

Electronic Supplementary Information

Cluster Carbonyls of the $[\text{Re}_6(\mu_3\text{-Se})_8]^{2+}$ Core: Synthesis, Structural Characterization, and Computational Analysis

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ADF Computational Studies

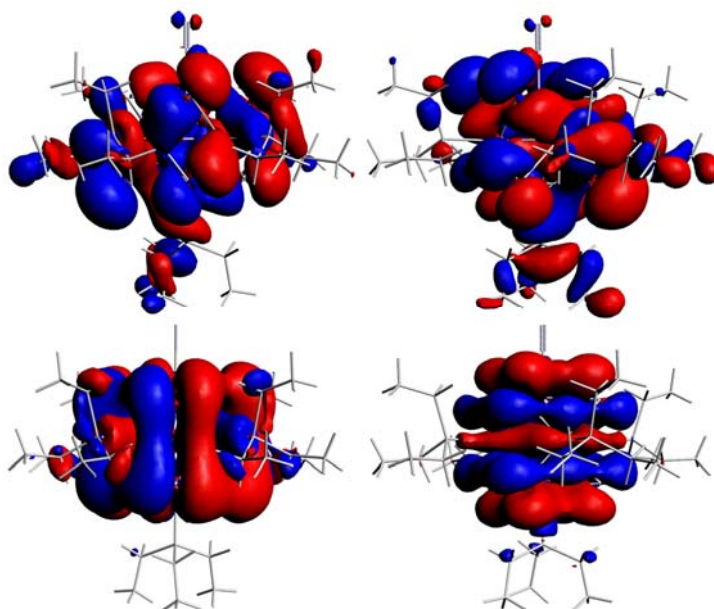


Figure 1. Orbital plots of the HOMO-3, HOMO-2, HOMO-1 and HOMO of compound **1**, clockwise from top left.

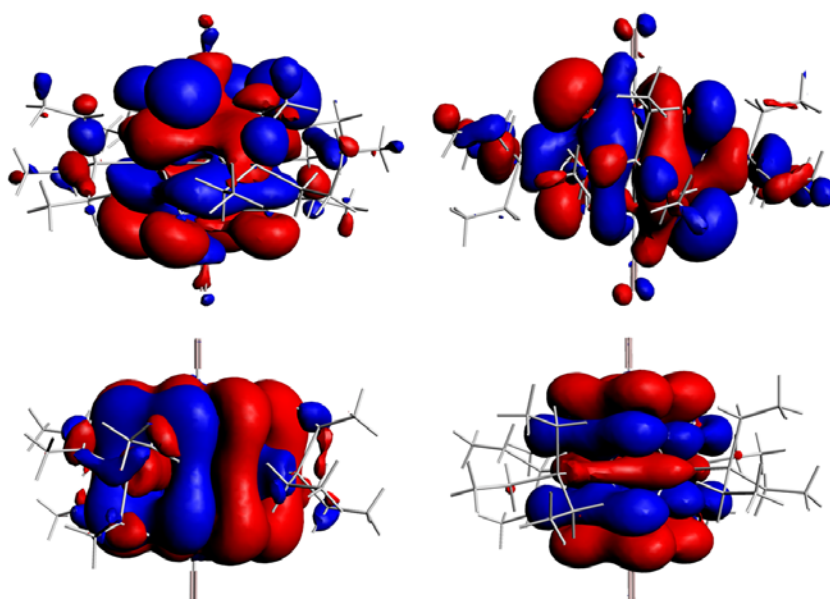


Figure 2. Orbital plots of the HOMO-4, HOMO-2, HOMO-1, and HOMO of compound **2**, clockwise from top left.

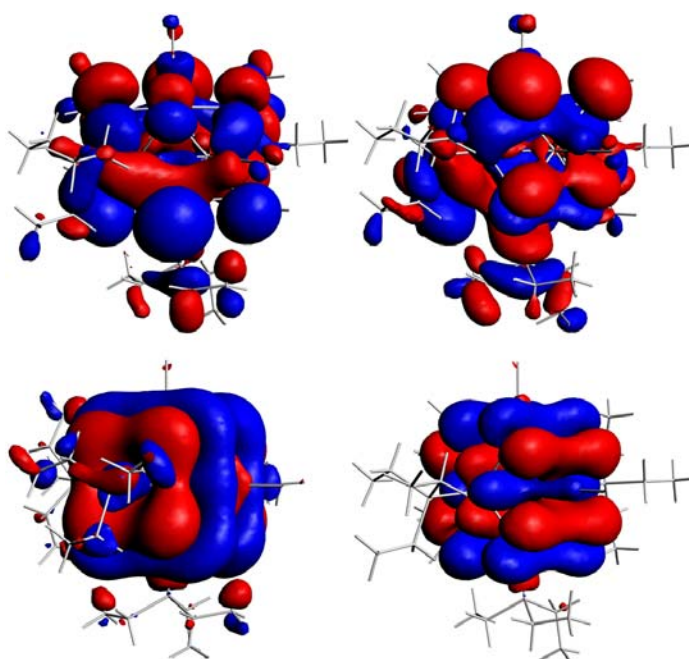


Figure 3. Orbital plots of the HOMO-4, HOMO-2, HOMO-1 and HOMO of compound **3**, clockwise from top left.

trans-[Re6Se8 (PEt3)4 (CO)2]

E (eV)	Occ	MO	%	SFO (first member)	E (eV)	Occ	Fragment
-10.673	2.00	244 A	10.60%	1 P:z	-6.559	1.33	8 Se
			10.32%	1 P:z	-6.559	1.33	7 Se
			5.65%	1 P:z	-6.559	1.33	13 Se
			5.37%	1 P:z	-6.559	1.33	14 Se
			4.43%	1 P:z	-6.559	1.33	11 Se
			4.10%	1 P:z	-6.559	1.33	12 Se
			4.10%	1 D:z2	-5.431	1.00	2 Re
			4.04%	1 D:z2	-5.431	1.00	1 Re
			2.17%	1 P:x	-6.559	1.33	13 Se
			2.12%	1 P:z	-6.559	1.33	9 Se
			2.11%	1 D:z2	-5.431	1.00	4 Re
			1.97%	1 D:z2	-5.431	1.00	3 Re
			1.91%	1 P:y	-6.559	1.33	14 Se
			1.83%	1 P:z	-6.559	1.33	10 Se
			1.81%	1 P:x	-6.559	1.33	9 Se
			1.67%	1 P:x	-6.559	1.33	10 Se
			1.64%	1 P:x	-6.559	1.33	11 Se
			1.55%	1 P:y	-6.559	1.33	13 Se
			1.48%	1 P:x	-6.559	1.33	14 Se
			1.40%	1 D:yz	-5.431	1.00	4 Re
			1.34%	1 P:x	-6.559	1.33	12 Se
			1.26%	1 D:xy	-5.431	1.00	1 Re
			1.16%	1 D:yz	-5.431	1.00	3 Re
			1.11%	1 D:yz	-5.431	1.00	1 Re
1.07%	1 P:x	-6.559	1.33	8 Se			
1.05%	1 D:xy	-5.431	1.00	2 Re			
-10.620	2.00	245 A	5.36%	1 D:x2-y2	-5.431	1.00	4 Re
			4.50%	1 P:y	-6.559	1.33	13 Se
			4.46%	1 D:x2-y2	-5.431	1.00	3 Re
			4.26%	1 P:x	-6.559	1.33	10 Se
			4.17%	1 P:y	-6.559	1.33	14 Se
			4.13%	1 P:x	-6.559	1.33	9 Se
			3.62%	1 P:x	-6.559	1.33	13 Se
			3.48%	1 P:y	-6.559	1.33	11 Se
			3.31%	1 P:x	-6.559	1.33	14 Se

			3.04%	1 P:y	-6.559	1.33	12 Se
			2.73%	1 D:xz	-5.431	1.00	4 Re
			2.73%	1 D:xz	-5.431	1.00	3 Re
			2.46%	1 P:z	-6.559	1.33	8 Se
			2.42%	1 P:z	-6.559	1.33	11 Se
			2.40%	1 P:y	-6.559	1.33	9 Se
			2.31%	1 P:y	-6.559	1.33	10 Se
			2.19%	1 P:y	-6.559	1.33	8 Se
			2.10%	1 P:y	-6.559	1.33	7 Se
			2.00%	1 P:z	-6.559	1.33	12 Se
			1.97%	1 P:z	-6.559	1.33	7 Se
			1.96%	1 D:z2	-5.431	1.00	4 Re
			1.51%	1 P:y	-5.520	1.00	45 P
			1.38%	1 D:z2	-5.431	1.00	3 Re
			1.14%	1 P:y	-5.520	1.00	43 P
			1.00%	1 P:z	-5.520	1.00	45 P
-10.597	2.00	246 A	8.11%	1 P:x	-6.559	1.33	9 Se
			7.49%	1 P:x	-6.559	1.33	10 Se
			5.54%	1 P:x	-6.559	1.33	12 Se
			5.36%	1 D:x2-y2	-5.431	1.00	2 Re
			5.35%	1 D:x2-y2	-5.431	1.00	1 Re
			4.83%	1 P:x	-6.559	1.33	11 Se
			3.95%	1 P:y	-6.559	1.33	11 Se
			3.62%	1 P:y	-6.559	1.33	12 Se
			2.33%	1 P:y	-6.559	1.33	8 Se
			2.09%	1 D:xz	-5.431	1.00	2 Re
			2.02%	1 D:xz	-5.431	1.00	1 Re
			1.70%	1 P:y	-6.559	1.33	13 Se
			1.64%	1 P:y	-6.559	1.33	14 Se
			1.59%	1 P:y	-6.559	1.33	10 Se
			1.50%	1 P:y	-5.520	1.00	46 P
			1.44%	1 P:x	-6.559	1.33	14 Se
			1.36%	1 P:y	-5.520	1.00	44 P
			1.34%	1 P:y	-6.559	1.33	7 Se
			1.28%	1 D:xy	-5.431	1.00	4 Re
			1.15%	1 D:xy	-5.431	1.00	3 Re
			1.13%	1 P:x	-6.559	1.33	7 Se
			1.12%	1 P:z	-6.559	1.33	14 Se
			1.07%	1 P:x	-6.559	1.33	13 Se
			1.05%	1 P:x	-6.559	1.33	8 Se

-9.974	2.00	247 A	1.00%	1 P:y	-6.559	1.33	9 Se
			11.44%	1 D:xz	-5.431	1.00	4 Re
			10.42%	1 D:xz	-5.431	1.00	3 Re
			9.30%	1 D:xz	-5.431	1.00	1 Re
			8.88%	1 D:xz	-5.431	1.00	2 Re
			3.90%	1 D:x ² -y ²	-5.431	1.00	3 Re
			3.38%	1 D:x ² -y ²	-5.431	1.00	4 Re
			3.22%	1 P:x	-6.559	1.33	7 Se
			3.07%	1 P:x	-6.559	1.33	8 Se
			2.96%	1 D:x ² -y ²	-5.431	1.00	1 Re
			2.93%	1 P:z	-6.559	1.33	10 Se
			2.89%	1 D:xz	-5.431	1.00	5 Re
			2.88%	1 D:xz	-5.431	1.00	6 Re
			2.78%	1 D:x ² -y ²	-5.431	1.00	2 Re
			2.59%	1 P:z	-6.559	1.33	9 Se
			2.11%	2 P:x	-0.424	0.00	5 Re
			2.01%	2 P:x	-0.424	0.00	6 Re
			1.85%	1 P:x	-6.559	1.33	11 Se
			1.82%	1 P:x	-6.559	1.33	12 Se
			-9.947	2.00	248 A	1.62%	1 D:yz
1.61%	2 P:z	-0.424				0.00	6 Re
1.58%	1 P:z	-6.559				1.33	14 Se
1.54%	2 P:z	-0.424				0.00	5 Re
1.52%	1 D:yz	-5.431				1.00	4 Re
1.30%	1 P:z	-6.559				1.33	13 Se
1.19%	1 P:y	-6.559				1.33	12 Se
1.05%	1 P:y	-6.559				1.33	11 Se
9.73%	1 D:yz	-5.431				1.00	5 Re
9.47%	1 D:yz	-5.431				1.00	6 Re
7.78%	1 D:xy	-5.431				1.00	6 Re
7.57%	1 D:xy	-5.431				1.00	5 Re
4.78%	1 D:yz	-5.431				1.00	2 Re
4.54%	1 D:yz	-5.431				1.00	1 Re
4.17%	1 D:xy	-5.431				1.00	2 Re
3.90%	1 D:xy	-5.431				1.00	1 Re
3.71%	1 D:yz	-5.431				1.00	4 Re
3.66%	1 D:yz	-5.431				1.00	3 Re
2.80%	1 P:y	-6.559	1.33	10 Se			
2.72%	1 P:y	-6.559	1.33	8 Se			
2.70%	1 D:xy	-5.431	1.00	4 Re			

			2.65%	1 P:y	-6.559	1.33	9 Se
			2.64%	1 D:xy	-5.431	1.00	3 Re
			2.59%	1 P:y	-6.559	1.33	7 Se
			2.43%	1 P:z	-6.559	1.33	12 Se
			2.23%	1 P:z	-6.559	1.33	11 Se
			2.22%	1 P:x	-6.559	1.33	14 Se
			2.07%	1 P:x	-6.559	1.33	13 Se
			1.63%	1 D:xz	-5.431	1.00	2 Re
			1.56%	1 D:xz	-5.431	1.00	1 Re
			1.33%	2 P:y	-0.424	0.00	4 Re
			1.30%	1 P:z	-6.559	1.33	13 Se
			1.29%	1 P:z	-6.559	1.33	14 Se
			1.24%	2 P:y	-0.424	0.00	3 Re
-8.139	0.00	249 A	7.78%	1 D:z2	-5.431	1.00	5 Re
			7.40%	1 D:z2	-5.431	1.00	6 Re
			6.91%	1 P:x	-6.559	1.33	7 Se
			6.60%	1 P:x	-6.559	1.33	8 Se
			6.41%	1 P:z	-6.559	1.33	10 Se
			6.32%	1 P:z	-6.559	1.33	9 Se
			4.91%	1 D:z2	-5.431	1.00	2 Re
			4.86%	1 D:z2	-5.431	1.00	1 Re
			3.38%	1 P:z	-5.375	0.67	17 C
			3.34%	1 D:xy	-5.431	1.00	2 Re
			3.32%	1 D:xy	-5.431	1.00	1 Re
			3.20%	1 P:z	-5.375	0.67	18 C
			2.69%	1 P:x	-5.375	0.67	17 C
			2.64%	1 D:yz	-5.431	1.00	2 Re
			2.61%	1 P:x	-5.375	0.67	18 C
			2.59%	1 D:x2-y2	-5.431	1.00	6 Re
			2.49%	1 D:x2-y2	-5.431	1.00	5 Re
			2.44%	1 D:xy	-5.431	1.00	3 Re
			2.41%	1 D:xy	-5.431	1.00	4 Re
			2.34%	1 P:z	-9.159	1.33	15 O
			2.29%	1 D:yz	-5.431	1.00	1 Re
			2.27%	1 D:z2	-5.431	1.00	4 Re
			2.25%	1 D:z2	-5.431	1.00	3 Re
			2.22%	1 P:z	-9.159	1.33	16 O
			1.86%	1 P:x	-9.159	1.33	15 O
			1.80%	1 P:x	-9.159	1.33	16 O
			1.51%	1 D:yz	-5.431	1.00	4 Re

			1.47%	1 D:yz	-5.431	1.00	3 Re
			1.13%	1 D:x2-y2	-5.431	1.00	2 Re
			1.12%	1 P:z	-6.559	1.33	14 Se
			1.12%	1 D:x2-y2	-5.431	1.00	1 Re
			1.09%	1 D:x2-y2	-5.431	1.00	3 Re
			1.09%	1 D:x2-y2	-5.431	1.00	4 Re
			1.06%	1 P:z	-6.559	1.33	13 Se
-8.116	0.00	250 A	6.04%	1 P:y	-5.375	0.67	17 C
			5.95%	1 P:y	-5.375	0.67	18 C
			5.90%	1 D:xy	-5.431	1.00	6 Re
			5.54%	1 D:xy	-5.431	1.00	5 Re
			4.85%	1 D:yz	-5.431	1.00	5 Re
			4.47%	1 D:yz	-5.431	1.00	6 Re
			4.17%	1 P:y	-9.159	1.33	15 O
			4.11%	1 P:y	-9.159	1.33	16 O
			4.10%	1 D:z2	-5.431	1.00	4 Re
			3.99%	1 D:z2	-5.431	1.00	3 Re
			3.75%	1 P:y	-6.559	1.33	11 Se
			3.69%	1 P:y	-6.559	1.33	12 Se
			3.48%	1 D:xy	-5.431	1.00	4 Re
			3.35%	1 D:xy	-5.431	1.00	3 Re
			3.25%	1 P:y	-6.559	1.33	13 Se
			3.14%	1 P:y	-6.559	1.33	14 Se
			2.97%	1 D:z2	-5.431	1.00	1 Re
			2.92%	1 D:z2	-5.431	1.00	2 Re
			2.86%	1 D:yz	-5.431	1.00	4 Re
			2.65%	1 D:yz	-5.431	1.00	3 Re
			2.12%	1 P:x	-6.559	1.33	13 Se
			2.09%	1 D:xy	-5.431	1.00	1 Re
			2.01%	1 D:xy	-5.431	1.00	2 Re
			1.95%	1 P:x	-6.559	1.33	14 Se
			1.70%	1 P:x	-6.559	1.33	11 Se
			1.63%	1 P:x	-6.559	1.33	12 Se
			1.62%	1 D:x2-y2	-5.431	1.00	4 Re
			1.57%	1 D:x2-y2	-5.431	1.00	3 Re
			1.52%	1 P:z	-6.559	1.33	11 Se
			1.52%	1 P:y	-6.559	1.33	10 Se
			1.49%	1 P:y	-6.559	1.33	9 Se
			1.44%	1 P:y	-6.559	1.33	8 Se
			1.41%	1 P:y	-6.559	1.33	7 Se

			1.38%	1	P:z	-6.559	1.33	12	Se	
			1.25%	1	D:yz	-5.431	1.00	2	Re	
			1.15%	1	D:yz	-5.431	1.00	1	Re	
			1.10%	1	P:z	-6.559	1.33	13	Se	
			1.08%	1	P:z	-6.559	1.33	14	Se	
-7.650	0.00	251	A	10.04%	1	D:yz	-5.431	1.00	6	Re
				9.93%	1	D:yz	-5.431	1.00	5	Re
				9.16%	1	D:xz	-5.431	1.00	4	Re
				8.48%	1	D:xz	-5.431	1.00	1	Re
				8.46%	1	D:xz	-5.431	1.00	3	Re
				7.93%	1	D:xy	-5.431	1.00	5	Re
				7.78%	1	D:xz	-5.431	1.00	2	Re
				7.70%	1	D:xy	-5.431	1.00	6	Re
				5.45%	1	D:x ² -y ²	-5.431	1.00	2	Re
				5.39%	1	D:x ² -y ²	-5.431	1.00	1	Re
				4.64%	1	D:x ² -y ²	-5.431	1.00	4	Re
				4.60%	1	D:x ² -y ²	-5.431	1.00	3	Re
				3.11%	1	D:yz	-5.431	1.00	4	Re
				3.07%	1	D:yz	-5.431	1.00	3	Re
				2.56%	1	D:xy	-5.431	1.00	1	Re
				2.32%	1	D:xy	-5.431	1.00	2	Re
				2.19%	1	D:yz	-5.431	1.00	1	Re
				1.89%	1	D:yz	-5.431	1.00	2	Re
				1.64%	1	D:xy	-5.431	1.00	4	Re
				1.61%	1	D:xy	-5.431	1.00	3	Re
				-1.01%	2	D:yz	4.925	0.00	6	Re
-7.568	0.00	252	A	9.55%	1	D:x ² -y ²	-5.431	1.00	1	Re
				9.48%	1	D:x ² -y ²	-5.431	1.00	4	Re
				9.27%	1	D:x ² -y ²	-5.431	1.00	2	Re
				9.04%	1	D:x ² -y ²	-5.431	1.00	3	Re
				8.42%	1	D:xz	-5.431	1.00	4	Re
				8.31%	1	D:xz	-5.431	1.00	1	Re
				5.80%	1	D:z ²	-5.431	1.00	4	Re
				5.34%	1	D:xz	-5.431	1.00	3	Re
				5.09%	1	D:xz	-5.431	1.00	2	Re
				4.90%	1	D:z ²	-5.431	1.00	1	Re
				4.71%	1	D:z ²	-5.431	1.00	2	Re
				4.58%	1	D:z ²	-5.431	1.00	3	Re
				3.30%	1	P:y	-6.559	1.33	8	Se
				3.10%	1	P:y	-6.559	1.33	9	Se

3.07%	1 P:y	-6.559	1.33	7 Se
2.92%	1 P:y	-6.559	1.33	10 Se
1.99%	1 P:z	-6.559	1.33	13 Se
1.83%	1 P:z	-6.559	1.33	11 Se
1.74%	1 P:z	-6.559	1.33	12 Se
1.54%	1 P:z	-6.559	1.33	14 Se
1.47%	1 P:x	-6.559	1.33	13 Se
-1.38%	2 D:x ² -y ²	4.925	0.00	4 Re
1.30%	1 P:x	-6.559	1.33	11 Se
-1.30%	2 D:x ² -y ²	4.925	0.00	1 Re
-1.26%	2 D:x ² -y ²	4.925	0.00	3 Re
-1.18%	2 D:x ² -y ²	4.925	0.00	2 Re
-1.18%	2 D:xz	4.925	0.00	1 Re
1.17%	1 P:x	-6.559	1.33	14 Se
1.15%	1 P:x	-6.559	1.33	12 Se
-1.10%	2 D:xz	4.925	0.00	4 Re

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M U L L I K E N P O P U L A T I O N S

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Atom	Charge	Spin density	S	P	D	F
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1 Re	0.1529		2.4463	6.7388	5.6580	14.0041
2 Re	0.1507		2.4548	6.7378	5.6527	14.0041
3 Re	0.1426		2.4339	6.7535	5.6659	14.0042
4 Re	0.1616		2.4340	6.7430	5.6573	14.0041
5 Re	-0.0568		2.7038	6.7311	5.6174	14.0046
6 Re	-0.0690		2.7035	6.7356	5.6252	14.0047
7 Se	-0.2051		2.0302	4.0508	10.1242	0.0000
8 Se	-0.1973		2.0273	4.0447	10.1253	0.0000
9 Se	-0.1794		2.0182	4.0420	10.1192	0.0000
10 Se	-0.1846		2.0195	4.0449	10.1202	0.0000
11 Se	-0.1558		2.0127	4.0206	10.1226	0.0000
12 Se	-0.1464		2.0111	4.0150	10.1203	0.0000
13 Se	-0.1872		2.0238	4.0434	10.1200	0.0000
14 Se	-0.1869		2.0248	4.0408	10.1213	0.0000
15 O	-0.3184		1.8955	4.3602	0.0628	0.0000
16 O	-0.3185		1.8956	4.3601	0.0628	0.0000

17	C	0.2948	1.4682	2.1445	0.0926	0.0000
18	C	0.2983	1.4670	2.1421	0.0926	0.0000
19	P	1.3975	1.3286	2.0007	0.2732	0.0000
20	P	1.4083	1.3309	1.9875	0.2733	0.0000
21	P	1.4044	1.3277	1.9946	0.2734	0.0000
22	P	1.4175	1.3294	1.9796	0.2735	0.0000
23	C	0.0090	1.1783	2.7606	0.0521	0.0000
24	C	0.3665	1.0146	2.5743	0.0446	0.0000
25	H	-0.1148	1.0386	0.0762	0.0000	0.0000
26	H	-0.1129	1.0374	0.0755	0.0000	0.0000
27	H	-0.1370	1.0602	0.0768	0.0000	0.0000
28	H	-0.1041	1.0238	0.0803	0.0000	0.0000
29	H	-0.1255	1.0460	0.0795	0.0000	0.0000
30	C	0.0093	1.1790	2.7599	0.0517	0.0000
31	C	0.3662	1.0151	2.5741	0.0445	0.0000
32	H	-0.1191	1.0413	0.0778	0.0000	0.0000
33	H	-0.1078	1.0286	0.0792	0.0000	0.0000
34	H	-0.1362	1.0595	0.0768	0.0000	0.0000
35	H	-0.1078	1.0275	0.0803	0.0000	0.0000
36	H	-0.1226	1.0428	0.0798	0.0000	0.0000
37	C	0.0093	1.1786	2.7600	0.0521	0.0000
38	C	0.3701	1.0153	2.5701	0.0446	0.0000
39	H	-0.1232	1.0481	0.0751	0.0000	0.0000
40	H	-0.1217	1.0439	0.0779	0.0000	0.0000
41	H	-0.1345	1.0578	0.0767	0.0000	0.0000
42	H	-0.1082	1.0278	0.0804	0.0000	0.0000
43	H	-0.1185	1.0381	0.0804	0.0000	0.0000
44	C	0.0105	1.1774	2.7602	0.0519	0.0000
45	C	0.3684	1.0152	2.5718	0.0446	0.0000
46	H	-0.1148	1.0354	0.0795	0.0000	0.0000
47	H	-0.1157	1.0382	0.0775	0.0000	0.0000
48	H	-0.1337	1.0570	0.0767	0.0000	0.0000
49	H	-0.1208	1.0402	0.0806	0.0000	0.0000
50	H	-0.1099	1.0291	0.0808	0.0000	0.0000
51	C	0.0121	1.1781	2.7577	0.0521	0.0000
52	C	0.3676	1.0149	2.5729	0.0446	0.0000
53	H	-0.1178	1.0401	0.0778	0.0000	0.0000
54	H	-0.1195	1.0450	0.0745	0.0000	0.0000
55	H	-0.1347	1.0579	0.0767	0.0000	0.0000
56	H	-0.1220	1.0421	0.0799	0.0000	0.0000

57	H	-0.1058	1.0253	0.0805	0.0000	0.0000
58	C	0.0079	1.1793	2.7608	0.0520	0.0000
59	C	0.3663	1.0151	2.5740	0.0446	0.0000
60	H	-0.1144	1.0386	0.0758	0.0000	0.0000
61	H	-0.1184	1.0420	0.0764	0.0000	0.0000
62	H	-0.1356	1.0589	0.0768	0.0000	0.0000
63	H	-0.1215	1.0419	0.0796	0.0000	0.0000
64	H	-0.1048	1.0245	0.0803	0.0000	0.0000
65	C	0.0100	1.1768	2.7612	0.0520	0.0000
66	C	0.3730	1.0143	2.5682	0.0446	0.0000
67	H	-0.1228	1.0429	0.0799	0.0000	0.0000
68	H	-0.1199	1.0439	0.0760	0.0000	0.0000
69	H	-0.1356	1.0589	0.0768	0.0000	0.0000
70	H	-0.1155	1.0347	0.0808	0.0000	0.0000
71	H	-0.1102	1.0292	0.0810	0.0000	0.0000
72	C	0.0082	1.1796	2.7600	0.0522	0.0000
73	C	0.3676	1.0156	2.5723	0.0446	0.0000
74	H	-0.1203	1.0439	0.0764	0.0000	0.0000
75	H	-0.1147	1.0400	0.0747	0.0000	0.0000
76	H	-0.1338	1.0572	0.0766	0.0000	0.0000
77	H	-0.1223	1.0423	0.0799	0.0000	0.0000
78	H	-0.1076	1.0269	0.0807	0.0000	0.0000
79	C	0.0108	1.1779	2.7593	0.0520	0.0000
80	C	0.3671	1.0154	2.5729	0.0446	0.0000
81	H	-0.1036	1.0278	0.0758	0.0000	0.0000
82	H	-0.1167	1.0391	0.0777	0.0000	0.0000
83	H	-0.1338	1.0571	0.0766	0.0000	0.0000
84	H	-0.1206	1.0404	0.0803	0.0000	0.0000
85	H	-0.1076	1.0273	0.0802	0.0000	0.0000
86	C	0.0123	1.1778	2.7579	0.0520	0.0000
87	C	0.3653	1.0156	2.5745	0.0446	0.0000
88	H	-0.1158	1.0384	0.0774	0.0000	0.0000
89	H	-0.1029	1.0273	0.0756	0.0000	0.0000
90	H	-0.1335	1.0569	0.0766	0.0000	0.0000
91	H	-0.1064	1.0264	0.0800	0.0000	0.0000
92	H	-0.1236	1.0435	0.0801	0.0000	0.0000
93	C	0.0096	1.1765	2.7619	0.0519	0.0000
94	C	0.3704	1.0146	2.5705	0.0445	0.0000
95	H	-0.1200	1.0438	0.0762	0.0000	0.0000
96	H	-0.1199	1.0394	0.0805	0.0000	0.0000

97 H	-0.1370	1.0601	0.0769	0.0000	0.0000
98 H	-0.1074	1.0264	0.0810	0.0000	0.0000
99 H	-0.1179	1.0378	0.0801	0.0000	0.0000
100 C	0.0045	1.1801	2.7633	0.0522	0.0000
101 C	0.3697	1.0147	2.5710	0.0446	0.0000
102 H	-0.1167	1.0423	0.0745	0.0000	0.0000
103 H	-0.1214	1.0446	0.0768	0.0000	0.0000
104 H	-0.1356	1.0589	0.0767	0.0000	0.0000
105 H	-0.1072	1.0266	0.0806	0.0000	0.0000
106 H	-0.1206	1.0405	0.0801	0.0000	0.0000

cis- [Re6Se8 (PEt3) 4 (CO) 2]

E (eV)	Occ	MO	%	SFO (first member)	E (eV)	Occ	Fragment
-10.660	2.00	244 A	10.56%	1 P:y	-6.559	1.33	14 Se
			7.22%	1 P:y	-6.559	1.33	12 Se
			6.62%	1 P:y	-6.559	1.33	13 Se
			4.79%	1 P:x	-6.559	1.33	14 Se
			4.15%	1 P:y	-6.559	1.33	11 Se
			4.04%	1 D:x ² -y ²	-5.431	1.00	4 Re
			3.78%	1 D:xy	-5.431	1.00	3 Re
			3.68%	1 P:y	-6.559	1.33	10 Se
			3.63%	1 P:x	-6.559	1.33	12 Se
			3.26%	1 P:x	-6.559	1.33	10 Se
			3.24%	1 P:y	-6.559	1.33	9 Se
			2.78%	1 D:x ² -y ²	-5.431	1.00	2 Re
			2.74%	1 P:x	-6.559	1.33	9 Se
			2.24%	1 P:y	-6.559	1.33	8 Se
			1.53%	1 D:z ²	-5.431	1.00	1 Re
			1.50%	1 D:xz	-5.431	1.00	2 Re
			1.43%	1 P:z	-6.559	1.33	12 Se
			1.30%	1 P:x	-6.559	1.33	11 Se
			1.21%	1 D:xy	-5.431	1.00	4 Re
			1.17%	2 P:y	-0.424	0.00	4 Re
1.15%	2 P:y	-0.424	0.00	3 Re			
1.08%	1 P:y	-6.559	1.33	7 Se			
1.06%	2 P:y	-0.424	0.00	1 Re			
-10.588	2.00	245 A	9.16%	1 P:x	-6.559	1.33	10 Se

			8.79%	1 P:x	-6.559	1.33	9 Se
			5.25%	1 P:x	-6.559	1.33	13 Se
			4.59%	1 P:y	-6.559	1.33	13 Se
			3.24%	1 P:x	-6.559	1.33	11 Se
			3.13%	1 P:z	-6.559	1.33	9 Se
			3.01%	1 P:z	-6.559	1.33	11 Se
			2.86%	1 P:x	-6.559	1.33	12 Se
			2.78%	1 D:x ² -y ²	-5.431	1.00	1 Re
			2.41%	1 D:z ²	-5.431	1.00	3 Re
			2.21%	1 D:yz	-5.431	1.00	3 Re
			2.04%	1 P:x	-6.559	1.33	14 Se
			1.91%	1 P:y	-5.520	1.00	16 P
			1.76%	1 P:y	-6.559	1.33	11 Se
			1.75%	1 P:x	-6.559	1.33	8 Se
			1.68%	1 D:x ² -y ²	-5.431	1.00	5 Re
			1.38%	2 P:x	-0.424	0.00	3 Re
			1.28%	1 D:x ² -y ²	-5.431	1.00	3 Re
			1.26%	1 P:z	-6.559	1.33	7 Se
			1.26%	1 D:xy	-5.431	1.00	3 Re
			1.22%	1 P:y	-6.559	1.33	14 Se
			1.15%	1 D:xy	-5.431	1.00	2 Re
			1.10%	1 P:x	-6.559	1.33	7 Se
			1.09%	2 P:x	-0.424	0.00	1 Re
			1.03%	1 P:y	-6.559	1.33	8 Se
-10.558	2.00	246 A	12.94%	1 P:z	-6.559	1.33	11 Se
			7.06%	1 P:z	-6.559	1.33	7 Se
			5.08%	1 P:z	-6.559	1.33	13 Se
			4.85%	1 P:z	-6.559	1.33	8 Se
			4.20%	1 D:z ²	-5.431	1.00	4 Re
			3.39%	1 P:y	-6.559	1.33	13 Se
			2.78%	1 P:z	-6.559	1.33	9 Se
			2.37%	1 D:z ²	-5.431	1.00	1 Re
			2.33%	1 D:yz	-5.431	1.00	2 Re
			2.27%	1 D:z ²	-5.431	1.00	3 Re
			2.26%	1 P:x	-5.520	1.00	17 P
			2.20%	1 P:z	-6.559	1.33	12 Se
			2.12%	1 P:z	-6.559	1.33	14 Se
			1.93%	2 P:z	-0.424	0.00	3 Re
			1.92%	2 P:z	-0.424	0.00	1 Re
			1.78%	1 D:z ²	-5.431	1.00	2 Re

			1.71%	1 P:z	-6.559	1.33	10	Se	
			1.65%	1 D:xy	-5.431	1.00	1	Re	
			1.32%	1 P:z	-5.520	1.00	15	P	
			1.30%	2 P:z	-0.424	0.00	4	Re	
			1.28%	1 P:z	-5.520	1.00	17	P	
			1.28%	1 D:yz	-5.431	1.00	4	Re	
			1.23%	1 P:x	-6.559	1.33	13	Se	
			1.22%	1 D:xy	-5.431	1.00	3	Re	
			1.09%	1 P:y	-5.520	1.00	15	P	
			1.08%	1 P:y	-6.559	1.33	8	Se	
-9.994	2.00	247	A	10.20%	1 D:xz	-5.431	1.00	2	Re
				10.19%	1 D:xz	-5.431	1.00	4	Re
				6.94%	1 D:xz	-5.431	1.00	1	Re
				5.01%	1 D:xz	-5.431	1.00	5	Re
				4.05%	1 D:yz	-5.431	1.00	2	Re
				3.96%	1 D:x ² -y ²	-5.431	1.00	4	Re
				3.69%	1 D:xz	-5.431	1.00	3	Re
				3.47%	1 D:yz	-5.431	1.00	3	Re
				3.40%	1 D:yz	-5.431	1.00	4	Re
				3.23%	1 D:x ² -y ²	-5.431	1.00	2	Re
				3.07%	1 P:x	-6.559	1.33	11	Se
				2.77%	1 P:x	-6.559	1.33	13	Se
				2.66%	1 D:yz	-5.431	1.00	6	Re
				2.49%	1 D:x ² -y ²	-5.431	1.00	5	Re
				2.44%	1 P:z	-6.559	1.33	10	Se
				2.38%	1 D:x ² -y ²	-5.431	1.00	1	Re
				2.32%	1 D:xz	-5.431	1.00	6	Re
				2.27%	1 P:z	-6.559	1.33	9	Se
				2.21%	1 P:z	-6.559	1.33	12	Se
				2.10%	1 P:z	-6.559	1.33	14	Se
				2.09%	1 P:x	-6.559	1.33	7	Se
				1.91%	1 P:x	-6.559	1.33	8	Se
				1.83%	2 P:x	-0.424	0.00	6	Re
				1.22%	2 P:x	-0.424	0.00	3	Re
				1.12%	1 D:x ² -y ²	-5.431	1.00	3	Re
				1.08%	2 P:z	-0.424	0.00	5	Re
-9.972	2.00	248	A	8.17%	1 D:yz	-5.431	1.00	3	Re
				7.81%	1 D:yz	-5.431	1.00	6	Re
				6.00%	1 D:xy	-5.431	1.00	3	Re
				5.11%	1 D:xy	-5.431	1.00	6	Re

			4.76%	1 D:xy	-5.431	1.00	1 Re
			4.40%	1 D:yz	-5.431	1.00	1 Re
			3.64%	1 D:xz	-5.431	1.00	1 Re
			3.63%	1 D:yz	-5.431	1.00	5 Re
			3.40%	1 D:xy	-5.431	1.00	5 Re
			3.32%	1 D:xz	-5.431	1.00	5 Re
			3.05%	1 D:yz	-5.431	1.00	2 Re
			3.02%	1 P:z	-6.559	1.33	13 Se
			2.82%	1 P:y	-6.559	1.33	10 Se
			2.55%	1 D:x2-y2	-5.431	1.00	1 Re
			2.35%	1 D:xy	-5.431	1.00	4 Re
			2.32%	1 P:y	-6.559	1.33	11 Se
			2.31%	1 D:x2-y2	-5.431	1.00	5 Re
			2.22%	1 P:y	-6.559	1.33	9 Se
			2.18%	1 P:x	-6.559	1.33	14 Se
			2.07%	1 P:x	-6.559	1.33	12 Se
			2.06%	1 P:z	-6.559	1.33	8 Se
			2.05%	1 P:y	-6.559	1.33	7 Se
			2.05%	1 D:yz	-5.431	1.00	4 Re
			1.72%	1 D:xy	-5.431	1.00	2 Re
			1.51%	2 P:y	-0.424	0.00	2 Re
			1.34%	2 P:y	-0.424	0.00	4 Re
			1.04%	1 D:x2-y2	-5.431	1.00	3 Re
-8.229	0.00	249 A	6.74%	1 D:xy	-5.431	1.00	6 Re
			6.59%	1 D:xy	-5.431	1.00	5 Re
			6.37%	1 D:z2	-5.431	1.00	3 Re
			6.25%	1 D:z2	-5.431	1.00	1 Re
			5.49%	1 D:z2	-5.431	1.00	6 Re
			5.24%	1 P:x	-6.559	1.33	7 Se
			5.04%	1 D:z2	-5.431	1.00	5 Re
			4.91%	1 P:x	-6.559	1.33	8 Se
			4.25%	1 P:z	-6.559	1.33	10 Se
			4.13%	1 P:z	-6.559	1.33	14 Se
			3.86%	1 P:x	-5.375	0.67	45 C
			3.18%	1 D:yz	-5.431	1.00	1 Re
			2.83%	1 P:x	-9.159	1.33	19 O
			2.59%	1 P:z	-5.375	0.67	46 C
			2.31%	1 P:y	-5.375	0.67	46 C
			2.21%	1 D:x2-y2	-5.431	1.00	5 Re
			2.14%	1 D:xz	-5.431	1.00	3 Re

			2.14%	1 P:z	-6.559	1.33	9 Se
			2.01%	1 P:z	-6.559	1.33	12 Se
			2.01%	1 D:xy	-5.431	1.00	3 Re
			1.99%	1 D:yz	-5.431	1.00	3 Re
			1.98%	1 D:xy	-5.431	1.00	1 Re
			1.92%	1 P:z	-5.375	0.67	45 C
			1.86%	1 P:y	-6.559	1.33	9 Se
			1.86%	1 P:z	-9.159	1.33	20 O
			1.69%	1 P:y	-6.559	1.33	8 Se
			1.67%	1 P:y	-9.159	1.33	20 O
			1.60%	1 D:x ² -y ²	-5.431	1.00	6 Re
			1.50%	1 D:xz	-5.431	1.00	1 Re
			-1.46%	2 D:xy	4.925	0.00	5 Re
			1.41%	1 P:y	-6.559	1.33	7 Se
			1.37%	1 P:z	-9.159	1.33	19 O
			-1.32%	2 D:xy	4.925	0.00	6 Re
			1.30%	1 P:y	-6.559	1.33	12 Se
			1.18%	1 P:x	-5.375	0.67	46 C
			1.01%	1 P:x	-6.559	1.33	11 Se
-8.008	0.00	250 A	8.94%	1 D:xy	-5.431	1.00	2 Re
			8.87%	1 D:yz	-5.431	1.00	4 Re
			6.51%	1 P:y	-5.375	0.67	46 C
			6.14%	1 D:x ² -y ²	-5.431	1.00	2 Re
			4.93%	1 P:x	-6.559	1.33	7 Se
			4.30%	1 D:xy	-5.431	1.00	6 Re
			4.21%	1 P:z	-6.559	1.33	10 Se
			4.21%	1 P:y	-9.159	1.33	20 O
			4.16%	1 P:x	-6.559	1.33	12 Se
			3.97%	1 D:yz	-5.431	1.00	6 Re
			3.39%	1 D:x ² -y ²	-5.431	1.00	4 Re
			3.03%	1 D:xy	-5.431	1.00	4 Re
			2.88%	1 D:xy	-5.431	1.00	3 Re
			2.86%	1 D:xz	-5.431	1.00	4 Re
			2.85%	1 P:y	-6.559	1.33	8 Se
			2.75%	1 D:z ²	-5.431	1.00	6 Re
			2.70%	1 D:z ²	-5.431	1.00	2 Re
			2.55%	1 D:x ² -y ²	-5.431	1.00	6 Re
			2.45%	1 P:y	-6.559	1.33	12 Se
			2.18%	1 D:yz	-5.431	1.00	3 Re
			2.14%	1 P:x	-5.375	0.67	46 C

			2.07%	1 P:z	-5.375	0.67	46 C
			1.93%	1 D:z2	-5.431	1.00	3 Re
			1.88%	1 D:z2	-5.431	1.00	4 Re
			1.83%	1 P:y	-6.559	1.33	9 Se
			-1.66%	2 D:xy	4.925	0.00	2 Re
			1.65%	1 D:x2-y2	-5.431	1.00	3 Re
			1.62%	1 P:y	-6.559	1.33	10 Se
			-1.58%	2 D:yz	4.925	0.00	4 Re
			1.52%	1 P:x	-6.559	1.33	14 Se
			1.38%	1 P:x	-9.159	1.33	20 O
			1.35%	1 P:z	-9.159	1.33	20 O
			1.33%	1 P:x	-6.559	1.33	8 Se
			1.09%	1 P:z	-6.559	1.33	8 Se
-7.977	0.00	251 A	9.93%	1 D:x2-y2	-5.431	1.00	2 Re
			6.84%	1 D:xz	-5.431	1.00	4 Re
			6.80%	1 D:z2	-5.431	1.00	2 Re
			6.11%	1 D:z2	-5.431	1.00	4 Re
			5.95%	1 D:x2-y2	-5.431	1.00	5 Re
			5.79%	1 P:y	-5.375	0.67	45 C
			5.43%	1 P:y	-6.559	1.33	7 Se
			5.39%	1 P:z	-6.559	1.33	14 Se
			5.01%	1 D:x2-y2	-5.431	1.00	1 Re
			3.93%	1 D:z2	-5.431	1.00	5 Re
			3.83%	1 P:y	-6.559	1.33	9 Se
			3.74%	1 P:y	-9.159	1.33	19 O
			3.42%	1 D:z2	-5.431	1.00	1 Re
			3.23%	1 D:x2-y2	-5.431	1.00	4 Re
			2.96%	1 P:z	-6.559	1.33	8 Se
			2.84%	1 P:z	-5.375	0.67	45 C
			2.54%	1 D:xz	-5.431	1.00	5 Re
			2.54%	1 P:x	-6.559	1.33	8 Se
			2.14%	1 D:yz	-5.431	1.00	4 Re
			2.08%	1 D:yz	-5.431	1.00	2 Re
			2.04%	1 P:y	-6.559	1.33	11 Se
			2.02%	1 P:x	-5.375	0.67	45 C
			-1.95%	2 D:x2-y2	4.925	0.00	2 Re
			1.83%	1 P:z	-6.559	1.33	13 Se
			1.83%	1 P:z	-9.159	1.33	19 O
			1.78%	1 D:xz	-5.431	1.00	1 Re
			-1.33%	2 D:xz	4.925	0.00	4 Re

			1.30%	1 P:x	-9.159	1.33	19 O
			-1.26%	2 D:z2	4.925	0.00	2 Re
-7.695	0.00	252 A	11.74%	1 D:xz	-5.431	1.00	4 Re
			11.61%	1 D:yz	-5.431	1.00	6 Re
			10.22%	1 D:yz	-5.431	1.00	3 Re
			9.95%	1 D:xz	-5.431	1.00	2 Re
			9.44%	1 D:xz	-5.431	1.00	5 Re
			9.43%	1 D:xz	-5.431	1.00	1 Re
			6.91%	1 D:xy	-5.431	1.00	6 Re
			5.61%	1 D:xy	-5.431	1.00	3 Re
			4.03%	1 D:x2-y2	-5.431	1.00	5 Re
			3.89%	1 D:yz	-5.431	1.00	4 Re
			3.76%	1 D:x2-y2	-5.431	1.00	1 Re
			3.37%	1 D:x2-y2	-5.431	1.00	2 Re
			3.31%	1 D:yz	-5.431	1.00	2 Re
			2.85%	1 D:x2-y2	-5.431	1.00	4 Re
			2.83%	1 D:xy	-5.431	1.00	5 Re
			2.34%	1 D:xy	-5.431	1.00	1 Re
			2.25%	1 D:yz	-5.431	1.00	1 Re
			1.80%	1 D:yz	-5.431	1.00	5 Re
			-1.18%	2 D:xz	4.925	0.00	4 Re
			-1.12%	2 D:yz	4.925	0.00	6 Re
			1.06%	1 D:z2	-5.431	1.00	3 Re
			1.04%	1 D:xy	-5.431	1.00	2 Re

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M U L L I K E N P O P U L A T I O N S

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Atom	Charge	Spin density	S	P	D	F
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1 Re	0.1215		2.4569	6.7494	5.6681	14.0040
2 Re	0.1795		2.4141	6.7402	5.6620	14.0041
3 Re	0.1532		2.4433	6.7357	5.6637	14.0041
4 Re	0.1871		2.4001	6.7491	5.6597	14.0040
5 Re	-0.0194		2.6736	6.7284	5.6127	14.0046
6 Re	-0.0182		2.6703	6.7340	5.6094	14.0046
7 Se	-0.0668		1.9895	3.9583	10.1190	0.0000
8 Se	-0.0819		1.9991	3.9616	10.1212	0.0000

9 Se	-0.1695	2.0214	4.0251	10.1230	0.0000
10 Se	-0.2109	2.0412	4.0460	10.1236	0.0000
11 Se	-0.3392	2.0678	4.1528	10.1185	0.0000
12 Se	-0.2072	2.0340	4.0488	10.1244	0.0000
13 Se	-0.3187	2.0645	4.1334	10.1208	0.0000
14 Se	-0.1982	2.0406	4.0330	10.1246	0.0000
15 P	1.5445	1.3473	1.8358	0.2724	0.0000
16 P	1.5222	1.3397	1.8641	0.2740	0.0000
17 P	1.5348	1.3563	1.8361	0.2728	0.0000
18 P	1.5284	1.3531	1.8459	0.2726	0.0000
19 O	-0.3144	1.8963	4.3553	0.0629	0.0000
20 O	-0.3140	1.8961	4.3550	0.0629	0.0000
21 C	-0.0218	1.1761	2.7940	0.0516	0.0000
22 H	-0.1027	1.0261	0.0767	0.0000	0.0000
23 H	-0.1091	1.0311	0.0780	0.0000	0.0000
24 C	0.3572	1.0089	2.5890	0.0448	0.0000
25 H	-0.1166	1.0403	0.0763	0.0000	0.0000
26 H	-0.1510	1.0731	0.0780	0.0000	0.0000
27 H	-0.1210	1.0438	0.0771	0.0000	0.0000
28 C	-0.0295	1.1892	2.7882	0.0522	0.0000
29 H	-0.1276	1.0520	0.0756	0.0000	0.0000
30 H	-0.0995	1.0248	0.0747	0.0000	0.0000
31 C	0.3636	1.0137	2.5776	0.0451	0.0000
32 H	-0.1356	1.0594	0.0762	0.0000	0.0000
33 H	-0.1473	1.0691	0.0782	0.0000	0.0000
34 H	-0.1026	1.0220	0.0806	0.0000	0.0000
35 C	-0.0389	1.1891	2.7979	0.0519	0.0000
36 H	-0.1000	1.0260	0.0740	0.0000	0.0000
37 H	-0.1321	1.0570	0.0751	0.0000	0.0000
38 C	0.3515	1.0198	2.5834	0.0453	0.0000
39 H	-0.0083	0.9234	0.0849	0.0000	0.0000
40 H	-0.1652	1.0859	0.0793	0.0000	0.0000
41 H	-0.1660	1.0882	0.0778	0.0000	0.0000
42 C	-0.0298	1.1831	2.7953	0.0513	0.0000
43 H	-0.0989	1.0233	0.0756	0.0000	0.0000
44 H	-0.1203	1.0467	0.0735	0.0000	0.0000
45 C	0.3714	1.0093	2.5741	0.0451	0.0000
46 H	-0.0930	1.0132	0.0798	0.0000	0.0000
47 H	-0.1478	1.0694	0.0785	0.0000	0.0000
48 H	-0.1325	1.0558	0.0767	0.0000	0.0000

49	C	0.0026	1.1811	2.7642	0.0521	0.0000
50	H	-0.1115	1.0362	0.0753	0.0000	0.0000
51	H	-0.1245	1.0462	0.0783	0.0000	0.0000
52	C	0.3579	1.0120	2.5853	0.0447	0.0000
53	H	-0.1248	1.0470	0.0778	0.0000	0.0000
54	H	-0.1366	1.0597	0.0769	0.0000	0.0000
55	H	-0.1166	1.0381	0.0785	0.0000	0.0000
56	C	-0.0138	1.1812	2.7812	0.0514	0.0000
57	H	-0.1034	1.0238	0.0796	0.0000	0.0000
58	H	-0.1247	1.0488	0.0759	0.0000	0.0000
59	C	0.3663	1.0125	2.5766	0.0445	0.0000
60	H	-0.1010	1.0221	0.0788	0.0000	0.0000
61	H	-0.1463	1.0688	0.0775	0.0000	0.0000
62	H	-0.1240	1.0451	0.0790	0.0000	0.0000
63	C	-0.0503	1.1907	2.8083	0.0513	0.0000
64	H	-0.1238	1.0484	0.0754	0.0000	0.0000
65	H	-0.1030	1.0296	0.0734	0.0000	0.0000
66	C	0.3655	1.0108	2.5785	0.0452	0.0000
67	H	-0.1375	1.0609	0.0766	0.0000	0.0000
68	H	-0.1601	1.0814	0.0787	0.0000	0.0000
69	H	-0.0778	0.9920	0.0858	0.0000	0.0000
70	C	-0.0274	1.1881	2.7874	0.0520	0.0000
71	H	-0.1013	1.0267	0.0747	0.0000	0.0000
72	H	-0.1218	1.0468	0.0750	0.0000	0.0000
73	C	0.3664	1.0119	2.5768	0.0450	0.0000
74	H	-0.1044	1.0243	0.0801	0.0000	0.0000
75	H	-0.1489	1.0706	0.0783	0.0000	0.0000
76	H	-0.1362	1.0588	0.0773	0.0000	0.0000
77	C	-0.0123	1.1751	2.7855	0.0517	0.0000
78	H	-0.1018	1.0232	0.0786	0.0000	0.0000
79	H	-0.1013	1.0251	0.0762	0.0000	0.0000
80	C	0.3554	1.0114	2.5884	0.0449	0.0000
81	H	-0.1190	1.0417	0.0772	0.0000	0.0000
82	H	-0.1520	1.0739	0.0781	0.0000	0.0000
83	H	-0.1153	1.0389	0.0764	0.0000	0.0000
84	C	-0.0290	1.1894	2.7879	0.0518	0.0000
85	H	-0.0993	1.0254	0.0739	0.0000	0.0000
86	H	-0.1264	1.0513	0.0751	0.0000	0.0000
87	C	0.3604	1.0121	2.5825	0.0451	0.0000
88	H	-0.1068	1.0267	0.0801	0.0000	0.0000

89	H	-0.1447	1.0665	0.0783	0.0000	0.0000
90	H	-0.1275	1.0516	0.0759	0.0000	0.0000
91	C	-0.0063	1.1752	2.7796	0.0515	0.0000
92	H	-0.1020	1.0243	0.0778	0.0000	0.0000
93	H	-0.1031	1.0266	0.0765	0.0000	0.0000
94	C	0.3539	1.0115	2.5898	0.0448	0.0000
95	H	-0.1182	1.0419	0.0764	0.0000	0.0000
96	H	-0.1473	1.0695	0.0778	0.0000	0.0000
97	H	-0.1171	1.0406	0.0766	0.0000	0.0000
98	C	-0.0343	1.1883	2.7942	0.0517	0.0000
99	H	-0.1282	1.0538	0.0744	0.0000	0.0000
100	H	-0.0993	1.0251	0.0742	0.0000	0.0000
101	C	0.3609	1.0139	2.5801	0.0452	0.0000
102	H	-0.1536	1.0763	0.0773	0.0000	0.0000
103	H	-0.1596	1.0804	0.0792	0.0000	0.0000
104	H	-0.0394	0.9582	0.0812	0.0000	0.0000
105	C	0.3088	1.4658	2.1334	0.0921	0.0000
106	C	0.3064	1.4651	2.1365	0.0920	0.0000

Re6Se8 (PEt3) 5 (CO)

E (eV)	Occ	MO	%	SFO (first member)	E (eV)	Occ	Fragment
-10.187	2.00	261 A	13.45%	1 P:y	-6.559	1.33	8 Se
			11.40%	1 P:y	-6.559	1.33	13 Se
			8.27%	1 D:yz	-5.431	1.00	3 Re
			5.01%	1 P:y	-6.559	1.33	14 Se
			4.27%	1 P:y	-6.559	1.33	10 Se
			4.11%	1 P:y	-6.559	1.33	9 Se
			3.83%	1 P:y	-6.559	1.33	7 Se
			3.49%	1 D:x2-y2	-5.431	1.00	1 Re
			3.28%	1 D:x2-y2	-5.431	1.00	6 Re
			2.78%	1 P:y	-6.559	1.33	11 Se
			2.65%	1 P:y	-6.559	1.33	12 Se
			2.39%	1 D:x2-y2	-5.431	1.00	2 Re
			2.36%	1 D:x2-y2	-5.431	1.00	5 Re
			1.79%	1 P:z	-6.559	1.33	8 Se
			1.69%	1 P:z	-6.559	1.33	14 Se

			1.37%	2 P:y	-0.424	0.00	3 Re
			1.15%	2 P:y	-0.424	0.00	1 Re
			1.15%	2 P:y	-0.424	0.00	2 Re
			1.03%	1 D:yz	-5.431	1.00	4 Re
			1.01%	1 P:y	-5.520	1.00	47 P
-10.159	2.00	262 A	10.72%	1 P:x	-6.559	1.33	7 Se
			5.54%	1 P:x	-6.559	1.33	9 Se
			5.23%	1 P:x	-6.559	1.33	11 Se
			4.80%	1 P:z	-6.559	1.33	7 Se
			4.58%	1 D:xz	-5.431	1.00	3 Re
			4.11%	1 P:z	-6.559	1.33	11 Se
			3.20%	1 D:x ² -y ²	-5.431	1.00	5 Re
			2.96%	1 D:x ² -y ²	-5.431	1.00	2 Re
			2.90%	1 P:x	-6.559	1.33	8 Se
			2.88%	1 P:x	-6.559	1.33	13 Se
			2.22%	1 P:z	-5.520	1.00	51 P
			2.00%	1 P:x	-6.559	1.33	10 Se
			1.99%	1 P:x	-6.559	1.33	14 Se
			1.93%	1 P:z	-6.559	1.33	13 Se
			1.93%	1 P:z	-6.559	1.33	10 Se
			1.78%	1 P:x	-6.559	1.33	12 Se
			1.73%	1 D:x ² -y ²	-5.431	1.00	1 Re
			1.69%	1 D:x ² -y ²	-5.431	1.00	6 Re
			1.65%	1 D:xz	-5.431	1.00	6 Re
			1.65%	1 P:z	-6.559	1.33	8 Se
			1.60%	1 D:xz	-5.431	1.00	2 Re
			1.51%	1 P:x	-5.520	1.00	50 P
			1.49%	1 P:y	-5.520	1.00	50 P
			1.29%	2 P:x	-0.424	0.00	6 Re
			1.26%	2 P:x	-0.424	0.00	2 Re
			1.02%	1 P:x	-5.520	1.00	47 P
			1.02%	1 P:y	-6.559	1.33	13 Se
			1.00%	1 P:z	-6.559	1.33	14 Se
-10.124	2.00	263 A	8.10%	1 P:x	-6.559	1.33	9 Se
			5.99%	1 P:z	-6.559	1.33	9 Se
			5.06%	1 P:z	-5.520	1.00	51 P
			4.88%	1 P:z	-6.559	1.33	12 Se
			3.63%	1 P:z	-6.559	1.33	13 Se
			3.45%	1 P:x	-6.559	1.33	12 Se
			3.36%	1 P:z	-6.559	1.33	10 Se

			3.25%	1 P:z	-6.559	1.33	8 Se
			2.76%	1 D:xz	-5.431	1.00	3 Re
			2.75%	1 P:z	-6.559	1.33	14 Se
			2.75%	1 D:xz	-5.431	1.00	5 Re
			2.64%	1 D:xz	-5.431	1.00	1 Re
			2.15%	2 P:z	-0.424	0.00	3 Re
			1.82%	1 D:yz	-5.431	1.00	5 Re
			1.66%	1 P:x	-6.559	1.33	7 Se
			1.58%	1 P:z	-6.559	1.33	7 Se
			1.57%	1 D:yz	-5.431	1.00	1 Re
			1.55%	1 D:yz	-5.431	1.00	6 Re
			1.51%	1 P:z	-6.559	1.33	11 Se
			1.40%	1 D:x ² -y ²	-5.431	1.00	1 Re
			1.37%	1 P:x	-6.559	1.33	13 Se
			1.37%	1 P:x	-5.520	1.00	49 P
			1.34%	1 D:yz	-5.431	1.00	2 Re
			1.33%	1 P:y	-5.520	1.00	49 P
			1.24%	1 P:x	-6.559	1.33	8 Se
			1.17%	1 D:x ² -y ²	-5.431	1.00	6 Re
			1.06%	2 P:x	-0.424	0.00	5 Re
			1.05%	1 P:x	-5.375	0.67	33 C
			1.04%	1 P:y	-5.520	1.00	48 P
			1.03%	1 P:x	-6.559	1.33	14 Se
			1.03%	1 P:x	-5.520	1.00	48 P
			1.03%	1 P:y	-6.559	1.33	13 Se
-9.525	2.00	264 A	15.33%	1 D:z ²	-5.431	1.00	1 Re
			14.61%	1 D:z ²	-5.431	1.00	6 Re
			13.13%	1 D:z ²	-5.431	1.00	2 Re
			12.89%	1 D:z ²	-5.431	1.00	5 Re
			5.82%	1 D:z ²	-5.431	1.00	3 Re
			3.54%	1 D:z ²	-5.431	1.00	4 Re
			3.50%	2 P:z	-0.424	0.00	4 Re
			2.73%	2 P:z	-0.424	0.00	3 Re
			2.20%	1 P:z	-6.559	1.33	9 Se
			2.19%	1 P:z	-6.559	1.33	8 Se
			2.18%	1 P:z	-6.559	1.33	7 Se
			2.04%	1 P:z	-6.559	1.33	13 Se
			1.96%	1 P:z	-6.559	1.33	11 Se
			1.80%	1 D:xy	-5.431	1.00	6 Re
			1.79%	1 P:z	-6.559	1.33	10 Se

			1.78%	1 P:z	-6.559	1.33	12 Se
			1.69%	1 P:z	-6.559	1.33	14 Se
			1.68%	1 D:xy	-5.431	1.00	1 Re
			-1.56%	2 D:z2	4.925	0.00	3 Re
			-1.32%	2 D:z2	4.925	0.00	5 Re
			-1.31%	2 D:z2	4.925	0.00	2 Re
			-1.19%	2 D:z2	4.925	0.00	4 Re
			1.09%	1 P:y	-6.559	1.33	13 Se
			1.09%	1 P:x	-6.559	1.33	7 Se
			-1.07%	2 D:z2	4.925	0.00	1 Re
			1.06%	1 P:y	-6.559	1.33	14 Se
			1.04%	1 P:y	-6.559	1.33	8 Se
			-1.01%	2 D:z2	4.925	0.00	6 Re
			1.01%	1 P:x	-6.559	1.33	11 Se
			1.00%	1 P:x	-6.559	1.33	9 Se
-9.516	2.00	265 A	19.01%	1 D:xy	-5.431	1.00	3 Re
			16.68%	1 D:xy	-5.431	1.00	4 Re
			8.50%	1 D:xy	-5.431	1.00	5 Re
			8.37%	1 D:xy	-5.431	1.00	2 Re
			6.96%	1 D:xy	-5.431	1.00	6 Re
			6.74%	1 D:xy	-5.431	1.00	1 Re
			3.37%	1 P:x	-6.559	1.33	13 Se
			3.30%	1 P:x	-6.559	1.33	14 Se
			3.15%	1 P:x	-6.559	1.33	8 Se
			3.01%	1 P:x	-6.559	1.33	10 Se
			2.85%	1 P:y	-6.559	1.33	7 Se
			2.84%	1 P:y	-6.559	1.33	12 Se
			2.72%	1 P:y	-6.559	1.33	9 Se
			2.61%	1 P:y	-6.559	1.33	11 Se
			2.02%	1 D:z2	-5.431	1.00	2 Re
			1.95%	1 D:z2	-5.431	1.00	5 Re
			-1.73%	2 D:xy	4.925	0.00	5 Re
			-1.67%	2 D:xy	4.925	0.00	2 Re
			-1.65%	2 D:xy	4.925	0.00	6 Re
			-1.63%	2 D:xy	4.925	0.00	1 Re
			1.19%	2 P:y	-0.424	0.00	1 Re
			1.13%	2 P:y	-0.424	0.00	6 Re
			1.11%	2 P:x	-0.424	0.00	1 Re
			1.10%	2 P:x	-0.424	0.00	6 Re
-7.629	0.00	266 A	12.84%	1 D:xz	-5.431	1.00	4 Re

			12.34%	1 P:x	-5.375	0.67	16 C
			8.42%	1 D:xz	-5.431	1.00	3 Re
			7.79%	1 P:x	-9.159	1.33	15 O
			5.94%	1 P:z	-6.559	1.33	11 Se
			5.41%	1 P:z	-6.559	1.33	12 Se
			4.96%	1 P:x	-6.559	1.33	11 Se
			4.55%	1 P:x	-6.559	1.33	12 Se
			4.46%	1 D:yz	-5.431	1.00	6 Re
			4.22%	1 D:yz	-5.431	1.00	1 Re
			4.22%	1 D:yz	-5.431	1.00	2 Re
			4.16%	1 D:yz	-5.431	1.00	5 Re
			3.91%	1 D:xz	-5.431	1.00	1 Re
			3.79%	1 D:xz	-5.431	1.00	6 Re
			3.78%	1 D:xz	-5.431	1.00	5 Re
			3.77%	1 D:xz	-5.431	1.00	2 Re
			-1.99%	2 D:xz	4.925	0.00	4 Re
			1.83%	1 P:x	-6.559	1.33	13 Se
			1.70%	1 P:x	-6.559	1.33	8 Se
			-1.27%	2 P:x	-0.424	0.00	4 Re
			1.10%	1 D:xy	-5.431	1.00	1 Re
			1.06%	1 D:xy	-5.431	1.00	5 Re
			1.03%	1 D:xy	-5.431	1.00	2 Re
			1.00%	1 P:x	-6.559	1.33	10 Se
-7.610	0.00	267 A	13.14%	1 D:yz	-5.431	1.00	4 Re
			12.39%	1 P:y	-5.375	0.67	16 C
			8.26%	1 D:yz	-5.431	1.00	3 Re
			7.79%	1 P:y	-9.159	1.33	15 O
			5.87%	1 P:z	-6.559	1.33	10 Se
			5.53%	1 P:z	-6.559	1.33	14 Se
			4.90%	1 P:y	-6.559	1.33	10 Se
			4.81%	1 P:y	-6.559	1.33	14 Se
			4.54%	1 D:xz	-5.431	1.00	2 Re
			4.43%	1 D:xz	-5.431	1.00	6 Re
			4.04%	1 D:yz	-5.431	1.00	2 Re
			3.98%	1 D:xz	-5.431	1.00	5 Re
			3.93%	1 D:xz	-5.431	1.00	1 Re
			3.80%	1 D:yz	-5.431	1.00	6 Re
			3.76%	1 D:yz	-5.431	1.00	1 Re
			3.69%	1 D:yz	-5.431	1.00	5 Re
			-2.13%	2 D:yz	4.925	0.00	4 Re

			1.84%	1 P:y	-6.559	1.33	7 Se
			1.59%	1 P:y	-6.559	1.33	9 Se
			-1.25%	2 P:y	-0.424	0.00	4 Re
			1.15%	1 D:xy	-5.431	1.00	2 Re
			1.12%	1 P:y	-6.559	1.33	12 Se
			1.11%	1 D:xy	-5.431	1.00	6 Re
			1.05%	1 D:xy	-5.431	1.00	5 Re
-7.221	0.00	268 A	20.20%	1 D:xy	-5.431	1.00	4 Re
			16.17%	1 D:xy	-5.431	1.00	3 Re
			14.34%	1 D:z2	-5.431	1.00	2 Re
			14.07%	1 D:z2	-5.431	1.00	6 Re
			13.62%	1 D:z2	-5.431	1.00	1 Re
			13.31%	1 D:z2	-5.431	1.00	5 Re
			4.63%	1 D:xy	-5.431	1.00	2 Re
			4.62%	1 D:xy	-5.431	1.00	1 Re
			4.60%	1 D:xy	-5.431	1.00	6 Re
			4.58%	1 D:xy	-5.431	1.00	5 Re
			-2.03%	2 D:xy	4.925	0.00	4 Re
			-1.59%	2 D:xy	4.925	0.00	3 Re
			-1.43%	2 D:z2	4.925	0.00	2 Re
			-1.37%	2 D:z2	4.925	0.00	6 Re
			-1.35%	2 D:z2	4.925	0.00	1 Re
			-1.31%	2 D:z2	4.925	0.00	5 Re
-7.152	0.00	269 A	23.00%	1 D:x2-y2	-5.431	1.00	2 Re
			22.08%	1 D:x2-y2	-5.431	1.00	6 Re
			21.42%	1 D:x2-y2	-5.431	1.00	1 Re
			20.55%	1 D:x2-y2	-5.431	1.00	5 Re
			3.65%	1 P:x	-6.559	1.33	8 Se
			3.58%	1 P:y	-6.559	1.33	7 Se
			3.42%	1 P:x	-6.559	1.33	13 Se
			-3.34%	2 D:x2-y2	4.925	0.00	2 Re
			3.30%	1 P:x	-6.559	1.33	10 Se
			3.16%	1 P:y	-6.559	1.33	12 Se
			-3.09%	2 D:x2-y2	4.925	0.00	1 Re
			3.08%	1 P:x	-6.559	1.33	14 Se
			3.08%	1 P:y	-6.559	1.33	9 Se
			-3.08%	2 D:x2-y2	4.925	0.00	6 Re
			2.98%	1 P:y	-6.559	1.33	11 Se
			-2.90%	2 D:x2-y2	4.925	0.00	5 Re

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M U L L I K E N P O P U L A T I O N S

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Atom	Charge	Spin density	S	P	D	F
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1 Re	0.1074		2.4754	6.7330	5.6801	14.0041
2 Re	0.1146		2.4609	6.7366	5.6837	14.0041
3 Re	0.0851		2.4952	6.7289	5.6867	14.0042
4 Re	-0.0573		2.6945	6.7338	5.6245	14.0046
5 Se	-0.3205		2.0533	4.1440	10.1232	0.0000
6 Se	-0.2810		2.0441	4.1125	10.1244	0.0000
7 Se	-0.2642		2.0376	4.1023	10.1242	0.0000
8 Se	-0.2227		2.0337	4.0652	10.1238	0.0000
9 Se	-0.2240		2.0332	4.0673	10.1235	0.0000
10 Se	-0.2431		2.0359	4.0832	10.1239	0.0000
11 O	-0.3241		1.8940	4.3677	0.0624	0.0000
12 C	0.2876		1.4693	2.1504	0.0927	0.0000
13 Re	0.1079		2.4696	6.7368	5.6815	14.0042
14 Re	0.1161		2.4621	6.7374	5.6803	14.0041
15 Se	-0.2774		2.0460	4.1085	10.1229	0.0000
16 Se	-0.2304		2.0343	4.0723	10.1237	0.0000
17 P	1.4145		1.3348	1.9763	0.2743	0.0000
18 P	1.4199		1.3318	1.9738	0.2745	0.0000
19 P	1.4158		1.3310	1.9789	0.2743	0.0000
20 P	1.4105		1.3368	1.9789	0.2738	0.0000
21 P	1.4404		1.3263	1.9578	0.2756	0.0000
22 C	0.0143		1.1778	2.7558	0.0521	0.0000
23 C	0.3667		1.0156	2.5729	0.0447	0.0000
24 H	-0.1226		1.0478	0.0748	0.0000	0.0000
25 H	-0.1218		1.0432	0.0786	0.0000	0.0000
26 H	-0.1407		1.0638	0.0769	0.0000	0.0000
27 H	-0.1062		1.0257	0.0805	0.0000	0.0000
28 H	-0.1261		1.0466	0.0795	0.0000	0.0000
29 C	0.0117		1.1787	2.7575	0.0521	0.0000
30 C	0.3634		1.0143	2.5775	0.0447	0.0000
31 H	-0.1180		1.0421	0.0759	0.0000	0.0000
32 H	-0.1089		1.0327	0.0762	0.0000	0.0000
33 H	-0.1435		1.0665	0.0770	0.0000	0.0000

34 H	-0.1058	1.0257	0.0801	0.0000	0.0000
35 H	-0.1263	1.0473	0.0790	0.0000	0.0000
36 C	0.0098	1.1783	2.7602	0.0517	0.0000
37 C	0.3636	1.0148	2.5770	0.0447	0.0000
38 H	-0.1225	1.0452	0.0773	0.0000	0.0000
39 H	-0.1069	1.0276	0.0794	0.0000	0.0000
40 H	-0.1385	1.0616	0.0769	0.0000	0.0000
41 H	-0.1089	1.0286	0.0803	0.0000	0.0000
42 H	-0.1246	1.0450	0.0796	0.0000	0.0000
43 C	0.0088	1.1783	2.7613	0.0517	0.0000
44 C	0.3646	1.0148	2.5759	0.0447	0.0000
45 H	-0.1209	1.0429	0.0781	0.0000	0.0000
46 H	-0.1047	1.0259	0.0788	0.0000	0.0000
47 H	-0.1375	1.0606	0.0768	0.0000	0.0000
48 H	-0.1091	1.0288	0.0803	0.0000	0.0000
49 H	-0.1257	1.0459	0.0798	0.0000	0.0000
50 C	0.0141	1.1774	2.7565	0.0520	0.0000
51 C	0.3678	1.0152	2.5723	0.0447	0.0000
52 H	-0.1237	1.0490	0.0747	0.0000	0.0000
53 H	-0.1202	1.0413	0.0789	0.0000	0.0000
54 H	-0.1409	1.0640	0.0769	0.0000	0.0000
55 H	-0.1051	1.0244	0.0807	0.0000	0.0000
56 H	-0.1248	1.0455	0.0793	0.0000	0.0000
57 C	0.0116	1.1792	2.7571	0.0521	0.0000
58 C	0.3665	1.0135	2.5752	0.0447	0.0000
59 H	-0.1215	1.0457	0.0758	0.0000	0.0000
60 H	-0.1174	1.0414	0.0760	0.0000	0.0000
61 H	-0.1427	1.0658	0.0769	0.0000	0.0000
62 H	-0.1058	1.0257	0.0801	0.0000	0.0000
63 H	-0.1253	1.0458	0.0794	0.0000	0.0000
64 C	0.0093	1.1774	2.7613	0.0520	0.0000
65 C	0.3614	1.0150	2.5788	0.0448	0.0000
66 H	-0.1179	1.0398	0.0781	0.0000	0.0000
67 H	-0.1066	1.0300	0.0766	0.0000	0.0000
68 H	-0.1424	1.0655	0.0769	0.0000	0.0000
69 H	-0.1066	1.0265	0.0800	0.0000	0.0000
70 H	-0.1272	1.0479	0.0793	0.0000	0.0000
71 C	0.0091	1.1771	2.7618	0.0519	0.0000
72 C	0.3641	1.0151	2.5761	0.0447	0.0000
73 H	-0.1212	1.0455	0.0757	0.0000	0.0000

74 H	-0.1148	1.0336	0.0812	0.0000	0.0000
75 H	-0.1405	1.0636	0.0770	0.0000	0.0000
76 H	-0.1084	1.0278	0.0806	0.0000	0.0000
77 H	-0.1243	1.0446	0.0797	0.0000	0.0000
78 C	0.0074	1.1802	2.7602	0.0523	0.0000
79 C	0.3617	1.0166	2.5769	0.0448	0.0000
80 H	-0.1227	1.0478	0.0749	0.0000	0.0000
81 H	-0.1202	1.0425	0.0777	0.0000	0.0000
82 H	-0.1401	1.0633	0.0768	0.0000	0.0000
83 H	-0.1055	1.0252	0.0803	0.0000	0.0000
84 H	-0.1264	1.0473	0.0791	0.0000	0.0000
85 C	0.0139	1.1769	2.7570	0.0521	0.0000
86 C	0.3685	1.0157	2.5710	0.0448	0.0000
87 H	-0.1181	1.0433	0.0748	0.0000	0.0000
88 H	-0.1184	1.0392	0.0792	0.0000	0.0000
89 H	-0.1382	1.0615	0.0768	0.0000	0.0000
90 H	-0.1091	1.0283	0.0808	0.0000	0.0000
91 H	-0.1256	1.0455	0.0801	0.0000	0.0000
92 C	0.0106	1.1794	2.7578	0.0522	0.0000
93 C	0.3651	1.0147	2.5755	0.0448	0.0000
94 H	-0.1187	1.0431	0.0756	0.0000	0.0000
95 H	-0.1168	1.0403	0.0764	0.0000	0.0000
96 H	-0.1441	1.0672	0.0769	0.0000	0.0000
97 H	-0.1050	1.0246	0.0804	0.0000	0.0000
98 H	-0.1254	1.0462	0.0792	0.0000	0.0000
99 C	0.0084	1.1776	2.7622	0.0518	0.0000
100 C	0.3662	1.0144	2.5748	0.0447	0.0000
101 H	-0.1228	1.0445	0.0782	0.0000	0.0000
102 H	-0.1096	1.0315	0.0781	0.0000	0.0000
103 H	-0.1377	1.0608	0.0769	0.0000	0.0000
104 H	-0.1092	1.0288	0.0804	0.0000	0.0000
105 H	-0.1227	1.0424	0.0802	0.0000	0.0000
106 C	0.0082	1.1782	2.7619	0.0517	0.0000
107 C	0.3662	1.0149	2.5742	0.0446	0.0000
108 H	-0.1073	1.0286	0.0788	0.0000	0.0000
109 H	-0.1224	1.0442	0.0781	0.0000	0.0000
110 H	-0.1374	1.0605	0.0768	0.0000	0.0000
111 H	-0.1240	1.0439	0.0802	0.0000	0.0000
112 H	-0.1100	1.0297	0.0803	0.0000	0.0000
113 C	0.0134	1.1776	2.7569	0.0520	0.0000

114	C	0.3684	1.0155	2.5713	0.0447	0.0000
115	H	-0.1205	1.0421	0.0785	0.0000	0.0000
116	H	-0.1245	1.0497	0.0749	0.0000	0.0000
117	H	-0.1392	1.0624	0.0768	0.0000	0.0000
118	H	-0.1251	1.0454	0.0797	0.0000	0.0000
119	H	-0.1066	1.0258	0.0808	0.0000	0.0000
120	C	0.0116	1.1792	2.7571	0.0520	0.0000
121	C	0.3654	1.0134	2.5765	0.0447	0.0000
122	H	-0.1111	1.0350	0.0761	0.0000	0.0000
123	H	-0.1221	1.0463	0.0758	0.0000	0.0000
124	H	-0.1436	1.0666	0.0770	0.0000	0.0000
125	H	-0.1247	1.0455	0.0791	0.0000	0.0000
126	H	-0.1060	1.0257	0.0802	0.0000	0.0000