

Supporting information

TDDFT Studies on Chiral Organophosphonate Substituted Divacant Keggin-Type Polyoxotungstate: Diplex Multistep-Redox-Triggered Chiroptical and NLO Switch

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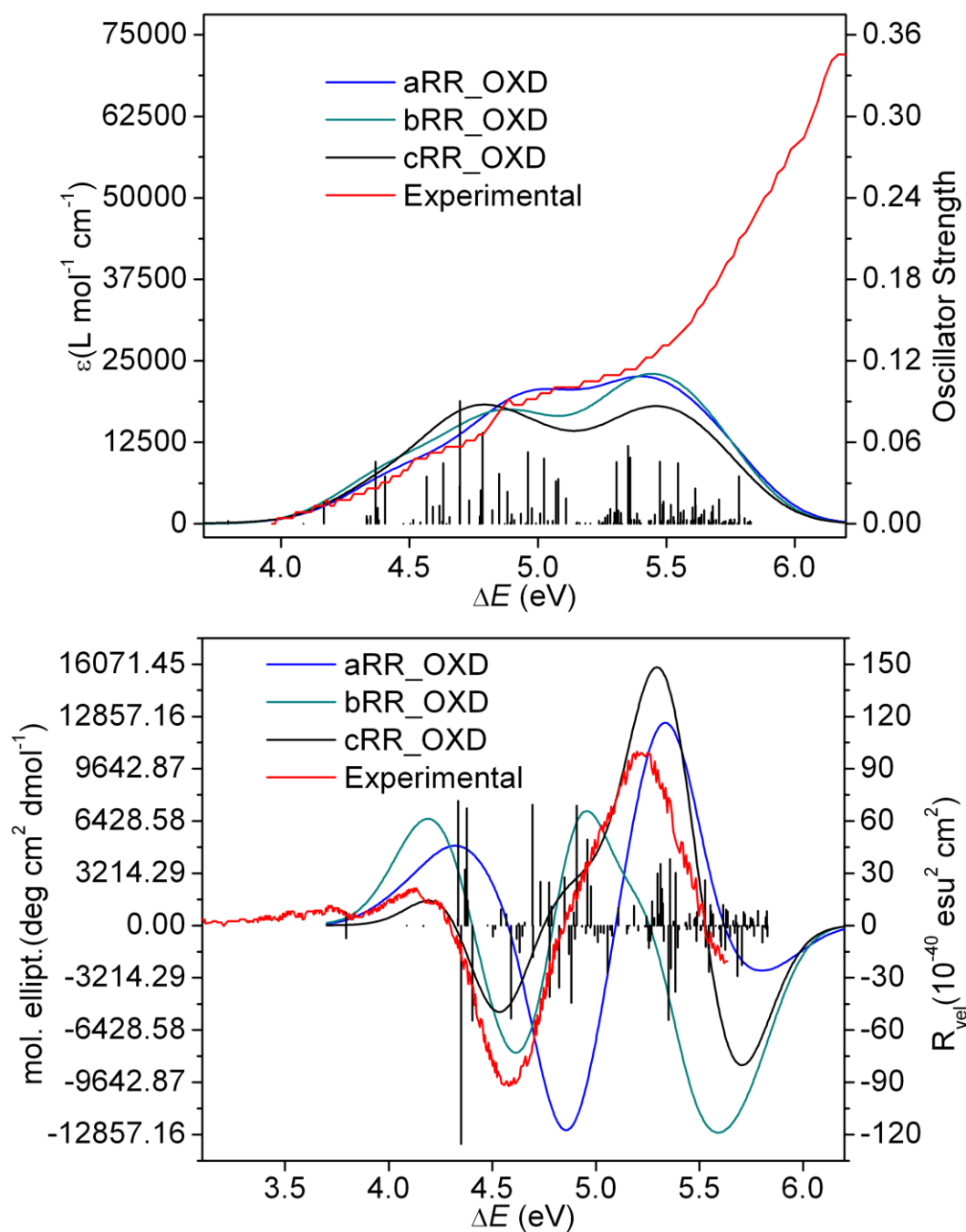


Figure S1 The UV-Vis and ECD spectra of three conformations for OXD. The simulated spectra are shifted by +0.2 eV.

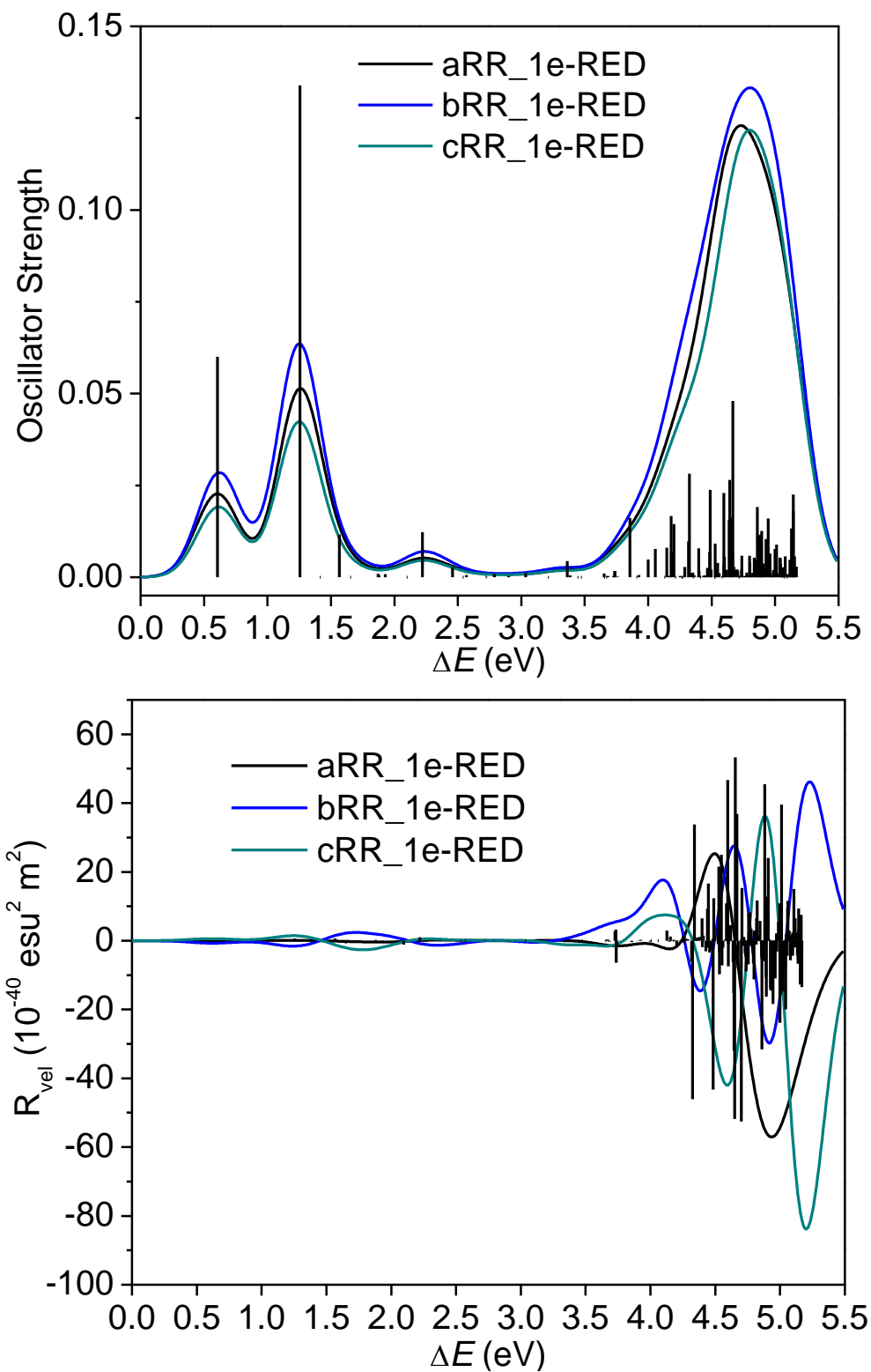


Figure S2 The UV-Vis and ECD spectra of three conformations for 1e-RED.

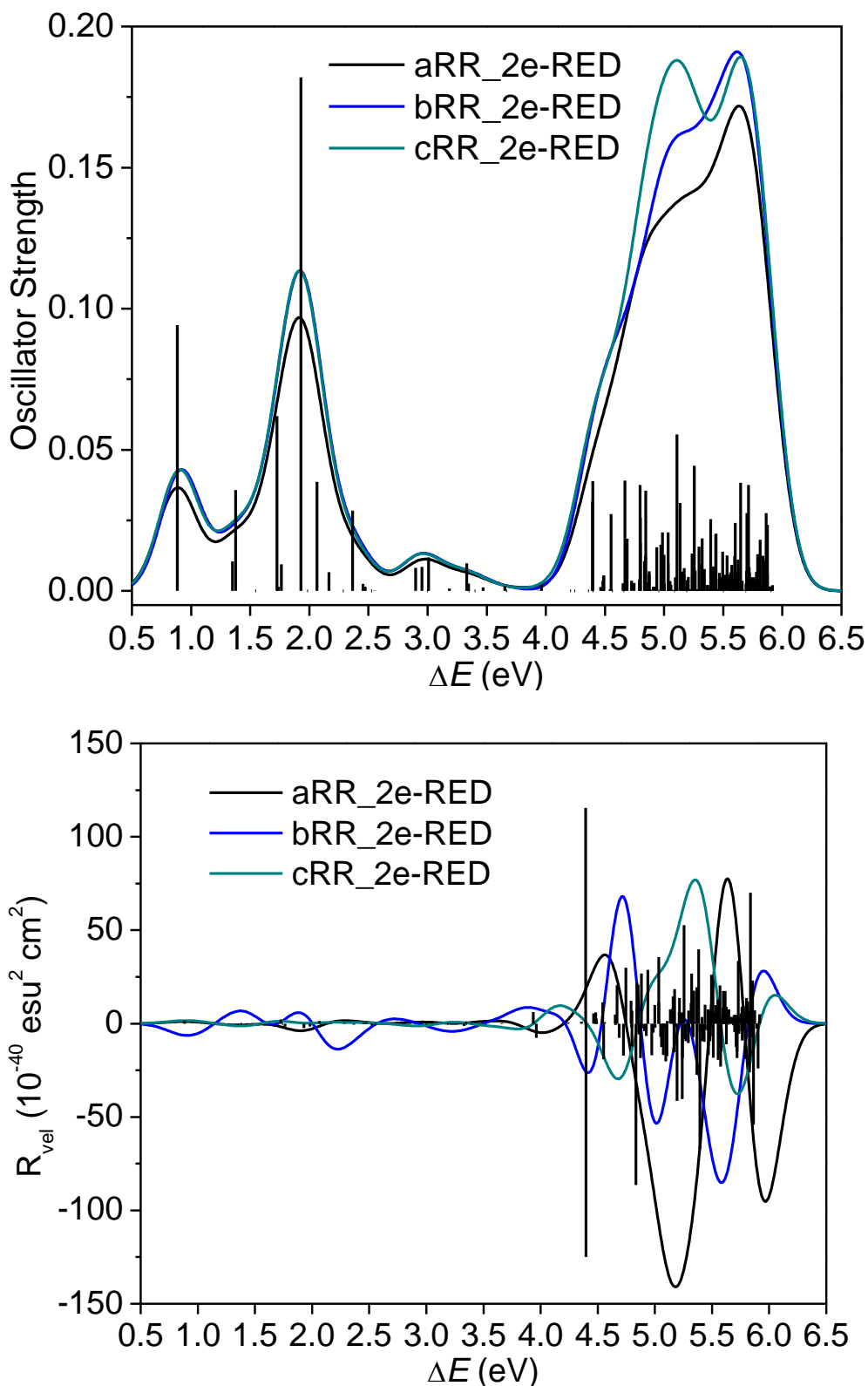
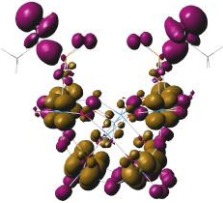
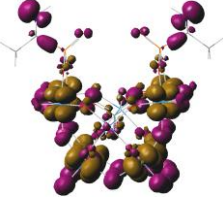
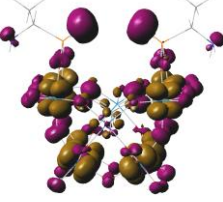
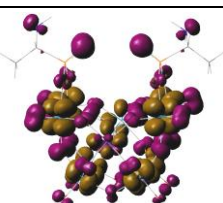
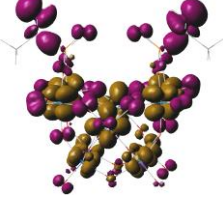
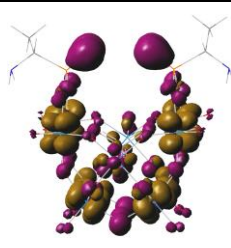
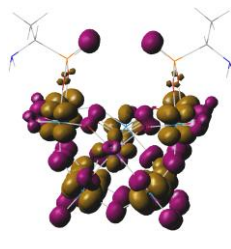
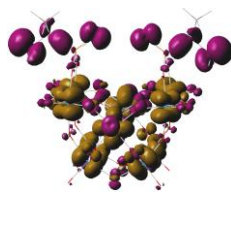
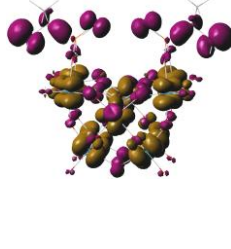
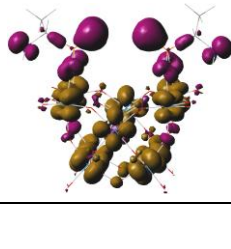


Figure S3 The UV-Vis and ECD spectra of three conformations for 2e-RED.

Table S1 The selected excited states for OXD.

excitation	symmetry	ΔE (eV)	f	MO	coefficient	EDDM
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6(cRR)	A	4.14	0.004	244 → 272	0.11502	
				258 → 272	0.26981	
				262 → 272	-0.10155	
				263 → 273	-0.17871	
				264 → 276	-0.12732	
				265 → 273	-0.20159	
				270 → 272	0.37233	
				271 → 273	-0.22234	
7(cRR)	A	4.15	0.006	258 → 272	0.37573	
				261 → 272	0.16676	
				262 → 272	0.11402	
				263 → 273	0.17130	
				264 → 276	-0.15407	
				265 → 273	-0.23258	
				270 → 272	-0.21772	
				271 → 273	0.12653	
10(bRR)	A	4.17	0.024	257 → 272	-0.19462	
				259 → 272	0.17115	
				259 → 276	-0.10166	
				262 → 273	-0.24446	
				263 → 272	0.29046	
				266 → 272	0.13032	
				267 → 273	0.18421	
				268 → 273	0.11782	
				269 → 272	0.21482	
11(cRR)	B	4.20	0.035	253 → 272	0.13724	
				253 → 276	0.10941	
				256 → 272	0.18511	
				257 → 272	0.13952	
				259 → 273	0.21894	
				260 → 273	0.14265	
				262 → 273	0.23208	
				263 → 272	-0.14600	
				264 → 277	-0.10385	
				265 → 275	-0.10444	
				267 → 272	0.10243	
				268 → 273	0.18661	
271 → 275	-0.13401					
18(cRR)	B	4.39	0.013	255 → 275	-0.14599	
				256 → 272	0.21591	
				259 → 273	0.11913	
				260 → 273	-0.26649	
				262 → 274	-0.12309	
				270 → 277	0.14735	

				271 → 275	0.31589	
30(bRR)	B	4.58	0.015	246 → 272	0.31585	
				250 → 272	0.13958	
				263 → 273	-0.13643	
				268 → 272	0.16343	
				268 → 276	-0.17288	
				269 → 273	0.31880	
31(bRR)	B	4.58	0.063	246 → 272	-0.15706	
				247 → 272	0.20699	
				253 → 275	0.11226	
				254 → 273	0.10812	
				256 → 272	-0.18391	
				262 → 272	-0.13286	
				264 → 273	0.12379	
				264 → 274	0.17820	
				265 → 276	-0.19609	
269 → 273	-0.14473					
44(bRR)	B	4.76	0.022	240 → 273	-0.14450	
				241 → 272	0.16887	
				244 → 272	-0.15880	
				249 → 275	-0.11406	
				250 → 275	-0.17512	
				254 → 274	0.14168	
				270 → 277	-0.17110	
				270 → 280	-0.16278	
				271 → 275	0.18707	
				271 → 279	0.21847	
				271 → 284	0.14835	
45(bRR)	B	4.76	0.038	243 → 272	0.10204	
				244 → 275	0.12852	
				246 → 272	0.18846	
				250 → 272	-0.17964	
				260 → 274	-0.11043	
				263 → 273	0.10233	
				270 → 277	-0.12496	
				270 → 280	-0.13628	
				271 → 275	0.14501	
				271 → 279	0.16694	
				271 → 284	0.13022	
71(bRR)	A	5.10	0.012	235 → 272	0.10759	
				248 → 274	0.12099	
				255 → 274	-0.12495	
				263 → 272	-0.11957	
				266 → 272	-0.11818	

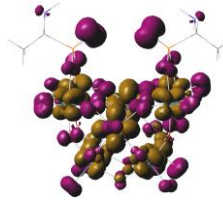
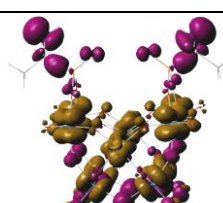
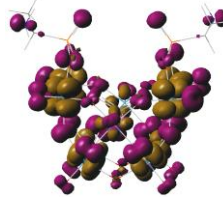
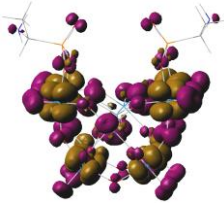
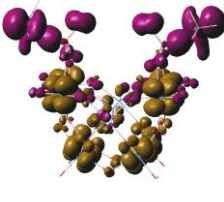

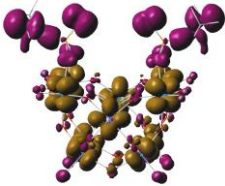
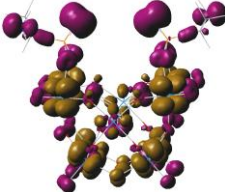
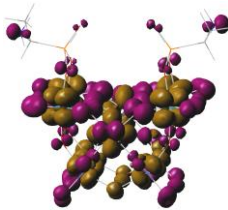
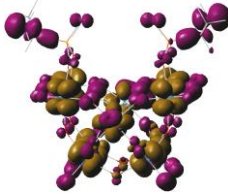
				268 → 273	-0.11888	
				268 → 277	0.10033	
				269 → 272	0.14714	
				269 → 275	0.18886	
				270 → 282	0.12230	
				271 → 287	-0.10686	
78(cRR)	B	5.16	0.049	231 → 275	-0.11647	
				246 → 275	0.10533	
				255 → 275	0.11659	
				256 → 275	-0.12430	
				258 → 274	-0.10344	
				259 → 274	-0.11423	
				260 → 274	0.13232	
				266 → 273	-0.13063	
				267 → 272	-0.13045	
126(cRR)	B	5.51	0.018	248 → 275	-0.10366	
				258 → 280	-0.18715	
				264 → 277	0.18842	
				270 → 277	0.12750	
				271 → 279	0.18571	

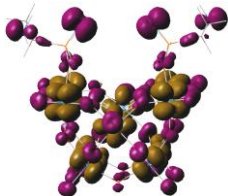
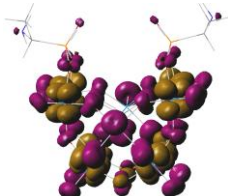
Table S2 The selected excited states of aRR conformation for 1e-RED.

excitation	$\Delta E(\text{eV})$	f	MO	coefficient	EDDM
54	4.32	0.028	249A → 275A	-0.12732	
			257A → 273A	0.13849	
			258A → 275A	-0.18034	
			261A → 273A	-0.21202	
			262A → 273A	0.26482	
			262A → 274A	0.11109	
			264A → 276A	-0.12777	
			265A → 277A	-0.11304	
			270A → 276A	0.10883	
			271A → 277A	0.11051	
			271A → 278A	0.10469	
			242B → 273B	-0.11752	
			246B → 272B	0.12182	
			249B → 272B	-0.11403	
			256B → 272B	-0.13945	
			257B → 272B	0.12710	
			257B → 275B	-0.11153	
			258B → 273B	0.13200	
			259B → 272B	-0.22036	
			259B → 276B	-0.10764	
261B → 273B	0.25754				

			262B → 277B	0.13407	
			264B → 273B	0.23695	
			264B → 274B	-0.11512	
			266B → 278B	0.13598	
			269B → 273B	-0.11812	
55	4.34	0.001	257A → 273A	-0.21348	
			259A → 273A	-0.14829	
			261A → 273A	-0.14067	
			263A → 275A	0.25164	
			264A → 273A	0.10224	
			266A → 273A	0.10446	
			241B → 273B	-0.11941	
			245B → 273B	-0.13658	
			248B → 273B	0.11634	
			250B → 272B	-0.13595	
			251B → 275B	-0.10053	
			254B → 273B	0.21764	
			257B → 272B	0.34289	
			258B → 273B	-0.22922	
			259B → 272B	0.16336	
			262B → 273B	-0.23521	
			263B → 272B	0.19468	
			263B → 276B	0.13667	
			266B → 276B	-0.14854	
71	4.48	0.007	251A → 273A	-0.12067	
			253A → 273A	-0.15188	
			260A → 275A	0.12922	
			265A → 274A	0.11058	
			251B → 273B	-0.11980	
			254B → 272B	-0.11116	
			257B → 273B	-0.12548	
			260B → 272B	-0.14931	
			267B → 273B	-0.10056	
			268B → 273B	0.16314	
			270B → 272B	0.41763	
			270B → 273B	-0.11314	
			271B → 273B	-0.32694	
			271B → 274B	-0.13982	
87	4.60	0.023	245A → 273A	0.10326	
			253A → 275A	0.10449	
			270A → 273A	-0.11898	
			270A → 274A	0.23217	
			271A → 275A	0.18934	
			238B → 273B	0.11671	

			239B → 272B	-0.12875	
			250B → 272B	-0.16682	
			254B → 273B	0.14018	
			256B → 275B	-0.16532	
			262B → 273B	0.17213	
			262B → 274B	0.14976	
			265B → 273B	-0.12340	
			266B → 272B	-0.12363	
			266B → 276B	0.17781	
			267B → 276B	0.15777	
96	4.65	0.016	238A → 273A	-0.12571	
			239A → 275A	0.10957	
			247A → 273A	0.15072	
			259A → 273A	-0.11133	
			266A → 273A	0.23689	
			267A → 275A	-0.14640	
			270A → 276A	0.14764	
			271A → 275A	-0.14166	
			271A → 277A	0.11807	
			271A → 278A	0.12051	
			239B → 272B	-0.12622	
			247B → 272B	0.14138	
			250B → 272B	-0.13931	
			254B → 273B	-0.10999	
			255B → 274B	-0.15379	
			256B → 275B	0.16289	
			261B → 277B	0.11055	
			262B → 274B	-0.14676	
			270B → 277B	0.18447	
			271B → 275B	0.25170	
			271B → 278B	0.12887	
97	4.65	0.016	236A → 273A	0.10127	
			239A → 273A	0.11873	
			244A → 273A	0.12617	
			248A → 273A	0.22276	
			250A → 273A	0.10606	
			263A → 273A	0.11916	
			264A → 275A	0.10237	
			265A → 273A	-0.11933	
			266A → 275A	0.10855	
			267A → 273A	-0.21869	
			271A → 276A	0.12296	
			239B → 273B	-0.16661	
			243B → 273B	-0.10626	

			247B → 273B	-0.11408	
			248B → 272B	0.10888	
			254B → 272B	-0.10372	
			255B → 272B	-0.10158	
			265B → 272B	-0.12438	
			266B → 273B	-0.10972	
			266B → 274B	0.12317	
			267B → 273B	0.10526	
			268B → 273B	-0.16116	
			269B → 272B	-0.10813	
			270B → 275B	0.13361	
			271B → 277B	0.11401	
103	4.70	0.002	238A → 275A	-0.11987	
			239A → 273A	0.14062	
			244A → 273A	-0.14198	
			244A → 274A	-0.10461	
			250A → 273A	0.19263	
			250A → 274A	0.18103	
			253A → 273A	0.18991	
			253A → 274A	0.10061	
			256A → 273A	-0.16894	
			260A → 277A	0.27891	
			260A → 278A	0.10077	
			270A → 275A	0.14286	
			244B → 274B	0.10400	
			245B → 272B	0.18469	
			250B → 273B	0.22772	
			252B → 275B	0.12807	
			253B → 273B	0.13837	
			260B → 275B	-0.15832	
			261B → 275B	-0.21421	
			263B → 274B	0.13291	
134	4.86	0.019	238A → 273A	0.11894	
			241A → 273A	-0.11185	
			245A → 273A	-0.20982	
			250A → 275A	-0.14643	
			253A → 275A	-0.11684	
			255A → 277A	-0.18018	
			256A → 275A	0.11691	
			259A → 273A	0.20846	
			260A → 276A	-0.11265	
			270A → 274A	-0.13965	
			272A → 308A	0.10397	
			244B → 272B	0.17896	

			250B → 272B	-0.17982	
			253B → 272B	-0.12327	
			263B → 272B	-0.17395	
			270B → 274B	0.21997	
			271B → 276B	0.14165	
137	4.88	0.012	235A → 273A	0.10377	
			238A → 273A	0.10286	
			244A → 275A	0.12847	
			245A → 273A	-0.13029	
			250A → 275A	-0.11325	
			251A → 277A	0.12802	
			255A → 277A	-0.13068	
			256A → 275A	0.12847	
			264A → 274A	-0.11205	
			265A → 275A	-0.13135	
			266A → 273A	0.19056	
			240B → 273B	-0.11409	
			241B → 274B	0.11194	
			244B → 272B	-0.15706	
			246B → 272B	0.13096	
			247B → 272B	0.18669	
			251B → 275B	-0.11160	
			255B → 273B	0.11512	
			256B → 275B	-0.11257	
			257B → 272B	0.11493	
			265B → 273B	0.15040	
			266B → 272B	0.13883	
			266B → 276B	0.12232	
			270B → 274B	-0.16825	
			271B → 276B	-0.11666	
161	5.00	0.008	237A → 273A	-0.10989	
			240A → 273A	0.16699	
			241A → 273A	0.24238	
			242A → 273A	-0.21982	
			246A → 275A	0.11294	
			247A → 273A	0.20895	
			249A → 275A	-0.11235	
			252A → 273A	0.26478	
			257A → 273A	-0.18467	
			262A → 273A	-0.19276	
			246B → 272B	0.10930	
			256B → 272B	0.23859	

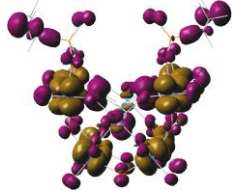
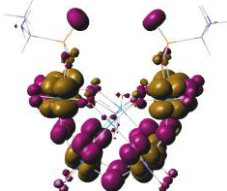
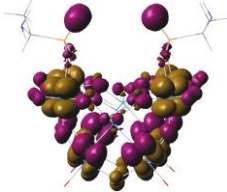

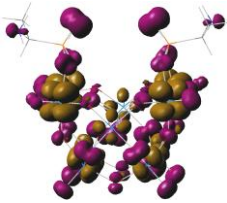
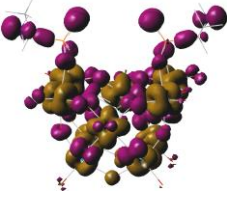
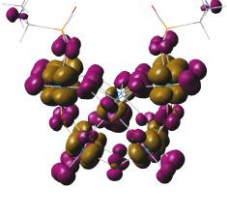
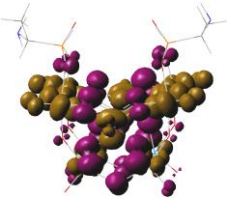
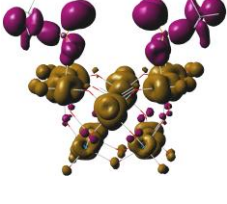
163	5.01	0.009	233A → 273A	0.16718	
			241A → 273A	-0.11465	
			244A → 275A	0.14249	
			245A → 273A	0.12650	
			247A → 273A	0.17715	
			248A → 275A	0.13198	
			263A → 275A	0.11713	
			246B → 272B	-0.13236	
			256B → 272B	-0.16448	
			270B → 281B	-0.12888	
271B → 278B	-0.13004				

Table S3 The selected excited states of aRR conformation for 2e-RED.

excitation	$\Delta E(\text{eV})$	f	MO	coefficient	EDDM
36	4.39	0.032	246 → 273	-0.18156	
			256 → 274	-0.14115	
			261 → 273	0.10072	
			263 → 273	0.39221	
			264 → 273	0.14306	
			265 → 273	-0.10835	
			267 → 274	-0.23719	
			269 → 273	0.10278	
37	4.40	0.039	247 → 274	0.10878	
			250 → 274	-0.10612	
			253 → 273	-0.10096	
			261 → 273	0.22463	
			263 → 273	-0.17136	
			264 → 273	0.37217	
			267 → 274	0.13761	
			267 → 278	0.12947	
269 → 273	0.20977				
55	4.83	0.011	246 → 273	-0.16936	
			254 → 275	-0.10750	
			257 → 277	-0.17688	
			260 → 275	-0.13345	
			270 → 273	-0.18057	
			270 → 275	0.26834	
			271 → 274	0.30007	
			271 → 282	-0.10380	
272 → 313	-0.17050				

90	5.20	0.004	236 → 273	0.17546	
			239 → 273	-0.12707	
			243 → 273	-0.10086	
			248 → 273	-0.14477	
			249 → 273	-0.12014	
			254 → 274	0.12813	
			256 → 273	-0.10251	
			260 → 274	0.10582	
			263 → 274	0.17487	
			264 → 277	0.13026	
			266 → 273	0.15715	
			267 → 273	0.12716	
269 → 277	0.10054				
97	5.25	0.044	244 → 278	0.10096	
			259 → 275	-0.12228	
			261 → 275	-0.12195	
			261 → 279	0.10079	
			264 → 276	-0.11498	
			267 → 281	0.13235	
			269 → 276	-0.11001	
			270 → 275	-0.10888	
271 → 274	0.10198				
114	5.39	0.025	232 → 273	0.15904	
			236 → 273	0.10947	
			242 → 274	-0.11298	
			245 → 274	0.12541	
			248 → 276	0.16757	
			252 → 273	0.10135	
			255 → 274	0.11243	
			256 → 276	0.12726	
			258 → 275	0.10608	
262 → 276	0.12780				
186	5.84	0.012	257 → 279	0.12067	
191	5.86	0.028	238 → 273	-0.10057	
			268 → 281	-0.13489	
			269 → 279	0.16163	
			270 → 289	-0.11357	
			271 → 278	0.10307	
			271 → 288	-0.14335	

Cartesian coordinates (Angstrom) of studied compounds:

aRR_OXD:

Atom	X	Y	Z
1.P	-0.087660	2.780665	3.987832
2.O	-0.056032	1.821154	5.136451
3.O	-1.369254	2.594877	3.059749
4.W	-1.759156	2.876172	1.107059
5.O	-0.046094	1.389213	0.958677
6.Si	0.000000	0.000000	0.107639
7.O	0.046094	-1.389213	0.958677
8.W	1.759156	-2.876172	1.107059
9.O	1.369254	-2.594877	3.059749
10.P	0.087660	-2.780665	3.987832
11.O	-2.942062	4.151450	1.314249
12.O	-0.134226	3.957286	1.084162
13.W	1.561139	2.992093	1.094639
14.O	1.197952	2.684489	3.054373
15.O	-2.909474	1.307719	1.111541
16.W	-3.598424	-0.122428	0.001658
17.O	-1.359164	-0.045419	-0.848037
18.W	-1.850643	-1.764865	-2.378217
19.O	0.059511	-1.765261	-2.683081
20.W	1.966117	-1.645136	-2.370055
21.O	1.359164	0.045419	-0.848037
22.W	1.850643	1.764865	-2.378217
23.O	2.065774	0.065620	-3.319005
24.O	-1.737545	2.814688	-0.817685
25.W	-1.966117	1.645136	-2.370055
26.O	-0.059511	1.765261	-2.683081
27.O	2.942062	-4.151450	1.314249
28.O	0.134226	-3.957286	1.084162
29.W	-1.561139	-2.992093	1.094639
30.O	-1.197952	-2.684489	3.054373
31.O	-2.656131	-4.343609	1.307835
32.O	-2.814581	-1.503575	1.108608
33.O	-1.545807	-2.924745	-0.824392
34.O	2.909474	-1.307719	1.111541
35.W	3.598424	0.122428	0.001658
36.O	3.540874	1.411158	-1.470125
37.O	1.737545	-2.814688	-0.817685
38.O	2.656131	4.343609	1.307835
39.O	2.814581	1.503575	1.108608

40.O	1.545807	2.924745	-0.824392
41.O	-5.281643	-0.183167	0.464981
42.O	-3.628829	1.170037	-1.467686
43.O	-3.540874	-1.411158	-1.470125
44.O	5.281643	0.183167	0.464981
45.O	3.628829	-1.170037	-1.467686
46.O	-2.577394	2.740699	-3.587150
47.O	-2.065774	-0.065620	-3.319005
48.O	-2.388118	-2.898158	-3.595653
49.O	2.577394	-2.740699	-3.587150
50.O	2.388118	2.898158	-3.595653
51.O	0.056032	-1.821154	5.136451
52.C	-0.136527	4.536109	4.545442
53.H	-0.323631	5.127321	3.636312
54.C	0.136527	-4.536109	4.545442
55.H	0.323631	-5.127321	3.636312
56.C	1.195827	4.973365	5.173016
57.H	2.029842	4.887499	4.463075
58.H	1.119078	6.023538	5.490175
59.H	1.427670	4.363766	6.058875
60.C	-1.195827	-4.973365	5.173016
61.H	-2.029842	-4.887499	4.463075
62.H	-1.119078	-6.023538	5.490175
63.H	-1.427670	-4.363766	6.058875
64.N	-1.311205	4.683784	5.424034
65.H	-1.131917	4.190070	6.303587
66.H	-1.415092	5.671387	5.672559
67.N	1.311205	-4.683784	5.424034
68.H	1.131917	-4.190070	6.303587
69.H	1.415092	-5.671387	5.672559

bRR_OXD:

Atom	X	Y	Z
1.P	-2.706924	0.175334	4.006683
2.O	-1.550646	0.096433	4.949307
3.O	-2.845699	-1.103418	3.057522
4.W	-3.054621	-1.475618	1.095217
5.O	-1.391255	0.086201	0.980735
6.Si	0.000000	0.000000	0.127964
7.O	1.391255	-0.086201	0.980735
8.W	3.054621	1.475618	1.095217
9.O	2.845699	1.103418	3.057522
10.P	2.706924	-0.175334	4.006683
11.O	-4.427820	-2.549822	1.264880
12.O	-3.969922	0.245538	1.028620

13.W	-2.850384	1.837021	1.083784
14.O	-2.668021	1.452778	3.049716
15.O	-1.586616	-2.753083	1.117172
16.W	-0.219630	-3.574452	0.010328
17.O	-0.084016	-1.351541	-0.838418
18.W	1.581368	-2.009997	-2.381417
19.O	1.760508	-0.109861	-2.694543
20.W	1.824577	1.798694	-2.373556
21.O	0.084016	1.351541	-0.838418
22.W	-1.581368	2.009997	-2.381417
23.O	0.131544	2.064148	-3.318442
24.O	-2.966834	-1.453117	-0.829078
25.W	-1.824577	-1.798694	-2.373556
26.O	-1.760508	0.109861	-2.694543
27.O	4.427820	2.549822	1.264880
28.O	3.969922	-0.245538	1.028620
29.W	2.850384	-1.837021	1.083784
30.O	2.668021	-1.452778	3.049716
31.O	4.085500	-3.066536	1.269951
32.O	1.236318	-2.930029	1.113371
33.O	2.763928	-1.813104	-0.835770
34.O	1.586616	2.753083	1.117172
35.W	0.219630	3.574452	0.010328
36.O	-1.064068	3.654511	-1.464910
37.O	2.966834	1.453117	-0.829078
38.O	-4.085500	3.066536	1.269951
39.O	-1.236318	2.930029	1.113371
40.O	-2.763928	1.813104	-0.835770
41.O	-0.325442	-5.254419	0.480292
42.O	-1.509399	-3.494144	-1.461169
43.O	1.064068	-3.654511	-1.464910
44.O	0.325442	5.254419	0.480292
45.O	1.509399	3.494144	-1.461169
46.O	-2.969967	-2.308143	-3.591954
47.O	-0.131544	-2.064148	-3.318442
48.O	2.654264	-2.659003	-3.599664
49.O	2.969967	2.308143	-3.591954
50.O	-2.654264	2.659003	-3.599664
51.O	1.550646	-0.096433	4.949307
52.C	-4.326236	0.325293	4.895668
53.H	-4.204162	1.244788	5.489862
54.C	4.326236	-0.325293	4.895668
55.H	4.204162	-1.244788	5.489862
56.C	-4.533567	-0.855437	5.846807
57.H	-3.676963	-0.974549	6.521208
58.H	-5.436592	-0.686862	6.449028
59.H	-4.664500	-1.791877	5.285391
60.C	4.533567	0.855437	5.846807
61.H	3.676963	0.974549	6.521208
62.H	5.436592	0.686862	6.449028

63.H	4.664500	1.791877	5.285391
64.N	-5.502883	0.502690	4.031682
65.H	-5.357170	1.289782	3.394652
66.H	-5.616631	-0.321978	3.434726
67.N	5.502883	-0.502690	4.031682
68.H	5.357170	-1.289782	3.394652
69.H	5.616631	0.321978	3.434726

cRR_OXD (BP86/6-31+G**/Lanl2DZ):

Atom	X	Y	Z
1.P	2.823009	-0.032871	4.039790
2.O	1.720017	-0.066614	5.069425
3.O	2.795717	1.270165	3.059818
4.W	2.960942	1.654907	1.109563
5.O	1.415288	-0.008450	1.017740
6.Si	0.000000	0.000000	0.158927
7.O	-1.415288	0.008450	1.017740
8.W	-2.960942	-1.654907	1.109563
9.O	-2.795717	-1.270165	3.059818
10.P	-2.823009	0.032871	4.039790
11.O	4.254368	2.802631	1.269247
12.O	3.965377	-0.005060	1.025760
13.W	2.980048	-1.674816	1.089495
14.O	2.819931	-1.323979	3.041541
15.O	1.414726	2.839150	1.118794
16.W	0.000000	3.575514	0.021517
17.O	0.001633	1.369875	-0.825502
18.W	-1.701328	1.906714	-2.367421
19.O	-1.768119	0.000993	-2.681184
20.W	-1.710943	-1.902599	-2.357839
21.O	-0.001633	-1.369875	-0.825502
22.W	1.701328	-1.906714	-2.367421
23.O	-0.007579	-2.066952	-3.290854
24.O	2.858185	1.637790	-0.810258
25.W	1.710943	1.902599	-2.357839
26.O	1.768119	-0.000993	-2.681184
27.O	-4.254368	-2.802631	1.269247
28.O	-3.965377	0.005060	1.025760
29.W	-2.980048	1.674816	1.089495
30.O	-2.819931	1.323979	3.041541
31.O	-4.278679	2.819053	1.221602
32.O	-1.433323	2.858176	1.104022
33.O	-2.859961	1.642581	-0.828503
34.O	-1.414726	-2.839150	1.118794
35.W	0.000000	-3.575514	0.021517
36.O	1.275100	-3.568969	-1.456012
37.O	-2.858185	-1.637790	-0.810258
38.O	4.278679	-2.819053	1.221602
39.O	1.433323	-2.858176	1.104022

40.O	2.859961	-1.642581	-0.828503
41.O	0.005162	5.247782	0.480742
42.O	1.283467	3.566353	-1.446488
43.O	-1.275100	3.568969	-1.456012
44.O	-0.005162	-5.247782	0.480742
45.O	-1.283467	-3.566353	-1.446488
46.O	2.814637	2.483548	-3.562436
47.O	0.007579	2.066952	-3.290854
48.O	-2.796058	2.486952	-3.580317
49.O	-2.814637	-2.483548	-3.562436
50.O	2.796058	-2.486952	-3.580317
51.O	-1.720017	0.066614	5.069425
52.C	4.487268	-0.022512	4.892966
53.H	4.540919	1.014828	5.298341
54.C	-4.487268	0.022512	4.892966
55.H	-4.540919	-1.014828	5.298341
56.C	5.691345	-0.263686	3.981978
57.H	5.720847	0.454062	3.139535
58.H	6.625885	-0.160383	4.571229
59.H	5.666029	-1.287298	3.553754
60.C	-5.691345	0.263686	3.981978
61.H	-5.720847	-0.454062	3.139535
62.H	-6.625885	0.160383	4.571229
63.H	-5.666029	1.287298	3.553754
64.N	4.487921	-0.953464	6.026634
65.H	3.609998	-0.826110	6.553412
66.H	4.446825	-1.920278	5.667890
67.N	-4.487921	0.953464	6.026634
68.H	-3.609998	0.826110	6.553412
69.H	-4.446825	1.920278	5.667890

cRR_OXD (BP86/TZ2P):

Atom	X	Y	Z
1.P	-2.749605	-0.253773	4.016028
2.O	-1.639922	-0.138998	5.012218
3.O	-2.622330	-1.527634	3.065034
4.W	-2.796087	-1.917850	1.101664
5.O	-1.387661	-0.124029	0.996041
6.Si	0.000000	0.000000	0.143419
7.O	1.387661	0.124029	0.996041
8.W	2.796087	1.917850	1.101664
9.O	2.622330	1.527634	3.065034
10.P	2.749605	0.253773	4.016028
11.O	-3.993117	-3.184672	1.277504
12.O	-3.959272	-0.357259	1.041237
13.W	-3.093848	1.385988	1.106761
14.O	-2.873331	1.028602	3.073894
15.O	-1.153205	-2.963185	1.125904
16.W	0.322257	-3.565133	0.023968

17.O	0.120932	-1.348192	-0.823751
18.W	1.870679	-1.745110	-2.361913
19.O	1.755823	0.158839	-2.682236
20.W	1.526865	2.054552	-2.363864
21.O	-0.120932	1.348192	-0.823751
22.W	-1.870679	1.745110	-2.361913
23.O	-0.186944	2.059808	-3.303919
24.O	-2.710267	-1.886753	-0.820217
25.W	-1.526865	-2.054552	-2.363864
26.O	-1.755823	-0.158839	-2.682236
27.O	3.993117	3.184672	1.277504
28.O	3.959272	0.357259	1.041237
29.W	3.093848	-1.385988	1.106761
30.O	2.873331	-1.028602	3.073894
31.O	4.492583	-2.426263	1.276333
32.O	1.660986	-2.705696	1.131647
33.O	3.002315	-1.371631	-0.815972
34.O	1.153205	2.963185	1.125904
35.W	-0.322257	3.565133	0.023968
36.O	-1.604650	3.450180	-1.448462
37.O	2.710267	1.886753	-0.820217
38.O	-4.492583	2.426263	1.276333
39.O	-1.660986	2.705696	1.131647
40.O	-3.002315	1.371631	-0.815972
41.O	0.472240	-5.241422	0.495536
42.O	-0.961279	-3.682752	-1.450679
43.O	1.604650	-3.450180	-1.448462
44.O	-0.472240	5.241422	0.495536
45.O	0.961279	3.682752	-1.450679
46.O	-2.581531	-2.731857	-3.582412
47.O	0.186944	-2.059808	-3.303919
48.O	3.031154	-2.225268	-3.578013
49.O	2.581531	2.731857	-3.582412
50.O	-3.031154	2.225268	-3.578013
51.O	1.639922	0.138998	5.012218
52.C	-4.372058	-0.436362	4.895262
53.H	-4.276967	-1.415130	5.392226
54.C	4.372058	0.436362	4.895262
55.H	4.276967	1.415130	5.392226
56.C	-5.597994	-0.450088	3.987659
57.H	-5.519257	-1.229373	3.220699
58.H	-6.496536	-0.640705	4.590433
59.H	-5.720468	0.517171	3.480115
60.C	5.597994	0.450088	3.987659
61.H	5.519257	1.229373	3.220699
62.H	6.496536	0.640705	4.590433
63.H	5.720468	-0.517171	3.480115
64.N	-4.521992	0.583726	5.948566
65.H	-3.663397	0.631346	6.504381
66.H	-4.629097	1.506865	5.516596

67.N	4.521992	-0.583726	5.948566
68.H	3.663397	-0.631346	6.504381
69.H	4.629097	-1.506865	5.516596

aRR_1e-RED:

Atom	X	Y	Z
1.P	-0.088566	2.846872	3.985010
2.O	-0.073965	2.000995	5.225962
3.O	-1.371363	2.572812	3.085746
4.W	-1.756200	2.870528	1.104198
5.O	-0.044057	1.392373	0.952879
6.Si	0.000146	0.000394	0.106454
7.O	0.044456	-1.390785	0.954648
8.W	1.755784	-2.869614	1.105339
9.O	1.371477	-2.579169	3.088123
10.P	0.087922	-2.850746	3.987344
11.O	-2.923046	4.162194	1.348838
12.O	-0.120824	3.941776	1.110337
13.W	1.577056	2.972912	1.106704
14.O	1.208566	2.649846	3.087066
15.O	-2.894254	1.302344	1.142488
16.W	-3.608706	-0.110307	-0.005563
17.O	-1.359415	-0.041798	-0.850660
18.W	-1.849164	-1.767185	-2.372049
19.O	0.054816	-1.767766	-2.685543
20.W	1.954981	-1.648935	-2.374496
21.O	1.359742	0.041987	-0.850683
22.W	1.849812	1.767126	-2.373124
23.O	2.102856	0.065259	-3.298266
24.O	-1.758659	2.825370	-0.806991
25.W	-1.954467	1.648392	-2.374491
26.O	-0.054244	1.767083	-2.686593
27.O	2.923906	-4.160833	1.347980
28.O	0.120287	-3.940586	1.110489
29.W	-1.577138	-2.970622	1.108441
30.O	-1.207803	-2.650221	3.088951
31.O	-2.667287	-4.328851	1.345405
32.O	-2.806999	-1.473067	1.144309
33.O	-1.580008	-2.925672	-0.803001
34.O	2.893530	-1.300769	1.144425
35.W	3.607637	0.110806	-0.004941
36.O	3.569384	1.416545	-1.433024
37.O	1.759374	-2.824322	-0.805013
38.O	2.666134	4.332261	1.343171
39.O	2.806387	1.474867	1.143623
40.O	1.580400	2.926685	-0.804944
41.O	-5.289070	-0.162774	0.491562
42.O	-3.649039	1.193662	-1.434215
43.O	-3.568684	-1.416431	-1.432973

44.O	5.288078	0.163387	0.492280
45.O	3.649637	-1.193788	-1.433588
46.O	-2.574802	2.742102	-3.593900
47.O	-2.102199	-0.066117	-3.298833
48.O	-2.400752	-2.898894	-3.590019
49.O	2.574773	-2.742291	-3.594413
50.O	2.401082	2.898165	-3.591754
51.O	0.074838	-2.010769	5.232201
52.C	-0.175284	4.655016	4.381832
53.H	-0.161288	5.177769	3.414347
54.C	0.171572	-4.660881	4.375817
55.H	0.144705	-5.179622	3.406379
56.C	1.023001	5.101324	5.218922
57.H	1.968986	4.875498	4.710468
58.H	0.970234	6.184818	5.394165
59.H	1.027440	4.592440	6.193749
60.C	-1.019120	-5.105685	5.224208
61.H	-1.969829	-4.874591	4.727104
62.H	-0.968381	-6.189948	5.395225
63.H	-1.010720	-4.599797	6.200541
64.N	-1.436883	5.005721	5.063985
65.H	-2.232114	4.708688	4.491168
66.H	-1.507671	4.467903	5.933938
67.N	1.438836	-5.020580	5.042650
68.H	2.228963	-4.718372	4.465495
69.H	1.518694	-4.492168	5.917604

bRR_1e-RED:

Atom	X	Y	Z
1.P	-2.710337	0.175102	4.016407
2.O	-1.616579	0.106645	5.039594
3.O	-2.786213	-1.111981	3.083636
4.W	-3.035458	-1.482462	1.099065
5.O	-1.389698	0.086969	0.966803
6.Si	0.000677	0.000199	0.115344
7.O	1.391921	-0.086751	0.965537
8.W	3.038796	1.482067	1.094802
9.O	2.791318	1.112915	3.080180
10.P	2.703712	-0.173032	4.012330
11.O	-4.420516	-2.543463	1.310687
12.O	-3.949725	0.241788	1.064356
13.W	-2.830307	1.840070	1.088504
14.O	-2.614005	1.453024	3.074799
15.O	-1.562714	-2.745606	1.145767
16.W	-0.220669	-3.590492	-0.002035
17.O	-0.083286	-1.352650	-0.850388
18.W	1.584616	-2.004737	-2.384644
19.O	1.760147	-0.109132	-2.700271
20.W	1.822726	1.792689	-2.380088

21.O	0.084194	1.352814	-0.850474
22.W	-1.585369	2.005562	-2.383617
23.O	0.131205	2.102776	-3.305398
24.O	-2.971245	-1.483631	-0.812130
25.W	-1.822994	-1.792069	-2.377084
26.O	-1.760765	0.109683	-2.698586
27.O	4.424074	2.542888	1.305502
28.O	3.951480	-0.242950	1.062073
29.W	2.831520	-1.840637	1.086866
30.O	2.612926	-1.453372	3.073839
31.O	4.083483	-3.055207	1.313241
32.O	1.219914	-2.921805	1.139467
33.O	2.767764	-1.840571	-0.820960
34.O	1.565573	2.745427	1.145301
35.W	0.222367	3.589665	-0.001573
36.O	-1.079276	3.679262	-1.433461
37.O	2.972119	1.484887	-0.815392
38.O	-4.083073	3.053849	1.314219
39.O	-1.218232	2.920198	1.140033
40.O	-2.768422	1.839804	-0.819518
41.O	-0.324844	-5.267712	0.499474
42.O	-1.525032	-3.518078	-1.430746
43.O	1.078270	-3.679597	-1.435592
44.O	0.324973	5.266736	0.500974
45.O	1.524168	3.518794	-1.432009
46.O	-2.972029	-2.313015	-3.593110
47.O	-0.133131	-2.102108	-3.305573
48.O	2.657952	-2.661753	-3.603556
49.O	2.969386	2.312365	-3.598534
50.O	-2.659961	2.661444	-3.602096
51.O	1.599038	-0.097914	5.023561
52.C	-4.369333	0.326849	4.834342
53.H	-4.265429	1.230089	5.456744
54.C	4.354747	-0.329016	4.844796
55.H	4.246417	-1.236470	5.460301
56.C	-4.640394	-0.872144	5.745394
57.H	-3.819060	-1.021731	6.456862
58.H	-5.569339	-0.707270	6.308417
59.H	-4.755409	-1.792313	5.154122
60.C	4.619181	0.863851	5.765743
61.H	3.795461	1.005964	6.476009
62.H	5.546588	0.696488	6.330606
63.H	4.734287	1.788880	5.182126
64.N	-5.505341	0.542661	3.922212
65.H	-5.305472	1.334867	3.305356
66.H	-5.593574	-0.266816	3.299818
67.N	5.497454	-0.538241	3.939410
68.H	5.304192	-1.328128	3.317524
69.H	5.588098	0.274244	3.321270

cRR_1e-RED:

Atom	X	Y	Z
1.P	-2.731814	-0.261803	4.021071
2.O	-1.657268	-0.161623	5.063521
3.O	-2.581768	-1.534940	3.082518
4.W	-2.785744	-1.922088	1.096967
5.O	-1.388495	-0.126114	0.980507
6.Si	0.000095	0.000082	0.130416
7.O	1.388657	0.126170	0.980510
8.W	2.785532	1.921552	1.096977
9.O	2.578790	1.536099	3.082889
10.P	2.728908	0.262038	4.019415
11.O	-3.998281	-3.177443	1.306033
12.O	-3.943553	-0.354290	1.072181
13.W	-3.076623	1.393317	1.112185
14.O	-2.822812	1.032297	3.100169
15.O	-1.139817	-2.953636	1.151242
16.W	0.320604	-3.579253	0.013141
17.O	0.121515	-1.349578	-0.836295
18.W	1.874033	-1.741002	-2.364481
19.O	1.758004	0.158067	-2.687005
20.W	1.527076	2.048084	-2.372574
21.O	-0.120944	1.349947	-0.836139
22.W	-1.873574	1.741165	-2.364063
23.O	-0.193311	2.097167	-3.292769
24.O	-2.714769	-1.916156	-0.811967
25.W	-1.526730	-2.048306	-2.372109
26.O	-1.757402	-0.158093	-2.685996
27.O	3.998761	3.176546	1.305565
28.O	3.943747	0.354052	1.073039
29.W	3.076747	-1.393882	1.111918
30.O	2.822645	-1.032424	3.099803
31.O	4.487013	-2.422146	1.320350
32.O	1.638376	-2.696922	1.160662
33.O	3.011549	-1.400581	-0.799187
34.O	1.140278	2.954064	1.150799
35.W	-0.319950	3.579425	0.013288
36.O	-1.622910	3.473824	-1.416111
37.O	2.714659	1.916101	-0.811708
38.O	-4.487690	2.420452	1.320672
39.O	-1.638140	2.697461	1.160751
40.O	-3.011659	1.401280	-0.799026
41.O	0.469436	-5.253080	0.516115
42.O	-0.973909	-3.707357	-1.423047
43.O	1.622508	-3.473770	-1.416788
44.O	-0.469458	5.253526	0.515477
45.O	0.973713	3.707821	-1.423674
46.O	-2.580158	-2.734147	-3.593027

47.O	0.193550	-2.097069	-3.292716
48.O	3.037943	-2.229675	-3.580024
49.O	2.579500	2.733849	-3.594201
50.O	-3.036685	2.228977	-3.580524
51.O	1.652867	0.161426	5.060261
52.C	-4.369223	-0.443389	4.874748
53.H	-4.282434	-1.419268	5.379724
54.C	4.365089	0.445109	4.874488
55.H	4.272632	1.416644	5.386994
56.C	-5.586690	-0.464733	3.956081
57.H	-5.500370	-1.252107	3.198272
58.H	-6.492932	-0.646035	4.551119
59.H	-5.700069	0.496668	3.435032
60.C	5.581871	0.480731	3.955360
61.H	5.490374	1.273723	3.204030
62.H	6.487494	0.662563	4.551166
63.H	5.700738	-0.475780	3.426728
64.N	-4.536545	0.582646	5.924024
65.H	-3.675274	0.640613	6.475561
66.H	-4.643781	1.500528	5.480425
67.N	4.539458	-0.588304	5.915157
68.H	3.678234	-0.658627	6.465267
69.H	4.655895	-1.501339	5.464101

aRR_2e-RED:

Atom	X	Y	Z
1.P	-0.084553	2.855819	3.982931
2.O	-0.070640	2.066339	5.265683
3.O	-1.372134	2.548761	3.107972
4.W	-1.758123	2.859855	1.105318
5.O	-0.043171	1.393656	0.945335
6.Si	0.000192	0.000008	0.100572
7.O	0.043249	-1.393826	0.945014
8.W	1.757494	-2.860062	1.105042
9.O	1.371930	-2.548705	3.107521
10.P	0.084357	-2.855991	3.982502
11.O	-2.915290	4.164422	1.367927
12.O	-0.119233	3.929756	1.128949
13.W	1.581396	2.963848	1.106329
14.O	1.216764	2.625283	3.107811
15.O	-2.882395	1.284693	1.168191
16.W	-3.621670	-0.111751	-0.008786
17.O	-1.360261	-0.041728	-0.856781
18.W	-1.843745	-1.767788	-2.373670
19.O	0.054504	-1.759944	-2.702127
20.W	1.949821	-1.651797	-2.374762
21.O	1.360815	0.041805	-0.856445
22.W	1.843911	1.768168	-2.373423
23.O	2.126217	0.065428	-3.286928

24.O	-1.774491	2.826098	-0.801264
25.W	-1.949592	1.651998	-2.373749
26.O	-0.054408	1.760187	-2.701335
27.O	2.915567	-4.164452	1.366225
28.O	0.119187	-3.930089	1.128493
29.W	-1.581213	-2.964448	1.105359
30.O	-1.216973	-2.626360	3.106862
31.O	-2.662422	-4.334899	1.356947
32.O	-2.799330	-1.460005	1.166542
33.O	-1.595982	-2.927082	-0.801472
34.O	2.882871	-1.285419	1.168236
35.W	3.621170	0.111313	-0.008568
36.O	3.596017	1.424492	-1.409138
37.O	1.774675	-2.824857	-0.801189
38.O	2.661091	4.335069	1.358770
39.O	2.799661	1.458787	1.167974
40.O	1.597042	2.926343	-0.800378
41.O	-5.300042	-0.163082	0.519315
42.O	-3.674963	1.201518	-1.407726
43.O	-3.595020	-1.424157	-1.409451
44.O	5.300073	0.162129	0.517869
45.O	3.675785	-1.201515	-1.409003
46.O	-2.583637	2.747011	-3.592368
47.O	-2.126619	-0.065024	-3.287298
48.O	-2.409399	-2.900161	-3.592016
49.O	2.583525	-2.746770	-3.593520
50.O	2.408786	2.901871	-3.590820
51.O	0.069307	-2.064574	5.264021
52.C	-0.171440	4.676238	4.325228
53.H	-0.133435	5.170102	3.343566
54.C	0.172694	-4.675560	4.329236
55.H	0.134881	-5.172680	3.349264
56.C	1.008631	5.145449	5.175168
57.H	1.964344	4.901091	4.693899
58.H	0.957401	6.234052	5.318326
59.H	0.990370	4.664609	6.164167
60.C	-1.006167	-5.143204	5.181914
61.H	-1.962839	-4.902529	4.700652
62.H	-0.952707	-6.231084	5.329493
63.H	-0.987810	-4.658253	6.168900
64.N	-1.447789	5.055080	4.968410
65.H	-2.227221	4.731006	4.387934
66.H	-1.536200	4.545763	5.854057
67.N	1.449963	-5.050753	4.972663
68.H	2.228064	-4.732408	4.387318
69.H	1.541735	-4.534091	5.853759

bRR_2e-RED:

Atom	X	Y	Z
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1.P	-2.709425	0.174157	4.018945
2.O	-1.658354	0.105430	5.091210
3.O	-2.751708	-1.119237	3.101843
4.W	-3.026451	-1.487903	1.096551
5.O	-1.392520	0.087349	0.952710
6.Si	0.000156	0.000258	0.104907
7.O	1.392728	-0.086884	0.952627
8.W	3.026660	1.488155	1.096322
9.O	2.751478	1.120949	3.101983
10.P	2.707006	-0.172770	4.018532
11.O	-4.425273	-2.535285	1.329776
12.O	-3.935605	0.240475	1.085182
13.W	-2.817963	1.842843	1.088130
14.O	-2.574773	1.456642	3.095751
15.O	-1.547612	-2.740340	1.168670
16.W	-0.223017	-3.606210	-0.007934
17.O	-0.083492	-1.354583	-0.858844
18.W	1.588795	-2.000657	-2.384504
19.O	1.758529	-0.109563	-2.710470
20.W	1.825036	1.786673	-2.380836
21.O	0.084108	1.354837	-0.859027
22.W	-1.588320	2.000802	-2.384701
23.O	0.132976	2.123314	-3.294463
24.O	-2.975563	-1.505238	-0.808695
25.W	-1.824771	-1.786820	-2.379826
26.O	-1.757710	0.109522	-2.709562
27.O	4.426006	2.534722	1.329608
28.O	3.935604	-0.240493	1.085348
29.W	2.818206	-1.842915	1.088034
30.O	2.570968	-1.455262	3.095786
31.O	4.086858	-3.042980	1.343603
32.O	1.203939	-2.914107	1.162137
33.O	2.770551	-1.862624	-0.814706
34.O	1.548019	2.741293	1.168442
35.W	0.223429	3.606098	-0.007753
36.O	-1.085537	3.707209	-1.410932
37.O	2.975147	1.506981	-0.808911
38.O	-4.088255	3.042026	1.341335
39.O	-1.203715	2.912980	1.161621
40.O	-2.770048	1.861832	-0.814412
41.O	-0.325905	-5.281482	0.523722
42.O	-1.534945	-3.544941	-1.407479
43.O	1.084626	-3.707849	-1.411325
44.O	0.325448	5.281525	0.523099
45.O	1.533965	3.546070	-1.408684
46.O	-2.973153	-2.318822	-3.598715
47.O	-0.133261	-2.123353	-3.294011
48.O	2.660322	-2.669182	-3.605869
49.O	2.972652	2.318878	-3.600233
50.O	-2.660762	2.667655	-3.606257

51.O	1.655298	-0.102628	5.089982
52.C	-4.389884	0.329949	4.796610
53.H	-4.298660	1.226183	5.431188
54.C	4.387149	-0.331780	4.796210
55.H	4.294025	-1.227178	5.431775
56.C	-4.696349	-0.874664	5.688453
57.H	-3.893060	-1.040303	6.416982
58.H	-5.636904	-0.708323	6.232254
59.H	-4.805329	-1.787062	5.083932
60.C	4.697912	0.873124	5.686193
61.H	3.896114	1.042241	6.415602
62.H	5.638759	0.704813	6.228868
63.H	4.808957	1.784375	5.080320
64.N	-5.503763	0.563863	3.857641
65.H	-5.274472	1.359886	3.254866
66.H	-5.565705	-0.235105	3.217748
67.N	5.499487	-0.569555	3.856460
68.H	5.268160	-1.366780	3.255982
69.H	5.561193	0.227704	3.214444

cRR_2e-RED:

Atom	X	Y	Z
1.P	-2.724336	-0.256476	4.024834
2.O	-1.688704	-0.153783	5.112603
3.O	-2.537793	-1.535196	3.107958
4.W	-2.771489	-1.923573	1.100565
5.O	-1.388763	-0.124616	0.970437
6.Si	0.000494	0.000238	0.121062
7.O	1.390970	0.125256	0.968428
8.W	2.772973	1.923095	1.098466
9.O	2.538250	1.535474	3.104602
10.P	2.719175	0.255739	4.021365
11.O	-3.998078	-3.169231	1.333235
12.O	-3.928143	-0.353118	1.098429
13.W	-3.066565	1.398577	1.109639
14.O	-2.787695	1.044417	3.119720
15.O	-1.121610	-2.942515	1.175924
16.W	0.322668	-3.592916	0.006022
17.O	0.121455	-1.351740	-0.844305
18.W	1.874447	-1.735892	-2.368815
19.O	1.753283	0.157692	-2.703746
20.W	1.531775	2.043098	-2.373950
21.O	-0.121073	1.352119	-0.844422
22.W	-1.874808	1.736199	-2.367276
23.O	-0.193921	2.120537	-3.281945
24.O	-2.715367	-1.931755	-0.804240
25.W	-1.532456	-2.043013	-2.371873
26.O	-1.753866	-0.157419	-2.702053
27.O	4.000268	3.169247	1.329924

28.O	3.930391	0.352973	1.096360
29.W	3.068839	-1.398459	1.106880
30.O	2.788945	-1.045350	3.117494
31.O	4.491986	-2.414813	1.334615
32.O	1.624094	-2.691153	1.180856
33.O	3.015028	-1.416679	-0.798712
34.O	1.123794	2.942642	1.174223
35.W	-0.321103	3.593292	0.005939
36.O	-1.633765	3.500251	-1.393790
37.O	2.716547	1.932876	-0.806584
38.O	-4.490778	2.413043	1.338680
39.O	-1.621955	2.691653	1.182098
40.O	-3.015280	1.417728	-0.796567
41.O	0.472944	-5.264707	0.539327
42.O	-0.981936	-3.734797	-1.398063
43.O	1.632812	-3.499621	-1.395507
44.O	-0.470585	5.265215	0.538997
45.O	0.981784	3.734976	-1.399631
46.O	-2.586864	-2.742288	-3.591448
47.O	0.192265	-2.120120	-3.281524
48.O	3.037759	-2.239018	-3.586142
49.O	2.584179	2.742280	-3.595119
50.O	-3.039347	2.238076	-3.583928
51.O	1.675140	0.154079	5.101033
52.C	-4.379752	-0.441969	4.845628
53.H	-4.294983	-1.406209	5.373542
54.C	4.368159	0.440811	4.854195
55.H	4.281310	1.408269	5.375801
56.C	-5.581453	-0.495428	3.907992
57.H	-5.474361	-1.300060	3.171198
58.H	-6.497632	-0.668365	4.491058
59.H	-5.691150	0.451320	3.359881
60.C	5.576528	0.485253	3.924856
61.H	5.476392	1.285002	3.181851
62.H	6.489140	0.659868	4.512963
63.H	5.687409	-0.465615	3.384121
64.N	-4.582021	0.604165	5.873052
65.H	-3.723191	0.691838	6.425298
66.H	-4.697035	1.507983	5.402717
67.N	4.559703	-0.599888	5.888768
68.H	3.696431	-0.681382	6.434988
69.H	4.675870	-1.506719	5.424677

γ -[SiW₁₂O₄₀]⁴⁺:

Atom	X	Y	Z (Angstrom)
1.W	0.000000	-1.526840	3.548077
2.W	0.000000	1.526840	3.548077
3.W	-1.698250	-3.000809	0.910494
4.W	-1.698250	3.000809	0.910494
5.W	1.698250	3.000809	0.910494

6.W	1.698250	-3.000809	0.910494
7.W	-3.588298	0.000000	-0.172366
8.W	3.588298	0.000000	-0.172366
9.W	-1.906131	-1.706344	-2.559313
10.W	-1.906131	1.706344	-2.559313
11.W	1.906131	1.706344	-2.559313
12.W	1.906131	-1.706344	-2.559313
13.Si	0.000000	0.000000	0.002552
14.O	0.000000	-1.357580	0.934935
15.O	0.000000	1.357580	0.934935
16.O	-1.343125	0.000000	-0.970977
17.O	1.343125	0.000000	-0.970977
18.O	-1.234979	0.000000	3.452601
19.O	1.234979	0.000000	3.452601
20.O	-2.896101	-1.446318	0.896461
21.O	-2.896101	1.446318	0.896461
22.O	2.896101	1.446318	0.896461
23.O	2.896101	-1.446318	0.896461
24.O	-1.611077	-2.859438	-1.002394
25.O	-1.611077	2.859438	-1.002394
26.O	1.611077	2.859438	-1.002394
27.O	1.611077	-2.859438	-1.002394
28.O	0.000000	-1.762475	-2.870518
29.O	0.000000	1.762475	-2.870518
30.O	-1.382254	-2.650291	2.826809
31.O	-1.382254	2.650291	2.826809
32.O	1.382254	2.650291	2.826809
33.O	1.382254	-2.650291	2.826809
34.O	0.000000	-3.962599	0.914087
35.O	0.000000	3.962599	0.914087
36.O	-3.574203	-1.280764	-1.667225
37.O	-3.574203	1.280764	-1.667225
38.O	3.574203	1.280764	-1.667225
39.O	3.574203	-1.280764	-1.667225
40.O	-2.038419	0.000000	-3.496516
41.O	2.038419	0.000000	-3.496516
42.O	0.000000	-1.953935	5.240551
43.O	0.000000	1.953935	5.240551
44.O	-2.828924	-4.322641	1.081562
45.O	-2.828924	4.322641	1.081562
46.O	2.828924	4.322641	1.081562
47.O	2.828924	-4.322641	1.081562
48.O	-5.280921	0.000000	0.265495
49.O	5.280921	0.000000	0.265495
50.O	-2.477633	-2.825676	-3.772933
51.O	-2.477633	2.825676	-3.772933
52.O	2.477633	2.825676	-3.772933
53.O	2.477633	-2.825676	-3.772933