0.00129	-0.01073	0.00588	0.01811
236	38	C	1S	-0.00516	0.00444	0.00193	0.00152	0.00109
237			2S	0.00808	-0.00855	-0.00625	-0.00458	-0.00793
238			3S	0.05380	-0.05487	0.01512	-0.01460	0.02996
239			4PX	0.00713	-0.00911	0.12187	-0.14265	0.31788
240			4PY	0.01770	-0.01444	-0.08606	0.09514	-0.21057
241			4PZ	0.01909	-0.02319	0.01135	-0.00917	0.02301
242			5PX	-0.04501	0.01423	0.10376	-0.10328	0.37808
243			5PY	-0.08202	0.00569	-0.05415	0.05881	-0.17741
244			5PZ	0.00951	-0.02561	0.02463	-0.00903	0.05083
245	39	H	1S	0.00774	-0.00905	-0.00667	0.00118	-0.00160
246			2S	0.02056	0.02328	-0.02723	0.01252	-0.04193
247	40	C	1S	0.00352	-0.00256	0.00069	0.00003	-0.00137
248			2S	-0.00375	0.00438	-0.00121	0.00042	0.00541
249			3S	-0.03223	0.03763	0.01849	-0.00374	-0.01189
250			4PX	-0.00476	0.00447	0.10154	-0.20094	-0.31023
251			4PY	-0.00918	0.00604	-0.06774	0.13297	0.20440
252			4PZ	0.01098	-0.01955	0.00547	-0.01556	-0.02478
253			5PX	0.03570	-0.00915	0.06345	-0.18307	-0.32660
254			5PY	0.06957	-0.01155	-0.05719	0.09171	0.16783
255			5PZ	-0.00616	-0.02564	-0.01888	0.01176	-0.00939

256	41	H	1S	-0.00531	0.00636	-0.00375	0.00263	0.00260
257			2S	-0.02539	-0.01842	-0.01742	0.02723	0.01600
258	42	C	1S	-0.00168	0.00130	-0.00103	0.00048	0.00050
259			2S	0.00286	-0.00173	0.00280	-0.00251	-0.00387
260			3S	0.02266	-0.02500	-0.00093	0.00403	0.02791
261			4PX	0.01686	0.00075	0.08995	-0.10272	0.31619
262			4PY	-0.00039	-0.00661	-0.04968	0.06443	-0.20230
263			4PZ	0.00048	0.00085	0.00509	-0.00765	0.01073
264			5PX	0.04137	-0.00354	0.08921	-0.12436	0.30775
265			5PY	0.04396	-0.01198	-0.08630	0.05664	-0.22323
266			5PZ	-0.01708	0.01108	0.01504	-0.02697	0.02334
267	43	H	1S	0.00022	-0.00158	-0.00246	0.00215	0.00091
268			2S	0.00446	0.00337	-0.00601	-0.01594	-0.00601

HOMO (#184) and LUMO(#185) for 4:

			181	182	183	184	185
			(A)--O	(A)--O	(A)--O	(A)--O	(A)--V
EIGENVALUES --			-0.23814	-0.23814	-0.23310	-0.23310	-0.08373
1	1	Zn 1S	-0.00091	0.00326	0.00179	0.00005	-0.00342
2		2S	-0.00449	0.01608	0.00912	0.00023	0.00781
3		3PX	-0.00069	0.00247	-0.01270	-0.00033	0.02242
4		3PY	-0.00712	0.02550	0.01148	0.00029	-0.01025
5		3PZ	-0.00005	0.00020	-0.02327	-0.00059	-0.00613
6		4PX	0.00185	-0.00662	-0.00957	-0.00024	-0.00390
7		4PY	-0.00707	0.02530	0.00766	0.00022	0.00126
8		4PZ	0.00408	-0.01457	0.08746	0.00224	-0.00033
9		5D 0	0.00128	-0.00459	-0.01609	-0.00041	0.00539
10		5D+1	0.00391	-0.01399	0.08128	0.00209	-0.00812
11		5D-1	0.01944	-0.06956	-0.01393	-0.00036	-0.00352
12		5D+2	0.00106	-0.00383	0.00592	0.00015	0.03011
13		5D-2	0.00575	-0.02056	-0.00032	-0.00001	-0.00459
14		6D 0	0.00027	-0.00097	-0.00296	-0.00008	0.00050
15		6D+1	0.00060	-0.00214	0.01257	0.00032	-0.00131
16		6D-1	0.00310	-0.01110	-0.00218	-0.00006	-0.00054
17		6D+2	0.00044	-0.00159	0.00050	0.00001	0.00438
18		6D-2	0.00122	-0.00436	-0.00039	-0.00001	-0.00004
19	2	Cl 1S	-0.00033	0.00117	-0.00791	-0.00020	-0.00110
20		2S	-0.00070	0.00249	-0.01895	-0.00049	-0.00330
21		3PX	-0.00936	0.03349	-0.25002	-0.00641	-0.00195
22		3PY	-0.11700	0.41865	0.07968	0.00204	0.00056

23		3PZ	0.00941	-0.03366	0.31100	0.00798	0.00578
24		4PX	-0.01082	0.03869	-0.28385	-0.00728	-0.00186
25		4PY	-0.13149	0.47050	0.08821	0.00226	0.00244
26		4PZ	0.00963	-0.03448	0.33990	0.00872	0.00927
27	3	Cl 1S	-0.00005	0.00018	0.00729	0.00019	-0.00280
28		2S	0.00090	-0.00321	0.02339	0.00060	-0.00748
29		3PX	0.02036	-0.07286	0.19984	0.00513	0.00237
30		3PY	0.06665	-0.23850	-0.00327	-0.00009	0.00358
31		3PZ	0.00176	-0.00627	0.25221	0.00647	-0.01136
32		4PX	0.02340	-0.08373	0.22798	0.00585	0.00352
33		4PY	0.07723	-0.27636	-0.00712	-0.00018	0.00271
34		4PZ	0.00198	-0.00705	0.27425	0.00704	-0.01679
35	4	O 1S	0.00001	-0.00005	0.00001	0.00000	-0.00020
36		2S	-0.00008	0.00024	-0.00009	-0.00001	0.00031
37		3S	0.00040	-0.00132	0.00071	0.00005	0.00252
38		4PX	0.00016	-0.00063	0.00074	0.00002	0.05228
39		4PY	0.00035	-0.00130	0.00124	0.00002	-0.13957
40		4PZ	0.00013	-0.00047	0.00036	0.00001	-0.04869
41		5PX	-0.00035	0.00141	0.00012	-0.00001	0.03778
42		5PY	-0.00012	0.00015	0.00082	0.00002	-0.10880
43		5PZ	0.00006	-0.00036	0.00040	0.00004	-0.03809
44	5	O 1S	-0.00005	-0.00001	0.00000	-0.00004	-0.00029
45		2S	-0.00014	-0.00002	-0.00001	0.00005	0.00146
46		3S	0.00264	0.00065	0.00005	0.00068	-0.00327
47		4PX	0.00433	0.00116	0.00004	0.00011	-0.06030
48		4PY	0.00595	0.00164	-0.00003	0.00235	-0.03104
49		4PZ	0.00201	0.00055	-0.00001	0.00082	-0.01284
50		5PX	0.00356	0.00096	0.00004	0.00025	-0.04796
51		5PY	0.00044	0.00009	-0.00011	0.00102	-0.02269
52		5PZ	0.00140	0.00038	0.00000	0.00061	-0.01167
53	6	N 1S	0.00035	-0.00124	0.00026	0.00001	-0.00262
54		2S	-0.00078	0.00278	-0.00111	-0.00003	0.00777
55		3S	-0.00149	0.00525	0.00263	0.00008	0.01296
56		4PX	-0.00093	0.00325	0.00502	0.00013	0.12617
57		4PY	-0.00149	0.00539	-0.00950	-0.00024	-0.19084
58		4PZ	-0.00058	0.00212	-0.00306	-0.00008	-0.08775
59		5PX	-0.00602	0.02151	0.00271	0.00005	0.11027
60		5PY	0.00142	-0.00505	-0.00906	-0.00024	-0.18007
61		5PZ	-0.00604	0.02168	-0.01780	-0.00047	-0.08187
62	7	N 1S	-0.00011	0.00036	-0.00008	0.00000	0.00071

63		2S	0.00017	-0.00046	0.00003	0.00000	-0.00236
64		3S	0.00045	-0.00182	0.00128	0.00009	0.00015
65		4PX	0.00065	-0.00258	0.00186	0.00003	-0.01838
66		4PY	-0.00008	0.00038	-0.00152	-0.00005	0.03317
67		4PZ	0.00006	-0.00023	-0.00024	-0.00001	0.01661
68		5PX	0.00130	-0.00495	0.00147	0.00022	-0.01403
69		5PY	0.00168	-0.00597	-0.00057	0.00007	0.06520
70		5PZ	-0.00340	0.01218	-0.00230	-0.00005	0.02530
71	8	H 1S	0.00022	-0.00077	0.00070	0.00002	0.00006
72		2S	0.00376	-0.01309	0.00336	0.00005	0.00195
73	9	N 1S	-0.00026	-0.00007	0.00000	0.00011	-0.00036
74		2S	0.00093	0.00026	-0.00001	0.00019	0.00104
75		3S	-0.00423	-0.00118	0.00017	-0.00401	0.00321
76		4PX	-0.00957	-0.00273	0.00008	-0.00194	0.01674
77		4PY	-0.00205	-0.00059	0.00003	-0.00070	0.00703
78		4PZ	-0.00025	-0.00008	-0.00002	0.00070	0.00419
79		5PX	-0.00482	-0.00142	-0.00001	-0.00153	0.02095
80		5PY	0.00389	0.00097	0.00016	-0.00170	0.01193
81		5PZ	-0.01882	-0.00519	0.00008	0.00060	0.00491
82	10	H 1S	0.00114	0.00032	-0.00003	0.00098	0.00114
83		2S	0.01523	0.00413	-0.00015	0.00196	0.00193
84	11	N 1S	-0.00540	-0.00151	0.00005	-0.00174	-0.00370
85		2S	0.01189	0.00332	-0.00010	0.00374	0.00854
86		3S	0.02564	0.00716	-0.00017	0.00690	0.02335
87		4PX	-0.02498	-0.00701	0.00032	-0.01195	-0.10068
88		4PY	0.01768	0.00493	-0.00008	0.00319	-0.02604
89		4PZ	-0.00701	-0.00197	0.00003	-0.00087	-0.02454
90		5PX	-0.00906	-0.00255	0.00040	-0.01463	-0.09343
91		5PY	0.02761	0.00771	-0.00033	0.01228	-0.03243
92		5PZ	-0.03055	-0.00854	0.00028	-0.01168	-0.02558
93	12	C 1S	0.00151	-0.00539	0.00316	0.00008	-0.00025
94		2S	-0.00202	0.00724	-0.00627	-0.00016	0.00043
95		3S	-0.02006	0.07144	-0.02914	-0.00070	0.01236
96		4PX	-0.00639	0.02290	-0.01169	-0.00030	-0.08073
97		4PY	-0.00103	0.00370	-0.00624	-0.00016	0.13385
98		4PZ	-0.00489	0.01750	-0.01592	-0.00041	0.06123
99		5PX	0.02174	-0.07782	0.00831	0.00027	-0.04944
100		5PY	0.01261	-0.04512	0.02575	0.00068	0.09817
101		5PZ	-0.00621	0.02211	-0.01721	-0.00041	0.04801
102	13	H 1S	-0.00263	0.00943	-0.00729	-0.00018	-0.00335

103		2S	0.00019	-0.00055	0.01347	0.00029	-0.01271
104	14	C 1S	-0.00068	0.00242	-0.00130	-0.00003	-0.00062
105		2S	0.00037	-0.00132	0.00161	0.00005	0.00191
106		3S	0.01743	-0.06205	0.02730	0.00062	0.00583
107		4PX	0.00182	-0.00655	0.00719	0.00018	-0.04294
108		4PY	0.00356	-0.01281	0.00092	0.00002	0.08601
109		4PZ	0.00069	-0.00255	-0.00134	-0.00003	0.03534
110		5PX	0.01235	-0.04405	0.01466	0.00035	-0.06300
111		5PY	0.00898	-0.03187	-0.00543	-0.00019	0.10730
112		5PZ	0.00062	-0.00236	-0.00191	0.00003	0.04634
113	15	H 1S	0.00032	-0.00115	0.00116	0.00003	-0.00352
114		2S	0.00197	-0.00691	0.00021	-0.00005	-0.00731
115	16	C 1S	0.00031	-0.00110	0.00043	0.00001	0.00054
116		2S	-0.00048	0.00164	-0.00017	0.00000	0.00000
117		3S	-0.00688	0.02474	-0.01124	-0.00045	-0.03050
118		4PX	-0.00141	0.00516	-0.00403	-0.00009	0.12671
119		4PY	0.00050	-0.00172	0.00398	0.00011	-0.24945
120		4PZ	-0.00182	0.00651	-0.00434	-0.00012	-0.09896
121		5PX	0.00489	-0.01785	-0.00276	0.00025	0.13445
122		5PY	-0.00152	0.00501	0.00450	0.00028	-0.23739
123		5PZ	0.01149	-0.04130	0.00311	0.00008	-0.09691
124	17	C 1S	0.00033	-0.00120	0.00109	0.00003	-0.00069
125		2S	-0.00030	0.00107	0.00009	0.00000	0.00243
126		3S	-0.00781	0.02786	-0.03513	-0.00088	-0.00461
127		4PX	-0.00044	0.00161	-0.00613	-0.00016	-0.04647
128		4PY	-0.00248	0.00882	0.00286	0.00007	0.08526
129		4PZ	-0.00052	0.00182	0.00299	0.00008	0.03282
130		5PX	-0.00800	0.02871	-0.01193	-0.00031	-0.05602
131		5PY	-0.01084	0.03879	-0.01254	-0.00031	0.09003
132		5PZ	0.00695	-0.02487	0.01551	0.00037	0.05409
133	18	H 1S	0.00003	-0.00011	-0.00069	-0.00002	-0.00281
134		2S	0.00111	-0.00388	0.00421	0.00008	0.00268
135	19	C 1S	-0.00057	0.00203	-0.00165	-0.00004	-0.00058
136		2S	0.00044	-0.00157	0.00215	0.00006	0.00152
137		3S	0.00486	-0.01738	0.02523	0.00059	0.01496
138		4PX	0.00216	-0.00768	0.00293	0.00007	-0.08477
139		4PY	-0.00021	0.00075	0.00393	0.00010	0.14159
140		4PZ	-0.00168	0.00602	-0.01050	-0.00027	0.05993
141		5PX	-0.01815	0.06493	-0.03490	-0.00086	-0.07188
142		5PY	-0.00677	0.02421	-0.01222	-0.00027	0.10539

143		5PZ	0.00027	-0.00089	-0.02026	-0.00057	0.02611
144	20	H 1S	0.00094	-0.00335	0.00485	0.00013	-0.00304
145		2S	0.00601	-0.02144	-0.00938	-0.00028	-0.01685
146	21	C 1S	0.00008	-0.00022	0.00021	0.00001	-0.00115
147		2S	-0.00038	0.00106	-0.00054	0.00001	0.00389
148		3S	-0.00030	0.00200	-0.00075	-0.00034	0.00917
149		4PX	-0.00051	0.00213	-0.00093	-0.00001	-0.06627
150		4PY	-0.00010	0.00056	-0.00107	-0.00002	0.17836
151		4PZ	-0.00029	0.00082	-0.00087	-0.00003	0.06810
152		5PX	-0.00008	-0.00042	-0.00420	0.00032	-0.02338
153		5PY	0.00007	0.00051	-0.00310	0.00000	0.08608
154		5PZ	0.00154	-0.00460	0.00182	0.00008	0.03546
155	22	C 1S	-0.00009	0.00015	-0.00008	0.00000	0.00143
156		2S	0.00005	-0.00016	0.00044	0.00003	-0.00282
157		3S	0.00098	-0.00066	-0.00209	-0.00012	-0.00970
158		4PX	0.00012	-0.00108	0.00061	-0.00001	0.00828
159		4PY	0.00012	-0.00067	0.00073	0.00001	-0.02079
160		4PZ	-0.00021	0.00042	-0.00036	-0.00002	-0.00462
161		5PX	-0.00013	-0.00018	-0.00150	0.00032	-0.01888
162		5PY	-0.00177	0.00038	-0.00038	0.00038	0.08248
163		5PZ	-0.00109	0.00168	0.00045	-0.00009	0.03904
164	23	H 1S	-0.00007	0.00004	0.00019	0.00001	-0.02765
165		2S	0.00105	-0.00046	-0.00027	0.00000	-0.09695
166	24	H 1S	0.00004	0.00003	-0.00018	0.00001	0.02358
167		2S	-0.00080	0.00039	-0.00030	0.00012	0.07312
168	25	C 1S	0.00005	-0.00006	0.00003	0.00001	-0.00104
169		2S	-0.00009	-0.00002	0.00001	-0.00004	0.00031
170		3S	0.00021	0.00170	-0.00008	0.00007	0.01771
171		4PX	0.00006	0.00055	-0.00021	0.00004	0.00543
172		4PY	0.00025	0.00031	-0.00017	0.00013	0.00001
173		4PZ	-0.00014	0.00022	-0.00011	-0.00007	0.00422
174		5PX	-0.00178	0.00025	-0.00139	0.00039	0.07040
175		5PY	0.00210	-0.00018	-0.00061	0.00008	-0.11384
176		5PZ	-0.00054	0.00006	0.00016	-0.00031	-0.02389
177	26	H 1S	-0.00007	-0.00001	0.00004	-0.00001	-0.00152
178		2S	0.00026	-0.00036	-0.00004	-0.00037	-0.05406
179	27	H 1S	0.00002	0.00005	-0.00007	0.00005	0.00277
180		2S	-0.00123	-0.00005	-0.00023	-0.00001	0.06333
181	28	C 1S	-0.00014	0.00003	-0.00003	0.00000	0.00461
182		2S	0.00028	-0.00004	0.00018	0.00001	-0.01139

183		3S	0.00255	-0.00007	-0.00058	0.00046	-0.03979
184		4PX	-0.00044	-0.00049	0.00024	0.00000	0.01457
185		4PY	0.00011	-0.00021	0.00012	-0.00013	0.00439
186		4PZ	0.00012	0.00016	-0.00007	0.00005	0.01354
187		5PX	0.00063	-0.00034	-0.00088	0.00096	-0.02582
188		5PY	-0.00408	-0.00089	-0.00057	-0.00022	0.09782
189		5PZ	0.00037	0.00017	-0.00020	0.00055	0.04512
190	29	H 1S	0.00016	0.00000	0.00005	-0.00001	0.00007
191		2S	0.00079	0.00013	0.00010	-0.00033	-0.05359
192	30	H 1S	0.00006	0.00000	0.00004	0.00016	0.00079
193		2S	-0.00268	-0.00038	-0.00007	-0.00066	0.06318
194	31	C 1S	-0.00024	-0.00011	0.00003	-0.00010	-0.00130
195		2S	0.00033	0.00019	-0.00004	0.00043	0.00212
196		3S	0.00327	0.00121	-0.00012	-0.00071	0.00526
197		4PX	-0.00007	0.00026	-0.00016	-0.00021	-0.00449
198		4PY	0.00192	0.00063	-0.00006	0.00098	-0.00236
199		4PZ	-0.00068	-0.00009	-0.00005	-0.00047	0.00117
200		5PX	-0.00146	-0.00036	-0.00074	0.00071	0.02947
201		5PY	0.00185	0.00048	0.00016	-0.00059	-0.03484
202		5PZ	-0.00424	-0.00116	-0.00035	0.00011	0.00946
203	32	H 1S	-0.00019	-0.00004	-0.00001	0.00001	0.00374
204		2S	-0.00248	-0.00073	-0.00005	-0.00070	0.00100
205	33	H 1S	-0.00046	-0.00022	0.00007	-0.00016	0.00867
206		2S	-0.00005	-0.00020	-0.00020	-0.00035	0.01021
207	34	C 1S	0.00016	0.00004	0.00000	0.00020	0.00017
208		2S	-0.00104	-0.00028	0.00006	-0.00035	-0.00286
209		3S	-0.00771	-0.00213	-0.00042	-0.00079	0.02849
210		4PX	-0.00066	-0.00015	-0.00001	0.00022	0.07509
211		4PY	-0.00260	-0.00074	0.00001	-0.00094	0.03966
212		4PZ	-0.00138	-0.00037	0.00002	-0.00067	0.01671
213		5PX	-0.00038	-0.00003	-0.00029	0.00126	0.05248
214		5PY	0.00103	0.00047	0.00061	-0.00272	0.00819
215		5PZ	0.00578	0.00148	0.00010	0.00115	0.00490
216	35	C 1S	0.00003	0.00001	0.00001	-0.00034	-0.00011
217		2S	0.00002	0.00001	0.00000	0.00037	0.00077
218		3S	-0.00320	-0.00082	-0.00037	0.01144	-0.00297
219		4PX	0.01044	0.00293	-0.00009	0.00328	-0.11658
220		4PY	0.00396	0.00110	-0.00005	0.00195	-0.04710
221		4PZ	-0.00412	-0.00115	0.00016	-0.00626	-0.02982
222		5PX	-0.01127	-0.00308	-0.00038	0.00725	-0.10844

223		5PY	0.00147	0.00035	0.00041	-0.00165	-0.05076
224		5PZ	0.07150	0.01994	0.00015	-0.00180	-0.02886
225	36	C 1S	-0.00266	-0.00074	0.00004	-0.00143	-0.00071
226		2S	0.00380	0.00106	-0.00003	0.00178	0.00132
227		3S	0.03686	0.01033	-0.00084	0.02698	0.00974
228		4PX	0.01644	0.00462	-0.00006	0.00169	0.03227
229		4PY	0.02370	0.00664	-0.00023	0.00879	0.01752
230		4PZ	0.00577	0.00162	-0.00005	0.00187	0.00773
231		5PX	-0.01128	-0.00314	0.00030	-0.01158	0.04133
232		5PY	0.06838	0.01910	-0.00032	0.00932	0.02522
233		5PZ	0.01353	0.00378	-0.00029	0.01614	0.01046
234	37	H 1S	-0.00144	-0.00040	-0.00001	0.00061	-0.00090
235		2S	0.00879	0.00246	0.00008	-0.00604	-0.00025
236	38	C 1S	0.00451	0.00126	-0.00007	0.00259	0.00142
237		2S	-0.00666	-0.00186	0.00012	-0.00454	-0.00499
238		3S	-0.03684	-0.01027	0.00092	-0.03287	-0.00244
239		4PX	0.00740	0.00207	-0.00013	0.00497	0.06859
240		4PY	-0.01634	-0.00457	0.00022	-0.00855	0.02692
241		4PZ	-0.00728	-0.00203	0.00032	-0.01233	0.02052
242		5PX	-0.05656	-0.01580	-0.00027	0.00934	0.05032
243		5PY	0.08060	0.02252	-0.00038	0.01670	0.02832
244		5PZ	0.00591	0.00166	0.00105	-0.03995	0.01682
245	39	H 1S	-0.00827	-0.00231	0.00018	-0.00693	-0.00219
246		2S	-0.02922	-0.00817	-0.00084	0.03048	-0.00722
247	40	C 1S	-0.00228	-0.00064	0.00007	-0.00271	0.00038
248		2S	0.00225	0.00064	-0.00012	0.00490	-0.00154
249		3S	0.02951	0.00814	-0.00099	0.03730	0.00371
250		4PX	-0.01683	-0.00470	0.00010	-0.00401	0.06869
251		4PY	-0.00186	-0.00052	-0.00022	0.00841	0.03238
252		4PZ	-0.01601	-0.00447	0.00047	-0.01844	0.01462
253		5PX	0.05243	0.01465	-0.00061	0.02353	0.05598
254		5PY	-0.07965	-0.02223	0.00050	-0.01775	0.00601
255		5PZ	0.02403	0.00675	0.00036	-0.01680	0.00364
256	41	H 1S	0.00237	0.00066	-0.00019	0.00749	-0.00100
257		2S	0.04251	0.01190	0.00032	-0.01470	-0.00154
258	42	C 1S	0.00030	0.00008	-0.00003	0.00119	-0.00017
259		2S	0.00073	0.00020	0.00001	-0.00042	0.00131
260		3S	-0.02235	-0.00623	0.00087	-0.03425	-0.01038
261		4PX	-0.01303	-0.00361	0.00001	-0.00081	0.04185
262		4PY	-0.00519	-0.00144	0.00013	-0.00529	0.01987

263		4PZ	-0.00251	-0.00069	-0.00003	0.00081	0.01106
264		5PX	0.00382	0.00100	0.00012	-0.00446	0.05008
265		5PY	-0.06321	-0.01754	0.00032	-0.01333	0.01742
266		5PZ	0.00131	0.00038	-0.00002	0.00013	0.01679
267	43	H 1S	-0.00199	-0.00056	0.00005	-0.00180	-0.00044
268		2S	-0.00934	-0.00259	0.00001	-0.00087	-0.00103
269	44	Zn 1S	-0.00326	-0.00091	0.00005	-0.00178	-0.00347
270		2S	-0.01608	-0.00450	0.00024	-0.00909	0.00789
271		3PX	0.00246	0.00069	0.00033	-0.01266	-0.02269
272		3PY	0.02543	0.00711	-0.00030	0.01148	0.01041
273		3PZ	0.00020	0.00006	0.00060	-0.02328	0.00621
274		4PX	-0.00663	-0.00186	0.00025	-0.00952	0.00394
275		4PY	0.02524	0.00705	-0.00018	0.00766	-0.00128
276		4PZ	-0.01455	-0.00406	-0.00224	0.08748	0.00033
277		5D 0	0.00460	0.00129	-0.00041	0.01606	0.00546
278		5D+1	0.01398	0.00391	0.00208	-0.08129	-0.00823
279		5D-1	0.06958	0.01944	-0.00036	0.01392	-0.00356
280		5D+2	0.00381	0.00107	0.00015	-0.00591	0.03048
281		5D-2	0.02052	0.00573	-0.00001	0.00031	-0.00463
282		6D 0	0.00097	0.00027	-0.00008	0.00295	0.00050
283		6D+1	0.00213	0.00060	0.00032	-0.01257	-0.00133
284		6D-1	0.01110	0.00310	-0.00006	0.00218	-0.00055
285		6D+2	0.00159	0.00044	0.00001	-0.00050	0.00443
286		6D-2	0.00435	0.00121	-0.00001	0.00039	-0.00004
287	45	Cl 1S	-0.00117	-0.00033	-0.00020	0.00791	-0.00111
288		2S	-0.00249	-0.00069	-0.00048	0.01896	-0.00334
289		3PX	0.03340	0.00933	0.00641	-0.24991	0.00198
290		3PY	0.41850	0.11696	-0.00205	0.07962	-0.00057
291		3PZ	-0.03359	-0.00939	-0.00797	0.31096	-0.00584
292		4PX	0.03859	0.01078	0.00728	-0.28373	0.00189
293		4PY	0.47035	0.13145	-0.00227	0.08814	-0.00249
294		4PZ	-0.03440	-0.00962	-0.00871	0.33986	-0.00937
295	46	Cl 1S	-0.00018	-0.00005	0.00019	-0.00729	-0.00284
296		2S	0.00320	0.00090	0.00060	-0.02338	-0.00757
297		3PX	-0.07289	-0.02037	-0.00513	0.19997	-0.00241
298		3PY	-0.23878	-0.06673	0.00008	-0.00326	-0.00364
299		3PZ	-0.00623	-0.00173	-0.00647	0.25229	0.01150
300		4PX	-0.08377	-0.02340	-0.00585	0.22814	-0.00357
301		4PY	-0.27666	-0.07732	0.00018	-0.00710	-0.00275
302		4PZ	-0.00701	-0.00195	-0.00704	0.27433	0.01700

303	47	O	1S	0.00005	0.00001	0.00000	-0.00001	-0.00020
304			2S	-0.00024	-0.00005	0.00001	0.00009	0.00031
305			3S	0.00133	0.00035	-0.00002	-0.00071	0.00258
306			4PX	-0.00062	-0.00020	-0.00001	0.00074	-0.05298
307			4PY	-0.00130	-0.00038	-0.00004	0.00124	0.14147
308			4PZ	-0.00047	-0.00013	-0.00001	0.00036	0.04934
309			5PX	0.00139	0.00043	-0.00002	0.00012	-0.03829
310			5PY	0.00019	-0.00002	-0.00002	0.00082	0.11029
311			5PZ	-0.00034	-0.00014	0.00002	0.00040	0.03860
312	48	O	1S	-0.00001	0.00005	0.00004	0.00000	-0.00028
313			2S	-0.00005	0.00013	-0.00005	0.00001	0.00146
314			3S	0.00082	-0.00259	-0.00068	-0.00008	-0.00330
315			4PX	-0.00126	0.00431	0.00011	0.00005	0.05978
316			4PY	-0.00168	0.00594	0.00234	0.00009	0.03079
317			4PZ	-0.00057	0.00200	0.00082	0.00003	0.01273
318			5PX	-0.00102	0.00355	0.00025	0.00006	0.04755
319			5PY	-0.00015	0.00042	0.00103	-0.00005	0.02251
320			5PZ	-0.00040	0.00140	0.00061	0.00004	0.01160
321	49	N	1S	0.00123	0.00034	0.00001	-0.00026	-0.00265
322			2S	-0.00276	-0.00077	-0.00003	0.00110	0.00786
323			3S	-0.00522	-0.00144	0.00005	-0.00264	0.01309
324			4PX	0.00321	0.00088	-0.00013	0.00504	-0.12784
325			4PY	0.00536	0.00151	0.00024	-0.00949	0.19339
326			4PZ	0.00212	0.00060	0.00008	-0.00306	0.08892
327			5PX	0.02146	0.00599	-0.00009	0.00273	-0.11174
328			5PY	-0.00509	-0.00141	0.00022	-0.00904	0.18247
329			5PZ	0.02169	0.00608	0.00045	-0.01781	0.08296
330	50	N	1S	-0.00037	-0.00009	0.00000	0.00008	0.00071
331			2S	0.00048	0.00009	0.00000	-0.00003	-0.00237
332			3S	0.00178	0.00056	-0.00003	-0.00127	0.00018
333			4PX	-0.00255	-0.00078	-0.00006	0.00186	0.01863
334			4PY	0.00037	0.00013	0.00003	-0.00152	-0.03363
335			4PZ	-0.00022	-0.00007	0.00000	-0.00024	-0.01682
336			5PX	-0.00490	-0.00145	0.00015	0.00148	0.01419
337			5PY	-0.00597	-0.00166	0.00010	-0.00057	-0.06611
338			5PZ	0.01218	0.00341	0.00007	-0.00230	-0.02563
339	51	H	1S	0.00078	0.00021	0.00001	-0.00070	0.00007
340			2S	0.01314	0.00357	0.00012	-0.00336	0.00200
341	52	N	1S	-0.00007	0.00026	-0.00011	0.00000	-0.00036
342			2S	0.00026	-0.00093	-0.00019	0.00000	0.00105

343		3S	-0.00119	0.00424	0.00402	0.00004	0.00316
344		4PX	0.00263	-0.00961	-0.00195	-0.00002	-0.01655
345		4PY	0.00056	-0.00206	-0.00070	-0.00001	-0.00695
346		4PZ	0.00006	-0.00026	0.00069	0.00002	-0.00413
347		5PX	0.00129	-0.00486	-0.00152	-0.00009	-0.02060
348		5PY	-0.00119	0.00382	-0.00171	0.00007	-0.01182
349		5PZ	0.00532	-0.01878	0.00060	0.00011	-0.00494
350	53	H 1S	0.00032	-0.00114	-0.00098	-0.00002	0.00114
351		2S	0.00436	-0.01516	-0.00196	0.00005	0.00183
352	54	N 1S	-0.00151	0.00540	0.00175	0.00004	-0.00365
353		2S	0.00333	-0.01191	-0.00374	-0.00009	0.00842
354		3S	0.00717	-0.02567	-0.00691	-0.00019	0.02304
355		4PX	0.00697	-0.02504	-0.01196	-0.00029	0.09971
356		4PY	-0.00496	0.01770	0.00321	0.00009	0.02584
357		4PZ	0.00195	-0.00702	-0.00087	-0.00002	0.02430
358		5PX	0.00252	-0.00911	-0.01464	-0.00035	0.09252
359		5PY	-0.00773	0.02765	0.01231	0.00030	0.03215
360		5PZ	0.00853	-0.03055	-0.01168	-0.00032	0.02530
361	55	C 1S	0.00539	0.00150	0.00008	-0.00316	-0.00025
362		2S	-0.00724	-0.00203	-0.00016	0.00627	0.00044
363		3S	-0.07146	-0.01988	-0.00079	0.02912	0.01252
364		4PX	0.02289	0.00641	0.00030	-0.01169	0.08181
365		4PY	0.00371	0.00104	0.00016	-0.00623	-0.13566
366		4PZ	0.01749	0.00489	0.00041	-0.01591	-0.06205
367		5PX	-0.07782	-0.02175	-0.00016	0.00830	0.05009
368		5PY	-0.04512	-0.01261	-0.00064	0.02575	-0.09950
369		5PZ	0.02215	0.00616	0.00048	-0.01723	-0.04868
370	56	H 1S	-0.00943	-0.00264	-0.00019	0.00729	-0.00339
371		2S	0.00057	0.00012	0.00040	-0.01348	-0.01289
372	57	C 1S	-0.00242	-0.00067	-0.00003	0.00130	-0.00063
373		2S	0.00133	0.00037	0.00003	-0.00161	0.00195
374		3S	0.06209	0.01726	0.00078	-0.02729	0.00594
375		4PX	-0.00655	-0.00184	-0.00019	0.00719	0.04353
376		4PY	-0.01281	-0.00360	-0.00002	0.00093	-0.08716
377		4PZ	-0.00254	-0.00073	0.00003	-0.00134	-0.03581
378		5PX	-0.04410	-0.01228	-0.00040	0.01467	0.06386
379		5PY	-0.03192	-0.00885	0.00009	-0.00543	-0.10874
380		5PZ	-0.00236	-0.00070	0.00012	-0.00189	-0.04696
381	58	H 1S	0.00114	0.00032	0.00003	-0.00116	-0.00356
382		2S	0.00692	0.00189	0.00006	-0.00020	-0.00740

383	59	C	1S	0.00110	0.00030	0.00001	-0.00043	0.00055
384			2S	-0.00165	-0.00045	-0.00001	0.00017	-0.00002
385			3S	-0.02468	-0.00693	-0.00013	0.01121	-0.03098
386			4PX	0.00515	0.00147	0.00011	-0.00403	-0.12844
387			4PY	-0.00174	-0.00046	-0.00010	0.00397	0.25279
388			4PZ	0.00650	0.00182	0.00011	-0.00434	0.10029
389			5PX	-0.01779	-0.00507	0.00039	-0.00275	-0.13630
390			5PY	0.00508	0.00131	0.00005	0.00451	0.24055
391			5PZ	-0.04129	-0.01159	-0.00008	0.00312	0.09827
392	60	C	1S	0.00120	0.00033	0.00003	-0.00109	-0.00070
393			2S	-0.00106	-0.00030	0.00000	-0.00009	0.00248
394			3S	-0.02788	-0.00777	-0.00092	0.03513	-0.00465
395			4PX	0.00159	0.00045	0.00015	-0.00613	0.04711
396			4PY	0.00882	0.00245	-0.00007	0.00286	-0.08644
397			4PZ	0.00182	0.00050	-0.00008	0.00298	-0.03327
398			5PX	0.02870	0.00804	0.00030	-0.01192	0.05672
399			5PY	0.03878	0.01084	0.00033	-0.01253	-0.09128
400			5PZ	-0.02485	-0.00695	-0.00042	0.01549	-0.05480
401	61	H	1S	0.00011	0.00003	-0.00002	0.00070	-0.00284
402			2S	0.00388	0.00106	0.00013	-0.00420	0.00273
403	62	C	1S	-0.00203	-0.00057	-0.00004	0.00165	-0.00059
404			2S	0.00156	0.00044	0.00005	-0.00215	0.00154
405			3S	0.01738	0.00485	0.00071	-0.02523	0.01510
406			4PX	-0.00768	-0.00214	-0.00008	0.00292	0.08586
407			4PY	0.00076	0.00021	-0.00010	0.00393	-0.14343
408			4PZ	0.00604	0.00169	0.00027	-0.01051	-0.06071
409			5PX	0.06495	0.01815	0.00093	-0.03490	0.07276
410			5PY	0.02424	0.00677	0.00035	-0.01221	-0.10680
411			5PZ	-0.00094	-0.00024	0.00047	-0.02025	-0.02646
412	63	H	1S	0.00335	0.00093	0.00012	-0.00485	-0.00308
413			2S	0.02147	0.00598	-0.00020	0.00938	-0.01708
414	64	C	1S	0.00023	0.00005	0.00000	-0.00021	-0.00116
415			2S	-0.00111	-0.00022	-0.00004	0.00054	0.00392
416			3S	-0.00187	-0.00078	0.00030	0.00077	0.00922
417			4PX	0.00208	0.00067	0.00004	-0.00093	0.06712
418			4PY	0.00054	0.00021	0.00004	-0.00107	-0.18079
419			4PZ	0.00086	0.00018	0.00002	-0.00087	-0.06900
420			5PX	-0.00031	-0.00029	0.00054	-0.00418	0.02363
421			5PY	0.00040	0.00033	0.00016	-0.00309	-0.08731
422			5PZ	-0.00473	-0.00107	-0.00002	0.00182	-0.03600

423	65	C	1S	-0.00017	0.00000	0.00000	0.00008	0.00143
424			2S	0.00016	0.00004	-0.00001	-0.00044	-0.00283
425			3S	0.00108	-0.00049	0.00001	0.00209	-0.00943
426			4PX	-0.00098	-0.00046	-0.00004	0.00061	-0.00836
427			4PY	-0.00064	-0.00024	-0.00002	0.00073	0.02110
428			4PZ	0.00047	0.00004	0.00000	-0.00036	0.00469
429			5PX	-0.00009	-0.00021	0.00040	-0.00148	0.01913
430			5PY	0.00125	-0.00132	0.00039	-0.00036	-0.08328
431			5PZ	0.00201	-0.00006	-0.00011	0.00044	-0.03942
432	66	H	1S	-0.00007	0.00004	0.00000	-0.00019	-0.02803
433			2S	0.00094	-0.00066	-0.00002	0.00027	-0.09813
434	67	H	1S	0.00000	-0.00005	-0.00002	0.00018	0.02392
435			2S	-0.00075	0.00048	-0.00014	0.00029	0.07395
436	68	C	1S	0.00007	-0.00001	-0.00001	-0.00003	-0.00106
437			2S	-0.00003	0.00009	0.00004	-0.00001	0.00034
438			3S	-0.00134	-0.00106	-0.00007	0.00008	0.01796
439			4PX	0.00044	0.00033	0.00005	-0.00021	-0.00549
440			4PY	0.00014	0.00037	0.00014	-0.00016	-0.00008
441			4PZ	0.00026	0.00000	-0.00007	-0.00011	-0.00427
442			5PX	0.00114	-0.00140	0.00046	-0.00137	-0.07097
443			5PY	-0.00125	0.00170	0.00011	-0.00060	0.11471
444			5PZ	0.00033	-0.00043	-0.00032	0.00015	0.02438
445	69	H	1S	-0.00003	0.00006	0.00001	-0.00004	-0.00157
446			2S	0.00044	-0.00003	0.00037	0.00006	-0.05472
447	70	H	1S	-0.00003	-0.00005	-0.00006	0.00006	0.00281
448			2S	-0.00059	0.00108	0.00000	0.00023	0.06381
449	71	C	1S	-0.00010	0.00011	0.00000	0.00003	0.00457
450			2S	0.00017	-0.00022	0.00000	-0.00018	-0.01132
451			3S	0.00139	-0.00215	-0.00049	0.00055	-0.03932
452			4PX	-0.00019	-0.00063	-0.00001	0.00024	-0.01437
453			4PY	-0.00024	-0.00002	-0.00014	0.00012	-0.00445
454			4PZ	0.00007	0.00018	0.00005	-0.00006	-0.01350
455			5PX	-0.00062	0.00037	0.00100	-0.00083	0.02599
456			5PY	0.00136	-0.00396	-0.00019	-0.00058	-0.09817
457			5PZ	-0.00004	0.00041	0.00056	-0.00018	-0.04531
458	72	H	1S	0.00008	-0.00014	0.00001	-0.00005	0.00011
459			2S	0.00030	-0.00075	0.00034	-0.00009	-0.05390
460	73	H	1S	0.00004	-0.00005	-0.00015	-0.00005	0.00072
461			2S	-0.00107	0.00249	0.00066	0.00011	0.06319
462	74	C	1S	-0.00003	0.00026	0.00010	-0.00003	-0.00130

463		2S	0.00001	-0.00038	-0.00043	0.00002	0.00211
464		3S	0.00066	-0.00343	0.00070	0.00016	0.00538
465		4PX	0.00026	0.00008	-0.00020	-0.00017	0.00440
466		4PY	-0.00046	0.00197	0.00098	-0.00001	0.00234
467		4PZ	0.00028	-0.00063	-0.00047	-0.00008	-0.00117
468		5PX	0.00045	-0.00144	0.00074	-0.00070	-0.02936
469		5PY	-0.00055	0.00184	-0.00060	0.00013	0.03483
470		5PZ	0.00121	-0.00423	0.00012	-0.00035	-0.00941
471	75	H 1S	-0.00006	0.00019	-0.00001	0.00001	0.00374
472		2S	-0.00066	0.00250	0.00070	0.00009	0.00099
473	76	H 1S	-0.00005	0.00051	0.00016	-0.00006	0.00858
474		2S	0.00015	0.00014	0.00034	0.00022	0.01004
475	77	C 1S	0.00005	-0.00015	-0.00020	-0.00001	0.00017
476		2S	-0.00030	0.00103	0.00035	-0.00005	-0.00287
477		3S	-0.00218	0.00770	0.00077	0.00046	0.02859
478		4PX	0.00021	-0.00065	0.00022	0.00000	-0.07443
479		4PY	0.00072	-0.00261	-0.00094	-0.00004	-0.03935
480		4PZ	0.00040	-0.00137	-0.00067	-0.00002	-0.01656
481		5PX	0.00018	-0.00034	0.00127	-0.00022	-0.05213
482		5PY	-0.00013	0.00112	-0.00275	0.00047	-0.00819
483		5PZ	-0.00173	0.00571	0.00114	0.00015	-0.00487
484	78	C 1S	0.00001	-0.00003	0.00034	0.00001	-0.00011
485		2S	0.00000	-0.00002	-0.00037	-0.00001	0.00076
486		3S	-0.00095	0.00313	-0.01148	-0.00022	-0.00302
487		4PX	-0.00291	0.01046	0.00328	0.00008	0.11547
488		4PY	-0.00111	0.00397	0.00195	0.00005	0.04664
489		4PZ	0.00115	-0.00411	-0.00626	-0.00017	0.02954
490		5PX	0.00321	-0.01122	0.00726	-0.00001	0.10731
491		5PY	-0.00046	0.00144	-0.00168	0.00032	0.05025
492		5PZ	-0.02002	0.07147	-0.00180	0.00006	0.02877
493	79	C 1S	-0.00074	0.00266	0.00143	0.00003	-0.00070
494		2S	0.00106	-0.00380	-0.00178	-0.00006	0.00130
495		3S	0.01027	-0.03685	-0.02698	-0.00054	0.00975
496		4PX	-0.00457	0.01646	0.00170	0.00003	-0.03200
497		4PY	-0.00661	0.02371	0.00880	0.00022	-0.01735
498		4PZ	-0.00160	0.00577	0.00187	0.00005	-0.00766
499		5PX	0.00317	-0.01128	-0.01158	-0.00030	-0.04098
500		5PY	-0.01912	0.06836	0.00934	0.00016	-0.02493
501		5PZ	-0.00379	0.01355	0.01614	0.00054	-0.01031
502	80	H 1S	-0.00040	0.00145	-0.00061	-0.00002	-0.00089

503		2S	0.00245	-0.00877	0.00604	0.00023	-0.00023
504	81	C 1S	0.00126	-0.00451	-0.00259	-0.00007	0.00140
505		2S	-0.00186	0.00665	0.00454	0.00011	-0.00493
506		3S	-0.01030	0.03677	0.03287	0.00077	-0.00241
507		4PX	-0.00206	0.00738	0.00497	0.00013	-0.06790
508		4PY	0.00457	-0.01634	-0.00855	-0.00022	-0.02666
509		4PZ	0.00203	-0.00725	-0.01232	-0.00032	-0.02030
510		5PX	0.01581	-0.05654	0.00934	0.00021	-0.04981
511		5PY	-0.02253	0.08057	0.01669	0.00048	-0.02800
512		5PZ	-0.00164	0.00591	-0.03996	-0.00100	-0.01667
513	82	H 1S	-0.00231	0.00826	0.00693	0.00018	-0.00216
514		2S	-0.00817	0.02924	-0.03048	-0.00072	-0.00713
515	83	C 1S	-0.00064	0.00227	0.00271	0.00007	0.00038
516		2S	0.00062	-0.00225	-0.00490	-0.00013	-0.00152
517		3S	0.00834	-0.02944	-0.03731	-0.00093	0.00360
518		4PX	0.00471	-0.01683	-0.00402	-0.00011	-0.06802
519		4PY	0.00053	-0.00187	0.00841	0.00021	-0.03206
520		4PZ	0.00448	-0.01602	-0.01845	-0.00048	-0.01449
521		5PX	-0.01465	0.05241	0.02354	0.00059	-0.05542
522		5PY	0.02228	-0.07963	-0.01776	-0.00041	-0.00605
523		5PZ	-0.00670	0.02409	-0.01676	-0.00050	-0.00365
524	84	H 1S	0.00066	-0.00236	-0.00749	-0.00020	-0.00099
525		2S	0.01187	-0.04253	0.01469	0.00043	-0.00153
526	85	C 1S	0.00008	-0.00029	-0.00119	-0.00003	-0.00017
527		2S	0.00021	-0.00073	0.00042	0.00001	0.00130
528		3S	-0.00626	0.02233	0.03425	0.00089	-0.01031
529		4PX	0.00366	-0.01301	-0.00081	-0.00003	-0.04147
530		4PY	0.00146	-0.00517	-0.00529	-0.00014	-0.01968
531		4PZ	0.00071	-0.00250	0.00081	0.00001	-0.01096
532		5PX	-0.00112	0.00379	-0.00446	-0.00011	-0.04953
533		5PY	0.01776	-0.06312	-0.01333	-0.00037	-0.01736
534		5PZ	-0.00035	0.00129	0.00010	-0.00002	-0.01661
535	86	H 1S	-0.00056	0.00199	0.00180	0.00005	-0.00043
536		2S	-0.00263	0.00933	0.00088	0.00004	-0.00100

HOMO (#184) and LUMO(#185) for 5:

	181	182	183	184	185
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--V
EIGENVALUES --	-0.22770	-0.22770	-0.22183	-0.22183	-0.08436
1 1 Zn 1S	0.00290	0.00079	0.00103	0.00003	0.00480

2	2S	0.01052	0.00288	0.00673	0.00016	-0.00656
3	3PX	0.00127	0.00035	-0.00958	-0.00024	-0.02525
4	3PY	0.02018	0.00553	0.00853	0.00021	0.01457
5	3PZ	0.00149	0.00041	-0.03957	-0.00097	0.00816
6	4PX	-0.00756	-0.00207	-0.00339	-0.00008	0.00503
7	4PY	0.01747	0.00478	0.00681	0.00019	0.00062
8	4PZ	-0.01137	-0.00311	0.08341	0.00206	-0.00146
9	5D 0	-0.00109	-0.00030	-0.01122	-0.00028	-0.00514
10	5D+1	-0.00514	-0.00141	0.07042	0.00174	0.00994
11	5D-1	-0.06156	-0.01684	-0.00483	-0.00012	0.00344
12	5D+2	0.00162	0.00044	0.00488	0.00012	-0.02823
13	5D-2	-0.01620	-0.00443	0.00285	0.00007	-0.00342
14	6D 0	-0.00033	-0.00009	-0.00168	-0.00004	-0.00031
15	6D+1	-0.00048	-0.00013	0.00805	0.00020	0.00144
16	6D-1	-0.00813	-0.00222	-0.00062	-0.00002	0.00053
17	6D+2	-0.00050	-0.00014	0.00033	0.00001	-0.00364
18	6D-2	-0.00314	-0.00086	-0.00013	0.00000	-0.00124
19 2	Br 1S	0.00060	0.00017	-0.00505	-0.00013	0.00029
20	2S	0.00274	0.00075	-0.02362	-0.00059	0.00229
21	3PX	-0.00959	-0.00262	-0.25290	-0.00625	0.00361
22	3PY	0.42253	0.11560	0.06015	0.00148	-0.00159
23	3PZ	-0.03975	-0.01088	0.31549	0.00781	-0.00381
24	4PX	-0.00811	-0.00222	-0.26830	-0.00664	0.00432
25	4PY	0.43672	0.11948	0.05971	0.00147	-0.00451
26	4PZ	-0.03729	-0.01021	0.31257	0.00774	-0.00635
27 3	Br 1S	0.00032	0.00009	0.00495	0.00012	0.00162
28	2S	-0.00062	-0.00017	0.02482	0.00062	0.00844
29	3PX	-0.04754	-0.01300	0.22818	0.00564	-0.00273
30	3PY	-0.27571	-0.07543	0.02402	0.00059	-0.00512
31	3PZ	0.00525	0.00145	0.26691	0.00660	0.01330
32	4PX	-0.05061	-0.01384	0.24260	0.00600	-0.00462
33	4PY	-0.29251	-0.08002	0.02066	0.00051	-0.00393
34	4PZ	0.00655	0.00180	0.26087	0.00646	0.01852
35 4	O 1S	-0.00004	-0.00001	-0.00001	0.00000	0.00016
36	2S	0.00025	0.00005	-0.00004	-0.00001	-0.00039
37	3S	-0.00129	-0.00030	0.00074	0.00005	-0.00106
38	4PX	-0.00014	-0.00006	0.00071	0.00002	-0.07180
39	4PY	-0.00177	-0.00051	0.00124	0.00002	0.14410
40	4PZ	-0.00056	-0.00016	0.00033	0.00001	0.04469
41	5PX	0.00138	0.00042	-0.00002	-0.00001	-0.05540

42		5PY	0.00003	-0.00009	0.00066	-0.00001	0.11185
43		5PZ	-0.00052	-0.00016	0.00047	0.00005	0.03463
44	5	O 1S	0.00001	-0.00003	0.00000	-0.00003	0.00014
45		2S	0.00006	-0.00018	-0.00001	-0.00001	-0.00094
46		3S	-0.00080	0.00257	0.00004	0.00097	0.00310
47		4PX	-0.00114	0.00396	0.00004	0.00003	0.03437
48		4PY	-0.00135	0.00486	-0.00001	0.00157	0.01805
49		4PZ	-0.00054	0.00192	-0.00001	0.00068	0.00773
50		5PX	-0.00096	0.00340	0.00004	0.00027	0.02702
51		5PY	-0.00012	0.00030	-0.00009	0.00058	0.01383
52		5PZ	-0.00041	0.00141	0.00000	0.00065	0.00761
53	6	N 1S	-0.00069	-0.00019	0.00003	0.00000	0.00241
54		2S	0.00154	0.00042	-0.00057	-0.00002	-0.00770
55		3S	0.00235	0.00062	0.00280	0.00009	-0.00922
56		4PX	0.00042	0.00010	0.00684	0.00017	-0.15165
57		4PY	0.00444	0.00123	-0.00870	-0.00021	0.20028
58		4PZ	0.00290	0.00080	-0.00323	-0.00008	0.09000
59		5PX	0.01517	0.00414	0.00752	0.00017	-0.13500
60		5PY	-0.00182	-0.00049	-0.00668	-0.00017	0.18835
61		5PZ	0.01549	0.00425	-0.00865	-0.00023	0.08205
62	7	N 1S	0.00038	0.00009	-0.00005	0.00000	-0.00056
63		2S	-0.00057	-0.00012	0.00014	0.00000	0.00198
64		3S	-0.00158	-0.00049	-0.00044	0.00007	0.00067
65		4PX	-0.00289	-0.00085	0.00167	0.00003	0.02414
66		4PY	0.00071	0.00021	-0.00124	-0.00003	-0.03750
67		4PZ	-0.00004	-0.00002	0.00009	0.00000	-0.01671
68		5PX	-0.00341	-0.00105	0.00033	0.00015	0.03122
69		5PY	-0.00460	-0.00128	-0.00048	0.00007	-0.06811
70		5PZ	0.01257	0.00341	-0.00279	-0.00007	-0.02002
71	8	H 1S	-0.00086	-0.00023	0.00079	0.00002	-0.00230
72		2S	-0.01240	-0.00327	0.00397	0.00007	-0.00897
73	9	N 1S	0.00009	-0.00033	0.00000	0.00012	0.00023
74		2S	-0.00024	0.00089	-0.00001	0.00005	-0.00127
75		3S	0.00060	-0.00227	0.00015	-0.00347	0.00104
76		4PX	0.00222	-0.00829	0.00006	-0.00123	-0.00959
77		4PY	0.00051	-0.00192	0.00003	-0.00077	-0.00481
78		4PZ	-0.00004	0.00009	-0.00002	0.00074	-0.00223
79		5PX	0.00087	-0.00355	-0.00004	-0.00016	-0.00982
80		5PY	-0.00109	0.00362	0.00014	-0.00116	-0.00580
81		5PZ	0.00524	-0.01875	0.00010	-0.00121	-0.00540

82	10	H	1S	-0.00032	0.00120	-0.00003	0.00103	-0.00101
83			2S	-0.00417	0.01466	-0.00015	0.00312	0.00319
84	11	N	1S	0.00127	-0.00465	0.00003	-0.00109	0.00384
85			2S	-0.00274	0.01001	-0.00006	0.00227	-0.00865
86			3S	-0.00665	0.02430	-0.00010	0.00444	-0.02405
87			4PX	0.00662	-0.02431	0.00031	-0.01213	0.05887
88			4PY	-0.00322	0.01173	0.00005	-0.00178	0.01126
89			4PZ	0.00208	-0.00763	0.00004	-0.00153	0.01583
90			5PX	0.00280	-0.01031	0.00043	-0.01653	0.05637
91			5PY	-0.00550	0.02008	-0.00017	0.00664	0.01661
92			5PZ	0.00671	-0.02456	0.00006	-0.00334	0.01919
93	12	C	1S	-0.00563	-0.00154	0.00325	0.00008	0.00082
94			2S	0.00908	0.00249	-0.00705	-0.00017	-0.00172
95			3S	0.06347	0.01727	-0.03062	-0.00071	-0.01722
96			4PX	0.02260	0.00620	-0.01204	-0.00030	0.10229
97			4PY	0.00677	0.00186	-0.00676	-0.00017	-0.13964
98			4PZ	0.01780	0.00487	-0.01584	-0.00039	-0.06273
99			5PX	-0.06098	-0.01668	0.00245	0.00012	0.06896
100			5PY	-0.03790	-0.01037	0.02147	0.00055	-0.09884
101			5PZ	0.01325	0.00359	-0.01494	-0.00033	-0.05132
102	13	H	1S	0.00933	0.00256	-0.00697	-0.00017	0.00369
103			2S	0.00394	0.00111	0.00996	0.00019	0.01177
104	14	C	1S	0.00244	0.00066	-0.00130	-0.00003	0.00081
105			2S	-0.00279	-0.00076	0.00224	0.00007	-0.00189
106			3S	-0.04653	-0.01269	0.02009	0.00041	-0.00890
107			4PX	-0.00506	-0.00139	0.00720	0.00018	0.05204
108			4PY	-0.01460	-0.00401	0.00124	0.00003	-0.08354
109			4PZ	-0.00285	-0.00080	-0.00167	-0.00004	-0.03610
110			5PX	-0.03335	-0.00907	0.01617	0.00038	0.07992
111			5PY	-0.03206	-0.00869	-0.00267	-0.00011	-0.10345
112			5PZ	0.00036	0.00007	0.00038	0.00007	-0.04191
113	15	H	1S	-0.00135	-0.00037	0.00138	0.00004	0.00401
114			2S	-0.00807	-0.00216	-0.00051	-0.00005	0.00562
115	16	C	1S	-0.00104	-0.00028	0.00028	0.00001	-0.00097
116			2S	0.00184	0.00049	-0.00036	-0.00001	0.00092
117			3S	0.01970	0.00546	-0.00382	-0.00024	0.03102
118			4PX	0.00542	0.00151	-0.00395	-0.00009	-0.15245
119			4PY	-0.00201	-0.00052	0.00350	0.00009	0.26233
120			4PZ	0.00643	0.00176	-0.00500	-0.00013	0.10495
121			5PX	-0.01691	-0.00468	-0.00111	0.00025	-0.14716

122		5PY	0.00262	0.00060	0.00239	0.00022	0.25395
123		5PZ	-0.03782	-0.01033	0.00554	0.00016	0.10573
124	17	C 1S	-0.00112	-0.00031	0.00113	0.00003	0.00092
125		2S	0.00147	0.00040	-0.00053	-0.00001	-0.00258
126		3S	0.02050	0.00562	-0.03102	-0.00072	-0.00272
127		4PX	0.00020	0.00006	-0.00629	-0.00016	0.05657
128		4PY	0.00952	0.00259	0.00166	0.00004	-0.09028
129		4PZ	0.00190	0.00051	0.00282	0.00007	-0.03495
130		5PX	0.02365	0.00650	-0.01289	-0.00030	0.06223
131		5PY	0.03494	0.00957	-0.01127	-0.00026	-0.09938
132		5PZ	-0.01690	-0.00463	0.01112	0.00026	-0.05190
133	18	H 1S	0.00011	0.00003	-0.00098	-0.00002	0.00396
134		2S	-0.00046	-0.00011	0.00161	0.00002	0.00084
135	19	C 1S	0.00216	0.00059	-0.00205	-0.00005	0.00062
136		2S	-0.00259	-0.00071	0.00308	0.00009	-0.00162
137		3S	-0.01822	-0.00499	0.03442	0.00077	-0.01239
138		4PX	-0.00760	-0.00207	0.00338	0.00008	0.10496
139		4PY	0.00005	0.00001	0.00482	0.00012	-0.14934
140		4PZ	0.00715	0.00196	-0.01316	-0.00033	-0.06197
141		5PX	0.05123	0.01402	-0.02785	-0.00065	0.08102
142		5PY	0.02400	0.00657	-0.01363	-0.00030	-0.11548
143		5PZ	-0.00667	-0.00180	-0.01500	-0.00042	-0.03271
144	20	H 1S	-0.00353	-0.00096	0.00517	0.00013	0.00370
145		2S	-0.02046	-0.00558	-0.00969	-0.00027	0.01647
146	21	C 1S	-0.00025	-0.00005	0.00022	0.00001	0.00027
147		2S	0.00112	0.00025	-0.00061	0.00002	-0.00086
148		3S	0.00354	0.00096	-0.00155	-0.00049	-0.00062
149		4PX	0.00192	0.00060	-0.00080	-0.00001	0.09237
150		4PY	0.00101	0.00032	-0.00115	-0.00002	-0.18304
151		4PZ	0.00103	0.00023	-0.00086	-0.00003	-0.05929
152		5PX	-0.00015	-0.00019	-0.00329	0.00030	0.04811
153		5PY	0.00013	0.00032	-0.00289	0.00012	-0.08584
154		5PZ	-0.00387	-0.00085	0.00156	0.00002	-0.02804
155	22	C 1S	0.00017	0.00001	-0.00008	0.00000	-0.00086
156		2S	-0.00016	-0.00006	0.00040	0.00002	0.00146
157		3S	-0.00152	0.00061	-0.00153	0.00010	0.01177
158		4PX	-0.00090	-0.00040	0.00055	-0.00002	-0.01051
159		4PY	-0.00079	-0.00028	0.00072	0.00001	0.02167
160		4PZ	0.00043	0.00004	-0.00038	-0.00002	0.00640
161		5PX	-0.00056	-0.00010	-0.00136	0.00042	0.03060

162		5PY	0.00117	-0.00129	-0.00051	0.00029	-0.07948
163		5PZ	0.00223	-0.00026	0.00008	-0.00022	-0.03147
164	23	H 1S	0.00008	0.00007	-0.00020	0.00001	-0.02721
165		2S	0.00080	-0.00047	-0.00029	0.00004	-0.08559
166	24	H 1S	0.00000	-0.00006	0.00015	0.00000	0.02788
167		2S	-0.00116	0.00066	-0.00012	0.00009	0.08885
168	25	C 1S	-0.00007	0.00000	0.00002	0.00001	-0.00009
169		2S	0.00002	-0.00002	0.00004	0.00001	0.00109
170		3S	0.00139	0.00069	-0.00018	-0.00028	-0.00376
171		4PX	0.00041	0.00023	-0.00014	0.00002	-0.00002
172		4PY	0.00018	0.00038	-0.00014	0.00010	-0.00029
173		4PZ	0.00026	0.00005	-0.00008	-0.00003	-0.00094
174		5PX	0.00141	-0.00155	-0.00134	0.00018	-0.06033
175		5PY	-0.00147	0.00155	-0.00039	0.00012	0.11253
176		5PZ	0.00020	-0.00048	0.00013	-0.00029	0.02890
177	26	H 1S	0.00001	-0.00009	0.00003	-0.00001	0.00221
178		2S	-0.00056	0.00001	0.00002	-0.00028	0.05365
179	27	H 1S	0.00006	0.00006	-0.00006	0.00003	-0.00314
180		2S	0.00077	-0.00092	-0.00035	0.00011	-0.06387
181	28	C 1S	0.00010	-0.00010	-0.00003	0.00001	-0.00254
182		2S	-0.00017	0.00022	0.00016	0.00001	0.00623
183		3S	-0.00119	0.00155	-0.00044	0.00009	0.02298
184		4PX	-0.00019	-0.00058	0.00021	0.00003	-0.00738
185		4PY	-0.00022	-0.00005	0.00011	-0.00013	-0.00539
186		4PZ	0.00010	0.00006	-0.00005	-0.00002	-0.00850
187		5PX	-0.00095	0.00070	-0.00077	0.00117	0.03166
188		5PY	0.00136	-0.00327	-0.00067	-0.00001	-0.08087
189		5PZ	0.00003	0.00038	-0.00029	0.00054	-0.03991
190	29	H 1S	-0.00007	0.00011	0.00004	-0.00002	-0.00129
191		2S	-0.00038	0.00050	0.00017	-0.00036	0.04749
192	30	H 1S	-0.00003	0.00003	0.00004	0.00013	0.00056
193		2S	0.00112	-0.00215	-0.00013	-0.00059	-0.05032
194	31	C 1S	0.00002	-0.00021	0.00003	-0.00006	0.00073
195		2S	0.00001	0.00030	-0.00003	0.00034	-0.00102
196		3S	-0.00052	0.00285	-0.00015	-0.00118	-0.00475
197		4PX	0.00024	0.00008	-0.00013	-0.00016	0.00304
198		4PY	-0.00037	0.00166	-0.00005	0.00072	0.00151
199		4PZ	0.00023	-0.00046	-0.00005	-0.00035	-0.00011
200		5PX	0.00031	-0.00082	-0.00071	0.00098	-0.01834
201		5PY	-0.00059	0.00176	0.00019	-0.00072	0.02646

202		5PZ	0.00079	-0.00321	-0.00037	0.00067	-0.00087
203	32	H 1S	0.00007	-0.00020	0.00000	0.00001	-0.00238
204		2S	0.00047	-0.00206	-0.00004	-0.00049	0.00237
205	33	H 1S	0.00004	-0.00043	0.00006	-0.00009	-0.00531
206		2S	-0.00015	-0.00003	-0.00017	-0.00038	-0.00548
207	34	C 1S	-0.00006	0.00020	0.00000	0.00021	-0.00037
208		2S	0.00032	-0.00114	0.00007	-0.00046	0.00310
209		3S	0.00243	-0.00851	-0.00041	-0.00171	-0.02108
210		4PX	0.00015	-0.00042	-0.00002	0.00034	-0.04135
211		4PY	0.00069	-0.00255	0.00001	-0.00085	-0.02323
212		4PZ	0.00045	-0.00159	0.00002	-0.00072	-0.00889
213		5PX	0.00019	-0.00054	-0.00029	0.00142	-0.03006
214		5PY	0.00035	-0.00038	0.00059	-0.00378	-0.00903
215		5PZ	-0.00135	0.00463	0.00011	0.00099	-0.00438
216	35	C 1S	-0.00007	0.00024	0.00001	-0.00028	0.00038
217		2S	0.00011	-0.00038	-0.00001	0.00046	-0.00130
218		3S	0.00192	-0.00682	-0.00026	0.00751	-0.00439
219		4PX	-0.00261	0.00955	-0.00006	0.00257	0.06469
220		4PY	-0.00109	0.00397	-0.00004	0.00180	0.03060
221		4PZ	0.00135	-0.00494	0.00016	-0.00663	0.01769
222		5PX	0.00353	-0.01262	-0.00033	0.00474	0.05837
223		5PY	-0.00003	0.00004	0.00039	-0.00186	0.03496
224		5PZ	-0.01889	0.06881	0.00010	0.00048	0.01368
225	36	C 1S	-0.00011	0.00039	-0.00003	0.00127	-0.00002
226		2S	0.00013	-0.00045	0.00003	-0.00109	-0.00110
227		3S	0.00220	-0.00805	0.00072	-0.02925	0.01358
228		4PX	0.00429	-0.01560	0.00000	-0.00036	-0.02543
229		4PY	0.00236	-0.00856	0.00015	-0.00636	-0.01489
230		4PZ	0.00112	-0.00408	-0.00001	0.00026	-0.00738
231		5PX	-0.00195	0.00683	0.00004	-0.00102	-0.03278
232		5PY	0.01630	-0.05916	0.00031	-0.01375	-0.01097
233		5PZ	-0.00068	0.00252	-0.00004	0.00108	-0.01150
234	37	H 1S	0.00051	-0.00187	0.00004	-0.00175	0.00041
235		2S	0.00246	-0.00890	-0.00002	0.00006	0.00105
236	38	C 1S	0.00073	-0.00266	0.00008	-0.00310	-0.00017
237		2S	-0.00118	0.00434	-0.00015	0.00614	0.00093
238		3S	-0.00734	0.02642	-0.00102	0.04053	-0.00404
239		4PX	0.00445	-0.01626	0.00010	-0.00400	-0.03588
240		4PY	0.00032	-0.00116	-0.00025	0.01016	-0.02063
241		4PZ	0.00455	-0.01662	0.00046	-0.01888	-0.00744

242		5PX	-0.01287	0.04700	-0.00049	0.01922	-0.03499
243		5PY	0.01605	-0.05853	0.00038	-0.01339	0.00702
244		5PZ	-0.00440	0.01618	0.00022	-0.01189	-0.00164
245	39	H 1S	-0.00106	0.00387	-0.00019	0.00765	0.00087
246		2S	-0.00921	0.03372	0.00020	-0.01049	-0.00145
247	40	C 1S	-0.00139	0.00509	-0.00006	0.00260	-0.00158
248		2S	0.00219	-0.00800	0.00012	-0.00486	0.00496
249		3S	0.01199	-0.04372	0.00090	-0.03343	0.00641
250		4PX	-0.00255	0.00934	-0.00015	0.00620	-0.04028
251		4PY	0.00463	-0.01692	0.00019	-0.00772	-0.01806
252		4PZ	0.00339	-0.01240	0.00035	-0.01405	-0.01585
253		5PX	0.01418	-0.05181	-0.00025	0.00855	-0.02928
254		5PY	-0.01676	0.06124	-0.00029	0.01358	-0.02743
255		5PZ	-0.00146	0.00538	0.00072	-0.02826	-0.00981
256	41	H 1S	0.00249	-0.00911	0.00015	-0.00608	0.00224
257		2S	0.00612	-0.02241	-0.00060	0.02176	0.00638
258	42	C 1S	0.00074	-0.00271	0.00003	-0.00129	0.00082
259		2S	-0.00132	0.00483	-0.00004	0.00206	-0.00180
260		3S	-0.00744	0.02732	-0.00066	0.02063	-0.01093
261		4PX	-0.00435	0.01598	-0.00004	0.00111	-0.01294
262		4PY	-0.00700	0.02564	-0.00020	0.00792	-0.01127
263		4PZ	-0.00169	0.00618	-0.00004	0.00156	-0.00357
264		5PX	0.00355	-0.01292	0.00026	-0.01035	-0.01343
265		5PY	-0.01718	0.06271	-0.00026	0.00744	-0.02089
266		5PZ	-0.00275	0.01004	-0.00016	0.01143	-0.00866
267	43	H 1S	0.00017	-0.00064	-0.00002	0.00102	0.00101
268		2S	-0.00271	0.00988	0.00002	-0.00369	0.00139
269	44	Zn 1S	0.00079	-0.00290	0.00003	-0.00104	0.00469
270		2S	0.00287	-0.01052	0.00017	-0.00674	-0.00643
271		3PX	-0.00035	0.00127	0.00024	-0.00960	0.02474
272		3PY	-0.00553	0.02022	-0.00021	0.00853	-0.01422
273		3PZ	-0.00041	0.00149	0.00099	-0.03957	-0.00797
274		4PX	0.00207	-0.00756	0.00009	-0.00340	-0.00493
275		4PY	-0.00478	0.01750	-0.00015	0.00682	-0.00061
276		4PZ	0.00311	-0.01137	-0.00207	0.08341	0.00142
277		5D 0	-0.00030	0.00108	-0.00028	0.01124	-0.00503
278		5D+1	-0.00141	0.00515	0.00174	-0.07043	0.00971
279		5D-1	-0.01684	0.06156	-0.00012	0.00483	0.00337
280		5D+2	0.00045	-0.00162	0.00012	-0.00489	-0.02766
281		5D-2	-0.00444	0.01622	0.00007	-0.00285	-0.00333

282	6D 0	-0.00009	0.00033	-0.00004	0.00169	-0.00031
283	6D+1	-0.00013	0.00049	0.00020	-0.00805	0.00140
284	6D-1	-0.00222	0.00813	-0.00002	0.00062	0.00052
285	6D+2	-0.00014	0.00050	0.00001	-0.00033	-0.00357
286	6D-2	-0.00086	0.00314	0.00000	0.00013	-0.00121
287 45	Br 1S	0.00017	-0.00060	-0.00012	0.00505	0.00029
288	2S	0.00075	-0.00274	-0.00058	0.02362	0.00226
289	3PX	0.00261	-0.00955	0.00626	-0.25294	-0.00352
290	3PY	-0.11562	0.42260	-0.00149	0.06020	0.00155
291	3PZ	0.01088	-0.03980	-0.00780	0.31551	0.00376
292	4PX	0.00221	-0.00806	0.00664	-0.26834	-0.00421
293	4PY	-0.11950	0.43679	-0.00148	0.05976	0.00440
294	4PZ	0.01021	-0.03733	-0.00773	0.31259	0.00626
295 46	Br 1S	0.00009	-0.00032	0.00012	-0.00495	0.00158
296	2S	-0.00017	0.00063	0.00061	-0.02482	0.00826
297	3PX	0.01302	-0.04756	-0.00564	0.22812	0.00267
298	3PY	0.07540	-0.27559	-0.00059	0.02400	0.00500
299	3PZ	-0.00142	0.00524	-0.00660	0.26688	-0.01302
300	4PX	0.01386	-0.05063	-0.00600	0.24255	0.00451
301	4PY	0.08000	-0.29239	-0.00051	0.02064	0.00384
302	4PZ	-0.00178	0.00653	-0.00645	0.26084	-0.01813
303 47	O 1S	-0.00001	0.00004	0.00000	0.00001	0.00015
304	2S	0.00008	-0.00024	0.00001	0.00004	-0.00038
305	3S	-0.00040	0.00127	-0.00001	-0.00074	-0.00101
306	4PX	0.00002	-0.00015	-0.00001	0.00071	0.07027
307	4PY	0.00046	-0.00178	-0.00004	0.00124	-0.14100
308	4PZ	0.00015	-0.00056	-0.00001	0.00033	-0.04373
309	5PX	-0.00034	0.00140	-0.00001	-0.00002	0.05421
310	5PY	-0.00009	-0.00002	-0.00004	0.00066	-0.10943
311	5PZ	0.00012	-0.00053	0.00002	0.00047	-0.03389
312 48	O 1S	0.00003	0.00001	0.00003	0.00000	0.00015
313	2S	0.00019	0.00003	0.00001	0.00001	-0.00095
314	3S	-0.00262	-0.00062	-0.00097	-0.00009	0.00304
315	4PX	0.00398	0.00103	0.00003	0.00004	-0.03481
316	4PY	0.00487	0.00131	0.00157	0.00006	-0.01826
317	4PZ	0.00193	0.00052	0.00068	0.00003	-0.00782
318	5PX	0.00341	0.00091	0.00026	0.00005	-0.02738
319	5PY	0.00032	0.00005	0.00058	-0.00006	-0.01397
320	5PZ	0.00142	0.00037	0.00065	0.00004	-0.00765
321 49	N 1S	-0.00019	0.00069	0.00000	-0.00003	0.00237

322		2S	0.00042	-0.00155	-0.00001	0.00057	-0.00755
323		3S	0.00066	-0.00235	0.00005	-0.00280	-0.00907
324		4PX	-0.00013	0.00042	-0.00017	0.00683	0.14837
325		4PY	-0.00121	0.00446	0.00022	-0.00870	-0.19593
326		4PZ	-0.00079	0.00290	0.00008	-0.00323	-0.08805
327		5PX	-0.00416	0.01518	-0.00021	0.00752	0.13209
328		5PY	0.00050	-0.00180	0.00016	-0.00669	-0.18426
329		5PZ	-0.00423	0.01549	0.00020	-0.00865	-0.08027
330	50	N 1S	0.00011	-0.00037	0.00000	0.00005	-0.00056
331		2S	-0.00019	0.00055	0.00001	-0.00014	0.00195
332		3S	-0.00039	0.00161	-0.00009	0.00044	0.00068
333		4PX	0.00074	-0.00292	-0.00005	0.00167	-0.02360
334		4PY	-0.00018	0.00071	0.00003	-0.00124	0.03668
335		4PZ	0.00001	-0.00004	-0.00001	0.00009	0.01636
336		5PX	0.00083	-0.00347	0.00013	0.00034	-0.03053
337		5PY	0.00124	-0.00461	0.00010	-0.00047	0.06661
338		5PZ	-0.00347	0.01256	0.00006	-0.00279	0.01959
339	51	H 1S	-0.00024	0.00086	0.00002	-0.00079	-0.00225
340		2S	-0.00350	0.01233	0.00012	-0.00397	-0.00875
341	52	N 1S	0.00033	0.00009	-0.00012	0.00000	0.00023
342		2S	-0.00089	-0.00025	-0.00005	0.00001	-0.00126
343		3S	0.00226	0.00064	0.00347	0.00002	0.00096
344		4PX	-0.00826	-0.00231	-0.00123	0.00000	0.00977
345		4PY	-0.00191	-0.00054	-0.00077	-0.00001	0.00491
346		4PZ	0.00010	0.00002	0.00074	0.00002	0.00229
347		5PX	-0.00350	-0.00106	-0.00016	-0.00005	0.01021
348		5PY	0.00367	0.00090	-0.00116	0.00008	0.00586
349		5PZ	-0.01881	-0.00504	-0.00122	0.00004	0.00530
350	53	H 1S	-0.00120	-0.00033	-0.00103	-0.00002	-0.00101
351		2S	-0.01475	-0.00388	-0.00313	0.00000	0.00306
352	54	N 1S	0.00465	0.00127	0.00109	0.00003	0.00393
353		2S	-0.01000	-0.00274	-0.00226	-0.00005	-0.00884
354		3S	-0.02428	-0.00664	-0.00443	-0.00012	-0.02458
355		4PX	-0.02428	-0.00667	-0.01212	-0.00029	-0.05976
356		4PY	0.01172	0.00320	-0.00178	-0.00004	-0.01129
357		4PZ	-0.00762	-0.00209	-0.00153	-0.00003	-0.01606
358		5PX	-0.01029	-0.00284	-0.01653	-0.00038	-0.05724
359		5PY	0.02007	0.00548	0.00663	0.00015	-0.01676
360		5PZ	-0.02456	-0.00673	-0.00333	-0.00010	-0.01953
361	55	C 1S	-0.00154	0.00563	0.00008	-0.00325	0.00081

362		2S	0.00248	-0.00908	-0.00018	0.00705	-0.00168
363		3S	0.01745	-0.06343	-0.00080	0.03061	-0.01688
364		4PX	-0.00617	0.02261	0.00030	-0.01204	-0.10012
365		4PY	-0.00185	0.00677	0.00017	-0.00676	0.13667
366		4PZ	-0.00487	0.01780	0.00039	-0.01584	0.06141
367		5PX	0.01669	-0.06098	0.00000	0.00246	-0.06749
368		5PY	0.01037	-0.03790	-0.00051	0.02146	0.09675
369		5PZ	-0.00365	0.01322	0.00041	-0.01492	0.05027
370	56	H 1S	0.00255	-0.00933	-0.00017	0.00697	0.00362
371		2S	0.00105	-0.00395	0.00030	-0.00994	0.01154
372	57	C 1S	0.00067	-0.00244	-0.00003	0.00130	0.00079
373		2S	-0.00076	0.00278	0.00005	-0.00224	-0.00185
374		3S	-0.01276	0.04651	0.00058	-0.02009	-0.00870
375		4PX	0.00138	-0.00506	-0.00018	0.00720	-0.05086
376		4PY	0.00397	-0.01460	-0.00003	0.00124	0.08166
377		4PZ	0.00077	-0.00286	0.00004	-0.00168	0.03529
378		5PX	0.00917	-0.03332	-0.00042	0.01616	-0.07814
379		5PY	0.00884	-0.03202	0.00002	-0.00267	0.10114
380		5PZ	-0.00013	0.00035	0.00005	0.00037	0.04094
381	58	H 1S	-0.00037	0.00135	0.00003	-0.00138	0.00393
382		2S	-0.00225	0.00805	0.00003	0.00050	0.00548
383	59	C 1S	-0.00029	0.00104	0.00000	-0.00028	-0.00094
384		2S	0.00051	-0.00183	-0.00001	0.00036	0.00089
385		3S	0.00533	-0.01975	0.00005	0.00383	0.03034
386		4PX	-0.00146	0.00543	0.00010	-0.00395	0.14914
387		4PY	0.00057	-0.00199	-0.00008	0.00350	-0.25665
388		4PZ	-0.00176	0.00643	0.00012	-0.00500	-0.10267
389		5PX	0.00458	-0.01694	0.00031	-0.00110	0.14393
390		5PY	-0.00082	0.00256	0.00010	0.00240	-0.24845
391		5PZ	0.01036	-0.03782	-0.00011	0.00553	-0.10342
392	60	C 1S	-0.00031	0.00112	0.00003	-0.00113	0.00090
393		2S	0.00040	-0.00147	-0.00001	0.00053	-0.00252
394		3S	0.00560	-0.02051	-0.00082	0.03102	-0.00265
395		4PX	-0.00005	0.00021	0.00015	-0.00629	-0.05539
396		4PY	-0.00262	0.00951	-0.00004	0.00166	0.08840
397		4PZ	-0.00053	0.00190	-0.00007	0.00282	0.03422
398		5PX	-0.00645	0.02367	0.00034	-0.01288	-0.06095
399		5PY	-0.00956	0.03495	0.00030	-0.01127	0.09729
400		5PZ	0.00462	-0.01692	-0.00029	0.01111	0.05080
401	61	H 1S	0.00003	-0.00011	-0.00003	0.00098	0.00387

402		2S	-0.00014	0.00045	0.00006	-0.00161	0.00084
403	62	C 1S	0.00059	-0.00216	-0.00005	0.00205	0.00061
404		2S	-0.00071	0.00259	0.00007	-0.00308	-0.00158
405		3S	-0.00498	0.01823	0.00093	-0.03441	-0.01213
406		4PX	0.00209	-0.00760	-0.00008	0.00338	-0.10264
407		4PY	-0.00001	0.00005	-0.00012	0.00482	0.14606
408		4PZ	-0.00196	0.00715	0.00032	-0.01316	0.06060
409		5PX	-0.01402	0.05123	0.00072	-0.02785	-0.07925
410		5PY	-0.00656	0.02400	0.00038	-0.01363	0.11286
411		5PZ	0.00184	-0.00664	0.00032	-0.01500	0.03200
412	63	H 1S	-0.00097	0.00353	0.00013	-0.00517	0.00362
413		2S	-0.00561	0.02045	-0.00021	0.00969	0.01608
414	64	C 1S	-0.00008	0.00024	0.00000	-0.00022	0.00028
415		2S	0.00036	-0.00109	-0.00005	0.00061	-0.00087
416		3S	0.00098	-0.00354	0.00042	0.00157	-0.00071
417		4PX	-0.00046	0.00195	0.00003	-0.00080	-0.09041
418		4PY	-0.00023	0.00103	0.00003	-0.00115	0.17908
419		4PZ	-0.00033	0.00100	0.00002	-0.00086	0.05804
420		5PX	-0.00009	-0.00022	0.00047	-0.00327	-0.04714
421		5PY	0.00021	0.00028	0.00026	-0.00288	0.08393
422		5PZ	0.00124	-0.00377	-0.00005	0.00156	0.02739
423	65	C 1S	0.00008	-0.00015	0.00000	0.00008	-0.00086
424		2S	-0.00003	0.00017	0.00000	-0.00040	0.00145
425		3S	-0.00130	0.00100	-0.00018	0.00153	0.01186
426		4PX	0.00011	-0.00098	-0.00004	0.00055	0.01031
427		4PY	0.00016	-0.00082	-0.00002	0.00072	-0.02117
428		4PZ	-0.00019	0.00039	0.00000	-0.00038	-0.00624
429		5PX	0.00020	-0.00053	0.00049	-0.00134	-0.02994
430		5PY	-0.00170	0.00035	0.00032	-0.00050	0.07803
431		5PZ	-0.00136	0.00179	-0.00023	0.00007	0.03094
432	66	H 1S	-0.00002	-0.00011	-0.00002	0.00020	-0.02660
433		2S	0.00081	-0.00045	-0.00006	0.00029	-0.08386
434	67	H 1S	0.00006	0.00003	0.00001	-0.00015	0.02727
435		2S	-0.00115	0.00066	-0.00009	0.00011	0.08704
436	68	C 1S	-0.00003	0.00006	-0.00001	-0.00002	-0.00010
437		2S	0.00003	-0.00001	0.00000	-0.00004	0.00110
438		3S	0.00012	-0.00154	0.00027	0.00020	-0.00365
439		4PX	-0.00001	0.00047	0.00003	-0.00014	0.00004
440		4PY	0.00024	0.00035	0.00011	-0.00013	0.00021
441		4PZ	-0.00009	0.00025	-0.00003	-0.00009	0.00092

442		5PX	-0.00205	0.00042	0.00025	-0.00133	0.05938
443		5PY	0.00208	-0.00048	0.00014	-0.00038	-0.11068
444		5PZ	-0.00052	-0.00008	-0.00029	0.00011	-0.02813
445	69	H 1S	0.00008	0.00003	0.00001	-0.00003	0.00213
446		2S	-0.00029	0.00048	0.00028	-0.00001	0.05253
447	70	H 1S	-0.00002	-0.00008	-0.00003	0.00006	-0.00307
448		2S	0.00118	-0.00020	-0.00013	0.00035	-0.06284
449	71	C 1S	0.00013	-0.00003	-0.00001	0.00003	-0.00257
450		2S	-0.00028	0.00004	0.00000	-0.00016	0.00629
451		3S	-0.00193	0.00023	-0.00011	0.00043	0.02332
452		4PX	-0.00040	-0.00046	0.00002	0.00021	0.00757
453		4PY	0.00007	-0.00022	-0.00013	0.00010	0.00528
454		4PZ	0.00000	0.00012	-0.00002	-0.00005	0.00853
455		5PX	0.00108	-0.00046	0.00120	-0.00071	-0.03116
456		5PY	-0.00351	-0.00050	0.00003	-0.00067	0.07997
457		5PZ	0.00031	0.00022	0.00055	-0.00026	0.03945
458	72	H 1S	-0.00013	0.00000	0.00002	-0.00004	-0.00123
459		2S	-0.00063	0.00007	0.00037	-0.00015	0.04686
460	73	H 1S	-0.00004	0.00001	-0.00013	-0.00004	0.00048
461		2S	0.00242	0.00013	0.00059	0.00016	-0.04996
462	74	C 1S	0.00019	0.00009	0.00006	-0.00002	0.00073
463		2S	-0.00025	-0.00016	-0.00035	0.00001	-0.00104
464		3S	-0.00272	-0.00100	0.00117	0.00021	-0.00462
465		4PX	-0.00005	0.00025	-0.00015	-0.00014	-0.00312
466		4PY	0.00162	0.00052	0.00072	-0.00001	-0.00151
467		4PZ	-0.00052	-0.00004	-0.00035	-0.00007	0.00012
468		5PX	-0.00086	-0.00015	0.00102	-0.00066	0.01838
469		5PY	0.00182	0.00039	-0.00073	0.00016	-0.02632
470		5PZ	-0.00317	-0.00095	0.00069	-0.00034	0.00099
471	75	H 1S	0.00021	0.00004	-0.00001	0.00000	-0.00238
472		2S	0.00201	0.00065	0.00049	0.00007	0.00233
473	76	H 1S	0.00039	0.00019	0.00010	-0.00005	-0.00538
474		2S	-0.00005	0.00015	0.00037	0.00019	-0.00564
475	77	C 1S	-0.00020	-0.00005	-0.00021	-0.00001	-0.00037
476		2S	0.00115	0.00031	0.00046	-0.00004	0.00307
477		3S	0.00856	0.00224	0.00168	0.00049	-0.02079
478		4PX	-0.00043	-0.00009	0.00034	0.00000	0.04192
479		4PY	-0.00255	-0.00071	-0.00085	-0.00004	0.02347
480		4PZ	-0.00159	-0.00042	-0.00072	-0.00002	0.00902
481		5PX	-0.00056	-0.00011	0.00144	-0.00022	0.03036

482		5PY	-0.00050	0.00011	-0.00380	0.00040	0.00893
483		5PZ	0.00467	0.00120	0.00098	0.00016	0.00435
484 78	C	1S	-0.00024	-0.00006	0.00028	0.00001	0.00038
485		2S	0.00038	0.00010	-0.00046	-0.00002	-0.00132
486		3S	0.00686	0.00183	-0.00750	-0.00011	-0.00462
487		4PX	0.00954	0.00262	0.00257	0.00006	-0.06563
488		4PY	0.00397	0.00108	0.00180	0.00004	-0.03103
489		4PZ	-0.00494	-0.00136	-0.00663	-0.00017	-0.01794
490		5PX	-0.01266	-0.00339	0.00475	-0.00010	-0.05935
491		5PY	0.00005	-0.00001	-0.00187	0.00030	-0.03554
492		5PZ	0.06884	0.01877	0.00047	0.00012	-0.01358
493 79	C	1S	-0.00039	-0.00011	-0.00127	-0.00003	-0.00002
494		2S	0.00046	0.00012	0.00109	0.00003	-0.00112
495		3S	0.00806	0.00221	0.02924	0.00073	0.01376
496		4PX	-0.01561	-0.00424	-0.00035	-0.00002	0.02581
497		4PY	-0.00858	-0.00233	-0.00636	-0.00017	0.01513
498		4PZ	-0.00408	-0.00111	0.00027	0.00000	0.00750
499		5PX	0.00687	0.00180	-0.00102	-0.00001	0.03346
500		5PY	-0.05923	-0.01608	-0.01375	-0.00037	0.01098
501		5PZ	0.00253	0.00070	0.00109	0.00001	0.01171
502 80	H	1S	0.00187	0.00051	0.00175	0.00004	0.00042
503		2S	0.00891	0.00241	-0.00007	0.00001	0.00111
504 81	C	1S	0.00266	0.00073	0.00310	0.00008	-0.00017
505		2S	-0.00434	-0.00119	-0.00614	-0.00016	0.00095
506		3S	-0.02648	-0.00713	-0.04054	-0.00098	-0.00424
507		4PX	-0.01626	-0.00444	-0.00399	-0.00010	0.03637
508		4PY	-0.00115	-0.00031	0.01016	0.00025	0.02092
509		4PZ	-0.01662	-0.00455	-0.01887	-0.00047	0.00751
510		5PX	0.04701	0.01285	0.01921	0.00046	0.03554
511		5PY	-0.05856	-0.01599	-0.01338	-0.00029	-0.00735
512		5PZ	0.01616	0.00445	-0.01190	-0.00036	0.00159
513 82	H	1S	-0.00387	-0.00106	-0.00765	-0.00019	0.00089
514		2S	-0.03371	-0.00924	0.01050	0.00031	-0.00148
515 83	C	1S	-0.00509	-0.00139	-0.00260	-0.00006	-0.00161
516		2S	0.00800	0.00219	0.00486	0.00012	0.00507
517		3S	0.04374	0.01194	0.03344	0.00076	0.00656
518		4PX	0.00935	0.00256	0.00620	0.00015	0.04093
519		4PY	-0.01692	-0.00463	-0.00772	-0.00019	0.01831
520		4PZ	-0.01241	-0.00339	-0.01405	-0.00035	0.01613
521		5PX	-0.05181	-0.01417	0.00856	0.00017	0.02974

522		5PY	0.06126	0.01675	0.01357	0.00039	0.02797
523		5PZ	0.00538	0.00148	-0.02826	-0.00067	0.00993
524 84	H	1S	0.00911	0.00249	0.00608	0.00015	0.00229
525		2S	0.02241	0.00614	-0.02177	-0.00048	0.00652
526 85	C	1S	0.00271	0.00074	0.00129	0.00003	0.00083
527		2S	-0.00483	-0.00132	-0.00206	-0.00006	-0.00184
528		3S	-0.02731	-0.00751	-0.02063	-0.00036	-0.01097
529		4PX	0.01597	0.00439	0.00110	0.00001	0.01302
530		4PY	0.02564	0.00703	0.00792	0.00019	0.01142
531		4PZ	0.00618	0.00170	0.00156	0.00004	0.00361
532		5PX	-0.01292	-0.00352	-0.01035	-0.00025	0.01347
533		5PY	0.06272	0.01714	0.00744	0.00011	0.02130
534		5PZ	0.01004	0.00274	0.01142	0.00040	0.00887
535 86	H	1S	0.00064	0.00018	-0.00102	-0.00003	0.00103
536		2S	-0.00989	-0.00270	0.00368	0.00017	0.00145

HOMO (#92) and LUMO(#93) for **6**:

			181	182	183	184	185
			(A)--O	(A)--O	(A)--O	(A)--O	(A)--V
EIGENVALUES --			-0.21233	-0.21233	-0.20762	-0.20762	-0.08597
1 1	Zn	1S	0.00038	0.00067	0.00056	-0.00010	0.00310
2		2S	0.00122	0.00213	0.00444	-0.00077	-0.01253
3		3PX	-0.00090	-0.00157	0.00330	-0.00056	0.02296
4		3PY	0.01394	0.02426	0.00336	-0.00055	-0.00815
5		3PZ	-0.00119	-0.00207	0.05278	-0.00863	0.00908
6		4PX	0.00028	0.00048	0.01788	-0.00295	-0.00191
7		4PY	0.01162	0.02018	-0.00045	0.00008	-0.00213
8		4PZ	0.00041	0.00073	-0.08912	0.01458	-0.00006
9		5D 0	-0.00198	-0.00345	0.00696	-0.00114	-0.00394
10		5D+1	-0.00161	-0.00281	0.06134	-0.01003	-0.00617
11		5D-1	0.02835	0.04932	0.00305	-0.00050	-0.00347
12		5D+2	-0.00081	-0.00140	-0.00647	0.00106	-0.02569
13		5D-2	0.00494	0.00859	0.00071	-0.00012	-0.00513
14		6D 0	-0.00029	-0.00050	0.00045	-0.00007	-0.00005
15		6D+1	-0.00024	-0.00041	0.00709	-0.00116	-0.00079
16		6D-1	0.00374	0.00651	0.00036	-0.00006	-0.00040
17		6D+2	-0.00023	-0.00040	-0.00102	0.00017	-0.00337
18		6D-2	0.00140	0.00244	0.00018	-0.00003	-0.00086
19 2	I	1S	0.00008	0.00014	0.00860	-0.00141	0.00095
20		2S	0.00010	0.00017	0.03101	-0.00508	0.00403

21		3PX	0.01065	0.01852	-0.17997	0.02944	-0.00073
22		3PY	-0.13057	-0.22718	-0.00945	0.00155	0.00050
23		3PZ	0.00551	0.00957	-0.29539	0.04832	-0.00741
24		4PX	0.01090	0.01897	-0.18914	0.03094	-0.00090
25		4PY	-0.13535	-0.23550	-0.01046	0.00171	0.00225
26		4PZ	0.00565	0.00983	-0.28300	0.04629	-0.01041
27	3	I 1S	-0.00007	-0.00013	-0.00811	0.00133	0.00202
28		2S	-0.00028	-0.00048	-0.02747	0.00450	0.00794
29		3PX	-0.00643	-0.01118	0.31863	-0.05212	-0.00013
30		3PY	0.23040	0.40089	0.01889	-0.00309	0.00315
31		3PZ	0.00051	0.00089	-0.25657	0.04197	0.01400
32		4PX	-0.00661	-0.01150	0.32214	-0.05269	0.00073
33		4PY	0.22654	0.39417	0.01872	-0.00306	0.00379
34		4PZ	-0.00010	-0.00018	-0.23910	0.03911	0.01891
35	4	O 1S	0.00008	0.00015	0.00006	-0.00001	0.00036
36		2S	-0.00010	-0.00020	-0.00006	0.00001	-0.00180
37		3S	-0.00127	-0.00210	-0.00099	0.00013	0.00189
38		4PX	0.00106	0.00187	0.00179	-0.00030	0.06264
39		4PY	0.00182	0.00318	-0.00009	0.00002	-0.06669
40		4PZ	-0.00112	-0.00190	0.00079	-0.00012	0.08881
41		5PX	0.00037	0.00069	0.00105	-0.00015	0.04666
42		5PY	0.00037	0.00096	-0.00027	0.00007	-0.05271
43		5PZ	-0.00121	-0.00207	0.00019	-0.00001	0.07423
44	5	O 1S	0.00007	-0.00004	-0.00001	-0.00005	0.00000
45		2S	0.00000	0.00001	0.00001	0.00004	0.00041
46		3S	-0.00230	0.00125	0.00010	0.00098	-0.00226
47		4PX	-0.00111	0.00062	0.00028	0.00172	0.03967
48		4PY	0.00218	-0.00129	0.00004	0.00025	0.06312
49		4PZ	0.00064	-0.00036	-0.00002	-0.00015	0.01153
50		5PX	0.00041	-0.00025	0.00012	0.00061	0.03160
51		5PY	0.00041	-0.00032	0.00002	0.00033	0.04930
52		5PZ	0.00135	-0.00070	0.00000	-0.00019	0.00963
53	6	N 1S	0.00223	0.00389	0.00103	-0.00017	0.00219
54		2S	-0.00482	-0.00839	-0.00236	0.00038	-0.00617
55		3S	-0.01121	-0.01945	-0.00287	0.00047	-0.00965
56		4PX	0.01038	0.01807	0.00711	-0.00116	0.15713
57		4PY	0.00416	0.00722	-0.00073	0.00012	-0.12953
58		4PZ	0.00359	0.00626	-0.00038	0.00006	0.05901
59		5PX	0.00588	0.01029	0.00948	-0.00155	0.14019
60		5PY	0.00873	0.01521	0.00414	-0.00070	-0.12433

61		5PZ	0.01507	0.02623	-0.00005	0.00000	0.05022
62	7	N 1S	0.00002	0.00005	-0.00016	0.00003	0.00040
63		2S	-0.00017	-0.00037	0.00003	-0.00002	-0.00121
64		3S	0.00186	0.00367	0.00384	-0.00057	-0.01227
65		4PX	0.00181	0.00317	-0.00079	0.00013	-0.01823
66		4PY	-0.00097	-0.00171	0.00039	-0.00008	0.01947
67		4PZ	0.00000	0.00003	-0.00205	0.00035	-0.01868
68		5PX	-0.00304	-0.00570	-0.00340	0.00044	-0.00716
69		5PY	0.00109	0.00142	-0.00006	-0.00007	0.02298
70		5PZ	0.00672	0.01185	-0.00108	0.00023	-0.06366
71	8	H 1S	-0.00086	-0.00150	-0.00113	0.00019	0.01678
72		2S	-0.00523	-0.00933	-0.00302	0.00040	0.06175
73	9	N 1S	-0.00011	0.00006	0.00002	0.00014	-0.00083
74		2S	-0.00028	0.00017	-0.00001	-0.00011	0.00122
75		3S	0.00629	-0.00377	-0.00051	-0.00282	0.01223
76		4PX	-0.00094	0.00055	-0.00015	-0.00092	-0.01508
77		4PY	-0.00125	0.00071	-0.00014	-0.00088	-0.02173
78		4PZ	0.00154	-0.00089	-0.00021	-0.00130	-0.00515
79		5PX	0.00381	-0.00221	-0.00029	-0.00068	-0.02216
80		5PY	-0.00113	0.00071	-0.00009	-0.00133	-0.03326
81		5PZ	-0.01389	0.00787	0.00004	-0.00007	-0.01380
82	10	H 1S	-0.00141	0.00081	0.00019	0.00115	-0.00254
83		2S	-0.01036	0.00591	0.00072	0.00398	-0.00981
84	11	N 1S	0.00262	-0.00150	-0.00009	-0.00055	-0.00478
85		2S	-0.00566	0.00325	0.00022	0.00131	0.01177
86		3S	-0.01268	0.00726	0.00010	0.00070	0.02940
87		4PX	-0.01306	0.00750	0.00030	0.00180	0.09182
88		4PY	0.00388	-0.00223	-0.00042	-0.00254	0.08361
89		4PZ	-0.00320	0.00184	-0.00043	-0.00261	0.00899
90		5PX	-0.01424	0.00820	0.00036	0.00216	0.08551
91		5PY	0.00732	-0.00423	-0.00081	-0.00496	0.08610
92		5PZ	-0.02555	0.01468	-0.00051	-0.00301	0.00579
93	12	C 1S	-0.00234	-0.00407	-0.00297	0.00049	-0.00042
94		2S	0.00350	0.00609	0.00580	-0.00095	0.00082
95		3S	0.01965	0.03435	0.03861	-0.00626	0.00368
96		4PX	-0.00527	-0.00917	-0.01144	0.00187	-0.09212
97		4PY	-0.00694	-0.01205	-0.00621	0.00102	0.08219
98		4PZ	0.00464	0.00808	0.01590	-0.00260	-0.03656
99		5PX	0.02893	0.05023	-0.00695	0.00113	-0.06141
100		5PY	0.02377	0.04133	0.01336	-0.00219	0.05203

101		5PZ	0.00652	0.01145	0.02991	-0.00489	-0.02692
102	13	H 1S	0.00389	0.00677	0.00689	-0.00113	0.00254
103		2S	0.00989	0.01707	-0.02180	0.00355	0.00513
104	14	C 1S	0.00124	0.00217	0.00134	-0.00022	-0.00064
105		2S	-0.00221	-0.00382	-0.00212	0.00035	0.00102
106		3S	-0.01638	-0.02865	-0.02358	0.00379	0.00579
107		4PX	-0.00308	-0.00539	0.00433	-0.00072	-0.06960
108		4PY	0.01158	0.02016	0.00537	-0.00088	0.07005
109		4PZ	-0.00236	-0.00410	0.00011	-0.00002	-0.03616
110		5PX	0.01550	0.02713	0.01407	-0.00228	-0.08725
111		5PY	0.02599	0.04538	0.00427	-0.00066	0.08595
112		5PZ	-0.00859	-0.01476	-0.01309	0.00220	-0.04578
113	15	H 1S	0.00020	0.00035	-0.00142	0.00023	-0.00098
114		2S	-0.00074	-0.00144	0.00580	-0.00099	0.00114
115	16	C 1S	0.00012	0.00022	0.00043	-0.00007	0.00045
116		2S	-0.00026	-0.00042	-0.00057	0.00010	-0.00019
117		3S	-0.00285	-0.00562	-0.01063	0.00164	-0.01012
118		4PX	-0.00351	-0.00609	-0.00192	0.00032	0.18251
119		4PY	0.00296	0.00514	0.00151	-0.00025	-0.16669
120		4PZ	0.00248	0.00431	0.00841	-0.00138	0.07973
121		5PX	0.00694	0.01127	-0.00373	0.00046	0.18801
122		5PY	-0.00425	-0.00803	-0.00265	0.00030	-0.14294
123		5PZ	-0.02940	-0.05125	0.00153	-0.00025	0.09425
124	17	C 1S	-0.00052	-0.00091	-0.00158	0.00026	0.00037
125		2S	0.00026	0.00046	0.00177	-0.00029	-0.00427
126		3S	0.01445	0.02517	0.03278	-0.00534	0.03651
127		4PX	0.00542	0.00943	-0.00291	0.00047	-0.04929
128		4PY	-0.00698	-0.01212	-0.00673	0.00111	0.04966
129		4PZ	0.00235	0.00408	-0.00104	0.00017	-0.02812
130		5PX	-0.01224	-0.02121	-0.00561	0.00090	-0.06595
131		5PY	-0.02621	-0.04558	-0.01080	0.00175	0.05623
132		5PZ	-0.00474	-0.00831	-0.00627	0.00101	-0.03330
133	18	H 1S	0.00103	0.00180	0.00224	-0.00037	0.00021
134		2S	0.00383	0.00653	-0.00114	0.00017	-0.01375
135	19	C 1S	0.00177	0.00308	0.00390	-0.00064	-0.00098
136		2S	-0.00243	-0.00420	-0.00704	0.00116	0.00377
137		3S	-0.01826	-0.03182	-0.05283	0.00859	-0.01902
138		4PX	0.00522	0.00908	0.00292	-0.00048	-0.11697
139		4PY	0.00077	0.00134	0.01263	-0.00206	0.11047
140		4PZ	0.01017	0.01770	0.02384	-0.00390	-0.04728

141		5PX	-0.03068	-0.05345	-0.01808	0.00294	-0.08924
142		5PY	-0.02954	-0.05155	-0.00867	0.00139	0.08474
143		5PZ	-0.01015	-0.01783	0.01817	-0.00299	-0.01825
144	20	H 1S	-0.00239	-0.00415	-0.00835	0.00137	0.00119
145		2S	-0.01716	-0.03001	0.01857	-0.00305	0.01422
146	21	C 1S	-0.00020	-0.00033	-0.00027	0.00005	0.00504
147		2S	0.00052	0.00105	0.00047	-0.00005	-0.01223
148		3S	0.00635	0.00960	0.00306	-0.00071	-0.07323
149		4PX	-0.00085	-0.00148	-0.00152	0.00024	-0.06920
150		4PY	-0.00085	-0.00146	0.00004	0.00000	0.09379
151		4PZ	0.00093	0.00164	-0.00002	0.00000	-0.12756
152		5PX	-0.00174	-0.00366	-0.00312	0.00033	-0.01852
153		5PY	-0.00067	-0.00220	-0.00308	0.00029	0.04995
154		5PZ	-0.00061	-0.00108	-0.00087	0.00008	-0.07932
155	22	C 1S	0.00010	0.00022	0.00006	0.00001	-0.00049
156		2S	-0.00022	-0.00040	-0.00033	0.00004	-0.00077
157		3S	-0.00128	-0.00213	0.00112	-0.00052	0.02882
158		4PX	0.00037	0.00042	0.00040	-0.00020	0.00393
159		4PY	0.00098	0.00169	0.00055	-0.00008	-0.01907
160		4PZ	0.00018	0.00038	0.00056	-0.00005	0.00976
161		5PX	0.00181	0.00019	-0.00098	-0.00041	-0.04974
162		5PY	0.00006	-0.00035	-0.00100	-0.00005	0.01042
163		5PZ	0.00217	0.00290	0.00070	0.00015	-0.01873
164	23	H 1S	0.00000	0.00002	0.00022	-0.00003	0.01940
165		2S	-0.00080	-0.00132	-0.00007	-0.00021	0.03985
166	24	H 1S	0.00014	0.00038	-0.00015	0.00007	-0.02540
167		2S	0.00172	0.00149	0.00019	-0.00009	-0.07537
168	25	C 1S	0.00003	-0.00001	-0.00002	-0.00003	-0.00184
169		2S	-0.00028	-0.00007	-0.00004	0.00012	0.00193
170		3S	0.00084	0.00009	0.00015	-0.00002	0.02623
171		4PX	-0.00020	0.00003	-0.00010	0.00019	-0.00771
172		4PY	0.00003	-0.00024	-0.00009	-0.00012	-0.00175
173		4PZ	0.00010	0.00025	-0.00001	0.00003	0.00279
174		5PX	-0.00098	-0.00315	-0.00167	-0.00065	0.02111
175		5PY	-0.00201	-0.00051	-0.00032	0.00007	-0.00543
176		5PZ	-0.00167	-0.00074	0.00027	0.00007	0.02697
177	26	H 1S	-0.00005	0.00001	0.00007	0.00003	0.00200
178		2S	-0.00088	-0.00015	0.00051	-0.00010	0.01070
179	27	H 1S	-0.00017	-0.00021	-0.00012	0.00003	0.00094
180		2S	0.00128	0.00068	0.00056	0.00002	-0.00634

181	28	C	1S	-0.00002	-0.00002	0.00002	0.00001	0.00396
182			2S	-0.00011	0.00011	-0.00005	0.00004	-0.00448
183			3S	0.00063	-0.00020	-0.00038	-0.00023	-0.07936
184			4PX	-0.00003	-0.00009	0.00009	-0.00019	-0.00463
185			4PY	0.00000	0.00021	0.00003	0.00001	-0.00576
186			4PZ	-0.00009	-0.00006	0.00004	0.00001	0.00862
187			5PX	0.00299	-0.00089	-0.00034	-0.00047	-0.02467
188			5PY	0.00160	0.00111	0.00052	0.00035	0.01483
189			5PZ	0.00103	-0.00072	-0.00026	0.00033	0.01389
190	29	H	1S	0.00000	-0.00001	0.00000	-0.00006	-0.00081
191			2S	-0.00038	0.00023	0.00026	-0.00050	0.00221
192	30	H	1S	-0.00004	-0.00010	-0.00006	0.00003	0.00241
193			2S	0.00181	0.00047	0.00043	-0.00007	0.02603
194	31	C	1S	0.00008	-0.00005	-0.00002	-0.00005	-0.00017
195			2S	-0.00034	0.00024	0.00006	0.00029	-0.00056
196			3S	0.00039	-0.00092	-0.00028	-0.00146	0.00103
197			4PX	-0.00063	0.00039	0.00006	0.00063	0.00085
198			4PY	0.00058	-0.00031	-0.00003	-0.00027	0.01139
199			4PZ	-0.00060	0.00038	0.00014	0.00060	0.00342
200			5PX	0.00088	-0.00144	-0.00088	-0.00151	-0.02994
201			5PY	-0.00181	0.00097	0.00030	0.00025	-0.02827
202			5PZ	-0.00120	-0.00014	-0.00022	-0.00006	0.01686
203	32	H	1S	0.00008	-0.00006	0.00001	0.00007	0.01625
204			2S	0.00126	-0.00043	0.00006	0.00015	0.05793
205	33	H	1S	0.00005	-0.00003	-0.00002	-0.00012	-0.00863
206			2S	0.00001	-0.00052	-0.00018	-0.00041	-0.00535
207	34	C	1S	-0.00022	0.00011	0.00004	0.00025	-0.00059
208			2S	0.00080	-0.00054	-0.00018	-0.00066	0.00081
209			3S	0.00882	-0.00392	0.00040	-0.00044	0.00878
210			4PX	0.00125	-0.00074	-0.00019	-0.00129	-0.04609
211			4PY	-0.00077	0.00047	0.00000	0.00008	-0.08352
212			4PZ	-0.00082	0.00046	0.00011	0.00059	-0.01556
213			5PX	0.00591	-0.00380	-0.00083	-0.00203	-0.02843
214			5PY	-0.00315	0.00221	0.00061	0.00195	-0.03633
215			5PZ	0.00209	-0.00128	-0.00024	-0.00193	-0.00617
216	35	C	1S	0.00050	-0.00029	-0.00005	-0.00034	0.00070
217			2S	-0.00126	0.00072	0.00007	0.00052	-0.00128
218			3S	-0.00816	0.00482	0.00101	0.00531	-0.01384
219			4PX	0.00106	-0.00062	0.00000	-0.00006	0.09317
220			4PY	0.00177	-0.00101	0.00013	0.00083	0.12653

221		4PZ	-0.00744	0.00428	0.00145	0.00888	0.00756
222		5PX	-0.00289	0.00139	-0.00047	-0.00063	0.08620
223		5PY	-0.00209	0.00132	0.00037	0.00080	0.12373
224		5PZ	0.05360	-0.03067	0.00074	0.00430	0.02588
225	36	C 1S	-0.00144	0.00083	0.00026	0.00158	-0.00101
226		2S	0.00129	-0.00073	-0.00037	-0.00223	0.00341
227		3S	0.03147	-0.01823	-0.00481	-0.02919	-0.01302
228		4PX	-0.00318	0.00184	-0.00109	-0.00666	-0.01678
229		4PY	-0.01379	0.00792	0.00047	0.00287	-0.02909
230		4PZ	0.00116	-0.00067	-0.00031	-0.00187	-0.00310
231		5PX	0.03562	-0.02051	-0.00160	-0.00972	-0.02143
232		5PY	-0.03856	0.02220	0.00052	0.00307	-0.04081
233		5PZ	0.01205	-0.00694	-0.00132	-0.00782	-0.01389
234	37	H 1S	0.00185	-0.00107	-0.00037	-0.00227	-0.00154
235		2S	0.00777	-0.00444	0.00035	0.00191	0.00782
236	38	C 1S	0.00408	-0.00235	-0.00063	-0.00387	0.00110
237		2S	-0.00568	0.00325	0.00115	0.00709	-0.00361
238		3S	-0.04630	0.02671	0.00858	0.05198	0.01016
239		4PX	-0.01141	0.00656	0.00116	0.00711	-0.07040
240		4PY	0.00317	-0.00182	-0.00141	-0.00860	-0.08592
241		4PZ	-0.02001	0.01150	0.00410	0.02509	-0.00630
242		5PX	0.06376	-0.03670	-0.00142	-0.00838	-0.05504
243		5PY	-0.04303	0.02479	0.00153	0.00909	-0.06895
244		5PZ	0.01525	-0.00881	0.00379	0.02351	0.01319
245	39	H 1S	-0.00575	0.00330	0.00136	0.00836	-0.00404
246		2S	-0.02361	0.01361	-0.00375	-0.02317	-0.01703
247	40	C 1S	-0.00347	0.00200	0.00048	0.00295	0.00032
248		2S	0.00488	-0.00280	-0.00094	-0.00575	-0.00016
249		3S	0.03038	-0.01750	-0.00657	-0.03973	0.00401
250		4PX	0.01096	-0.00630	-0.00183	-0.01121	-0.04758
251		4PY	-0.00671	0.00386	0.00102	0.00625	-0.06206
252		4PZ	-0.00652	0.00375	0.00286	0.01747	-0.00779
253		5PX	-0.05480	0.03144	0.00025	0.00184	-0.03549
254		5PY	0.03025	-0.01737	-0.00152	-0.00947	-0.03108
255		5PZ	-0.01357	0.00787	0.00474	0.02876	-0.01336
256	41	H 1S	0.00599	-0.00345	-0.00118	-0.00720	-0.00268
257		2S	0.01705	-0.00973	0.00338	0.02028	-0.00462
258	42	C 1S	0.00184	-0.00106	-0.00024	-0.00143	-0.00081
259		2S	-0.00317	0.00181	0.00032	0.00202	0.00149
260		3S	-0.02532	0.01468	0.00446	0.02645	0.00915

261		4PX	0.00073	-0.00042	0.00118	0.00726	-0.03271
262		4PY	0.01739	-0.01000	-0.00026	-0.00160	-0.05224
263		4PZ	-0.00014	0.00008	0.00011	0.00064	-0.00417
264		5PX	-0.03518	0.02026	0.00203	0.01213	-0.05491
265		5PY	0.03990	-0.02294	-0.00043	-0.00244	-0.06107
266		5PZ	0.01261	-0.00721	-0.00159	-0.01038	0.00051
267	43	H 1S	0.00019	-0.00011	0.00024	0.00150	-0.00178
268		2S	-0.00066	0.00040	-0.00061	-0.00412	-0.00332
269	44	Zn 1S	-0.00067	0.00038	-0.00009	-0.00056	-0.00387
270		2S	-0.00212	0.00122	-0.00069	-0.00445	0.01562
271		3PX	-0.00157	0.00090	0.00052	0.00331	0.02873
272		3PY	0.02427	-0.01395	0.00055	0.00336	-0.01019
273		3PZ	-0.00207	0.00119	0.00864	0.05278	0.01136
274		4PX	0.00048	-0.00028	0.00290	0.01789	-0.00233
275		4PY	0.02021	-0.01159	-0.00007	-0.00045	-0.00277
276		4PZ	0.00073	-0.00042	-0.01457	-0.08912	-0.00017
277		5D 0	0.00345	-0.00198	-0.00114	-0.00696	0.00493
278		5D+1	0.00281	-0.00161	-0.01003	-0.06134	0.00772
279		5D-1	-0.04932	0.02835	-0.00050	-0.00305	0.00435
280		5D+2	0.00140	-0.00081	0.00106	0.00647	0.03212
281		5D-2	-0.00860	0.00494	-0.00012	-0.00071	0.00645
282		6D 0	0.00050	-0.00029	-0.00007	-0.00045	0.00007
283		6D+1	0.00041	-0.00024	-0.00116	-0.00709	0.00098
284		6D-1	-0.00650	0.00374	-0.00006	-0.00036	0.00050
285		6D+2	0.00040	-0.00023	0.00017	0.00102	0.00421
286		6D-2	-0.00244	0.00140	-0.00003	-0.00018	0.00107
287	45	I 1S	-0.00014	0.00008	-0.00141	-0.00861	-0.00120
288		2S	-0.00017	0.00010	-0.00507	-0.03102	-0.00507
289		3PX	0.01852	-0.01064	-0.02943	-0.17995	-0.00092
290		3PY	-0.22714	0.13054	-0.00155	-0.00945	0.00065
291		3PZ	0.00958	-0.00550	-0.04831	-0.29538	-0.00927
292		4PX	0.01897	-0.01090	-0.03093	-0.18912	-0.00115
293		4PY	-0.23546	0.13533	-0.00171	-0.01047	0.00285
294		4PZ	0.00984	-0.00565	-0.04629	-0.28299	-0.01301
295	46	I 1S	0.00013	-0.00007	0.00133	0.00811	-0.00252
296		2S	0.00048	-0.00027	0.00449	0.02747	-0.00991
297		3PX	-0.01119	0.00643	0.05212	0.31863	-0.00016
298		3PY	0.40091	-0.23042	0.00310	0.01890	0.00395
299		3PZ	0.00089	-0.00051	-0.04197	-0.25659	0.01752
300		4PX	-0.01151	0.00661	0.05269	0.32215	0.00091

301		4PY	0.39419	-0.22655	0.00307	0.01872	0.00474
302		4PZ	-0.00017	0.00010	-0.03911	-0.23912	0.02366
303	47	O 1S	-0.00015	0.00009	-0.00001	-0.00005	-0.00040
304		2S	0.00019	-0.00012	0.00001	0.00006	0.00226
305		3S	0.00215	-0.00118	0.00019	0.00098	-0.00325
306		4PX	0.00185	-0.00108	0.00029	0.00179	0.07863
307		4PY	0.00317	-0.00183	-0.00001	-0.00009	-0.08361
308		4PZ	-0.00192	0.00107	0.00014	0.00078	0.11133
309		5PX	0.00067	-0.00041	0.00019	0.00105	0.05840
310		5PY	0.00080	-0.00065	-0.00002	-0.00028	-0.06568
311		5PZ	-0.00209	0.00118	0.00005	0.00018	0.09284
312	48	O 1S	-0.00004	-0.00007	0.00005	-0.00001	-0.00004
313		2S	-0.00001	0.00001	-0.00004	0.00000	-0.00022
314		3S	0.00136	0.00224	-0.00096	0.00021	0.00178
315		4PX	-0.00064	-0.00110	0.00172	-0.00028	0.03192
316		4PY	0.00123	0.00221	0.00025	-0.00004	0.05101
317		4PZ	0.00037	0.00063	-0.00015	0.00003	0.00927
318		5PX	0.00023	0.00042	0.00062	-0.00008	0.02557
319		5PY	0.00019	0.00048	0.00032	-0.00009	0.03992
320		5PZ	0.00081	0.00129	-0.00018	0.00006	0.00735
321	49	N 1S	-0.00389	0.00223	-0.00017	-0.00103	-0.00273
322		2S	0.00839	-0.00483	0.00039	0.00236	0.00771
323		3S	0.01948	-0.01116	0.00047	0.00287	0.01196
324		4PX	0.01807	-0.01040	0.00117	0.00711	0.19663
325		4PY	0.00723	-0.00414	-0.00012	-0.00073	-0.16213
326		4PZ	0.00625	-0.00360	-0.00006	-0.00038	0.07384
327		5PX	0.01027	-0.00593	0.00155	0.00948	0.17550
328		5PY	0.01520	-0.00875	0.00066	0.00415	-0.15553
329		5PZ	0.02623	-0.01508	-0.00002	-0.00004	0.06289
330	50	N 1S	-0.00004	0.00003	0.00002	0.00016	-0.00050
331		2S	0.00034	-0.00023	0.00001	-0.00004	0.00153
332		3S	-0.00345	0.00224	-0.00068	-0.00383	0.01502
333		4PX	0.00316	-0.00183	-0.00013	-0.00079	-0.02282
334		4PY	-0.00170	0.00099	0.00005	0.00040	0.02440
335		4PZ	0.00001	-0.00002	-0.00033	-0.00206	-0.02330
336		5PX	-0.00550	0.00340	-0.00066	-0.00336	-0.00948
337		5PY	0.00166	-0.00068	-0.00009	-0.00004	0.02812
338		5PZ	0.01178	-0.00686	-0.00013	-0.00110	-0.07942
339	51	H 1S	0.00150	-0.00086	0.00018	0.00113	-0.02097
340		2S	0.00921	-0.00543	0.00058	0.00299	-0.07721

341	52	N	1S	0.00006	0.00011	-0.00014	0.00003	0.00077
342			2S	0.00015	0.00029	0.00011	-0.00003	-0.00113
343			3S	-0.00354	-0.00642	0.00283	-0.00041	-0.01072
344			4PX	-0.00054	-0.00095	-0.00092	0.00015	-0.01220
345			4PY	-0.00072	-0.00124	-0.00088	0.00015	-0.01720
346			4PZ	0.00088	0.00154	-0.00130	0.00022	-0.00399
347			5PX	0.00218	0.00383	-0.00073	-0.00006	-0.01985
348			5PY	-0.00062	-0.00119	-0.00129	0.00034	-0.02534
349			5PZ	-0.00804	-0.01379	-0.00005	0.00006	-0.00911
350	53	H	1S	0.00081	0.00141	-0.00115	0.00019	0.00199
351			2S	0.00598	0.01032	-0.00400	0.00058	0.00624
352	54	N	1S	-0.00151	-0.00262	0.00055	-0.00009	0.00382
353			2S	0.00325	0.00566	-0.00131	0.00021	-0.00941
354			3S	0.00730	0.01265	-0.00070	0.00013	-0.02345
355			4PX	-0.00750	-0.01305	0.00180	-0.00029	0.07356
356			4PY	0.00223	0.00388	-0.00254	0.00042	0.06704
357			4PZ	-0.00184	-0.00320	-0.00261	0.00043	0.00721
358			5PX	-0.00817	-0.01425	0.00216	-0.00035	0.06855
359			5PY	0.00420	0.00734	-0.00496	0.00081	0.06899
360			5PZ	-0.01469	-0.02555	-0.00301	0.00048	0.00465
361	55	C	1S	0.00406	-0.00234	0.00049	0.00297	0.00052
362			2S	-0.00609	0.00350	-0.00095	-0.00580	-0.00103
363			3S	-0.03427	0.01978	-0.00636	-0.03859	-0.00470
364			4PX	-0.00917	0.00527	-0.00187	-0.01144	-0.11523
365			4PY	-0.01206	0.00692	-0.00101	-0.00621	0.10282
366			4PZ	0.00808	-0.00464	0.00260	0.01590	-0.04571
367			5PX	0.05028	-0.02884	-0.00115	-0.00694	-0.07698
368			5PY	0.04134	-0.02374	0.00218	0.01336	0.06499
369			5PZ	0.01139	-0.00661	0.00489	0.02992	-0.03348
370	56	H	1S	-0.00677	0.00389	-0.00113	-0.00689	-0.00317
371			2S	-0.01714	0.00977	0.00358	0.02179	-0.00623
372	57	C	1S	-0.00216	0.00125	-0.00022	-0.00133	0.00080
373			2S	0.00383	-0.00219	0.00034	0.00212	-0.00127
374			3S	0.02858	-0.01651	0.00392	0.02356	-0.00729
375			4PX	-0.00538	0.00311	0.00070	0.00433	-0.08718
376			4PY	0.02015	-0.01159	0.00088	0.00537	0.08770
377			4PZ	-0.00410	0.00235	0.00002	0.00011	-0.04523
378			5PX	0.02704	-0.01563	0.00232	0.01406	-0.10904
379			5PY	0.04530	-0.02613	0.00074	0.00426	0.10780
380			5PZ	-0.01485	0.00843	-0.00208	-0.01311	-0.05710

381	58	H	1S	-0.00035	0.00020	0.00023	0.00142	0.00123
382			2S	0.00136	-0.00087	-0.00091	-0.00581	-0.00125
383	59	C	1S	-0.00022	0.00013	-0.00007	-0.00043	-0.00055
384			2S	0.00044	-0.00023	0.00009	0.00057	0.00020
385			3S	0.00528	-0.00342	0.00183	0.01060	0.01324
386			4PX	-0.00610	0.00350	-0.00031	-0.00193	0.22844
387			4PY	0.00515	-0.00295	0.00025	0.00151	-0.20860
388			4PZ	0.00431	-0.00247	0.00137	0.00841	0.09980
389			5PX	0.01167	-0.00624	-0.00075	-0.00369	0.23430
390			5PY	-0.00771	0.00480	-0.00056	-0.00261	-0.17990
391			5PZ	-0.05120	0.02948	0.00025	0.00153	0.11749
392	60	C	1S	0.00091	-0.00052	0.00026	0.00158	-0.00046
393			2S	-0.00045	0.00027	-0.00029	-0.00177	0.00529
394			3S	-0.02515	0.01448	-0.00538	-0.03277	-0.04526
395			4PX	0.00943	-0.00541	-0.00048	-0.00291	-0.06166
396			4PY	-0.01213	0.00696	-0.00109	-0.00673	0.06214
397			4PZ	0.00408	-0.00234	-0.00017	-0.00103	-0.03520
398			5PX	-0.02125	0.01216	-0.00094	-0.00561	-0.08193
399			5PY	-0.04559	0.02619	-0.00178	-0.01080	0.07066
400			5PZ	-0.00828	0.00479	-0.00104	-0.00627	-0.04190
401	61	H	1S	-0.00180	0.00104	-0.00037	-0.00224	-0.00027
402			2S	-0.00659	0.00372	0.00020	0.00113	0.01753
403	62	C	1S	-0.00308	0.00177	-0.00064	-0.00390	0.00123
404			2S	0.00421	-0.00241	0.00115	0.00704	-0.00470
405			3S	0.03179	-0.01830	0.00869	0.05281	0.02334
406			4PX	0.00908	-0.00522	0.00048	0.00292	-0.14641
407			4PY	0.00134	-0.00077	0.00207	0.01262	0.13828
408			4PZ	0.01770	-0.01017	0.00390	0.02384	-0.05920
409			5PX	-0.05342	0.03074	-0.00298	-0.01808	-0.11175
410			5PY	-0.05147	0.02967	-0.00145	-0.00867	0.10605
411			5PZ	-0.01775	0.01030	0.00295	0.01817	-0.02309
412	63	H	1S	0.00416	-0.00239	0.00136	0.00835	-0.00149
413			2S	0.02994	-0.01729	-0.00302	-0.01857	-0.01757
414	64	C	1S	0.00034	-0.00019	0.00004	0.00027	-0.00622
415			2S	-0.00098	0.00064	-0.00010	-0.00046	0.01498
416			3S	-0.01032	0.00510	-0.00030	-0.00313	0.09151
417			4PX	-0.00148	0.00085	-0.00026	-0.00151	-0.08635
418			4PY	-0.00147	0.00083	0.00001	0.00004	0.11779
419			4PZ	0.00163	-0.00094	-0.00001	-0.00002	-0.15949
420			5PX	-0.00335	0.00229	-0.00068	-0.00307	-0.02388

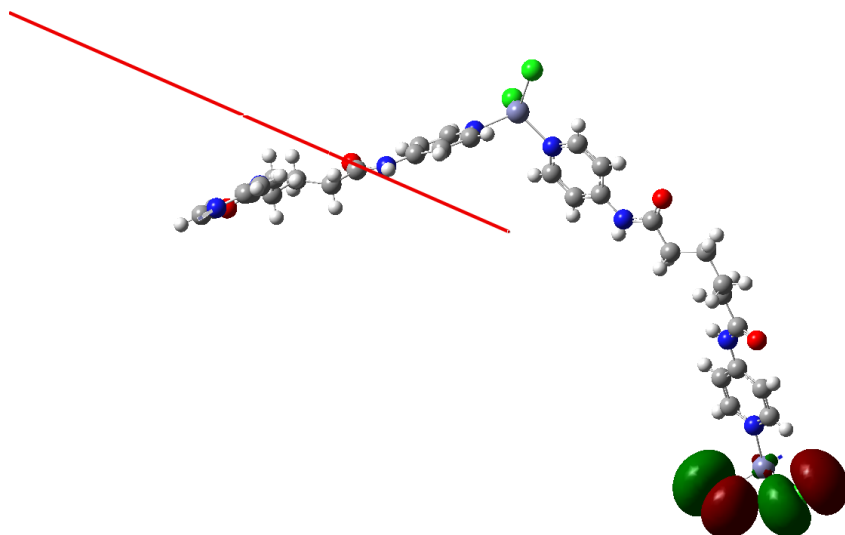
421		5PY	-0.00168	0.00156	-0.00070	-0.00301	0.06274
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423	65	C 1S	-0.00019	0.00014	-0.00003	-0.00005	0.00072
424		2S	0.00039	-0.00023	0.00007	0.00032	0.00053
425		3S	0.00218	-0.00120	0.00013	-0.00123	-0.03588
426		4PX	0.00053	-0.00018	-0.00006	0.00044	0.00543
427		4PY	0.00169	-0.00097	0.00010	0.00055	-0.02400
428		4PZ	0.00034	-0.00024	0.00013	0.00055	0.01229
429		5PX	0.00166	0.00074	-0.00070	-0.00080	-0.06337
430		5PY	-0.00012	0.00033	-0.00036	-0.00093	0.01359
431		5PZ	0.00333	-0.00141	0.00037	0.00062	-0.02691
432	66	H 1S	-0.00001	0.00002	-0.00004	-0.00021	-0.02436
433		2S	0.00136	-0.00073	0.00022	0.00000	-0.05192
434	67	H 1S	-0.00031	0.00026	-0.00002	0.00016	0.03211
435		2S	-0.00223	0.00043	0.00003	-0.00021	0.09673
436	68	C 1S	-0.00003	-0.00002	0.00003	0.00001	0.00233
437		2S	0.00027	0.00008	-0.00010	0.00008	-0.00239
438		3S	-0.00077	-0.00034	-0.00003	-0.00015	-0.03374
439		4PX	-0.00016	-0.00013	0.00015	-0.00016	-0.00990
440		4PY	-0.00009	0.00022	-0.00014	-0.00004	-0.00063
441		4PZ	0.00021	-0.00016	0.00002	-0.00002	0.00372
442		5PX	-0.00243	0.00222	-0.00115	-0.00137	0.02831
443		5PY	-0.00199	-0.00057	-0.00003	-0.00033	-0.00204
444		5PZ	-0.00181	-0.00020	0.00015	0.00023	0.04276
445	69	H 1S	0.00004	0.00003	-0.00005	-0.00006	-0.00187
446		2S	0.00084	0.00031	-0.00007	-0.00052	-0.01934
447	70	H 1S	0.00025	-0.00009	0.00001	0.00013	-0.00164
448		2S	-0.00145	-0.00006	-0.00020	-0.00052	0.01035
449	71	C 1S	0.00002	-0.00001	-0.00002	-0.00002	-0.00391
450		2S	0.00004	0.00015	-0.00003	0.00006	0.00388
451		3S	-0.00044	-0.00049	0.00034	0.00029	0.08589
452		4PX	-0.00007	0.00007	-0.00015	0.00015	-0.00120
453		4PY	0.00011	-0.00018	0.00002	0.00003	-0.00749
454		4PZ	-0.00011	0.00001	0.00003	0.00004	0.00807
455		5PX	0.00213	0.00228	-0.00055	-0.00017	-0.02933
456		5PY	0.00194	-0.00016	0.00050	0.00038	0.00016
457		5PZ	0.00053	0.00114	0.00023	-0.00035	0.00655
458	72	H 1S	0.00000	-0.00001	0.00005	-0.00002	0.00081
459		2S	0.00021	0.00039	0.00039	-0.00040	-0.01016
460	73	H 1S	0.00008	-0.00006	-0.00001	0.00007	-0.00230

461		2S	-0.00180	-0.00050	-0.00007	-0.00043	-0.01970
462	74	C 1S	-0.00005	-0.00008	0.00005	0.00000	0.00034
463		2S	0.00017	0.00038	-0.00029	0.00003	0.00065
464		3S	0.00012	-0.00100	0.00147	-0.00020	-0.00912
465		4PX	-0.00035	-0.00066	0.00061	-0.00014	-0.00011
466		4PY	0.00034	0.00056	-0.00026	0.00006	0.00943
467		4PZ	-0.00033	-0.00063	0.00062	-0.00006	0.00332
468		5PX	0.00004	0.00169	-0.00172	-0.00035	-0.02401
469		5PY	-0.00108	-0.00175	0.00034	0.00021	-0.02123
470		5PZ	-0.00111	-0.00048	-0.00013	-0.00019	0.02114
471	75	H 1S	-0.00004	-0.00009	-0.00007	0.00002	-0.01349
472		2S	-0.00087	-0.00100	-0.00016	-0.00001	-0.04706
473	76	H 1S	-0.00003	-0.00005	0.00012	-0.00002	0.00711
474		2S	0.00026	-0.00046	0.00045	0.00004	0.00078
475	77	C 1S	0.00014	0.00020	-0.00025	0.00004	0.00023
476		2S	-0.00042	-0.00087	0.00068	-0.00004	-0.00027
477		3S	-0.00565	-0.00783	0.00029	-0.00052	0.00014
478		4PX	0.00071	0.00127	-0.00128	0.00023	-0.03626
479		4PY	-0.00043	-0.00079	0.00007	-0.00003	-0.06775
480		4PZ	-0.00048	-0.00081	0.00060	-0.00008	-0.01196
481		5PX	0.00319	0.00625	-0.00219	-0.00014	-0.02409
482		5PY	-0.00161	-0.00350	0.00205	-0.00004	-0.02981
483		5PZ	0.00116	0.00215	-0.00190	0.00039	-0.00298
484	78	C 1S	-0.00029	-0.00050	0.00034	-0.00006	-0.00062
485		2S	0.00073	0.00125	-0.00051	0.00010	0.00116
486		3S	0.00462	0.00827	-0.00535	0.00073	0.01054
487		4PX	0.00061	0.00107	-0.00006	0.00002	0.07492
488		4PY	0.00102	0.00176	0.00083	-0.00014	0.10121
489		4PZ	-0.00428	-0.00744	0.00888	-0.00146	0.00606
490		5PX	-0.00179	-0.00266	-0.00075	-0.00024	0.06704
491		5PY	-0.00114	-0.00219	0.00088	0.00009	0.10077
492		5PZ	0.03088	0.05349	0.00431	-0.00066	0.01941
493	79	C 1S	0.00083	0.00144	-0.00158	0.00026	0.00082
494		2S	-0.00074	-0.00128	0.00223	-0.00036	-0.00268
495		3S	-0.01802	-0.03160	0.02920	-0.00474	0.00929
496		4PX	-0.00183	-0.00319	-0.00666	0.00109	-0.01353
497		4PY	-0.00792	-0.01378	0.00287	-0.00047	-0.02337
498		4PZ	0.00067	0.00116	-0.00187	0.00030	-0.00250
499		5PX	0.02045	0.03566	-0.00973	0.00158	-0.01682
500		5PY	-0.02215	-0.03859	0.00307	-0.00049	-0.03297

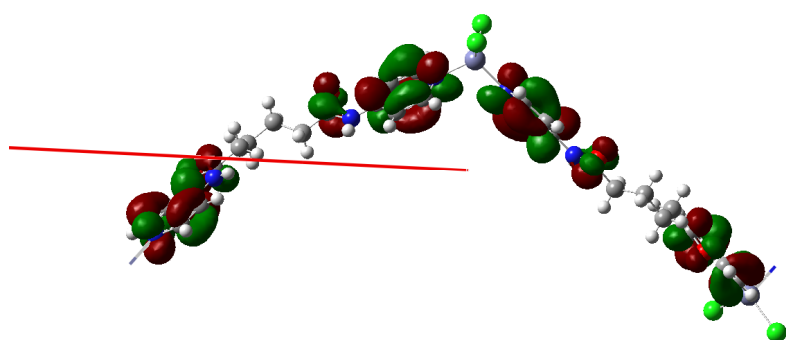
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502	80	H 1S	-0.00106	-0.00185	0.00227	-0.00037	0.00122
503		2S	-0.00448	-0.00775	-0.00193	0.00028	-0.00645
504	81	C 1S	-0.00234	-0.00408	0.00387	-0.00063	-0.00088
505		2S	0.00327	0.00567	-0.00709	0.00117	0.00291
506		3S	0.02656	0.04639	-0.05200	0.00843	-0.00774
507		4PX	-0.00656	-0.01141	0.00712	-0.00116	-0.05632
508		4PY	0.00182	0.00317	-0.00861	0.00141	-0.06885
509		4PZ	-0.01150	-0.02001	0.02510	-0.00411	-0.00505
510		5PX	0.03662	0.06381	-0.00840	0.00132	-0.04427
511		5PY	-0.02470	-0.04308	0.00911	-0.00145	-0.05509
512		5PZ	0.00873	0.01528	0.02350	-0.00389	0.01003
513	82	H 1S	0.00331	0.00575	-0.00836	0.00137	0.00324
514		2S	0.01355	0.02364	0.02316	-0.00383	0.01316
515	83	C 1S	0.00200	0.00347	-0.00295	0.00048	-0.00027
516		2S	-0.00280	-0.00488	0.00575	-0.00094	0.00014
517		3S	-0.01744	-0.03042	0.03975	-0.00643	-0.00259
518		4PX	0.00630	0.01096	-0.01121	0.00184	-0.03805
519		4PY	-0.00386	-0.00671	0.00625	-0.00103	-0.04980
520		4PZ	-0.00375	-0.00653	0.01747	-0.00286	-0.00623
521		5PX	-0.03152	-0.05476	0.00182	-0.00035	-0.02848
522		5PY	0.01740	0.03024	-0.00946	0.00158	-0.02492
523		5PZ	-0.00776	-0.01363	0.02878	-0.00467	-0.01072
524	84	H 1S	-0.00344	-0.00600	0.00720	-0.00118	0.00212
525		2S	-0.00984	-0.01699	-0.02031	0.00326	0.00352
526	85	C 1S	-0.00106	-0.00184	0.00143	-0.00023	0.00068
527		2S	0.00183	0.00316	-0.00201	0.00034	-0.00119
528		3S	0.01449	0.02544	-0.02650	0.00420	-0.00758
529		4PX	0.00042	0.00073	0.00726	-0.00119	-0.02629
530		4PY	0.00999	0.01739	-0.00160	0.00026	-0.04181
531		4PZ	-0.00008	-0.00014	0.00064	-0.00010	-0.00325
532		5PX	-0.02020	-0.03522	0.01215	-0.00194	-0.04343
533		5PY	0.02293	0.03991	-0.00246	0.00037	-0.04945
534		5PZ	0.00727	0.01258	-0.01035	0.00180	0.00140
535	86	H 1S	-0.00011	-0.00019	-0.00150	0.00025	0.00143
536		2S	0.00037	0.00068	0.00410	-0.00073	0.00197

MO diagrams

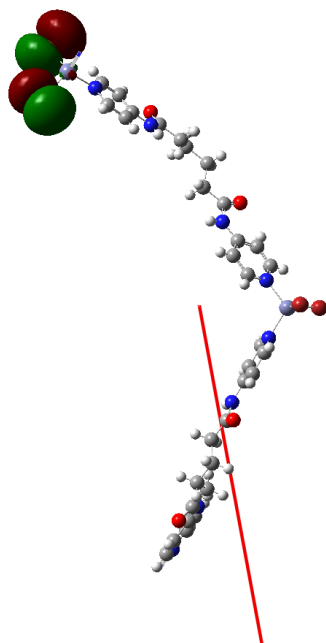
HOMO for **1** (red line in the figure represents the repeating unit of the polymeric structure):



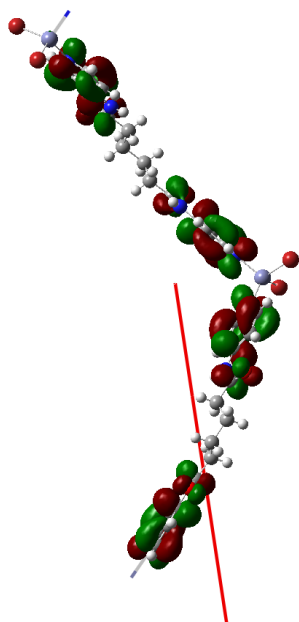
LUMO for **1** (red line in the figure represents the repeating unit of the polymeric structure):



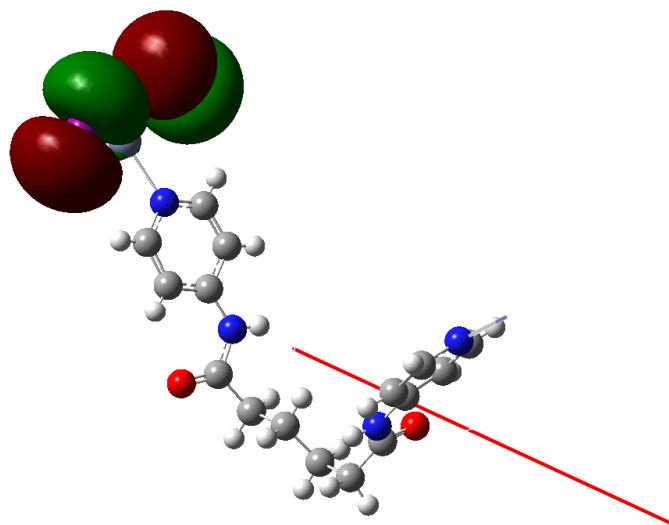
HOMO for **2** (red line in the figure represents the repeating unit of the polymeric structure):



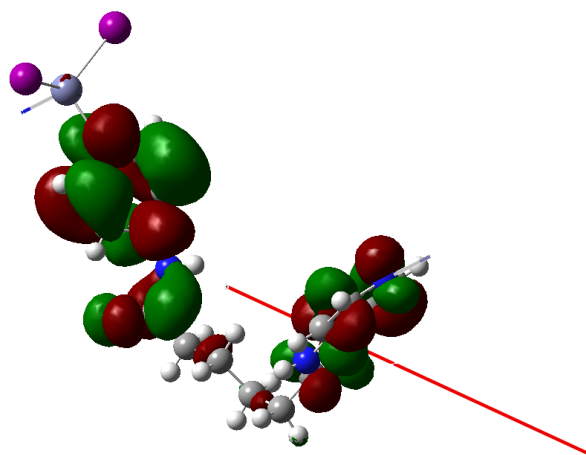
LUMO for **2** (red line in the figure represents the repeating unit of the polymeric structure):



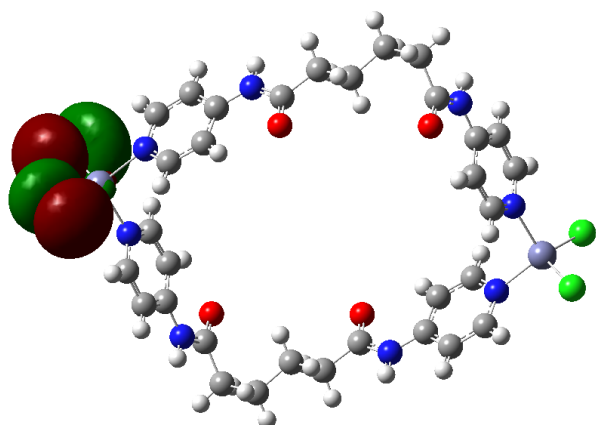
HOMO for **3** (red line in the figure represents the repeating unit of the polymeric structure):



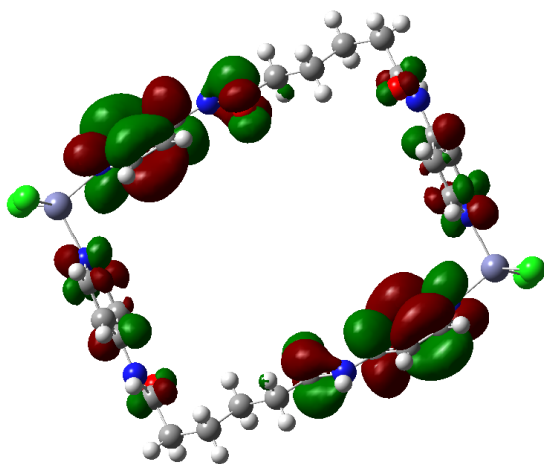
LUMO for **3** (red line in the figure represents the repeating unit of the polymeric structure):



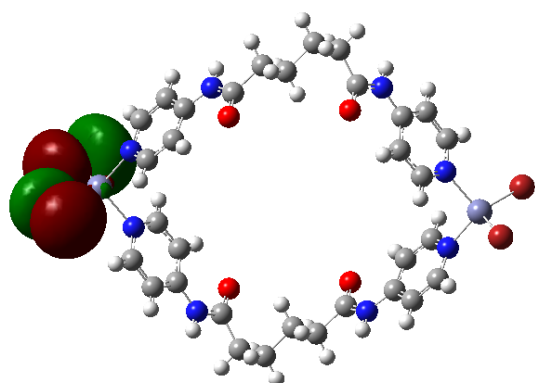
HOMO for **4**:



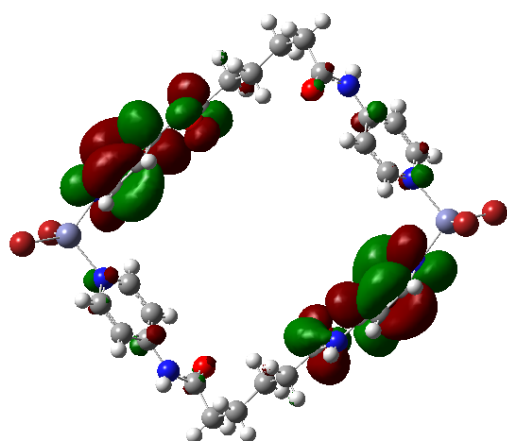
LUMO for 4:



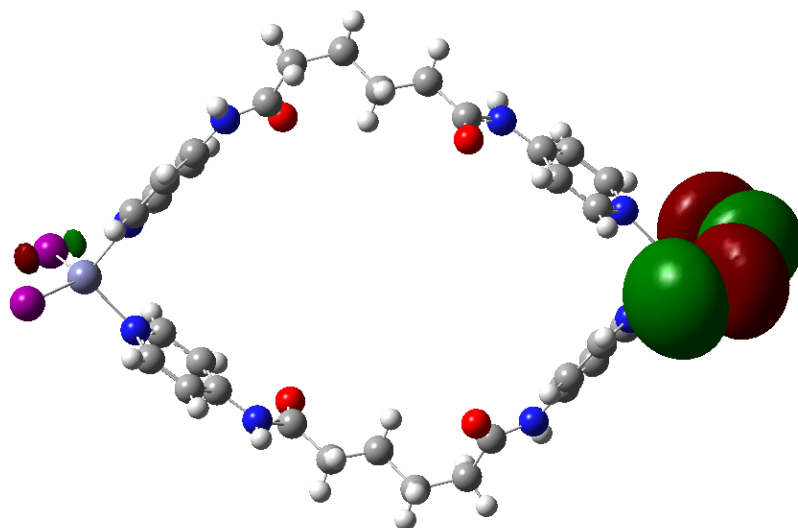
HOMO for 5:



LUMO for 5:



HOMO for 6:



LUMO for 6:

