

Relativistic effects at the Cu-O core – a density functional theory study - Supporting Information

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S1. Cartesian Coordinates of **C1**, **C2** and **C3** for O and P core for the nonrelativistic minimum energy wave function, TPSSh/cc-pVTZ.

		O			P		
Atoms		x	y	z	x	y	z
C1	N	-2.775837	1.337149	-0.100573	-3.184819	1.379334	-0.112774
	C	-4.076975	0.70109	0.28925	-4.460585	0.702896	0.288366
	C	-4.077043	-0.701059	-0.289052	-4.460656	-0.702874	-0.288174
	N	-2.775847	-1.337151	0.100534	-3.184817	-1.379339	0.112692
	Cu	-1.357797	-0.000007	-0.000075	-1.744335	-0.000004	-0.000091
	O	0	1.160158	-0.080826	0.000001	0.733892	-0.058881
	O	0	-1.160164	0.080785	-0.000001	-0.733894	0.05885
	Cu	1.357797	0.000001	0.000025	1.744335	0.000001	0.000043
	N	2.775843	1.337151	-0.100513	3.184819	1.379338	-0.112688
	C	4.077014	0.701071	0.289168	4.460631	0.70288	0.288273
	C	4.077006	-0.701071	-0.289153	4.46061	-0.702888	-0.28827
	N	2.775842	-1.33715	0.100556	3.184817	-1.379335	0.112772
	H	-2.812358	1.692039	-1.056904	-3.261263	1.734551	-1.06556
	H	-2.555101	2.138664	0.489304	-3.01795	2.195863	0.472061
	H	-4.114286	0.677172	1.378811	-4.48502	0.674313	1.378518
	H	-4.921414	1.288847	-0.07132	-5.328946	1.264645	-0.056662
	H	-4.921429	-1.288799	0.071667	-5.328953	-1.26461	0.057034
	H	-4.114547	-0.677138	-1.378606	-4.485321	-0.674286	-1.37832
	H	-2.555235	-2.138648	-0.489415	-3.01805	-2.195818	-0.472241
	H	-2.812222	-1.692091	1.056851	-3.261091	-1.734638	1.065461
	H	2.555171	2.138647	0.489414	3.018014	2.19583	0.472216
	H	2.812274	1.692076	-1.056833	3.261155	1.734615	-1.06546
	H	4.114435	0.677134	1.378724	4.485215	0.674291	1.378422
	H	4.921423	1.288823	-0.071479	5.328952	1.264621	-0.05687
	H	4.114404	-0.677135	-1.37871	4.485126	-0.674302	-1.37842
	H	4.921422	-1.288825	0.071475	5.328948	-1.264634	0.05682
	H	2.812297	-1.692077	1.056874	3.2612	-1.734578	1.065553
	H	2.555154	-2.138643	-0.489369	3.017986	-2.195848	-0.472096
C2	Cu	-0.000083	-1.389177	0.019945	0.000711	1.771715	-0.00327
	Cu	0.00002	1.389134	-0.019941	-0.000711	-1.771716	0.003269
	O	1.157132	-0.00007	0.000084	0.745622	-0.0003	-0.000006
	O	-1.157212	0.000019	0.000046	-0.745621	0.000301	0.00001
	N	1.432183	-2.69069	0.100266	1.497432	3.001141	-0.092462
	N	2.81102	-1.823489	-1.572846	2.87104	1.960321	1.469527
	N	3.778457	-2.825152	0.271195	3.844493	3.143154	-0.274254
	N	-1.432434	-2.690651	0.100402	-1.49505	3.002309	-0.092425
	N	-2.811276	-1.82322	-1.572605	-2.869455	1.962513	1.469542
	N	-3.778719	-2.825079	0.271323	-3.842004	3.14609	-0.274235
	N	-1.432207	2.690726	-0.1002	-1.497433	-3.00114	0.092464
	N	-2.810981	1.823352	1.57289	-2.871041	-1.960321	-1.469526
	N	-3.778481	2.825309	-0.270965	-3.844495	-3.143155	0.274255

N	1.432339	2.690601	-0.100403	1.495051	-3.00231	0.092423
N	2.811308	1.823171	1.572454	2.869455	-1.962513	-1.469544
N	3.778593	2.824965	-0.271617	3.842006	-3.14609	0.274233
C	1.260294	-3.892518	0.92501	1.286151	4.265256	-0.810921
C	-0.000112	-4.651965	0.549346	0.001948	4.959604	-0.364307
C	-1.260543	-3.892575	0.925019	-1.282809	4.266261	-0.810886
C	2.645911	-2.43191	-0.375504	2.711584	2.706142	0.343069
C	3.88558	-0.870327	-1.810559	3.946757	0.990304	1.618326
C	1.760012	-1.816717	-2.573864	1.842872	1.902083	2.496164
C	4.953948	-3.32216	-0.442475	5.035206	3.557619	0.464637
C	3.867073	-2.862378	1.724804	3.917376	3.275877	-1.724418
C	-2.646165	-2.431776	-0.375307	-2.709427	2.70822	0.343089
C	-1.760336	-1.816549	-2.573686	-1.841342	1.903504	2.49619
C	-3.8854	-0.869478	-1.809941	-3.945863	0.993256	1.618291
C	-3.867471	-2.862426	1.724924	-3.914785	3.278891	-1.724397
C	-4.954327	-3.321721	-0.442405	-5.032418	3.561415	0.464653
C	-1.260375	3.892667	-0.9248	-1.286151	-4.265254	0.810924
C	0.000133	4.651995	-0.549241	-0.001949	-4.959603	0.364308
C	1.260447	3.892482	-0.925074	1.28281	-4.266262	0.810885
C	-2.645924	2.431898	0.375597	-2.711585	-2.706142	-0.343067
C	-3.885248	0.869815	1.810402	-3.946759	-0.990305	-1.618324
C	-1.759867	1.816453	2.573806	-1.842872	-1.902081	-2.496162
C	-4.953981	3.322111	0.442831	-5.035206	-3.557622	-0.464636
C	-3.867219	2.86281	-1.724563	-3.917379	-3.275877	1.724419
C	2.646129	2.431732	0.375208	2.709429	-2.70822	-0.343091
C	1.760523	1.816573	2.573706	1.841342	-1.903505	-2.496192
C	3.885988	0.870156	1.810109	3.945862	-0.993254	-1.618293
C	3.867084	2.862109	-1.725242	3.914787	-3.278891	1.724395
C	4.954196	3.321958	0.441866	5.03242	-3.561413	-0.464655
H	1.215568	-3.639608	1.990667	1.239198	4.097953	-1.893218
H	2.126402	-4.539317	0.777876	2.133103	4.928314	-0.621197
H	-0.000094	-4.882578	-0.518619	0.002011	5.080134	0.722104
H	-0.000094	-5.599674	1.093797	0.002335	5.961634	-0.801699
H	-2.126644	-4.53936	0.777791	-2.129239	4.929978	-0.621132
H	-1.215853	-3.639776	1.990704	-1.236018	4.09893	-1.893185
H	4.518443	-0.800584	-0.931437	4.581974	1.008162	0.738139
H	3.443152	0.107945	-2.004949	3.515049	-0.00943	1.724191
H	4.48973	-1.167706	-2.670254	4.551111	1.206252	2.502311
H	1.118488	-2.680752	-2.423538	1.2132	2.78531	2.422814
H	2.219294	-1.876806	-3.562294	2.325852	1.886783	3.475533
H	1.167668	-0.89926	-2.511416	1.229452	1.001123	2.394762
H	4.718343	-3.440291	-1.496714	4.817604	3.572457	1.529392
H	5.23269	-4.29433	-0.029889	5.316704	4.564664	0.148828
H	5.805191	-2.644998	-0.334132	5.879213	2.888906	0.274984
H	3.018369	-2.337827	2.155188	3.073552	2.76123	-2.177911
H	4.788731	-2.364026	2.034436	4.844045	2.813292	-2.072696
H	3.888845	-3.88712	2.10464	3.915439	4.32142	-2.042541

H	-1.167896	-0.899145	-2.511304	-1.228572	1.002104	2.394775
H	-2.219689	-1.876604	-3.56209	-2.324347	1.888528	3.475552
H	-1.118885	-2.68064	-2.423395	-1.211031	2.786277	2.422872
H	-4.518827	-0.800495	-0.931169	-4.581074	1.01162	0.738111
H	-4.489056	-1.165816	-2.670336	-4.550055	1.209583	2.502293
H	-3.442567	0.108885	-2.002982	-3.514867	-0.006793	1.724091
H	-3.018691	-2.33814	2.155478	-3.07134	2.763631	-2.177899
H	-3.889544	-3.887209	2.10463	-3.912079	4.324437	-2.042502
H	-4.789036	-2.363877	2.034524	-4.841794	2.816995	-2.072685
H	-5.805502	-2.644539	-0.333639	-5.876916	2.893331	0.274972
H	-5.233084	-4.294043	-0.030183	-5.31317	4.568676	0.148869
H	-4.718877	-3.439408	-1.496726	-4.814817	3.57606	1.529412
H	-1.215813	3.63991	-1.990502	-1.239195	-4.09795	1.893221
H	-2.126439	4.539474	-0.77745	-2.133103	-4.928312	0.621202
H	0.000272	4.882553	0.518736	-0.002014	-5.080135	-0.722103
H	0.000131	5.59973	-1.093645	-0.002336	-5.961634	0.801701
H	2.12663	4.539197	-0.778017	2.129239	-4.92998	0.621129
H	1.21558	3.639625	-1.990741	1.236021	-4.09893	1.893184
H	-4.518845	0.800958	0.931743	-4.581976	-1.008164	-0.738138
H	-3.44258	-0.108638	2.003367	-3.515051	0.009429	-1.72419
H	-4.488693	1.166275	2.670903	-4.551112	-1.206253	-2.502309
H	-1.118581	2.680714	2.42376	-1.2132	-2.785308	-2.422812
H	-2.219097	1.876045	3.562288	-2.325851	-1.886781	-3.475531
H	-1.167301	0.899166	2.510974	-1.229453	-1.001121	-2.394758
H	-4.718486	3.439658	1.497157	-4.817603	-3.572458	-1.529392
H	-5.232567	4.294523	0.030706	-5.316703	-4.564668	-0.148829
H	-5.805286	2.645099	0.334024	-5.879214	-2.88891	-0.274984
H	-3.018483	2.338476	-2.155151	-3.073554	-2.761232	2.177913
H	-4.788832	2.364386	-2.034221	-4.844047	-2.813291	2.072696
H	-3.889174	3.887632	-2.104169	-3.915444	-4.32142	2.042542
H	1.16834	0.898984	2.511698	1.22857	-1.002105	-2.394775
H	2.219978	1.8771	3.562035	2.324346	-1.888526	-3.475554
H	1.118801	2.680417	2.423171	1.211032	-2.786279	-2.422874
H	4.518688	0.800325	0.930875	4.581075	-1.01162	-0.738114
H	4.49029	1.167696	2.669645	4.550051	-1.209579	-2.502297
H	3.443698	-0.108129	2.004739	3.514864	0.006795	-1.724089
H	3.018232	2.337733	-2.155547	3.071343	-2.763631	2.177898
H	3.889043	3.886841	-2.105093	3.912079	-4.324438	2.0425
H	4.788614	2.363557	-2.034939	4.841796	-2.816996	2.072683
H	4.71888	3.439772	1.496203	4.814818	-3.576061	-1.529414
H	5.805501	2.644944	0.333081	5.876917	-2.893327	-0.274976
H	5.232686	4.294289	0.029482	5.313174	-4.568673	-0.148869
C3						
Cu	-1.274357	-0.294276	-0.281801	1.692894	-0.063081	-0.097938
Cu	1.365385	0.499736	0.421588	-1.769658	0.089026	0.126979
O	-0.110026	-0.265432	1.081055	0.030557	0.800689	0.302145
O	0.118164	0.697408	-0.874873	-0.047646	-0.577831	0.739775
N	-4.39051	0.551835	-0.078311	4.139069	-1.071125	-1.074679

N	-3.275151	1.213681	0.328045	2.986503	-1.51788	-0.498869
N	-3.726657	-1.748101	-0.187067	4.417896	0.992751	0.093875
N	-2.503745	-1.699938	0.41762	3.28443	1.026287	0.845335
N	2.790338	-1.413935	-0.637719	-3.281882	-1.091016	0.671599
N	3.972042	-1.399135	0.031333	-4.29644	-1.161486	-0.232037
N	2.927416	1.510182	-0.22434	-3.051554	1.475979	-0.516062
N	4.149032	0.985534	0.090379	-4.08115	0.978412	-1.255318
C	-4.269215	-0.610816	-0.918949	4.408287	0.35423	-1.207682
C	-3.721583	2.181292	1.138135	3.127496	-2.847282	-0.350038
C	-5.132176	2.119309	1.252096	4.384521	-3.239111	-0.850985
C	-5.525798	1.065665	0.468978	5.001749	-2.091995	-1.286321
C	-2.795937	3.214963	1.734537	3.627152	1.60617	2.004047
C	-2.442464	-2.785536	1.229268	4.998273	1.944794	1.978435
C	-3.64113	-3.513606	1.104022	5.470775	1.535207	0.756259
C	-4.430683	-2.825019	0.220675	-4.207218	-0.451342	-1.496556
C	-1.33733	-3.112948	2.213923	-4.946239	1.959417	-1.603262
C	4.307288	-0.249645	0.841958	-4.456844	3.131873	-1.079818
C	5.142732	1.748094	-0.416978	-3.272474	2.79608	-0.394244
C	4.555558	2.803918	-1.066602	-5.347617	-1.850946	0.272087
C	3.164695	2.635549	-0.928246	-4.996416	-2.247025	1.539949
C	2.088968	3.557551	-1.449284	-3.698016	-1.746733	1.766887
C	4.830396	-2.357742	-0.415755	5.416595	0.435993	-1.604846
C	4.166264	-3.041366	-1.400599	4.788719	-4.234996	-0.881243
C	2.905055	-2.409206	-1.525652	5.56643	2.423177	2.756307
C	1.858965	-2.651005	-2.590571	-5.162346	-0.592676	-1.995523
H	-5.275237	-0.902978	-1.208662	-4.902767	4.106527	-1.166233
H	-5.773085	2.765428	1.825634	-5.600756	-2.817413	2.222457
H	-3.894596	-4.426854	1.610264	3.446355	1.040621	-2.157374
H	5.367789	-0.328087	1.067346	3.90727	1.761683	-3.247985
H	5.060537	3.610918	-1.565858	2.142561	0.944268	-1.861755
H	4.540595	-3.877495	-1.964553	2.981328	2.412219	-4.057545
C	-3.47243	-0.322524	-2.165232	4.9673	1.820103	-3.458865
C	-4.098345	-0.174498	-3.392033	1.252256	1.578539	-2.63458
N	-2.143942	-0.201571	-2.033666	1.631628	2.322001	-3.742677
C	-3.327488	0.106568	-4.514589	0.215909	1.483723	-2.338867
H	-5.17329	-0.275534	-3.464417	0.881101	2.819986	-4.341284
C	-1.394275	0.07135	-3.110587	-3.100954	-0.993042	-2.384943
C	-1.952785	0.22959	-4.368525	-3.404122	-1.619357	-3.585181
H	-3.795241	0.224806	-5.483496	-1.847591	-0.842408	-1.940215
C	3.55511	-0.184455	2.151446	-2.358218	-2.113101	-4.359139
C	4.180316	-0.487444	3.350235	-4.431539	-1.723141	-3.91045
N	2.269467	0.190529	2.11182	-0.848296	-1.321412	-2.685971
C	3.45711	-0.385546	4.533985	-1.056405	-1.961579	-3.900942
H	5.218371	-0.793094	3.356277	0.149541	-1.1914	-2.285962
C	1.563396	0.298131	3.247236	-0.214955	-2.334584	-4.469186
C	2.130829	0.02165	4.480527	5.972323	-1.920956	-1.722633
H	3.927869	-0.61222	5.481939	6.450373	1.586732	0.309534

H	-6.496473	0.64945	0.252891	-6.245332	-2.003105	-0.304573
H	-5.43035	-3.004336	-0.140087	-5.828478	1.74635	-2.18455
H	5.818503	-2.471127	0.000281	-2.560461	-2.608048	-5.30027
H	6.17657	1.481931	-0.268952	3.31202	2.98334	-4.915458
C	0.461936	-2.770657	-1.97266	2.626966	1.840005	3.111677
H	-0.290005	-2.840092	-2.761759	3.350018	2.365374	4.358724
H	0.384281	-3.659828	-1.348239	3.842208	3.320463	4.164562
H	0.245913	-1.898132	-1.3542	2.624755	2.522918	5.158182
C	1.904485	-1.442522	-3.548627	4.096896	1.654463	4.718012
H	1.712923	-0.516955	-3.002575	1.909961	0.523753	3.459016
H	2.884526	-1.359313	-4.021574	1.333521	0.143427	2.615184
H	1.157165	-1.561708	-4.337015	2.624362	-0.241585	3.768155
C	2.176379	-3.931695	-3.372374	1.215982	0.695573	4.284247
H	2.191545	-4.804804	-2.716928	1.597762	2.884544	2.640188
H	1.411304	-4.094963	-4.133323	0.879084	3.073806	3.440227
H	3.139135	-3.862413	-3.881895	2.086774	3.828261	2.390316
C	0.021763	-3.32886	1.531042	1.05493	2.526085	1.766134
H	0.767685	-3.553943	2.296688	2.087841	-3.717439	0.31655
H	-0.025219	-4.181873	0.852499	1.918915	-3.251134	1.775578
H	0.349109	-2.450017	0.983491	2.869321	-3.302544	2.30952
C	-1.272775	-1.974572	3.250387	1.547406	-2.227322	1.829343
H	-1.050868	-1.023272	2.766757	1.205479	-3.899838	2.28584
H	-2.221692	-1.883195	3.782542	2.561303	-5.177486	0.310031
H	-0.490133	-2.194321	3.980034	3.498137	-5.297755	0.857163
C	-1.695297	-4.410439	2.959977	1.81017	-5.800596	0.796987
H	-1.7742	-5.259463	2.278231	2.69889	-5.551162	-0.706782
H	-0.902817	-4.631994	3.675869	0.748724	-3.623603	-0.433533
H	-2.62862	-4.315638	3.517634	0.863233	-3.934051	-1.474374
C	-2.427483	4.213292	0.618875	0.019182	-4.283584	0.039117
H	-3.319053	4.716333	0.240359	0.349648	-2.610062	-0.406264
H	-1.746355	4.973353	1.007617	-2.842671	-1.887758	3.003698
H	-1.943627	3.6978	-0.21163	-2.285055	-0.516555	3.423819
C	-1.524496	2.545752	2.27379	-1.601952	-0.112273	2.674306
H	-1.770836	1.835021	3.06674	-3.08918	0.2013	3.593752
H	-1.001317	2.006972	1.485137	-1.720028	-0.62464	4.351196
H	-0.856632	3.306163	2.684832	-3.688792	-2.458513	4.149959
C	-3.499946	3.962207	2.874759	-4.069845	-3.453152	3.910582
H	-2.815698	4.692856	3.309256	-3.070756	-2.547852	5.044166
H	-4.376655	4.505601	2.517933	-4.53295	-1.808061	4.387259
H	-3.813883	3.278393	3.666231	-1.682089	-2.852514	2.696466
C	1.381701	2.894373	-2.646042	-1.054276	-2.962227	3.582723
H	2.092837	2.661602	-3.441001	-2.058888	-3.838684	2.418286
H	0.88538	1.975669	-2.329231	-1.064737	-2.471557	1.884192
H	0.627919	3.576081	-3.045305	-2.357177	3.710771	0.385894
C	1.078518	3.870216	-0.335372	-2.112698	3.128658	1.788818
H	1.576075	4.298901	0.536733	-3.055089	2.978653	2.318149
H	0.351518	4.595473	-0.702036	-1.580236	2.177384	1.744604

H	0.529317	2.978692	-0.032734	-1.500676	3.821223	2.368146
C	2.731424	4.871924	-1.920441	-1.021925	3.864845	-0.367577
H	1.947251	5.544997	-2.268721	-1.184863	4.282704	-1.363285
H	3.267902	5.370026	-1.110556	-0.366426	4.541371	0.183637
H	3.420277	4.709853	-2.751497	-0.513604	2.906094	-0.465697
H	-0.334919	0.16535	-2.9269	-3.013234	5.091766	0.525175
H	-1.311199	0.444941	-5.21174	-2.358602	5.744263	1.104164
H	0.533595	0.603468	3.134494	-3.17344	5.561058	-0.447544
H	1.535632	0.128132	5.376837	-3.970879	5.028803	1.045345

S2. Diagonal Matrix Elements of the relativistic non-relativistic Overlap Difference dS_{ij} for C1, C2 and C3

	MO _i	O			P		
		dS _{ii}	S _{ii} ^(nr-DKH)	S _{ii} ^(nr)	dS _{ii}	S _{ii} ^(nr-DKH)	S _{ii} ^(nr)
C1	1	0.63	-0.37	1.00	0.32	-0.68	1.00
	2	0.26	0.74	1.00	0.06	0.94	1.00
	3	0.05	0.95	1.00	0.00	-1.00	1.00
	4	0.05	-0.95	1.00	0.00	1.00	1.00
	5	0.52	0.48	1.00	0.00	1.00	1.00
	6	0.62	-0.38	1.00	0.00	-1.00	1.00
	7	0.27	0.73	1.00	0.02	-0.98	1.00
	8	0.25	-0.75	1.00	0.03	0.97	1.00
	9	0.35	-0.65	1.00	0.12	-0.88	1.00
	10	0.32	0.68	1.00	0.11	0.89	1.00
	11	0.00	1.00	1.00	0.00	1.00	1.00
	12	0.00	1.00	1.00	0.00	1.00	1.00
	13	0.15	-0.85	1.00	0.02	-0.98	1.00
	14	0.30	0.70	1.00	0.02	0.98	1.00
	15	0.35	0.65	1.00	0.03	-0.97	1.00
	16	0.22	0.78	1.00	0.03	0.97	1.00
	17	0.16	-0.84	1.00	0.01	-0.99	1.00
	18	0.16	0.84	1.00	0.01	0.99	1.00
	19	0.05	0.95	1.00	0.02	0.98	1.00
	20	0.05	-0.95	1.00	0.02	-0.98	1.00
	21	0.00	1.00	1.00	0.01	-0.99	1.00
	22	0.00	-1.00	1.00	0.01	0.99	1.00
	23	0.00	-1.00	1.00	0.00	-1.00	1.00
	24	0.00	1.00	1.00	0.00	1.00	1.00
	25	0.00	1.00	1.00	0.00	1.00	1.00
	26	0.00	-1.00	1.00	0.00	-1.00	1.00
	27	0.00	1.00	1.00	0.72	-0.28	1.00
	28	0.00	-1.00	1.00	0.71	0.29	1.00
	29	0.00	1.00	1.00	0.00	1.00	1.00
	30	0.00	1.00	1.00	0.00	-1.00	1.00
	31	0.00	1.00	1.00	0.00	1.00	1.00
	32	0.00	1.00	1.00	0.00	1.00	1.00
	33	0.00	1.00	1.00	0.00	-1.00	1.00
	34	0.00	1.00	1.00	0.00	1.00	1.00
	35	0.00	1.00	1.00	0.00	-1.00	1.00
	36	0.00	1.00	1.00	0.00	1.00	1.00
	37	0.00	1.00	1.00	0.87	-0.13	1.00
	38	0.00	1.00	1.00	0.87	0.13	1.00
	39	0.00	1.00	1.00	0.95	-0.05	1.00
	40	0.00	1.00	1.00	0.95	0.05	1.00
	41	0.00	1.00	1.00	0.00	1.00	1.00

42	0.00	1.00	1.00	0.00	-1.00	1.00
43	0.00	1.00	1.00	0.00	1.00	1.00
44	0.00	1.00	1.00	0.00	-1.00	1.00
45	0.00	-1.00	1.00	0.00	1.00	1.00
46	0.00	1.00	1.00	0.00	1.00	1.00
47	0.00	1.00	1.00	0.00	-1.00	1.00
48	0.00	1.00	1.00	0.00	1.00	1.00
49	0.00	1.00	1.00	0.00	1.00	1.00
50	0.01	0.99	1.00	0.00	1.00	1.00
51	0.01	0.99	1.00	0.00	1.00	1.00
52	0.00	1.00	1.00	0.00	-1.00	1.00
53	0.00	1.00	1.00	0.00	1.00	1.00
54	0.00	-1.00	1.00	0.00	1.00	1.00
55	0.00	1.00	1.00	0.00	1.00	1.00
56	0.01	0.99	1.00	0.00	1.00	1.00
57	0.12	-0.88	1.00	0.00	1.00	1.00
58	0.12	0.88	1.00	0.00	-1.00	1.00
59	0.01	-0.99	1.00	0.00	-1.00	1.00
60	0.01	0.99	1.00	0.00	1.00	1.00
61	0.02	0.98	1.00	0.00	1.00	1.00
62	0.02	0.98	1.00	0.00	1.00	1.00
63	0.00	-1.00	1.00	0.08	0.92	1.00
64	0.00	1.00	1.00	0.08	-0.92	1.00
65	0.00	-1.00	1.00	0.00	1.00	1.00
66	0.00	1.00	1.00	0.00	1.00	1.00
67	0.00	-1.00	1.00	0.00	1.00	1.00
68	0.00	1.00	1.00	0.00	1.00	1.00
69	0.00	1.00	1.00	0.00	1.00	1.00
70	0.00	1.00	1.00	0.00	1.00	1.00
C2						
1	0.00	1.00	1.00	0.00	1.00	1.00
2	0.00	1.00	1.00	0.00	1.00	1.00
3	0.00	1.00	1.00	0.00	1.00	1.00
4	0.00	1.00	1.00	0.00	1.00	1.00
5	0.00	1.00	1.00	0.00	1.00	1.00
6	0.00	1.00	1.00	0.00	1.00	1.00
7	0.00	1.00	1.00	0.00	1.00	1.00
8	0.00	1.00	1.00	0.00	1.00	1.00
9	0.00	1.00	1.00	0.00	1.00	1.00
10	0.00	1.00	1.00	0.00	1.00	1.00
11	0.00	1.00	1.00	0.00	1.00	1.00
12	0.00	1.00	1.00	0.00	1.00	1.00
13	0.00	1.00	1.00	0.00	1.00	1.00
14	0.00	1.00	1.00	0.00	1.00	1.00
15	0.00	1.00	1.00	0.00	1.00	1.00
16	0.00	1.00	1.00	0.00	1.00	1.00
17	0.00	1.00	1.00	0.00	1.00	1.00
18	0.00	1.00	1.00	0.00	1.00	1.00

19	0.00	1.00	1.00	0.00	1.00	1.00
20	0.00	1.00	1.00	0.00	1.00	1.00
21	0.00	1.00	1.00	0.04	0.96	1.00
22	0.00	1.00	1.00	0.04	0.96	1.00
23	0.00	1.00	1.00	0.10	0.90	1.00
24	0.00	1.00	1.00	0.10	0.90	1.00
25	0.00	1.00	1.00	0.06	0.94	1.00
26	0.00	1.00	1.00	0.06	0.94	1.00
27	0.00	1.00	1.00	0.06	0.94	1.00
28	0.00	1.00	1.00	0.06	0.94	1.00
29	0.00	1.00	1.00	0.00	1.00	1.00
30	0.00	1.00	1.00	0.00	1.00	1.00
31	0.00	1.00	1.00	0.00	1.00	1.00
32	0.00	1.00	1.00	0.00	1.00	1.00
33	0.00	1.00	1.00	0.00	1.00	1.00
34	0.00	1.00	1.00	0.49	-0.51	1.00
35	0.00	1.00	1.00	0.49	0.51	1.00
36	0.00	1.00	1.00	0.00	1.00	1.00
37	0.00	1.00	1.00	0.00	1.00	1.00
38	0.00	1.00	1.00	0.00	1.00	1.00
39	0.00	1.00	1.00	0.00	1.00	1.00
40	0.00	1.00	1.00	0.00	1.00	1.00
41	0.00	1.00	1.00	0.00	1.00	1.00
42	0.00	1.00	1.00	0.00	1.00	1.00
43	0.00	1.00	1.00	0.00	1.00	1.00
44	0.00	1.00	1.00	0.00	1.00	1.00
45	0.00	1.00	1.00	0.00	1.00	1.00
46	0.00	1.00	1.00	0.00	1.00	1.00
47	0.00	1.00	1.00	0.00	1.00	1.00
48	0.00	1.00	1.00	0.00	1.00	1.00
49	0.00	1.00	1.00	0.00	1.00	1.00
50	0.00	1.00	1.00	0.00	1.00	1.00
51	0.00	1.00	1.00	0.00	1.00	1.00
52	0.00	1.00	1.00	0.00	1.00	1.00
53	0.00	1.00	1.00	0.00	1.00	1.00
54	0.00	1.00	1.00	0.00	1.00	1.00
55	0.00	1.00	1.00	0.00	1.00	1.00
56	0.00	1.00	1.00	0.00	1.00	1.00
57	0.00	1.00	1.00	0.00	1.00	1.00
58	0.00	1.00	1.00	0.00	1.00	1.00
59	0.00	1.00	1.00	0.00	1.00	1.00
60	0.00	1.00	1.00	0.00	1.00	1.00
61	0.00	1.00	1.00	0.00	1.00	1.00
62	0.00	1.00	1.00	0.00	-1.00	1.00
63	0.00	1.00	1.00	0.00	-1.00	1.00
64	0.00	1.00	1.00	0.00	1.00	1.00
65	0.00	1.00	1.00	0.00	1.00	1.00

66	0.00	1.00	1.00	0.00	1.00	1.00
67	0.00	1.00	1.00	0.00	1.00	1.00
68	0.00	1.00	1.00	0.00	1.00	1.00
69	0.00	-1.00	1.00	0.00	1.00	1.00
70	0.00	1.00	1.00	0.00	1.00	1.00
71	0.00	1.00	1.00	0.00	1.00	1.00
72	0.00	1.00	1.00	0.00	1.00	1.00
73	0.00	1.00	1.00	0.00	1.00	1.00
74	0.00	1.00	1.00	0.00	1.00	1.00
75	0.00	1.00	1.00	0.00	1.00	1.00
76	0.00	1.00	1.00	0.00	1.00	1.00
77	0.00	1.00	1.00	0.00	1.00	1.00
78	0.00	1.00	1.00	0.00	1.00	1.00
79	0.00	1.00	1.00	0.00	1.00	1.00
80	0.00	1.00	1.00	0.00	1.00	1.00
81	0.00	1.00	1.00	0.00	1.00	1.00
82	0.00	1.00	1.00	0.00	1.00	1.00
83	0.00	1.00	1.00	0.00	1.00	1.00
84	0.00	1.00	1.00	0.00	1.00	1.00
85	0.00	1.00	1.00	0.00	1.00	1.00
86	0.00	1.00	1.00	0.00	1.00	1.00
87	0.00	1.00	1.00	0.00	1.00	1.00
88	0.00	1.00	1.00	0.00	-1.00	1.00
89	0.00	1.00	1.00	0.00	1.00	1.00
90	0.00	1.00	1.00	0.00	1.00	1.00
91	0.00	1.00	1.00	0.00	1.00	1.00
92	0.00	1.00	1.00	0.00	1.00	1.00
93	0.00	1.00	1.00	0.00	1.00	1.00
94	0.00	1.00	1.00	0.00	1.00	1.00
95	0.00	1.00	1.00	0.00	1.00	1.00
96	0.00	1.00	1.00	0.00	1.00	1.00
97	0.00	1.00	1.00	0.00	-1.00	1.00
98	0.00	1.00	1.00	0.00	-1.00	1.00
99	0.00	-1.00	1.00	0.00	1.00	1.00
100	0.00	1.00	1.00	0.00	-1.00	1.00
101	0.00	1.00	1.00	0.00	1.00	1.00
102	0.00	1.00	1.00	0.00	1.00	1.00
103	0.00	1.00	1.00	0.00	1.00	1.00
104	0.00	1.00	1.00	0.00	1.00	1.00
105	0.00	1.00	1.00	0.00	1.00	1.00
106	0.00	1.00	1.00	0.00	1.00	1.00
107	0.00	1.00	1.00	0.00	-1.00	1.00
108	0.00	1.00	1.00	0.00	-1.00	1.00
109	0.00	1.00	1.00	0.00	1.00	1.00
110	0.00	1.00	1.00	0.00	1.00	1.00
111	0.00	1.00	1.00	0.00	1.00	1.00
112	0.00	1.00	1.00	0.00	1.00	1.00

113	0.00	-1.00	1.00	0.00	1.00	1.00
114	0.00	1.00	1.00	0.00	1.00	1.00
115	0.00	1.00	1.00	0.00	1.00	1.00
116	0.00	1.00	1.00	0.00	1.00	1.00
117	0.00	1.00	1.00	0.00	1.00	1.00
118	0.00	1.00	1.00	0.00	1.00	1.00
119	0.00	1.00	1.00	0.00	1.00	1.00
120	0.00	-1.00	1.00	0.00	1.00	1.00
121	0.00	1.00	1.00	0.00	1.00	1.00
122	0.00	1.00	1.00	0.00	1.00	1.00
123	0.00	1.00	1.00	0.00	1.00	1.00
124	0.00	1.00	1.00	0.00	1.00	1.00
125	0.00	1.00	1.00	0.00	1.00	1.00
126	0.00	1.00	1.00	0.00	1.00	1.00
127	0.00	1.00	1.00	0.00	1.00	1.00
128	0.00	1.00	1.00	0.00	1.00	1.00
129	0.00	1.00	1.00	0.00	1.00	1.00
130	0.00	1.00	1.00	0.00	1.00	1.00
131	0.01	0.99	1.00	0.00	1.00	1.00
132	0.00	1.00	1.00	0.00	1.00	1.00
133	0.00	1.00	1.00	0.00	1.00	1.00
134	0.00	1.00	1.00	0.00	1.00	1.00
135	0.01	0.99	1.00	0.00	1.00	1.00
136	0.01	0.99	1.00	0.00	1.00	1.00
137	0.00	1.00	1.00	1.00	0.00	1.00
138	0.00	1.00	1.00	1.00	0.00	1.00
139	0.00	1.00	1.00	0.00	1.00	1.00
140	0.00	1.00	1.00	0.01	0.99	1.00
141	0.00	1.00	1.00	0.01	0.99	1.00
142	0.00	1.00	1.00	0.01	0.99	1.00
143	0.00	1.00	1.00	0.00	1.00	1.00
144	0.00	1.00	1.00	0.00	1.00	1.00
145	0.00	-1.00	1.00	0.00	1.00	1.00
146	0.00	1.00	1.00	0.00	1.00	1.00
147	0.00	1.00	1.00	0.00	1.00	1.00
148	0.01	-0.99	1.00	0.00	1.00	1.00
149	0.00	1.00	1.00	0.00	1.00	1.00
150	0.01	0.99	1.00	0.00	1.00	1.00
151	0.00	1.00	1.00	1.00	0.00	1.00
152	0.89	0.11	1.00	1.00	0.00	1.00
153	0.89	0.11	1.00	0.00	1.00	1.00
154	0.00	1.00	1.00	0.00	1.00	1.00
155	0.00	1.00	1.00	0.00	-1.00	1.00
156	0.00	1.00	1.00	0.00	1.00	1.00
157	0.00	-1.00	1.00	0.00	1.00	1.00
158	0.01	0.99	1.00	0.00	1.00	1.00
159	0.00	-1.00	1.00	0.00	1.00	1.00

160	0.00	1.00	1.00	0.00	1.00	1.00
161	1.00	0.00	1.00	0.00	1.00	1.00
162	1.00	0.00	1.00	0.00	-1.00	1.00
163	0.00	1.00	1.00	0.00	1.00	1.00
164	0.03	0.97	1.00	0.00	1.00	1.00
165	0.03	0.97	1.00	0.00	1.00	1.00
166	0.00	1.00	1.00	0.02	0.98	1.00
167	0.00	1.00	1.00	0.01	0.99	1.00
168	0.00	1.00	1.00	0.01	0.99	1.00
169	0.00	1.00	1.00	0.02	0.98	1.00
170	0.00	1.00	1.00	0.00	1.00	1.00
171	0.00	1.00	1.00	0.02	0.98	1.00
172	0.00	1.00	1.00	0.02	0.98	1.00
173	0.00	1.00	1.00	0.00	1.00	1.00
174	0.00	-1.00	1.00	0.00	1.00	1.00
175	0.00	-1.00	1.00	0.00	1.00	1.00
176	0.00	1.00	1.00	0.01	0.99	1.00
177	0.00	1.00	1.00	0.00	1.00	1.00
178	0.00	1.00	1.00	0.00	1.00	1.00
179	0.00	1.00	1.00	0.00	1.00	1.00
180	0.00	1.00	1.00	0.05	-0.95	1.00
181	0.00	1.00	1.00	0.05	0.95	1.00
182	0.00	1.00	1.00	0.00	1.00	1.00
183	0.03	0.97	1.00	0.00	1.00	1.00
184	0.00	-1.00	1.00	0.00	-1.00	1.00
185	0.03	-0.97	1.00	0.00	1.00	1.00
186	0.00	1.00	1.00	0.00	1.00	1.00
C3						
1	0.00	1.00	1.00	0.00	1.00	1.00
2	0.00	1.00	1.00	0.00	1.00	1.00
3	0.00	1.00	1.00	0.00	1.00	1.00
4	0.00	1.00	1.00	0.00	1.00	1.00
5	0.00	1.00	1.00	0.00	1.00	1.00
6	0.00	1.00	1.00	0.00	1.00	1.00
7	0.00	1.00	1.00	0.00	1.00	1.00
8	0.00	1.00	1.00	0.00	1.00	1.00
9	0.00	1.00	1.00	1.00	0.00	1.00
10	0.00	1.00	1.00	1.00	0.00	1.00
11	0.00	1.00	1.00	0.00	1.00	1.00
12	0.00	1.00	1.00	0.00	1.00	1.00
13	0.00	1.00	1.00	0.00	1.00	1.00
14	0.00	1.00	1.00	0.00	1.00	1.00
15	0.00	1.00	1.00	0.00	1.00	1.00
16	0.00	1.00	1.00	0.00	1.00	1.00
17	0.00	1.00	1.00	0.00	1.00	1.00
18	0.00	1.00	1.00	0.00	1.00	1.00
19	0.00	1.00	1.00	0.00	1.00	1.00
20	0.00	1.00	1.00	0.00	1.00	1.00

21	0.00	1.00	1.00	0.00	1.00	1.00
22	0.00	1.00	1.00	0.00	1.00	1.00
23	0.00	1.00	1.00	0.00	1.00	1.00
24	0.00	1.00	1.00	0.00	1.00	1.00
25	0.00	1.00	1.00	0.00	1.00	1.00
26	0.00	1.00	1.00	0.00	1.00	1.00
27	0.00	1.00	1.00	0.00	1.00	1.00
28	0.00	1.00	1.00	0.00	1.00	1.00
29	0.00	1.00	1.00	0.00	1.00	1.00
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34	0.00	1.00	1.00	0.00	1.00	1.00
35	0.00	1.00	1.00	0.00	1.00	1.00
36	0.00	1.00	1.00	0.00	1.00	1.00
37	0.00	1.00	1.00	0.00	1.00	1.00
38	0.00	1.00	1.00	0.00	1.00	1.00
39	0.00	1.00	1.00	0.00	1.00	1.00
40	0.00	1.00	1.00	0.00	1.00	1.00
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42	0.00	1.00	1.00	0.00	1.00	1.00
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44	0.00	1.00	1.00	0.00	1.00	1.00
45	0.00	1.00	1.00	0.00	1.00	1.00
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53	0.00	1.00	1.00	0.00	1.00	1.00
54	0.00	1.00	1.00	1.00	0.00	1.00
55	0.00	1.00	1.00	1.00	0.00	1.00
56	0.97	-0.03	1.00	0.00	1.00	1.00
57	0.97	0.03	1.00	0.00	1.00	1.00
58	0.00	1.00	1.00	0.00	1.00	1.00
59	0.00	1.00	1.00	0.00	1.00	1.00
60	0.00	1.00	1.00	0.00	1.00	1.00
61	0.00	1.00	1.00	0.00	1.00	1.00
62	0.00	1.00	1.00	0.00	1.00	1.00
63	0.00	1.00	1.00	0.00	1.00	1.00
64	0.00	1.00	1.00	0.00	1.00	1.00
65	0.00	1.00	1.00	0.00	1.00	1.00
66	0.00	1.00	1.00	0.00	1.00	1.00
67	0.00	1.00	1.00	0.00	1.00	1.00

68	0.00	1.00	1.00	0.00	1.00	1.00
69	0.00	1.00	1.00	0.00	1.00	1.00
70	0.00	1.00	1.00	0.00	1.00	1.00
71	0.00	1.00	1.00	0.00	1.00	1.00
72	0.00	1.00	1.00	0.00	1.00	1.00
73	0.00	1.00	1.00	0.00	1.00	1.00
74	0.00	1.00	1.00	0.00	1.00	1.00
75	0.00	1.00	1.00	0.00	1.00	1.00
76	0.00	1.00	1.00	0.00	1.00	1.00
77	0.00	1.00	1.00	0.00	1.00	1.00
78	0.00	1.00	1.00	0.00	1.00	1.00
79	0.00	1.00	1.00	0.00	1.00	1.00
80	0.00	1.00	1.00	0.00	1.00	1.00
81	0.00	1.00	1.00	0.00	1.00	1.00
82	0.00	-1.00	1.00	0.00	1.00	1.00
83	0.00	1.00	1.00	0.00	1.00	1.00
84	0.00	1.00	1.00	0.01	0.99	1.00
85	0.00	1.00	1.00	0.01	0.99	1.00
86	0.00	1.00	1.00	0.00	1.00	1.00
87	0.00	1.00	1.00	0.00	1.00	1.00
88	0.00	1.00	1.00	0.00	1.00	1.00
89	0.00	1.00	1.00	0.00	1.00	1.00
90	0.00	1.00	1.00	0.00	1.00	1.00
91	0.00	1.00	1.00	0.00	1.00	1.00
92	0.00	1.00	1.00	0.00	1.00	1.00
93	0.00	1.00	1.00	0.00	1.00	1.00
94	0.00	1.00	1.00	0.00	1.00	1.00
95	0.00	1.00	1.00	0.00	1.00	1.00
96	0.00	1.00	1.00	0.00	1.00	1.00
97	0.00	1.00	1.00	0.00	1.00	1.00
98	0.00	1.00	1.00	0.00	1.00	1.00
99	0.00	1.00	1.00	0.00	1.00	1.00
100	0.00	1.00	1.00	0.00	1.00	1.00
101	0.00	1.00	1.00	0.01	-0.99	1.00
102	0.00	1.00	1.00	0.01	0.99	1.00
103	0.00	1.00	1.00	0.00	1.00	1.00
104	0.00	1.00	1.00	0.00	1.00	1.00
105	0.00	1.00	1.00	0.00	1.00	1.00
106	0.00	1.00	1.00	0.00	1.00	1.00
107	0.00	1.00	1.00	0.00	1.00	1.00
108	0.00	1.00	1.00	0.00	1.00	1.00
109	0.00	1.00	1.00	0.00	1.00	1.00
110	0.00	1.00	1.00	0.00	1.00	1.00
111	0.00	1.00	1.00	0.00	1.00	1.00
112	0.00	1.00	1.00	0.00	1.00	1.00
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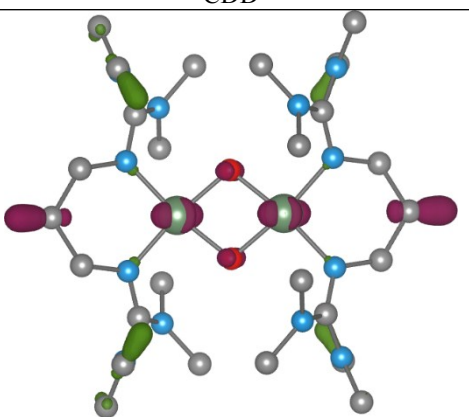
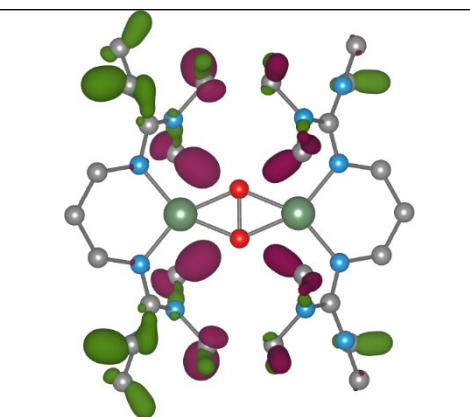
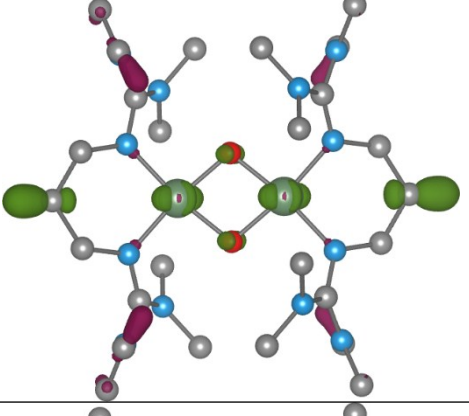
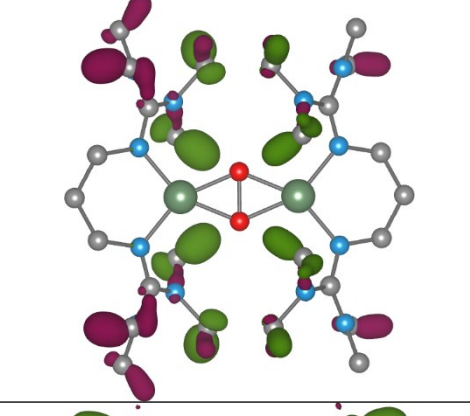
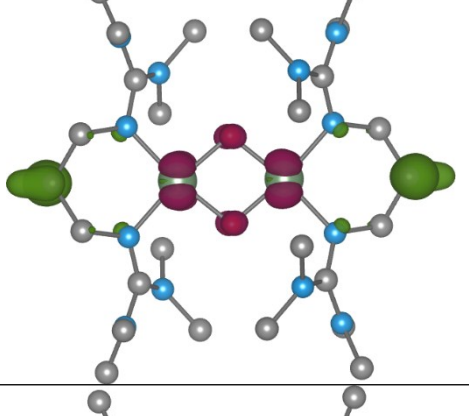
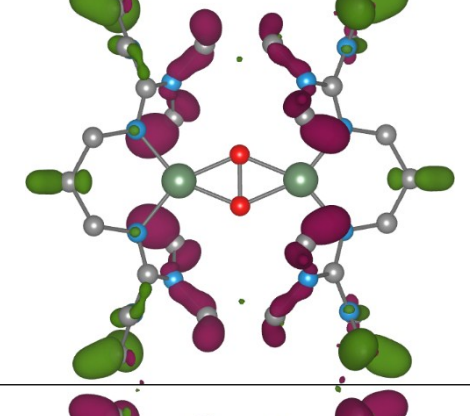
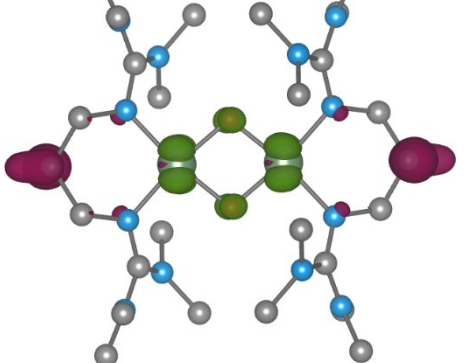
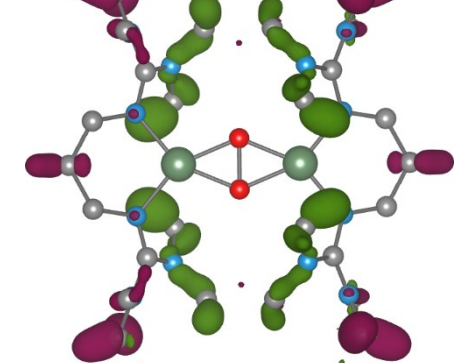
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116	0.00	1.00	1.00	0.00	1.00	1.00
117	0.00	1.00	1.00	0.00	1.00	1.00
118	0.00	1.00	1.00	0.00	1.00	1.00
119	0.00	1.00	1.00	0.00	1.00	1.00
120	0.00	1.00	1.00	0.00	1.00	1.00
121	0.00	1.00	1.00	0.00	1.00	1.00
122	0.00	1.00	1.00	0.00	1.00	1.00
123	0.00	1.00	1.00	0.00	1.00	1.00
124	0.00	1.00	1.00	0.00	1.00	1.00
125	0.00	1.00	1.00	0.00	1.00	1.00
126	0.03	0.97	1.00	0.00	1.00	1.00
127	0.03	0.97	1.00	0.00	1.00	1.00
128	0.00	1.00	1.00	0.00	1.00	1.00
129	0.00	1.00	1.00	0.00	-1.00	1.00
130	0.00	1.00	1.00	0.00	1.00	1.00
131	0.01	-0.99	1.00	0.00	1.00	1.00
132	0.02	-0.98	1.00	0.00	1.00	1.00
133	0.03	-0.97	1.00	0.00	1.00	1.00
134	0.03	-0.97	1.00	0.00	1.00	1.00
135	0.00	1.00	1.00	0.00	1.00	1.00
136	0.00	1.00	1.00	0.00	1.00	1.00
137	0.00	1.00	1.00	0.00	1.00	1.00
138	0.00	-1.00	1.00	0.00	1.00	1.00
139	0.00	1.00	1.00	0.00	1.00	1.00
140	0.00	1.00	1.00	0.00	1.00	1.00
141	0.01	-0.99	1.00	0.01	0.99	1.00
142	0.02	0.98	1.00	0.00	1.00	1.00
143	0.00	1.00	1.00	0.00	1.00	1.00
144	0.00	1.00	1.00	0.07	-0.93	1.00
145	0.00	1.00	1.00	0.06	0.94	1.00
146	0.00	1.00	1.00	0.00	1.00	1.00
147	0.01	0.99	1.00	0.00	1.00	1.00
148	0.01	0.99	1.00	0.01	0.99	1.00
149	0.00	1.00	1.00	0.00	1.00	1.00
150	0.00	1.00	1.00	0.00	1.00	1.00
151	0.00	1.00	1.00	0.00	1.00	1.00
152	0.00	1.00	1.00	0.00	1.00	1.00
153	0.00	1.00	1.00	0.00	1.00	1.00
154	0.00	1.00	1.00	0.00	1.00	1.00
155	0.00	1.00	1.00	0.01	0.99	1.00
156	0.00	1.00	1.00	0.01	0.99	1.00
157	0.00	1.00	1.00	0.01	0.99	1.00
158	0.00	1.00	1.00	0.00	1.00	1.00
159	0.00	1.00	1.00	0.00	1.00	1.00
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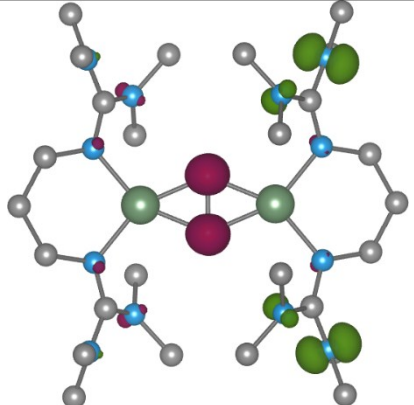
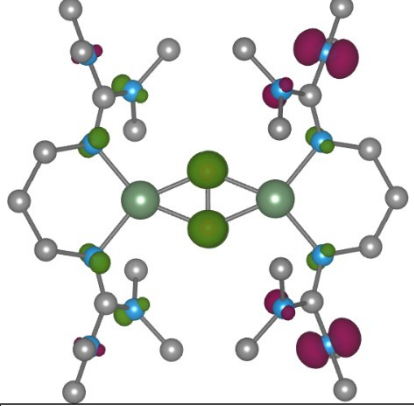
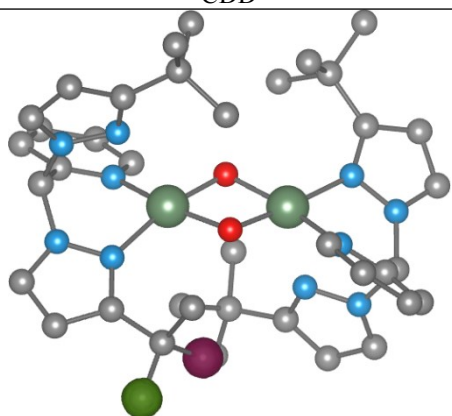
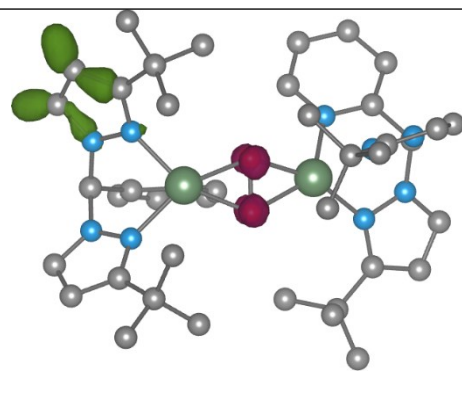
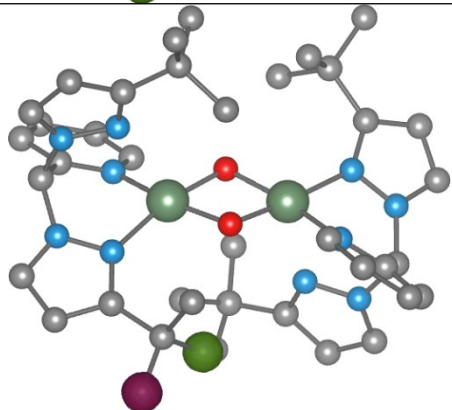
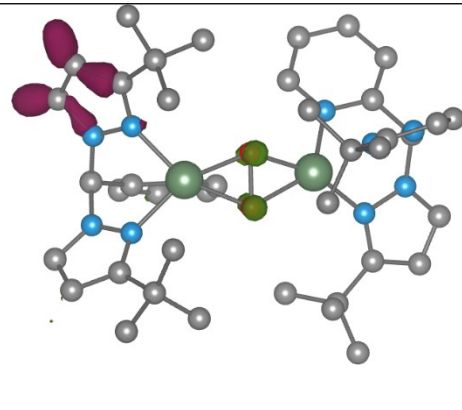
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163	0.02	-0.98	1.00	0.00	1.00	1.00
164	0.02	0.98	1.00	0.01	-0.99	1.00
165	0.02	0.98	1.00	0.00	1.00	1.00
166	0.01	0.99	1.00	0.01	0.99	1.00
167	0.01	0.99	1.00	0.00	1.00	1.00
168	0.01	0.99	1.00	0.00	1.00	1.00
169	0.02	0.98	1.00	0.00	1.00	1.00
170	0.05	0.95	1.00	0.00	1.00	1.00
171	0.09	0.91	1.00	0.00	1.00	1.00
172	0.11	0.89	1.00	0.00	1.00	1.00
173	0.02	0.98	1.00	0.00	1.00	1.00
174	0.01	-0.99	1.00	0.00	1.00	1.00
175	0.49	-0.51	1.00	0.00	1.00	1.00
176	0.52	0.48	1.00	0.00	1.00	1.00
177	0.83	0.17	1.00	0.00	1.00	1.00
178	0.88	0.12	1.00	0.02	-0.98	1.00
179	0.62	0.38	1.00	0.05	0.95	1.00
180	0.46	-0.54	1.00	0.00	1.00	1.00
181	0.03	0.97	1.00	0.03	0.97	1.00
182	0.01	0.99	1.00	0.01	0.99	1.00
183	0.01	0.99	1.00	0.01	0.99	1.00
184	0.02	0.98	1.00	0.01	0.99	1.00
185	0.00	-1.00	1.00	0.02	0.98	1.00
186	0.00	1.00	1.00	0.06	0.94	1.00
187	0.00	1.00	1.00	0.01	-0.99	1.00
188	0.00	1.00	1.00	0.06	0.94	1.00
189	0.00	1.00	1.00	0.04	-0.96	1.00
190	0.00	1.00	1.00	0.06	-0.94	1.00
191	0.00	1.00	1.00	0.15	0.85	1.00
192	0.01	0.99	1.00	0.29	-0.71	1.00
193	0.00	-1.00	1.00	0.33	-0.67	1.00
194	0.00	-1.00	1.00	0.06	0.94	1.00
195	0.00	1.00	1.00	0.02	0.98	1.00
196	0.00	1.00	1.00	0.09	0.91	1.00
197	0.00	-1.00	1.00	0.17	0.83	1.00
198	0.00	-1.00	1.00	0.22	-0.78	1.00
199	0.00	1.00	1.00	0.07	0.93	1.00
200	0.00	-1.00	1.00	0.09	0.91	1.00
201	0.00	1.00	1.00	0.06	0.94	1.00
202	0.00	1.00	1.00	0.09	0.91	1.00
203	0.00	-1.00	1.00	0.05	0.95	1.00
204	0.00	1.00	1.00	0.01	0.99	1.00
205	0.00	1.00	1.00	0.05	0.95	1.00
206	0.00	1.00	1.00	0.05	0.95	1.00
207	0.00	1.00	1.00	0.00	1.00	1.00
208	0.00	-1.00	1.00	0.02	0.98	1.00

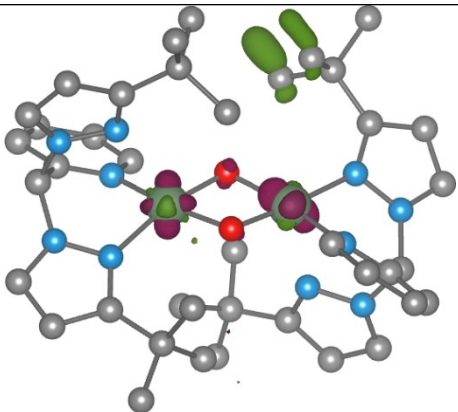
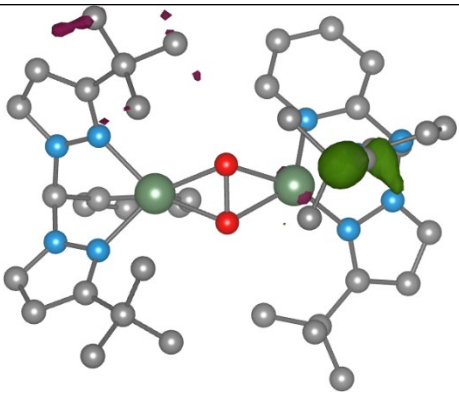
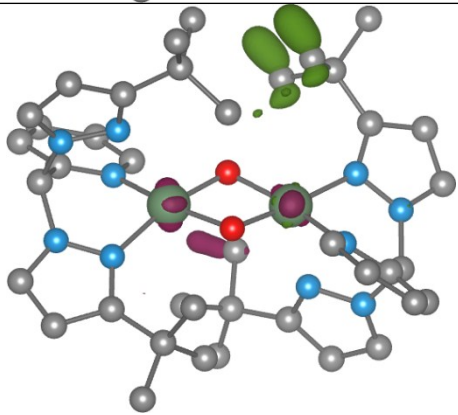
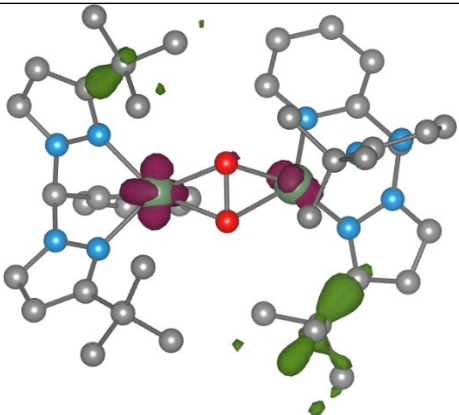
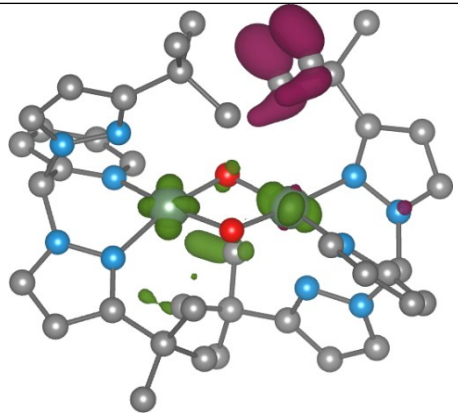
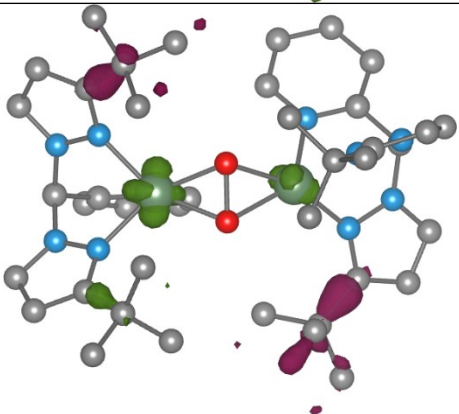
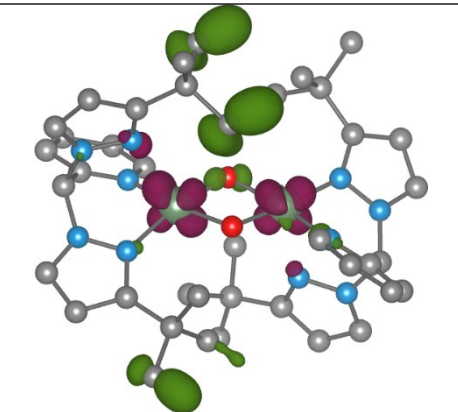
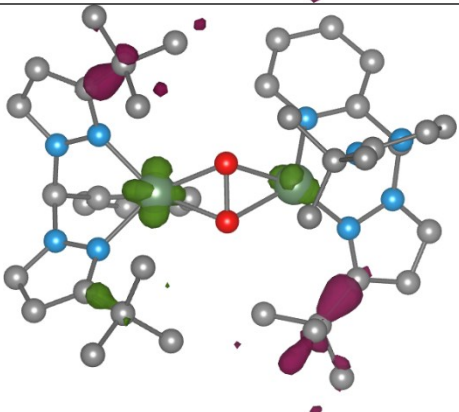
209	0.00	1.00	1.00	0.04	0.96	1.00
210	0.00	1.00	1.00	0.64	-0.36	1.00
211	0.00	1.00	1.00	0.62	0.38	1.00
212	0.00	1.00	1.00	0.01	0.99	1.00
213	0.01	0.99	1.00	0.03	0.97	1.00
214	0.00	1.00	1.00	0.00	1.00	1.00
215	0.00	1.00	1.00	0.02	0.98	1.00
216	0.00	1.00	1.00	0.01	0.99	1.00
217	0.00	1.00	1.00	0.01	0.99	1.00
218	0.00	1.00	1.00	0.00	1.00	1.00

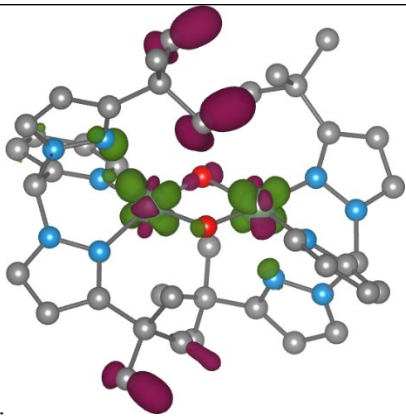
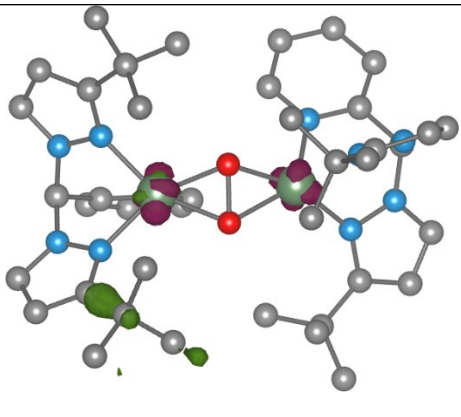
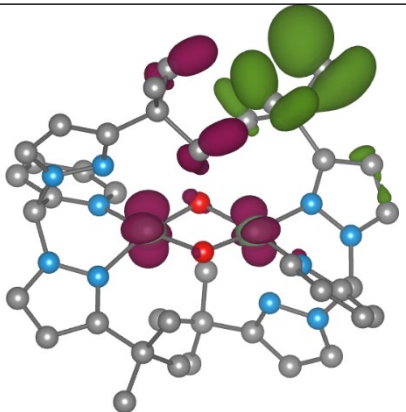
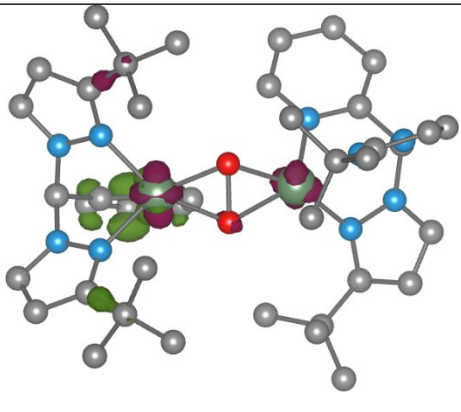
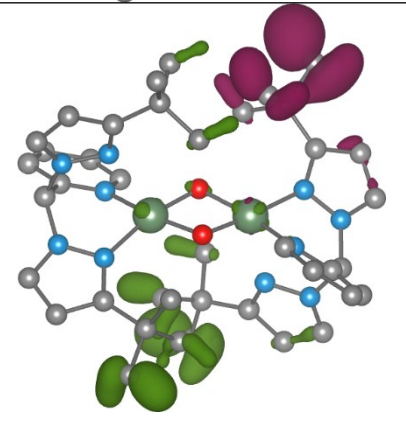
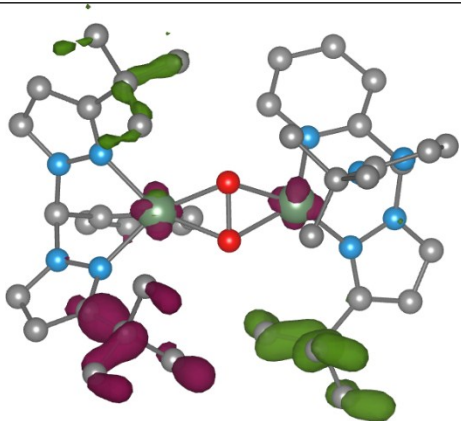
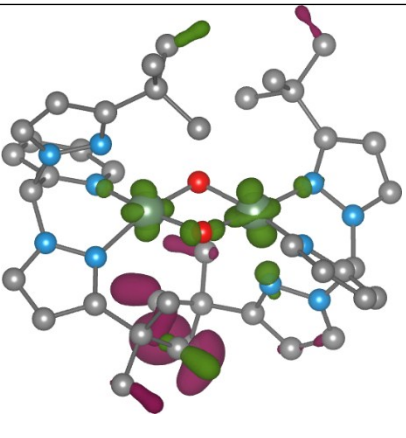
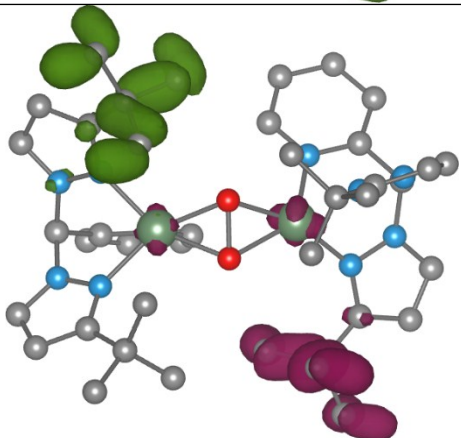
S3: Charge Density Difference (CDD) Plots ($|\varphi_i^{nr}|^2 - |\varphi_i^{DKH}|^2$) for relevant MOs for all Complexes based on the DKH approximation

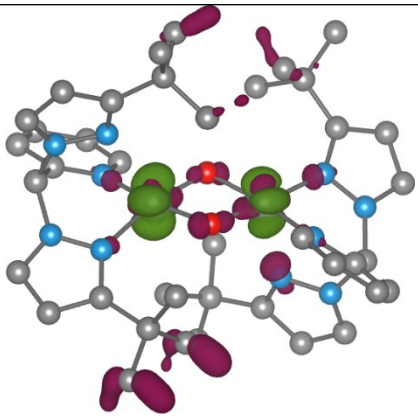
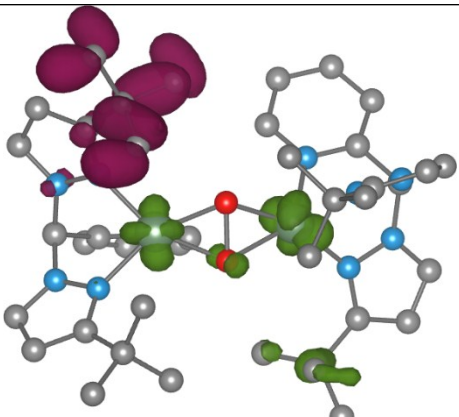
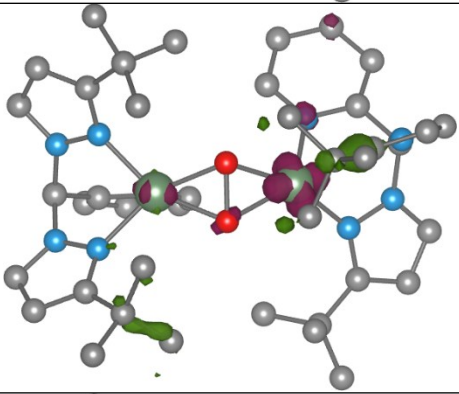
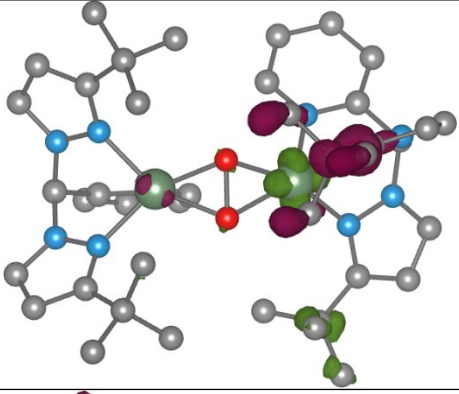
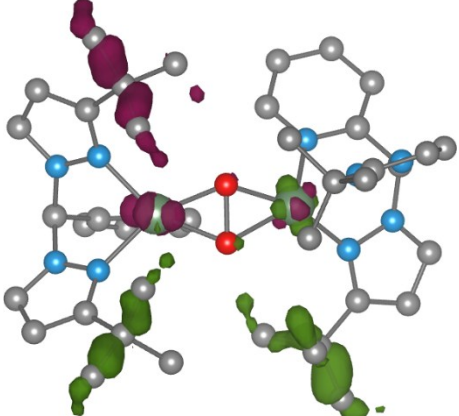
	MO	CDD		MO
C1 O	57		C1 P	27
	58			28
				37
				38
				39
				40
				63
				64

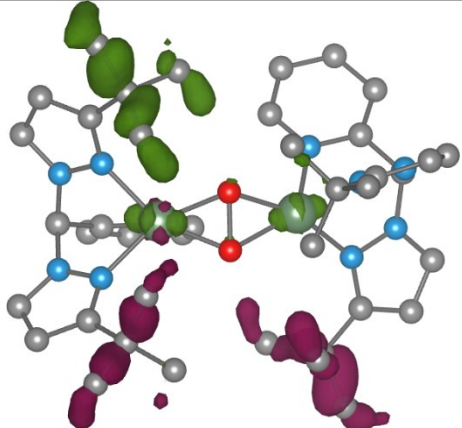
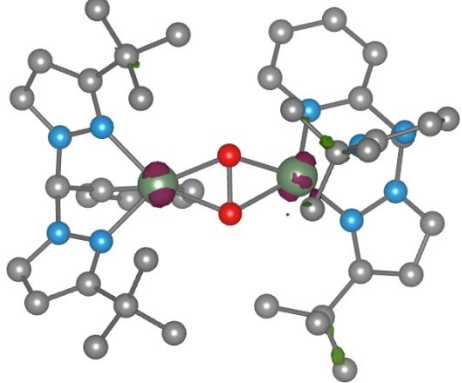
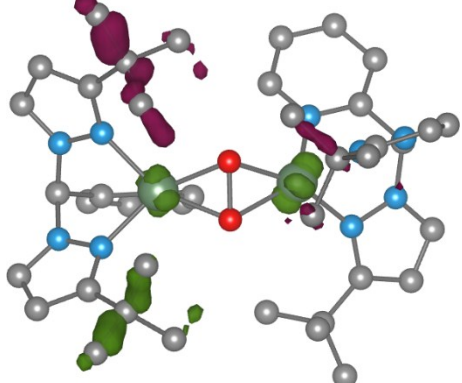
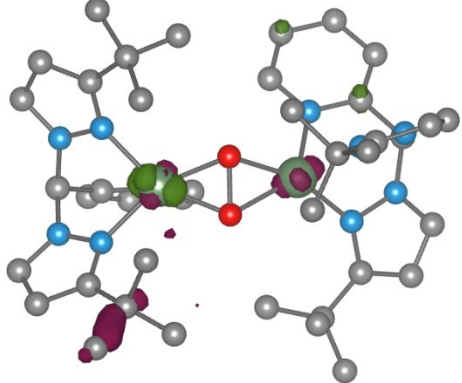
	MO	CDD		MO	
C2 O	52		C2 P	137	
	53			138	
	61			151	
	62			152	

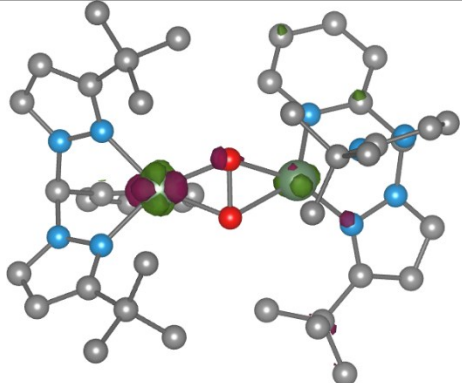
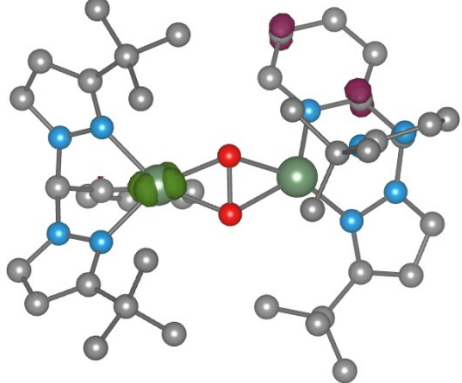
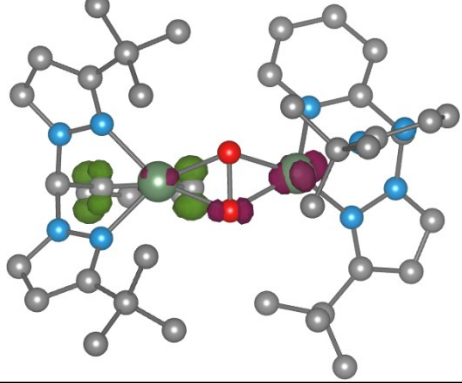
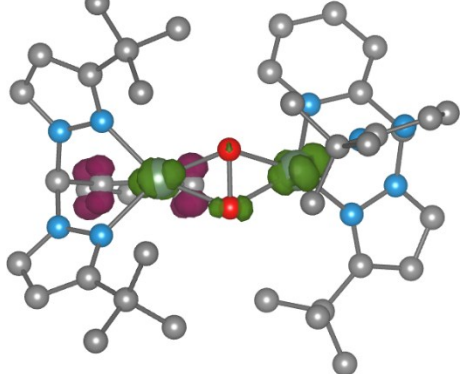
					180	
					181	
C3	MO	CDD		C3	MO	
O	56			P	144	
	57				145	

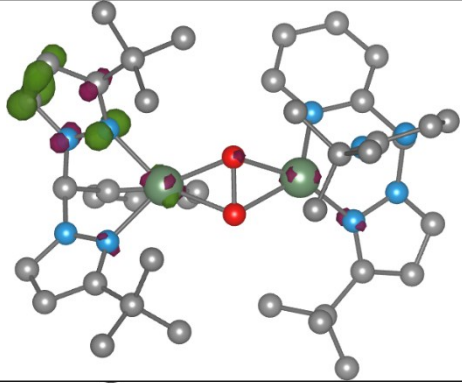
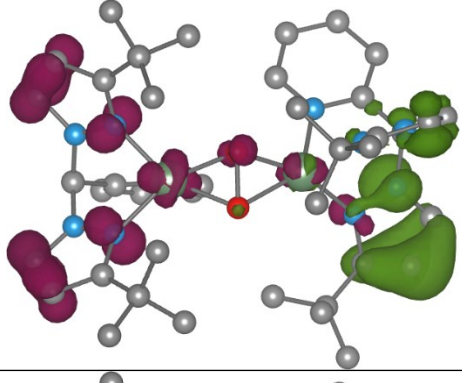
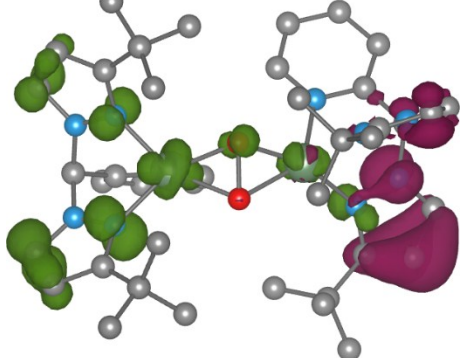
170		179	
171		186	
172		188	
175		188	

176	 <p>A ball-and-stick model of a complex organic molecule, possibly a porphyrin derivative, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces, likely representing electron density or electrostatic potential. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>	189	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>
177	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>	190	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>
178	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>	191	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>
179	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>	192	 <p>A ball-and-stick model of a complex organic molecule, similar to the one in 176, with a central metal atom (grey). The structure is surrounded by large purple and green isosurfaces. The atoms are colored: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).</p>

	180			193	
				194	
				196	
				197	

			198	
			199	
			200	
			201	

			202	
			203	
			205	
			206	

			209	 A ball-and-stick model of a complex organic molecule. The structure features a central core with several fused and branched rings. Atoms are color-coded: carbon is grey, oxygen is red, nitrogen is blue, and sulfur is green. The molecule has a complex, multi-ring architecture.
			210	 A ball-and-stick model of a complex organic molecule, similar in structure to 209. It features a central core with fused and branched rings. Atoms are color-coded: carbon is grey, oxygen is red, nitrogen is blue, sulfur is green, and phosphorus is purple. The molecule has a complex, multi-ring architecture.
			211	 A ball-and-stick model of a complex organic molecule, similar in structure to 209 and 210. It features a central core with fused and branched rings. Atoms are color-coded: carbon is grey, oxygen is red, nitrogen is blue, sulfur is green, and phosphorus is purple. The molecule has a complex, multi-ring architecture.

S4: Total Overlap Population for Cu (Fr. 1) and O (Fr. 2) and N ligand (Fr. 3) fragments for all Complexes

C1 O non-relativistic

Alpha MO: 1 2 3 4 5 6 7 8 9 10
 HOMO-69 HOMO-68 HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60
 Energy(eV): -8792.9 -8792.9 -1062.0 -1062.0 -930.85 -930.85 -930.84 -930.84 -930.27 -930.27
 Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 100.05 100.03 100.00 100.00 100.00 100.00 100.00 100.00
 Net pop.(%) 100.00 100.00 100.10 100.05 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 -0.03 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
 HOMO-59 HOMO-58 HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50
 Energy(eV): -525.73 -525.73 -396.70 -396.70 -396.70 -396.70 -283.65 -283.65 -283.65 -283.65
 Symmetry: A A A A A A A A A A

FRAG# 1: 0.01 0.01 0.00 0.00 0.01 0.01 0.02 0.01 0.00 0.00

FRAG# 2: 99.99 99.99 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 Net pop.(%) 99.99 99.98 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 99.99 100.00 99.98 99.99 100.00 100.00
 Net pop.(%) 0.00 0.00 99.99 100.00 99.98 99.99 99.97 99.98 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
 HOMO-49 HOMO-48 HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40
 Energy(eV): -126.12 -126.12 -85.29 -85.27 -85.23 -85.22 -84.36 -84.36 -32.72 -32.66
 Symmetry: A A A A A A A A A A

FRAG# 1: 100.38 100.30 100.04 99.97 100.01 99.98 100.00 100.00 3.68 1.49
 Net pop.(%) 100.78 100.61 100.08 99.95 100.02 99.97 100.00 100.00 0.84 0.33

FRAG# 2: -0.13 -0.07 0.01 0.03 0.01 0.09 0.01 0.00 7.58 -0.03
 Net pop.(%) 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 6.51 0.01

FRAG# 3: -0.26 -0.23 -0.05 0.00 -0.02 -0.07 0.00 0.00 88.73 98.54
 Net pop.(%) 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00 86.44 97.41

OP(1 & 2) -0.003 -0.002 0.000 0.001 0.000 0.002 0.000 0.000 0.016 0.000
 OP(1 & 3) -0.005 -0.005 -0.001 0.000 0.000 -0.002 0.000 0.000 0.041 0.023
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.005 -0.001

Alpha MO: 31 32 33 34 35 36 37 38 39 40
HOMO-39 HOMO-38 HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30
Energy(eV): -31.90 -31.74 -31.74 -30.93 -27.05 -27.04 -23.90 -23.90 -21.67 -21.67
Symmetry: A A A A A A A A A A

FRAG# 1: 5.74 1.41 1.56 4.69 0.71 0.44 0.77 0.91 1.94 2.08
Net pop.(%) 2.30 0.30 0.33 2.25 0.28 0.18 0.30 0.40 0.83 1.01

FRAG# 2: 84.84 0.76 0.12 94.60 0.03 0.16 0.08 0.03 0.13 0.06
Net pop.(%) 81.08 0.74 0.02 92.10 0.02 0.27 0.02 0.02 0.06 0.03

FRAG# 3: 9.41 97.83 98.33 0.71 99.27 99.40 99.15 99.06 97.93 97.86
Net pop.(%) 10.88 96.46 96.98 0.61 98.85 99.17 98.62 98.55 96.75 96.77

OP(1 & 2) 0.087 -0.003 0.000 0.048 0.000 -0.001 0.000 0.000 0.000 0.000
OP(1 & 3) -0.018 0.025 0.025 0.000 0.008 0.006 0.010 0.010 0.022 0.021
OP(2 & 3) -0.012 0.003 0.002 0.001 0.000 -0.001 0.001 0.000 0.002 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
HOMO-29 HOMO-28 HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20
Energy(eV): -21.43 -21.41 -21.13 -21.12 -19.37 -19.35 -19.08 -18.99 -18.91 -18.79
Symmetry: A A A A A A A A A A

FRAG# 1: 4.70 3.54 4.52 4.02 28.04 33.99 3.76 8.30 17.71 29.30
Net pop.(%) 2.90 1.93 2.87 2.18 20.25 28.83 3.22 7.02 15.41 25.36

FRAG# 2: 0.52 0.01 0.50 0.10 16.94 11.51 0.33 1.14 2.40 8.87
Net pop.(%) 0.46 0.00 0.50 0.06 11.91 8.98 0.55 1.00 2.57 7.05

FRAG# 3: 94.78 96.45 94.98 95.88 55.02 54.51 95.91 90.55 79.89 61.84
Net pop.(%) 92.91 94.85 93.29 94.06 49.86 51.95 95.32 89.79 77.24 59.72

OP(1 & 2) 0.000 0.000 0.000 0.001 0.077 0.051 -0.003 0.007 -0.005 0.036
OP(1 & 3) 0.036 0.032 0.033 0.036 0.079 0.052 0.014 0.019 0.051 0.042
OP(2 & 3) 0.001 0.000 0.000 0.000 0.024 -0.001 -0.002 -0.004 0.002 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
HOMO-19 HOMO-18 HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10
Energy(eV): -18.45 -18.07 -17.68 -17.61 -17.46 -17.20 -17.03 -16.96 -16.79 -16.72
Symmetry: A A A A A A A A A A

FRAG# 1: 40.07 21.09 31.81 71.15 28.57 60.29 71.89 25.50 33.01 39.11
Net pop.(%) 38.88 19.54 29.64 66.22 27.71 57.62 72.43 24.41 32.54 38.55

FRAG# 2: 25.54 16.52 9.20 24.88 15.45 11.13 0.26 0.44 3.61 1.98
Net pop.(%) 24.27 14.10 8.12 19.43 13.86 8.72 0.21 0.42 3.31 1.95

FRAG# 3: 34.38 62.38 58.99 3.97 55.98 28.58 27.84 74.06 63.38 58.90
Net pop.(%) 35.87 63.79 57.22 4.23 59.93 28.22 28.33 73.03 63.37 58.43

OP(1 & 2) 0.040 0.054 0.015 0.106 0.064 0.047 0.000 0.001 0.008 0.001
OP(1 & 3) -0.016 -0.023 0.029 -0.008 -0.047 0.006 -0.011 0.021 0.002 0.010
OP(2 & 3) -0.014 -0.005 0.007 0.003 -0.032 0.001 0.001 0.000 -0.002 -0.001

Alpha MO: 61 62 63 64 65 66 67 68 69 70
 HOMO-9 HOMO-8 HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO
 Energy(eV): -16.54 -16.52 -16.48 -15.90 -15.76 -15.04 -15.00 -14.70 -14.31 -13.60
 Symmetry: A A A A A A A A A A

FRAG# 1: 10.72 93.51 79.55 49.49 58.74 31.20 48.15 13.62 35.31 17.40
 Net pop.(%) 6.72 93.92 80.36 48.62 58.36 30.56 52.12 13.04 35.32 20.69

FRAG# 2: 26.60 1.27 0.12 3.72 -0.05 51.08 51.31 40.62 63.03 82.29
 Net pop.(%) 22.34 1.00 0.01 4.22 0.40 52.08 52.69 39.48 62.63 85.40

FRAG# 3: 62.67 5.22 20.34 46.79 41.31 17.72 0.54 45.76 1.66 0.32
 Net pop.(%) 57.95 5.67 21.25 45.74 40.85 23.78 2.30 47.48 2.38 0.19

OP(1 & 2) 0.035 0.003 0.002 -0.007 -0.005 0.057 -0.036 0.034 0.011 -0.065
 OP(1 & 3) 0.045 -0.011 -0.018 0.024 0.013 -0.044 -0.043 -0.023 -0.011 -0.001
 OP(2 & 3) 0.050 0.002 0.000 -0.003 -0.004 -0.077 0.008 -0.011 -0.003 0.003

C1 O DKH

Alpha MO: 1 2 3 4 5 6 7 8 9 10
 HOMO-69 HOMO-68 HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60
 Energy(eV): -8888.9 -8888.9 -1083.9 -1083.9 -935.64 -935.64 -935.64 -935.64 -935.07 -935.07
 Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 100.04 100.02 100.00 100.00 100.00 100.00 100.00 100.00
 Net pop.(%) 100.00 100.00 100.09 100.05 100.00 100.01 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 -0.02 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 -0.03 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
 HOMO-59 HOMO-58 HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50
 Energy(eV): -526.07 -526.07 -396.92 -396.92 -396.92 -396.92 -283.75 -283.75 -283.75 -283.75
 Symmetry: A A A A A A A A A A

FRAG# 1: 0.01 0.01 0.00 0.00 0.01 0.01 0.02 0.01 0.00 0.00

FRAG# 2: 99.99 99.99 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 Net pop.(%) 99.99 99.98 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 99.99 99.99 99.98 99.99 100.00 100.00
 Net pop.(%) 0.00 0.00 99.99 100.00 99.98 99.99 99.97 99.98 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
HOMO-49 HOMO-48 HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40
Energy(eV): -129.90 -129.90 -86.39 -86.37 -86.33 -86.32 -85.43 -85.43 -32.76 -32.69
Symmetry: A A A A A A A A A A

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FRAG# 1:	100.31	100.25	100.04	99.98	100.01	99.99	100.00	100.00	3.90	1.58
Net pop.(%)	100.64	100.51	100.09	99.96	100.02	99.98	100.00	100.01	0.90	0.34

FRAG# 2:	-0.10	-0.06	0.00	0.03	0.00	0.09	0.01	0.00	8.19	-0.03
Net pop.(%)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.03	0.01

FRAG# 3:	-0.21	-0.19	-0.05	0.00	-0.01	-0.07	0.00	0.00	87.91	98.45
Net pop.(%)	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	85.53	97.25

OP(1 & 2)	-0.002	-0.001	0.000	0.001	0.000	0.002	0.000	0.000	0.018	0.000
OP(1 & 3)	-0.004	-0.004	-0.001	0.000	0.000	-0.001	0.000	0.000	0.042	0.025
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.005	-0.001

Alpha MO: 31 32 33 34 35 36 37 38 39 40
HOMO-39 HOMO-38 HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30
Energy(eV): -31.95 -31.78 -31.77 -30.96 -27.08 -27.06 -23.91 -23.91 -21.68 -21.67
Symmetry: A A A A A A A A A A

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FRAG# 1:	5.82	1.39	1.56	4.61	0.72	0.45	0.77	0.90	1.91	2.04
Net pop.(%)	2.29	0.30	0.33	2.20	0.29	0.18	0.29	0.39	0.80	0.97

FRAG# 2:	84.01	0.80	0.12	94.64	0.03	0.16	0.08	0.03	0.14	0.06
Net pop.(%)	80.13	0.78	0.02	92.19	0.02	0.28	0.02	0.02	0.06	0.03

FRAG# 3:	10.16	97.81	98.32	0.75	99.24	99.39	99.15	99.07	97.95	97.90
Net pop.(%)	11.71	96.45	96.96	0.66	98.82	99.15	98.62	98.56	96.76	96.81

OP(1 & 2)	0.090	-0.002	0.000	0.048	0.000	-0.001	0.000	0.000	0.000	0.000
OP(1 & 3)	-0.019	0.024	0.025	0.000	0.008	0.006	0.010	0.010	0.022	0.021
OP(2 & 3)	-0.012	0.003	0.002	0.001	0.000	-0.001	0.001	0.000	0.002	0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
HOMO-29 HOMO-28 HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20
Energy(eV): -21.44 -21.42 -21.14 -21.13 -19.41 -19.33 -19.09 -18.99 -18.91 -18.78
Symmetry: A A A A A A A A A A

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FRAG# 1:	4.71	3.63	4.38	4.01	27.56	30.64	3.25	9.19	16.66	23.77
Net pop.(%)	2.87	1.93	2.73	2.12	19.57	25.82	2.74	7.74	14.37	19.77

FRAG# 2:	0.52	0.02	0.48	0.13	17.16	10.61	0.26	1.38	2.21	6.11
Net pop.(%)	0.48	0.01	0.50	0.08	11.99	8.27	0.46	1.20	2.37	5.01

FRAG# 3:	94.76	96.35	95.14	95.87	55.28	58.75	96.49	89.43	81.13	70.12
Net pop.(%)	92.83	94.66	93.44	94.00	50.11	56.29	95.94	88.58	78.52	67.41

OP(1 & 2)	0.000	0.000	-0.001	0.001	0.080	0.047	-0.002	0.008	-0.005	0.024
OP(1 & 3)	0.037	0.034	0.034	0.037	0.080	0.050	0.013	0.021	0.051	0.056
OP(2 & 3)	0.001	0.000	0.000	0.000	0.024	0.000	-0.002	-0.004	0.002	-0.002

Alpha MO: 51 52 53 54 55 56 57 58 59 60
 HOMO-19 HOMO-18 HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10
 Energy(eV): -18.43 -18.05 -17.64 -17.53 -17.44 -17.14 -16.97 -16.93 -16.75 -16.68
 Symmetry: A A A A A A A A A A

FRAG# 1: 44.18 22.64 30.94 71.14 24.86 50.60 47.66 43.48 35.76 37.80
 Net pop.(%) 42.93 20.79 28.67 65.91 23.90 48.03 47.52 43.04 35.00 37.13

FRAG# 2: 29.69 17.88 8.73 26.55 16.55 9.80 0.08 0.42 5.66 1.96
 Net pop.(%) 27.69 15.24 7.77 20.78 14.75 7.70 0.04 0.39 4.91 2.01

FRAG# 3: 26.14 59.48 60.33 2.31 58.59 39.59 52.25 56.10 58.58 60.24
 Net pop.(%) 28.10 60.87 58.34 2.57 62.72 38.99 52.23 55.64 58.79 59.57

OP(1 & 2) 0.052 0.059 0.012 0.113 0.069 0.041 0.002 0.000 0.017 0.000
 OP(1 & 3) -0.027 -0.022 0.033 -0.008 -0.050 0.011 0.001 0.009 -0.002 0.014
 OP(2 & 3) -0.012 -0.006 0.007 0.003 -0.033 0.001 -0.001 0.001 -0.002 -0.001

Alpha MO: 61 62 63 64 65 66 67 68 69 70
 HOMO-9 HOMO-8 HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO
 Energy(eV): -16.57 -16.39 -16.38 -15.87 -15.73 -15.03 -14.98 -14.69 -14.26 -13.55
 Symmetry: A A A A A A A A A A

FRAG# 1: 7.16 97.34 85.70 57.91 61.36 34.39 49.84 13.99 36.65 18.31
 Net pop.(%) 2.82 97.95 86.51 57.29 61.11 33.82 53.95 13.31 36.80 21.74

FRAG# 2: 27.43 0.12 0.13 3.94 0.37 48.57 49.49 41.88 61.65 81.36
 Net pop.(%) 22.96 0.03 0.02 4.45 1.08 49.28 50.84 40.65 61.38 84.61

FRAG# 3: 65.40 2.54 14.17 38.16 38.27 17.03 0.67 44.13 1.70 0.33
 Net pop.(%) 60.39 3.23 15.09 37.30 37.90 23.17 2.59 45.82 2.45 0.20

OP(1 & 2) 0.038 0.002 0.002 -0.008 -0.008 0.060 -0.036 0.036 0.009 -0.068
 OP(1 & 3) 0.049 -0.014 -0.018 0.020 0.013 -0.048 -0.047 -0.022 -0.012 -0.001
 OP(2 & 3) 0.051 0.000 0.000 -0.003 -0.006 -0.074 0.008 -0.011 -0.003 0.003

C1 P non-relativistic

Alpha MO: 1 2 3 4 5 6 7 8 9 10
 HOMO-69 HOMO-68 HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60
 Energy(eV): -8791.2 -8791.2 -1060.0 -1060.0 -928.77 -928.77 -928.77 -928.77 -928.49 -928.49
 Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 100.03 100.02 100.00 100.00 100.00 100.00 100.00 100.00
 Net pop.(%) 100.00 100.00 100.05 100.04 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 FRAG# 3: 0.00 0.00 -0.02 -0.02 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
HOMO-59 HOMO-58 HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50
Energy(eV): -527.34 -527.34 -396.03 -396.03 -396.03 -396.03 -283.18 -283.18 -283.18 -283.18
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.00 0.00 0.01 0.00 0.00 0.00 0.02 0.01 0.00 0.00

FRAG# 2: 100.00 100.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 100.01 100.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 99.99 100.00 100.00 100.00 99.98 99.99 100.00 100.00
Net pop.(%) 0.00 0.00 99.99 99.99 100.00 100.00 99.97 99.98 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
HOMO-49 HOMO-48 HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40
Energy(eV): -124.37 -124.37 -83.47 -83.47 -83.37 -83.37 -82.94 -82.94 -36.30 -32.02
Symmetry: A A A A A A A A A A

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FRAG# 1: 100.36 100.23 100.00 100.01 100.03 100.02 100.00 100.00 1.32 1.37
Net pop.(%) 100.74 100.46 100.00 100.03 100.05 100.04 99.99 99.99 1.03 0.27

FRAG# 2: -0.15 -0.05 0.03 -0.01 0.02 0.05 0.01 0.00 98.77 -0.03
Net pop.(%) 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 98.49 0.01

FRAG# 3: -0.22 -0.18 -0.02 -0.01 -0.04 -0.07 0.00 0.00 -0.09 98.66
Net pop.(%) 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.04 97.57

OP(1 & 2) -0.003 -0.001 0.000 0.000 0.000 0.001 0.000 0.000 0.007 0.000
OP(1 & 3) -0.005 -0.004 -0.001 0.000 -0.001 -0.001 0.000 0.000 -0.001 0.022
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 -0.001 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
HOMO-39 HOMO-38 HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30
Energy(eV): -32.02 -31.18 -31.18 -29.04 -26.53 -26.53 -23.36 -23.36 -21.07 -21.06
Symmetry: A A A A A A A A A A

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FRAG# 1: 1.28 1.39 0.96 2.58 0.25 0.45 0.59 0.57 1.41 1.38
Net pop.(%) 0.25 0.25 0.21 0.87 0.11 0.11 0.19 0.18 0.53 0.50

FRAG# 2: 0.06 0.04 0.00 97.39 0.02 0.01 0.00 0.01 0.01 0.01
Net pop.(%) 0.14 0.01 0.00 95.65 0.01 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 98.66 98.57 99.03 0.03 99.73 99.55 99.41 99.42 98.58 98.61
Net pop.(%) 97.59 97.37 98.26 0.01 99.58 99.21 99.01 99.02 97.69 97.72

OP(1 & 2) -0.001 0.000 0.000 0.034 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.022 0.023 0.015 0.000 0.003 0.007 0.008 0.008 0.018 0.018
OP(2 & 3) 0.000 0.001 0.000 0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
HOMO-29 HOMO-28 HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20
Energy(eV): -20.87 -20.81 -20.63 -20.53 -19.98 -18.89 -18.61 -18.57 -18.34 -18.26
Symmetry: A A A A A A A A A A

FRAG# 1: 7.63 2.21 6.66 3.00 13.01 10.53 7.54 2.37 12.87 7.85
Net pop.(%) 4.16 1.16 3.75 1.64 8.50 7.41 5.94 1.82 10.34 6.24

FRAG# 2: 6.22 0.10 8.32 0.13 58.37 82.89 1.87 0.51 2.57 0.44
Net pop.(%) 5.00 0.19 6.91 0.33 52.30 80.15 1.41 0.51 2.02 0.53

FRAG# 3: 86.16 97.69 85.02 96.87 28.62 6.58 90.59 97.12 84.56 91.72
Net pop.(%) 83.81 96.54 83.34 95.34 30.23 5.87 89.41 96.61 82.76 89.99

OP(1 & 2) 0.023 -0.002 0.026 -0.004 0.122 0.052 0.009 0.000 0.013 -0.002
OP(1 & 3) 0.046 0.023 0.032 0.031 -0.032 0.011 0.023 0.011 0.038 0.034
OP(2 & 3) 0.001 0.000 0.002 0.000 0.000 0.003 0.000 0.000 -0.002 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
HOMO-19 HOMO-18 HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10
Energy(eV): -18.20 -17.99 -17.95 -17.19 -16.48 -16.44 -16.43 -15.99 -15.89 -15.59
Symmetry: A A A A A A A A A A

FRAG# 1: 19.29 5.77 8.44 35.66 32.72 3.33 3.27 21.15 27.28 5.98
Net pop.(%) 13.71 3.43 6.05 31.79 29.37 2.57 2.40 19.27 25.35 2.30

FRAG# 2: 79.12 7.91 3.51 25.73 0.65 0.20 0.02 0.25 0.99 29.48
Net pop.(%) 73.40 8.38 4.30 21.91 0.93 0.17 0.02 0.75 1.58 26.28

FRAG# 3: 1.59 86.32 88.05 38.61 66.63 96.46 96.71 78.60 71.73 64.54
Net pop.(%) 1.62 84.10 86.17 39.00 62.76 95.72 95.84 76.31 69.58 61.06

OP(1 & 2) 0.113 -0.004 -0.003 0.081 -0.008 0.001 0.000 -0.009 -0.008 0.034
OP(1 & 3) -0.002 0.050 0.050 -0.003 0.075 0.015 0.017 0.047 0.047 0.040
OP(2 & 3) 0.001 -0.006 -0.013 -0.004 0.002 0.000 0.000 -0.001 -0.004 0.030

Alpha MO: 61 62 63 64 65 66 67 68 69 70
HOMO-9 HOMO-8 HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO
Energy(eV): -15.34 -15.26 -15.12 -15.06 -15.03 -14.71 -14.63 -14.55 -13.22 -12.99
Symmetry: A A A A A A A A A A

FRAG# 1: 84.82 98.17 96.77 73.51 89.32 85.75 91.55 82.44 12.31 59.23
Net pop.(%) 83.72 98.46 97.33 75.25 93.86 85.85 91.71 86.95 13.86 67.19

FRAG# 2: 11.54 0.25 0.09 6.89 6.80 0.81 3.00 16.03 87.51 2.22
Net pop.(%) 9.81 0.04 0.04 7.93 10.26 0.89 2.54 20.05 89.05 5.57

FRAG# 3: 3.64 1.58 3.14 19.61 3.88 13.44 5.45 1.53 0.18 38.56
Net pop.(%) 4.32 2.07 3.75 21.30 4.92 13.46 5.95 2.11 0.13 43.92

OP(1 & 2) 0.035 0.004 0.001 -0.011 -0.070 -0.002 0.008 -0.079 -0.031 -0.059
OP(1 & 3) -0.013 -0.010 -0.012 -0.024 -0.021 0.000 -0.011 -0.011 0.000 -0.100
OP(2 & 3) 0.000 0.000 0.000 -0.010 0.000 0.000 0.001 -0.001 0.001 -0.008

C1 P DKH

Alpha MO: 1 2 3 4 5 6 7 8 9 10
HOMO-69 HOMO-68 HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60
Energy(eV): -8887.1 -8887.1 -1081.9 -1081.9 -933.54 -933.54 -933.54 -933.27 -933.27
Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 100.02 100.02 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 100.05 100.04 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00
FRAG# 3: 0.00 0.00 -0.02 -0.02 0.00 0.00 0.00 0.00 0.00 0.00
OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
HOMO-59 HOMO-58 HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50
Energy(eV): -527.68 -527.67 -396.26 -396.26 -396.26 -396.26 -283.29 -283.29 -283.28 -283.28
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.01 0.01 0.00 0.00 0.02 0.01 0.00 0.00

FRAG# 2: 100.00 100.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 100.00 100.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 99.99 99.99 100.00 100.00 99.98 99.99 100.00 100.00
Net pop.(%) 0.00 0.00 99.99 99.99 100.00 100.00 99.97 99.99 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
HOMO-49 HOMO-48 HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40
Energy(eV): -128.12 -128.12 -84.54 -84.54 -84.44 -84.43 -84.00 -84.00 -36.33 -32.06
Symmetry: A A A A A A A A A A

FRAG# 1: 100.30 100.18 100.00 100.02 100.03 100.02 100.00 99.99 1.36 1.43
Net pop.(%) 100.61 100.37 100.01 100.04 100.05 100.04 100.00 99.99 1.01 0.28

FRAG# 2: -0.12 -0.04 0.02 -0.01 0.02 0.05 0.00 0.01 98.73 -0.03
Net pop.(%) 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 98.39 0.01

FRAG# 3: -0.18 -0.14 -0.02 -0.01 -0.04 -0.07 0.00 0.00 -0.09 98.60
Net pop.(%) 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.04 97.46

OP(1 & 2) -0.002 -0.001 0.000 0.000 0.000 0.001 0.000 0.000 0.008 0.000
OP(1 & 3) -0.004 -0.003 -0.001 0.000 -0.001 -0.001 0.000 0.000 -0.001 0.023
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 -0.001 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
HOMO-39 HOMO-38 HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30
Energy(eV): -32.06 -31.22 -31.22 -29.07 -26.55 -26.55 -23.38 -23.38 -21.08 -21.08
Symmetry: A A A A A A A A A A

FRAG# 1: 1.32 1.40 0.95 2.54 0.26 0.45 0.57 0.58 1.36 1.40
Net pop.(%) 0.26 0.25 0.20 0.85 0.12 0.11 0.18 0.19 0.49 0.52

FRAG# 2: 0.06 0.04 0.01 97.43 0.03 0.01 0.01 0.00 0.01 0.01
Net pop.(%) 0.14 0.01 0.00 95.71 0.01 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 98.62 98.56 99.04 0.03 99.71 99.54 99.42 99.41 98.62 98.59
Net pop.(%) 97.52 97.35 98.29 0.01 99.55 99.20 99.02 99.01 97.73 97.70

OP(1 & 2) -0.001 0.000 0.000 0.034 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.023 0.023 0.015 0.000 0.003 0.007 0.008 0.008 0.018 0.018
OP(2 & 3) 0.000 0.001 0.000 0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
HOMO-29 HOMO-28 HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20
Energy(eV): -20.89 -20.83 -20.65 -20.55 -20.01 -18.87 -18.62 -18.58 -18.34 -18.26
Symmetry: A A A A A A A A A A

FRAG# 1: 8.47 2.26 6.45 3.00 12.61 10.44 6.46 2.14 12.18 7.22
Net pop.(%) 4.58 1.16 3.59 1.61 8.05 7.28 5.03 1.62 9.69 5.67

FRAG# 2: 7.30 0.09 8.37 0.12 56.77 82.31 1.58 0.34 2.36 0.15
Net pop.(%) 5.84 0.20 6.93 0.32 50.60 79.59 1.19 0.36 1.85 0.25

FRAG# 3: 84.23 97.65 85.17 96.88 30.63 7.25 91.96 97.52 85.46 92.63
Net pop.(%) 81.67 96.45 83.58 95.32 32.28 6.45 90.88 97.02 83.65 90.93

OP(1 & 2) 0.028 -0.002 0.027 -0.004 0.124 0.051 0.007 0.000 0.012 -0.002
OP(1 & 3) 0.050 0.024 0.030 0.032 -0.033 0.012 0.021 0.010 0.038 0.033
OP(2 & 3) 0.001 0.000 0.002 0.000 0.000 0.004 0.000 0.000 -0.002 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
HOMO-19 HOMO-18 HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10
Energy(eV): -18.16 -18.02 -17.97 -17.15 -16.45 -16.44 -16.44 -16.00 -15.89 -15.61
Symmetry: A A A A A A A A A A

FRAG# 1: 18.98 5.77 8.21 36.30 31.40 2.92 2.94 17.83 22.29 6.15
Net pop.(%) 13.34 3.33 5.77 32.13 27.88 2.17 2.07 15.96 20.29 2.33

FRAG# 2: 80.16 8.76 3.90 26.63 0.60 0.17 0.02 0.24 1.27 29.67
Net pop.(%) 74.40 9.25 4.74 22.72 0.86 0.15 0.03 0.80 2.02 26.40

FRAG# 3: 0.86 85.47 87.89 37.07 68.00 96.91 97.04 81.92 76.44 64.18
Net pop.(%) 0.89 83.16 85.98 37.31 64.00 96.17 96.17 79.59 74.13 60.66

OP(1 & 2) 0.114 -0.004 -0.003 0.083 -0.007 0.000 0.000 -0.010 -0.011 0.036
OP(1 & 3) -0.001 0.052 0.052 0.000 0.078 0.015 0.017 0.048 0.051 0.041
OP(2 & 3) 0.001 -0.006 -0.014 -0.005 0.002 0.000 0.000 -0.001 -0.004 0.030

Alpha MO: 61 62 63 64 65 66 67 68 69 70
 HOMO-9 HOMO-8 HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO
 Energy(eV): -15.22 -15.13 -14.98 -14.97 -14.91 -14.62 -14.54 -14.43 -13.17 -12.90
 Symmetry: A A A A A A A A A A

FRAG# 1: 83.99 98.25 93.12 81.84 89.81 89.50 93.60 83.11 13.63 61.15
 Net pop.(%) 82.76 98.54 93.88 83.41 94.35 89.69 93.80 87.63 15.30 69.28

FRAG# 2: 12.89 0.25 1.30 5.02 6.57 0.80 2.74 15.36 86.17 2.31
 Net pop.(%) 11.04 0.03 1.44 5.69 10.01 0.86 2.27 19.39 87.84 5.80

FRAG# 3: 3.11 1.50 5.58 13.13 3.63 9.70 3.66 1.53 0.20 36.54
 Net pop.(%) 3.77 2.00 6.36 14.74 4.69 9.82 4.28 2.12 0.15 41.95

OP(1 & 2) 0.038 0.004 -0.001 -0.006 -0.069 -0.001 0.009 -0.080 -0.034 -0.062
 OP(1 & 3) -0.013 -0.010 -0.014 -0.025 -0.022 -0.002 -0.013 -0.011 0.000 -0.101
 OP(2 & 3) 0.000 0.000 -0.002 -0.007 0.000 0.000 0.001 -0.001 0.001 -0.008

C2 O non-relativistic

Alpha MO: 1 2 3 4 5 6 7 8 9 10
 Energy(eV): -8790.0 -8790.0 -1059.1 -1059.1 -927.95 -927.95 -927.95 -927.95 -927.39 -927.39
 Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 99.98 99.98 100.00 100.00 100.00 100.00 100.00 100.00
 Net pop.(%) 100.00 100.00 99.98 99.96 100.01 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 0.02 0.01 0.00 0.00 0.00 0.00 0.00 0.00
 Net pop.(%) 0.00 0.00 0.03 0.01 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
 Energy(eV): -522.92 -522.92 -393.63 -393.63 -393.63 -393.63 -393.60 -393.60 -393.60 -393.60
 Symmetry: A A A A A A A A A A

FRAG# 1: 0.02 0.02 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 99.98 99.98 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 Net pop.(%) 99.97 99.97 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00
 Net pop.(%) 0.00 0.00 100.00 100.00 100.00 100.00 99.99 99.99 99.99 99.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
 Energy(eV): -392.82 -392.82 -392.82 -392.82 -283.14 -283.14 -283.14 -283.14 -280.92 -280.92
 Symmetry: A A A A A A A A A A

FRAG# 1: 0.01 0.01 0.01 0.01 -0.02 -0.02 -0.02 -0.02 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 99.99 99.99 99.99 99.99 100.02 100.02 100.02 100.02 100.00 100.00
 Net pop.(%) 99.98 99.98 99.98 99.98 100.03 100.03 100.03 100.03 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
 OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
Energy(eV): -280.92 -280.92 -280.91 -280.91 -280.91 -280.91 -280.84 -280.84 -280.84 -280.84
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 -0.01 -0.01 -0.01 0.01 0.00 0.01 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.01 100.00 100.01 99.99 100.00 99.99 100.00
Net pop.(%) 100.00 100.00 100.01 100.02 100.01 100.02 99.99 100.00 99.98 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.81 -280.81 -280.81 -280.81 -280.80 -280.80 -280.80 -280.80 -279.88 -279.88
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.01

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 100.00 100.00 100.01 100.01 100.00 100.00 99.99 99.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -123.20 -123.20 -82.35 -82.33 -82.31 -82.31 -81.47 -81.46 -31.80 -31.78
Symmetry: A A A A A A A A A A

FRAG# 1: 100.40 100.37 100.01 99.94 99.91 99.93 100.03 99.98 -0.22 0.02
Net pop.(%) 100.83 100.75 100.04 99.90 99.84 99.87 100.08 99.97 0.06 0.04

FRAG# 2: -0.10 -0.08 0.01 0.02 0.07 0.10 0.00 0.00 0.40 -0.03

Net pop.(%) 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.27 0.00

FRAG# 3: -0.30 -0.29 -0.03 0.04 0.02 -0.02 -0.03 0.02 99.82 100.01

Net pop.(%) 0.02 0.01 0.01 0.01 0.01 0.01 0.03 0.01 100.06 100.05

OP(1 & 2) -0.002 -0.002 0.000 0.000 0.001 0.002 0.000 0.000 0.001 0.000

OP(1 & 3) -0.006 -0.006 -0.001 0.000 0.000 -0.001 -0.001 0.000 -0.007 0.000

OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.002 -0.001

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -31.77 -31.76 -29.59 -29.58 -29.57 -29.57 -29.26 -28.89 -28.79 -28.55
Symmetry: A A A A A A A A A A

FRAG# 1: -0.38 -0.16 0.48 0.37 0.06 0.13 7.52 0.52 -0.03 -0.07

Net pop.(%) 0.02 0.03 0.13 0.02 0.01 0.02 2.41 0.17 0.50 0.13

FRAG# 2: 0.16 0.06 4.66 0.00 0.01 0.42 69.36 -0.03 18.27 2.33

Net pop.(%) 0.10 0.01 4.27 0.00 0.00 0.36 65.17 0.01 18.26 2.19

FRAG# 3: 100.22 100.11 94.87 99.64 99.93 99.45 23.13 99.51 81.76 97.75

Net pop.(%) 100.55 100.24 94.62 99.29 99.88 99.33 22.54 99.19 83.69 97.61

OP(1 & 2) 0.000 0.000 0.005 0.000 0.000 0.000 0.087 0.000 0.014 -0.002

OP(1 & 3) -0.008 -0.004 0.002 0.007 0.001 0.002 0.015 0.007 -0.025 -0.002

OP(2 & 3) 0.001 0.001 0.003 0.000 0.000 0.001 -0.003 -0.001 -0.014 0.005

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -28.54 -28.12 -25.68 -25.67 -24.51 -24.48 -24.38 -24.36 -24.16 -24.14
Symmetry: A A A A A A A A A A

FRAG# 1: 0.10 4.41 -0.24 -0.11 0.13 0.12 -0.02 0.10 0.08 0.10
Net pop.(%) 0.17 2.00 0.07 0.04 0.02 0.02 0.01 0.01 0.03 0.03

FRAG# 2: 0.06 92.45 0.00 0.09 0.01 0.00 0.01 0.03 0.00 0.02
Net pop.(%) 0.01 90.06 0.01 0.12 0.01 0.00 0.00 0.04 0.00 0.04

FRAG# 3: 99.84 3.13 100.24 100.03 99.87 99.88 100.01 99.87 99.91 99.88
Net pop.(%) 99.84 3.23 100.55 100.21 99.75 99.78 100.04 99.80 99.87 99.80

OP(1 & 2) 0.000 0.049 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 -0.001 -0.006 -0.003 0.002 0.002 -0.001 0.002 0.001 0.002
OP(2 & 3) 0.001 -0.001 0.000 -0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -24.04 -23.95 -23.93 -23.88 -23.64 -23.63 -22.48 -22.46 -22.40 -22.35
Symmetry: A A A A A A A A A A

FRAG# 1: -0.05 0.00 0.03 0.08 0.17 0.05 0.41 0.28 0.02 0.18
Net pop.(%) 0.01 0.01 0.02 0.02 0.12 0.09 0.23 0.17 0.06 0.04

FRAG# 2: 0.01 0.00 0.01 0.00 0.01 0.06 0.05 0.09 0.02 0.02
Net pop.(%) 0.00 0.00 0.01 0.00 0.01 0.11 0.07 0.03 0.01 0.03

FRAG# 3: 100.04 100.00 99.96 99.92 99.83 99.89 99.55 99.62 99.96 99.80
Net pop.(%) 100.08 100.01 99.93 99.87 99.79 99.95 99.41 99.42 100.00 99.65

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 0.000 0.000 0.001 0.001 0.000 0.003 0.002 -0.001 0.003
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 -0.001 -0.001 0.002 0.000 0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -22.22 -22.19 -20.61 -20.60 -19.54 -19.52 -19.38 -19.32 -19.00 -18.97
Symmetry: A A A A A A A A A A

FRAG# 1: 0.01 -0.02 0.52 0.61 1.13 1.82 0.28 0.46 1.52 2.21
Net pop.(%) 0.03 0.02 0.27 0.27 0.50 0.73 0.37 0.51 0.90 1.04

FRAG# 2: -0.01 0.01 0.07 0.10 0.06 0.18 0.03 0.02 0.13 0.40
Net pop.(%) 0.00 0.01 0.10 0.05 0.15 0.10 0.04 0.01 0.35 0.23

FRAG# 3: 100.00 100.01 99.40 99.29 98.81 98.01 99.69 99.52 98.35 97.39
Net pop.(%) 100.04 100.06 99.19 98.94 98.13 96.94 99.76 99.58 97.73 96.21

OP(1 & 2) 0.000 0.000 0.000 0.000 -0.001 0.001 0.000 0.000 -0.002 0.002
OP(1 & 3) 0.000 -0.001 0.005 0.006 0.014 0.021 -0.001 -0.001 0.015 0.022
OP(2 & 3) 0.000 0.000 -0.001 0.001 0.000 0.001 0.000 0.000 -0.002 0.002

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -18.68 -18.65 -18.53 -18.47 -18.29 -18.20 -18.12 -18.06 -17.81 -17.78
Symmetry: A A A A A A A A A A

FRAG# 1: 0.72 0.37 0.38 1.15 3.89 2.84 2.68 1.53 -0.02 0.26
Net pop.(%) 0.42 0.17 0.30 0.78 2.82 2.07 1.75 1.04 0.18 0.19

FRAG# 2: 0.05 0.09 0.15 0.31 0.25 0.16 2.04 0.78 0.42 1.09
Net pop.(%) 0.03 0.04 0.07 0.19 0.16 0.23 1.21 0.83 0.47 0.62

FRAG# 3: 99.23 99.54 99.47 98.54 95.86 97.00 95.28 97.69 99.60 98.65
Net pop.(%) 98.94 99.31 99.30 98.16 94.88 96.11 94.12 97.24 99.82 98.24

OP(1 & 2) 0.000 0.000 0.000 0.001 0.002 -0.002 0.006 0.000 0.000 0.001
OP(1 & 3) 0.006 0.004 0.002 0.006 0.020 0.017 0.012 0.010 -0.004 0.000
OP(2 & 3) 0.000 0.001 0.002 0.001 0.000 0.000 0.011 -0.001 -0.001 0.008

Alpha MO: 111 112 113 114 115 116 117 118 119 120
HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68 HOMO-67 HOMO-66
Energy(eV): -17.27 -17.26 -17.10 -17.03 -16.98 -16.96 -16.87 -16.87 -16.70 -16.69
Symmetry: A A A A A A A A A A

FRAG# 1: 1.29 0.98 2.65 0.19 0.90 0.40 1.05 0.74 1.41 4.60
Net pop.(%) 0.78 0.60 1.62 0.13 0.71 0.35 0.82 0.56 1.07 3.72

FRAG# 2: 0.78 0.29 1.68 0.32 0.24 0.20 0.20 0.01 0.18 0.68
Net pop.(%) 0.45 0.20 1.11 0.17 0.33 0.15 0.13 0.03 0.13 0.56

FRAG# 3: 97.93 98.73 95.67 99.48 98.87 99.40 98.75 99.24 98.41 94.72
Net pop.(%) 97.29 98.26 94.68 99.29 98.77 99.36 98.55 99.07 98.03 94.09

OP(1 & 2) 0.002 0.000 0.006 0.000 0.000 0.001 0.001 0.000 0.000 0.004
OP(1 & 3) 0.008 0.007 0.014 0.001 0.004 0.000 0.004 0.004 0.007 0.014
OP(2 & 3) 0.005 0.002 0.005 0.003 -0.002 0.000 0.000 0.000 0.001 -0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58 HOMO-57 HOMO-56
Energy(eV): -16.60 -16.58 -16.46 -16.45 -16.29 -16.27 -16.14 -15.95 -15.90 -15.80
Symmetry: A A A A A A A A A A

FRAG# 1: 0.89 1.31 1.89 0.37 3.01 0.98 9.48 7.90 40.52 2.65
Net pop.(%) 0.63 1.05 1.41 0.23 2.44 0.69 7.20 6.64 35.91 2.33

FRAG# 2: 0.37 0.08 1.13 0.29 0.37 0.60 7.34 2.42 16.14 0.41
Net pop.(%) 0.32 0.12 0.76 0.17 0.28 0.34 5.47 1.99 13.52 0.42

FRAG# 3: 98.74 98.62 96.99 99.34 96.63 98.42 83.18 89.68 43.33 96.94
Net pop.(%) 98.43 98.33 96.61 99.14 96.06 97.86 82.08 88.95 42.40 96.61

OP(1 & 2) 0.000 -0.001 0.005 0.001 0.001 0.000 0.031 0.010 0.063 0.000
OP(1 & 3) 0.005 0.006 0.005 0.002 0.011 0.006 0.015 0.016 0.029 0.007
OP(2 & 3) 0.001 0.000 0.003 0.002 0.001 0.005 0.007 -0.001 -0.011 0.000

Alpha MO: 131 132 133 134 135 136 137 138 139 140
HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48 HOMO-47 HOMO-46
Energy(eV): -15.78 -15.72 -15.68 -15.62 -15.59 -15.56 -15.52 -15.49 -15.41 -15.36
Symmetry: A A A A A A A A A A

FRAG# 1: 40.32 2.20 9.56 7.64 11.69 4.83 6.21 1.60 0.35 3.35
Net pop.(%) 37.28 1.71 8.13 7.15 9.80 4.04 5.40 1.47 0.26 2.93

FRAG# 2: 27.67 0.29 1.16 3.09 7.30 4.43 6.53 0.81 0.01 1.86
Net pop.(%) 24.02 0.20 1.01 2.75 5.79 3.47 5.36 0.84 0.00 1.48

FRAG# 3: 32.00 97.51 89.28 89.26 81.02 90.74 87.26 97.60 99.65 94.79
Net pop.(%) 32.69 97.04 87.99 89.53 80.73 90.53 87.18 97.52 99.55 94.78

OP(1 & 2) 0.074 0.001 0.003 0.011 0.031 0.015 0.019 0.000 0.000 0.008
OP(1 & 3) -0.013 0.009 0.026 -0.001 0.007 0.000 -0.003 0.002 0.002 0.001
OP(2 & 3) -0.001 0.001 0.000 -0.004 -0.001 0.004 0.004 -0.001 0.000 0.000

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38 HOMO-37 HOMO-36
Energy(eV): -15.34 -15.26 -15.26 -15.24 -15.15 -15.09 -15.06 -14.99 -14.93 -14.91
Symmetry: A A A A A A A A A A

FRAG# 1: 2.08 1.41 0.97 11.53 1.93 0.09 2.50 9.52 2.11 9.89
Net pop.(%) 1.74 1.05 0.71 10.52 1.39 0.07 2.34 8.69 1.69 8.86

FRAG# 2: 0.27 1.56 0.65 2.56 0.05 0.00 2.70 1.92 5.65 3.05
Net pop.(%) 0.41 1.29 0.45 2.48 0.14 0.00 2.45 1.52 4.64 2.55

FRAG# 3: 97.65 97.02 98.38 85.91 98.02 99.91 94.80 88.57 92.24 87.06
Net pop.(%) 97.33 96.94 98.09 84.84 97.43 99.90 94.93 88.27 91.94 86.67

OP(1 & 2) -0.001 0.006 0.002 0.000 -0.001 0.000 0.005 0.009 0.011 0.012
OP(1 & 3) 0.008 0.002 0.003 0.020 0.012 0.000 -0.002 0.007 -0.003 0.009
OP(2 & 3) -0.001 0.000 0.002 0.001 0.000 0.000 0.000 -0.001 0.009 -0.001

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28 HOMO-27 HOMO-26
Energy(eV): -14.90 -14.83 -14.80 -14.79 -14.76 -14.68 -14.61 -14.61 -14.39 -14.33
Symmetry: A A A A A A A A A A

FRAG# 1: 4.68 26.86 7.07 0.98 2.18 0.92 4.35 39.86 22.24 25.21
Net pop.(%) 4.20 24.99 6.30 0.85 1.36 0.86 4.02 37.92 20.58 23.71

FRAG# 2: 0.03 7.71 0.25 0.01 8.53 0.12 1.84 8.47 1.67 7.08
Net pop.(%) 0.15 6.13 0.69 0.01 6.95 0.14 1.45 6.93 2.30 6.07

FRAG# 3: 95.28 65.44 92.68 99.02 89.29 98.96 93.81 51.67 76.09 67.71
Net pop.(%) 94.73 65.37 91.67 98.88 88.38 98.92 93.47 51.74 74.27 67.41

OP(1 & 2) -0.002 0.034 -0.007 0.000 0.015 0.000 0.004 0.035 -0.008 0.022
OP(1 & 3) 0.012 0.004 0.022 0.003 0.001 0.001 0.003 0.003 0.041 0.008
OP(2 & 3) -0.001 -0.002 -0.002 0.000 0.017 0.000 0.004 -0.005 -0.005 -0.002

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18 HOMO-17 HOMO-16
Energy(eV): -14.26 -14.22 -13.97 -13.91 -13.81 -13.65 -13.46 -13.37 -13.31 -13.16
Symmetry: A A A A A A A A A A

FRAG# 1: 68.73 6.69 50.61 42.44 61.14 80.26 5.41 23.94 48.94 13.33
Net pop.(%) 66.21 6.33 51.63 41.83 60.97 80.62 5.08 24.11 50.63 14.16

FRAG# 2: 12.62 1.67 0.11 3.87 3.88 0.37 3.48 5.62 3.86 1.00
Net pop.(%) 10.21 1.72 0.08 3.53 4.01 0.35 2.86 6.50 3.98 1.70

FRAG# 3: 18.65 91.64 49.28 53.69 34.98 19.36 91.12 70.44 47.20 85.67
Net pop.(%) 19.11 91.78 50.49 53.36 35.49 19.82 90.55 72.69 47.90 86.90

OP(1 & 2) 0.054 0.005 0.002 0.006 0.005 0.001 0.004 0.012 -0.011 -0.003
OP(1 & 3) -0.004 0.003 -0.023 0.006 -0.002 -0.008 0.003 -0.015 -0.023 -0.014
OP(2 & 3) -0.006 -0.006 -0.002 0.001 -0.008 -0.001 0.009 -0.030 0.009 -0.011

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8 HOMO-7 HOMO-6
Energy(eV): -12.86 -12.85 -12.60 -12.45 -12.34 -11.82 -11.78 -11.14 -11.10 -11.05
Symmetry: A A A A A A A A A A

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FRAG# 1:	26.67	35.05	4.01	46.32	41.39	6.97	25.51	3.16	4.17	0.30
Net pop.(%)	25.36	34.13	2.51	45.49	42.38	6.36	25.24	4.18	4.08	0.37

FRAG# 2:	3.80	-0.14	13.80	43.52	44.75	38.31	48.05	26.40	0.26	1.28
Net pop.(%)	4.34	0.14	13.26	42.97	46.26	36.53	48.85	27.35	0.59	1.53

FRAG# 3:	69.52	65.09	82.19	10.16	13.86	54.73	26.44	70.44	95.58	98.42
Net pop.(%)	68.01	64.07	82.12	15.36	13.88	54.22	28.17	70.74	95.30	99.02

OP(1 & 2)	-0.007	-0.004	0.020	0.066	-0.025	0.019	0.012	-0.017	-0.005	0.003
OP(1 & 3)	0.034	0.022	0.010	-0.049	0.005	-0.007	-0.007	-0.004	0.007	-0.004
OP(2 & 3)	-0.003	-0.002	-0.009	-0.055	-0.005	0.017	-0.028	-0.002	-0.001	-0.008

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1 LUMO+2 LUMO+3
Energy(eV): -10.98 -10.96 -10.93 -10.90 -10.87 -10.76 -8.45 -8.01 -5.18 -5.18
Symmetry: A A A A A A A A A A

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FRAG# 1:	4.31	2.58	5.52	1.96	11.74	11.50	36.07	38.05	7.05	10.17
Net pop.(%)	5.23	2.93	6.49	2.32	15.77	13.33	48.10	49.70	9.54	12.18

FRAG# 2:	2.86	2.51	37.34	1.08	17.75	14.98	44.35	34.05	0.24	1.57
Net pop.(%)	3.45	2.87	39.05	1.14	18.39	16.89	53.85	43.31	0.46	4.15

FRAG# 3:	92.83	94.91	57.14	96.96	70.51	73.52	19.58	27.90	92.71	88.26
Net pop.(%)	93.84	95.40	57.31	97.49	72.18	75.74	23.33	40.30	95.54	88.16

OP(1 & 2)	-0.005	-0.002	-0.025	0.001	-0.030	-0.015	-0.178	-0.085	0.001	-0.047
OP(1 & 3)	-0.013	-0.005	0.006	-0.008	-0.051	-0.021	-0.063	-0.148	-0.051	0.007
OP(2 & 3)	-0.007	-0.005	-0.009	-0.002	0.017	-0.023	-0.012	-0.100	-0.006	-0.005

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.90 -280.90 -280.90 -280.90 -280.88 -280.88 -280.88 -280.88 -279.97 -279.97
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.01
FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 99.99 99.99
Net pop.(%) 100.00 100.00 100.00 100.00 100.01 100.01 100.00 100.00 99.99 99.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -127.00 -127.00 -83.46 -83.45 -83.42 -83.42 -82.55 -82.55 -31.82 -31.80
Symmetry: A A A A A A A A A A

FRAG# 1: 100.30 100.27 100.02 99.94 99.91 99.93 100.03 99.98 -0.19 0.04
Net pop.(%) 100.61 100.54 100.05 99.90 99.84 99.87 100.09 99.96 0.07 0.04

FRAG# 2: -0.07 -0.05 0.01 0.02 0.06 0.09 0.00 0.00 0.42 -0.03
Net pop.(%) 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.00 0.28 0.00

FRAG# 3: -0.22 -0.22 -0.03 0.04 0.02 -0.02 -0.03 0.02 99.77 99.99
Net pop.(%) 0.01 0.01 0.01 0.01 0.01 0.01 0.04 0.01 99.97 100.02

OP(1 & 2) -0.002 -0.001 0.000 0.000 0.001 0.002 0.000 0.000 0.001 0.000
OP(1 & 3) -0.005 -0.005 -0.001 0.000 0.000 -0.001 -0.001 0.000 -0.006 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.002 -0.001

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -31.78 -31.77 -29.61 -29.60 -29.59 -29.58 -29.32 -28.91 -28.82 -28.58
Symmetry: A A A A A A A A A A

FRAG# 1: -0.38 -0.16 0.64 0.37 0.06 0.13 7.63 0.58 -0.08 -0.09
Net pop.(%) 0.02 0.03 0.17 0.02 0.01 0.02 2.47 0.17 0.45 0.13

FRAG# 2: 0.16 0.06 6.00 0.00 0.01 0.44 69.64 -0.03 16.48 2.63
Net pop.(%) 0.10 0.01 5.51 0.00 0.00 0.37 65.38 0.01 16.50 2.48

FRAG# 3: 100.23 100.10 93.37 99.62 99.93 99.44 22.73 99.44 83.60 97.46
Net pop.(%) 100.57 100.23 93.08 99.27 99.88 99.31 22.35 99.07 85.43 97.34

OP(1 & 2) 0.000 0.000 0.007 0.000 0.000 0.000 0.090 0.000 0.013 -0.002
OP(1 & 3) -0.008 -0.004 0.003 0.007 0.001 0.002 0.013 0.008 -0.023 -0.002
OP(2 & 3) 0.001 0.001 0.003 0.000 0.000 0.001 -0.005 -0.001 -0.013 0.005

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -28.56 -28.16 -25.69 -25.69 -24.52 -24.49 -24.39 -24.37 -24.16 -24.15
Symmetry: A A A A A A A A A A

FRAG# 1: 0.09 4.33 -0.25 -0.11 0.13 0.12 -0.02 0.10 0.08 0.10
Net pop.(%) 0.17 1.95 0.07 0.04 0.02 0.02 0.01 0.01 0.03 0.03

FRAG# 2: 0.06 92.22 0.00 0.09 0.01 0.00 0.01 0.03 0.00 0.02
Net pop.(%) 0.01 89.89 0.01 0.12 0.01 0.00 0.00 0.04 0.00 0.04

FRAG# 3: 99.85 3.45 100.24 100.03 99.86 99.88 100.01 99.86 99.92 99.88
Net pop.(%) 99.85 3.58 100.57 100.21 99.75 99.77 100.04 99.79 99.87 99.80

OP(1 & 2) 0.000 0.048 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 -0.001 -0.006 -0.003 0.002 0.002 -0.001 0.002 0.001 0.002
OP(2 & 3) 0.001 -0.002 0.000 -0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -24.05 -23.96 -23.94 -23.89 -23.65 -23.64 -22.49 -22.47 -22.40 -22.36
Symmetry: A A A A A A A A A A

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FRAG# 1:	-0.04	0.00	0.03	0.08	0.18	0.06	0.40	0.28	0.02	0.18
Net pop.(%)	0.01	0.01	0.02	0.02	0.13	0.09	0.23	0.17	0.06	0.04

FRAG# 2:	0.01	0.00	0.01	0.00	0.01	0.06	0.05	0.10	0.02	0.02
Net pop.(%)	0.00	0.00	0.01	0.00	0.01	0.12	0.07	0.03	0.01	0.03

FRAG# 3:	100.03	99.99	99.95	99.92	99.81	99.87	99.55	99.62	99.96	99.80
Net pop.(%)	100.08	100.00	99.93	99.86	99.76	99.91	99.43	99.42	100.00	99.65

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	-0.001	0.000	0.000	0.001	0.001	0.000	0.003	0.002	-0.001	0.003
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	-0.001	-0.001	0.002	0.000	0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -22.23 -22.20 -20.62 -20.60 -19.54 -19.53 -19.39 -19.32 -19.01 -18.98
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.01	-0.02	0.52	0.61	1.20	2.00	0.27	0.44	1.62	2.37
Net pop.(%)	0.03	0.02	0.26	0.27	0.53	0.80	0.36	0.50	0.93	1.11

FRAG# 2:	-0.01	0.00	0.07	0.10	0.07	0.21	0.03	0.02	0.14	0.44
Net pop.(%)	0.00	0.01	0.10	0.05	0.17	0.12	0.04	0.01	0.37	0.25

FRAG# 3:	100.01	100.01	99.41	99.29	98.73	97.79	99.70	99.54	98.24	97.19
Net pop.(%)	100.04	100.06	99.20	98.93	98.00	96.61	99.78	99.61	97.55	95.93

OP(1 & 2)	0.000	0.000	0.000	0.000	-0.002	0.001	0.000	0.000	-0.002	0.002
OP(1 & 3)	0.000	-0.001	0.005	0.006	0.015	0.023	-0.002	-0.001	0.016	0.023
OP(2 & 3)	0.000	0.000	-0.001	0.001	0.000	0.001	0.000	0.000	-0.002	0.002

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -18.68 -18.65 -18.53 -18.47 -18.29 -18.20 -18.12 -18.05 -17.80 -17.78
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.71	0.37	0.37	1.10	3.71	2.74	2.78	1.52	-0.02	0.26
Net pop.(%)	0.41	0.17	0.29	0.75	2.67	1.98	1.80	1.01	0.18	0.18

FRAG# 2:	0.05	0.09	0.15	0.31	0.23	0.15	2.13	0.77	0.42	1.09
Net pop.(%)	0.03	0.04	0.08	0.19	0.15	0.22	1.26	0.83	0.47	0.61

FRAG# 3:	99.25	99.54	99.48	98.59	96.06	97.11	95.09	97.72	99.60	98.65
Net pop.(%)	98.95	99.31	99.31	98.22	95.10	96.25	93.91	97.25	99.83	98.24

OP(1 & 2)	0.000	0.000	0.000	0.001	0.002	-0.002	0.007	0.000	0.000	0.001
OP(1 & 3)	0.006	0.004	0.002	0.006	0.019	0.017	0.013	0.010	-0.004	0.000
OP(2 & 3)	0.000	0.001	0.002	0.001	0.000	0.000	0.011	-0.001	-0.001	0.008

Alpha MO: 111 112 113 114 115 116 117 118 119 120
HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68 HOMO-67 HOMO-66
Energy(eV): -17.27 -17.26 -17.10 -17.03 -16.98 -16.95 -16.87 -16.87 -16.70 -16.68
Symmetry: A A A A A A A A A A

FRAG# 1: 1.37 0.99 2.74 0.18 0.85 0.38 0.99 0.71 1.35 4.13
Net pop.(%) 0.83 0.61 1.67 0.12 0.66 0.33 0.77 0.52 1.01 3.31

FRAG# 2: 0.79 0.31 1.80 0.32 0.22 0.20 0.20 0.01 0.17 0.58
Net pop.(%) 0.46 0.21 1.18 0.17 0.33 0.15 0.13 0.03 0.12 0.48

FRAG# 3: 97.83 98.71 95.47 99.49 98.92 99.42 98.81 99.28 98.48 95.29
Net pop.(%) 97.17 98.23 94.47 99.30 98.81 99.38 98.61 99.11 98.10 94.68

OP(1 & 2) 0.002 0.000 0.007 0.000 0.000 0.001 0.001 0.000 0.000 0.003
OP(1 & 3) 0.009 0.008 0.015 0.001 0.004 0.000 0.004 0.004 0.007 0.013
OP(2 & 3) 0.004 0.002 0.005 0.003 -0.002 0.000 0.000 0.000 0.001 -0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58 HOMO-57 HOMO-56
Energy(eV): -16.60 -16.58 -16.46 -16.44 -16.29 -16.27 -16.15 -15.95 -15.86 -15.79
Symmetry: A A A A A A A A A A

FRAG# 1: 0.89 1.22 2.03 0.35 2.83 0.90 9.42 5.59 38.52 2.32
Net pop.(%) 0.63 0.97 1.52 0.21 2.27 0.60 7.08 4.48 33.96 2.02

FRAG# 2: 0.38 0.07 1.24 0.28 0.34 0.67 7.65 1.35 15.29 0.35
Net pop.(%) 0.33 0.11 0.85 0.17 0.26 0.38 5.68 1.13 12.84 0.36

FRAG# 3: 98.72 98.71 96.73 99.36 96.83 98.43 82.94 93.06 46.19 97.32
Net pop.(%) 98.41 98.43 96.35 99.16 96.28 97.85 81.93 92.27 45.20 97.01

OP(1 & 2) 0.000 -0.001 0.005 0.001 0.001 0.000 0.033 0.005 0.060 0.000
OP(1 & 3) 0.005 0.006 0.005 0.002 0.010 0.006 0.014 0.017 0.031 0.006
OP(2 & 3) 0.001 0.000 0.003 0.002 0.001 0.006 0.006 -0.001 -0.011 0.000

Alpha MO: 131 132 133 134 135 136 137 138 139 140
HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48 HOMO-47 HOMO-46
Energy(eV): -15.76 -15.72 -15.68 -15.61 -15.59 -15.56 -15.51 -15.49 -15.41 -15.35
Symmetry: A A A A A A A A A A

FRAG# 1: 38.84 2.21 9.08 9.88 12.05 3.04 7.46 1.73 0.37 2.90
Net pop.(%) 35.67 1.70 7.65 9.24 10.06 2.45 6.48 1.59 0.28 2.50

FRAG# 2: 28.32 0.27 1.09 4.68 8.32 3.30 7.47 0.96 0.01 1.76
Net pop.(%) 24.58 0.19 0.94 4.14 6.62 2.53 6.16 0.98 0.00 1.40

FRAG# 3: 32.84 97.52 89.82 85.44 79.64 93.66 85.07 97.31 99.62 95.34
Net pop.(%) 33.37 97.04 88.52 85.84 79.57 93.40 85.00 97.24 99.52 95.35

OP(1 & 2) 0.075 0.001 0.003 0.016 0.036 0.011 0.022 0.000 0.000 0.008
OP(1 & 3) -0.011 0.009 0.026 -0.003 0.004 0.001 -0.003 0.002 0.002 0.000
OP(2 & 3) 0.000 0.001 0.000 -0.005 -0.002 0.004 0.004 -0.001 0.000 0.000

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38 HOMO-37 HOMO-36
Energy(eV): -15.33 -15.26 -15.25 -15.23 -15.15 -15.09 -15.06 -14.98 -14.92 -14.90
Symmetry: A A A A A A A A A A

FRAG# 1: 2.02 1.15 0.89 11.24 2.02 0.10 2.71 5.73 2.22 7.17
Net pop.(%) 1.69 0.81 0.62 10.17 1.45 0.08 2.52 5.18 1.75 6.30

FRAG# 2: 0.31 1.38 0.67 2.50 0.04 0.00 2.96 1.13 6.13 2.48
Net pop.(%) 0.45 1.13 0.46 2.40 0.13 0.00 2.68 0.91 5.05 2.09

FRAG# 3: 97.67 97.47 98.45 86.26 97.94 99.90 94.34 93.14 91.65 90.34
Net pop.(%) 97.34 97.38 98.16 85.14 97.31 99.89 94.48 92.91 91.34 89.98

OP(1 & 2) -0.001 0.005 0.002 0.000 -0.001 0.000 0.006 0.005 0.012 0.009
OP(1 & 3) 0.008 0.002 0.003 0.021 0.013 0.000 -0.002 0.005 -0.003 0.008
OP(2 & 3) -0.002 0.000 0.002 0.002 0.000 0.000 0.000 -0.001 0.009 -0.001

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28 HOMO-27 HOMO-26
Energy(eV): -14.90 -14.81 -14.81 -14.78 -14.76 -14.67 -14.61 -14.57 -14.38 -14.31
Symmetry: A A A A A A A A A A

FRAG# 1: 4.39 6.42 25.43 0.84 2.26 0.88 3.02 42.53 18.56 22.33
Net pop.(%) 3.91 5.67 23.51 0.72 1.40 0.82 2.76 40.09 16.91 20.69

FRAG# 2: 0.03 0.31 7.42 0.01 8.73 0.12 1.57 10.71 1.72 7.99
Net pop.(%) 0.17 0.73 5.92 0.01 7.11 0.13 1.24 8.78 2.40 6.80

FRAG# 3: 95.59 93.27 67.15 99.15 89.01 99.00 95.41 46.77 79.72 69.69
Net pop.(%) 95.03 92.29 66.93 99.02 88.10 98.95 95.11 46.79 77.90 69.46

OP(1 & 2) -0.002 -0.006 0.032 0.000 0.016 0.000 0.003 0.044 -0.009 0.026
OP(1 & 3) 0.012 0.021 0.006 0.003 0.002 0.001 0.002 0.005 0.042 0.007
OP(2 & 3) -0.001 -0.002 -0.002 0.000 0.017 0.000 0.004 -0.005 -0.005 -0.002

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18 HOMO-17 HOMO-16
Energy(eV): -14.21 -14.18 -13.92 -13.88 -13.73 -13.55 -13.46 -13.34 -13.25 -13.14
Symmetry: A A A A A A A A A A

FRAG# 1: 6.27 68.64 55.71 27.33 73.60 80.09 6.26 21.21 48.43 16.04
Net pop.(%) 5.86 65.91 56.60 26.78 73.15 80.29 5.89 21.29 50.16 16.89

FRAG# 2: 1.73 13.41 0.27 5.59 2.25 0.35 3.68 6.86 4.03 1.06
Net pop.(%) 1.76 10.87 0.22 5.20 2.41 0.34 3.04 7.73 4.12 1.74

FRAG# 3: 91.99 17.95 44.03 67.08 24.14 19.56 90.06 71.93 47.54 82.90
Net pop.(%) 92.09 18.30 45.25 66.99 24.23 19.87 89.53 74.38 48.21 84.16

OP(1 & 2) 0.005 0.056 0.004 0.009 0.004 0.001 0.005 0.015 -0.011 -0.003
OP(1 & 3) 0.004 -0.002 -0.022 0.003 0.005 -0.005 0.003 -0.017 -0.023 -0.014
OP(2 & 3) -0.005 -0.005 -0.003 -0.001 -0.007 -0.001 0.008 -0.033 0.010 -0.011

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8 HOMO-7 HOMO-6
Energy(eV): -12.86 -12.84 -12.61 -12.44 -12.32 -11.83 -11.76 -11.13 -11.10 -11.05
Symmetry: A A A A A A A A A A

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FRAG# 1:	28.86	41.26	4.07	51.36	43.13	7.27	25.83	2.61	4.33	0.31
Net pop.(%)	27.68	40.53	2.57	50.68	44.17	6.57	25.51	3.43	4.30	0.39

FRAG# 2:	4.95	-0.08	13.35	39.49	42.61	39.30	45.85	22.18	0.29	1.25
Net pop.(%)	5.69	0.31	12.81	38.69	44.04	37.46	46.67	22.99	0.63	1.49

FRAG# 3:	66.19	58.81	82.58	9.15	14.26	53.43	28.33	75.21	95.38	98.44
Net pop.(%)	64.79	58.01	82.54	14.31	14.32	52.91	29.85	75.49	95.12	99.04

OP(1 & 2)	-0.010	-0.005	0.020	0.066	-0.024	0.020	0.010	-0.013	-0.006	0.003
OP(1 & 3)	0.033	0.019	0.010	-0.053	0.003	-0.006	-0.004	-0.003	0.006	-0.004
OP(2 & 3)	-0.005	-0.003	-0.009	-0.050	-0.005	0.017	-0.027	-0.003	-0.001	-0.008

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1 LUMO+2 LUMO+3
Energy(eV): -10.97 -10.96 -10.92 -10.89 -10.85 -10.74 -8.38 -7.94 -5.19 -5.19
Symmetry: A A A A A A A A A A

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FRAG# 1:	4.73	2.74	2.28	2.13	16.58	12.70	37.12	38.86	7.42	10.29
Net pop.(%)	5.71	3.11	2.68	2.52	21.55	14.71	49.45	50.79	9.94	12.37

FRAG# 2:	2.95	2.55	25.24	1.08	33.16	15.77	43.31	33.56	0.26	1.64
Net pop.(%)	3.55	2.91	26.49	1.14	34.53	17.72	53.00	42.84	0.51	4.27

FRAG# 3:	92.32	94.70	72.48	96.79	50.26	71.53	19.57	27.58	92.32	88.07
Net pop.(%)	93.38	95.21	72.82	97.36	51.82	73.85	23.44	40.27	95.14	87.95

OP(1 & 2)	-0.005	-0.002	-0.013	0.001	-0.048	-0.016	-0.181	-0.085	0.000	-0.048
OP(1 & 3)	-0.014	-0.005	0.005	-0.009	-0.051	-0.024	-0.065	-0.153	-0.051	0.007
OP(2 & 3)	-0.007	-0.005	-0.012	-0.002	0.020	-0.023	-0.012	-0.100	-0.005	-0.004

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.71 -280.71 -280.71 -280.71 -280.68 -280.68 -280.68 -280.68 -279.76 -279.76
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 0.00 0.01 0.00 0.01 0.00 0.01 0.01
FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 99.99 100.00 99.99 100.00 99.99 99.99
Net pop.(%) 100.00 100.00 100.00 100.00 99.97 100.00 99.97 100.00 99.98 99.98

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -122.31 -121.67 -81.51 -81.45 -80.63 -80.63 -80.57 -80.43 -33.40 -31.63
Symmetry: A A A A A A A A A A

FRAG# 1: 100.29 100.29 99.99 99.98 99.99 99.98 99.96 100.00 0.89 -0.19
Net pop.(%) 100.60 100.58 99.99 99.97 99.99 99.97 99.93 100.00 0.95 0.03

FRAG# 2: -0.04 -0.04 0.03 0.04 0.00 0.03 0.05 0.00 99.17 0.06
Net pop.(%) 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 99.28 0.08

FRAG# 3: -0.26 -0.25 -0.02 -0.02 0.00 -0.01 -0.01 0.00 -0.06 100.13
Net pop.(%) 0.01 0.01 0.01 0.00 0.01 0.01 0.01 0.01 0.14 100.38

OP(1 & 2) -0.001 -0.001 0.000 0.001 0.000 0.001 0.001 0.000 0.000 0.000
OP(1 & 3) -0.005 -0.005 -0.001 -0.001 0.000 0.000 0.000 0.000 -0.001 -0.004
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 -0.003 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -31.62 -31.61 -31.60 -29.46 -29.45 -29.45 -29.45 -28.68 -28.64 -28.39
Symmetry: A A A A A A A A A A

FRAG# 1: -0.16 -0.21 -0.23 0.12 0.09 0.09 0.08 0.21 0.23 0.04
Net pop.(%) 0.03 0.02 0.02 0.01 0.01 0.01 0.01 0.15 0.15 0.16

FRAG# 2: 0.05 0.01 0.00 0.00 0.00 0.02 0.01 0.01 0.01 0.01
Net pop.(%) 0.07 0.01 0.00 0.00 0.01 0.02 0.01 0.03 0.03 0.00

FRAG# 3: 100.12 100.20 100.22 99.88 99.91 99.89 99.90 99.78 99.76 99.95
Net pop.(%) 100.33 100.43 100.47 99.76 99.84 99.82 99.84 99.73 99.69 100.05

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.004 -0.005 -0.005 0.002 0.002 0.001 0.001 0.001 0.002 -0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -28.35 -26.53 -25.49 -25.48 -24.36 -24.35 -24.27 -24.26 -24.13 -24.09
Symmetry: A A A A A A A A A A

FRAG# 1: 0.04 2.63 -0.01 -0.18 0.10 0.15 0.13 -0.01 0.12 0.12
Net pop.(%) 0.14 0.82 0.05 0.05 0.02 0.02 0.01 0.01 0.03 0.03

FRAG# 2: 0.01 97.10 0.00 0.01 0.00 0.00 0.01 0.03 0.04 -0.01
Net pop.(%) 0.00 95.16 0.00 0.00 0.00 0.00 0.01 0.01 0.06 0.00

FRAG# 3: 99.94 0.28 100.01 100.18 99.90 99.85 99.87 99.98 99.84 99.88
Net pop.(%) 100.02 0.22 100.06 100.40 99.82 99.72 99.76 99.98 99.76 99.80

OP(1 & 2) 0.000 0.037 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.002 -0.001 -0.001 -0.005 0.002 0.003 0.002 0.000 0.002 0.002
OP(2 & 3) 0.000 0.002 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -23.94 -23.89 -23.83 -23.82 -23.51 -23.50 -22.35 -22.33 -22.27 -22.26
Symmetry: A A A A A A A A A A

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FRAG# 1:	-0.01	-0.01	0.04	0.07	0.04	-0.01	0.24	0.19	0.01	0.07
Net pop.(%)	0.00	0.00	0.02	0.02	0.09	0.09	0.13	0.10	0.04	0.03

FRAG# 2:	0.00	0.01	0.00	0.00	0.01	0.03	0.00	0.01	0.01	0.00
Net pop.(%)	0.00	0.00	0.00	0.00	0.02	0.01	0.01	0.01	0.01	0.00

FRAG# 3:	100.01	100.01	99.96	99.93	99.95	99.98	99.76	99.81	99.98	99.93
Net pop.(%)	100.03	100.02	99.94	99.88	100.00	100.08	99.66	99.72	100.01	99.90

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.001	-0.001	-0.002	0.002	0.002	-0.001	0.001
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -22.11 -22.09 -20.47 -20.44 -19.37 -19.35 -19.29 -19.24 -18.84 -18.81
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.01	0.02	0.61	0.28	0.88	1.33	0.24	0.30	2.87	2.08
Net pop.(%)	0.02	0.02	0.19	0.16	0.40	0.55	0.28	0.32	1.40	1.00

FRAG# 2:	0.01	0.00	0.05	0.06	0.11	0.40	0.01	0.01	1.89	0.90
Net pop.(%)	0.01	0.00	0.03	0.04	0.10	0.29	0.01	0.01	1.47	0.79

FRAG# 3:	99.98	99.98	99.34	99.66	99.01	98.27	99.75	99.69	95.24	97.02
Net pop.(%)	100.00	99.99	98.91	99.52	98.52	97.54	99.77	99.70	93.88	95.98

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.005	0.001
OP(1 & 3)	0.000	0.000	0.008	0.002	0.010	0.014	-0.001	0.000	0.024	0.020
OP(2 & 3)	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.003	0.001

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -18.61 -18.55 -18.36 -18.35 -18.13 -18.05 -17.97 -17.94 -17.70 -17.68
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.59	0.43	0.84	0.78	3.55	1.89	2.23	1.60	0.00	0.24
Net pop.(%)	0.30	0.19	0.42	0.41	2.50	1.22	1.40	0.82	0.02	0.12

FRAG# 2:	0.00	0.01	0.24	0.16	0.11	0.03	8.05	2.00	0.08	0.24
Net pop.(%)	0.00	0.01	0.19	0.13	0.09	0.05	6.60	1.75	0.17	0.13

FRAG# 3:	99.40	99.56	98.92	99.05	96.34	98.08	89.71	96.40	99.92	99.52
Net pop.(%)	99.11	99.32	98.46	98.68	95.30	97.39	88.80	95.46	100.00	99.35

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	-0.001	0.014	0.001	0.000	0.001
OP(1 & 3)	0.006	0.005	0.008	0.007	0.021	0.014	0.003	0.015	0.000	0.002
OP(2 & 3)	0.000	0.000	0.001	0.000	0.000	0.000	0.015	0.004	-0.002	0.002

Alpha MO: 111 112 113 114 115 116 117 118 119 120
HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68 HOMO-67 HOMO-66
Energy(eV): -17.35 -17.14 -17.12 -16.92 -16.91 -16.90 -16.81 -16.78 -16.75 -16.61
Symmetry: A A A A A A A A A A

FRAG# 1: 13.62 1.02 0.44 0.06 1.67 0.06 3.50 0.61 0.74 1.86
Net pop.(%) 9.54 0.45 0.27 0.04 0.98 0.06 2.62 0.42 0.54 1.38

FRAG# 2: 49.67 2.09 1.07 0.18 4.06 0.03 14.54 0.03 0.10 0.06
Net pop.(%) 45.02 1.60 0.98 0.09 3.84 0.06 13.92 0.04 0.09 0.05

FRAG# 3: 36.71 96.89 98.49 99.76 94.27 99.91 81.96 99.36 99.16 98.08
Net pop.(%) 37.32 96.10 98.16 99.65 93.43 99.94 82.78 99.17 98.99 97.61

OP(1 & 2) 0.093 0.003 -0.001 0.000 0.001 0.000 0.023 0.000 0.000 0.000
OP(1 & 3) -0.012 0.009 0.004 0.000 0.013 0.000 -0.006 0.004 0.004 0.009
OP(2 & 3) 0.000 0.007 0.002 0.002 0.004 -0.001 -0.011 0.000 0.000 0.000

Alpha MO: 121 122 123 124 125 126 127 128 129 130
HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58 HOMO-57 HOMO-56
Energy(eV): -16.57 -16.45 -16.44 -16.41 -16.39 -16.18 -16.11 -16.08 -15.84 -15.80
Symmetry: A A A A A A A A A A

FRAG# 1: 1.66 0.49 0.49 0.49 0.44 8.68 1.68 0.59 3.68 0.66
Net pop.(%) 1.15 0.29 0.38 0.34 0.25 6.78 1.33 0.38 2.53 0.32

FRAG# 2: 0.07 2.48 0.03 0.14 1.66 70.64 0.03 0.04 9.64 6.19
Net pop.(%) 0.05 2.35 0.04 0.09 1.45 69.20 0.03 0.03 8.82 6.20

FRAG# 3: 98.27 97.03 99.48 99.37 97.90 20.68 98.29 99.36 86.67 93.15
Net pop.(%) 97.78 96.77 99.37 99.22 97.58 21.57 97.96 99.14 86.06 92.90

OP(1 & 2) 0.000 0.001 0.000 0.000 0.001 0.042 0.000 0.000 0.014 0.001
OP(1 & 3) 0.010 0.003 0.002 0.002 0.003 -0.004 0.007 0.004 0.009 0.006
OP(2 & 3) 0.000 0.002 0.000 0.001 0.003 -0.014 0.000 0.000 0.003 -0.001

Alpha MO: 131 132 133 134 135 136 137 138 139 140
HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48 HOMO-47 HOMO-46
Energy(eV): -15.73 -15.72 -15.67 -15.61 -15.59 -15.49 -15.35 -15.35 -15.29 -15.27
Symmetry: A A A A A A A A A A

FRAG# 1: 9.32 4.85 2.76 0.48 10.51 3.54 0.76 0.51 1.53 6.70
Net pop.(%) 6.69 4.30 2.29 0.24 9.08 2.60 0.66 0.29 1.17 5.92

FRAG# 2: 33.52 0.75 0.84 0.97 1.10 0.26 0.18 0.35 3.39 3.13
Net pop.(%) 30.56 0.62 0.64 1.07 0.94 0.25 0.18 0.38 3.32 2.44

FRAG# 3: 57.15 94.40 96.40 98.55 88.39 96.19 99.06 99.14 95.08 90.18
Net pop.(%) 55.95 93.97 96.08 98.41 87.26 95.36 98.97 98.92 95.05 89.73

OP(1 & 2) 0.044 0.003 0.004 0.000 0.005 0.001 0.000 0.000 0.004 0.010
OP(1 & 3) 0.009 0.009 0.006 0.005 0.024 0.018 0.002 0.005 0.003 0.005
OP(2 & 3) 0.015 0.000 0.001 -0.002 -0.001 -0.001 0.000 0.000 -0.003 0.004

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38 HOMO-37 HOMO-36
Energy(eV): -15.25 -15.24 -15.23 -15.19 -15.04 -15.03 -14.97 -14.93 -14.86 -14.81
Symmetry: A A A A A A A A A A

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FRAG# 1:	1.94	9.20	1.15	7.54	1.30	2.15	3.20	2.40	4.66	0.23
Net pop.(%)	1.59	8.35	0.84	6.09	0.81	1.79	2.95	1.71	3.58	0.10

FRAG# 2:	6.11	2.43	0.95	20.43	0.41	0.07	0.78	0.51	0.47	0.49
Net pop.(%)	6.11	2.05	1.01	20.14	0.44	0.09	0.69	0.59	0.43	0.49

FRAG# 3:	91.95	88.37	97.90	72.03	98.29	97.77	96.01	97.08	94.86	99.27
Net pop.(%)	92.06	88.02	97.67	73.02	97.79	97.37	95.93	96.47	93.89	99.20

OP(1 & 2)	0.005	0.009	0.000	0.027	-0.001	0.000	0.003	0.000	0.002	0.001
OP(1 & 3)	0.002	0.008	0.006	0.002	0.010	0.008	0.002	0.014	0.020	0.002
OP(2 & 3)	-0.005	-0.001	-0.001	-0.022	0.000	0.000	-0.001	-0.002	-0.001	-0.001

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28 HOMO-27 HOMO-26
Energy(eV): -14.79 -14.78 -14.72 -14.66 -14.63 -14.61 -14.59 -14.30 -14.26 -14.19
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.63	0.56	2.44	1.44	6.67	2.97	6.37	15.76	9.98	5.89
Net pop.(%)	0.52	0.42	2.26	1.28	5.60	2.37	5.46	14.59	8.86	5.15

FRAG# 2:	0.01	0.00	1.31	0.69	1.03	0.41	1.02	21.03	0.60	1.96
Net pop.(%)	0.01	0.00	1.10	0.59	1.27	0.37	1.29	17.64	0.67	2.29

FRAG# 3:	99.37	99.44	96.25	97.86	92.30	96.63	92.60	63.22	89.43	92.15
Net pop.(%)	99.26	99.30	96.30	97.78	91.12	96.11	91.64	63.78	88.43	91.26

OP(1 & 2)	0.000	0.000	0.004	0.002	-0.004	0.001	-0.003	0.051	0.000	-0.005
OP(1 & 3)	0.002	0.003	-0.001	0.001	0.025	0.011	0.021	-0.028	0.022	0.020
OP(2 & 3)	0.000	0.000	0.000	0.000	-0.001	0.000	-0.002	0.017	-0.002	-0.002

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18 HOMO-17 HOMO-16
Energy(eV): -14.07 -13.98 -13.48 -13.41 -13.19 -13.06 -12.96 -12.95 -12.82 -12.70
Symmetry: A A A A A A A A A A

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FRAG# 1:	11.15	11.26	23.60	12.80	41.19	40.83	20.03	53.51	56.58	69.32
Net pop.(%)	9.47	9.59	22.27	11.78	39.62	39.98	19.61	53.02	57.20	69.17

FRAG# 2:	0.37	1.07	2.61	0.93	5.89	0.73	0.13	4.55	1.26	3.09
Net pop.(%)	0.55	1.41	2.11	0.82	5.82	0.84	0.15	3.92	1.41	2.77

FRAG# 3:	88.48	87.68	73.79	86.27	52.92	58.44	79.84	41.94	42.17	27.59
Net pop.(%)	86.69	85.91	72.58	85.39	51.46	57.50	79.33	42.24	42.51	27.74

OP(1 & 2)	-0.003	-0.004	0.006	0.002	0.002	-0.002	-0.001	0.014	-0.004	0.006
OP(1 & 3)	0.036	0.038	0.020	0.018	0.030	0.019	0.010	-0.004	-0.008	-0.003
OP(2 & 3)	-0.001	-0.002	0.004	0.000	0.000	0.000	0.001	-0.002	0.001	0.000

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8 HOMO-7 HOMO-6
Energy(eV): -12.66 -12.59 -12.38 -12.36 -12.14 -12.03 -10.99 -10.98 -10.96 -10.94
Symmetry: A A A A A A A A A A

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FRAG# 1:	85.63	64.34	5.75	76.52	73.62	82.84	4.42	0.82	0.56	1.06
Net pop.(%)	89.20	65.08	4.21	76.65	77.21	83.16	5.02	1.02	0.50	1.15

FRAG# 2:	6.59	8.49	18.53	0.72	14.16	0.78	1.10	0.06	0.16	22.66
Net pop.(%)	9.42	9.88	17.51	0.71	17.66	0.77	1.27	0.10	0.25	22.56

FRAG# 3:	7.79	27.17	75.72	22.75	12.22	16.38	94.48	99.11	99.28	76.27
Net pop.(%)	8.52	27.62	74.52	22.86	13.17	16.64	94.84	99.27	99.27	75.88

OP(1 & 2)	-0.057	-0.017	0.014	0.000	-0.061	-0.001	-0.004	-0.001	0.000	-0.004
OP(1 & 3)	-0.015	0.002	0.017	-0.002	-0.010	-0.006	-0.008	-0.003	0.002	0.002
OP(2 & 3)	0.000	-0.011	0.007	0.000	-0.009	0.001	0.001	0.000	-0.001	0.006

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1 LUMO+2 LUMO+3
Energy(eV): -10.92 -10.85 -10.73 -10.72 -10.61 -10.44 -7.77 -5.31 -5.14 -5.08
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.70	9.45	7.64	12.70	14.64	38.95	50.52	11.45	14.07	17.20
Net pop.(%)	0.78	9.92	9.00	14.32	18.04	44.89	63.02	8.78	18.57	20.00

FRAG# 2:	39.78	0.17	2.56	2.01	24.59	7.83	28.77	70.22	0.06	0.59
Net pop.(%)	40.08	0.64	2.74	2.97	25.43	10.75	37.88	66.05	0.64	3.12

FRAG# 3:	59.52	90.38	89.81	85.29	60.78	53.21	20.71	18.33	85.88	82.21
Net pop.(%)	59.73	90.69	91.02	86.36	62.88	57.06	27.60	16.94	89.54	82.79

OP(1 & 2)	-0.002	-0.006	-0.003	-0.015	-0.021	-0.050	-0.147	0.054	-0.014	-0.047
OP(1 & 3)	0.000	-0.003	-0.024	-0.017	-0.047	-0.069	-0.103	-0.001	-0.076	-0.009
OP(2 & 3)	-0.004	-0.003	0.000	-0.004	0.005	-0.008	-0.035	0.029	0.003	-0.003

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.80 -280.80 -280.80 -280.80 -280.77 -280.77 -280.77 -280.77 -279.85 -279.85
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 0.00 0.01 0.00 0.01 0.00 0.01 0.01
FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 99.99 100.00 99.99 100.00 99.99 99.99
Net pop.(%) 100.00 100.00 100.00 100.00 99.97 100.00 99.97 100.00 99.98 99.98

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -126.10 -125.42 -82.62 -82.56 -81.72 -81.70 -81.63 -81.50 -33.43 -31.65
Symmetry: A A A A A A A A A A

FRAG# 1: 100.23 100.22 99.99 99.98 99.99 99.98 99.96 99.99 0.94 -0.18
Net pop.(%) 100.46 100.45 100.00 99.97 99.99 99.97 99.92 100.00 0.94 0.03

FRAG# 2: -0.02 -0.02 0.02 0.04 0.00 0.03 0.05 0.00 99.14 0.06
Net pop.(%) 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 99.22 0.08

FRAG# 3: -0.20 -0.19 -0.02 -0.02 0.00 -0.01 0.00 0.00 -0.08 100.12
Net pop.(%) 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.14 100.34

OP(1 & 2) -0.001 0.000 0.000 0.001 0.000 0.000 0.001 0.000 0.001 0.000
OP(1 & 3) -0.004 -0.004 -0.001 0.000 0.000 0.000 0.000 0.000 -0.001 -0.004
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 -0.003 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -31.64 -31.63 -31.62 -29.47 -29.47 -29.47 -29.46 -28.71 -28.67 -28.42
Symmetry: A A A A A A A A A A

FRAG# 1: -0.15 -0.22 -0.23 0.12 0.09 0.09 0.08 0.24 0.26 0.03
Net pop.(%) 0.03 0.02 0.02 0.01 0.01 0.01 0.01 0.15 0.15 0.16

FRAG# 2: 0.05 0.01 0.00 0.00 0.00 0.02 0.01 0.01 0.01 0.01
Net pop.(%) 0.07 0.01 0.00 0.00 0.01 0.02 0.01 0.03 0.03 0.00

FRAG# 3: 100.10 100.21 100.23 99.88 99.91 99.89 99.90 99.75 99.73 99.96
Net pop.(%) 100.30 100.44 100.47 99.76 99.83 99.82 99.83 99.66 99.63 100.07

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.004 -0.005 -0.005 0.002 0.002 0.001 0.001 0.002 0.002 -0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -28.37 -26.56 -25.50 -25.49 -24.37 -24.36 -24.27 -24.26 -24.14 -24.10
Symmetry: A A A A A A A A A A

FRAG# 1: 0.03 2.61 -0.01 -0.18 0.10 0.15 0.13 0.00 0.12 0.12
Net pop.(%) 0.14 0.81 0.05 0.05 0.02 0.02 0.01 0.01 0.03 0.03

FRAG# 2: 0.01 97.12 0.00 0.01 0.00 0.00 0.01 0.03 0.04 -0.01
Net pop.(%) 0.01 95.20 0.00 0.00 0.00 0.00 0.01 0.01 0.05 0.00

FRAG# 3: 99.95 0.27 100.01 100.17 99.90 99.85 99.86 99.97 99.84 99.89
Net pop.(%) 100.04 0.22 100.07 100.40 99.82 99.71 99.74 99.96 99.75 99.80

OP(1 & 2) 0.000 0.037 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.002 -0.001 -0.001 -0.005 0.002 0.003 0.002 0.000 0.002 0.002
OP(2 & 3) 0.000 0.002 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -23.95 -23.90 -23.84 -23.83 -23.53 -23.51 -22.36 -22.34 -22.27 -22.27
Symmetry: A A A A A A A A A A

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FRAG# 1:	-0.01	-0.01	0.04	0.07	0.05	0.01	0.24	0.18	0.01	0.06
Net pop.(%)	0.00	0.00	0.02	0.02	0.09	0.09	0.13	0.10	0.05	0.04

FRAG# 2:	0.00	0.01	0.00	0.00	0.01	0.03	0.00	0.01	0.01	0.00
Net pop.(%)	0.00	0.00	0.00	0.00	0.02	0.02	0.01	0.01	0.01	0.00

FRAG# 3:	100.01	100.00	99.96	99.93	99.93	99.96	99.76	99.81	99.98	99.93
Net pop.(%)	100.02	100.01	99.93	99.88	99.97	100.04	99.66	99.73	100.02	99.90

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.001	-0.001	-0.002	0.002	0.002	-0.001	0.001
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -22.11 -22.10 -20.48 -20.45 -19.38 -19.36 -19.29 -19.24 -18.85 -18.82
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.01	0.01	0.62	0.28	1.03	1.43	0.24	0.29	3.28	2.09
Net pop.(%)	0.02	0.02	0.19	0.16	0.46	0.59	0.28	0.31	1.58	0.99

FRAG# 2:	0.01	0.00	0.05	0.07	0.16	0.45	0.01	0.01	2.31	0.77
Net pop.(%)	0.01	0.00	0.03	0.04	0.14	0.33	0.01	0.01	1.77	0.71

FRAG# 3:	99.98	99.98	99.33	99.65	98.81	98.11	99.75	99.70	94.41	97.13
Net pop.(%)	100.01	99.99	98.90	99.50	98.23	97.33	99.78	99.71	92.89	96.06

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.007	0.001
OP(1 & 3)	0.000	0.000	0.008	0.002	0.011	0.015	-0.001	0.000	0.027	0.021
OP(2 & 3)	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.000	0.004	0.000

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -18.61 -18.55 -18.36 -18.35 -18.13 -18.05 -17.98 -17.94 -17.70 -17.68
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.59	0.42	0.83	0.76	3.45	1.82	2.53	1.62	0.00	0.24
Net pop.(%)	0.29	0.19	0.41	0.40	2.41	1.17	1.54	0.82	0.02	0.11

FRAG# 2:	0.00	0.01	0.24	0.15	0.11	0.03	8.95	1.93	0.08	0.23
Net pop.(%)	0.00	0.01	0.19	0.12	0.09	0.05	7.33	1.69	0.17	0.13

FRAG# 3:	99.41	99.56	98.94	99.09	96.44	98.15	88.52	96.45	99.92	99.53
Net pop.(%)	99.12	99.32	98.47	98.73	95.42	97.47	87.58	95.50	100.00	99.36

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	-0.001	0.017	0.001	0.000	0.001
OP(1 & 3)	0.006	0.005	0.008	0.007	0.020	0.014	0.003	0.015	0.000	0.002
OP(2 & 3)	0.000	0.000	0.001	0.000	0.000	0.000	0.016	0.004	-0.002	0.001

Alpha MO: 111 112 113 114 115 116 117 118 119 120
HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68 HOMO-67 HOMO-66
Energy(eV): -17.37 -17.13 -17.12 -16.92 -16.91 -16.89 -16.81 -16.78 -16.75 -16.60
Symmetry: A A A A A A A A A A

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FRAG# 1:	13.43	0.92	0.45	0.06	1.68	0.05	3.28	0.57	0.71	1.81
Net pop.(%)	9.17	0.40	0.28	0.04	0.98	0.06	2.40	0.39	0.51	1.33

FRAG# 2:	48.64	1.97	1.01	0.18	3.86	0.03	13.91	0.02	0.10	0.06
Net pop.(%)	43.89	1.50	0.92	0.09	3.67	0.06	13.29	0.03	0.09	0.04

FRAG# 3:	37.93	97.11	98.55	99.76	94.46	99.91	82.81	99.40	99.18	98.13
Net pop.(%)	38.67	96.35	98.23	99.65	93.60	99.95	83.61	99.22	99.02	97.67

OP(1 & 2)	0.097	0.002	-0.001	0.000	0.000	0.000	0.023	0.000	0.000	0.000
OP(1 & 3)	-0.012	0.008	0.004	0.000	0.014	0.000	-0.005	0.004	0.004	0.009
OP(2 & 3)	-0.003	0.007	0.002	0.002	0.004	-0.001	-0.011	0.000	0.000	0.000

Alpha MO: 121 122 123 124 125 126 127 128 129 130
HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58 HOMO-57 HOMO-56
Energy(eV): -16.56 -16.45 -16.44 -16.41 -16.39 -16.16 -16.12 -16.09 -15.83 -15.80
Symmetry: A A A A A A A A A A

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FRAG# 1:	1.59	0.46	0.46	0.45	0.43	8.58	1.59	0.57	3.22	0.71
Net pop.(%)	1.08	0.26	0.35	0.31	0.24	6.66	1.25	0.36	2.17	0.35

FRAG# 2:	0.06	2.22	0.02	0.14	1.61	70.48	0.03	0.05	7.55	6.96
Net pop.(%)	0.05	2.09	0.04	0.09	1.41	69.05	0.03	0.03	6.95	6.97

FRAG# 3:	98.35	97.31	99.52	99.41	97.96	20.94	98.37	99.38	89.23	92.33
Net pop.(%)	97.86	97.05	99.41	99.26	97.63	21.75	98.05	99.16	88.65	92.08

OP(1 & 2)	0.000	0.001	0.000	0.000	0.001	0.042	0.000	0.000	0.011	0.001
OP(1 & 3)	0.010	0.003	0.002	0.002	0.003	-0.003	0.007	0.004	0.010	0.006
OP(2 & 3)	0.000	0.002	0.000	0.001	0.003	-0.013	0.000	0.000	0.001	-0.001

Alpha MO: 131 132 133 134 135 136 137 138 139 140
HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48 HOMO-47 HOMO-46
Energy(eV): -15.71 -15.71 -15.67 -15.60 -15.59 -15.49 -15.35 -15.35 -15.29 -15.26
Symmetry: A A A A A A A A A A

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FRAG# 1:	9.03	4.14	2.50	0.48	10.09	3.30	0.52	0.61	1.13	4.88
Net pop.(%)	6.40	3.64	2.05	0.23	8.65	2.38	0.30	0.51	0.84	4.24

FRAG# 2:	34.26	0.65	0.76	1.10	1.01	0.21	0.37	0.13	2.38	2.45
Net pop.(%)	31.15	0.55	0.57	1.20	0.86	0.20	0.39	0.14	2.33	1.88

FRAG# 3:	56.71	95.21	96.74	98.43	88.91	96.49	99.12	99.26	96.48	92.67
Net pop.(%)	55.43	94.82	96.43	98.29	87.75	95.66	98.89	99.18	96.41	92.25

OP(1 & 2)	0.045	0.002	0.003	0.000	0.004	0.001	0.000	0.000	0.003	0.008
OP(1 & 3)	0.008	0.008	0.006	0.005	0.024	0.017	0.005	0.002	0.003	0.005
OP(2 & 3)	0.018	0.000	0.001	-0.002	-0.001	-0.001	0.000	0.000	-0.002	0.004

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38 HOMO-37 HOMO-36
Energy(eV): -15.24 -15.23 -15.23 -15.17 -15.04 -15.03 -14.96 -14.93 -14.86 -14.81
Symmetry: A A A A A A A A A A

FRAG# 1: 1.73 11.09 1.07 8.27 1.39 1.99 3.34 2.45 4.35 0.23
Net pop.(%) 1.43 10.04 0.77 6.59 0.86 1.63 3.06 1.72 3.28 0.10

FRAG# 2: 5.10 2.98 0.92 24.63 0.43 0.06 0.78 0.61 0.41 0.54
Net pop.(%) 5.11 2.51 0.98 24.22 0.46 0.08 0.68 0.70 0.37 0.54

FRAG# 3: 93.16 85.93 98.01 67.11 98.18 97.95 95.88 96.93 95.24 99.23
Net pop.(%) 93.19 85.48 97.77 68.24 97.64 97.57 95.77 96.29 94.27 99.16

OP(1 & 2) 0.003 0.011 0.000 0.032 -0.001 0.000 0.003 0.000 0.001 0.001
OP(1 & 3) 0.003 0.010 0.006 0.001 0.011 0.007 0.003 0.015 0.020 0.002
OP(2 & 3) -0.003 -0.001 -0.001 -0.024 0.000 0.000 -0.001 -0.002 -0.001 -0.001

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28 HOMO-27 HOMO-26
Energy(eV): -14.78 -14.78 -14.72 -14.66 -14.64 -14.61 -14.59 -14.29 -14.25 -14.19
Symmetry: A A A A A A A A A A

FRAG# 1: 0.53 0.54 2.43 1.48 6.23 2.80 5.93 16.89 9.23 5.41
Net pop.(%) 0.39 0.44 2.24 1.31 5.18 2.21 5.07 15.55 8.10 4.64

FRAG# 2: 0.00 0.01 1.23 0.68 1.03 0.40 1.10 22.12 0.61 1.88
Net pop.(%) 0.01 0.01 1.04 0.58 1.28 0.36 1.40 18.57 0.70 2.20

FRAG# 3: 99.47 99.45 96.34 97.84 92.74 96.80 92.97 60.99 90.15 92.71
Net pop.(%) 99.33 99.35 96.37 97.74 91.55 96.29 92.04 61.56 89.14 91.81

OP(1 & 2) 0.000 0.000 0.004 0.002 -0.004 0.001 -0.004 0.055 0.000 -0.005
OP(1 & 3) 0.003 0.002 0.000 0.002 0.025 0.011 0.021 -0.028 0.022 0.020
OP(2 & 3) 0.000 0.000 0.000 0.000 -0.001 0.000 -0.002 0.016 -0.002 -0.002

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18 HOMO-17 HOMO-16
Energy(eV): -14.07 -13.99 -13.46 -13.39 -13.14 -13.02 -12.95 -12.89 -12.74 -12.61
Symmetry: A A A A A A A A A A

FRAG# 1: 9.84 10.28 18.27 10.37 36.91 27.76 15.35 58.85 67.42 71.14
Net pop.(%) 8.18 8.61 17.01 9.39 35.21 26.81 14.64 58.12 67.97 70.69

FRAG# 2: 0.34 1.16 2.62 0.73 6.13 0.53 0.13 5.40 1.59 3.78
Net pop.(%) 0.53 1.54 2.13 0.64 6.06 0.65 0.19 4.64 1.81 3.40

FRAG# 3: 89.82 88.55 79.11 88.90 56.96 71.71 84.52 35.75 30.99 25.08
Net pop.(%) 88.03 86.76 77.92 88.04 55.40 70.66 83.70 35.94 31.22 24.96

OP(1 & 2) -0.003 -0.005 0.006 0.002 0.002 -0.002 -0.002 0.017 -0.005 0.007
OP(1 & 3) 0.036 0.038 0.020 0.017 0.032 0.021 0.016 -0.002 -0.006 0.002
OP(2 & 3) -0.001 -0.003 0.004 0.000 -0.001 0.000 0.001 -0.002 0.001 0.000

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8 HOMO-7 HOMO-6
Energy(eV): -12.56 -12.53 -12.39 -12.30 -12.04 -11.95 -10.98 -10.98 -10.96 -10.93
Symmetry: A A A A A A A A A A

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FRAG# 1:	83.98	67.87	7.62	81.51	73.64	87.49	3.99	0.97	0.60	0.68
Net pop.(%)	87.16	68.98	6.12	81.80	77.21	87.88	4.53	1.17	0.55	0.77

FRAG# 2:	6.52	7.42	17.45	0.63	13.79	0.58	1.05	0.06	0.17	5.92
Net pop.(%)	9.02	8.92	16.45	0.62	17.34	0.48	1.19	0.10	0.27	5.82

FRAG# 3:	9.50	24.71	74.93	17.86	12.57	11.93	94.96	98.97	99.23	93.40
Net pop.(%)	10.35	25.18	73.84	18.15	13.44	12.35	95.29	99.13	99.22	93.20

OP(1 & 2)	-0.048	-0.021	0.014	0.000	-0.063	0.001	-0.003	-0.001	0.000	-0.002
OP(1 & 3)	-0.015	-0.001	0.016	-0.006	-0.009	-0.009	-0.007	-0.003	0.002	0.000
OP(2 & 3)	-0.002	-0.009	0.006	0.000	-0.008	0.001	0.001	0.000	-0.001	0.004

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1 LUMO+2 LUMO+3
Energy(eV): -10.91 -10.85 -10.72 -10.70 -10.58 -10.41 -7.65 -5.29 -5.16 -5.09
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.70	10.31	8.48	14.22	16.28	40.71	51.86	11.55	15.25	17.35
Net pop.(%)	0.71	10.92	9.93	16.05	19.91	46.88	64.67	8.84	20.39	20.23

FRAG# 2:	51.29	0.20	2.67	2.21	28.99	8.48	28.00	69.52	0.05	0.64
Net pop.(%)	51.52	0.70	2.86	3.23	29.97	11.59	37.22	65.36	0.90	3.20

FRAG# 3:	48.01	89.49	88.85	83.57	54.73	50.82	20.14	18.93	84.70	82.01
Net pop.(%)	48.07	89.90	90.15	84.78	56.87	54.77	27.22	17.46	88.68	82.63

OP(1 & 2)	-0.002	-0.007	-0.003	-0.016	-0.025	-0.053	-0.149	0.054	-0.020	-0.048
OP(1 & 3)	0.002	-0.005	-0.026	-0.020	-0.048	-0.070	-0.107	0.000	-0.083	-0.009
OP(2 & 3)	-0.003	-0.003	0.000	-0.004	0.005	-0.009	-0.035	0.029	0.003	-0.003

Alpha MO: 31 32 33 34 35 36 37 38 39 40
Energy(eV): -281.47 -281.46 -281.43 -281.35 -281.29 -281.20 -281.15 -281.11 -281.01 -281.00
Symmetry: A A A A A A A A A A

FRAG# 1: -0.01 -0.01 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 100.00 100.00 100.00 100.00 100.01 100.00 100.01 100.00
Net pop.(%) 100.02 100.03 100.01 100.02 100.01 100.01 100.02 100.01 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.73 -280.58 -280.44 -280.42 -280.22 -280.19 -280.17 -279.96 -279.77 -279.64
Symmetry: A A A A A A A A A A

FRAG# 1: -0.01 -0.01 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00
p orbitals: 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 100.00 99.99 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.01 100.02 99.99 99.99 100.00 99.99 100.00 100.00 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -279.34 -279.33 -279.30 -279.29 -279.28 -279.19 -279.19 -279.17 -279.10 -279.03
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00 0.01 0.00
FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 99.99 99.99 100.00 100.00 100.00 100.00 99.99 100.00
Net pop.(%) 99.99 100.00 99.99 99.99 100.00 100.00 100.00 100.00 99.99 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -278.94 -278.83 -123.78 -123.68 -82.96 -82.93 -82.88 -82.81 -81.98 -81.86
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 100.31 100.22 99.86 99.94 99.84 99.92 99.90 99.84
Net pop.(%) 0.00 0.00 100.63 100.46 99.74 99.88 99.71 99.85 99.84 99.73

FRAG# 2: 0.00 0.00 -0.09 -0.07 0.05 0.08 0.07 0.05 0.01 0.02

FRAG# 3: 100.00 100.00 -0.22 -0.15 0.09 -0.02 0.08 0.03 0.09 0.14
Net pop.(%) 100.00 100.00 0.01 0.01 0.02 0.01 0.02 0.01 0.02 0.04

OP(1 & 2) 0.000 0.000 -0.002 -0.001 0.001 0.001 0.001 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 -0.005 -0.003 0.001 0.000 0.001 0.000 0.001 0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -33.92 -33.84 -32.92 -32.83 -31.69 -31.51 -30.28 -28.98 -28.90 -28.86
Symmetry: A A A A A A A A A A

FRAG# 1: -0.84 -0.89 -0.26 -0.35 -0.91 -0.70 4.44 -0.16 3.11 -0.28
Net pop.(%) 0.06 0.05 0.02 0.04 0.21 0.16 2.45 0.13 1.67 0.12

FRAG# 2: 0.01 0.01 0.00 0.00 0.73 0.67 92.13 2.23 90.48 3.05
Net pop.(%) 0.01 0.01 0.00 0.00 0.58 0.54 88.81 2.21 88.33 3.04

FRAG# 3: 100.83 100.88 100.26 100.35 100.18 100.04 3.42 97.93 6.41 97.23
Net pop.(%) 101.73 101.82 100.54 100.73 101.13 100.78 3.40 98.34 5.68 97.71

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.053 0.001 0.029 0.001
OP(1 & 3) -0.018 -0.019 -0.006 -0.008 -0.022 -0.017 -0.013 -0.007 0.000 -0.009
OP(2 & 3) 0.000 0.000 0.000 0.000 0.003 0.002 0.013 -0.001 0.014 -0.001

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -27.45 -27.33 -27.27 -27.13 -26.74 -26.60 -26.46 -26.44 -25.97 -25.90
Symmetry: A A A A A A A A A A

FRAG# 1: 0.13 -0.08 0.30 0.22 0.01 0.11 0.11 0.05 -0.17 0.02
Net pop.(%) 0.05 0.04 0.13 0.11 0.07 0.08 0.10 0.07 0.03 0.02

FRAG# 2: 0.07 0.15 0.14 0.12 0.13 0.11 0.05 0.10 0.07 0.01
Net pop.(%) 0.07 0.17 0.18 0.15 0.15 0.12 0.08 0.13 0.09 0.01

FRAG# 3: 99.81 99.93 99.56 99.66 99.86 99.78 99.83 99.85 100.10 99.97
Net pop.(%) 99.74 100.07 99.42 99.59 99.94 99.75 99.82 99.87 100.33 99.96

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.002 -0.002 0.003 0.002 -0.001 0.001 0.000 0.000 -0.004 0.000
OP(2 & 3) 0.000 0.000 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -25.83 -25.74 -25.38 -25.28 -23.82 -23.69 -22.91 -22.77 -22.73 -22.67
Symmetry: A A A A A A A A A A

FRAG# 1: -0.02 0.07 0.04 0.04 -0.02 0.00 0.75 0.77 -0.19 0.11
Net pop.(%) 0.03 0.01 0.02 0.02 0.04 0.03 0.29 0.26 0.02 0.02

FRAG# 2: 0.06 0.01 0.01 0.02 0.01 0.01 0.17 0.20 0.05 0.02
Net pop.(%) 0.08 0.01 0.01 0.02 0.01 0.01 0.14 0.15 0.02 0.01

FRAG# 3: 99.96 99.92 99.95 99.93 100.01 100.00 99.08 99.03 100.15 99.87
Net pop.(%) 100.02 99.86 99.93 99.90 100.07 100.04 98.60 98.49 100.34 99.77

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 0.001 0.000 0.001 -0.001 -0.001 0.009 0.010 -0.004 0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.001 0.001 0.001 0.000

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -22.64 -22.60 -22.55 -22.51 -22.40 -22.29 -22.24 -22.16 -21.53 -21.45
Symmetry: A A A A A A A A A A

FRAG# 1: -0.04 0.00 0.07 0.06 0.00 0.32 0.03 0.33 0.30 0.25
Net pop.(%) 0.02 0.03 0.02 0.02 0.01 0.26 0.01 0.25 0.12 0.09

FRAG# 2: 0.15 0.09 0.12 0.01 0.04 0.06 0.00 0.05 0.07 0.07
Net pop.(%) 0.16 0.06 0.13 0.01 0.03 0.07 0.00 0.05 0.08 0.07

FRAG# 3: 99.89 99.91 99.81 99.93 99.96 99.61 99.96 99.62 99.63 99.69
Net pop.(%) 99.95 99.91 99.76 99.88 99.96 99.57 99.94 99.56 99.43 99.51

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 -0.001 0.001 0.001 0.000 0.001 0.000 0.001 0.004 0.003
OP(2 & 3) 0.000 0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 111 112 113 114 115 116 117 118 119 120
Energy(eV): -21.26 -21.14 -20.82 -20.73 -20.55 -20.42 -19.99 -19.91 -19.66 -19.49
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.08 0.09 0.06 0.17 1.26 0.98 2.65 2.19 1.77 1.24
Net pop.(%) 0.06 0.06 0.05 0.08 0.63 0.54 1.66 1.36 0.85 0.60

FRAG# 2: 0.02 0.01 0.01 0.05 0.38 0.37 0.18 0.17 0.36 0.25
Net pop.(%) 0.01 0.01 0.01 0.04 0.40 0.40 0.10 0.08 0.24 0.24

FRAG# 3: 99.90 99.90 99.93 99.78 98.36 98.65 97.17 97.64 97.86 98.50
Net pop.(%) 99.88 99.87 99.92 99.70 97.76 98.23 96.08 96.71 96.92 97.78

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.001 -0.001
OP(1 & 3) 0.000 0.001 0.000 0.002 0.012 0.009 0.020 0.017 0.018 0.014
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.002 0.002 0.001 0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
Energy(eV): -19.32 -19.21 -18.88 -18.79 -18.58 -18.42 -18.42 -18.26 -17.81 -17.64
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.35 0.36 0.39 0.28 0.29 1.11 0.44 1.22 4.87 2.21
Net pop.(%) 0.16 0.18 0.32 0.25 0.20 0.82 0.33 0.89 4.21 1.65

FRAG# 2: 0.02 0.02 0.20 0.20 0.11 0.35 0.22 0.36 5.14 2.37
Net pop.(%) 0.01 0.01 0.15 0.17 0.09 0.24 0.17 0.25 3.81 1.70

FRAG# 3: 99.62 99.62 99.41 99.51 99.60 98.54 99.34 98.41 89.98 95.42
Net pop.(%) 99.42 99.43 99.31 99.43 99.46 98.30 99.22 98.12 89.13 94.64

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.002 0.000 0.002 0.011 0.005
OP(1 & 3) 0.004 0.004 0.001 0.001 0.002 0.004 0.002 0.005 0.002 0.007
OP(2 & 3) 0.000 0.000 0.001 0.001 0.001 0.001 0.001 0.001 0.015 0.009

Alpha MO: 131 132 133 134 135 136 137 138 139 140
Energy(eV): -17.45 -17.41 -17.23 -17.19 -17.15 -17.07 -17.02 -16.93 -16.85 -16.76
Symmetry: A A A A A A A A A A

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FRAG# 1: 1.55 5.26 6.74 8.20 10.52 3.50 7.24 12.99 12.24 8.78
Net pop.(%) 0.99 3.59 5.25 5.72 8.97 2.78 6.10 11.25 10.66 7.28

FRAG# 2: 0.57 4.34 3.31 4.89 2.79 0.88 2.25 9.60 5.28 2.64
Net pop.(%) 0.54 3.15 2.50 3.65 2.36 0.76 1.88 7.93 4.55 2.24

FRAG# 3: 97.88 90.40 89.95 86.91 86.69 95.61 90.50 77.41 82.48 88.57
Net pop.(%) 97.38 89.18 88.85 85.12 85.82 95.07 89.84 76.33 81.80 87.13

OP(1 & 2) 0.001 0.016 0.012 0.019 0.011 0.003 0.008 0.023 0.016 0.005
OP(1 & 3) 0.010 0.017 0.018 0.030 0.020 0.011 0.014 0.011 0.015 0.025
OP(2 & 3) 0.000 0.007 0.004 0.005 -0.003 -0.001 -0.001 0.010 -0.002 0.003

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-77 HOMO-76 HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68
Energy(eV): -16.68 -16.65 -16.59 -16.52 -16.46 -16.42 -16.33 -16.27 -16.25 -16.08
Symmetry: A A A A A A A A A A

FRAG# 1: 4.36 10.44 5.67 4.70 5.28 6.05 17.87 4.75 3.91 7.80
Net pop.(%) 3.87 8.70 4.50 4.15 4.28 5.32 16.34 3.99 3.12 6.68

FRAG# 2: 5.47 7.07 7.68 5.17 1.94 4.36 14.69 3.13 2.80 5.34
Net pop.(%) 4.39 6.13 6.18 4.65 1.78 3.75 12.95 2.84 2.08 4.39

FRAG# 3: 90.17 82.49 86.65 90.12 92.77 89.58 67.44 92.13 93.29 86.86
Net pop.(%) 89.56 81.37 85.25 90.05 91.97 89.46 68.31 91.99 92.63 86.13

OP(1 & 2) 0.010 0.016 0.013 0.010 0.004 0.012 0.041 0.009 0.008 0.013
OP(1 & 3) 0.000 0.019 0.011 0.001 0.016 0.002 -0.011 0.006 0.007 0.009
OP(2 & 3) 0.012 0.003 0.017 0.000 0.000 0.000 -0.007 -0.003 0.006 0.006

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58
Energy(eV): -16.05 -15.99 -15.97 -15.91 -15.89 -15.80 -15.77 -15.70 -15.67 -15.55
Symmetry: A A A A A A A A A A

FRAG# 1: 3.44 4.75 4.13 6.74 3.77 2.09 7.58 2.95 2.52 9.26
Net pop.(%) 3.05 4.36 3.63 5.73 3.19 1.80 6.70 2.66 2.32 9.09

FRAG# 2: 2.25 2.42 1.35 3.16 1.31 1.48 4.68 1.97 1.77 1.79
Net pop.(%) 2.03 2.16 1.15 2.62 1.20 1.30 3.79 1.61 1.38 1.99

FRAG# 3: 94.31 92.84 94.52 90.10 94.92 96.43 87.74 95.08 95.72 88.96
Net pop.(%) 94.25 92.84 94.26 89.40 94.56 96.38 87.28 94.84 95.52 89.63

OP(1 & 2) 0.006 0.006 0.004 0.008 0.003 0.004 0.013 0.004 0.004 0.006
OP(1 & 3) 0.002 0.001 0.006 0.012 0.008 0.001 0.004 0.002 0.000 -0.003
OP(2 & 3) -0.001 -0.001 0.000 0.002 -0.001 0.000 0.005 0.003 0.004 -0.010

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48
Energy(eV): -15.51 -15.43 -15.35 -15.30 -15.24 -15.17 -15.14 -15.12 -14.85 -14.75
Symmetry: A A A A A A A A A A

FRAG# 1: 7.87 5.14 21.80 17.28 14.16 3.60 9.12 26.34 40.86 53.02
Net pop.(%) 7.10 4.86 19.63 16.12 12.67 3.27 8.63 25.51 39.87 52.94

FRAG# 2: 4.23 2.13 9.45 7.03 4.39 1.20 3.50 8.47 8.68 3.92
Net pop.(%) 3.57 1.85 8.36 6.01 3.83 1.05 3.34 8.21 7.33 3.50

FRAG# 3: 87.90 92.73 68.76 75.68 81.46 95.20 87.37 65.19 50.46 43.06
Net pop.(%) 87.72 92.88 68.06 75.54 80.45 95.05 87.32 67.24 50.06 43.28

OP(1 & 2) 0.013 0.007 0.026 0.020 0.010 0.003 0.006 0.031 0.019 0.007
OP(1 & 3) 0.003 -0.002 0.018 0.003 0.019 0.003 0.004 -0.015 0.001 -0.006
OP(2 & 3) 0.001 -0.002 -0.004 0.000 0.001 0.000 -0.003 -0.026 0.008 0.001

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38
Energy(eV): -14.68 -14.66 -14.55 -14.43 -14.36 -14.31 -14.27 -14.24 -14.24 -14.22
Symmetry: A A A A A A A A A A

FRAG# 1: 26.75 9.57 14.56 21.97 71.86 25.46 56.92 2.68 7.40 21.89
Net pop.(%) 25.95 9.39 14.26 20.84 70.55 25.28 56.48 2.47 6.82 20.88

FRAG# 2: 3.92 1.55 1.81 7.17 2.01 2.59 2.37 0.10 1.44 4.89
Net pop.(%) 3.41 1.50 1.62 6.64 1.93 2.54 2.11 0.11 1.48 5.58

FRAG# 3: 69.34 88.88 83.63 70.86 26.14 71.95 40.71 97.22 91.16 73.22
Net pop.(%) 69.75 88.75 83.72 69.48 25.02 71.80 40.36 96.99 90.67 72.99

OP(1 & 2) 0.017 0.001 0.006 0.003 0.003 0.001 0.003 0.000 0.001 0.001
OP(1 & 3) -0.001 0.003 0.000 0.020 0.023 0.003 0.005 0.005 0.011 0.019
OP(2 & 3) -0.007 0.000 -0.002 0.008 -0.001 0.000 0.002 0.000 -0.001 -0.015

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28
Energy(eV): -14.16 -14.11 -14.00 -13.98 -13.89 -13.81 -13.76 -13.62 -13.54 -13.45
Symmetry: A A A A A A A A A A

FRAG# 1: 9.94 28.09 4.29 4.43 12.16 10.36 12.26 6.87 4.27 4.52
Net pop.(%) 9.45 26.80 3.80 4.28 11.51 10.03 10.98 6.76 4.09 4.58

FRAG# 2: 3.07 1.28 1.39 0.71 5.44 1.91 11.95 1.96 2.73 1.51
Net pop.(%) 3.44 1.14 1.16 0.58 5.22 1.86 11.55 1.90 2.59 1.58

FRAG# 3: 86.99 70.63 94.32 94.87 82.41 87.74 75.79 91.17 92.99 93.97
Net pop.(%) 86.87 69.26 93.54 94.53 81.70 87.40 75.62 91.16 92.80 93.97

OP(1 & 2) 0.000 0.001 -0.001 -0.001 0.002 0.000 0.015 0.002 0.001 -0.001
OP(1 & 3) 0.010 0.025 0.010 0.004 0.011 0.006 0.010 0.001 0.002 0.000
OP(2 & 3) -0.007 0.002 0.005 0.003 0.003 0.001 -0.007 0.000 0.002 0.000

Alpha MO: 191 192 193 194 195 196 197 198 199 200
HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18
Energy(eV): -13.37 -13.33 -13.29 -13.23 -13.21 -13.16 -13.09 -13.02 -12.99 -12.88
Symmetry: A A A A A A A A A A

FRAG# 1: 6.19 7.52 5.67 8.45 1.61 20.54 8.31 7.12 1.51 5.71
Net pop.(%) 6.57 7.74 5.74 8.47 1.63 21.33 8.42 7.36 1.52 6.01

FRAG# 2: 2.43 2.46 5.22 7.47 1.22 12.56 5.40 4.83 0.61 2.44
Net pop.(%) 2.52 2.57 5.41 7.83 1.33 12.99 5.54 4.82 0.61 2.38

FRAG# 3: 91.37 90.01 89.12 84.08 97.17 66.91 86.29 88.06 97.88 91.85
Net pop.(%) 92.33 90.38 89.60 85.58 97.41 66.84 86.28 87.86 97.80 92.26

OP(1 & 2) 0.005 0.001 0.002 0.011 0.001 -0.013 -0.003 -0.004 -0.001 0.002
OP(1 & 3) -0.012 -0.005 -0.004 -0.012 -0.001 -0.003 0.000 -0.001 0.001 -0.008
OP(2 & 3) -0.007 -0.003 -0.006 -0.018 -0.003 0.004 0.000 0.005 0.001 -0.001

Alpha MO: 201 202 203 204 205 206 207 208 209 210
HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8
Energy(eV): -12.85 -12.79 -12.71 -12.67 -12.56 -12.50 -12.41 -12.31 -12.02 -11.96
Symmetry: A A A A A A A A A A

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FRAG# 1:	2.94	6.75	3.69	3.83	16.33	15.70	14.29	18.63	5.60	11.95
Net pop.(%)	3.16	6.96	3.88	3.86	17.40	16.23	14.78	19.14	6.43	13.28

FRAG# 2:	1.16	4.90	2.89	3.79	19.28	16.16	17.41	9.06	2.07	2.64
Net pop.(%)	1.50	5.14	2.91	3.98	21.07	17.86	18.86	9.75	2.15	2.59

FRAG# 3:	95.90	88.35	93.43	92.38	64.39	68.14	68.30	72.30	92.33	85.42
Net pop.(%)	96.27	88.65	93.82	92.61	66.50	70.40	70.25	73.26	93.25	86.91

OP(1 & 2)	-0.002	-0.002	0.002	0.000	-0.008	0.000	0.000	-0.002	0.000	0.002
OP(1 & 3)	-0.003	-0.003	-0.006	-0.001	-0.014	-0.011	-0.010	-0.008	-0.017	-0.029
OP(2 & 3)	-0.005	-0.003	-0.002	-0.004	-0.028	-0.034	-0.029	-0.011	-0.002	-0.001

Alpha MO: 211 212 213 214 215 216 217 218 219 220
HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1
Energy(eV): -11.88 -11.84 -11.75 -11.57 -11.41 -11.30 -11.29 -11.15 -9.18 -8.91
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.39	3.12	25.52	17.45	0.38	0.82	0.16	0.03	31.98	42.44
Net pop.(%)	0.61	3.60	29.78	20.73	0.43	0.91	0.28	0.10	43.32	54.47

FRAG# 2:	0.66	4.42	33.73	72.32	0.18	0.44	0.19	0.12	53.84	36.13
Net pop.(%)	0.70	4.73	37.26	76.68	0.20	0.49	0.21	0.13	63.04	44.98

FRAG# 3:	98.94	92.46	40.75	10.22	99.45	98.73	99.65	99.85	14.18	21.43
Net pop.(%)	99.09	92.96	43.47	11.80	99.52	98.84	99.76	99.92	19.05	31.52

OP(1 & 2)	-0.001	-0.003	-0.051	-0.061	0.000	0.000	0.000	0.000	-0.157	-0.108
OP(1 & 3)	-0.003	-0.007	-0.034	-0.005	-0.001	-0.002	-0.002	-0.001	-0.070	-0.133
OP(2 & 3)	0.000	-0.003	-0.020	-0.027	0.000	-0.001	0.000	0.000	-0.027	-0.069

C3 O DKH

Alpha MO: 1 2 3 4 5 6 7 8 9 10
Energy(eV): -8886.6 -8886.5 -1081.6 -1081.4 -933.31 -933.30 -933.22 -933.18 -932.69 -932.58
Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 99.94 99.91 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 99.92 99.89 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 0.01 0.02 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 0.05 0.07 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 0.00 0.00 0.04 0.06 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
Energy(eV): -524.25 -524.20 -395.82 -395.71 -395.19 -395.10 -395.05 -394.87 -394.84 -394.80
Symmetry: A A A A A A A A A A

FRAG# 1: 0.03 0.02 0.00 0.00 0.00 0.00 0.01 0.01 0.01 0.01

FRAG# 2: 99.97 99.98 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 99.94 99.95 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 100.00 100.00 99.99 99.99 99.98 99.99
Net pop.(%) 0.00 0.00 100.01 100.00 100.00 99.99 99.98 99.99 99.97 99.99

OP(1 & 2) 0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
Energy(eV): -393.44 -393.34 -283.87 -283.73 -282.70 -282.54 -282.22 -282.00 -281.75 -281.68
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 -0.01 0.00 0.00 -0.02 -0.02 -0.01 -0.01 -0.01 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.01 100.00 100.00 100.02 100.02 100.01 100.01 100.01 100.01
Net pop.(%) 100.00 100.01 100.00 100.00 100.04 100.05 100.02 100.02 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
Energy(eV): -281.57 -281.56 -281.53 -281.44 -281.38 -281.30 -281.25 -281.20 -281.10 -281.09
Symmetry: A A A A A A A A A A

FRAG# 1: -0.01 -0.01 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 100.00 100.01 100.00 100.00 100.01 100.00 100.00 100.00
Net pop.(%) 100.02 100.03 100.01 100.02 100.01 100.01 100.02 100.01 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.82 -280.67 -280.53 -280.51 -280.32 -280.28 -280.26 -280.05 -279.86 -279.72
Symmetry: A A A A A A A A A A

FRAG# 1: -0.01 -0.01 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 99.99 99.99 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.01 100.02 99.99 99.99 100.00 99.99 100.00 100.00 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -279.42 -279.42 -279.38 -279.37 -279.37 -279.28 -279.28 -279.26 -279.18 -279.12
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00 0.01 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 99.99 99.99 100.00 100.00 100.00 100.00 99.99 100.00
Net pop.(%) 99.99 100.00 99.99 99.99 100.00 100.00 100.00 100.00 99.99 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -279.03 -278.92 -127.57 -127.47 -84.07 -84.04 -83.99 -83.92 -83.06 -82.95
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 100.21 100.12 99.86 99.94 99.85 99.92 99.90 99.84
Net pop.(%) 0.00 0.00 100.42 100.25 99.75 99.88 99.71 99.86 99.83 99.73

FRAG# 2: 0.00 0.00 -0.06 -0.05 0.04 0.08 0.07 0.05 0.01 0.01

FRAG# 3: 100.00 100.00 -0.15 -0.08 0.09 -0.01 0.08 0.03 0.09 0.14
Net pop.(%) 100.00 100.00 0.00 0.00 0.02 0.01 0.02 0.01 0.03 0.04

OP(1 & 2) 0.000 0.000 -0.001 -0.001 0.001 0.001 0.001 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 -0.003 -0.002 0.001 0.000 0.001 0.000 0.001 0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -33.95 -33.86 -32.94 -32.85 -31.71 -31.54 -30.33 -29.00 -28.94 -28.87
Symmetry: A A A A A A A A A A

FRAG# 1: -0.83 -0.89 -0.27 -0.36 -0.91 -0.70 4.62 -0.12 3.05 -0.31
Net pop.(%) 0.06 0.05 0.02 0.04 0.21 0.16 2.45 0.15 1.64 0.10

FRAG# 2: 0.01 0.01 0.00 0.00 0.77 0.70 91.93 3.25 90.77 1.79
Net pop.(%) 0.01 0.01 0.00 0.00 0.62 0.58 88.47 3.20 88.66 1.81

FRAG# 3: 100.82 100.87 100.27 100.36 100.14 100.00 3.45 96.86 6.18 98.51
Net pop.(%) 101.71 101.81 100.56 100.75 101.07 100.75 3.50 97.27 5.44 98.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.057 0.002 0.028 0.001
OP(1 & 3) -0.018 -0.019 -0.006 -0.008 -0.022 -0.017 -0.013 -0.007 0.000 -0.009
OP(2 & 3) 0.000 0.000 0.000 0.000 0.003 0.002 0.012 -0.001 0.014 -0.001

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -27.46 -27.34 -27.29 -27.15 -26.76 -26.61 -26.47 -26.45 -25.98 -25.91
Symmetry: A A A A A A A A A A

FRAG# 1: 0.12 -0.08 0.31 0.22 0.01 0.12 0.10 0.05 -0.18 0.02
Net pop.(%) 0.05 0.04 0.14 0.11 0.07 0.08 0.10 0.07 0.03 0.02

FRAG# 2: 0.07 0.14 0.15 0.12 0.13 0.10 0.06 0.10 0.07 0.01
Net pop.(%) 0.08 0.17 0.19 0.15 0.14 0.12 0.08 0.13 0.09 0.01

FRAG# 3: 99.81 99.94 99.55 99.65 99.86 99.78 99.84 99.85 100.11 99.97
Net pop.(%) 99.75 100.08 99.39 99.57 99.93 99.74 99.83 99.87 100.34 99.95

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.001 -0.002 0.004 0.002 -0.001 0.001 0.000 0.000 -0.004 0.000
OP(2 & 3) 0.000 0.000 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -25.84 -25.75 -25.39 -25.29 -23.83 -23.70 -22.92 -22.78 -22.73 -22.68
Symmetry: A A A A A A A A A A

FRAG# 1: -0.03 0.07 0.04 0.04 -0.01 0.00 0.76 0.79 -0.19 0.12
Net pop.(%) 0.03 0.01 0.02 0.02 0.04 0.03 0.29 0.26 0.02 0.02

FRAG# 2: 0.06 0.01 0.01 0.02 0.01 0.01 0.16 0.19 0.05 0.02
Net pop.(%) 0.08 0.01 0.01 0.02 0.01 0.01 0.13 0.15 0.02 0.01

FRAG# 3: 99.96 99.92 99.95 99.93 100.01 99.99 99.08 99.01 100.14 99.86
Net pop.(%) 100.03 99.86 99.93 99.90 100.06 100.03 98.58 98.46 100.34 99.76

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 0.001 0.000 0.001 -0.001 -0.001 0.009 0.010 -0.004 0.002
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.001 0.001 0.001 0.000

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -22.64 -22.61 -22.55 -22.51 -22.40 -22.30 -22.24 -22.17 -21.54 -21.45
Symmetry: A A A A A A A A A A

FRAG# 1: -0.05 0.00 0.07 0.06 0.00 0.34 0.03 0.33 0.30 0.26
Net pop.(%) 0.02 0.03 0.02 0.02 0.01 0.26 0.01 0.25 0.12 0.09

FRAG# 2: 0.15 0.09 0.11 0.01 0.04 0.07 0.01 0.06 0.07 0.07
Net pop.(%) 0.16 0.05 0.13 0.00 0.03 0.08 0.00 0.06 0.08 0.07

FRAG# 3: 99.90 99.91 99.82 99.92 99.96 99.60 99.96 99.61 99.62 99.68
Net pop.(%) 99.96 99.91 99.76 99.88 99.96 99.54 99.94 99.54 99.42 99.49

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 -0.001 0.001 0.001 0.000 0.001 0.000 0.002 0.004 0.004
OP(2 & 3) 0.000 0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 111 112 113 114 115 116 117 118 119 120
Energy(eV): -21.27 -21.15 -20.82 -20.73 -20.56 -20.43 -19.99 -19.92 -19.66 -19.50
Symmetry: A A A A A A A A A A

FRAG# 1: 0.10 0.10 0.07 0.18 1.40 1.05 2.60 2.16 1.85 1.29
Net pop.(%) 0.06 0.07 0.05 0.08 0.67 0.55 1.61 1.31 0.89 0.62

FRAG# 2: 0.02 0.01 0.01 0.06 0.41 0.38 0.18 0.17 0.38 0.26
Net pop.(%) 0.02 0.01 0.01 0.05 0.42 0.42 0.10 0.08 0.26 0.25

FRAG# 3: 99.88 99.89 99.92 99.76 98.20 98.57 97.22 97.68 97.78 98.45
Net pop.(%) 99.85 99.86 99.91 99.66 97.50 98.09 96.13 96.75 96.80 97.70

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.001 -0.001
OP(1 & 3) 0.001 0.001 0.000 0.002 0.014 0.010 0.020 0.017 0.018 0.014
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 -0.001 0.002 0.002 0.001 0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
Energy(eV): -19.32 -19.21 -18.88 -18.80 -18.58 -18.43 -18.42 -18.27 -17.81 -17.65
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.35	0.36	0.38	0.27	0.29	1.30	0.32	1.26	4.53	2.14
Net pop.(%)	0.16	0.18	0.30	0.24	0.19	0.93	0.25	0.90	3.91	1.58

FRAG# 2:	0.02	0.02	0.19	0.20	0.11	0.44	0.18	0.39	4.97	2.36
Net pop.(%)	0.02	0.01	0.14	0.17	0.09	0.30	0.14	0.27	3.66	1.69

FRAG# 3:	99.62	99.62	99.43	99.53	99.60	98.26	99.50	98.35	90.50	95.50
Net pop.(%)	99.42	99.43	99.34	99.46	99.47	97.95	99.41	98.03	89.69	94.73

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.002	0.011	0.005
OP(1 & 3)	0.004	0.004	0.001	0.001	0.002	0.006	0.001	0.005	0.001	0.007
OP(2 & 3)	0.000	0.000	0.001	0.001	0.001	0.001	0.001	0.001	0.015	0.009

Alpha MO: 131 132 133 134 135 136 137 138 139 140
Energy(eV): -17.45 -17.43 -17.24 -17.20 -17.15 -17.07 -17.02 -16.93 -16.84 -16.76
Symmetry: A A A A A A A A A A

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FRAG# 1:	2.48	5.65	7.50	5.81	8.36	3.16	6.22	12.46	11.24	8.27
Net pop.(%)	1.61	3.82	5.63	4.02	7.07	2.47	5.20	10.62	9.70	6.75

FRAG# 2:	1.32	4.62	4.21	3.28	1.97	0.72	1.79	8.68	4.83	2.52
Net pop.(%)	1.08	3.36	3.14	2.46	1.68	0.64	1.51	7.19	4.17	2.21

FRAG# 3:	96.19	89.73	88.30	90.91	89.67	96.11	91.98	78.86	83.93	89.20
Net pop.(%)	95.46	88.47	87.03	89.59	88.88	95.57	91.35	77.63	83.19	87.66

OP(1 & 2)	0.004	0.018	0.017	0.013	0.008	0.002	0.007	0.021	0.015	0.003
OP(1 & 3)	0.014	0.018	0.021	0.023	0.018	0.012	0.014	0.016	0.016	0.027
OP(2 & 3)	0.001	0.007	0.005	0.003	-0.002	-0.001	-0.001	0.009	-0.001	0.003

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-77 HOMO-76 HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68
Energy(eV): -16.68 -16.65 -16.59 -16.52 -16.45 -16.41 -16.32 -16.26 -16.24 -16.07
Symmetry: A A A A A A A A A A

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FRAG# 1:	3.10	12.68	6.32	4.82	5.13	5.03	18.13	6.21	3.55	7.54
Net pop.(%)	2.76	10.63	5.06	4.20	4.12	4.37	16.41	5.34	2.80	6.44

FRAG# 2:	3.94	9.86	8.45	5.29	1.83	3.69	15.25	4.65	2.68	5.26
Net pop.(%)	3.12	8.42	6.83	4.77	1.67	3.16	13.38	4.19	1.99	4.34

FRAG# 3:	92.96	77.47	85.23	89.89	93.04	91.29	66.62	89.14	93.78	87.21
Net pop.(%)	92.47	76.23	83.82	89.77	92.22	91.14	67.33	89.17	93.14	86.55

OP(1 & 2)	0.007	0.022	0.015	0.010	0.003	0.010	0.043	0.014	0.008	0.013
OP(1 & 3)	0.000	0.019	0.010	0.002	0.017	0.003	-0.009	0.004	0.007	0.008
OP(2 & 3)	0.010	0.006	0.018	0.000	0.000	0.000	-0.006	-0.004	0.006	0.005

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58
Energy(eV): -16.04 -15.98 -15.96 -15.91 -15.88 -15.79 -15.76 -15.69 -15.66 -15.53
Symmetry: A A A A A A A A A A

FRAG# 1: 3.14 4.38 4.27 6.16 3.07 1.76 6.69 2.34 2.52 8.78
Net pop.(%) 2.75 4.02 3.71 5.18 2.55 1.51 5.84 2.10 2.33 8.56

FRAG# 2: 2.26 2.44 1.45 3.05 1.20 1.27 4.38 1.77 2.06 1.82
Net pop.(%) 2.04 2.20 1.25 2.51 1.07 1.14 3.53 1.45 1.60 2.05

FRAG# 3: 94.60 93.18 94.27 90.80 95.73 96.97 88.93 95.89 95.41 89.40
Net pop.(%) 94.52 93.26 94.00 90.12 95.40 96.94 88.41 95.68 95.20 90.08

OP(1 & 2) 0.005 0.007 0.005 0.008 0.003 0.003 0.012 0.004 0.004 0.007
OP(1 & 3) 0.002 0.000 0.006 0.011 0.007 0.001 0.005 0.001 -0.001 -0.002
OP(2 & 3) -0.001 -0.002 -0.001 0.002 -0.001 -0.001 0.005 0.003 0.005 -0.011

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48
Energy(eV): -15.50 -15.42 -15.35 -15.28 -15.23 -15.16 -15.13 -15.10 -14.82 -14.70
Symmetry: A A A A A A A A A A

FRAG# 1: 7.01 4.44 18.93 15.38 14.28 3.41 9.00 26.71 32.53 41.62
Net pop.(%) 6.28 4.18 16.52 14.28 12.73 3.05 8.47 25.69 31.53 41.46

FRAG# 2: 3.97 2.04 9.87 7.34 5.50 1.38 3.40 10.14 8.15 2.72
Net pop.(%) 3.36 1.78 8.84 6.18 4.73 1.18 3.18 9.78 6.83 2.46

FRAG# 3: 89.03 93.52 71.20 77.28 80.22 95.21 87.60 63.15 59.32 55.65
Net pop.(%) 88.85 93.67 69.76 77.31 79.50 95.05 87.55 65.51 58.66 55.68

OP(1 & 2) 0.012 0.007 0.020 0.023 0.016 0.004 0.007 0.037 0.017 0.004
OP(1 & 3) 0.003 -0.002 0.028 -0.001 0.015 0.003 0.004 -0.017 0.003 -0.001
OP(2 & 3) 0.001 -0.001 0.001 0.000 0.000 0.000 -0.003 -0.030 0.010 0.001

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38
Energy(eV): -14.65 -14.64 -14.53 -14.41 -14.30 -14.29 -14.24 -14.23 -14.21 -14.19
Symmetry: A A A A A A A A A A

FRAG# 1: 20.86 26.57 22.46 18.53 16.31 53.75 2.23 6.53 27.45 64.73
Net pop.(%) 20.05 26.32 21.88 17.37 15.84 52.44 2.09 6.23 26.27 64.24

FRAG# 2: 3.51 3.19 3.36 7.57 4.71 1.87 0.22 1.41 3.91 1.26
Net pop.(%) 3.04 2.93 2.91 6.92 4.50 1.88 0.22 1.29 4.48 1.15

FRAG# 3: 75.63 70.24 74.19 73.91 78.98 44.38 97.55 92.07 68.64 34.02
Net pop.(%) 75.76 70.50 74.50 72.54 78.76 43.15 97.40 91.76 68.11 33.68

OP(1 & 2) 0.014 0.008 0.013 0.004 0.005 0.001 0.000 0.001 0.001 0.002
OP(1 & 3) 0.002 -0.003 -0.002 0.019 0.005 0.026 0.003 0.005 0.023 0.007
OP(2 & 3) -0.005 -0.002 -0.005 0.009 0.000 -0.001 0.000 0.001 -0.012 0.000

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28
Energy(eV): -14.15 -14.08 -13.99 -13.97 -13.88 -13.80 -13.75 -13.61 -13.53 -13.44
Symmetry: A A A A A A A A A A

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FRAG# 1:	16.73	31.87	3.46	7.16	13.77	13.62	13.86	7.42	4.58	4.93
Net pop.(%)	15.94	30.74	3.04	6.91	13.14	13.25	12.54	7.28	4.40	4.98

FRAG# 2:	4.90	0.92	0.98	0.90	5.05	1.82	11.08	1.71	2.48	1.18
Net pop.(%)	5.46	0.90	0.82	0.75	4.86	1.78	10.66	1.65	2.34	1.23

FRAG# 3:	78.37	67.21	95.56	91.94	81.19	84.55	75.06	90.87	92.94	93.89
Net pop.(%)	78.18	66.06	94.96	91.47	80.50	84.16	74.81	90.82	92.75	93.93

OP(1 & 2)	0.000	0.000	0.000	-0.001	0.001	0.000	0.015	0.002	0.001	-0.001
OP(1 & 3)	0.016	0.023	0.009	0.006	0.011	0.007	0.011	0.001	0.002	0.000
OP(2 & 3)	-0.012	0.000	0.003	0.004	0.003	0.001	-0.007	0.000	0.002	0.000

Alpha MO: 191 192 193 194 195 196 197 198 199 200
HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18
Energy(eV): -13.36 -13.32 -13.29 -13.22 -13.20 -13.14 -13.08 -13.01 -12.99 -12.87
Symmetry: A A A A A A A A A A

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FRAG# 1:	6.99	8.35	5.91	9.46	1.63	22.35	8.24	7.18	1.61	5.76
Net pop.(%)	7.37	8.57	5.98	9.51	1.63	23.21	8.34	7.39	1.62	6.04

FRAG# 2:	2.60	2.30	4.42	6.89	0.96	11.90	4.94	4.60	0.65	2.22
Net pop.(%)	2.68	2.35	4.59	7.22	1.04	12.29	5.08	4.55	0.64	2.16

FRAG# 3:	90.41	89.35	89.66	83.65	97.41	65.75	86.82	88.22	97.74	92.02
Net pop.(%)	91.41	89.76	90.10	85.17	97.57	65.69	86.81	88.00	97.65	92.42

OP(1 & 2)	0.005	0.001	0.002	0.011	0.001	-0.013	-0.003	-0.004	-0.001	0.002
OP(1 & 3)	-0.013	-0.006	-0.003	-0.012	-0.001	-0.004	0.000	0.000	0.001	-0.008
OP(2 & 3)	-0.007	-0.002	-0.005	-0.018	-0.002	0.005	0.000	0.005	0.001	-0.001

Alpha MO: 201 202 203 204 205 206 207 208 209 210
HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8
Energy(eV): -12.84 -12.79 -12.71 -12.66 -12.54 -12.48 -12.39 -12.29 -12.02 -11.95
Symmetry: A A A A A A A A A A

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FRAG# 1:	2.93	7.13	4.63	3.52	16.92	16.14	14.58	21.32	6.45	12.82
Net pop.(%)	3.15	7.35	4.90	3.56	17.96	16.58	15.07	22.01	7.35	14.17

FRAG# 2:	1.04	4.72	3.35	2.88	19.66	16.33	17.04	9.29	1.87	2.38
Net pop.(%)	1.41	5.03	3.46	3.00	21.36	17.95	18.39	10.03	1.94	2.30

FRAG# 3:	96.02	88.14	92.02	93.60	63.43	67.54	68.38	69.39	91.68	84.80
Net pop.(%)	96.42	88.44	92.51	93.78	65.49	69.82	70.31	70.50	92.67	86.35

OP(1 & 2)	-0.002	-0.002	0.001	0.000	-0.007	0.002	0.001	-0.003	0.000	0.003
OP(1 & 3)	-0.002	-0.002	-0.006	-0.001	-0.014	-0.011	-0.011	-0.011	-0.018	-0.030
OP(2 & 3)	-0.005	-0.004	-0.003	-0.003	-0.027	-0.035	-0.028	-0.011	-0.002	-0.001

Alpha MO: 211 212 213 214 215 216 217 218 219 220
HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1
Energy(eV): -11.88 -11.84 -11.71 -11.53 -11.41 -11.30 -11.28 -11.14 -9.12 -8.83
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.32	2.36	28.45	18.46	0.40	0.94	0.17	0.03	33.11	43.22
Net pop.(%)	0.52	2.73	33.09	21.89	0.46	1.04	0.30	0.10	44.77	55.50

FRAG# 2:	0.47	2.70	36.09	71.93	0.18	0.52	0.20	0.12	52.73	35.57
Net pop.(%)	0.49	2.85	39.90	76.37	0.20	0.57	0.22	0.13	62.08	44.42

FRAG# 3:	99.21	94.94	35.46	9.61	99.42	98.55	99.63	99.85	14.17	21.21
Net pop.(%)	99.37	95.36	38.39	11.12	99.50	98.68	99.75	99.92	19.14	31.57

OP(1 & 2)	-0.001	-0.001	-0.055	-0.064	0.000	0.000	0.000	0.000	-0.160	-0.108
OP(1 & 3)	-0.003	-0.006	-0.038	-0.005	-0.001	-0.002	-0.002	-0.001	-0.073	-0.138
OP(2 & 3)	0.000	-0.002	-0.021	-0.025	0.000	-0.001	0.000	0.000	-0.027	-0.069

C3 P non-relativistic

Alpha MO: 1 2 3 4 5 6 7 8 9 10
Energy(eV): -8789.2 -8789.0 -1058.0 -1057.8 -927.00 -926.70 -926.63 -926.59 -926.34 -926.34
Symmetry: A A A A A A A A A A

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FRAG# 1: 100.00 100.00 99.93 99.96 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 99.93 99.96 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 0.06 0.03 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 0.00 0.00 0.06 0.05 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
Energy(eV): -525.05 -524.91 -395.49 -395.46 -395.42 -395.16 -394.32 -394.25 -394.16 -394.15
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.01 0.01 0.00 0.00 0.00 0.00 0.01 0.01 0.01 0.00

FRAG# 2: 99.99 99.99 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 99.98 99.99 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 100.00 100.00 99.99 99.99 99.99 100.00
Net pop.(%) 0.00 0.00 100.01 100.00 100.01 100.00 99.98 99.98 99.98 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
Energy(eV): -393.71 -393.66 -283.72 -283.68 -282.29 -282.14 -281.88 -281.73 -281.53 -281.51
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.00 0.00 0.00 0.00 -0.02 -0.02 0.00 0.01 -0.01 -0.01

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 100.02 100.02 100.00 99.99 100.01 100.00
Net pop.(%) 99.99 100.00 100.00 100.00 100.04 100.04 100.01 99.99 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
Energy(eV): -281.46 -281.27 -281.26 -281.22 -281.21 -281.18 -281.13 -281.10 -281.03 -280.98
Symmetry: A A A A A A A A A A

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FRAG# 1: 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 100.01 100.00 100.00 100.01 100.00 100.00 100.00 100.00
Net pop.(%) 100.01 100.02 100.02 100.00 100.01 100.02 100.01 100.00 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.87 -280.84 -280.37 -280.36 -280.25 -280.12 -280.11 -280.04 -280.01 -279.80
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.01 100.00 99.99 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.02 99.99 99.99 100.00 100.00 100.00 100.00 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -279.38 -279.38 -279.27 -279.22 -279.22 -279.16 -279.12 -279.11 -279.00 -279.00
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 99.99 100.00 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 99.99 99.99 100.00 100.00 100.00 100.00 100.00 99.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -278.97 -278.83 -122.63 -121.99 -82.14 -81.57 -80.98 -80.93 -80.86 -80.67
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 100.14 100.18 99.90 99.87 99.77 99.93 99.91 99.90
Net pop.(%) 0.00 0.00 100.28 100.37 99.82 99.76 99.61 99.88 99.84 99.83

FRAG# 2: 0.00 0.00 0.00 0.00 0.05 0.03 0.10 0.03 0.01 0.01

FRAG# 3: 99.99 100.00 -0.14 -0.18 0.05 0.10 0.12 0.04 0.08 0.08
Net pop.(%) 99.99 100.00 0.00 0.01 0.02 0.02 0.06 0.01 0.01 0.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 -0.003 -0.004 0.001 0.002 0.001 0.001 0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -34.17 -33.94 -33.83 -33.20 -33.01 -31.25 -31.00 -28.96 -28.88 -27.55
Symmetry: A A A A A A A A A A

FRAG# 1: -0.11 -0.88 -0.87 -0.67 -0.53 -0.83 -0.53 -0.54 -0.67 -0.18
Net pop.(%) 0.98 0.07 0.06 0.06 0.05 0.09 0.04 0.14 0.14 0.04

FRAG# 2: 97.99 1.12 0.45 0.00 0.00 0.03 0.01 0.01 0.01 0.14
Net pop.(%) 98.20 1.17 0.48 0.00 0.00 0.02 0.01 0.01 0.01 0.13

FRAG# 3: 2.11 99.76 100.42 100.67 100.53 100.80 100.52 100.53 100.66 100.04
Net pop.(%) 1.32 100.69 101.33 101.40 101.11 101.71 101.09 101.21 101.47 100.24

OP(1 & 2) -0.021 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.001 -0.018 -0.018 -0.015 -0.012 -0.018 -0.011 -0.014 -0.016 -0.004
OP(2 & 3) 0.017 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -27.41 -27.02 -26.87 -26.66 -26.63 -26.58 -26.34 -26.33 -26.16 -25.92
Symmetry: A A A A A A A A A A

FRAG# 1: -0.13 0.16 0.16 1.65 0.04 0.40 0.15 0.10 0.02 0.10
Net pop.(%) 0.03 0.06 0.04 0.61 0.09 0.15 0.08 0.08 0.08 0.05

FRAG# 2: 0.11 0.33 0.04 81.29 2.99 10.37 0.05 1.41 0.35 0.01
Net pop.(%) 0.10 0.32 0.04 79.60 2.93 10.25 0.06 1.43 0.36 0.01

FRAG# 3: 100.02 99.50 99.80 17.06 96.97 89.24 99.80 98.50 99.63 99.90
Net pop.(%) 100.17 99.39 99.67 16.48 97.05 89.13 99.73 98.49 99.68 99.85

OP(1 & 2) 0.000 0.000 0.000 0.022 0.001 0.003 0.000 0.000 0.000 0.000
OP(1 & 3) -0.003 0.002 0.002 -0.001 -0.002 0.002 0.001 0.000 -0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.012 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -25.79 -25.74 -25.44 -25.31 -23.78 -23.71 -22.71 -22.67 -22.64 -22.63
Symmetry: A A A A A A A A A A

FRAG# 1: -0.27 -0.05 0.12 0.05 0.03 0.01 0.04 -0.07 0.11 0.15
Net pop.(%) 0.03 0.02 0.02 0.03 0.06 0.05 0.12 0.02 0.08 0.09

FRAG# 2: 0.02 0.00 0.11 0.04 0.01 0.01 0.06 0.03 0.05 0.03
Net pop.(%) 0.02 0.01 0.12 0.04 0.01 0.01 0.04 0.03 0.05 0.03

FRAG# 3: 100.25 100.05 99.76 99.91 99.96 99.98 99.89 100.04 99.83 99.82
Net pop.(%) 100.55 100.13 99.69 99.88 99.98 100.03 99.95 100.13 99.79 99.77

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.006 -0.001 0.002 0.000 -0.001 -0.001 -0.002 -0.002 0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -22.55 -22.52 -22.48 -22.39 -22.32 -22.28 -22.06 -21.99 -21.51 -21.44
Symmetry: A A A A A A A A A A

FRAG# 1: 0.26 0.16 0.12 0.41 -0.05 0.02 -0.01 -0.01 0.28 0.42
Net pop.(%) 0.07 0.04 0.05 0.13 0.01 0.01 0.12 0.06 0.15 0.15

FRAG# 2: 0.04 0.07 0.00 0.04 0.04 0.03 0.02 0.00 0.01 0.03
Net pop.(%) 0.05 0.09 0.01 0.02 0.03 0.02 0.02 0.00 0.04 0.03

FRAG# 3: 99.70 99.78 99.87 99.55 100.01 99.95 99.99 100.01 99.71 99.55
Net pop.(%) 99.51 99.67 99.81 99.26 100.07 99.93 100.11 100.08 99.55 99.28

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.004 0.002 0.001 0.006 -0.001 0.000 -0.003 -0.001 0.003 0.005
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 111 112 113 114 115 116 117 118 119 120
Energy(eV): -21.33 -21.17 -20.98 -20.84 -20.38 -20.35 -19.83 -19.80 -19.72 -19.50
Symmetry: A A A A A A A A A A

FRAG# 1: 0.04 0.05 0.05 0.06 0.16 0.78 2.01 1.52 1.50 1.00
Net pop.(%) 0.03 0.05 0.03 0.04 0.30 0.38 1.14 0.66 0.78 0.48

FRAG# 2: 0.00 0.01 0.00 0.01 0.20 0.52 0.08 0.19 0.04 0.11
Net pop.(%) 0.00 0.00 0.00 0.01 0.20 0.37 0.06 0.14 0.02 0.08

FRAG# 3: 99.96 99.94 99.95 99.93 99.64 98.70 97.91 98.29 98.46 98.89
Net pop.(%) 99.95 99.93 99.93 99.91 99.77 98.26 97.03 97.45 97.72 98.33

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.001 0.000 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 -0.003 0.007 0.017 0.016 0.014 0.011
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.002 0.000 0.000 0.000 0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
Energy(eV): -19.45 -19.42 -18.74 -18.69 -18.48 -18.46 -18.24 -18.18 -17.88 -17.58
Symmetry: A A A A A A A A A A

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FRAG# 1:	1.17	1.03	0.09	0.37	0.28	0.19	0.91	0.71	14.74	0.88
Net pop.(%)	0.47	0.38	0.06	0.23	0.19	0.13	0.60	0.42	11.70	0.55

FRAG# 2:	0.16	0.12	0.05	0.15	0.18	0.17	2.10	0.93	61.91	4.29
Net pop.(%)	0.12	0.09	0.05	0.12	0.15	0.13	1.81	0.79	55.79	3.89

FRAG# 3:	98.67	98.85	99.86	99.48	99.53	99.64	97.00	98.36	23.35	94.83
Net pop.(%)	97.94	98.19	99.83	99.32	99.40	99.56	96.77	98.18	24.05	94.23

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.003	0.099	0.001
OP(1 & 3)	0.014	0.013	0.001	0.003	0.002	0.001	0.002	0.003	-0.038	0.005
OP(2 & 3)	0.001	0.000	0.000	0.000	0.001	0.001	0.002	0.000	0.024	0.007

Alpha MO: 131 132 133 134 135 136 137 138 139 140
Energy(eV): -17.47 -17.44 -17.33 -17.12 -17.04 -16.98 -16.93 -16.90 -16.73 -16.67
Symmetry: A A A A A A A A A A

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FRAG# 1:	2.12	0.90	1.23	0.39	0.92	1.96	0.89	4.91	0.61	1.32
Net pop.(%)	1.47	0.49	0.95	0.29	0.59	1.28	0.64	3.69	0.39	0.94

FRAG# 2:	5.34	1.16	3.64	0.15	1.11	3.67	0.81	44.94	0.26	1.34
Net pop.(%)	4.89	1.10	3.52	0.13	0.98	3.49	0.78	42.98	0.25	1.17

FRAG# 3:	92.54	97.94	95.13	99.46	97.97	94.38	98.31	50.15	99.13	97.34
Net pop.(%)	92.03	97.57	95.24	99.36	97.63	93.76	98.09	48.70	98.90	96.94

OP(1 & 2)	0.006	0.001	0.005	0.000	0.001	0.002	0.000	0.017	0.000	0.001
OP(1 & 3)	0.007	0.007	0.000	0.002	0.005	0.011	0.004	0.007	0.004	0.006
OP(2 & 3)	0.003	0.000	-0.003	0.000	0.001	0.001	0.000	0.022	0.000	0.002

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-77 HOMO-76 HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68
Energy(eV): -16.59 -16.58 -16.47 -16.44 -16.44 -16.35 -16.29 -16.25 -16.18 -16.12
Symmetry: A A A A A A A A A A

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FRAG# 1:	0.99	1.48	3.97	5.19	1.86	4.61	1.28	4.30	0.51	1.88
Net pop.(%)	0.69	1.15	3.00	3.77	1.17	3.41	0.88	3.10	0.27	1.18

FRAG# 2:	12.25	2.00	0.40	19.00	4.25	11.90	4.69	11.73	0.62	2.06
Net pop.(%)	11.70	1.79	0.36	17.16	3.92	11.57	4.66	11.44	0.59	2.06

FRAG# 3:	86.76	96.52	95.63	75.81	93.88	83.49	94.03	83.97	98.87	96.05
Net pop.(%)	86.28	96.14	94.73	74.53	93.18	82.90	93.98	83.45	98.63	95.59

OP(1 & 2)	0.004	0.002	0.001	0.020	0.003	0.010	0.004	0.010	0.000	0.002
OP(1 & 3)	0.002	0.005	0.018	0.009	0.011	0.015	0.004	0.014	0.004	0.012
OP(2 & 3)	0.007	0.003	0.000	0.017	0.003	-0.003	-0.003	-0.004	0.000	-0.002

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58
Energy(eV): -16.04 -15.96 -15.94 -15.88 -15.82 -15.81 -15.78 -15.69 -15.66 -15.61
Symmetry: A A A A A A A A A A

FRAG# 1: 4.13 0.77 1.30 2.30 25.33 2.38 1.68 0.57 2.84 1.27
Net pop.(%) 3.37 0.64 0.99 1.87 22.35 1.98 1.33 0.45 2.40 1.00

FRAG# 2: 8.73 0.49 2.46 5.10 6.76 5.02 2.90 0.72 2.11 0.97
Net pop.(%) 8.30 0.47 2.37 4.95 5.96 4.89 2.99 0.69 2.13 1.09

FRAG# 3: 87.15 98.74 96.23 92.59 67.91 92.61 95.42 98.71 95.05 97.76
Net pop.(%) 87.01 98.67 96.00 92.61 65.81 92.68 95.40 98.70 94.86 97.65

OP(1 & 2) 0.010 0.001 0.002 0.006 0.017 0.006 0.002 0.001 0.002 0.000
OP(1 & 3) 0.005 0.002 0.005 0.003 0.043 0.002 0.005 0.001 0.006 0.005
OP(2 & 3) -0.002 0.000 0.000 -0.003 -0.001 -0.003 -0.004 -0.001 -0.003 -0.003

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48
Energy(eV): -15.49 -15.47 -15.37 -15.22 -15.13 -15.11 -15.04 -14.92 -14.78 -14.65
Symmetry: A A A A A A A A A A

FRAG# 1: 1.31 4.04 8.43 4.64 3.31 6.90 1.36 22.52 22.02 0.77
Net pop.(%) 1.00 3.42 7.55 3.57 2.74 4.83 1.02 17.67 17.78 0.62

FRAG# 2: 0.77 5.87 3.63 2.91 1.62 5.78 0.12 3.65 1.91 0.23
Net pop.(%) 0.74 6.33 4.02 3.51 1.71 6.51 0.19 3.18 1.86 0.18

FRAG# 3: 97.92 90.09 87.94 92.45 95.07 87.33 98.52 73.83 76.07 99.01
Net pop.(%) 97.71 90.36 87.65 92.00 94.84 85.75 98.15 69.81 71.94 98.83

OP(1 & 2) 0.001 0.004 0.002 0.000 0.002 -0.002 -0.001 0.013 0.002 0.000
OP(1 & 3) 0.005 0.008 0.016 0.021 0.009 0.044 0.008 0.084 0.083 0.003
OP(2 & 3) -0.001 -0.014 -0.010 -0.012 -0.004 -0.012 0.000 -0.004 -0.001 0.001

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38
Energy(eV): -14.58 -14.48 -14.40 -14.30 -14.21 -14.20 -14.10 -13.98 -13.95 -13.93
Symmetry: A A A A A A A A A A

FRAG# 1: 0.89 4.65 28.32 0.78 0.81 0.75 0.86 9.81 14.39 3.70
Net pop.(%) 0.75 4.08 25.54 0.60 0.73 0.58 0.70 8.68 12.87 3.36

FRAG# 2: 0.55 0.65 3.94 0.85 0.48 0.13 0.08 6.15 11.25 0.80
Net pop.(%) 0.60 0.64 3.61 0.76 0.42 0.13 0.09 5.25 9.72 0.74

FRAG# 3: 98.56 94.70 67.75 98.38 98.71 99.12 99.06 84.03 74.36 95.50
Net pop.(%) 98.54 94.28 65.09 98.19 98.68 98.96 98.92 83.27 73.77 95.31

OP(1 & 2) 0.001 0.002 0.004 0.001 0.001 0.000 0.000 0.013 0.024 0.002
OP(1 & 3) 0.002 0.010 0.051 0.003 0.001 0.003 0.003 0.010 0.006 0.005
OP(2 & 3) -0.002 -0.001 0.002 0.001 0.000 0.000 0.000 0.005 0.006 -0.001

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28
Energy(eV): -13.91 -13.82 -13.75 -13.64 -13.58 -13.49 -13.41 -13.38 -13.32 -13.27
Symmetry: A A A A A A A A A A

FRAG# 1: 4.94 13.68 18.79 9.98 37.17 61.69 9.86 10.60 31.79 28.08
Net pop.(%) 4.28 12.21 16.54 9.54 36.58 60.85 9.66 10.21 31.26 27.37

FRAG# 2: 4.82 1.55 1.69 1.04 1.59 2.41 1.36 1.15 1.11 2.34
Net pop.(%) 4.13 1.34 1.59 0.97 1.72 2.68 1.58 1.09 1.30 2.41

FRAG# 3: 90.24 84.78 79.52 88.98 61.24 35.90 88.78 88.24 67.11 69.58
Net pop.(%) 89.92 83.29 77.24 88.54 60.49 34.93 88.60 87.93 66.43 68.78

OP(1 & 2) 0.010 0.002 0.001 0.001 -0.003 -0.004 -0.002 0.001 -0.003 -0.002
OP(1 & 3) 0.003 0.027 0.044 0.008 0.015 0.021 0.006 0.006 0.014 0.016
OP(2 & 3) 0.003 0.002 0.001 0.001 0.000 -0.001 -0.002 0.000 0.000 0.000

Alpha MO: 191 192 193 194 195 196 197 198 199 200
HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18
Energy(eV): -13.23 -13.20 -13.18 -13.12 -13.06 -13.03 -12.96 -12.95 -12.86 -12.83
Symmetry: A A A A A A A A A A

FRAG# 1: 20.50 12.63 8.32 35.22 4.59 23.91 22.25 14.27 10.48 22.17
Net pop.(%) 20.60 12.69 8.34 36.08 4.53 24.63 22.43 14.24 10.60 22.63

FRAG# 2: 1.29 0.85 0.90 2.90 0.15 1.42 1.65 0.60 0.26 0.48
Net pop.(%) 1.70 0.94 1.11 3.67 0.20 2.09 2.14 1.03 0.35 0.60

FRAG# 3: 78.21 86.52 90.78 61.88 95.26 74.67 76.10 85.13 89.26 77.36
Net pop.(%) 77.94 86.42 90.60 62.01 95.16 75.04 76.52 85.02 89.38 77.87

OP(1 & 2) -0.008 -0.003 -0.004 -0.015 -0.001 -0.010 -0.002 -0.005 -0.001 -0.001
OP(1 & 3) 0.006 0.001 0.004 -0.002 0.002 -0.004 -0.001 0.006 -0.002 -0.008
OP(2 & 3) 0.000 0.001 0.000 0.000 0.000 -0.003 -0.007 -0.004 -0.001 -0.002

Alpha MO: 201 202 203 204 205 206 207 208 209 210
HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8
Energy(eV): -12.74 -12.72 -12.62 -12.56 -12.52 -12.44 -12.05 -11.89 -11.84 -11.80
Symmetry: A A A A A A A A A A

FRAG# 1: 28.46 48.87 4.85 6.52 20.41 29.34 27.19 23.49 9.12 20.94
Net pop.(%) 28.91 49.78 4.98 6.50 21.01 30.16 28.27 25.08 9.92 23.05

FRAG# 2: 1.46 3.75 0.70 1.28 3.47 8.38 1.19 7.99 1.54 4.66
Net pop.(%) 1.60 4.31 0.95 1.93 3.81 9.04 1.23 8.35 1.84 5.39

FRAG# 3: 70.08 47.39 94.45 92.20 76.12 62.29 71.63 68.52 89.34 74.40
Net pop.(%) 70.42 47.95 94.55 92.55 76.53 63.17 72.69 69.68 89.92 75.88

OP(1 & 2) -0.002 -0.009 -0.003 -0.003 -0.005 -0.006 -0.001 -0.008 -0.005 -0.013
OP(1 & 3) -0.006 -0.009 0.000 0.003 -0.007 -0.010 -0.021 -0.024 -0.011 -0.029
OP(2 & 3) 0.000 -0.002 -0.002 -0.010 -0.001 -0.007 0.000 0.001 -0.001 -0.001

Alpha MO: 211 212 213 214 215 216 217 218 219 220
HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1
Energy(eV): -11.79 -11.67 -11.51 -11.48 -11.43 -11.30 -11.26 -10.88 -8.37 -7.05
Symmetry: A A A A A A A A A A

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FRAG# 1:	4.57	13.35	21.93	0.31	22.58	2.38	50.09	20.18	53.10	1.25
Net pop.(%)	5.26	14.68	24.38	0.41	25.79	2.73	55.59	24.78	64.11	2.35

FRAG# 2:	1.14	12.76	1.26	0.03	8.27	0.81	3.82	68.41	33.65	0.08
Net pop.(%)	1.13	12.31	1.51	0.03	8.48	0.82	5.12	72.03	41.05	0.16

FRAG# 3:	94.28	73.89	76.80	99.66	69.16	96.81	46.08	11.41	13.25	98.67
Net pop.(%)	95.01	75.93	79.01	99.76	72.03	97.12	50.72	14.00	18.38	99.67

OP(1 & 2)	0.000	0.012	-0.005	0.000	-0.005	-0.001	-0.022	-0.056	-0.133	-0.002
OP(1 & 3)	-0.014	-0.038	-0.044	-0.002	-0.059	-0.006	-0.088	-0.036	-0.087	-0.020
OP(2 & 3)	0.000	-0.003	0.000	0.000	0.001	0.000	-0.004	-0.016	-0.015	0.000

C3 P DKH

Alpha MO: 1 2 3 4 5 6 7 8 9 10
Energy(eV): -8885.2 -8885.1 -1079.9 -1079.7 -931.79 -931.49 -931.41 -931.38 -931.13 -931.13
Symmetry: A A A A A A A A A A

FRAG# 1: 100.00 100.00 99.93 99.95 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 99.93 99.96 100.00 100.00 100.00 100.00 100.00 100.00

FRAG# 2: 0.00 0.00 0.01 0.01 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 0.06 0.04 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 0.00 0.00 0.07 0.05 0.00 0.00 0.00 0.00 0.00 0.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 11 12 13 14 15 16 17 18 19 20
Energy(eV): -525.34 -525.20 -395.68 -395.65 -395.62 -395.35 -394.54 -394.47 -394.37 -394.36
Symmetry: A A A A A A A A A A

FRAG# 1: 0.01 0.01 0.00 0.00 0.00 0.00 0.01 0.01 0.01 0.00

FRAG# 2: 99.99 100.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
Net pop.(%) 99.98 99.99 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 0.00 0.00 100.00 100.00 100.00 100.00 99.99 99.99 99.99 100.00
Net pop.(%) 0.00 0.00 100.01 100.00 100.01 100.00 99.98 99.98 99.98 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 21 22 23 24 25 26 27 28 29 30
Energy(eV): -393.91 -393.87 -283.82 -283.78 -282.38 -282.23 -281.98 -281.82 -281.62 -281.61
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.00 0.00 -0.02 -0.02 0.00 0.01 -0.01 -0.01

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 100.02 100.02 100.00 99.99 100.01 100.01
Net pop.(%) 99.99 100.00 100.00 100.00 100.04 100.04 100.01 99.99 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 31 32 33 34 35 36 37 38 39 40
Energy(eV): -281.56 -281.37 -281.36 -281.31 -281.30 -281.27 -281.23 -281.19 -281.12 -281.07
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.01 100.01 100.01 100.00 100.00 100.01 100.00 100.00 100.00 100.00
Net pop.(%) 100.01 100.02 100.02 100.00 100.01 100.02 100.01 100.00 100.01 100.01

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 41 42 43 44 45 46 47 48 49 50
Energy(eV): -280.96 -280.94 -280.46 -280.45 -280.34 -280.21 -280.21 -280.14 -280.10 -279.90
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 -0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.01 100.00 99.99 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.01 100.02 99.99 99.99 100.00 100.00 100.00 100.00 100.00 100.00

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 51 52 53 54 55 56 57 58 59 60
Energy(eV): -279.47 -279.46 -279.35 -279.31 -279.30 -279.25 -279.21 -279.20 -279.09 -279.08
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00
FRAG# 2: 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

FRAG# 3: 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00 100.00
Net pop.(%) 100.00 100.00 99.99 100.00 99.99 100.00 100.00 100.00 100.00 99.99

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 61 62 63 64 65 66 67 68 69 70
Energy(eV): -279.05 -278.92 -126.42 -125.74 -83.26 -82.67 -82.04 -81.99 -81.94 -81.73
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 0.00 100.06 100.10 99.90 99.86 99.78 99.93 99.91 99.90
Net pop.(%) 0.00 0.00 100.12 100.21 99.82 99.75 99.62 99.87 99.83 99.82

FRAG# 2: 0.00 0.00 0.01 0.01 0.05 0.03 0.10 0.03 0.01 0.01

FRAG# 3: 99.99 100.00 -0.07 -0.11 0.05 0.11 0.13 0.04 0.08 0.09
Net pop.(%) 99.99 100.00 0.00 0.00 0.02 0.02 0.06 0.01 0.02 0.02

OP(1 & 2) 0.000 0.000 0.000 0.000 0.001 0.001 0.002 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 -0.001 -0.002 0.001 0.002 0.001 0.001 0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 71 72 73 74 75 76 77 78 79 80
Energy(eV): -34.17 -33.97 -33.86 -33.23 -33.04 -31.27 -31.02 -28.98 -28.90 -27.57
Symmetry: A A A A A A A A A A

FRAG# 1: 0.00 -0.89 -0.87 -0.70 -0.54 -0.83 -0.53 -0.53 -0.66 -0.19
Net pop.(%) 0.97 0.07 0.06 0.06 0.05 0.09 0.04 0.13 0.14 0.04

FRAG# 2: 97.47 1.49 0.56 0.00 0.00 0.03 0.01 0.01 0.01 0.14
Net pop.(%) 97.61 1.55 0.60 0.00 0.00 0.03 0.01 0.01 0.01 0.12

FRAG# 3: 2.53 99.40 100.31 100.70 100.54 100.81 100.52 100.52 100.64 100.05
Net pop.(%) 1.72 100.33 101.21 101.45 101.14 101.71 101.08 101.19 101.44 100.26

OP(1 & 2) -0.019 -0.001 -0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.000 -0.018 -0.018 -0.015 -0.012 -0.018 -0.011 -0.013 -0.016 -0.004
OP(2 & 3) 0.016 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 81 82 83 84 85 86 87 88 89 90
Energy(eV): -27.43 -27.03 -26.89 -26.66 -26.65 -26.59 -26.36 -26.34 -26.18 -25.94
Symmetry: A A A A A A A A A A

FRAG# 1: -0.13 0.17 0.17 1.43 0.18 0.51 0.14 0.09 0.01 0.09
Net pop.(%) 0.03 0.06 0.04 0.53 0.13 0.18 0.08 0.07 0.08 0.05

FRAG# 2: 0.10 0.31 0.04 71.77 8.46 14.31 0.04 1.56 0.35 0.01
Net pop.(%) 0.09 0.30 0.04 70.26 8.30 14.13 0.05 1.58 0.36 0.01

FRAG# 3: 100.03 99.52 99.79 26.80 91.35 85.18 99.82 98.35 99.64 99.90
Net pop.(%) 100.18 99.40 99.66 26.30 91.36 85.03 99.75 98.35 99.70 99.85

OP(1 & 2) 0.000 0.000 0.000 0.019 0.002 0.004 0.000 0.000 0.000 0.000
OP(1 & 3) -0.003 0.002 0.003 -0.001 -0.001 0.003 0.001 0.000 -0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.011 0.001 0.000 0.000 0.000 0.000 0.000

Alpha MO: 91 92 93 94 95 96 97 98 99 100
Energy(eV): -25.81 -25.74 -25.45 -25.32 -23.79 -23.73 -22.72 -22.67 -22.65 -22.64
Symmetry: A A A A A A A A A A

FRAG# 1: -0.27 -0.05 0.12 0.05 0.03 0.01 0.07 -0.06 0.11 0.15
Net pop.(%) 0.03 0.02 0.02 0.03 0.06 0.06 0.13 0.03 0.08 0.10

FRAG# 2: 0.02 0.00 0.12 0.04 0.01 0.01 0.06 0.03 0.05 0.03
Net pop.(%) 0.02 0.01 0.12 0.05 0.00 0.01 0.04 0.03 0.04 0.03

FRAG# 3: 100.25 100.06 99.77 99.91 99.96 99.98 99.87 100.03 99.84 99.81
Net pop.(%) 100.56 100.14 99.69 99.89 99.99 100.03 99.91 100.11 99.79 99.75

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) -0.006 -0.001 0.002 0.000 -0.001 -0.001 -0.001 -0.002 0.001 0.001
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 101 102 103 104 105 106 107 108 109 110
Energy(eV): -22.55 -22.52 -22.48 -22.40 -22.32 -22.29 -22.07 -21.99 -21.51 -21.44
Symmetry: A A A A A A A A A A

FRAG# 1: 0.28 0.14 0.12 0.42 -0.05 0.02 -0.01 -0.01 0.29 0.43
Net pop.(%) 0.08 0.04 0.05 0.13 0.01 0.01 0.12 0.06 0.15 0.16

FRAG# 2: 0.05 0.06 0.00 0.04 0.04 0.03 0.02 0.01 0.01 0.03
Net pop.(%) 0.06 0.08 0.01 0.02 0.03 0.01 0.02 0.01 0.04 0.03

FRAG# 3: 99.68 99.80 99.88 99.54 100.02 99.95 99.99 100.01 99.70 99.54
Net pop.(%) 99.48 99.70 99.82 99.25 100.08 99.93 100.11 100.08 99.55 99.26

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
OP(1 & 3) 0.004 0.002 0.001 0.006 -0.001 0.000 -0.002 -0.001 0.003 0.006
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

Alpha MO: 111 112 113 114 115 116 117 118 119 120
Energy(eV): -21.33 -21.18 -20.99 -20.85 -20.40 -20.36 -19.84 -19.81 -19.73 -19.51
Symmetry: A A A A A A A A A A

FRAG# 1: 0.04 0.05 0.05 0.06 0.28 0.90 2.01 1.57 1.48 1.00
Net pop.(%) 0.03 0.05 0.03 0.04 0.31 0.41 1.12 0.67 0.75 0.48

FRAG# 2: 0.00 0.01 0.00 0.01 0.22 0.56 0.08 0.20 0.04 0.10
Net pop.(%) 0.00 0.00 0.00 0.01 0.21 0.39 0.06 0.14 0.02 0.07

FRAG# 3: 99.96 99.94 99.95 99.92 99.50 98.55 97.91 98.24 98.48 98.90
Net pop.(%) 99.95 99.93 99.93 99.90 99.53 98.03 97.02 97.37 97.74 98.34

OP(1 & 2) 0.000 0.000 0.000 0.000 0.000 0.001 0.000 0.001 0.000 0.000
OP(1 & 3) 0.000 0.000 0.000 0.000 -0.001 0.008 0.018 0.017 0.014 0.011
OP(2 & 3) 0.000 0.000 0.000 0.000 0.000 0.002 0.000 0.000 0.000 0.001

Alpha MO: 121 122 123 124 125 126 127 128 129 130
Energy(eV): -19.46 -19.43 -18.74 -18.69 -18.48 -18.46 -18.25 -18.18 -17.89 -17.58
Symmetry: A A A A A A A A A A

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FRAG# 1:	1.24	1.04	0.09	0.37	0.29	0.19	1.06	0.79	14.78	0.81
Net pop.(%)	0.49	0.39	0.06	0.22	0.19	0.13	0.69	0.47	11.47	0.50

FRAG# 2:	0.18	0.13	0.05	0.14	0.18	0.17	2.43	1.10	60.34	3.72
Net pop.(%)	0.13	0.09	0.05	0.12	0.15	0.13	2.08	0.93	54.02	3.37

FRAG# 3:	98.59	98.83	99.86	99.49	99.53	99.64	96.51	98.11	24.89	95.47
Net pop.(%)	97.81	98.17	99.83	99.33	99.39	99.57	96.26	97.92	25.63	94.91

OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.005	0.003	0.104	0.001
OP(1 & 3)	0.015	0.013	0.001	0.003	0.002	0.001	0.003	0.003	-0.037	0.005
OP(2 & 3)	0.001	0.000	0.000	0.000	0.001	0.001	0.002	0.000	0.023	0.006

Alpha MO: 131 132 133 134 135 136 137 138 139 140
Energy(eV): -17.47 -17.44 -17.33 -17.12 -17.04 -16.98 -16.93 -16.88 -16.73 -16.67
Symmetry: A A A A A A A A A A

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FRAG# 1:	2.02	0.92	1.19	0.38	0.87	1.95	0.86	4.88	0.60	1.30
Net pop.(%)	1.39	0.49	0.91	0.28	0.55	1.29	0.61	3.59	0.37	0.93

FRAG# 2:	5.02	1.23	3.46	0.12	0.89	2.64	0.89	42.87	0.28	1.20
Net pop.(%)	4.58	1.16	3.33	0.10	0.77	2.51	0.86	40.95	0.27	1.05

FRAG# 3:	92.95	97.85	95.35	99.50	98.25	95.41	98.26	52.25	99.11	97.50
Net pop.(%)	92.45	97.47	95.48	99.40	97.91	94.79	98.03	50.65	98.88	97.11

OP(1 & 2)	0.006	0.001	0.005	0.000	0.001	0.002	0.001	0.016	0.000	0.001
OP(1 & 3)	0.007	0.007	0.000	0.002	0.005	0.011	0.004	0.010	0.004	0.006
OP(2 & 3)	0.003	0.000	-0.003	0.000	0.001	0.001	0.000	0.022	0.000	0.002

Alpha MO: 141 142 143 144 145 146 147 148 149 150
HOMO-77 HOMO-76 HOMO-75 HOMO-74 HOMO-73 HOMO-72 HOMO-71 HOMO-70 HOMO-69 HOMO-68
Energy(eV): -16.59 -16.58 -16.47 -16.44 -16.43 -16.34 -16.29 -16.25 -16.18 -16.12
Symmetry: A A A A A A A A A A

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FRAG# 1:	1.04	1.39	3.84	3.72	2.75	4.57	1.14	4.51	0.52	1.79
Net pop.(%)	0.72	1.08	2.86	2.55	1.84	3.33	0.77	3.21	0.27	1.07

FRAG# 2:	13.47	1.85	0.23	10.69	9.24	13.31	4.16	13.81	0.70	2.11
Net pop.(%)	12.84	1.69	0.20	9.72	8.32	12.91	4.11	13.42	0.66	2.11

FRAG# 3:	85.49	96.77	95.93	85.59	88.01	82.12	94.70	81.68	98.78	96.10
Net pop.(%)	84.90	96.44	95.00	84.55	87.03	81.48	94.62	81.10	98.53	95.60

OP(1 & 2)	0.004	0.001	0.001	0.011	0.008	0.010	0.003	0.011	0.000	0.002
OP(1 & 3)	0.003	0.005	0.019	0.012	0.010	0.015	0.004	0.015	0.005	0.012
OP(2 & 3)	0.009	0.002	0.000	0.008	0.010	-0.002	-0.002	-0.003	0.000	-0.002

Alpha MO: 151 152 153 154 155 156 157 158 159 160
HOMO-67 HOMO-66 HOMO-65 HOMO-64 HOMO-63 HOMO-62 HOMO-61 HOMO-60 HOMO-59 HOMO-58
Energy(eV): -16.03 -15.96 -15.93 -15.87 -15.81 -15.80 -15.77 -15.69 -15.65 -15.60
Symmetry: A A A A A A A A A A

FRAG# 1: 3.81 0.64 1.20 2.15 22.82 3.14 2.46 0.61 2.97 1.28
Net pop.(%) 3.12 0.53 0.89 1.73 19.97 2.63 2.04 0.48 2.50 0.99

FRAG# 2: 9.25 0.48 2.49 5.25 6.15 6.11 3.46 0.92 2.29 1.14
Net pop.(%) 8.75 0.47 2.38 5.07 5.53 5.91 3.48 0.89 2.31 1.24

FRAG# 3: 86.93 98.88 96.31 92.60 71.04 90.76 94.08 98.47 94.74 97.58
Net pop.(%) 86.84 98.82 96.06 92.59 68.99 90.80 94.01 98.47 94.52 97.47

OP(1 & 2) 0.011 0.001 0.002 0.006 0.014 0.007 0.003 0.002 0.002 0.001
OP(1 & 3) 0.003 0.002 0.004 0.002 0.043 0.003 0.005 0.001 0.007 0.005
OP(2 & 3) -0.001 0.000 0.001 -0.002 -0.002 -0.004 -0.004 -0.001 -0.003 -0.003

Alpha MO: 161 162 163 164 165 166 167 168 169 170
HOMO-57 HOMO-56 HOMO-55 HOMO-54 HOMO-53 HOMO-52 HOMO-51 HOMO-50 HOMO-49 HOMO-48
Energy(eV): -15.48 -15.47 -15.36 -15.22 -15.13 -15.12 -15.03 -14.91 -14.79 -14.65
Symmetry: A A A A A A A A A A

FRAG# 1: 1.15 4.18 8.08 5.37 2.82 6.13 1.19 21.92 22.06 0.69
Net pop.(%) 0.84 3.48 7.12 4.04 2.32 4.27 0.88 17.09 17.82 0.55

FRAG# 2: 0.60 6.39 4.17 3.30 1.37 6.78 0.09 3.60 1.83 0.23
Net pop.(%) 0.56 6.84 4.57 4.03 1.43 7.48 0.15 3.15 1.80 0.18

FRAG# 3: 98.24 89.42 87.74 91.33 95.81 87.08 98.72 74.48 76.11 99.08
Net pop.(%) 98.00 89.62 87.41 90.59 95.61 85.89 98.39 70.51 71.94 98.91

OP(1 & 2) 0.001 0.005 0.002 -0.001 0.002 0.000 -0.001 0.013 0.001 0.000
OP(1 & 3) 0.005 0.010 0.017 0.028 0.008 0.038 0.007 0.083 0.084 0.003
OP(2 & 3) 0.000 -0.013 -0.010 -0.013 -0.003 -0.014 0.000 -0.004 0.000 0.001

Alpha MO: 171 172 173 174 175 176 177 178 179 180
HOMO-47 HOMO-46 HOMO-45 HOMO-44 HOMO-43 HOMO-42 HOMO-41 HOMO-40 HOMO-39 HOMO-38
Energy(eV): -14.57 -14.47 -14.38 -14.30 -14.21 -14.19 -14.09 -13.97 -13.93 -13.92
Symmetry: A A A A A A A A A A

FRAG# 1: 0.75 3.45 28.18 0.91 0.72 0.70 0.73 5.07 12.84 2.82
Net pop.(%) 0.63 2.99 25.21 0.70 0.65 0.54 0.58 4.39 11.35 2.55

FRAG# 2: 0.56 0.60 3.90 0.97 0.45 0.13 0.06 3.01 10.51 0.69
Net pop.(%) 0.61 0.61 3.54 0.87 0.40 0.12 0.06 2.55 9.03 0.68

FRAG# 3: 98.69 95.95 67.92 98.12 98.83 99.17 99.21 91.93 76.66 96.49
Net pop.(%) 98.69 95.63 65.09 97.92 98.80 99.02 99.07 91.42 76.03 96.38

OP(1 & 2) 0.001 0.001 0.005 0.001 0.001 0.000 0.000 0.006 0.023 0.002
OP(1 & 3) 0.002 0.008 0.054 0.003 0.000 0.003 0.003 0.007 0.006 0.004
OP(2 & 3) -0.002 -0.002 0.002 0.001 0.000 0.000 0.000 0.003 0.006 -0.002

Alpha MO: 181 182 183 184 185 186 187 188 189 190
HOMO-37 HOMO-36 HOMO-35 HOMO-34 HOMO-33 HOMO-32 HOMO-31 HOMO-30 HOMO-29 HOMO-28
Energy(eV): -13.90 -13.81 -13.73 -13.62 -13.54 -13.43 -13.39 -13.36 -13.29 -13.24
Symmetry: A A A A A A A A A A

FRAG# 1: 9.40 10.57 20.35 4.37 35.28 39.59 5.88 24.98 21.97 17.46
Net pop.(%) 8.10 9.34 17.65 4.09 34.45 38.84 5.71 24.41 21.42 16.49

FRAG# 2: 9.86 1.86 1.59 0.81 1.43 1.47 0.95 1.90 0.43 1.24
Net pop.(%) 8.45 1.61 1.47 0.71 1.57 1.60 1.15 1.87 0.51 1.14

FRAG# 3: 80.74 87.56 78.06 94.82 63.29 58.94 93.17 73.12 77.60 81.30
Net pop.(%) 80.22 86.37 75.33 94.53 62.36 58.10 93.05 72.65 77.05 80.42

OP(1 & 2) 0.022 0.003 0.001 0.001 -0.002 -0.002 -0.002 0.001 -0.001 0.002
OP(1 & 3) 0.004 0.022 0.053 0.005 0.019 0.017 0.005 0.010 0.012 0.018
OP(2 & 3) 0.006 0.002 0.002 0.001 0.000 0.000 -0.003 -0.001 -0.001 0.000

Alpha MO: 191 192 193 194 195 196 197 198 199 200
HOMO-27 HOMO-26 HOMO-25 HOMO-24 HOMO-23 HOMO-22 HOMO-21 HOMO-20 HOMO-19 HOMO-18
Energy(eV): -13.21 -13.18 -13.15 -13.08 -13.05 -12.99 -12.94 -12.92 -12.84 -12.79
Symmetry: A A A A A A A A A A

FRAG# 1: 11.43 5.47 43.46 20.35 2.71 33.52 14.86 22.07 4.14 33.79
Net pop.(%) 11.40 5.40 43.61 20.68 2.62 34.60 14.87 22.34 4.14 34.35

FRAG# 2: 0.69 0.27 3.68 1.56 0.09 2.51 1.76 1.09 0.22 0.32
Net pop.(%) 0.92 0.27 4.28 2.03 0.11 3.53 2.32 1.69 0.33 0.39

FRAG# 3: 87.89 94.26 52.86 78.08 97.20 63.98 83.38 76.84 95.64 65.89
Net pop.(%) 87.71 94.23 52.26 77.95 97.10 64.50 83.69 76.81 95.62 66.42

OP(1 & 2) -0.004 0.000 -0.014 -0.009 0.000 -0.016 -0.002 -0.009 -0.001 -0.001
OP(1 & 3) 0.004 0.001 0.011 0.003 0.002 -0.006 0.002 0.003 0.001 -0.010
OP(2 & 3) -0.001 0.000 0.001 0.000 0.000 -0.005 -0.009 -0.003 -0.001 0.000

Alpha MO: 201 202 203 204 205 206 207 208 209 210
HOMO-17 HOMO-16 HOMO-15 HOMO-14 HOMO-13 HOMO-12 HOMO-11 HOMO-10 HOMO-9 HOMO-8
Energy(eV): -12.70 -12.65 -12.61 -12.55 -12.50 -12.39 -12.02 -11.86 -11.83 -11.78
Symmetry: A A A A A A A A A A

FRAG# 1: 30.52 47.70 13.06 6.69 11.29 48.45 26.95 19.89 7.80 5.95
Net pop.(%) 30.93 48.32 13.30 6.65 11.59 49.73 28.03 21.27 8.40 6.55

FRAG# 2: 1.23 2.85 1.32 1.44 0.97 10.92 1.42 5.62 0.96 2.37
Net pop.(%) 1.48 2.82 1.67 2.16 1.13 11.90 1.45 5.96 1.12 2.37

FRAG# 3: 68.26 49.45 85.62 91.87 87.74 40.63 71.63 74.49 91.25 91.68
Net pop.(%) 68.55 50.04 85.82 92.20 87.90 41.75 72.69 75.49 91.72 92.37

OP(1 & 2) -0.004 0.000 -0.004 -0.004 -0.003 -0.011 -0.001 -0.007 -0.003 0.001
OP(1 & 3) -0.005 -0.012 -0.001 0.004 -0.003 -0.014 -0.021 -0.020 -0.009 -0.013
OP(2 & 3) -0.001 0.000 -0.003 -0.011 0.000 -0.008 0.000 0.000 0.000 -0.001

Alpha MO: 211 212 213 214 215 216 217 218 219 220
HOMO-7 HOMO-6 HOMO-5 HOMO-4 HOMO-3 HOMO-2 HOMO-1 HOMO LUMO LUMO+1
Energy(eV): -11.77 -11.65 -11.49 -11.48 -11.40 -11.29 -11.18 -10.81 -8.25 -7.05
Symmetry: A A A A A A A A A A

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FRAG# 1:	24.99	15.47	21.18	0.36	28.97	2.94	54.44	20.90	54.51	1.28
Net pop.(%)	27.58	16.83	23.47	0.46	32.74	3.38	60.24	25.62	65.78	2.40

FRAG# 2:	3.85	15.03	1.10	0.01	9.17	1.24	3.92	68.19	32.46	0.09
Net pop.(%)	4.80	14.52	1.29	0.01	9.52	1.26	5.27	71.87	39.96	0.18

FRAG# 3:	71.15	69.50	77.72	99.63	61.86	95.82	41.64	10.91	13.04	98.63
Net pop.(%)	72.81	71.65	79.85	99.73	65.19	96.19	46.54	13.53	18.31	99.64

OP(1 & 2)	-0.019	0.013	-0.004	0.000	-0.008	-0.001	-0.023	-0.058	-0.135	-0.002
OP(1 & 3)	-0.033	-0.040	-0.042	-0.002	-0.067	-0.008	-0.094	-0.037	-0.090	-0.021
OP(2 & 3)	0.000	-0.003	0.000	0.000	0.001	0.000	-0.004	-0.016	-0.015	0.000