IPC ACTIVE SPACES FOR CHAPTER 3: MULTIREFERENCE GROUND AND EXCITED STATE ELECTRONIC STRUCTURES OF FREE- VERSUS IRON PORPHYRIN-CARBENES

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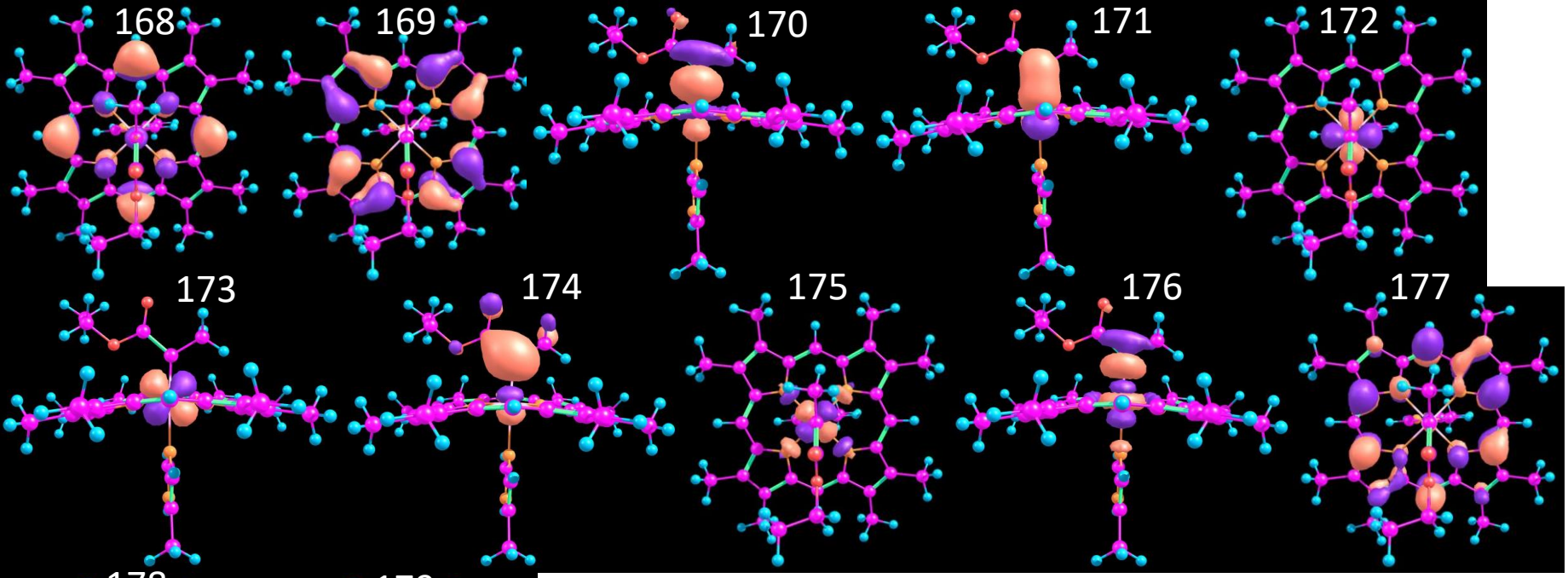
Stroscio, G. D.; Srnec, M.*; Hadt, R. G.* Multireference Ground and Excited State Electronic Structures of Free- versus Iron Porphyrin-Carbenes. *Inorg. Chem.* **2020**, *59* (13), 8707–8715. https://doi.org/10.1021/acs.inorgchem.0c00249.

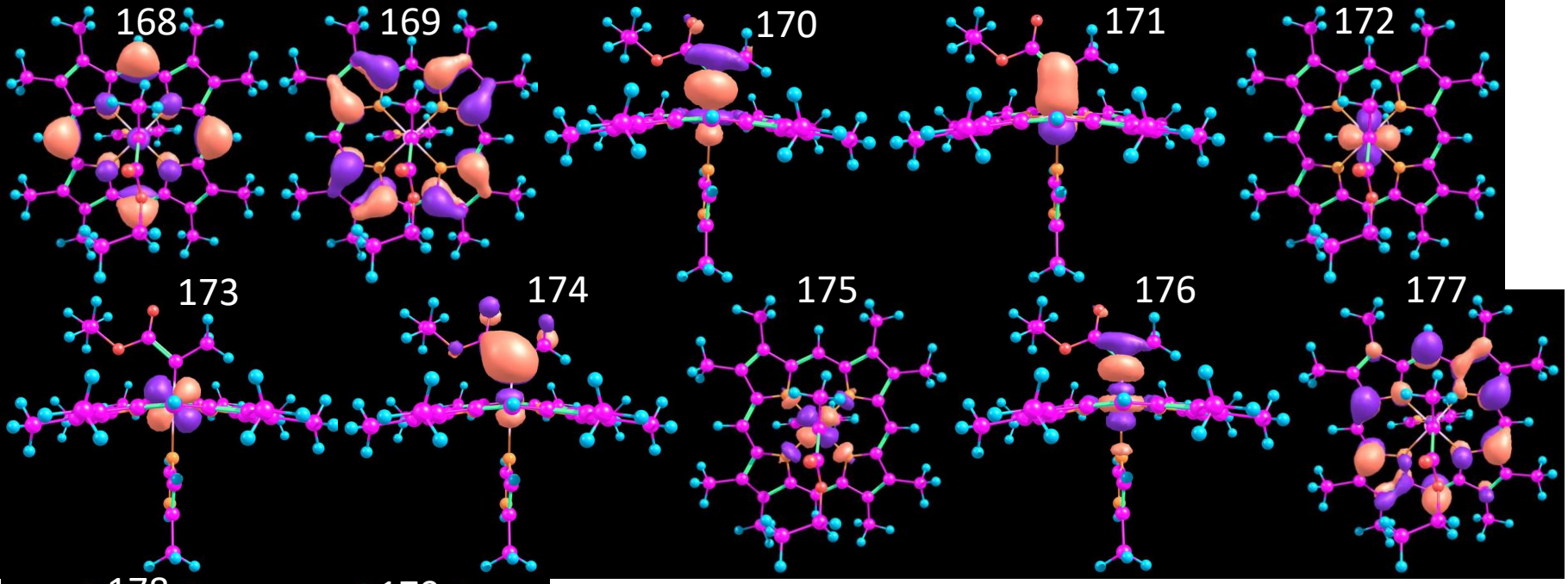
*Corresponding author.

Active Space for QD-NEVPT2 on RKS DFT Geometries: MeImid.



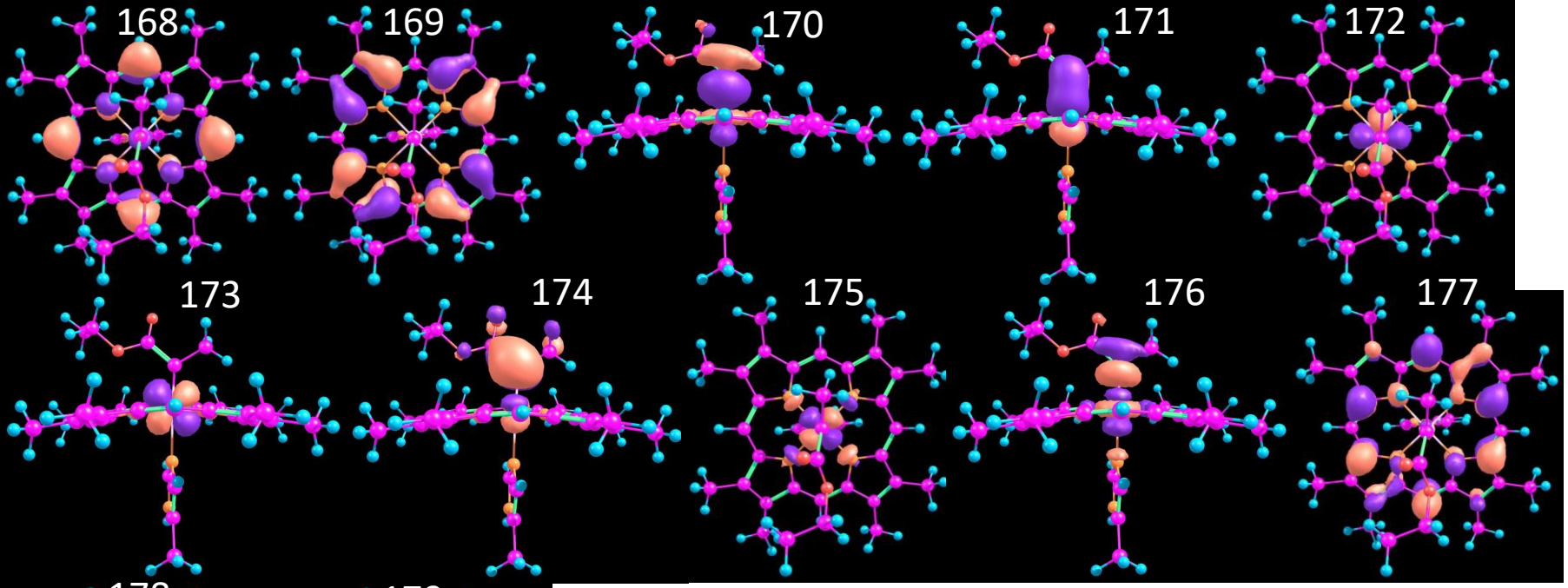
NO	OCC	E(Eh)	E(eV)
168	1.9380	-0.235231	-6.4010
169	1.9149	-0.187628	-5.1056
170	1.8734	-0.418025	-11.3750
171	1.7499	-0.375791	-10.2258
172	1.4922	-0.319947	-8.7062
173	1.3061	-0.246755	-6.7146
174	0.8675	-0.055571	-1.5122
175	0.5693	0.131237	3.5711
176	0.1341	0.259773	7.0688
177	0.0745	0.048897	1.3306
178	0.0734	0.051364	1.3977
179	0.0068	0.196915	5.3583

0 degrees;
1 Quintet,
5 Triplets,
2 Singlets



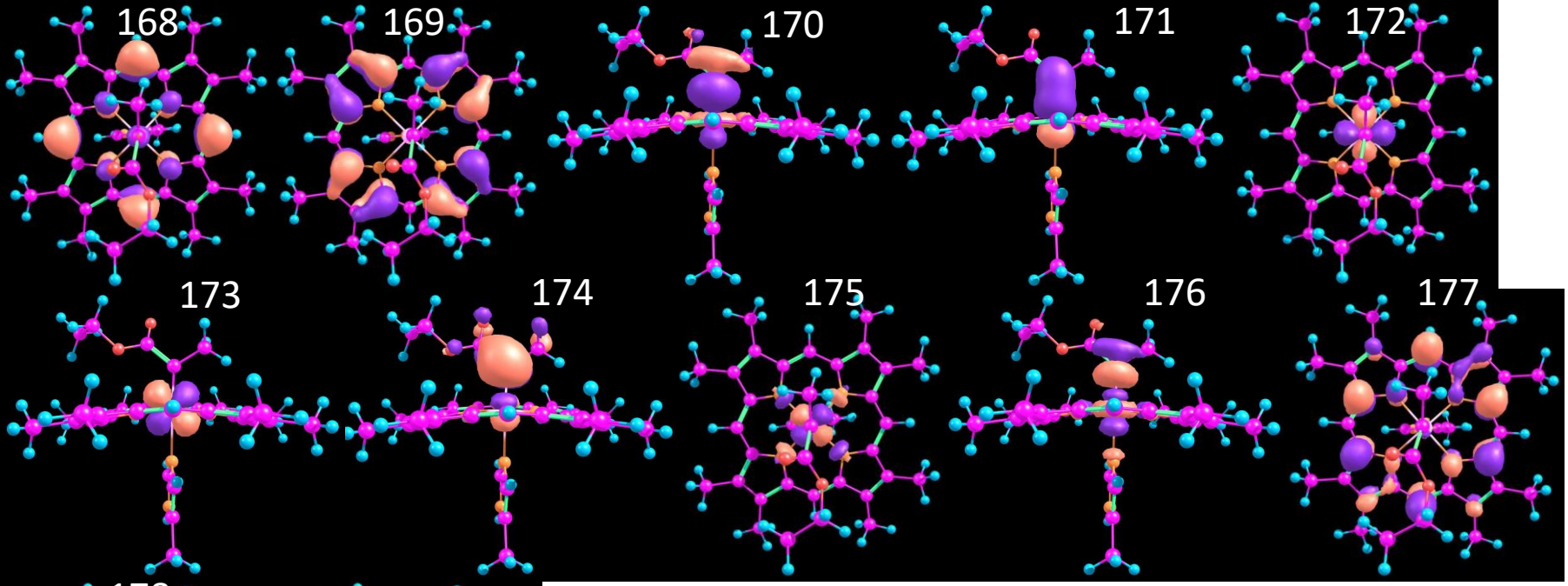
NO	OCC	E(Eh)	E(eV)
168	1.9379	-0.234817	-6.3897
169	1.9150	-0.187686	-5.1072
170	1.8734	-0.417677	-11.3656
171	1.7537	-0.377235	-10.2651
172	1.4883	-0.318038	-8.6543
173	1.3062	-0.246477	-6.7070
174	0.8670	-0.054086	-1.4717
175	0.5698	0.131183	3.5697
176	0.1339	0.260459	7.0875
177	0.0745	0.048867	1.3297
178	0.0734	0.051315	1.3964

10 degrees;
1 Quintet,
5 Triplets,
2 Singlets



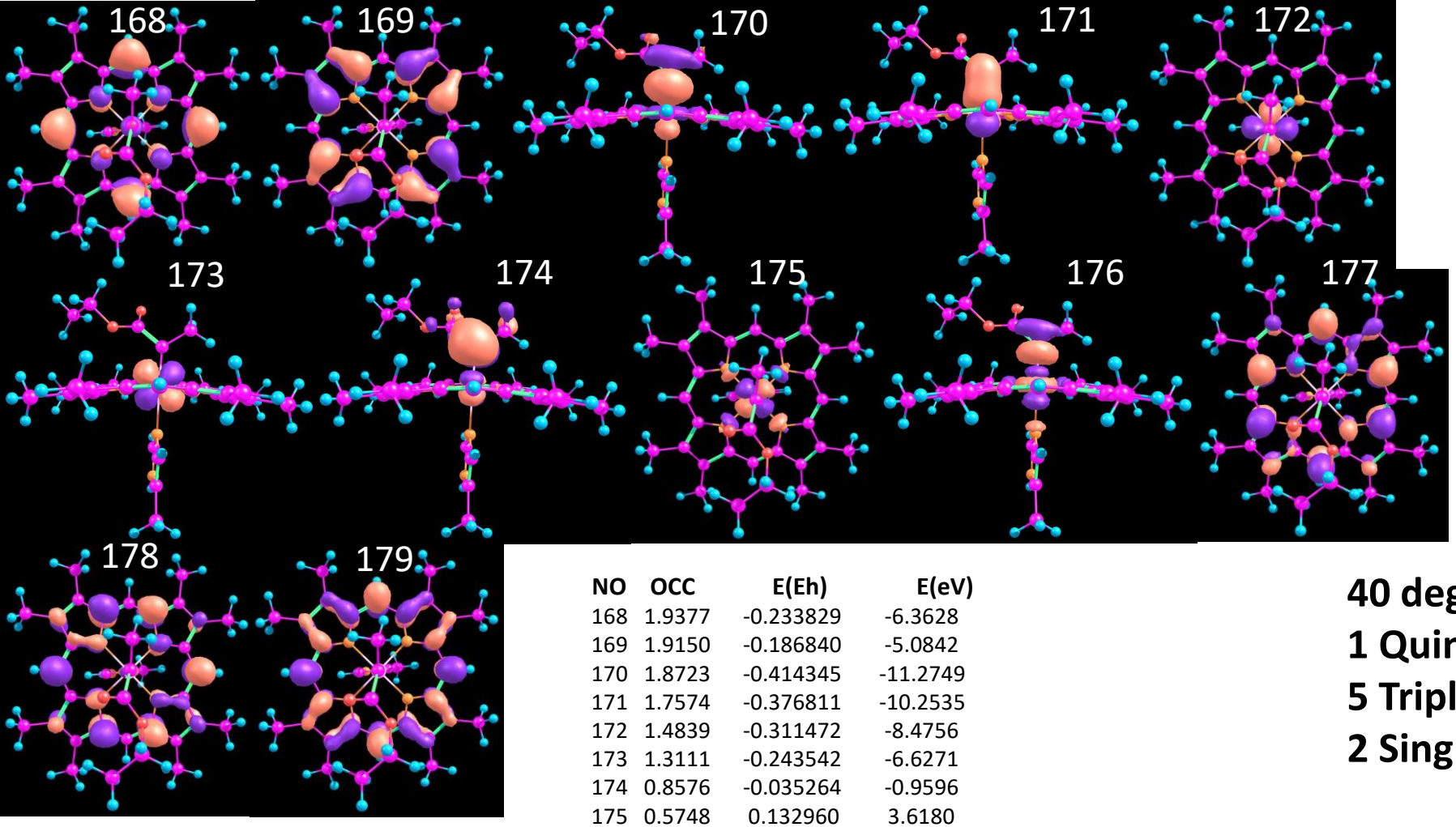
NO	OCC	E(Eh)	E(eV)
168	1.9378	-0.234442	-6.3795
169	1.9150	-0.187547	-5.1034
170	1.8729	-0.416865	-11.3435
171	1.7565	-0.378063	-10.2876
172	1.4855	-0.315805	-8.5935
173	1.3072	-0.245623	-6.6838
174	0.8649	-0.049455	-1.3457
175	0.5711	0.131383	3.5751
176	0.1343	0.261549	7.1171
177	0.0745	0.049003	1.3334
178	0.0734	0.051484	1.4009
179	0.0068	0.194882	5.3030

20 degrees;
1 Quintet,
5 Triplets,
2 Singlets



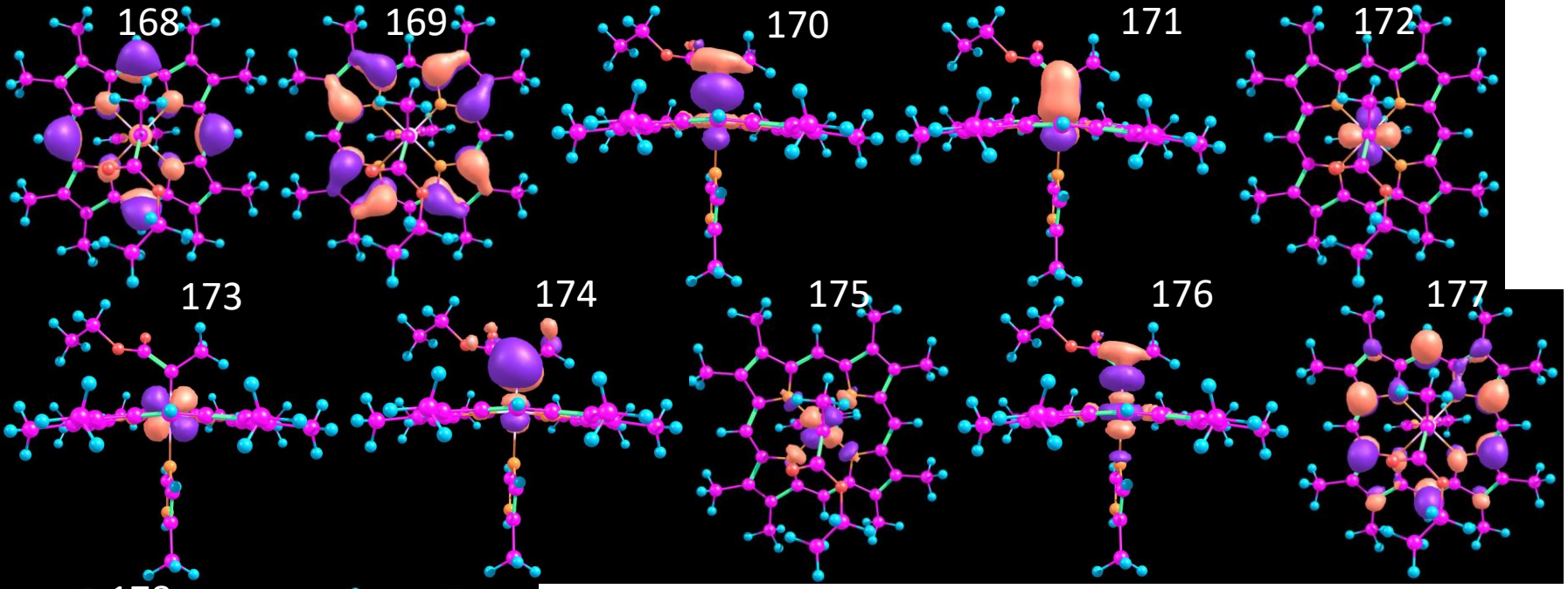
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.234233	-6.3738
169	1.9149	-0.187166	-5.0930
170	1.8728	-0.415730	-11.3126
171	1.7562	-0.377364	-10.2686
172	1.4857	-0.314081	-8.5466
173	1.3090	-0.244625	-6.6566
174	0.8617	-0.042763	-1.1636
175	0.5727	0.132329	3.6008
176	0.1345	0.263718	7.1761
177	0.0747	0.049169	1.3380
178	0.0734	0.051868	1.4114
179	0.0068	0.195394	5.3169

30 degrees;
1 Quintet,
5 Triplets,
2 Singlets



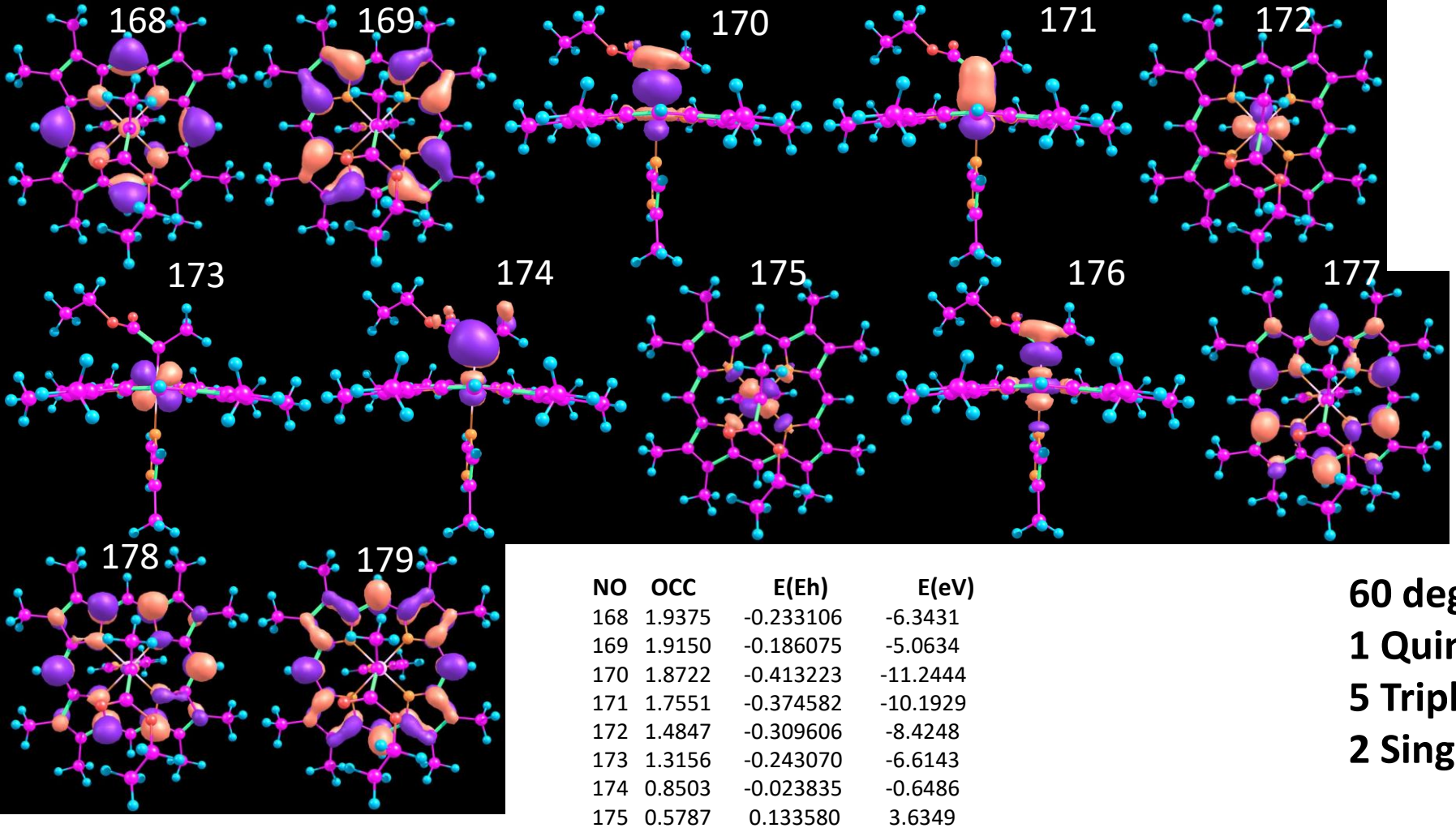
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233829	-6.3628
169	1.9150	-0.186840	-5.0842
170	1.8723	-0.414345	-11.2749
171	1.7574	-0.376811	-10.2535
172	1.4839	-0.311472	-8.4756
173	1.3111	-0.243542	-6.6271
174	0.8576	-0.035264	-0.9596
175	0.5748	0.132960	3.6180
176	0.1355	0.265206	7.2166
177	0.0748	0.049460	1.3459
178	0.0733	0.052307	1.4233
179	0.0068	0.196253	5.3403

40 degrees;
1 Quintet,
5 Triplets,
2 Singlets



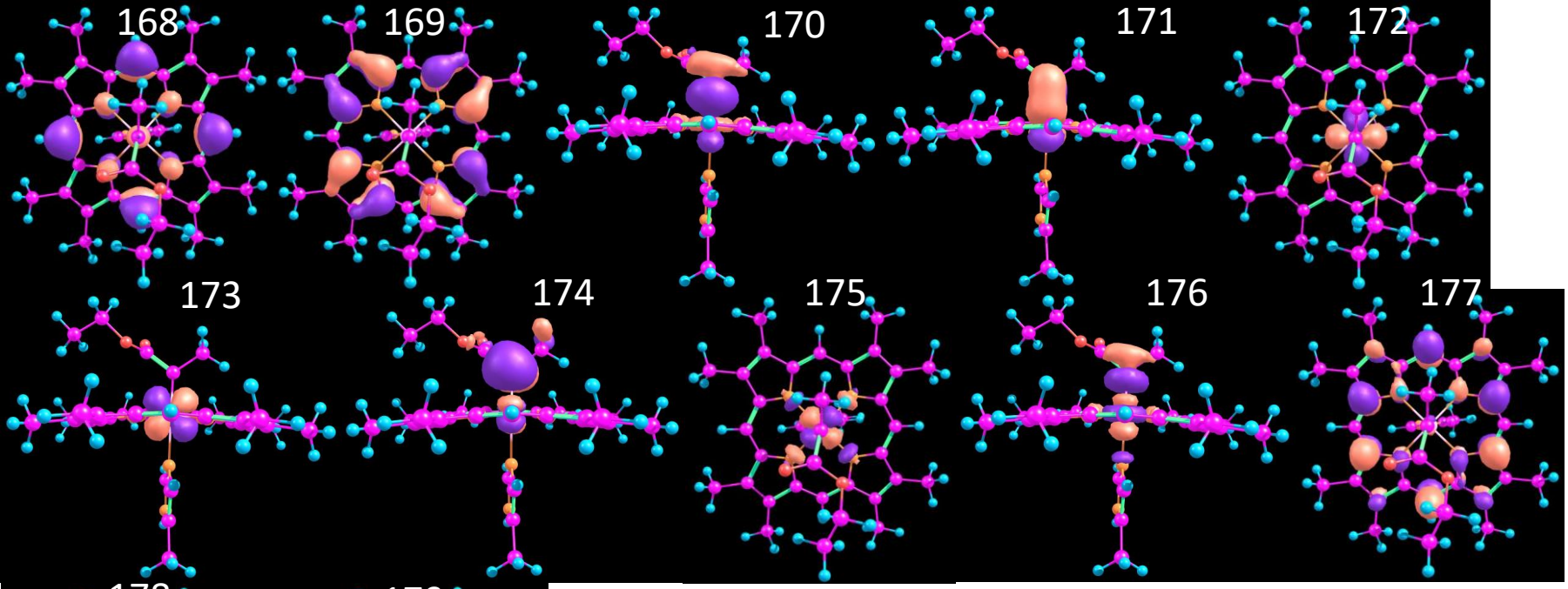
NO	OCC	E(Eh)	E(eV)
168	1.9376	-0.233576	-6.3559
169	1.9150	-0.186415	-5.0726
170	1.8724	-0.413432	-11.2501
171	1.7590	-0.376296	-10.2395
172	1.4813	-0.308914	-8.4060
173	1.3133	-0.242907	-6.6098
174	0.8531	-0.028653	-0.7797
175	0.5770	0.133381	3.6295
176	0.1364	0.266530	7.2526
177	0.0748	0.049906	1.3580
178	0.0733	0.052877	1.4389
179	0.0068	0.197603	5.3771

50 degrees;
1 Quintet,
5 Triplets,
2 Singlets



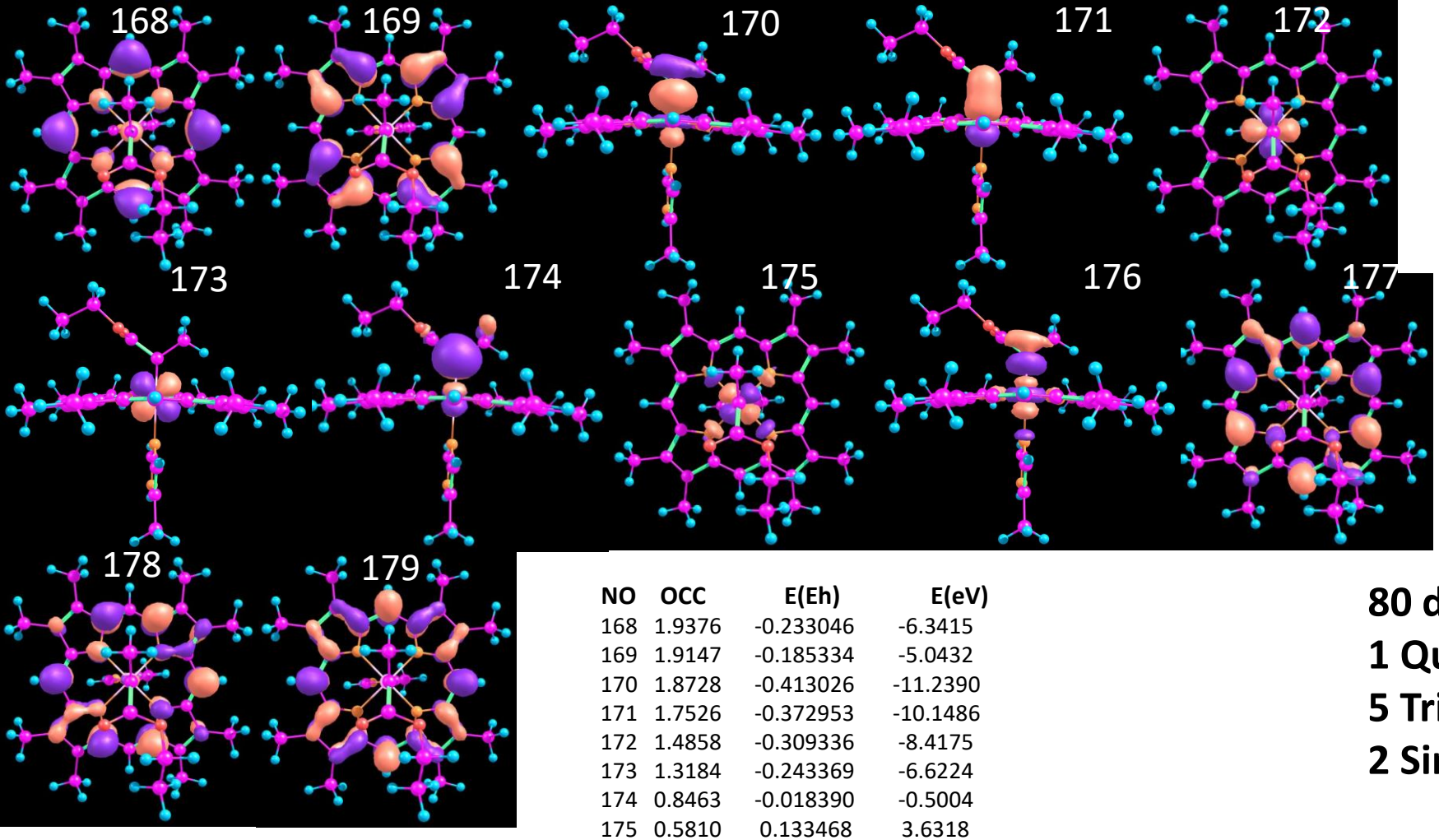
NO	OCC	E(Eh)	E(eV)
168	1.9375	-0.233106	-6.3431
169	1.9150	-0.186075	-5.0634
170	1.8722	-0.413223	-11.2444
171	1.7551	-0.374582	-10.1929
172	1.4847	-0.309606	-8.4248
173	1.3156	-0.243070	-6.6143
174	0.8503	-0.023835	-0.6486
175	0.5787	0.133580	3.6349
176	0.1358	0.268057	7.2942
177	0.0748	0.050278	1.3681
178	0.0734	0.052978	1.4416
179	0.0068	0.197011	5.3610

60 degrees;
1 Quintet,
5 Triplets,
2 Singlets



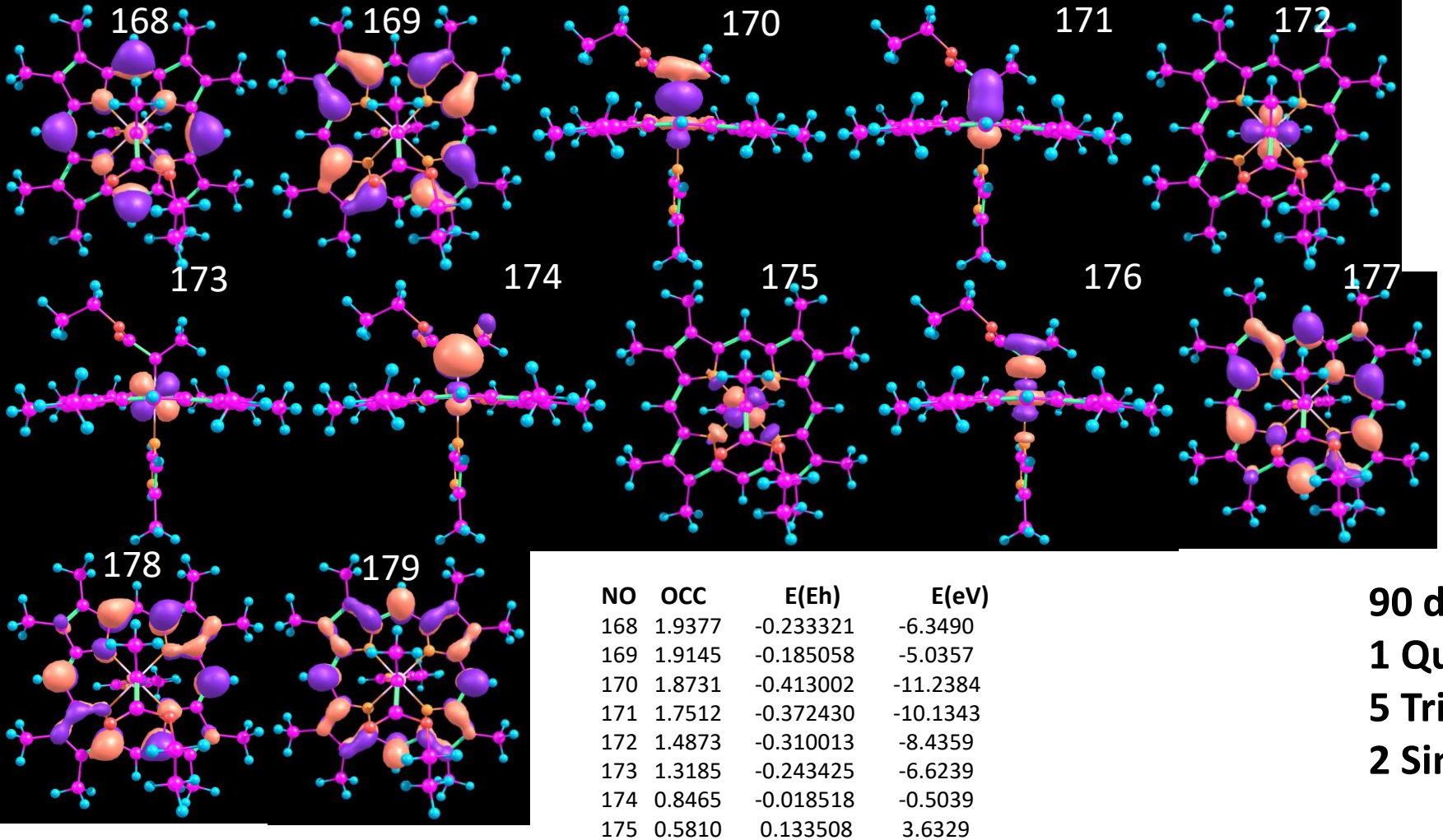
NO	OCC	E(Eh)	E(eV)
168	1.9375	-0.232904	-6.3376
169	1.9150	-0.185687	-5.0528
170	1.8726	-0.412888	-11.2352
171	1.7562	-0.374225	-10.1832
172	1.4822	-0.308005	-8.3812
173	1.3172	-0.243035	-6.6133
174	0.8468	-0.019973	-0.5435
175	0.5803	0.133300	3.6273
176	0.1371	0.267903	7.2900
177	0.0748	0.050724	1.3803
178	0.0735	0.053392	1.4529
179	0.0068	0.197771	5.3816

70 degrees;
1 Quintet,
5 Triplets,
2 Singlets



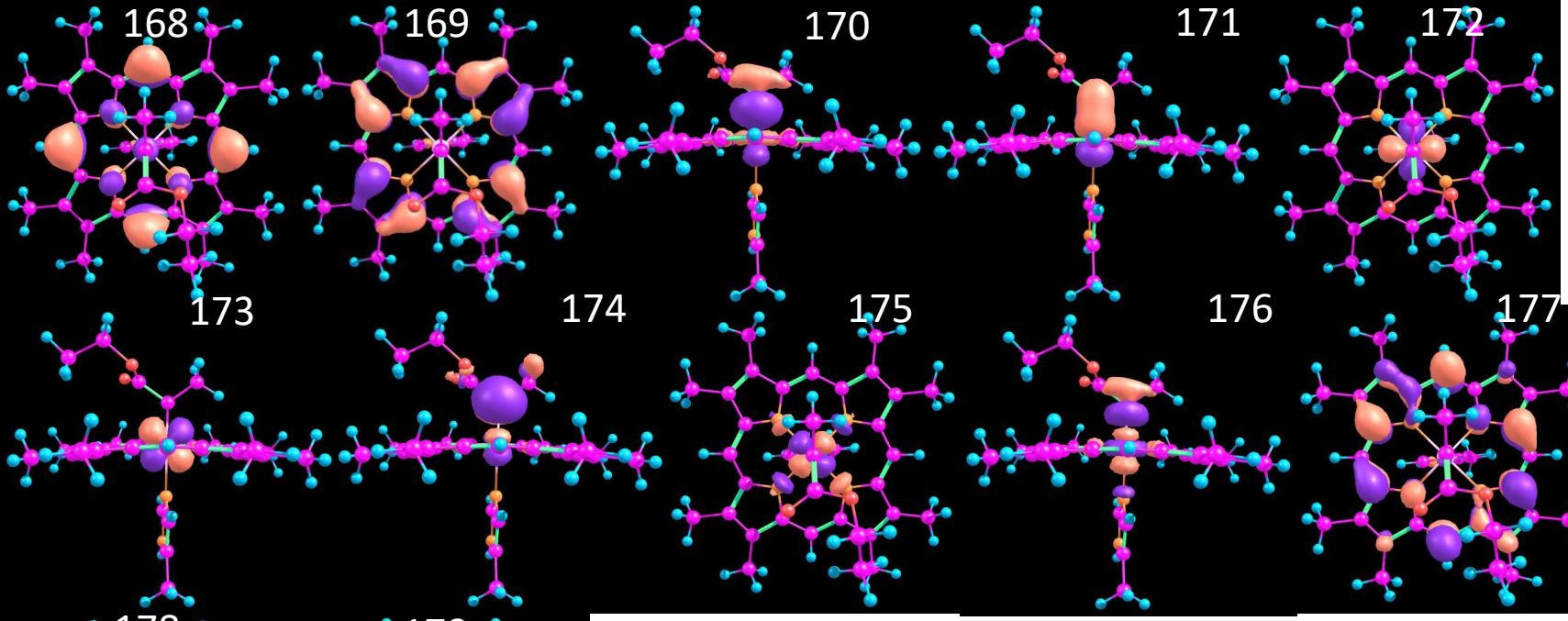
NO	OCC	E(Eh)	E(eV)
168	1.9376	-0.233046	-6.3415
169	1.9147	-0.185334	-5.0432
170	1.8728	-0.413026	-11.2390
171	1.7526	-0.372953	-10.1486
172	1.4858	-0.309336	-8.4175
173	1.3184	-0.243369	-6.6224
174	0.8463	-0.018390	-0.5004
175	0.5810	0.133468	3.6318
176	0.1357	0.269622	7.3368
177	0.0749	0.050858	1.3839
178	0.0734	0.053530	1.4566
179	0.0068	0.198577	5.4036

80 degrees;
1 Quintet,
5 Triplets,
2 Singlets



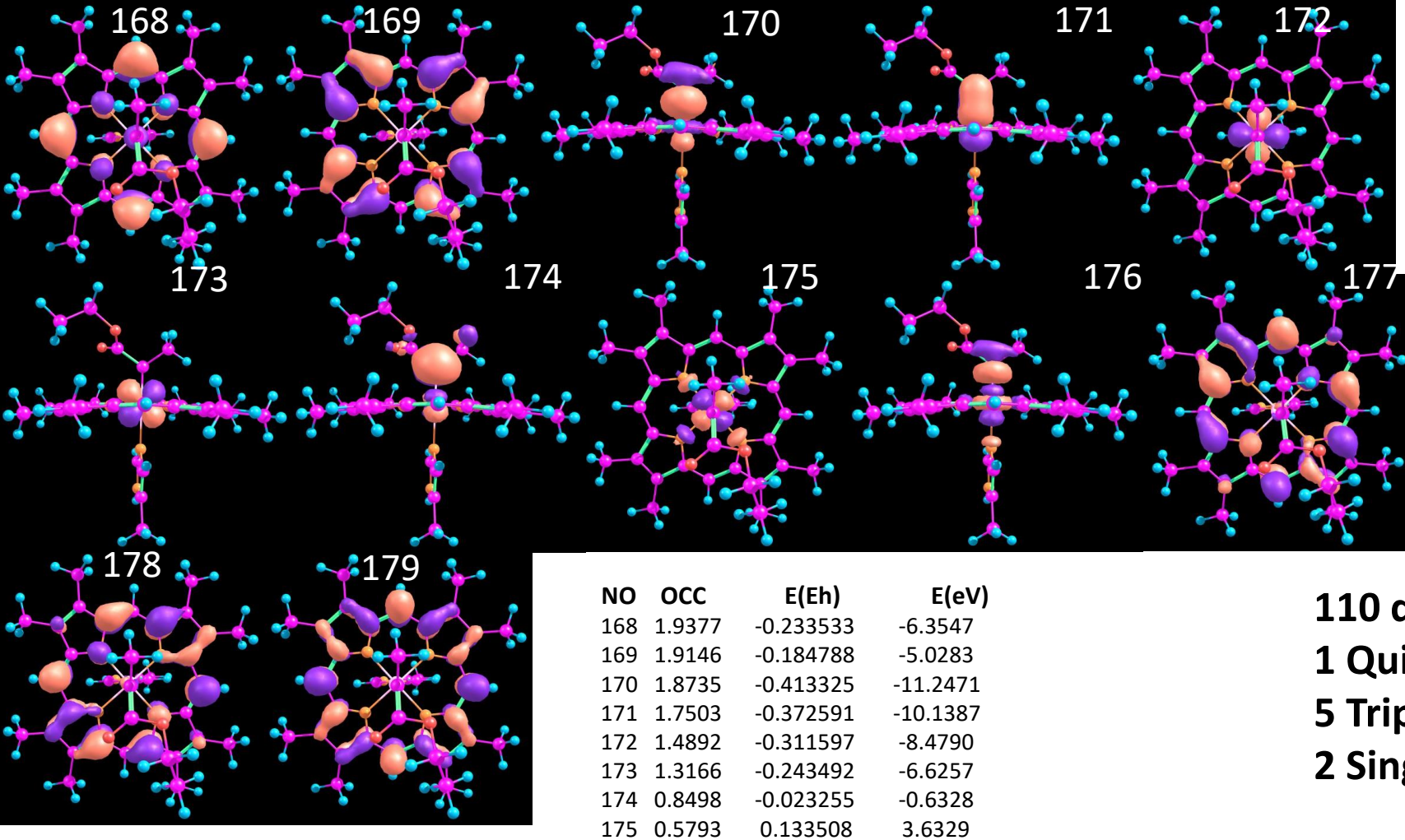
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233321	-6.3490
169	1.9145	-0.185058	-5.0357
170	1.8731	-0.413002	-11.2384
171	1.7512	-0.372430	-10.1343
172	1.4873	-0.310013	-8.4359
173	1.3185	-0.243425	-6.6239
174	0.8465	-0.018518	-0.5039
175	0.5810	0.133508	3.6329
176	0.1349	0.270587	7.3631
177	0.0749	0.051107	1.3907
178	0.0735	0.053753	1.4627
179	0.0068	0.199935	5.4405

90 degrees;
1 Quintet,
5 Triplets,
2 Singlets



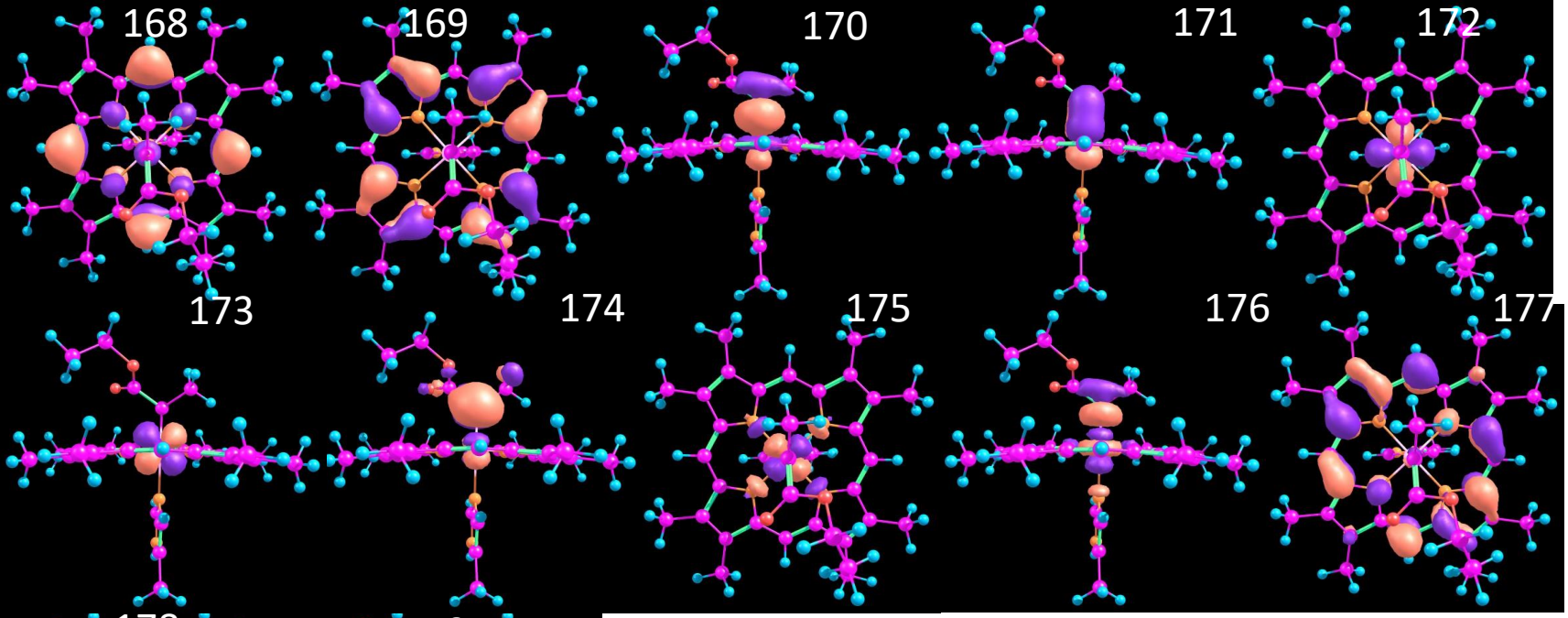
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233227	-6.3464
169	1.9146	-0.185028	-5.0349
170	1.8731	-0.413174	-11.2430
171	1.7505	-0.372558	-10.1378
172	1.4884	-0.310869	-8.4592
173	1.3179	-0.243578	-6.6281
174	0.8478	-0.020189	-0.5494
175	0.5805	0.133352	3.6287
176	0.1343	0.270630	7.3642
177	0.0749	0.051164	1.3922
178	0.0735	0.053687	1.4609
179	0.0067	0.198604	5.4043

100 degrees;
1 Quintet,
5 Triplets,
2 Singlets



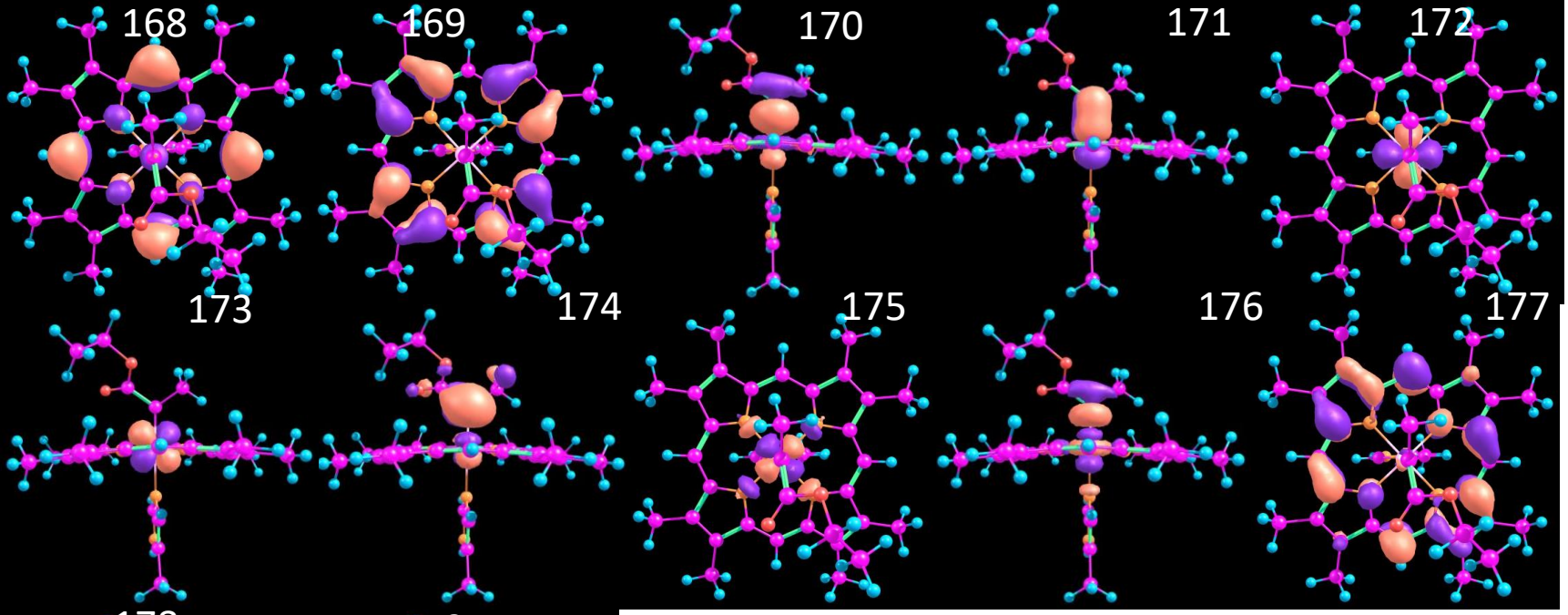
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233533	-6.3547
169	1.9146	-0.184788	-5.0283
170	1.8735	-0.413325	-11.2471
171	1.7503	-0.372591	-10.1387
172	1.4892	-0.311597	-8.4790
173	1.3166	-0.243492	-6.6257
174	0.8498	-0.023255	-0.6328
175	0.5793	0.133508	3.6329
176	0.1340	0.270512	7.3610
177	0.0749	0.051513	1.4017
178	0.0735	0.053897	1.4666
179	0.0068	0.200224	5.4484

110 degrees;
1 Quintet,
5 Triplets,
2 Singlets



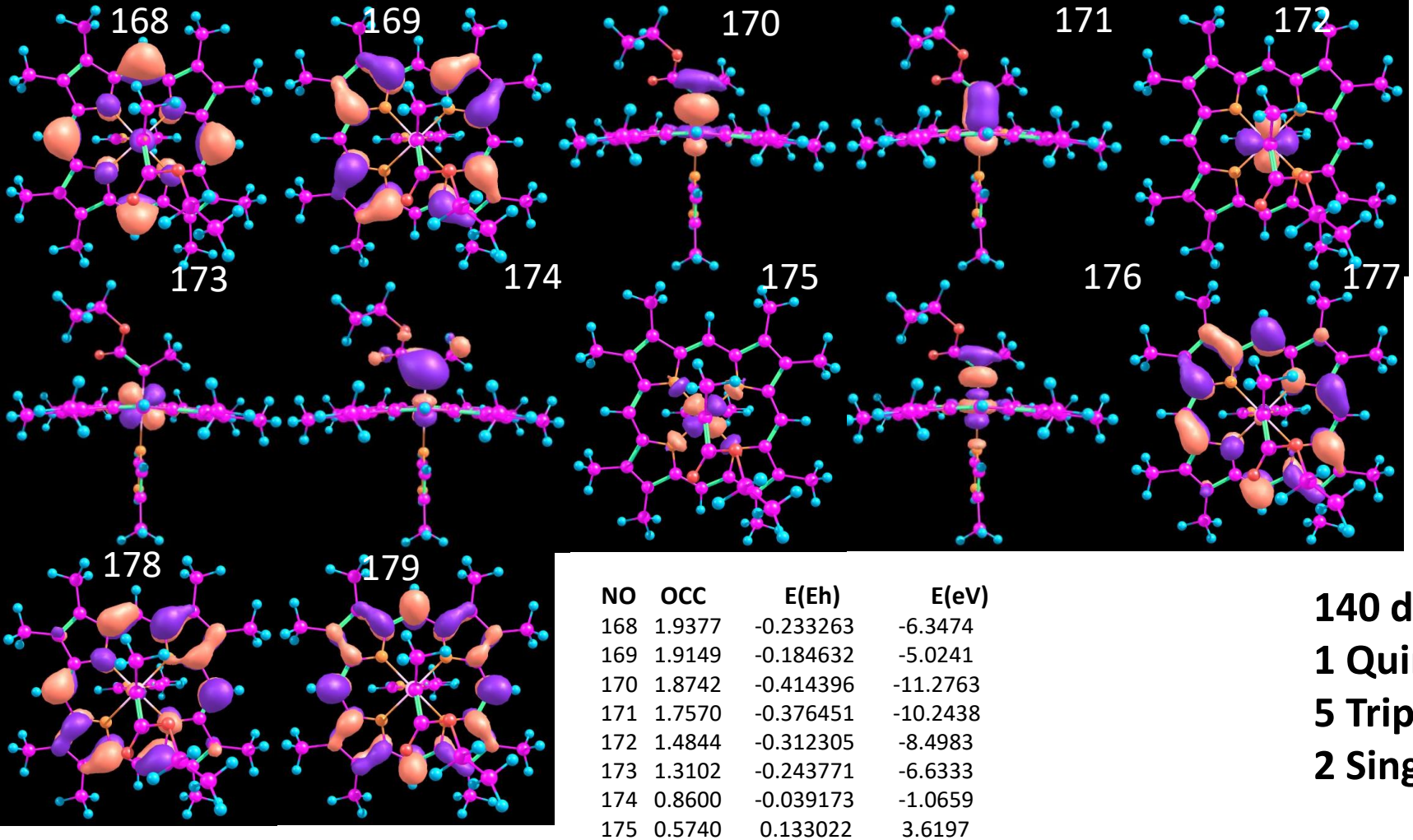
NO	OCC	E(Eh)	E(eV)
168	1.9378	-0.233483	-6.3534
169	1.9146	-0.184689	-5.0256
170	1.8737	-0.413893	-11.2626
171	1.7509	-0.373435	-10.1617
172	1.4893	-0.312390	-8.5006
173	1.3149	-0.243634	-6.6296
174	0.8526	-0.027597	-0.7509
175	0.5777	0.133469	3.6319
176	0.1335	0.269743	7.3401
177	0.0747	0.051703	1.4069
178	0.0736	0.053879	1.4661
179	0.0068	0.200322	5.4510

120 degrees;
1 Quintet,
5 Triplets,
2 Singlets



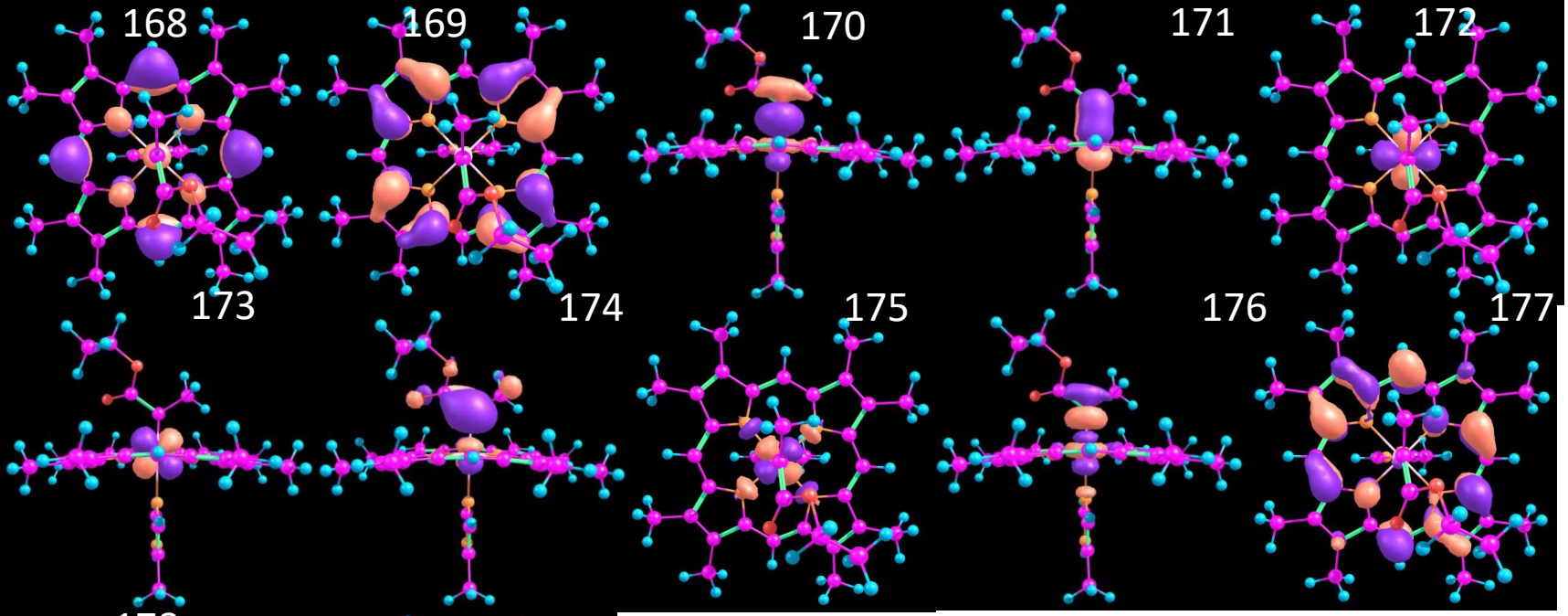
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233438	-6.3522
169	1.9148	-0.184678	-5.0254
170	1.8739	-0.414274	-11.2730
171	1.7524	-0.374323	-10.1859
172	1.4883	-0.313128	-8.5206
173	1.3129	-0.243931	-6.6377
174	0.8556	-0.033205	-0.9036
175	0.5761	0.132962	3.6181
176	0.1334	0.268444	7.3047
177	0.0746	0.051969	1.4141
178	0.0736	0.053908	1.4669
179	0.0068	0.201040	5.4706

130 degrees;
1 Quintet,
5 Triplets,
2 Singlets



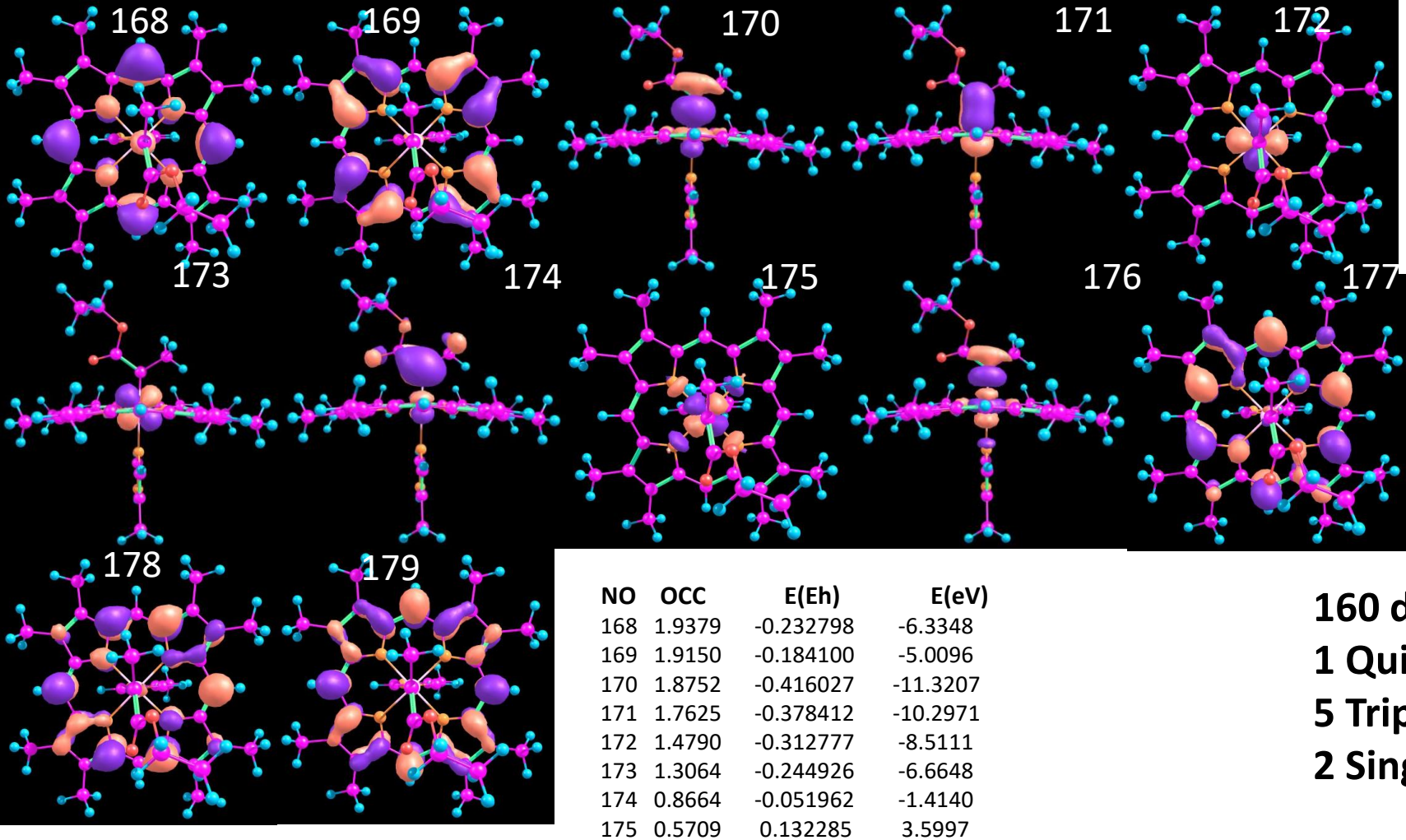
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233263	-6.3474
169	1.9149	-0.184632	-5.0241
170	1.8742	-0.414396	-11.2763
171	1.7570	-0.376451	-10.2438
172	1.4844	-0.312305	-8.4983
173	1.3102	-0.243771	-6.6333
174	0.8600	-0.039173	-1.0659
175	0.5740	0.133022	3.6197
176	0.1327	0.267907	7.2901
177	0.0745	0.052181	1.4199
178	0.0736	0.054053	1.4709
179	0.0068	0.201168	5.4741

140 degrees;
1 Quintet,
5 Triplets,
2 Singlets



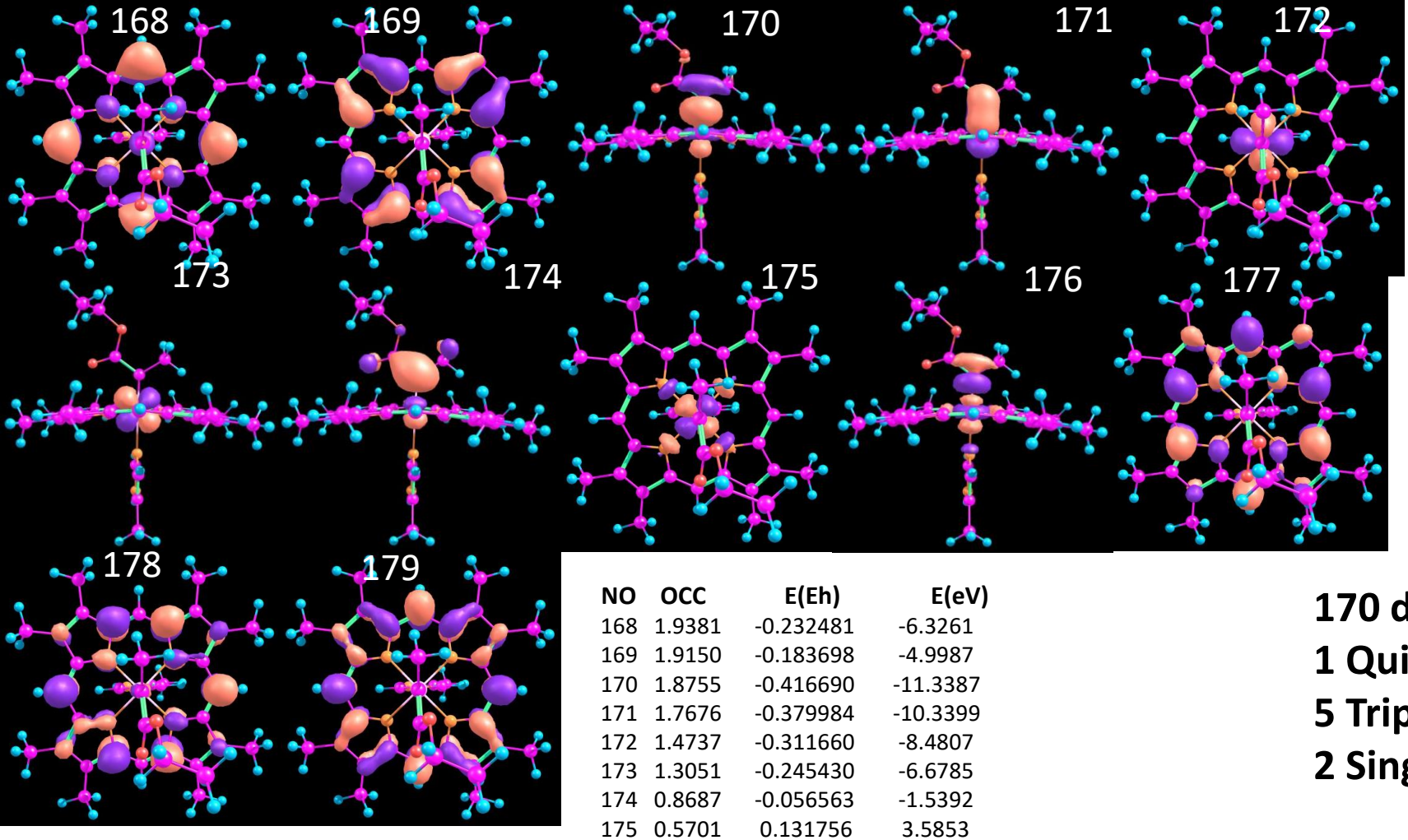
NO	OCC	E(Eh)	E(eV)
168	1.9378	-0.233030	-6.3411
169	1.9150	-0.184405	-5.0179
170	1.8748	-0.414918	-11.2905
171	1.7588	-0.377160	-10.2631
172	1.4828	-0.312933	-8.5153
173	1.3080	-0.244237	-6.6460
174	0.8636	-0.045878	-1.2484
175	0.5721	0.132817	3.6141
176	0.1323	0.266734	7.2582
177	0.0744	0.052606	1.4315
178	0.0736	0.054356	1.4791
179	0.0068	0.202224	5.5028

150 degrees;
1 Quintet,
5 Triplets,
2 Singlets



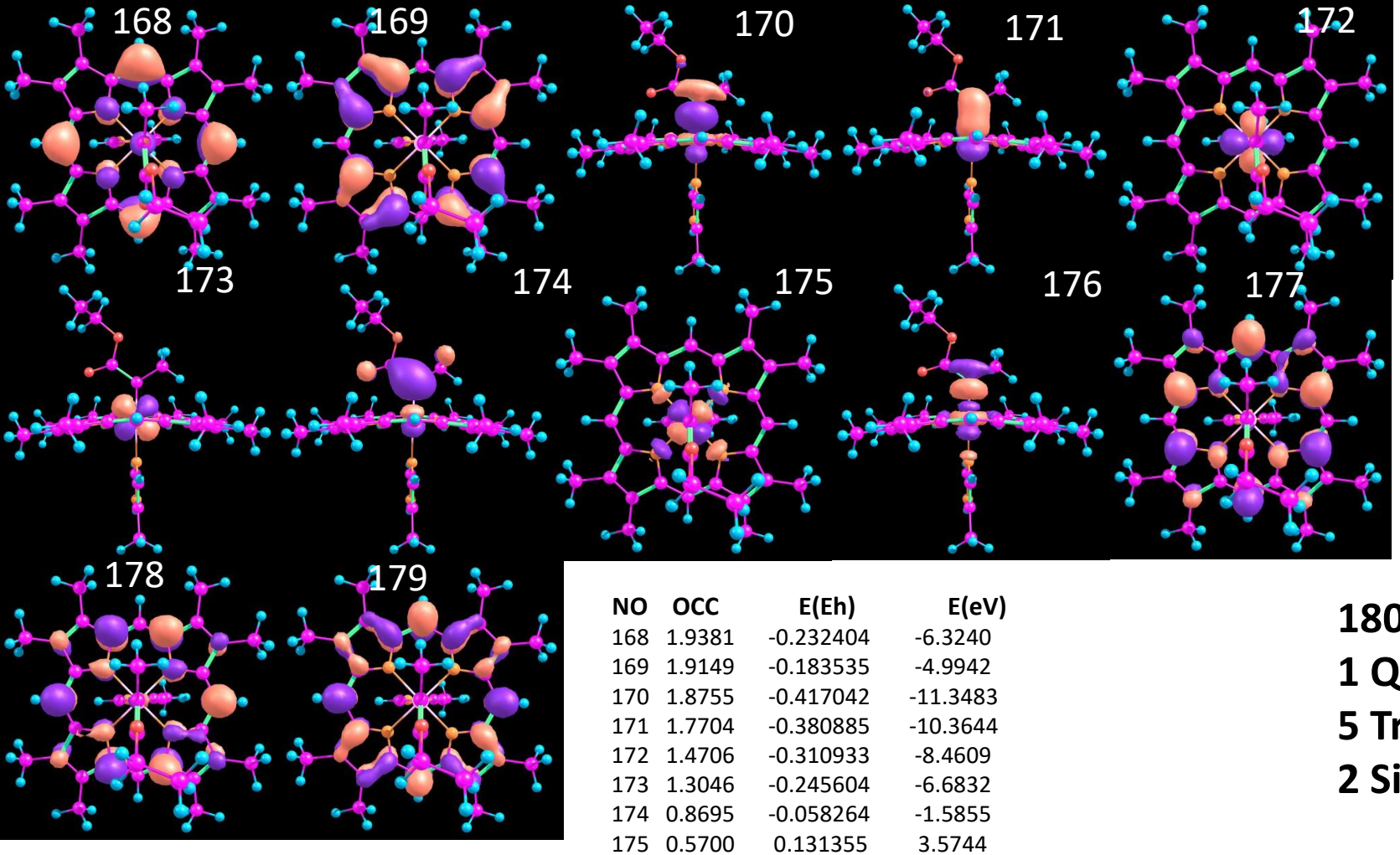
NO	OCC	E(Eh)	E(eV)
168	1.9379	-0.232798	-6.3348
169	1.9150	-0.184100	-5.0096
170	1.8752	-0.416027	-11.3207
171	1.7625	-0.378412	-10.2971
172	1.4790	-0.312777	-8.5111
173	1.3064	-0.244926	-6.6648
174	0.8664	-0.051962	-1.4140
175	0.5709	0.132285	3.5997
176	0.1320	0.265526	7.2253
177	0.0742	0.052905	1.4396
178	0.0736	0.054779	1.4906
179	0.0068	0.203534	5.5384

160 degrees;
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
168	1.9381	-0.232481	-6.3261
169	1.9150	-0.183698	-4.9987
170	1.8755	-0.416690	-11.3387
171	1.7676	-0.379984	-10.3399
172	1.4737	-0.311660	-8.4807
173	1.3051	-0.245430	-6.6785
174	0.8687	-0.056563	-1.5392
175	0.5701	0.131756	3.5853
176	0.1317	0.264777	7.2050
177	0.0742	0.053239	1.4487
178	0.0736	0.055298	1.5047
179	0.0068	0.203695	5.5428

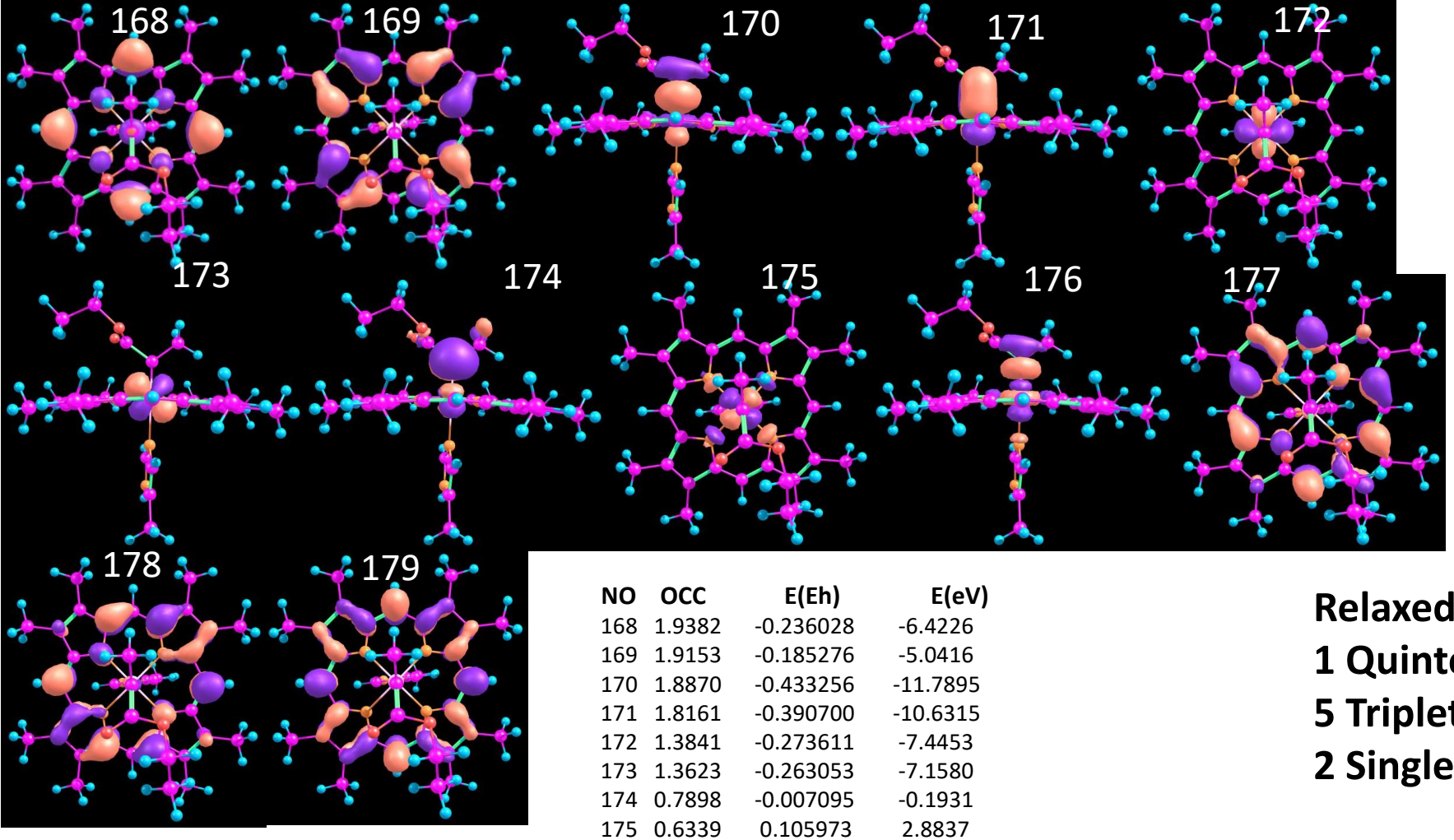
170 degrees;
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
168	1.9381	-0.232404	-6.3240
169	1.9149	-0.183535	-4.9942
170	1.8755	-0.417042	-11.3483
171	1.7704	-0.380885	-10.3644
172	1.4706	-0.310933	-8.4609
173	1.3046	-0.245604	-6.6832
174	0.8695	-0.058264	-1.5855
175	0.5700	0.131355	3.5744
176	0.1317	0.264450	7.1960
177	0.0742	0.053332	1.4512
178	0.0736	0.055460	1.5092
179	0.0068	0.204377	5.5614

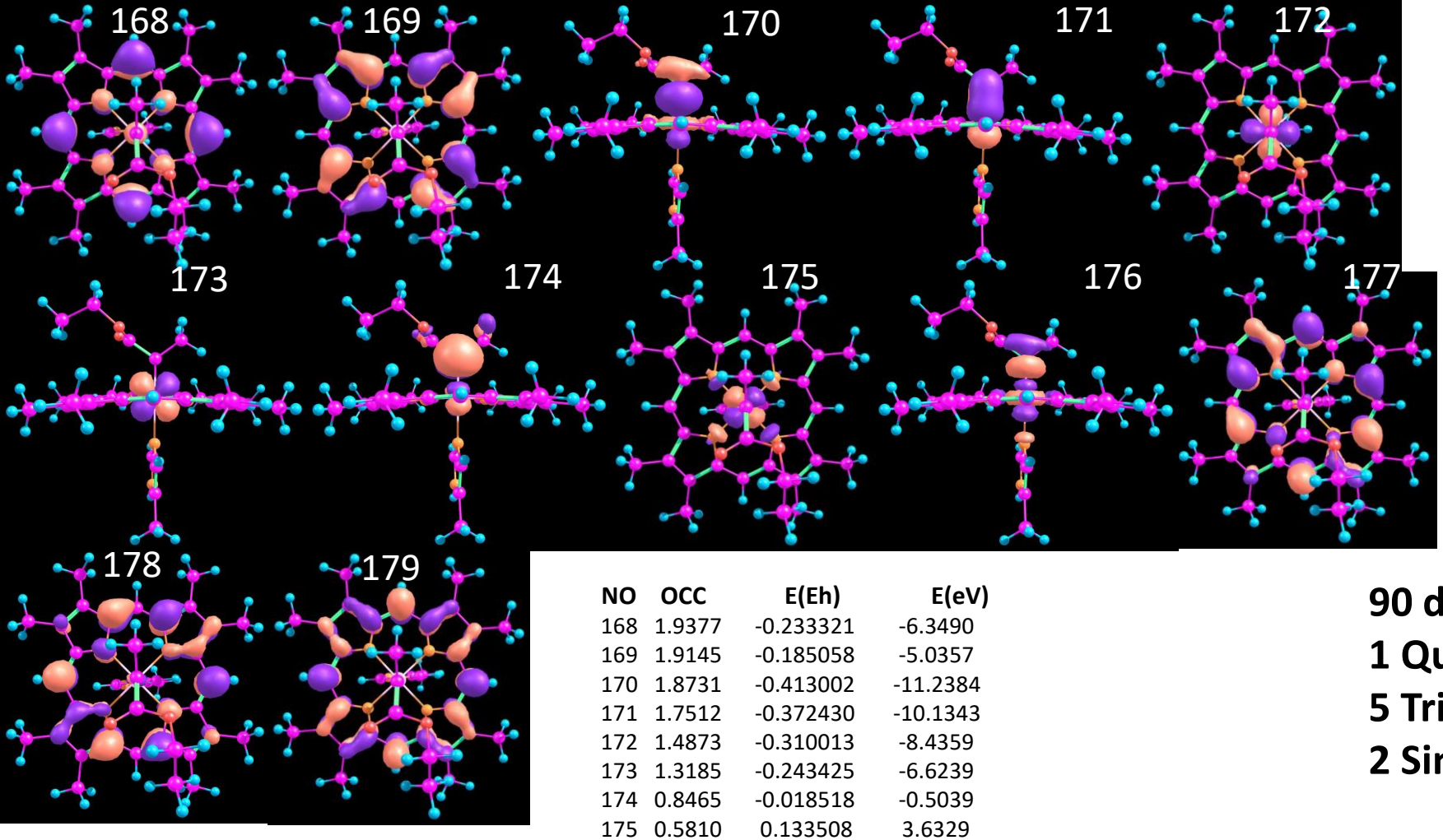
180 degrees;
1 Quintet,
5 Triplets,
2 Singlets

Active Space for QD-NEVPT2 on RKS DFT Geometries;Relaxed Scan of Fe-C: MeImid.



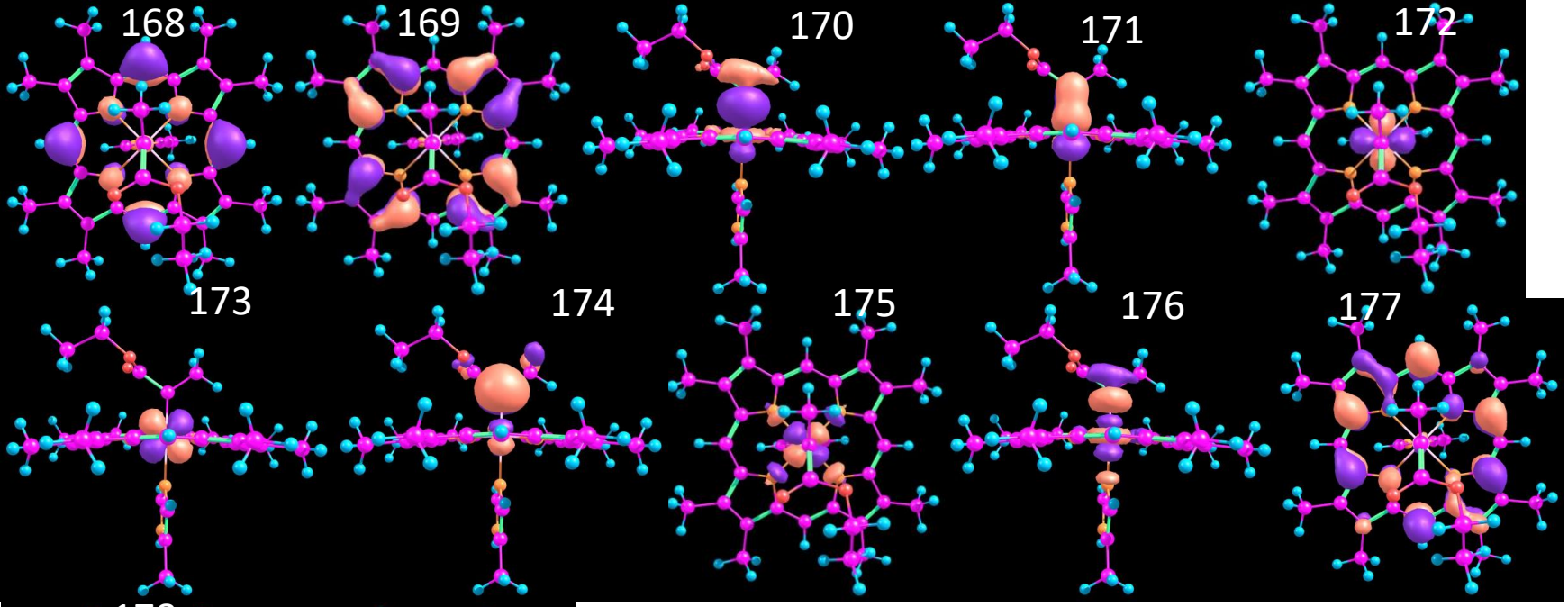
NO	OCC	E(Eh)	E(eV)
168	1.9382	-0.236028	-6.4226
169	1.9153	-0.185276	-5.0416
170	1.8870	-0.433256	-11.7895
171	1.8161	-0.390700	-10.6315
172	1.3841	-0.273611	-7.4453
173	1.3623	-0.263053	-7.1580
174	0.7898	-0.007095	-0.1931
175	0.6339	0.105973	2.8837
176	0.1192	0.296511	8.0685
177	0.0742	0.052416	1.4263
178	0.0731	0.052981	1.4417
179	0.0067	0.197820	5.3830

Relaxed; 1.7 Å
1 Quintet,
5 Triplets,
2 Singlets



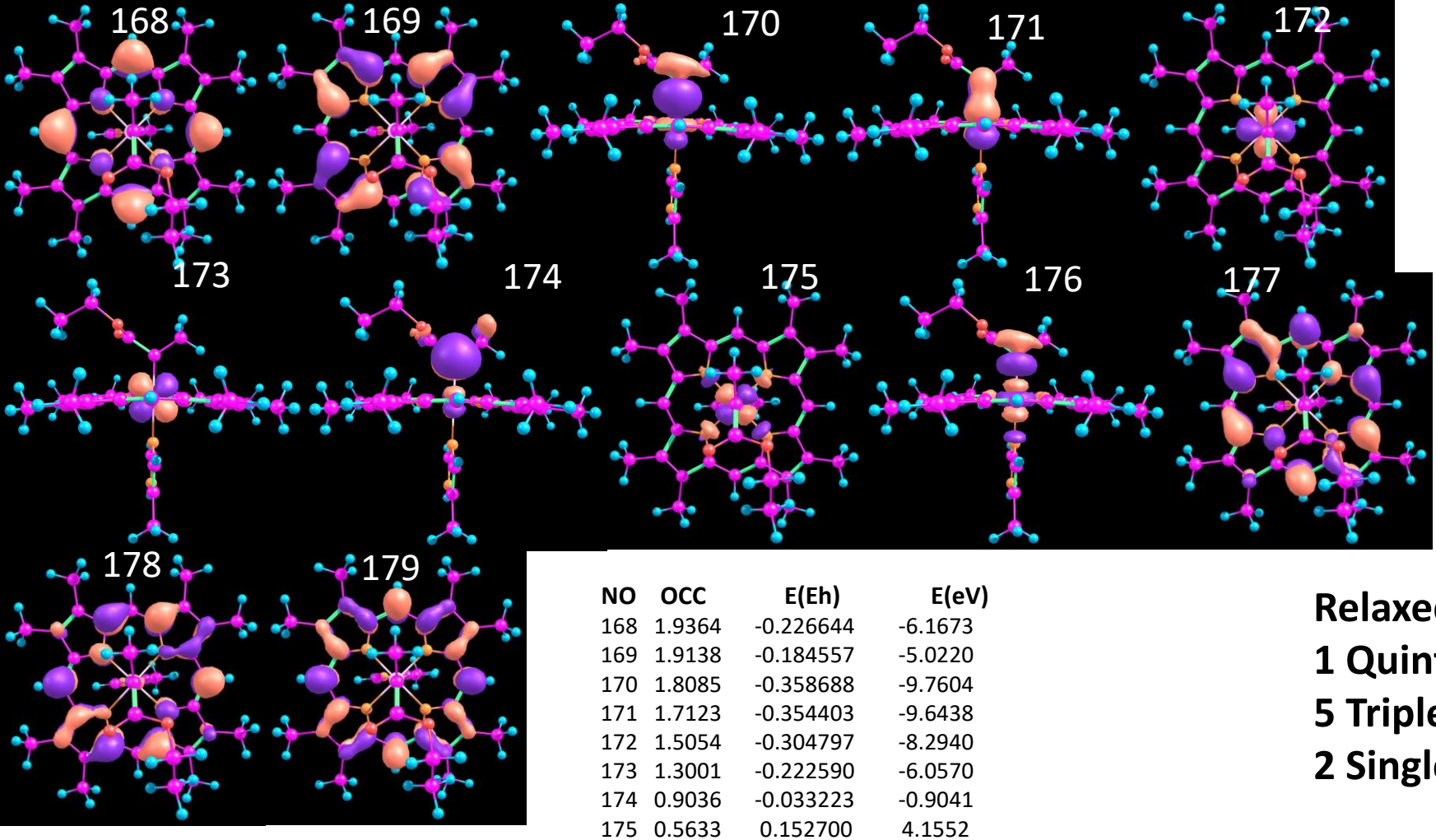
NO	OCC	E(Eh)	E(eV)
168	1.9377	-0.233321	-6.3490
169	1.9145	-0.185058	-5.0357
170	1.8731	-0.413002	-11.2384
171	1.7512	-0.372430	-10.1343
172	1.4873	-0.310013	-8.4359
173	1.3185	-0.243425	-6.6239
174	0.8465	-0.018518	-0.5039
175	0.5810	0.133508	3.6329
176	0.1349	0.270587	7.3631
177	0.0749	0.051107	1.3907
178	0.0735	0.053753	1.4627
179	0.0068	0.199935	5.4405

90 degrees;
1 Quintet,
5 Triplets,
2 Singlets



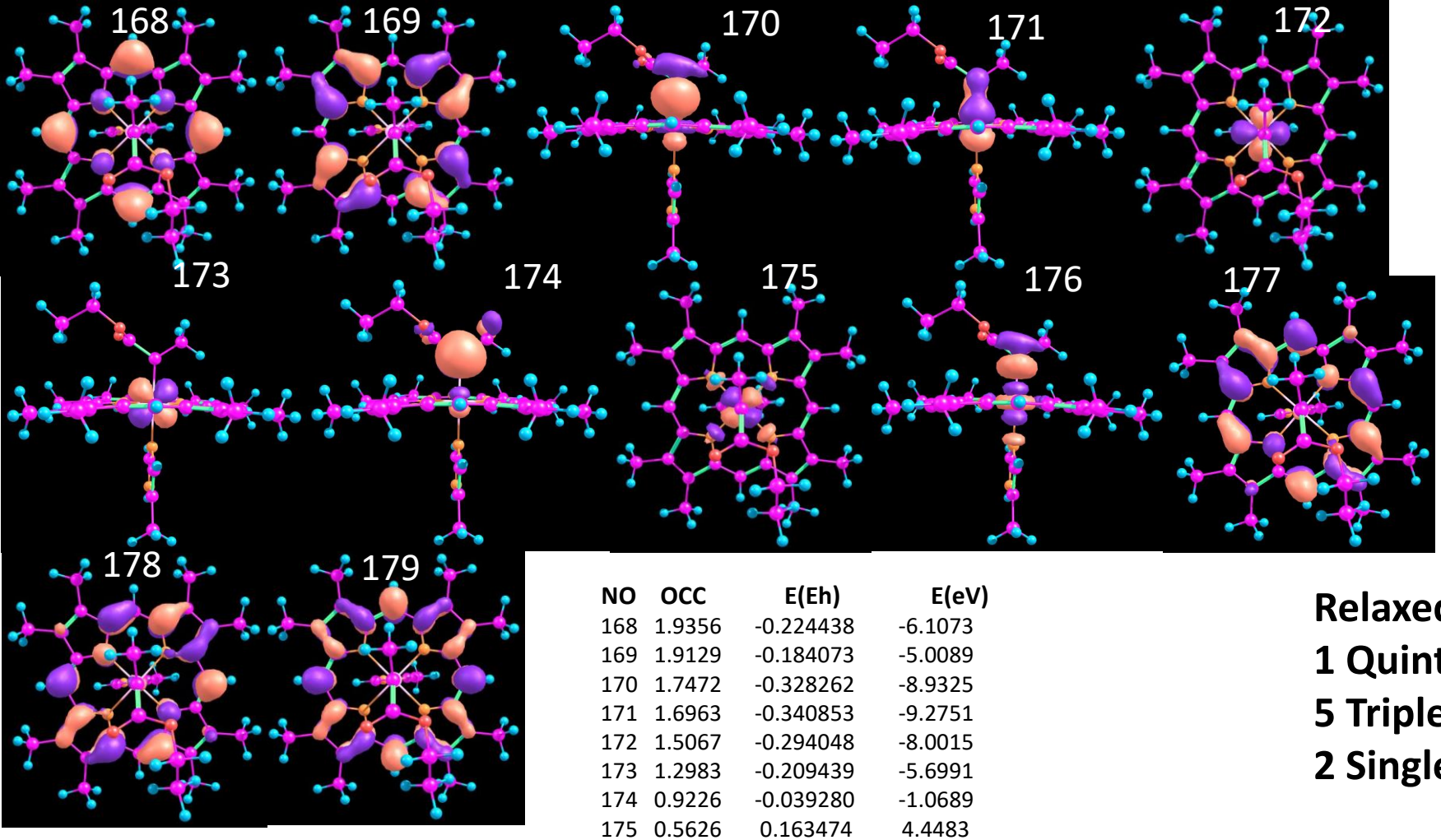
NO	OCC	E(Eh)	E(eV)
168	1.9371	-0.229692	-6.2502
169	1.9143	-0.184848	-5.0300
170	1.8470	-0.385460	-10.4889
171	1.7300	-0.364510	-9.9188
172	1.5021	-0.311003	-8.4628
173	1.3038	-0.232414	-6.3243
174	0.8815	-0.027427	-0.7463
175	0.5664	0.144345	3.9278
176	0.1618	0.241042	6.5591
177	0.0754	0.050491	1.3739
178	0.0738	0.054250	1.4762
179	0.0068	0.200407	5.4533

Relaxed; 1.9 Å
1 Quintet,
5 Triplets,
2 Singlets



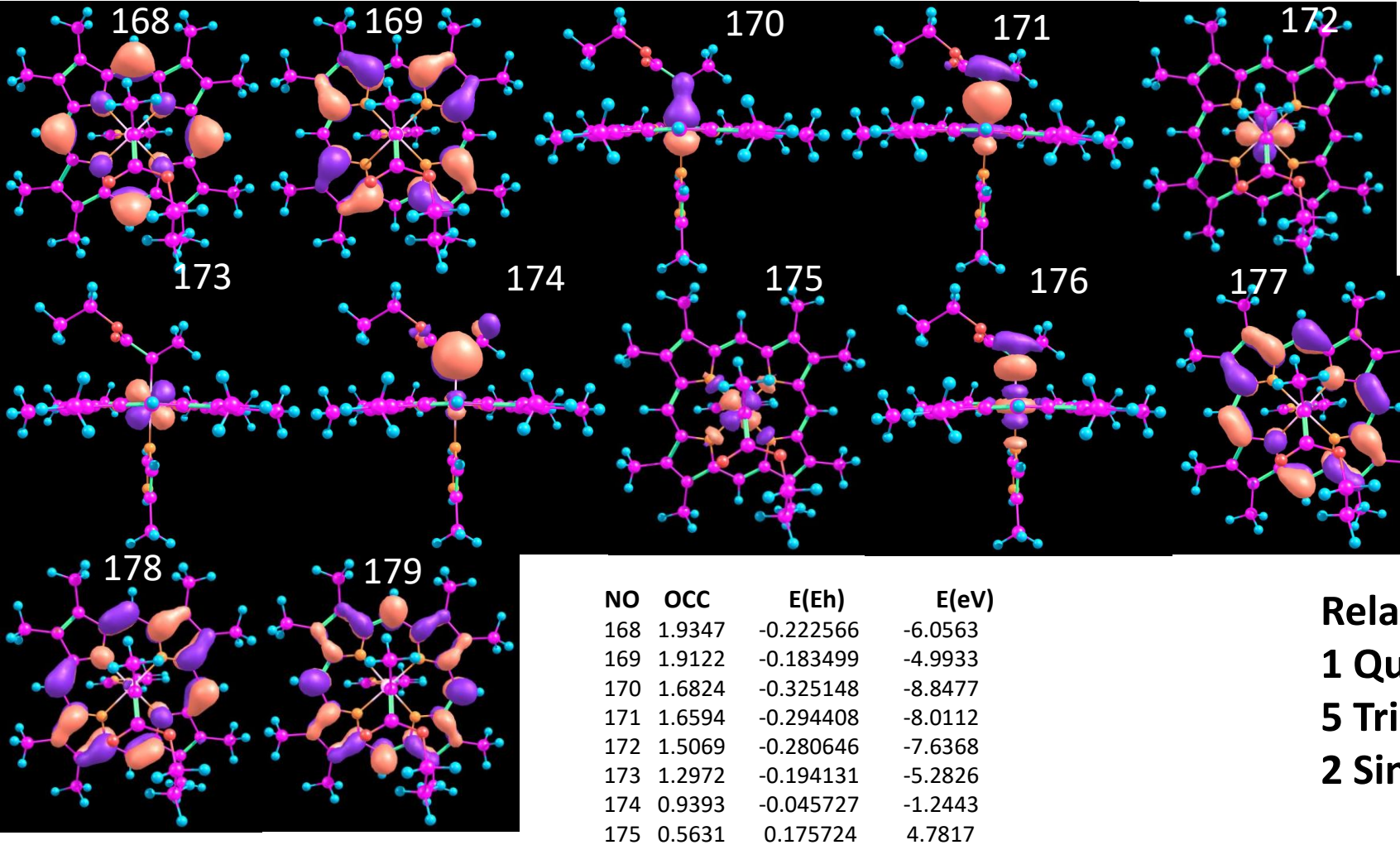
NO	OCC	E(Eh)	E(eV)
168	1.9364	-0.226644	-6.1673
169	1.9138	-0.184557	-5.0220
170	1.8085	-0.358688	-9.7604
171	1.7123	-0.354403	-9.6438
172	1.5054	-0.304797	-8.2940
173	1.3001	-0.222590	-6.0570
174	0.9036	-0.033223	-0.9041
175	0.5633	0.152700	4.1552
176	0.1999	0.212958	5.7949
177	0.0756	0.050247	1.3673
178	0.0744	0.053754	1.4627
179	0.0068	0.199383	5.4255

Relaxed; 2.0 Å
1 Quintet,
5 Triplets,
2 Singlets



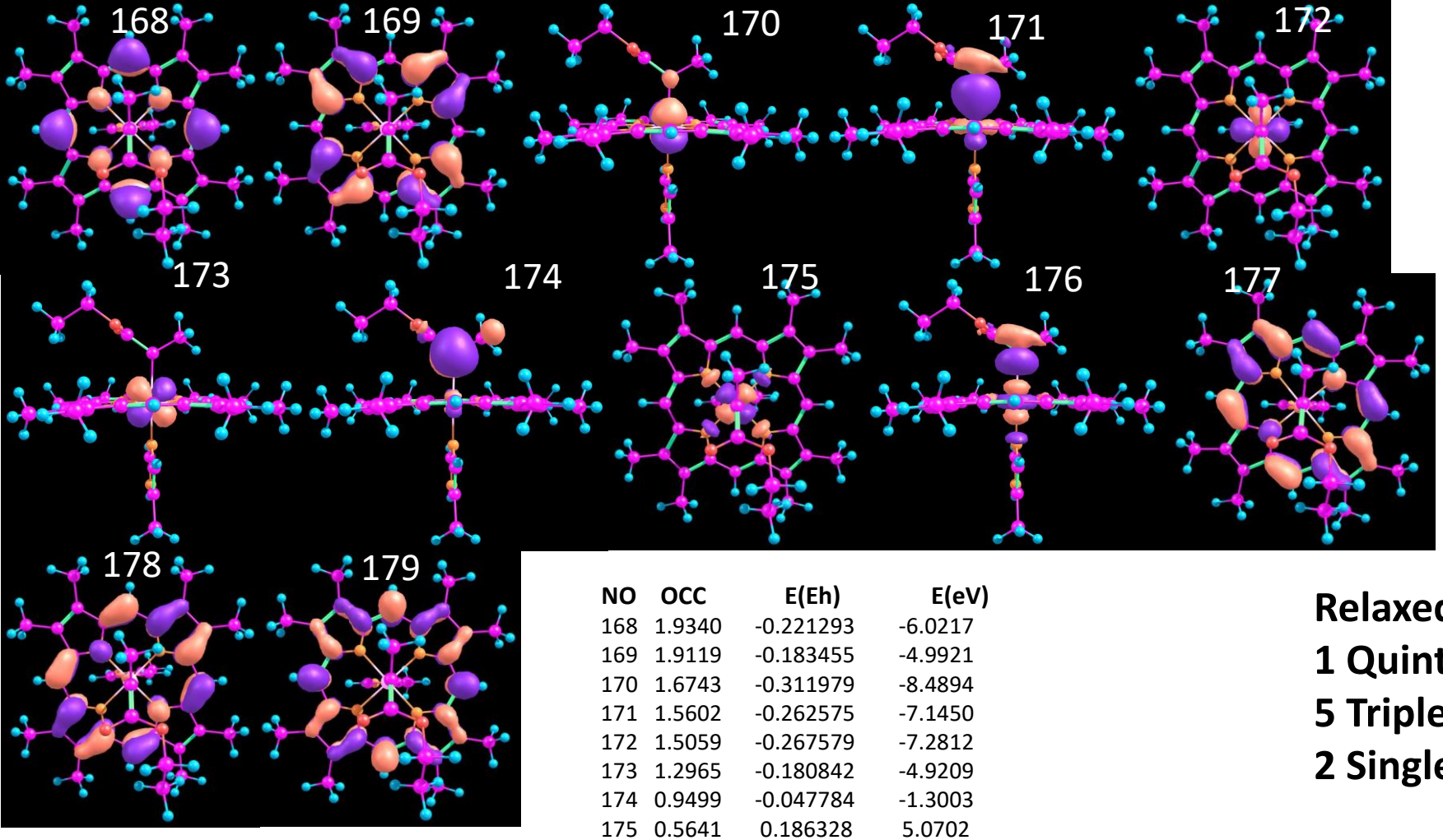
NO	OCC	E(Eh)	E(eV)
168	1.9356	-0.224438	-6.1073
169	1.9129	-0.184073	-5.0089
170	1.7472	-0.328262	-8.9325
171	1.6963	-0.340853	-9.2751
172	1.5067	-0.294048	-8.0015
173	1.2983	-0.209439	-5.6991
174	0.9226	-0.039280	-1.0689
175	0.5626	0.163474	4.4483
176	0.2605	0.180812	4.9202
177	0.0759	0.050240	1.3671
178	0.0748	0.052923	1.4401
179	0.0068	0.200150	5.4463

Relaxed; 2.1 Å
1 Quintet,
5 Triplets,
2 Singlets



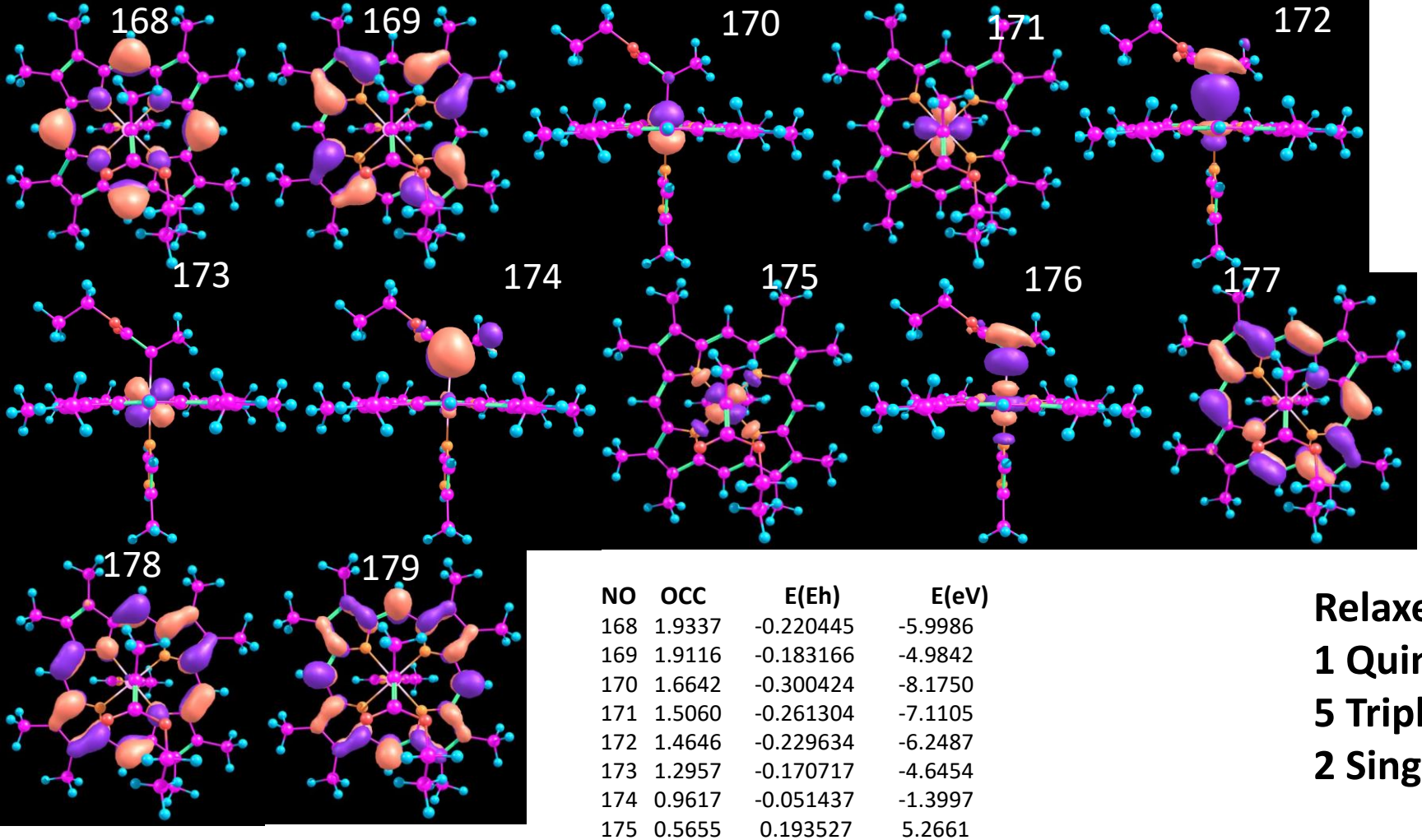
NO	OCC	E(Eh)	E(eV)
168	1.9347	-0.222566	-6.0563
169	1.9122	-0.183499	-4.9933
170	1.6824	-0.325148	-8.8477
171	1.6594	-0.294408	-8.0112
172	1.5069	-0.280646	-7.6368
173	1.2972	-0.194131	-5.2826
174	0.9393	-0.045727	-1.2443
175	0.5631	0.175724	4.7817
176	0.3470	0.145274	3.9531
177	0.0760	0.050481	1.3737
178	0.0751	0.052020	1.4155
179	0.0067	0.200588	5.4583

Relaxed; 2.2 Å
1 Quintet,
5 Triplets,
2 Singlets



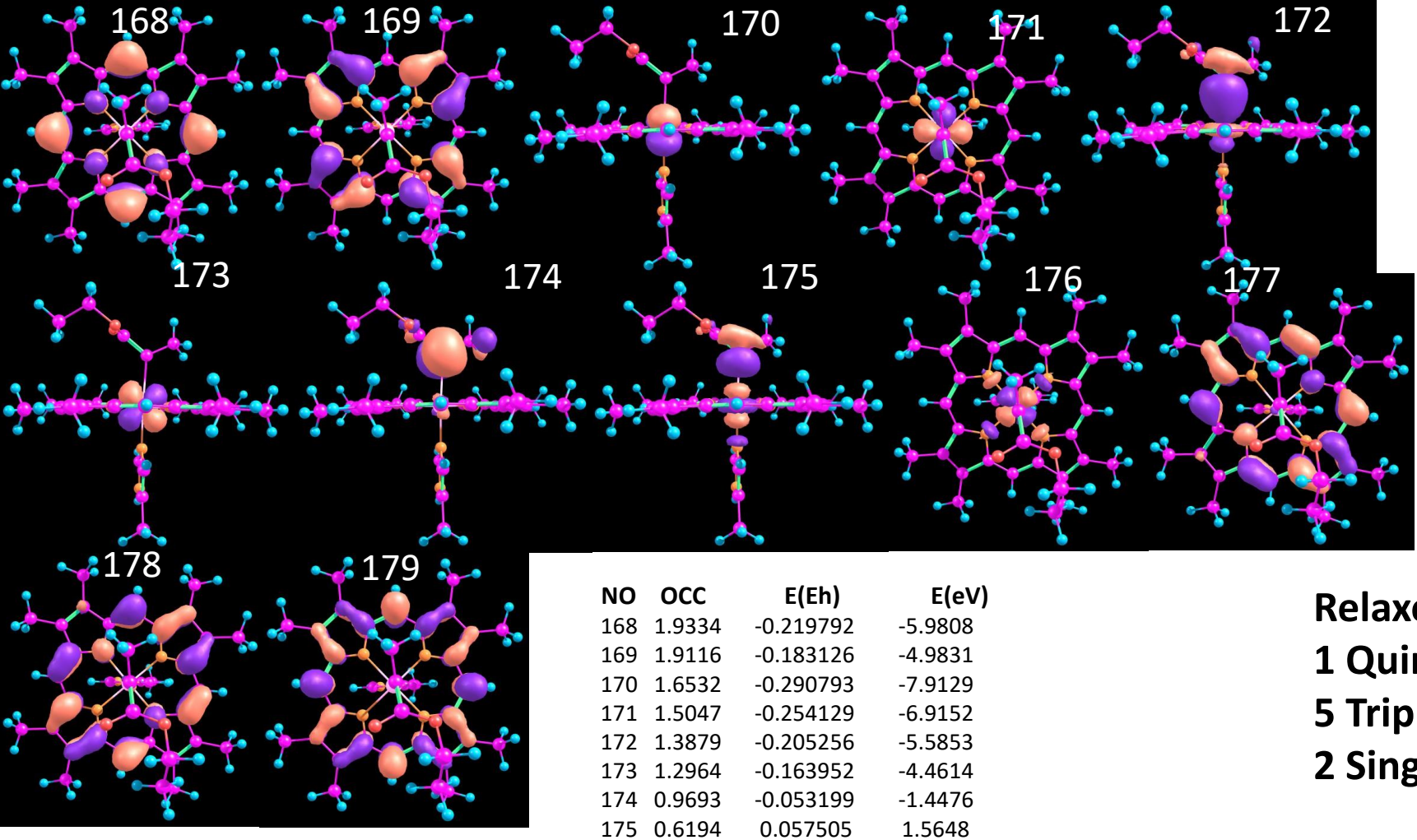
NO	OCC	E(Eh)	E(eV)
168	1.9340	-0.221293	-6.0217
169	1.9119	-0.183455	-4.9921
170	1.6743	-0.311979	-8.4894
171	1.5602	-0.262575	-7.1450
172	1.5059	-0.267579	-7.2812
173	1.2965	-0.180842	-4.9209
174	0.9499	-0.047784	-1.3003
175	0.5641	0.186328	5.0702
176	0.4456	0.111395	3.0312
177	0.0758	0.050472	1.3734
178	0.0752	0.051152	1.3919
179	0.0067	0.198749	5.4082

Relaxed; 2.3 Å
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
168	1.9337	-0.220445	-5.9986
169	1.9116	-0.183166	-4.9842
170	1.6642	-0.300424	-8.1750
171	1.5060	-0.261304	-7.1105
172	1.4646	-0.229634	-6.2487
173	1.2957	-0.170717	-4.6454
174	0.9617	-0.051437	-1.3997
175	0.5655	0.193527	5.2661
176	0.5395	0.081934	2.2295
177	0.0758	0.050452	1.3729
178	0.0751	0.051154	1.3920
179	0.0065	0.201379	5.4798

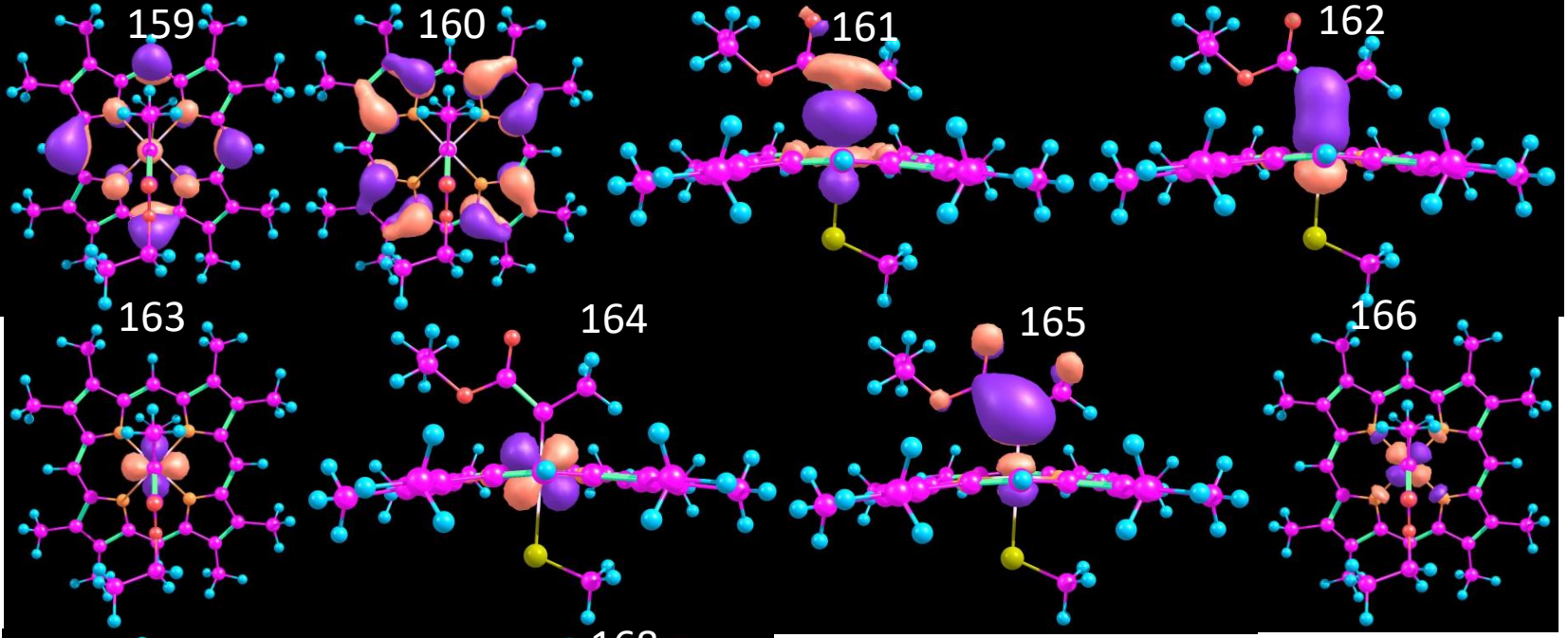
Relaxed; 2.4 Å
1 Quintet,
5 Triplets,
2 Singlets

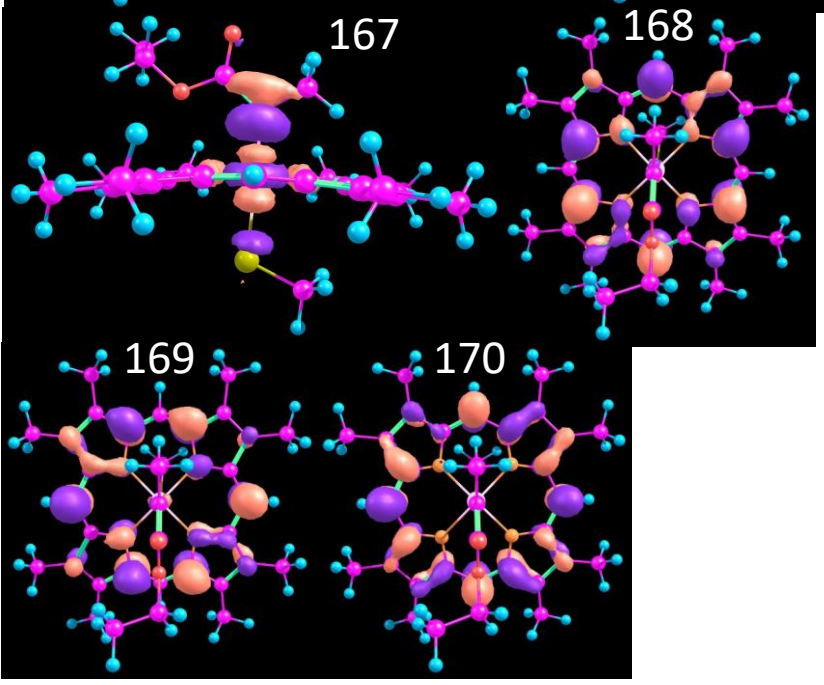


NO	OCC	E(Eh)	E(eV)
168	1.9334	-0.219792	-5.9808
169	1.9116	-0.183126	-4.9831
170	1.6532	-0.290793	-7.9129
171	1.5047	-0.254129	-6.9152
172	1.3879	-0.205256	-5.5853
173	1.2964	-0.163952	-4.4614
174	0.9693	-0.053199	-1.4476
175	0.6194	0.057505	1.5648
176	0.5668	0.199257	5.4221
177	0.0758	0.050385	1.3710
178	0.0749	0.051223	1.3938
179	0.0066	0.199115	5.4182

Relaxed; 2.5 Å
1 Quintet,
5 Triplets,
2 Singlets

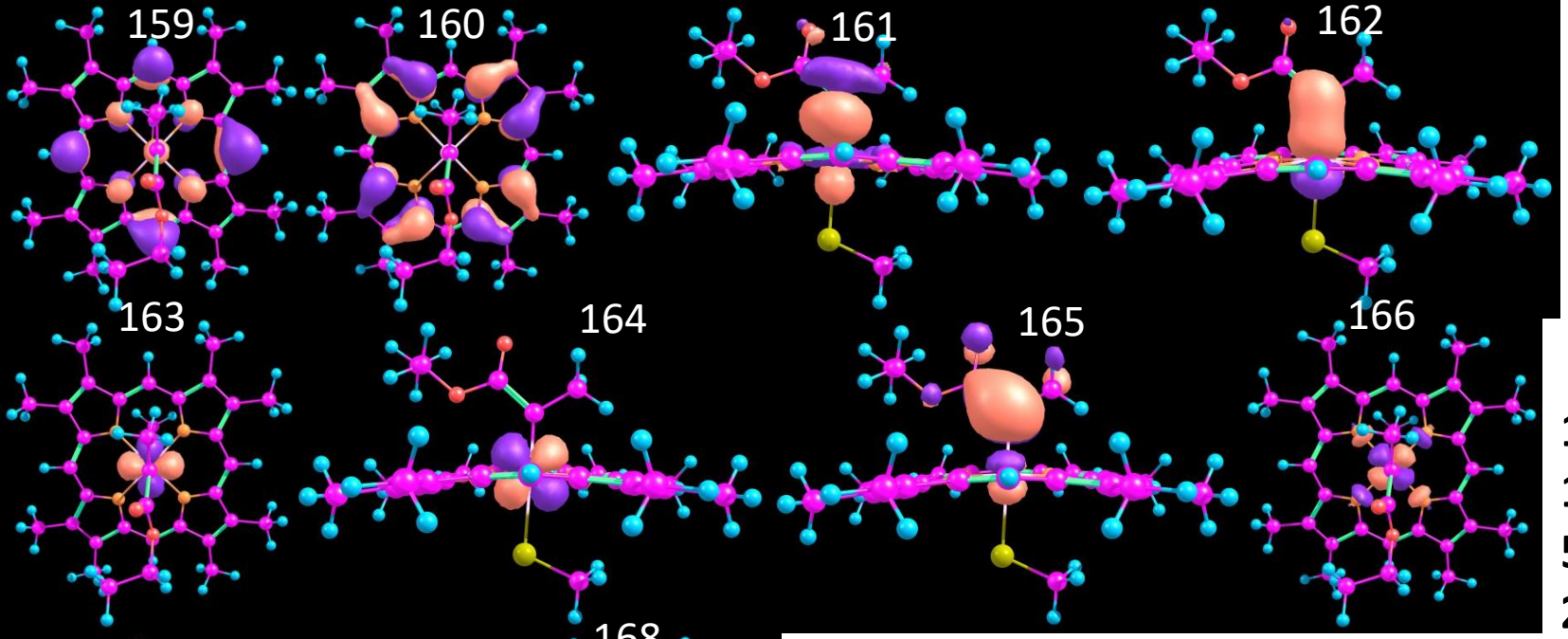
Active Space for QD-NEVPT2 on RKS DFT Geometries: Thiolate

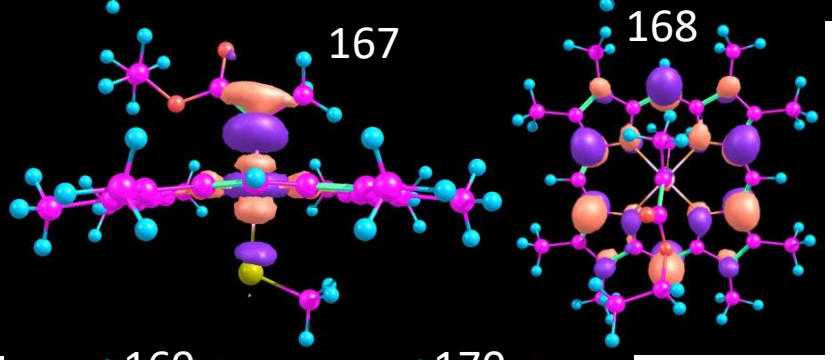


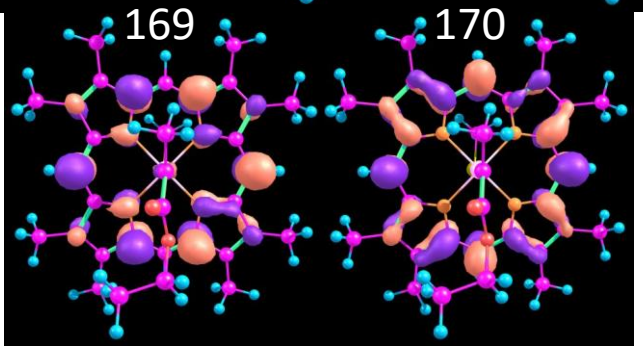


0 degrees;
1 Quintet,
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
159	1.9358	-0.136329	-3.7097
160	1.9165	-0.090491	-2.4624
161	1.8923	-0.319893	-8.7047
162	1.7250	-0.268024	-7.2933
163	1.4996	-0.228634	-6.2214
164	1.3043	-0.152014	-4.1365
165	0.8870	0.029568	0.8046
166	0.5666	0.226885	6.1739
167	0.1169	0.356642	9.7047
168	0.0750	0.147299	4.0082
169	0.0735	0.150381	4.0921
170	0.0074	0.302632	8.2350

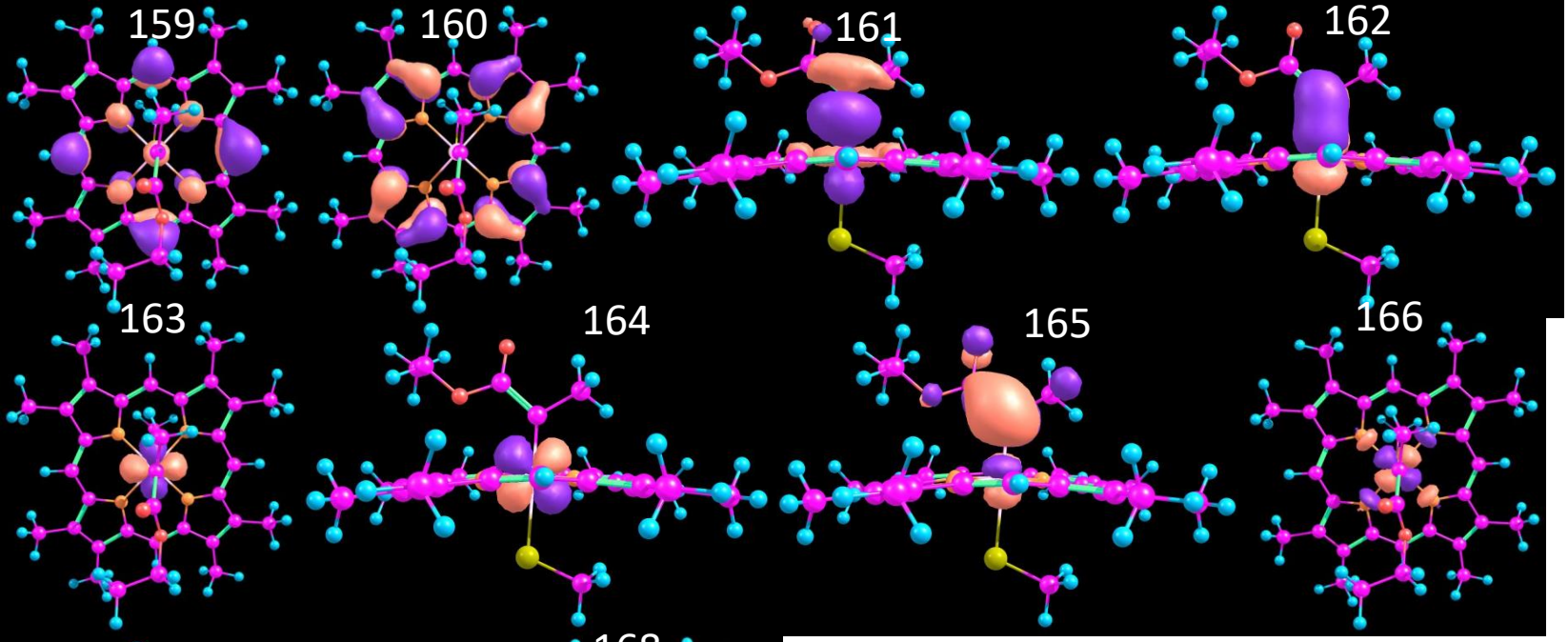


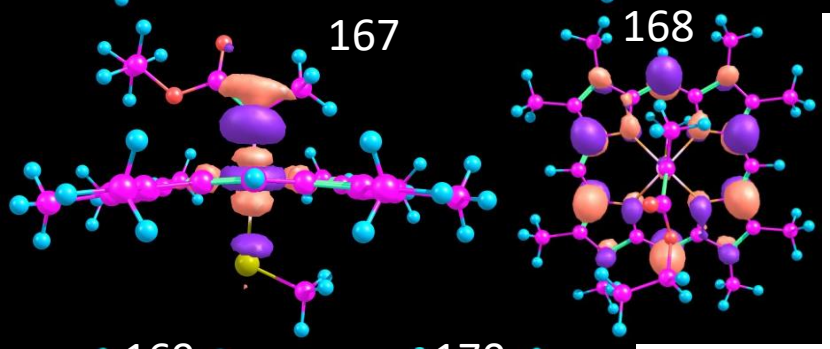


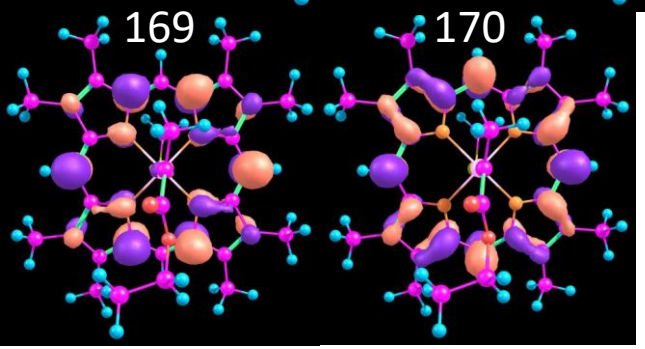


10 degrees;
1 Quintet,
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.135730	-3.6934
160	1.9167	-0.090573	-2.4646
161	1.8924	-0.319818	-8.7027
162	1.7270	-0.268993	-7.3197
163	1.4980	-0.227531	-6.1914
164	1.3045	-0.151679	-4.1274
165	0.8861	0.031420	0.8550
166	0.5671	0.226890	6.1740
167	0.1167	0.357228	9.7207
168	0.0750	0.147158	4.0044
169	0.0736	0.150313	4.0902
170	0.0073	0.300222	8.1695

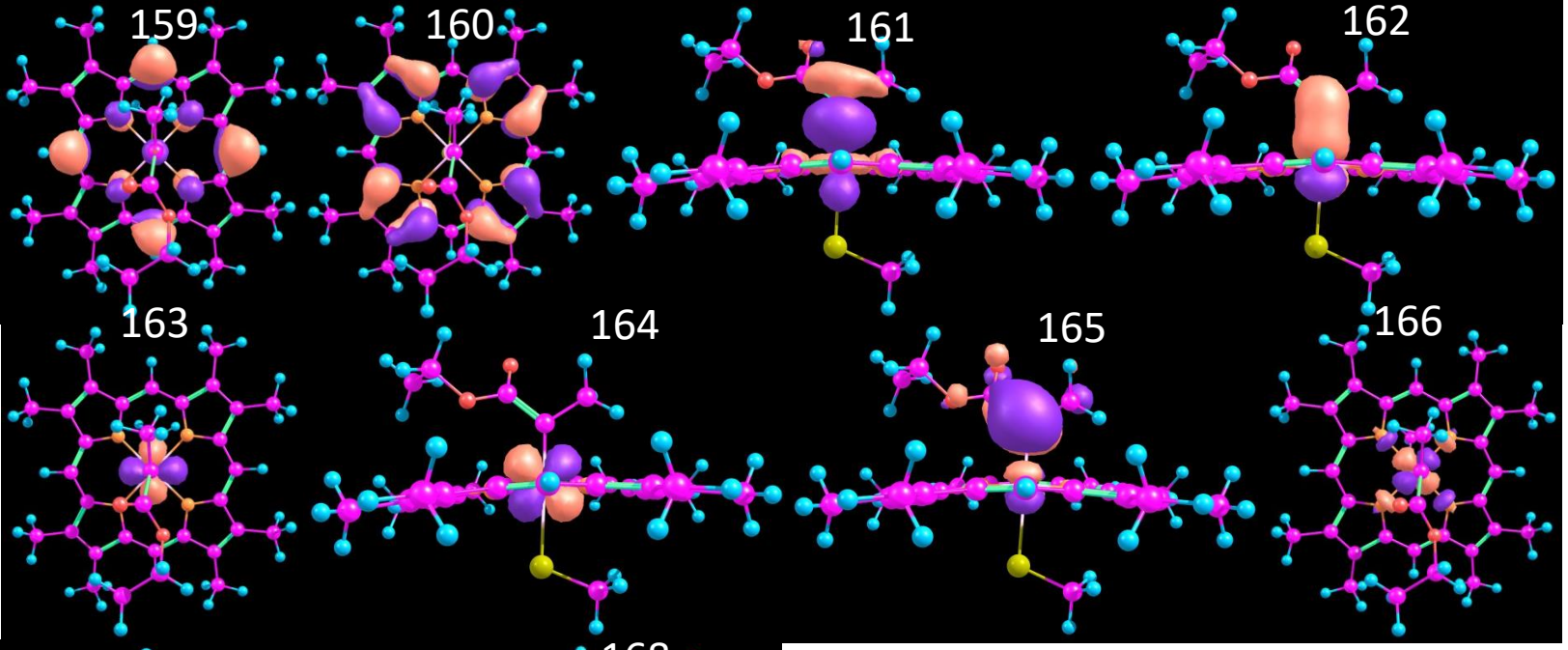


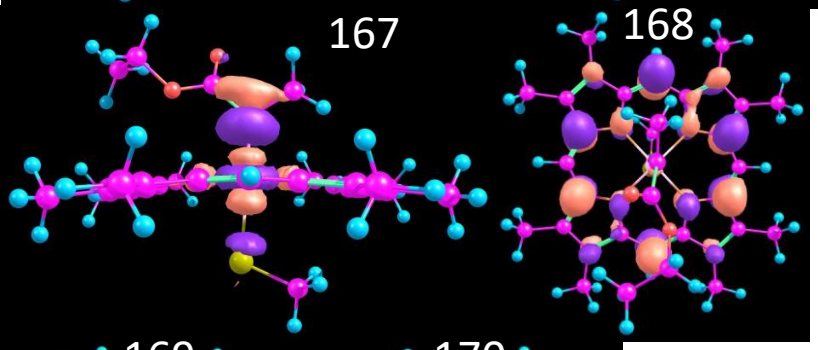


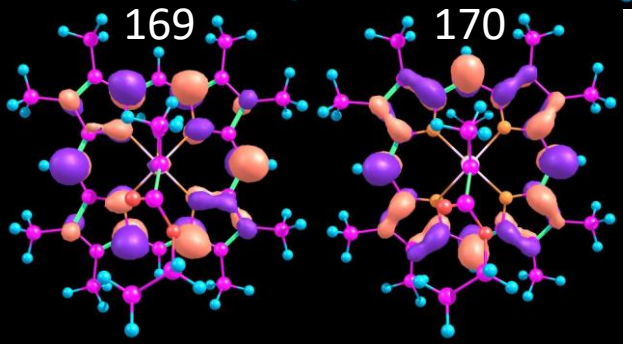


20 degrees;
1 Quintet,
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
159	1.9358	-0.135960	-3.6997
160	1.9169	-0.090559	-2.4642
161	1.8930	-0.318542	-8.6680
162	1.7248	-0.267707	-7.2847
163	1.4975	-0.227219	-6.1830
164	1.3045	-0.151486	-4.1222
165	0.8836	0.034503	0.9389
166	0.5670	0.226863	6.1733
167	0.1210	0.353547	9.6205
168	0.0750	0.147396	4.0108
169	0.0736	0.150484	4.0949
170	0.0072	0.298358	8.1187

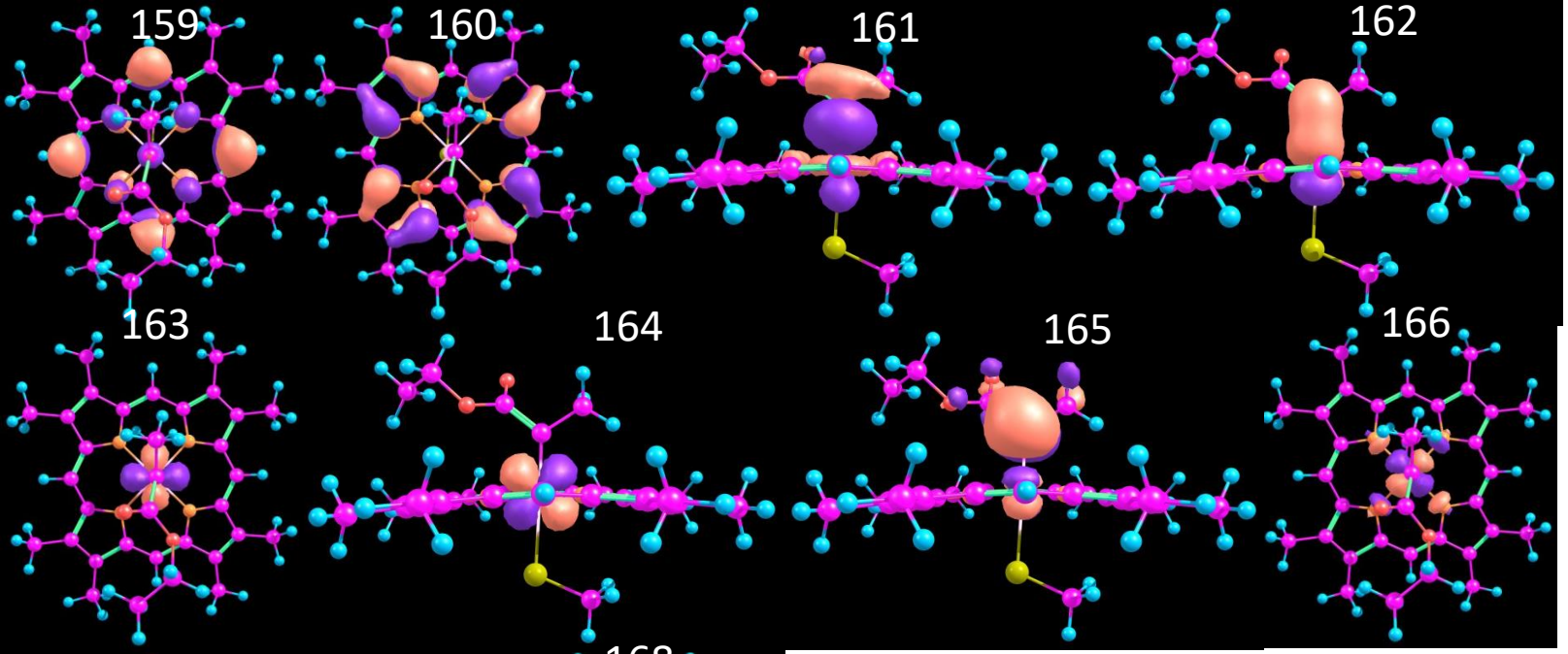


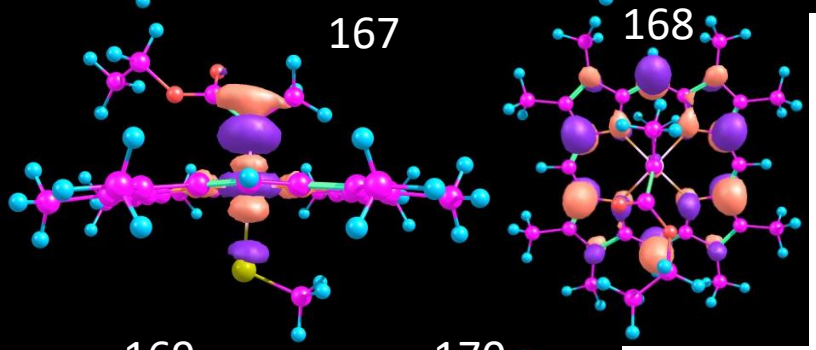


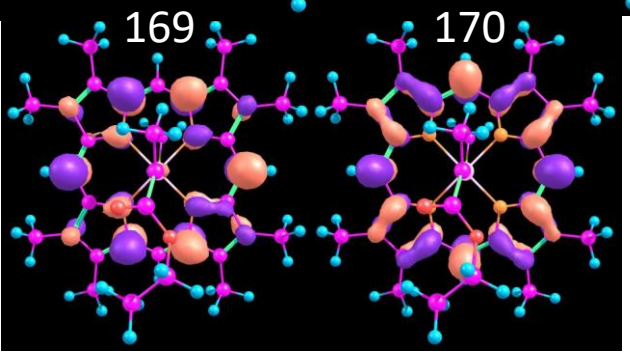


30 degrees;
1 Quintet,
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134812	-3.6684
160	1.9167	-0.090127	-2.4525
161	1.8925	-0.318039	-8.6543
162	1.7306	-0.269994	-7.3469
163	1.4957	-0.223521	-6.0823
164	1.3064	-0.149374	-4.0647
165	0.8813	0.043005	1.1702
166	0.5692	0.228512	6.2181
167	0.1162	0.361148	9.8273
168	0.0754	0.147151	4.0042
169	0.0734	0.150622	4.0986
170	0.0071	0.292862	7.9692

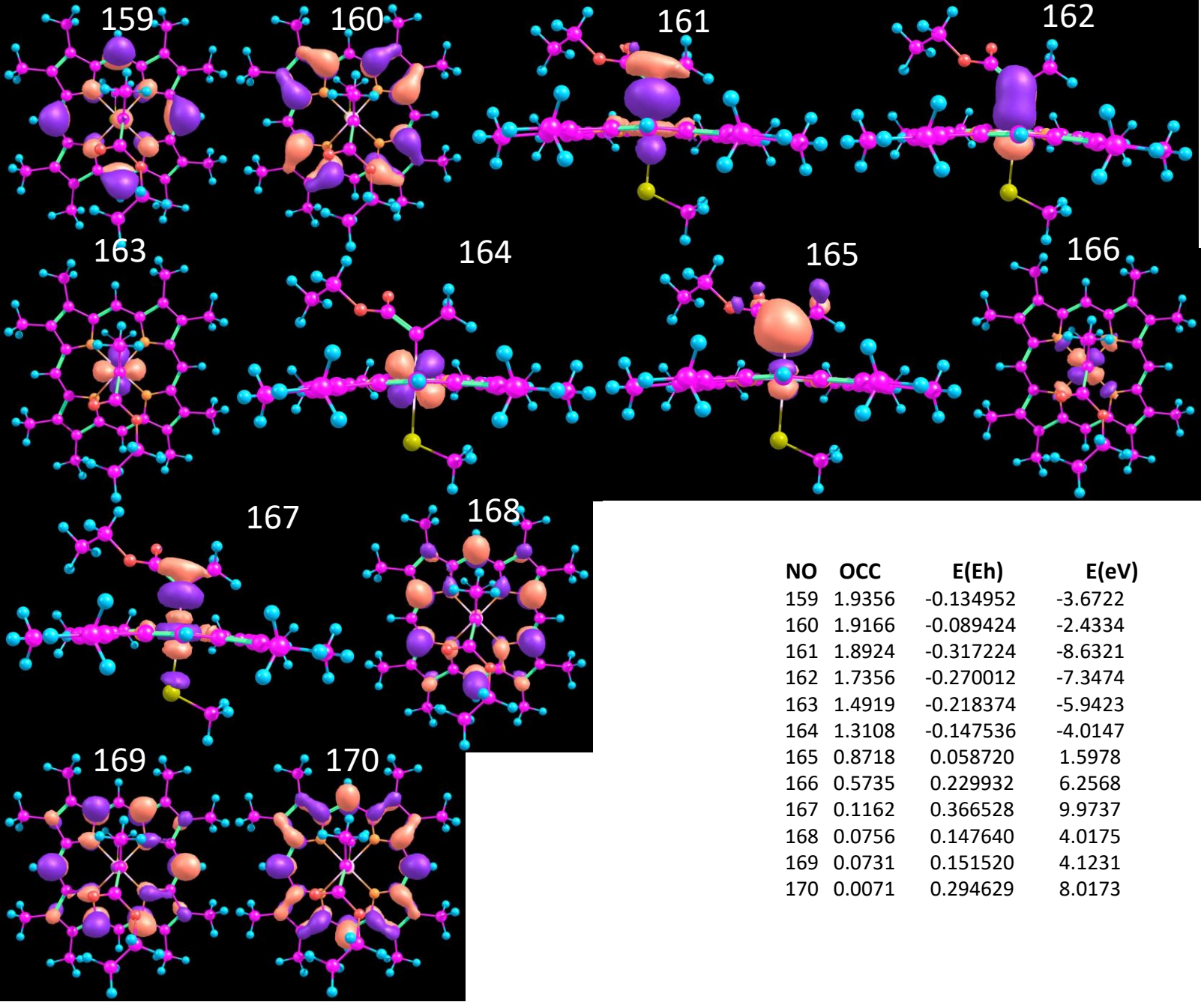






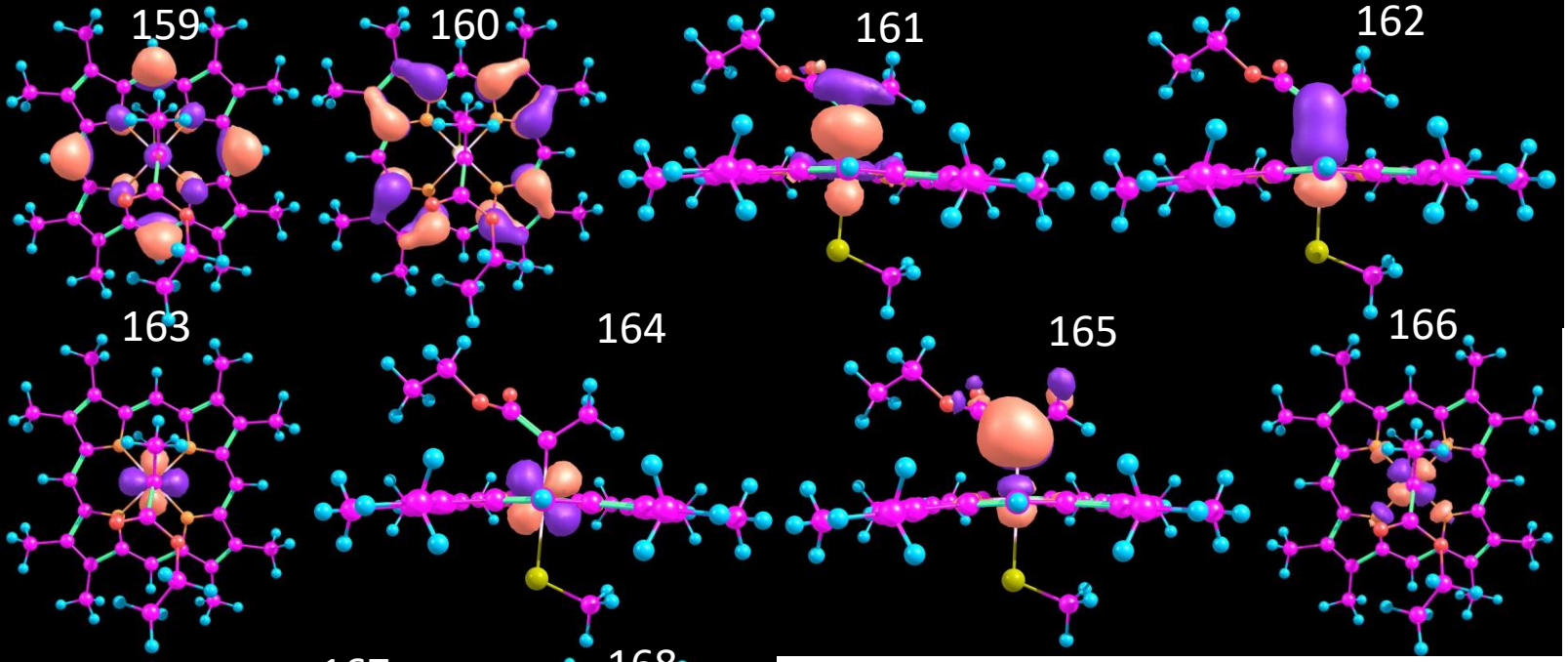
40 degrees;
1 Quintet,
5 Triplets,
2 Singlets

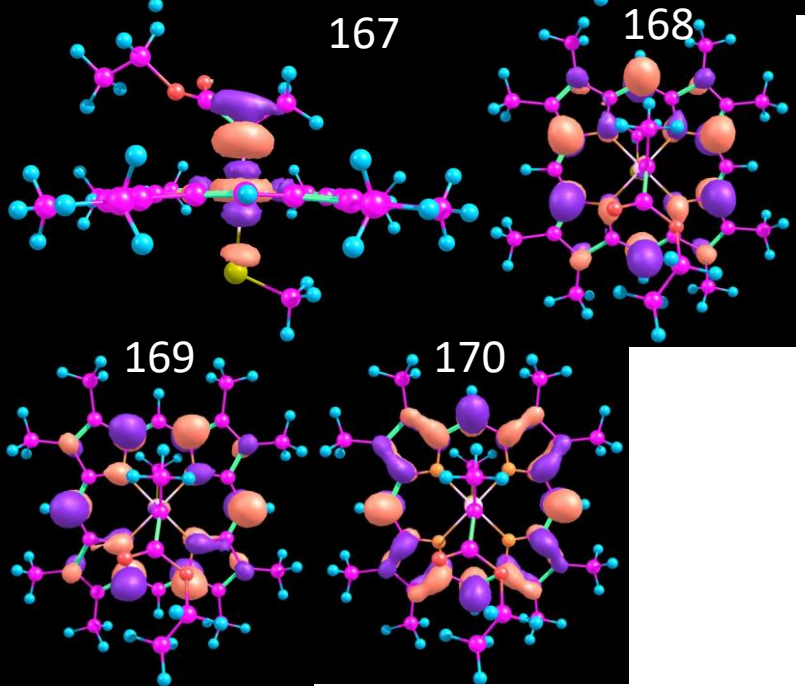
NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134787	-3.6677
160	1.9165	-0.089743	-2.4420
161	1.8923	-0.317698	-8.6450
162	1.7347	-0.270485	-7.3603
163	1.4926	-0.220047	-5.9878
164	1.3086	-0.148079	-4.0294
165	0.8757	0.052032	1.4159
166	0.5715	0.229357	6.2411
167	0.1166	0.364012	9.9053
168	0.0755	0.147273	4.0075
169	0.0733	0.151055	4.1104
170	0.0071	0.292522	7.9599



50 degrees;
1 Quintet,
5 Triplets,
2 Singlets

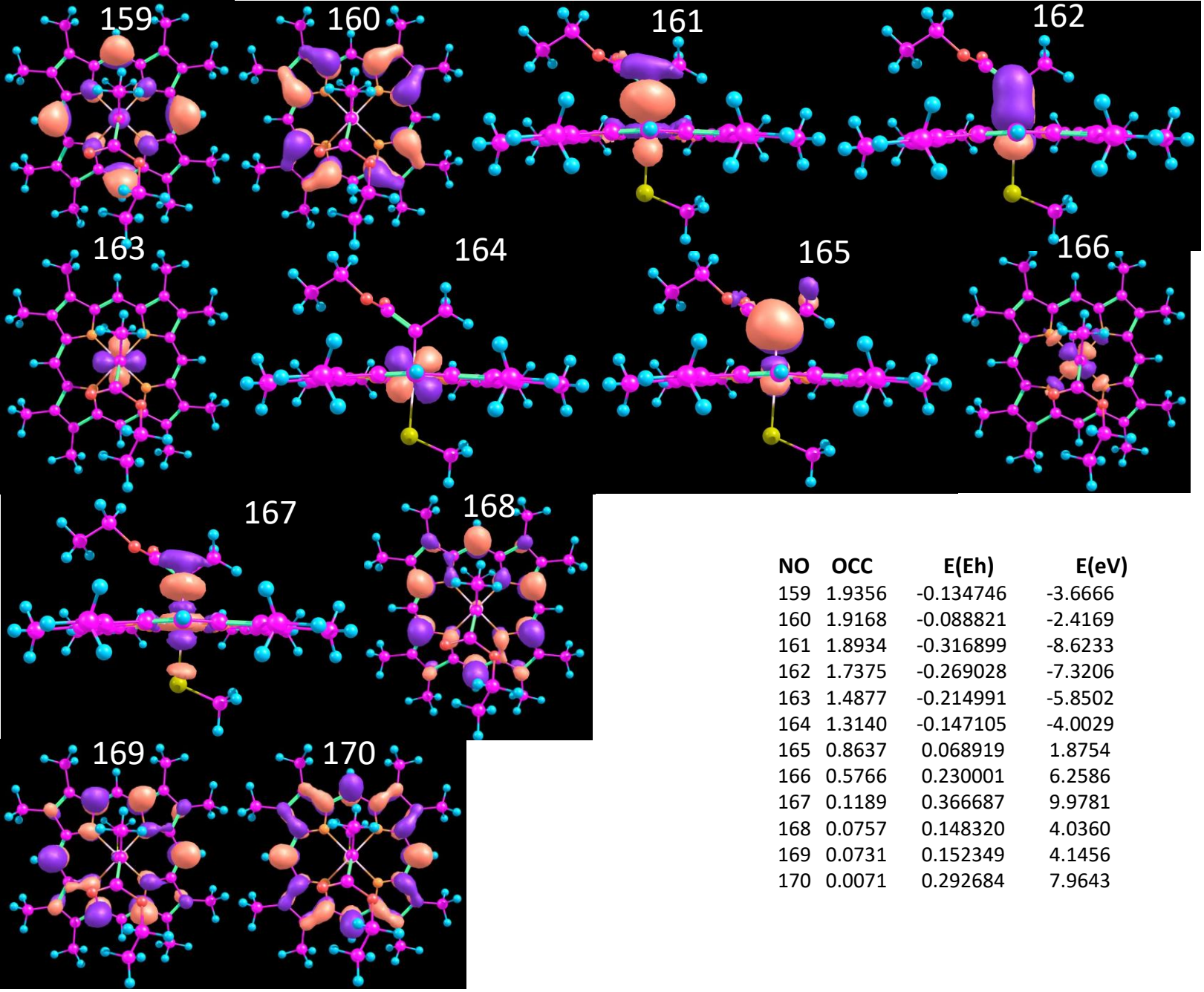
NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134952	-3.6722
160	1.9166	-0.089424	-2.4334
161	1.8924	-0.317224	-8.6321
162	1.7356	-0.270012	-7.3474
163	1.4919	-0.218374	-5.9423
164	1.3108	-0.147536	-4.0147
165	0.8718	0.058720	1.5978
166	0.5735	0.229932	6.2568
167	0.1162	0.366528	9.9737
168	0.0756	0.147640	4.0175
169	0.0731	0.151520	4.1231
170	0.0071	0.294629	8.0173





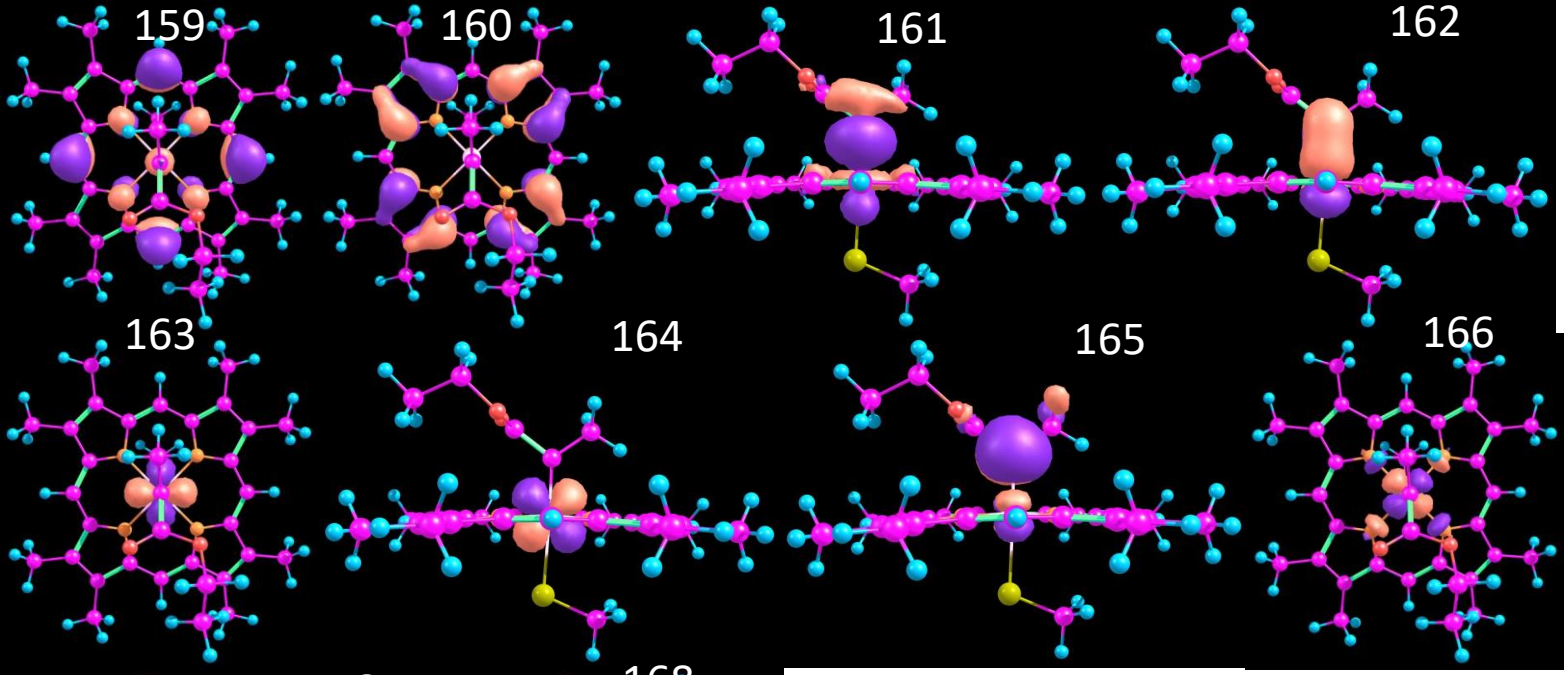
60 degrees;
1 Quintet,
5 Triplets,
2 Singlets

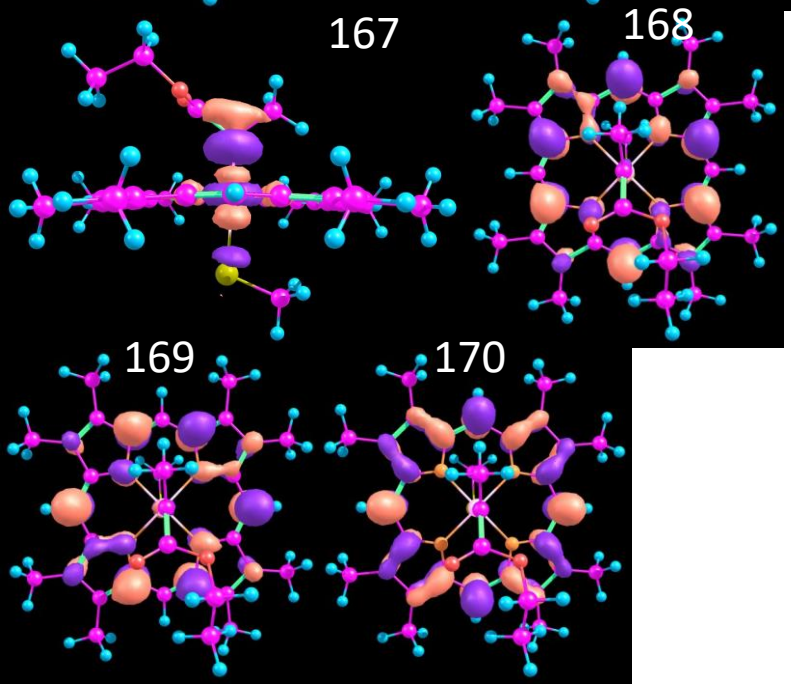
NO	OCC	E(Eh)	E(eV)
159	1.9355	-0.134526	-3.6606
160	1.9166	-0.089118	-2.4250
161	1.8927	-0.316995	-8.6259
162	1.7355	-0.269515	-7.3339
163	1.4917	-0.217420	-5.9163
164	1.3126	-0.147386	-4.0106
165	0.8689	0.064154	1.7457
166	0.5750	0.230267	6.2659
167	0.1156	0.368264	10.0210
168	0.0758	0.147737	4.0201
169	0.0731	0.151787	4.1303
170	0.0071	0.291661	7.9365



70 degrees;
1 Quintet,
5 Triplets,
2 Singlets

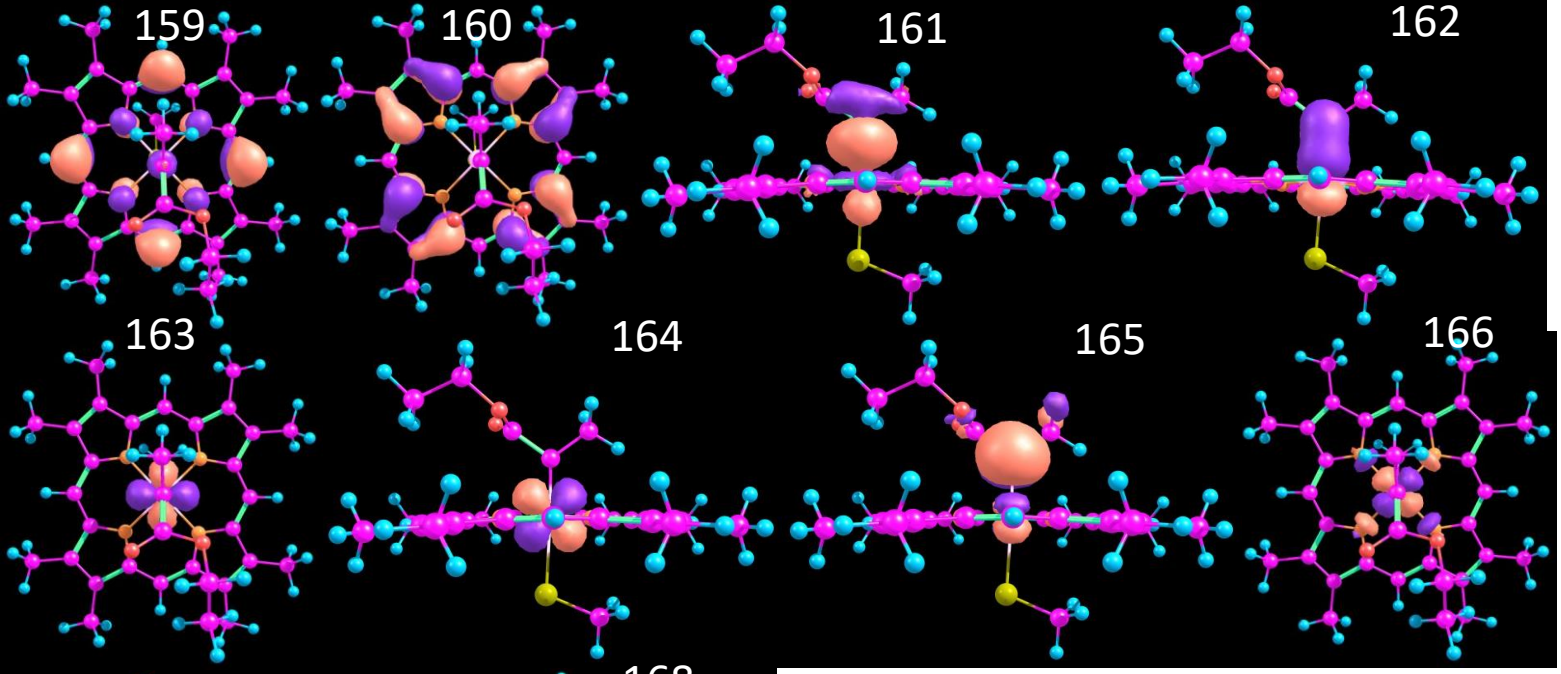
NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134746	-3.6666
160	1.9168	-0.088821	-2.4169
161	1.8934	-0.316899	-8.6233
162	1.7375	-0.269028	-7.3206
163	1.4877	-0.214991	-5.8502
164	1.3140	-0.147105	-4.0029
165	0.8637	0.068919	1.8754
166	0.5766	0.230001	6.2586
167	0.1189	0.366687	9.9781
168	0.0757	0.148320	4.0360
169	0.0731	0.152349	4.1456
170	0.0071	0.292684	7.9643

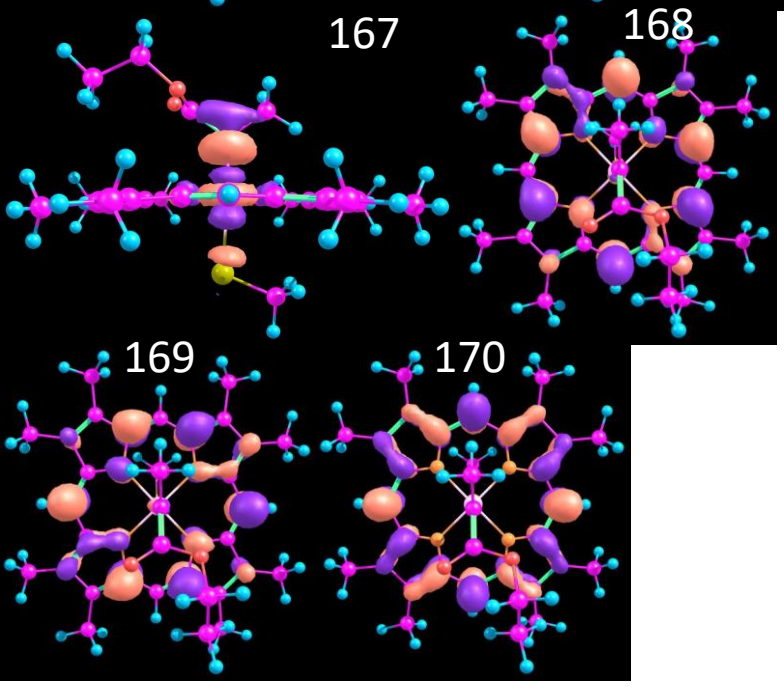




80 degrees;
1 Quintet,
5 Triplets,
2 Singlets

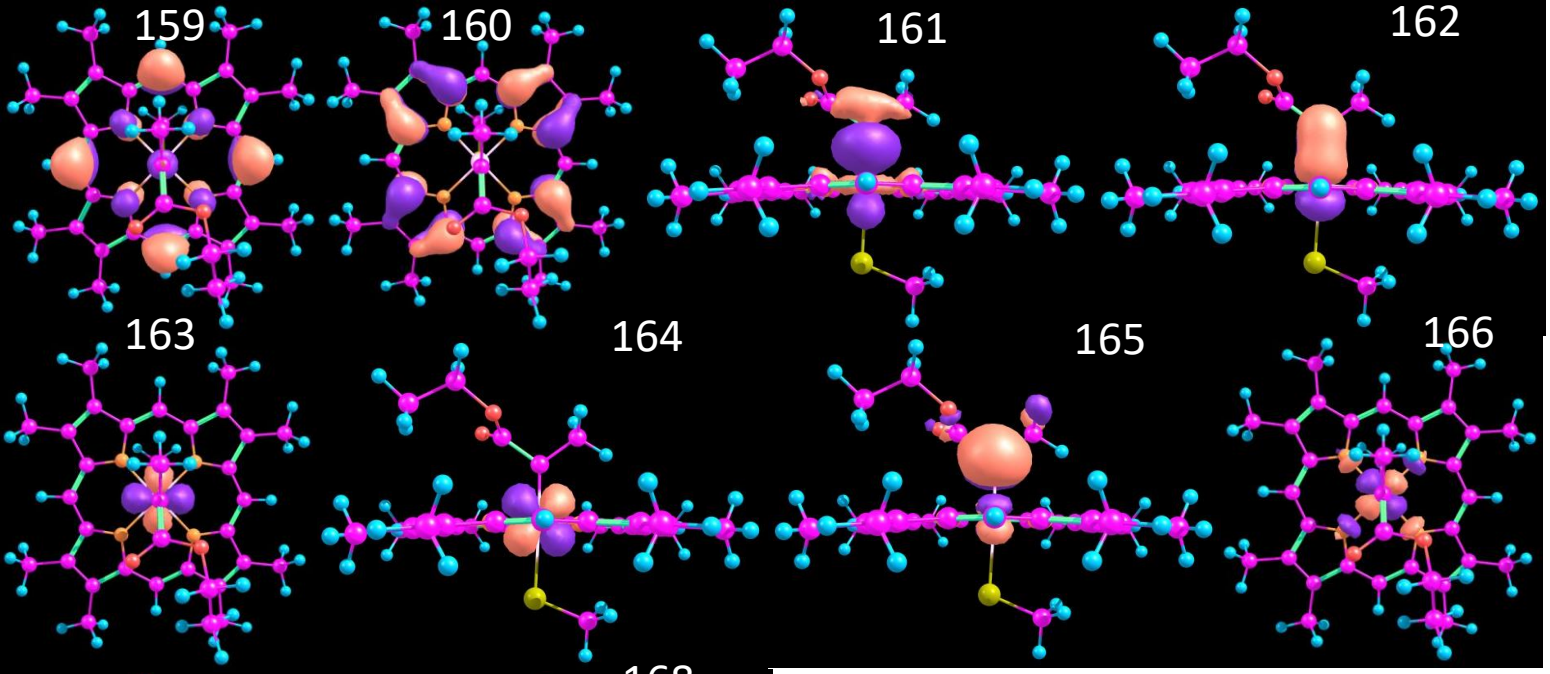
NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134590	-3.6624
160	1.9164	-0.088534	-2.4091
161	1.8933	-0.317113	-8.6291
162	1.7363	-0.268630	-7.3098
163	1.4897	-0.215481	-5.8635
164	1.3153	-0.147295	-4.0081
165	0.8639	0.070625	1.9218
166	0.5775	0.230319	6.2673
167	0.1160	0.370016	10.0687
168	0.0759	0.148074	4.0293
169	0.0730	0.152501	4.1498
170	0.0071	0.291643	7.9360

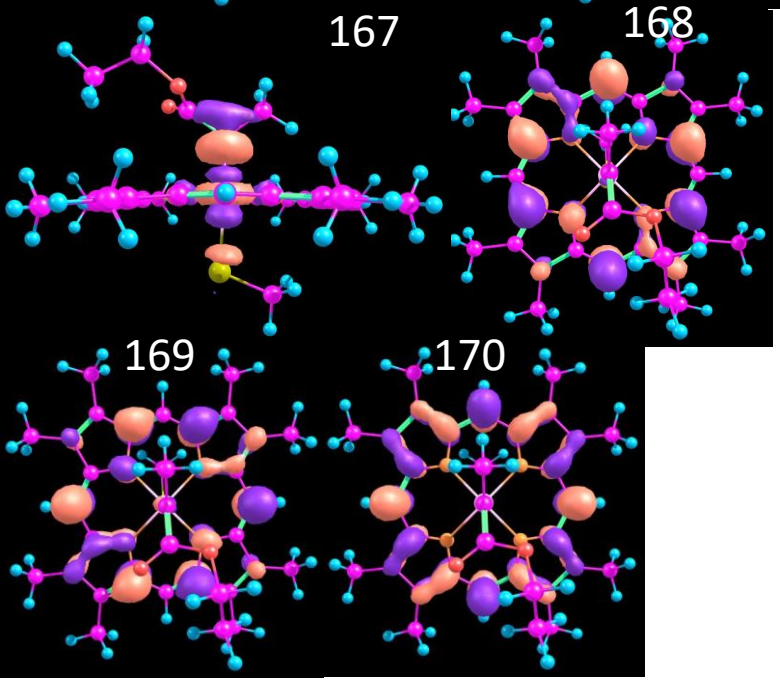




90 degrees;
1 Quintet,
5 Triplets,
2 Singlets

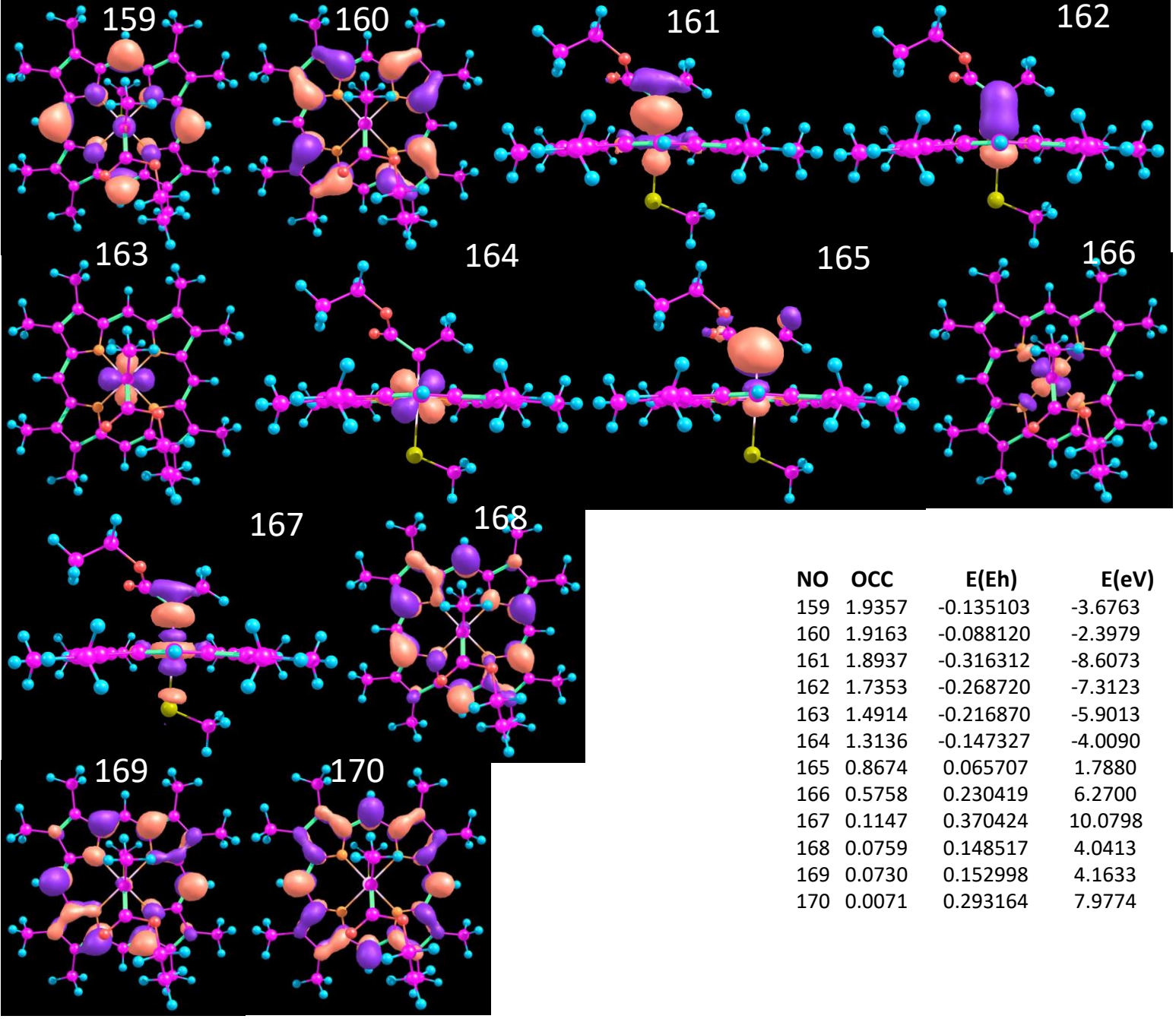
NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.134961	-3.6725
160	1.9164	-0.088328	-2.4035
161	1.8935	-0.316766	-8.6196
162	1.7363	-0.268412	-7.3039
163	1.4897	-0.215407	-5.8615
164	1.3155	-0.147310	-4.0085
165	0.8636	0.070590	1.9208
166	0.5777	0.230315	6.2672
167	0.1157	0.370774	10.0893
168	0.0760	0.148263	4.0344
169	0.0729	0.152744	4.1564
170	0.0071	0.292252	7.9526





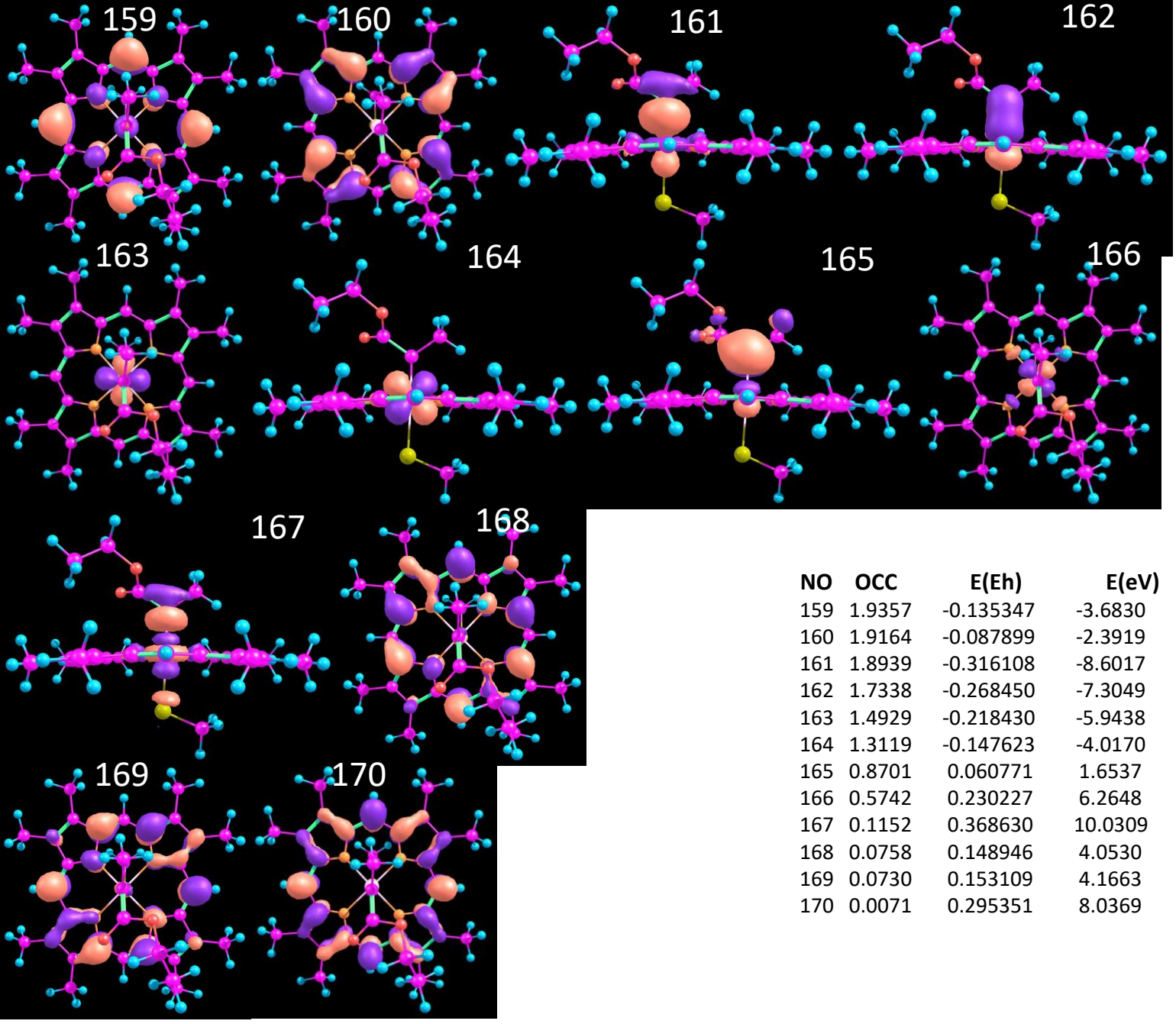
NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.135010	-3.6738
160	1.9164	-0.088259	-2.4016
161	1.8936	-0.316490	-8.6121
162	1.7359	-0.268570	-7.3082
163	1.4904	-0.216036	-5.8786
164	1.3149	-0.147365	-4.0100
165	0.8650	0.068833	1.8730
166	0.5771	0.230305	6.2669
167	0.1152	0.370768	10.0891
168	0.0760	0.148344	4.0366
169	0.0729	0.152847	4.1592
170	0.0071	0.291980	7.9452

100 degrees;
1 Quintet,
5 Triplets,
2 Singlets



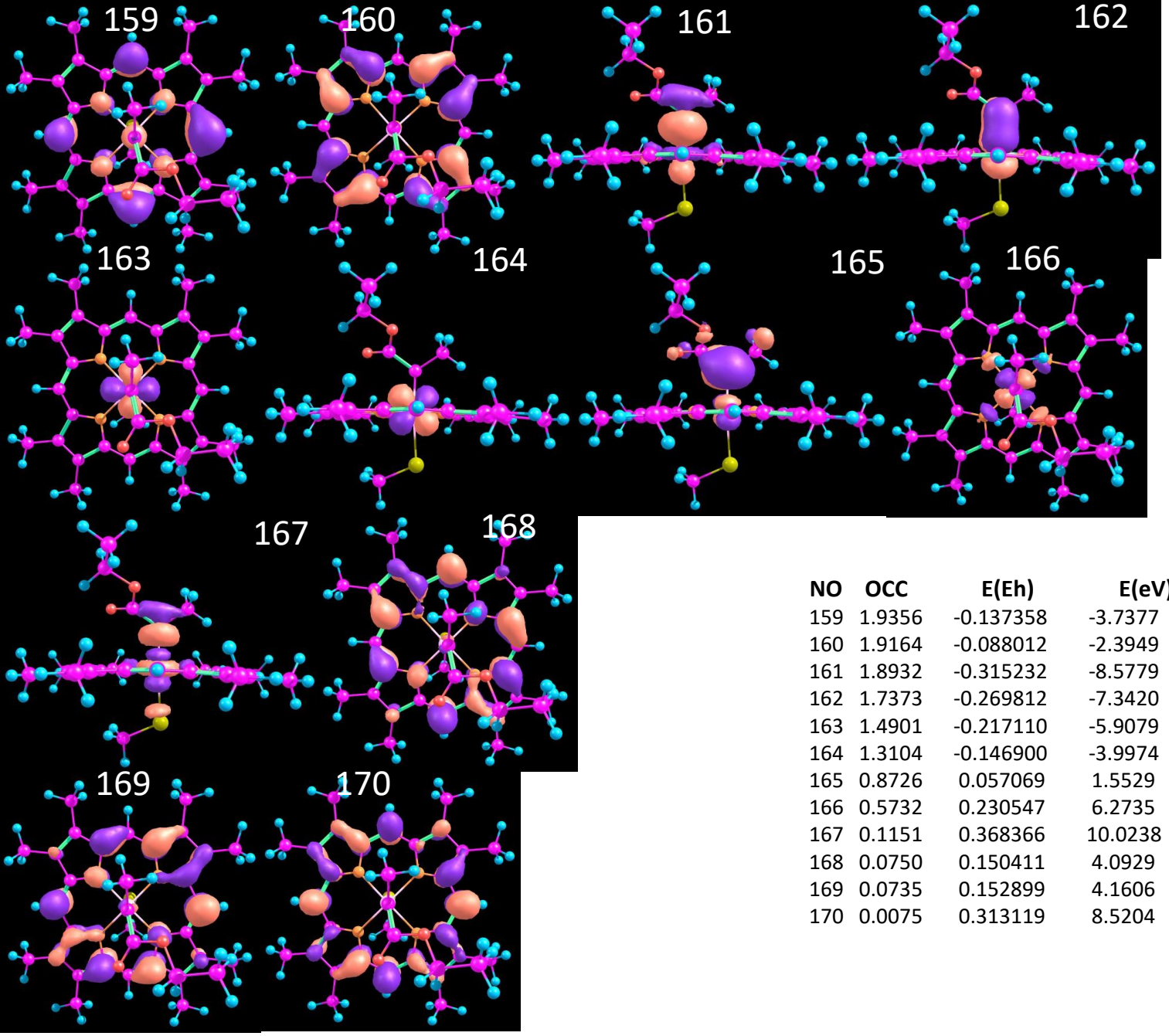
NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.135103	-3.6763
160	1.9163	-0.088120	-2.3979
161	1.8937	-0.316312	-8.6073
162	1.7353	-0.268720	-7.3123
163	1.4914	-0.216870	-5.9013
164	1.3136	-0.147327	-4.0090
165	0.8674	0.065707	1.7880
166	0.5758	0.230419	6.2700
167	0.1147	0.370424	10.0798
168	0.0759	0.148517	4.0413
169	0.0730	0.152998	4.1633
170	0.0071	0.293164	7.9774

110 degrees;
1 Quintet,
5 Triplets,
2 Singlets



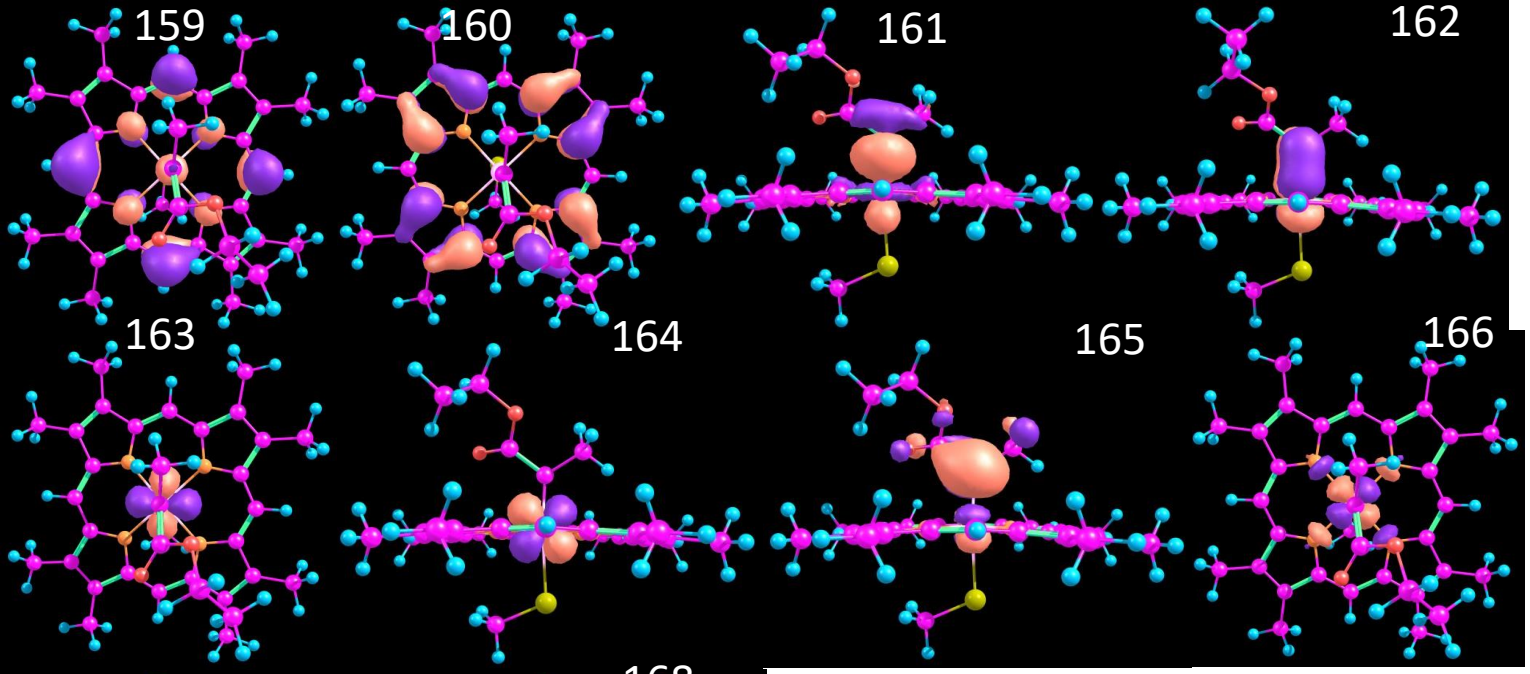
NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.135347	-3.6830
160	1.9164	-0.087899	-2.3919
161	1.8939	-0.316108	-8.6017
162	1.7338	-0.268450	-7.3049
163	1.4929	-0.218430	-5.9438
164	1.3119	-0.147623	-4.0170
165	0.8701	0.060771	1.6537
166	0.5742	0.230227	6.2648
167	0.1152	0.368630	10.0309
168	0.0758	0.148946	4.0530
169	0.0730	0.153109	4.1663
170	0.0071	0.295351	8.0369

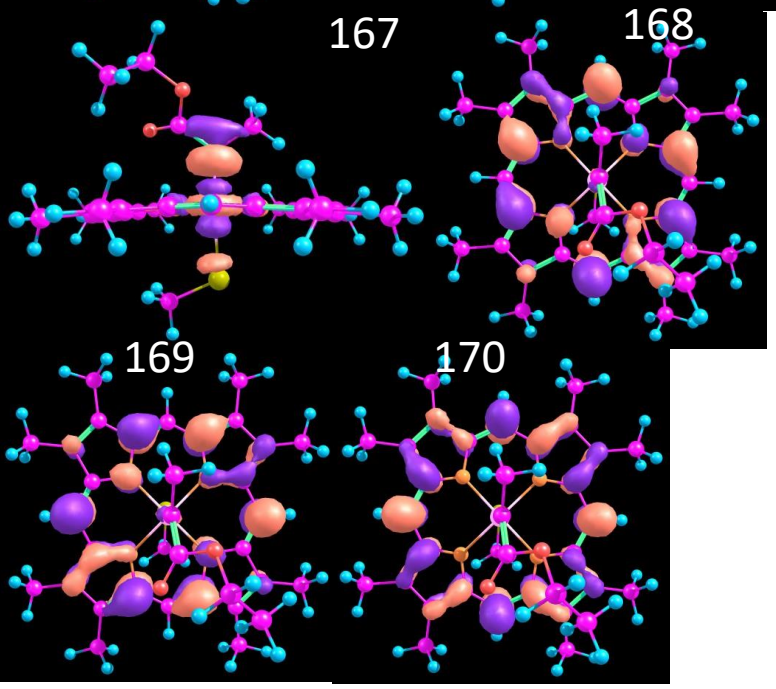
120 degrees;
1 Quintet,
5 Triplets,
2 Singlets



130 degrees;
1 Quintet,
5 Triplets,
2 Singlets

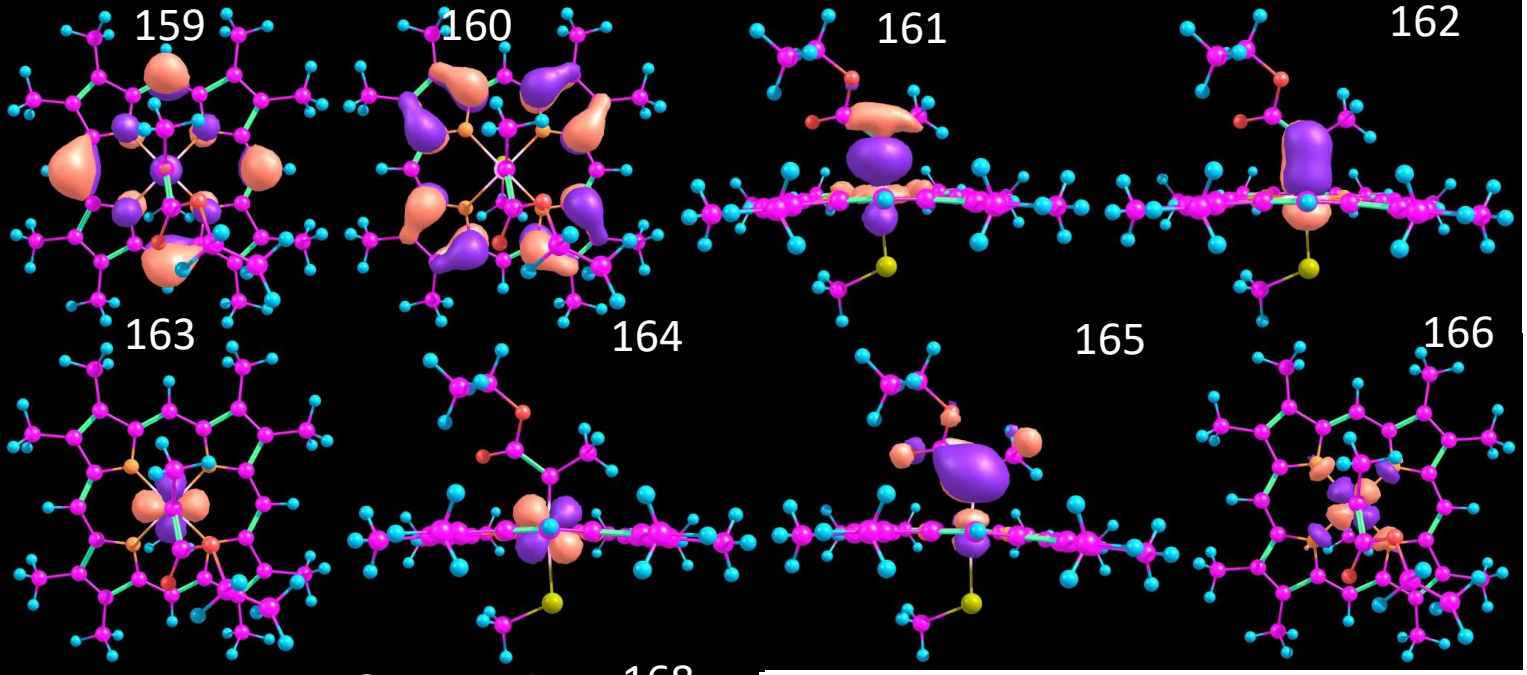
NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.137358	-3.7377
160	1.9164	-0.088012	-2.3949
161	1.8932	-0.315232	-8.5779
162	1.7373	-0.269812	-7.3420
163	1.4901	-0.217110	-5.9079
164	1.3104	-0.146900	-3.9974
165	0.8726	0.057069	1.5529
166	0.5732	0.230547	6.2735
167	0.1151	0.368366	10.0238
168	0.0750	0.150411	4.0929
169	0.0735	0.152899	4.1606
170	0.0075	0.313119	8.5204

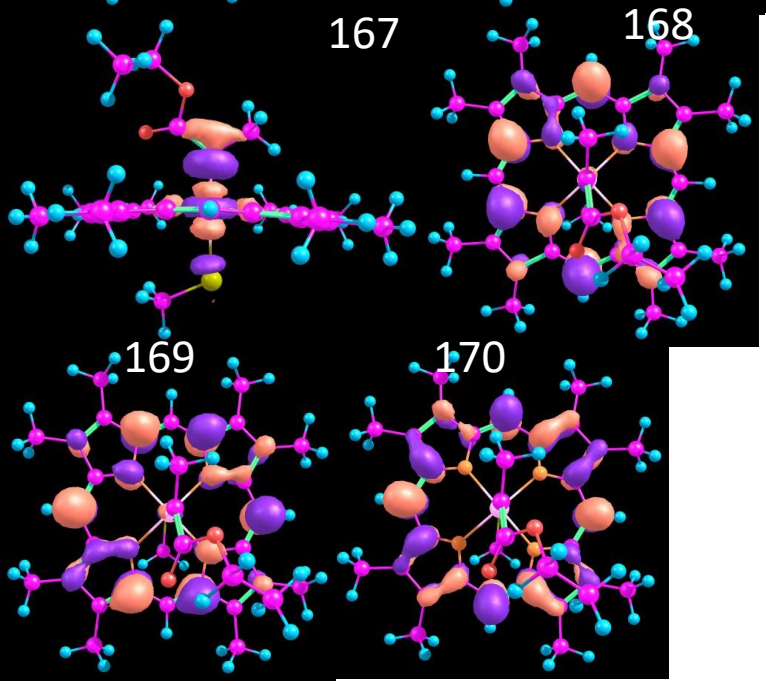




NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.135520	-3.6877
160	1.9168	-0.087866	-2.3910
161	1.8937	-0.316355	-8.6084
162	1.7315	-0.268445	-7.3048
163	1.4949	-0.221672	-6.0320
164	1.3082	-0.148531	-4.0417
165	0.8773	0.048006	1.3063
166	0.5707	0.229505	6.2451
167	0.1156	0.364901	9.9295
168	0.0750	0.150105	4.0846
169	0.0735	0.152987	4.1630
170	0.0072	0.302324	8.2267

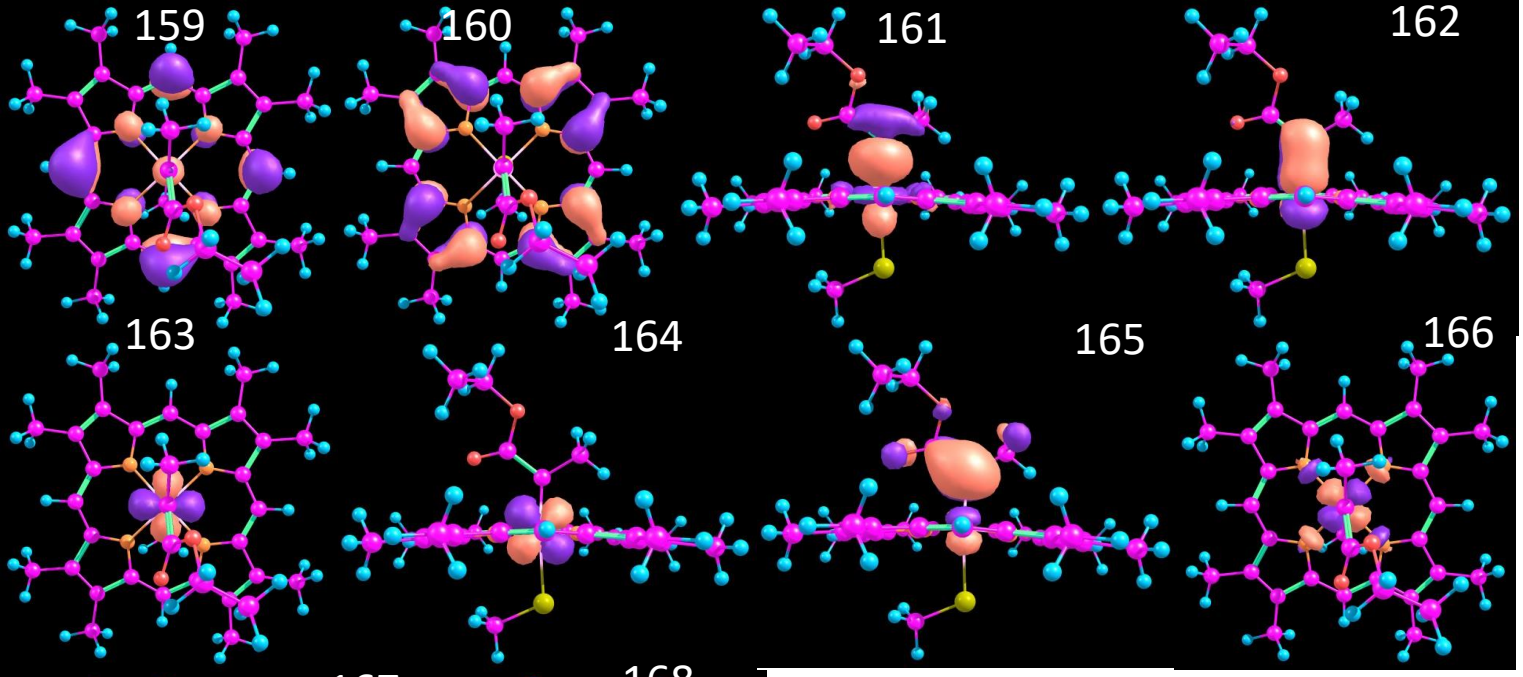
140 degrees;
1 Quintet,
5 Triplets,
2 Singlets

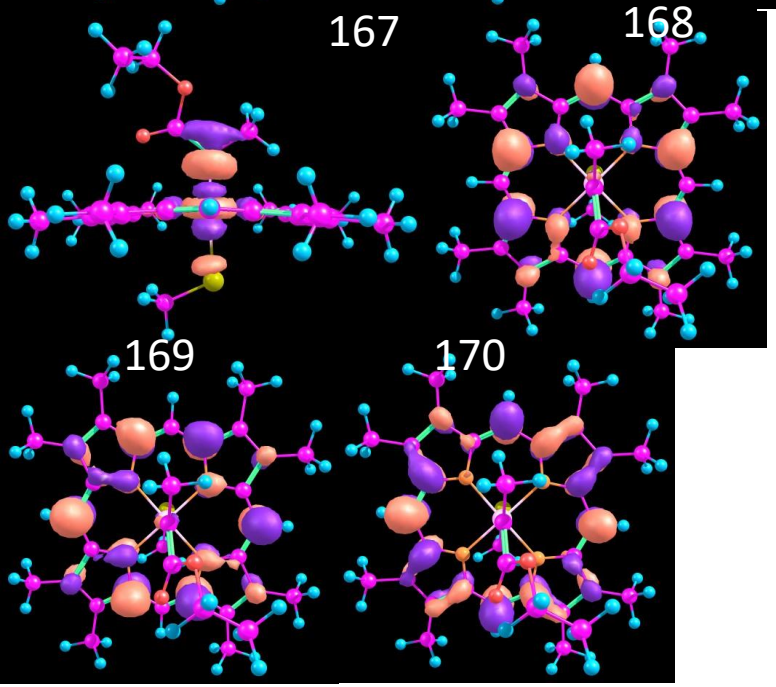




NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.135303	-3.6818
160	1.9169	-0.087826	-2.3899
161	1.8937	-0.316474	-8.6117
162	1.7304	-0.267996	-7.2926
163	1.4953	-0.223160	-6.0725
164	1.3062	-0.149123	-4.0578
165	0.8817	0.040268	1.0957
166	0.5688	0.229285	6.2392
167	0.1158	0.362925	9.8757
168	0.0746	0.150861	4.1051
169	0.0737	0.153188	4.1685
170	0.0073	0.307107	8.3568

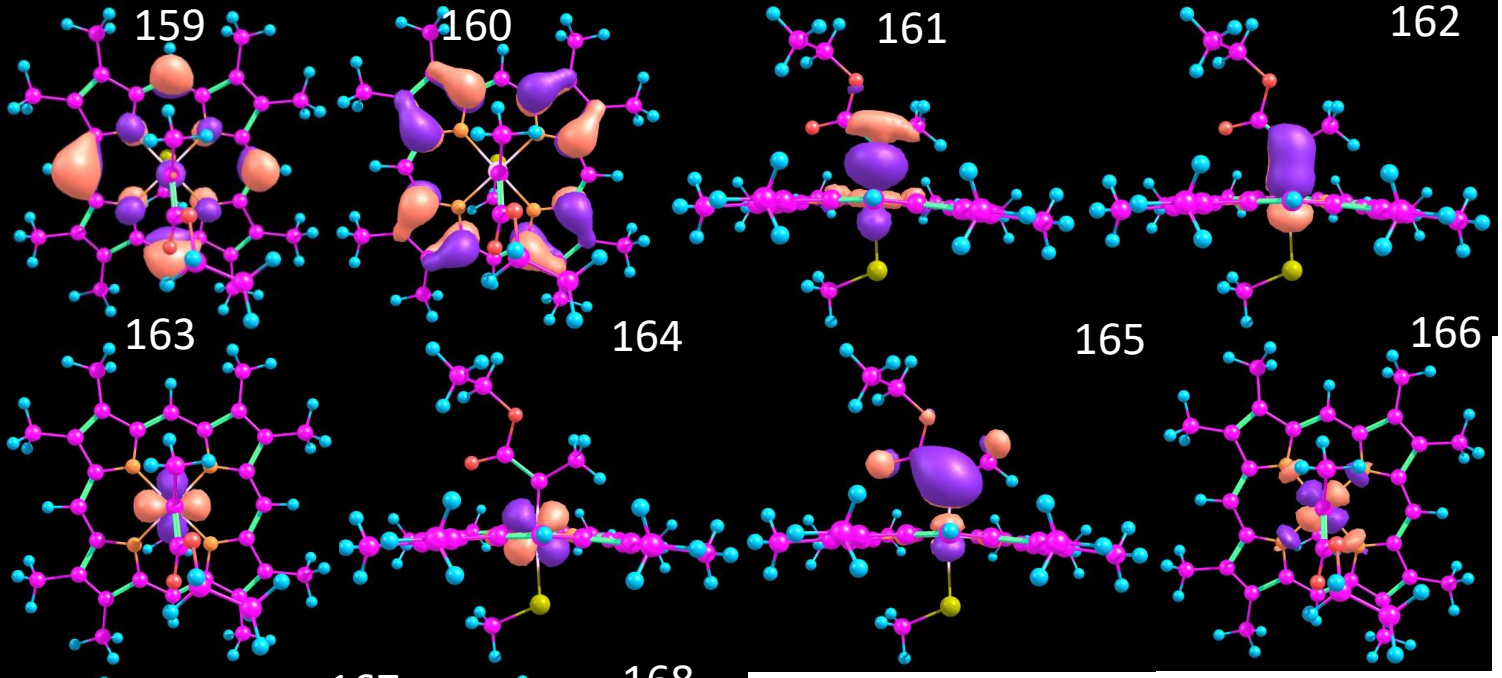
150 degrees;
1 Quintet,
5 Triplets,
2 Singlets

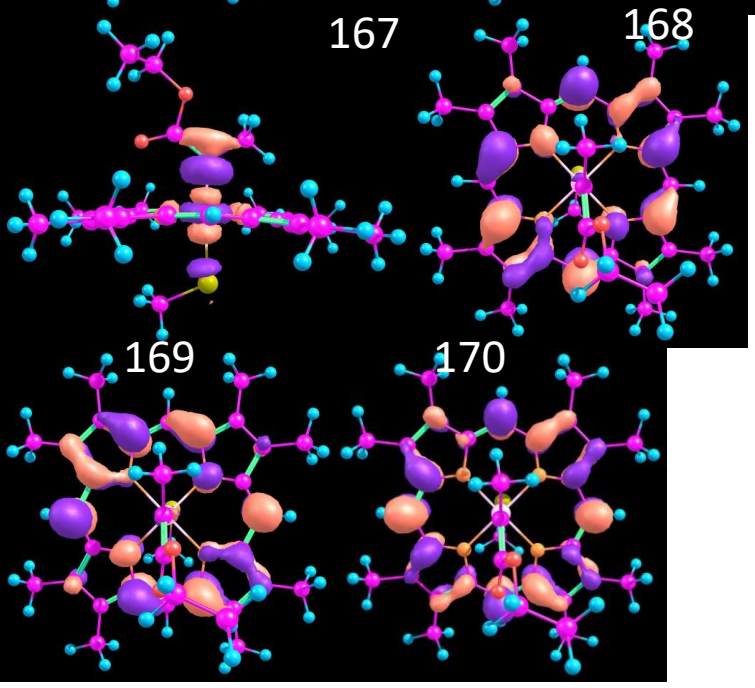




NO	OCC	E(Eh)	E(eV)
159	1.9356	-0.134774	-3.6674
160	1.9169	-0.087499	-2.3810
161	1.8937	-0.317360	-8.6358
162	1.7279	-0.266851	-7.2614
163	1.4968	-0.225298	-6.1307
164	1.3049	-0.150159	-4.0860
165	0.8852	0.033170	0.9026
166	0.5673	0.228752	6.2247
167	0.1160	0.360830	9.8187
168	0.0744	0.151506	4.1227
169	0.0739	0.153433	4.1751
170	0.0074	0.310029	8.4363

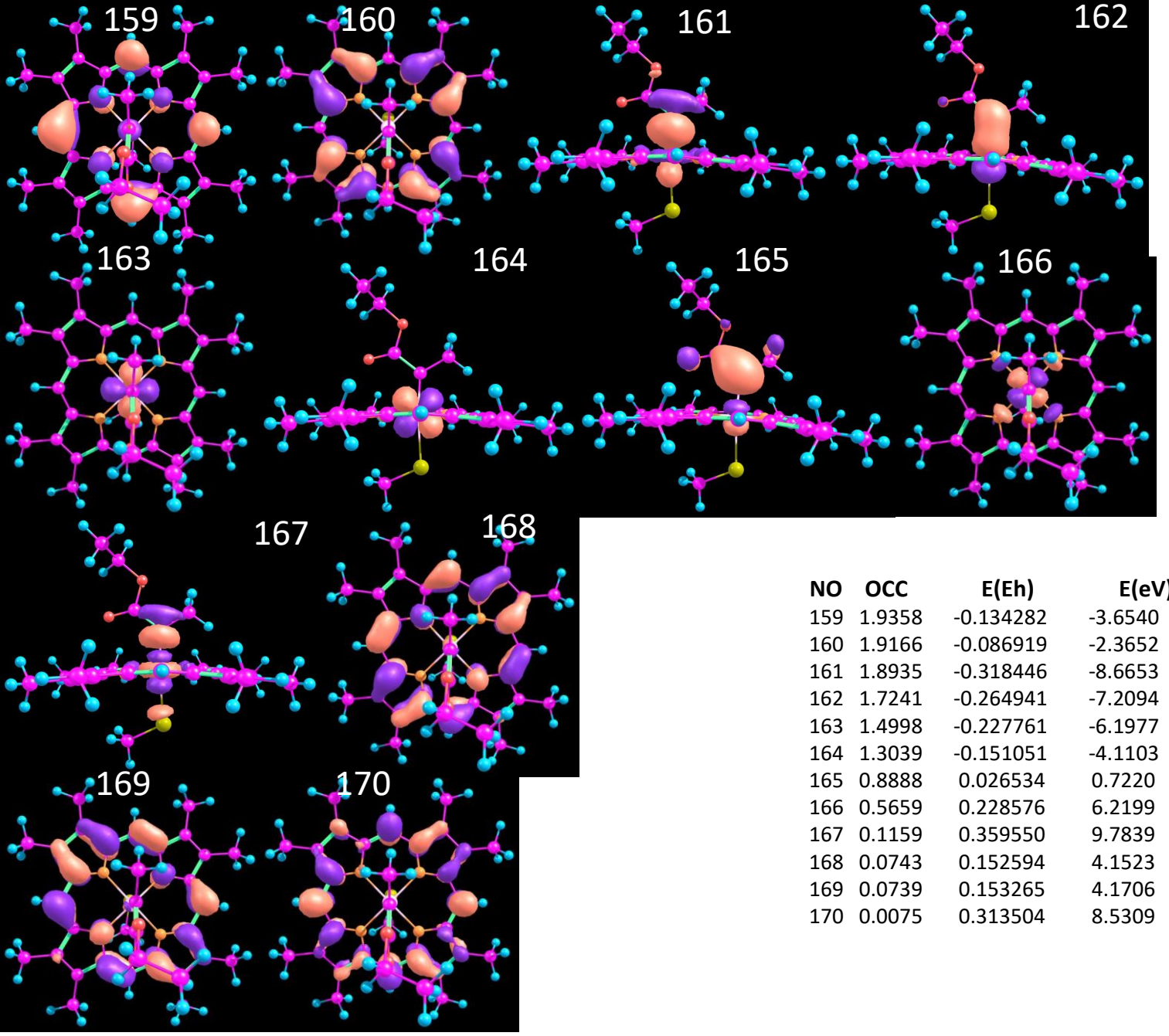
160 degrees;
1 Quintet,
5 Triplets,
2 Singlets





NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.134319	-3.6550
160	1.9167	-0.087119	-2.3706
161	1.8936	-0.318159	-8.6576
162	1.7258	-0.265809	-7.2330
163	1.4983	-0.226878	-6.1737
164	1.3042	-0.150908	-4.1064
165	0.8878	0.028227	0.7681
166	0.5663	0.228492	6.2176
167	0.1158	0.359872	9.7926
168	0.0743	0.152111	4.1392
169	0.0740	0.153480	4.1764
170	0.0075	0.312081	8.4922

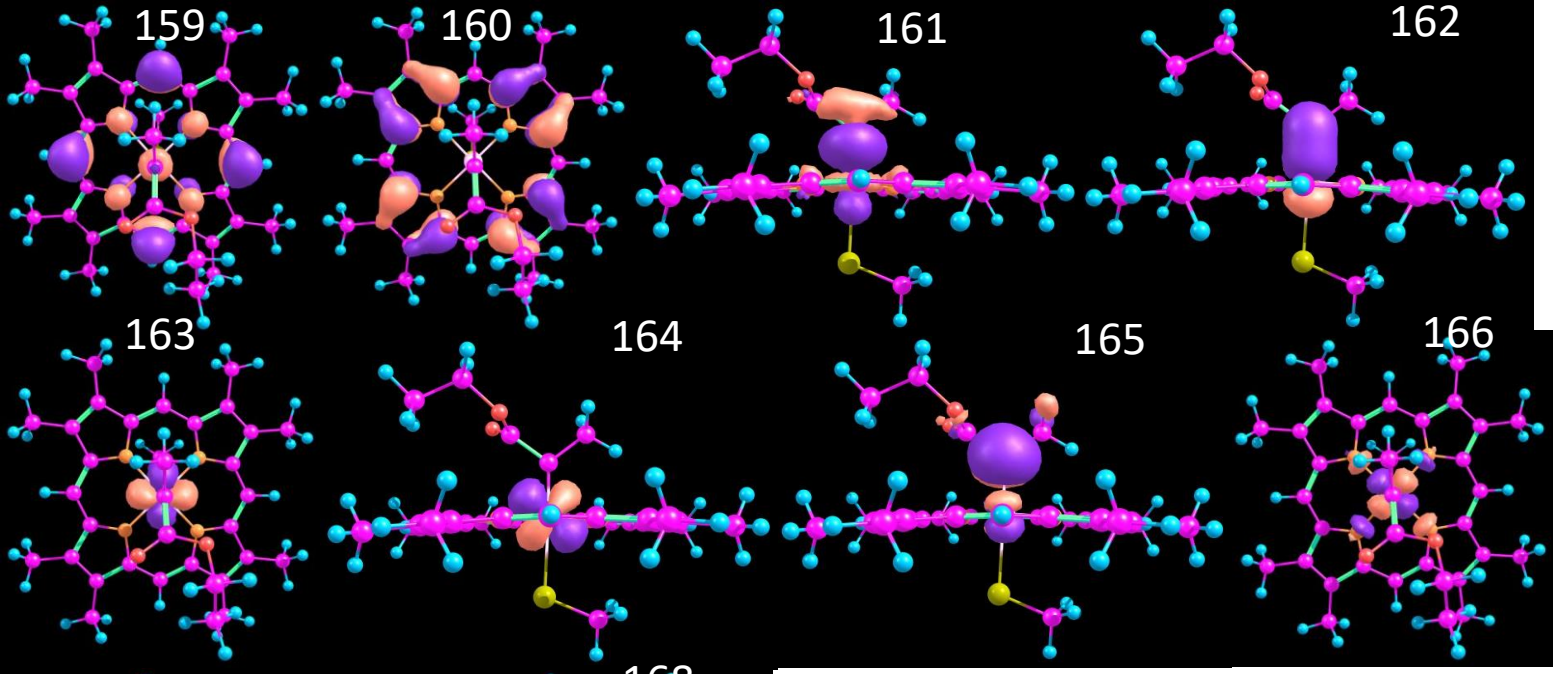
170 degrees;
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
159	1.9358	-0.134282	-3.6540
160	1.9166	-0.086919	-2.3652
161	1.8935	-0.318446	-8.6653
162	1.7241	-0.264941	-7.2094
163	1.4998	-0.227761	-6.1977
164	1.3039	-0.151051	-4.1103
165	0.8888	0.026534	0.7220
166	0.5659	0.228576	6.2199
167	0.1159	0.359550	9.7839
168	0.0743	0.152594	4.1523
169	0.0739	0.153265	4.1706
170	0.0075	0.313504	8.5309

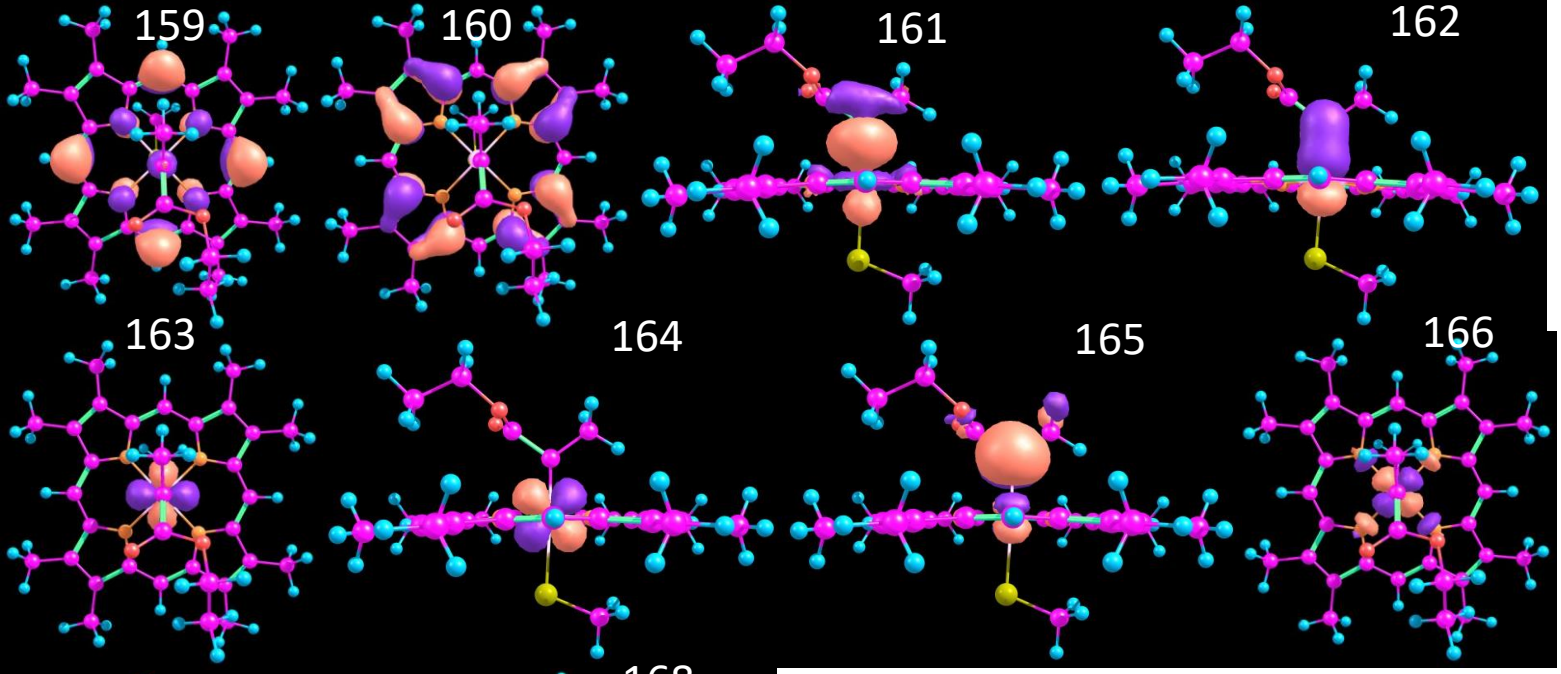
180 degrees;
1 Quintet,
5 Triplets,
2 Singlets

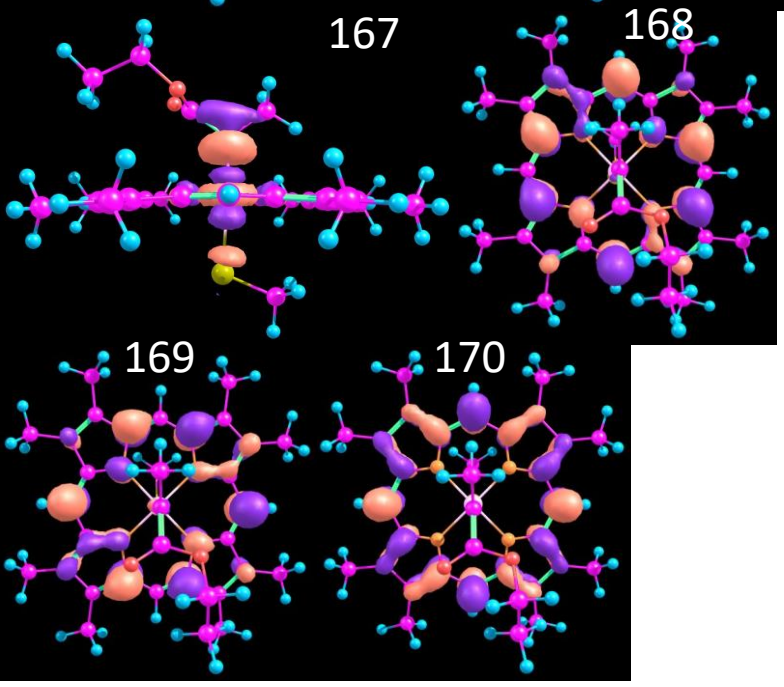
Active Space for QD-NEVPT2 on RKS DFT Geometries;Relaxed Scan of Fe-C: Thiolate



NO	OCC	E(Eh)	E(eV)
159	1.9362	-0.140075	-3.8116
160	1.9170	-0.088768	-2.4155
161	1.9007	-0.338460	-9.2100
162	1.8092	-0.288570	-7.8524
163	1.3836	-0.177411	-4.8276
164	1.3618	-0.167453	-4.5566
165	0.7976	0.083366	2.2685
166	0.6340	0.201499	5.4831
167	0.1053	0.400110	10.8876
168	0.0750	0.149628	4.0716
169	0.0726	0.151169	4.1135
170	0.0070	0.291693	7.9374

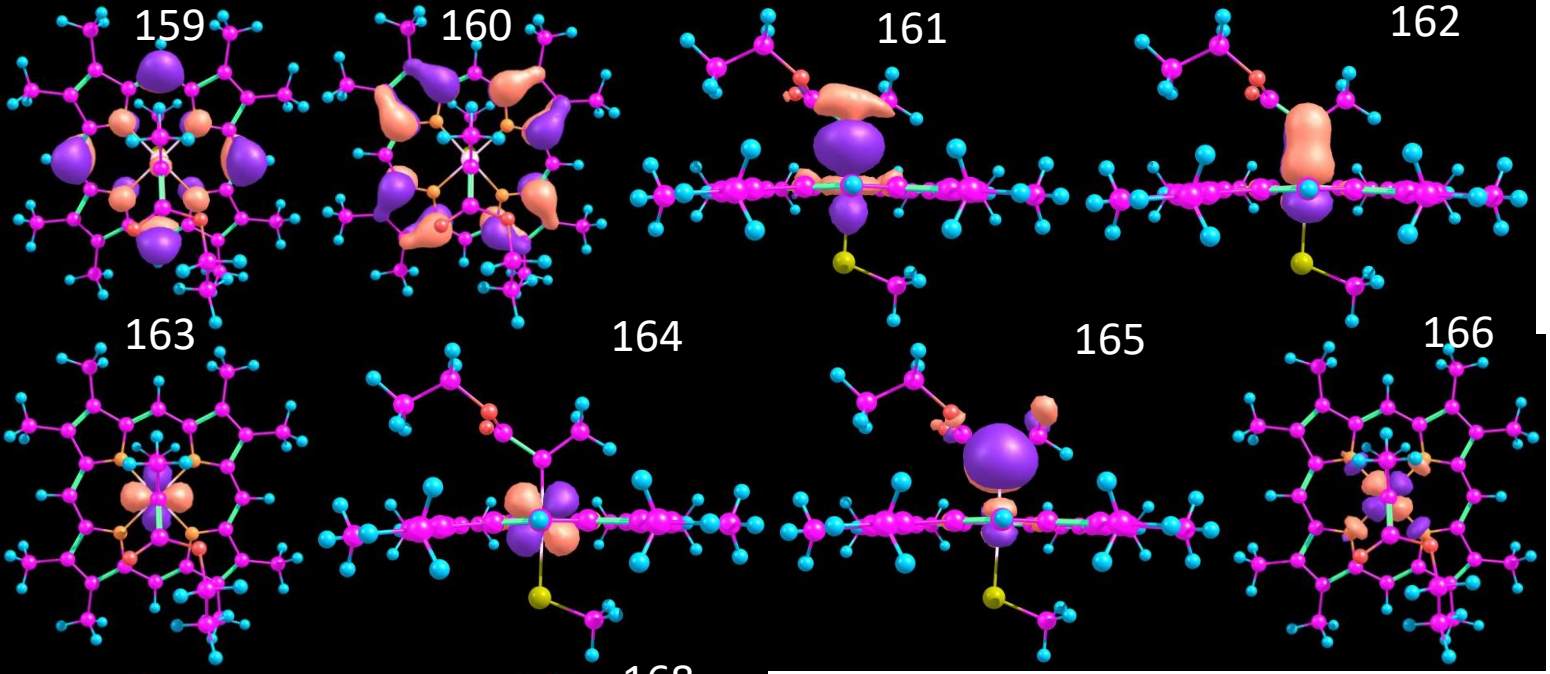
1.7 Å;
1 Quintet,
5 Triplets,
2 Singlets

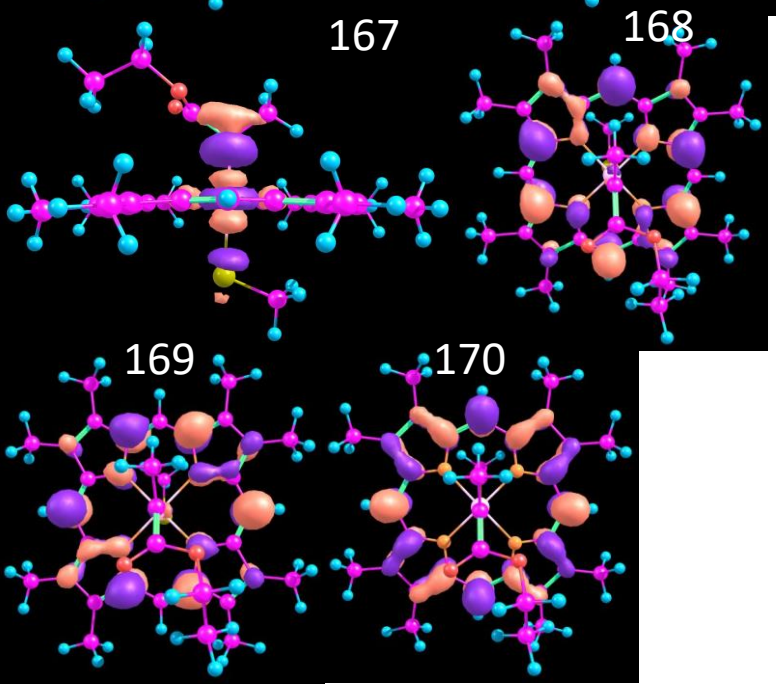




90 degrees;
1 Quintet,
5 Triplets,
2 Singlets

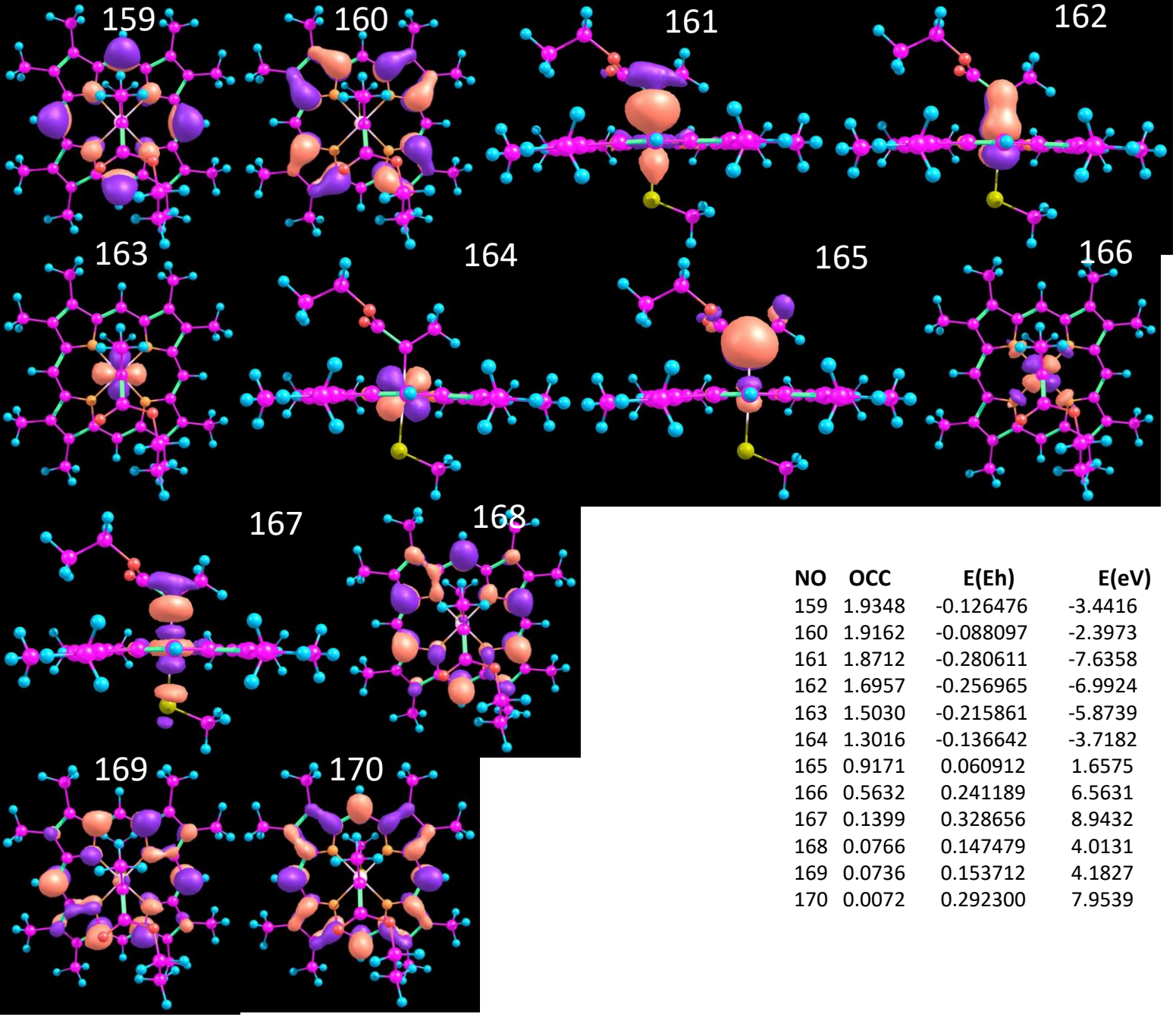
NO	OCC	E(Eh)	E(eV)
159	1.9357	-0.134961	-3.6725
160	1.9164	-0.088328	-2.4035
161	1.8935	-0.316766	-8.6196
162	1.7363	-0.268412	-7.3039
163	1.4897	-0.215407	-5.8615
164	1.3155	-0.147310	-4.0085
165	0.8636	0.070590	1.9208
166	0.5777	0.230315	6.2672
167	0.1157	0.370774	10.0893
168	0.0760	0.148263	4.0344
169	0.0729	0.152744	4.1564
170	0.0071	0.292252	7.9526





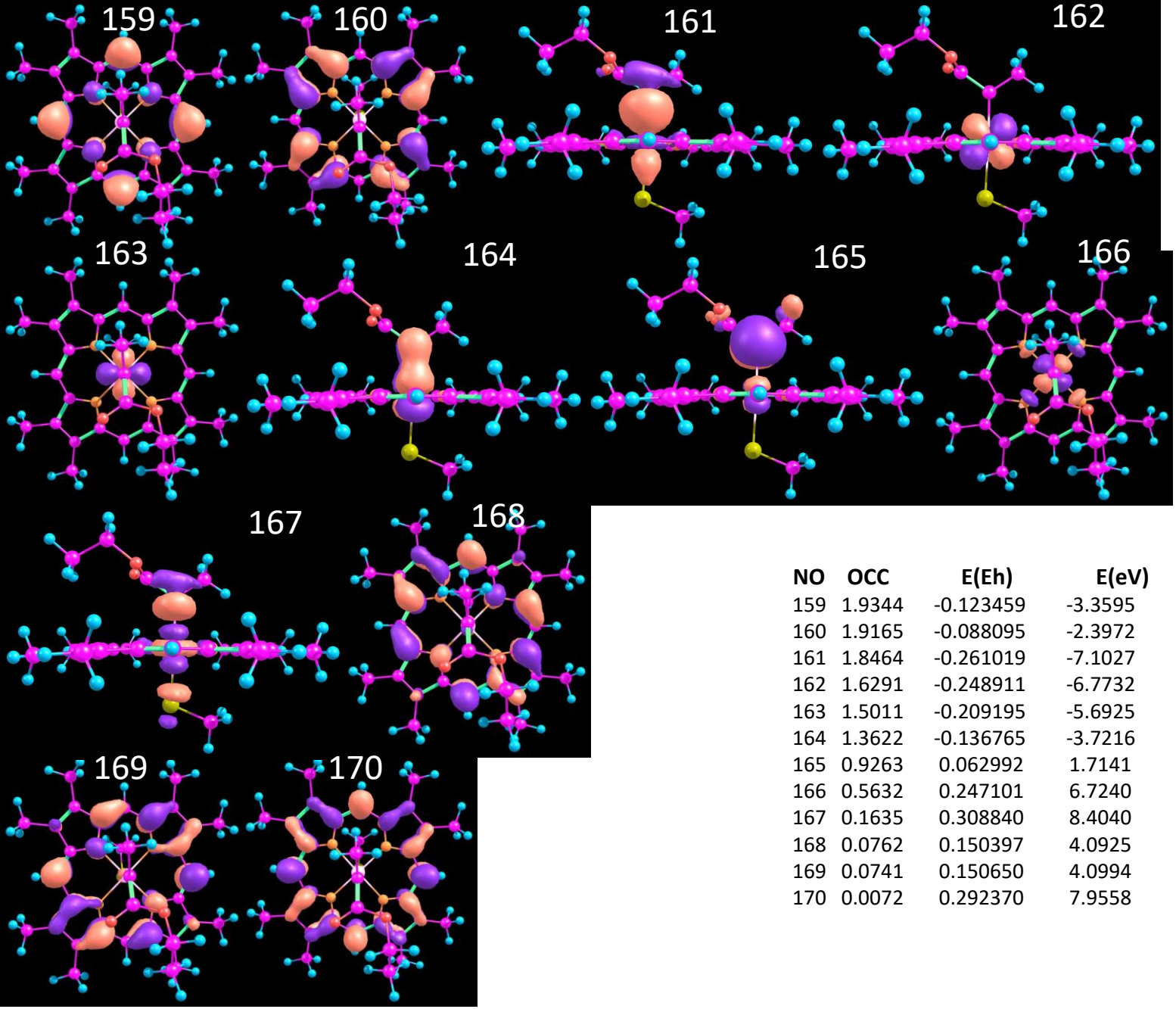
NO	OCC	E(Eh)	E(eV)
159	1.9353	-0.130587	-3.5534
160	1.9164	-0.088188	-2.3997
161	1.8850	-0.299229	-8.1424
162	1.7162	-0.263127	-7.1600
163	1.4997	-0.217512	-5.9188
164	1.3052	-0.141313	-3.8453
165	0.8931	0.064544	1.7563
166	0.5670	0.236765	6.4427
167	0.1254	0.350056	9.5255
168	0.0763	0.147836	4.0228
169	0.0732	0.153607	4.1798
170	0.0071	0.292423	7.9572

1.9 Å;
1 Quintet,
5 Triplets,
2 Singlets



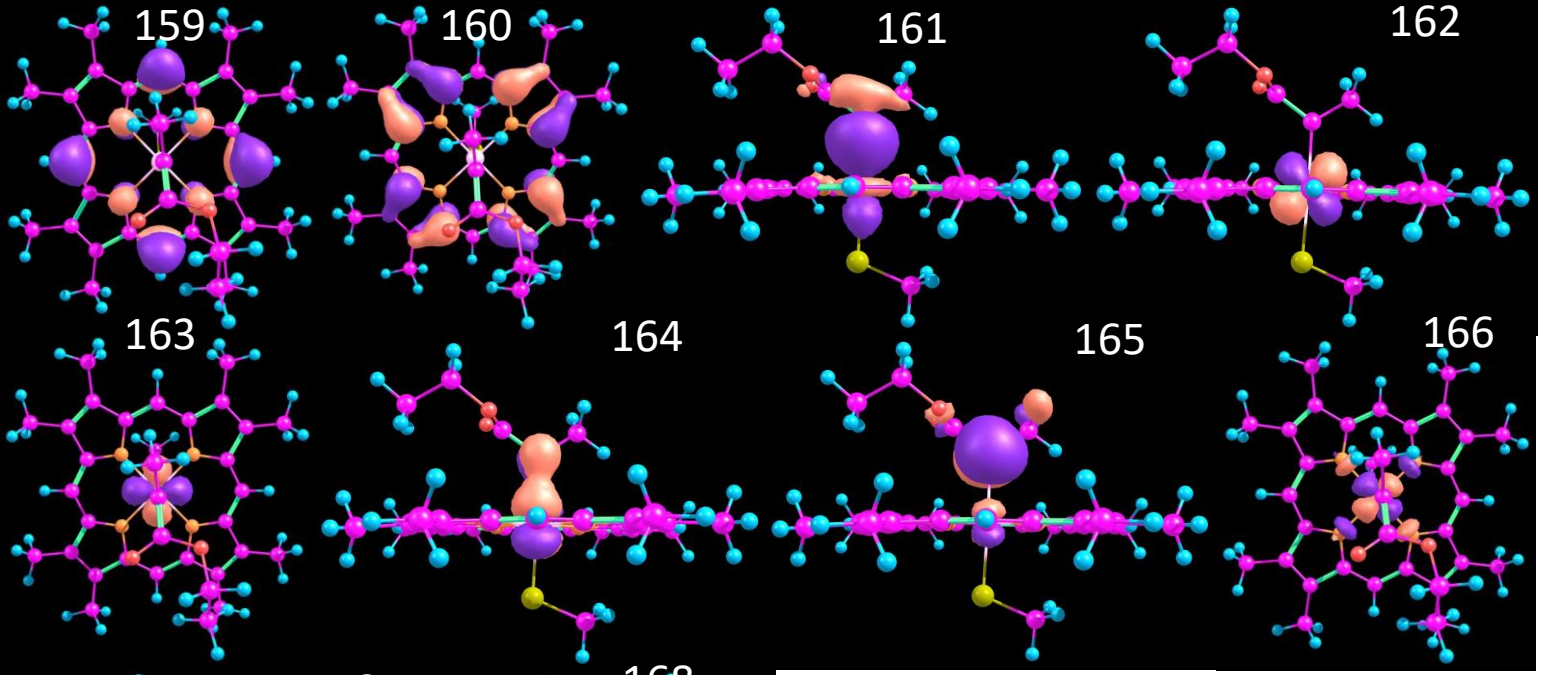
NO	OCC	E(Eh)	E(eV)
159	1.9348	-0.126476	-3.4416
160	1.9162	-0.088097	-2.3973
161	1.8712	-0.280611	-7.6358
162	1.6957	-0.256965	-6.9924
163	1.5030	-0.215861	-5.8739
164	1.3016	-0.136642	-3.7182
165	0.9171	0.060912	1.6575
166	0.5632	0.241189	6.5631
167	0.1399	0.328656	8.9432
168	0.0766	0.147479	4.0131
169	0.0736	0.153712	4.1827
170	0.0072	0.292300	7.9539

2.0 Å;
1 Quintet,
5 Triplets,
2 Singlets



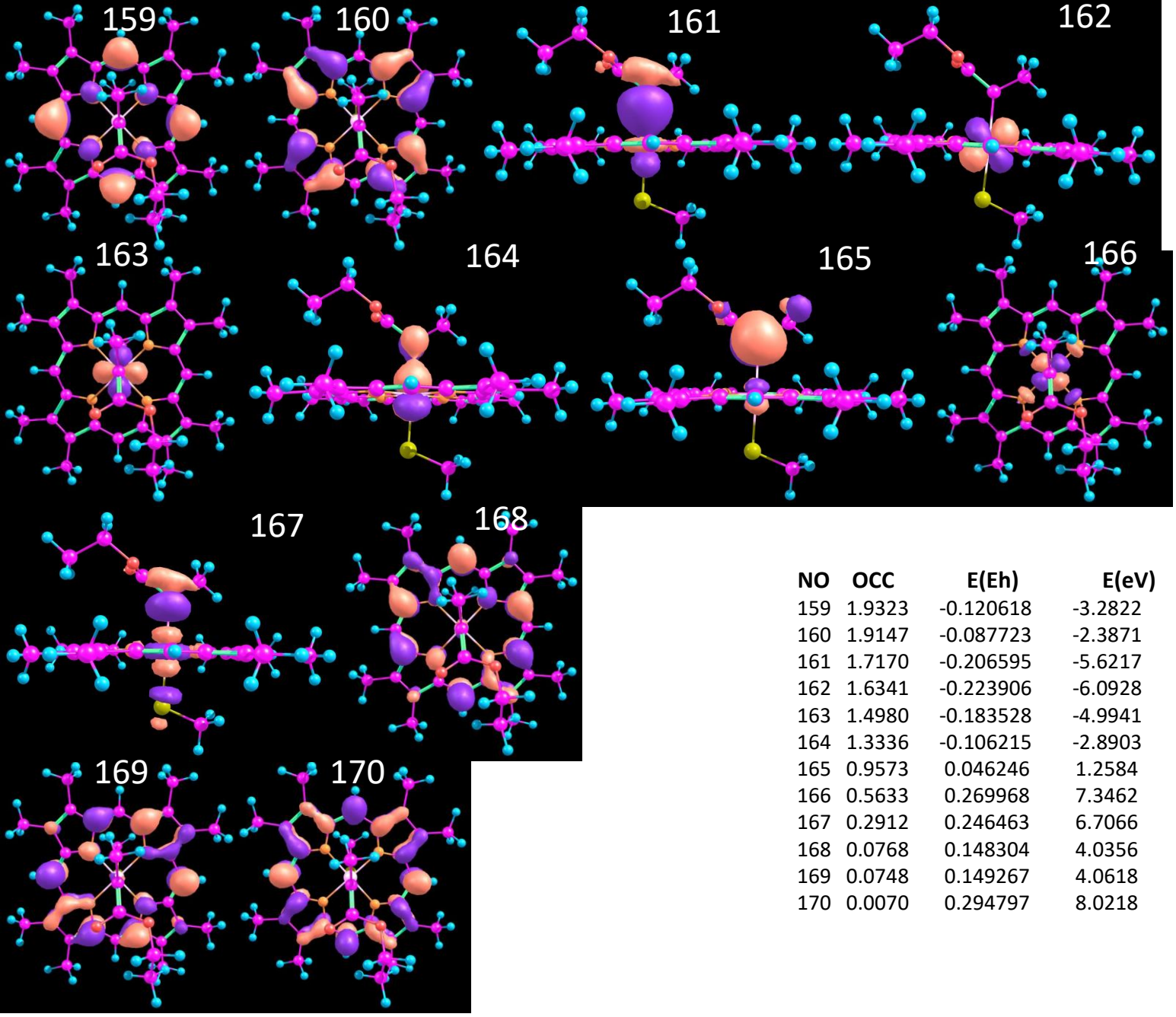
NO	OCC	E(Eh)	E(eV)
159	1.9344	-0.123459	-3.3595
160	1.9165	-0.088095	-2.3972
161	1.8464	-0.261019	-7.1027
162	1.6291	-0.248911	-6.7732
163	1.5011	-0.209195	-5.6925
164	1.3622	-0.136765	-3.7216
165	0.9263	0.062992	1.7141
166	0.5632	0.247101	6.7240
167	0.1635	0.308840	8.4040
168	0.0762	0.150397	4.0925
169	0.0741	0.150650	4.0994
170	0.0072	0.292370	7.9558

2.1 Å;
1 Quintet,
5 Triplets,
2 Singlets



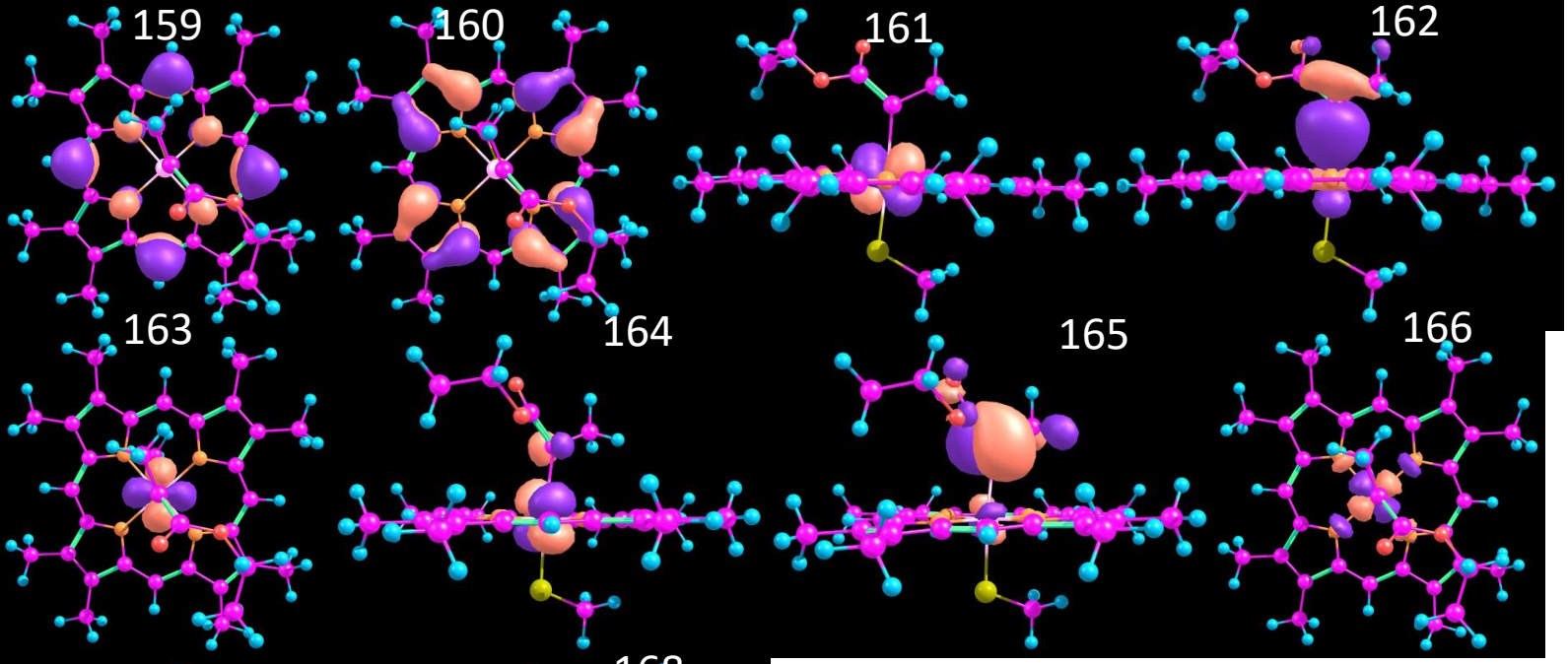
NO	OCC	E(Eh)	E(eV)
159	1.9334	-0.121703	-3.3117
160	1.9156	-0.088038	-2.3956
161	1.8038	-0.238117	-6.4795
162	1.6309	-0.240167	-6.5353
163	1.5007	-0.200841	-5.4652
164	1.3454	-0.124558	-3.3894
165	0.9435	0.056532	1.5383
166	0.5628	0.255106	6.9418
167	0.2057	0.282340	7.6829
168	0.0765	0.149769	4.0754
169	0.0746	0.149327	4.0634
170	0.0071	0.292493	7.9591

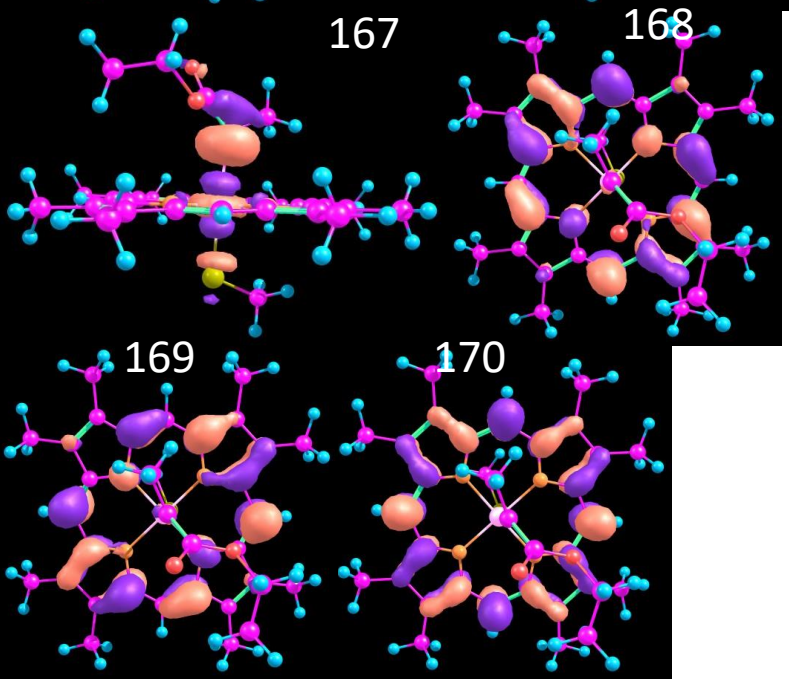
2.2 Å;
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
159	1.9323	-0.120618	-3.2822
160	1.9147	-0.087723	-2.3871
161	1.7170	-0.206595	-5.6217
162	1.6341	-0.223906	-6.0928
163	1.4980	-0.183528	-4.9941
164	1.3336	-0.106215	-2.8903
165	0.9573	0.046246	1.2584
166	0.5633	0.269968	7.3462
167	0.2912	0.246463	6.7066
168	0.0768	0.148304	4.0356
169	0.0748	0.149267	4.0618
170	0.0070	0.294797	8.0218

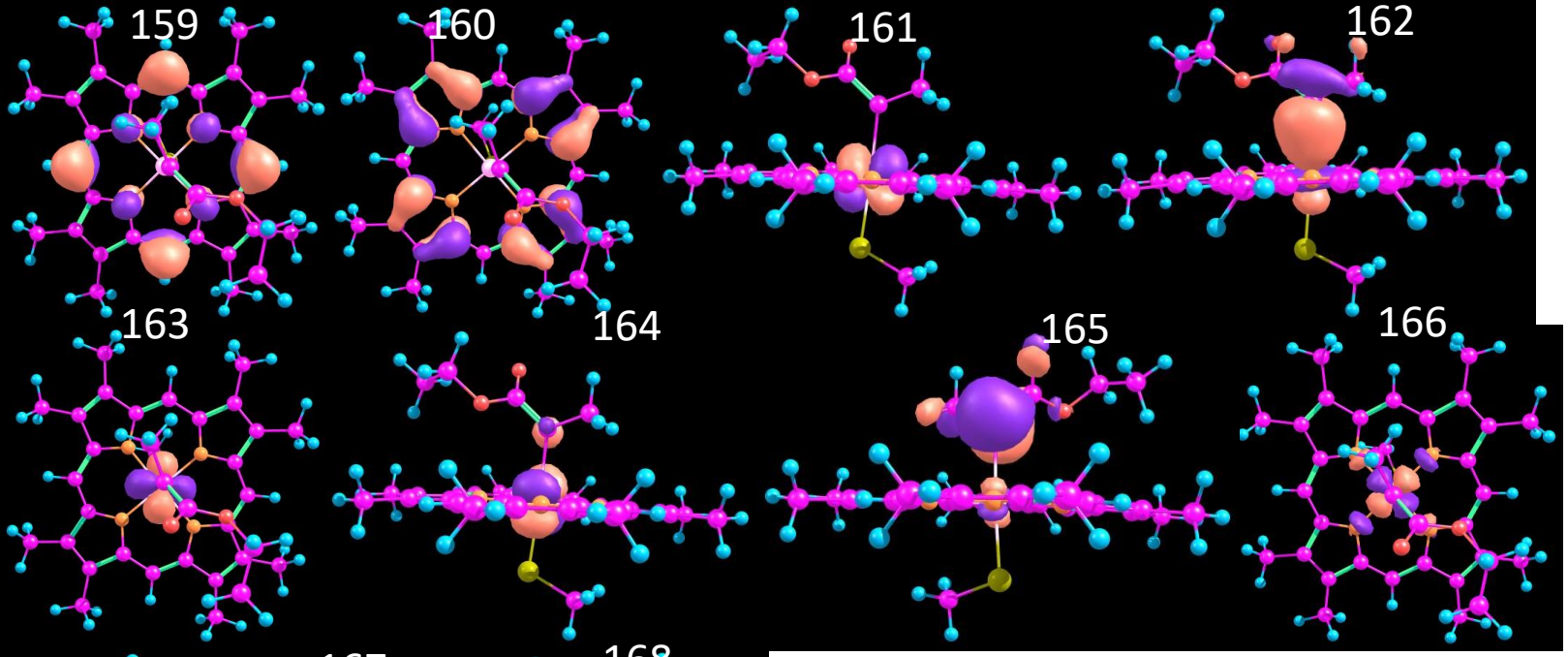
2.3 Å;
1 Quintet,
5 Triplets,
2 Singlets

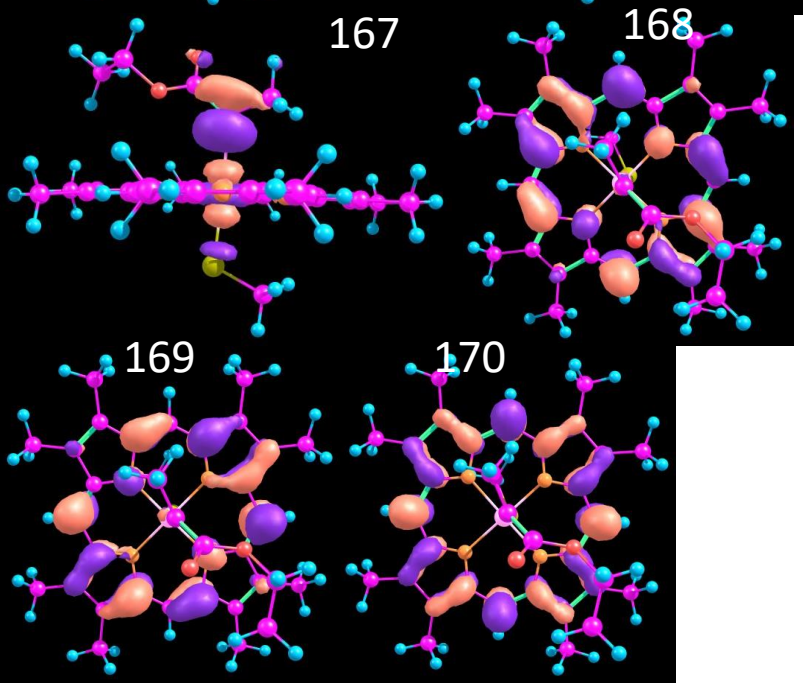




NO	OCC	E(Eh)	E(eV)
159	1.9310	-0.119900	-3.2626
160	1.9147	-0.088744	-2.4148
161	1.6486	-0.210897	-5.7388
162	1.6116	-0.174190	-4.7400
163	1.4851	-0.160147	-4.3578
164	1.3177	-0.085503	-2.3267
165	0.9650	0.024371	0.6632
166	0.5641	0.285675	7.7736
167	0.4036	0.208695	5.6789
168	0.0767	0.146539	3.9875
169	0.0749	0.148577	4.0430
170	0.0070	0.290922	7.9164

2.4 Å;
1 Quintet,
5 Triplets,
2 Singlets

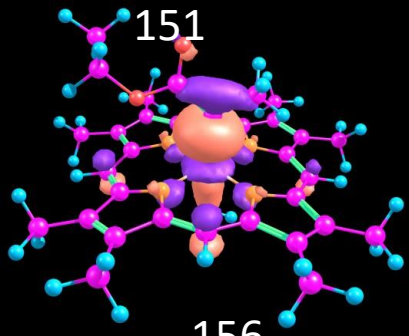


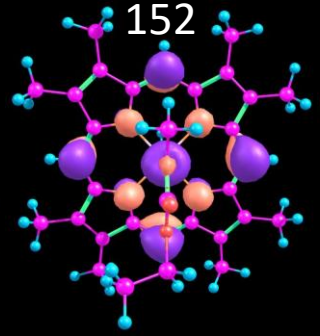


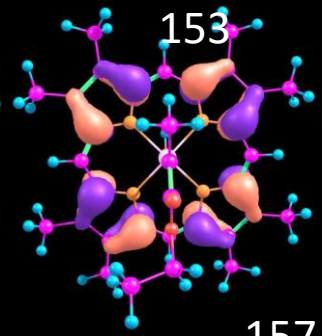
NO	OCC	E(Eh)	E(eV)
159	1.9306	-0.119489	-3.2515
160	1.9144	-0.088328	-2.4035
161	1.6525	-0.197670	-5.3789
162	1.4950	-0.139662	-3.8004
163	1.4815	-0.145041	-3.9468
164	1.3064	-0.068513	-1.8643
165	0.9727	0.013754	0.3743
166	0.5654	0.297386	8.0923
167	0.5233	0.172993	4.7074
168	0.0766	0.146493	3.9863
169	0.0747	0.148512	4.0412
170	0.0069	0.291511	7.9324

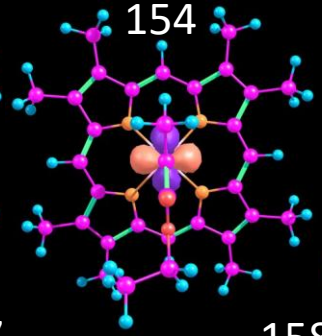
2.5 Å;
1 Quintet,
5 Triplets,
2 Singlets

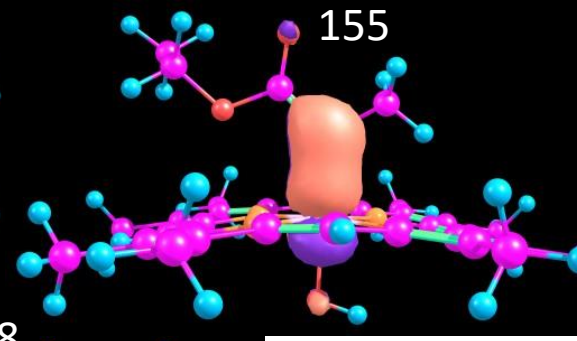
Active Space for QD-NEVPT2 on RKS DFT Geometries: Hydroxide

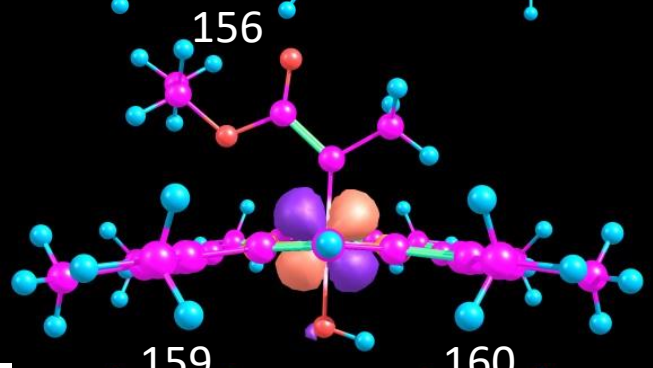


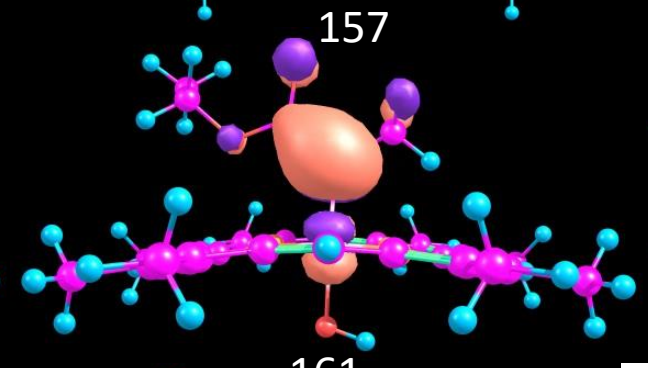


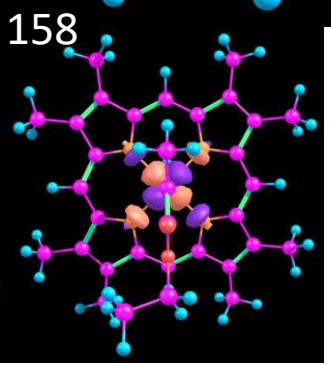




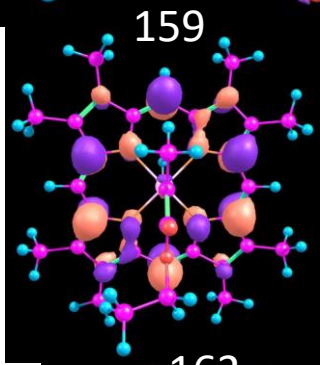


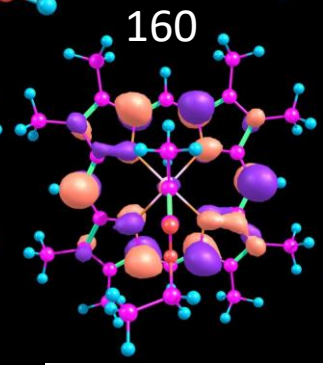


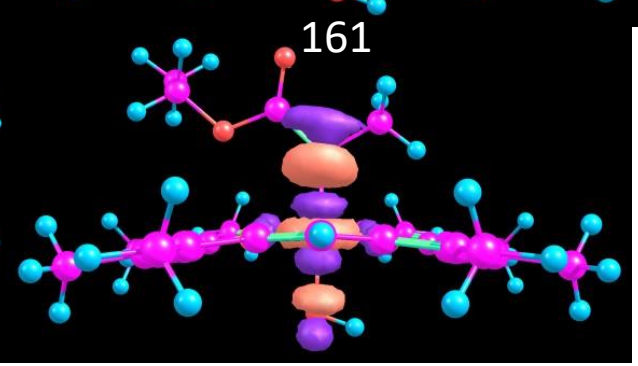


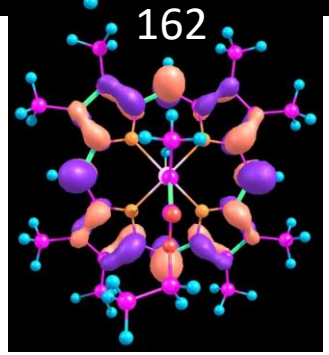


0 degrees; 5 Triplets, 2 Singlets

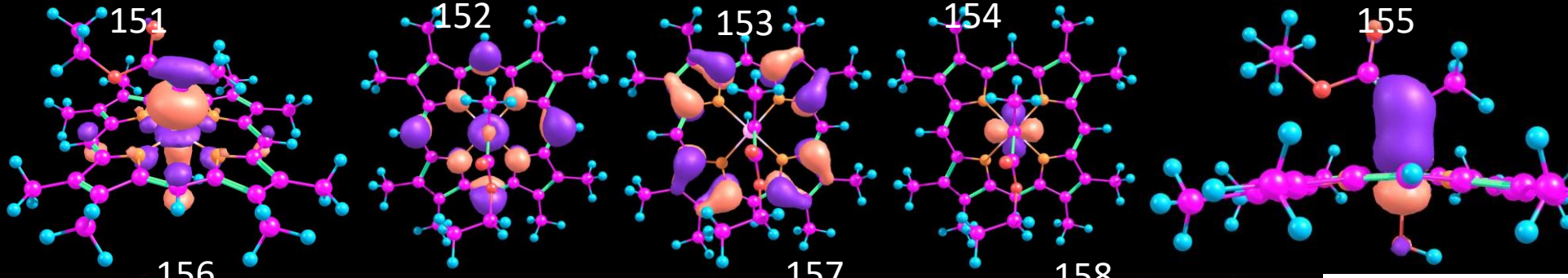


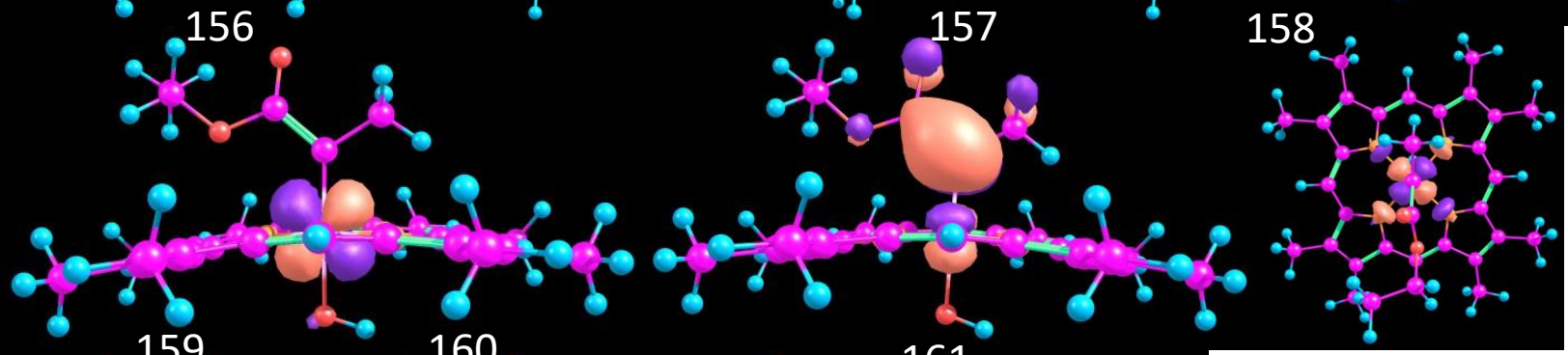


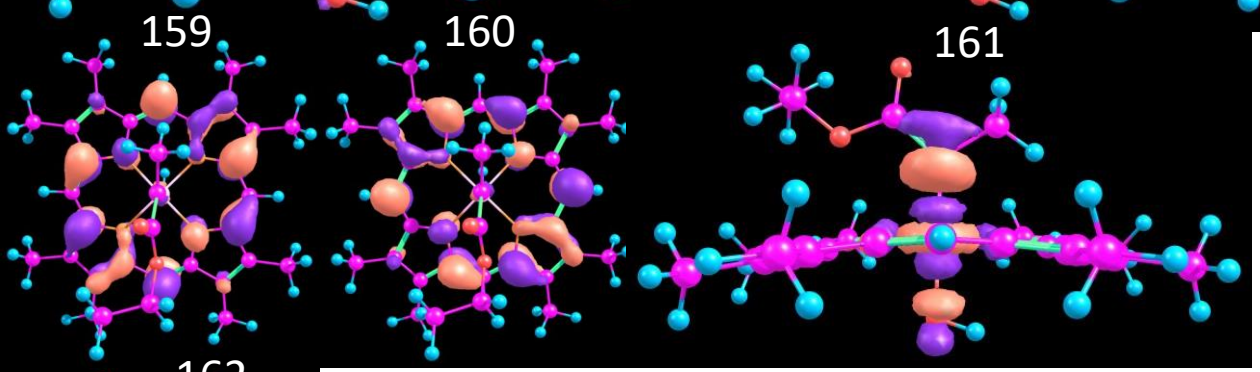


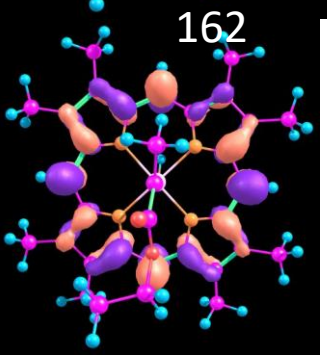


NO	OCC	E(Eh)	E(eV)
151	1.9407	-0.298276	-8.1165
152	1.9290	-0.146233	-3.9792
153	1.9175	-0.084720	-2.3053
154	1.7476	-0.310703	-8.4547
155	1.5922	-0.199023	-5.4157
156	1.4576	-0.189890	-5.1672
157	0.8307	0.060404	1.6437
158	0.3557	0.328651	8.9430
159	0.0748	0.156093	4.2475
160	0.0743	0.155229	4.2240
161	0.0727	0.434232	11.8161
162	0.0072	0.299892	8.1605



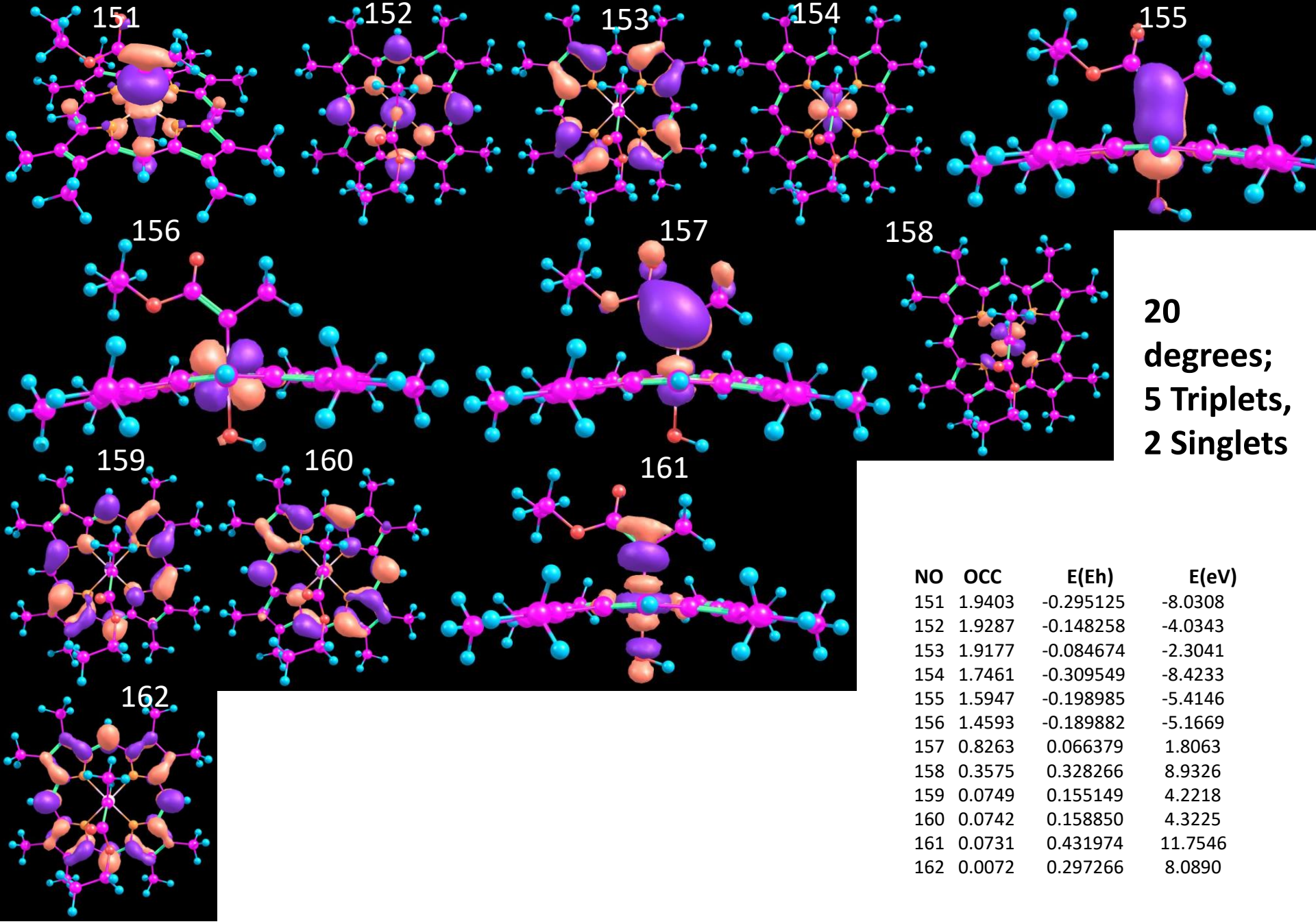






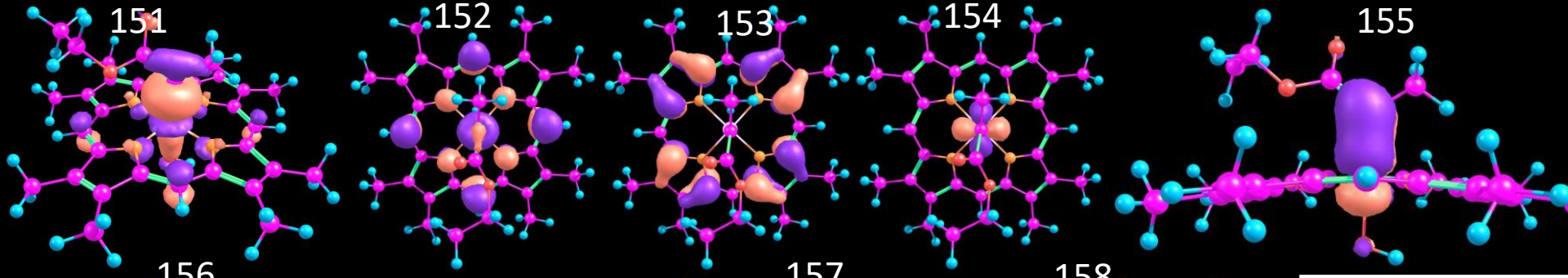
10 degrees; 5 Triplets, 2 Singlets

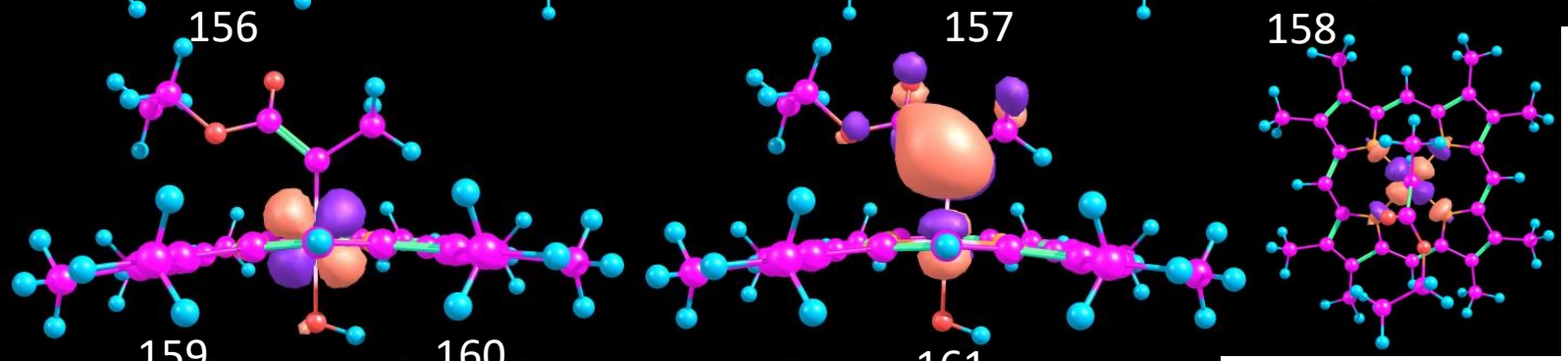
NO	OCC	E(Eh)	E(eV)
151	1.9405	-0.297412	-8.0930
152	1.9289	-0.147112	-4.0031
153	1.9176	-0.084794	-2.3074
154	1.7472	-0.310393	-8.4462
155	1.5928	-0.199005	-5.4152
156	1.4581	-0.189879	-5.1669
157	0.8297	0.061936	1.6854
158	0.3561	0.328599	8.9416
159	0.0748	0.155727	4.2376
160	0.0743	0.156433	4.2567
161	0.0729	0.433525	11.7968
162	0.0073	0.302205	8.2234

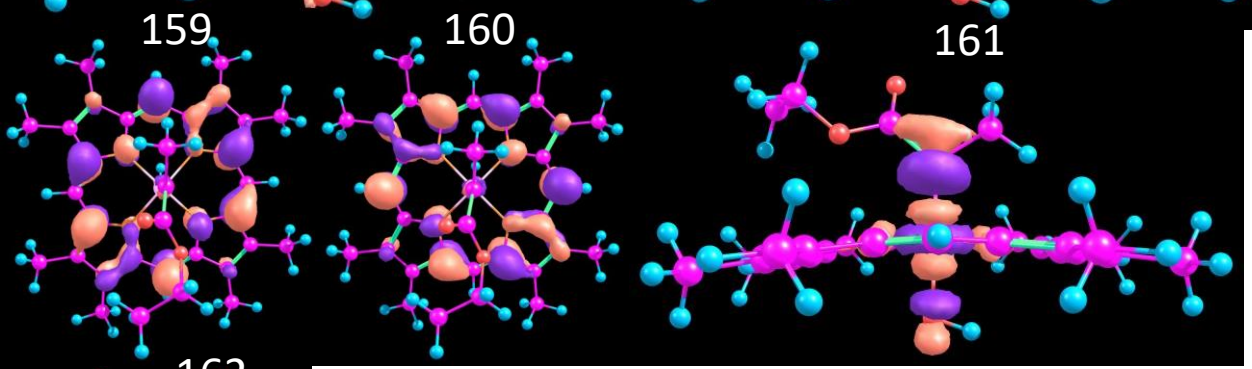


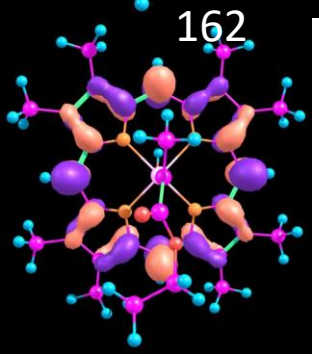
20 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9403	-0.295125	-8.0308
152	1.9287	-0.148258	-4.0343
153	1.9177	-0.084674	-2.3041
154	1.7461	-0.309549	-8.4233
155	1.5947	-0.198985	-5.4146
156	1.4593	-0.189882	-5.1669
157	0.8263	0.066379	1.8063
158	0.3575	0.328266	8.9326
159	0.0749	0.155149	4.2218
160	0.0742	0.158850	4.3225
161	0.0731	0.431974	11.7546
162	0.0072	0.297266	8.0890



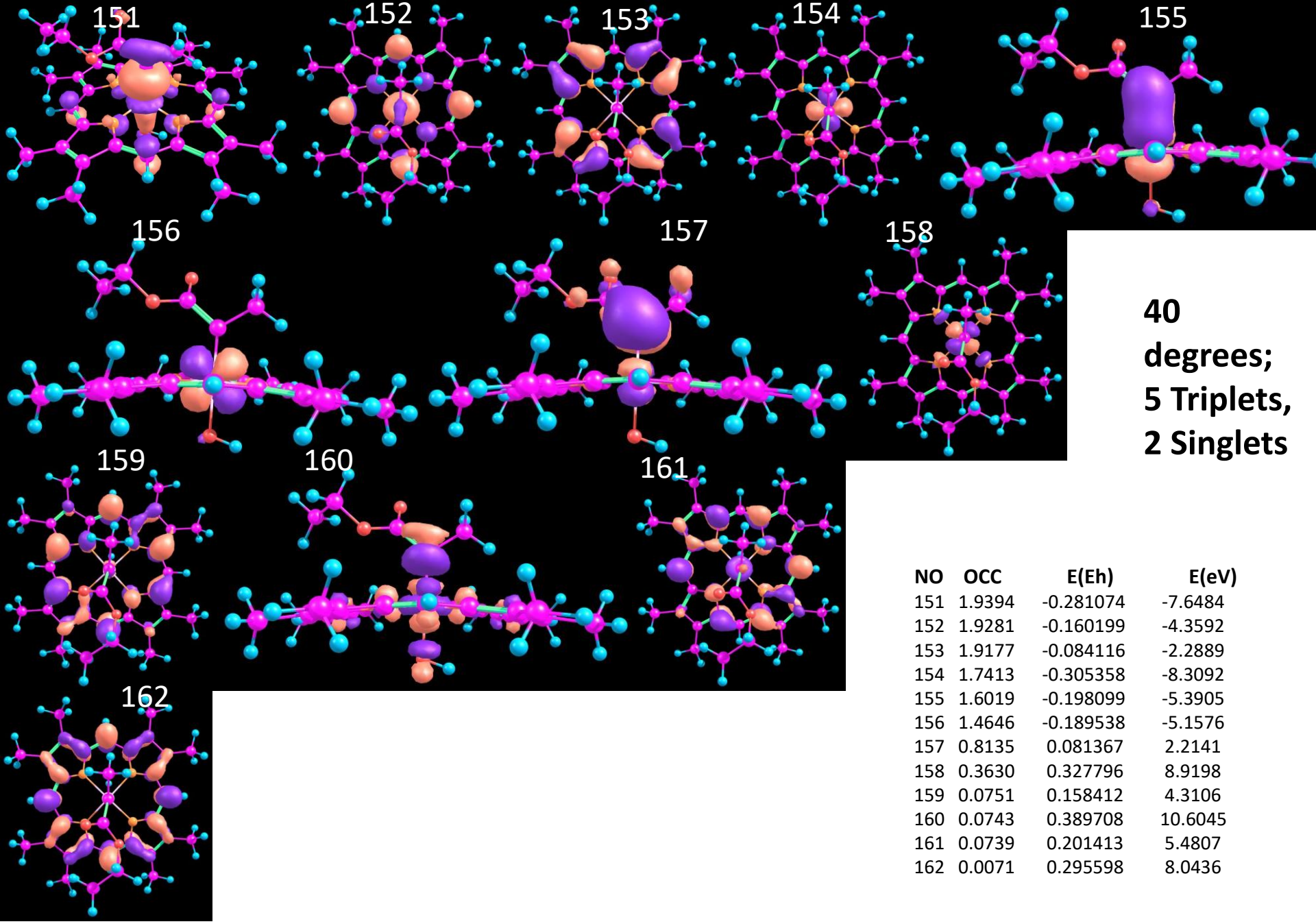






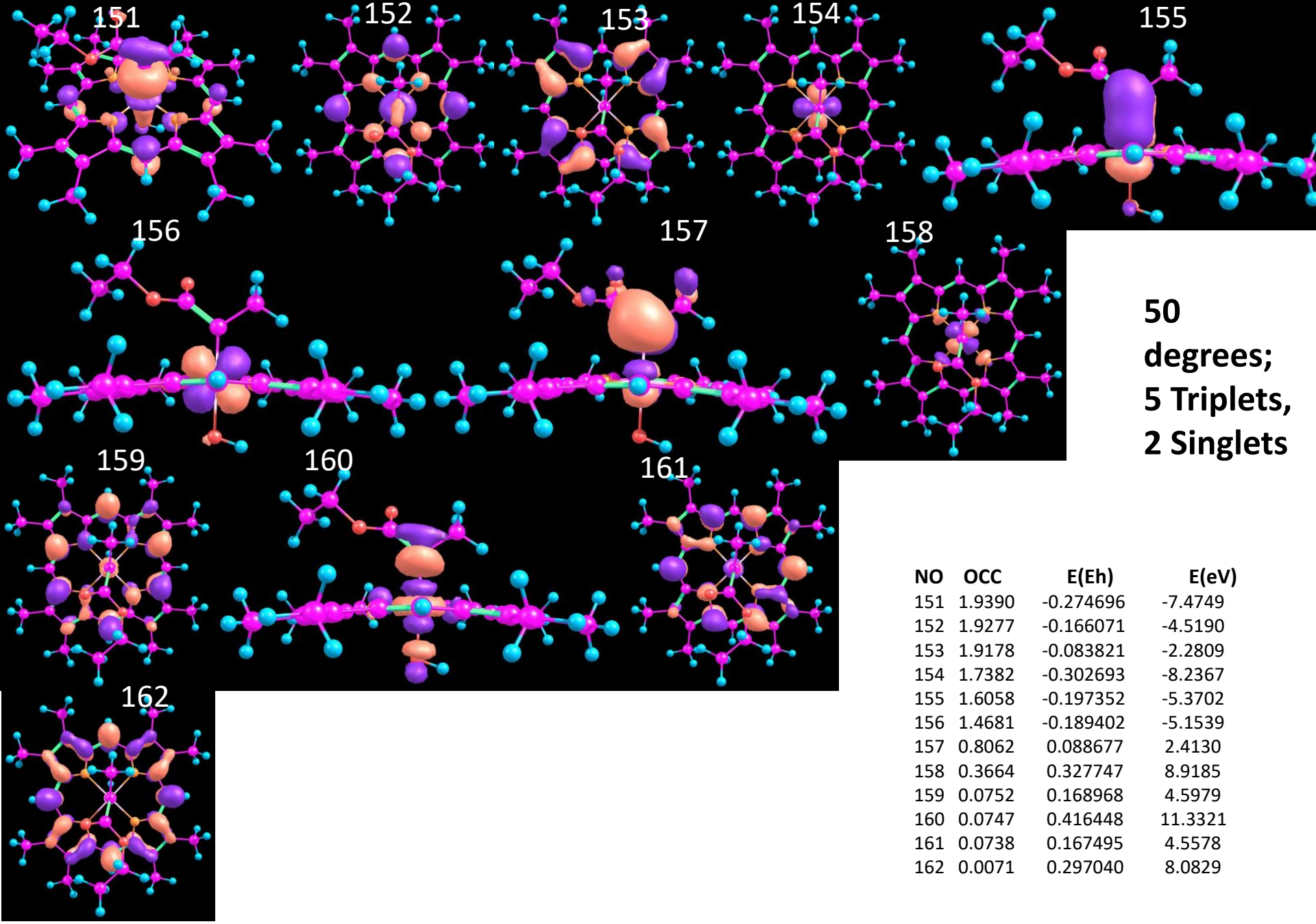
30 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9399	-0.289671	-7.8823
152	1.9284	-0.153098	-4.1660
153	1.9176	-0.084375	-2.2959
154	1.7440	-0.307766	-8.3747
155	1.5982	-0.198715	-5.4073
156	1.4617	-0.189816	-5.1652
157	0.8204	0.073187	1.9915
158	0.3599	0.328016	8.9258
159	0.0751	0.156370	4.2551
160	0.0741	0.159018	4.3271
161	0.0735	0.432485	11.7685
162	0.0071	0.296965	8.0808



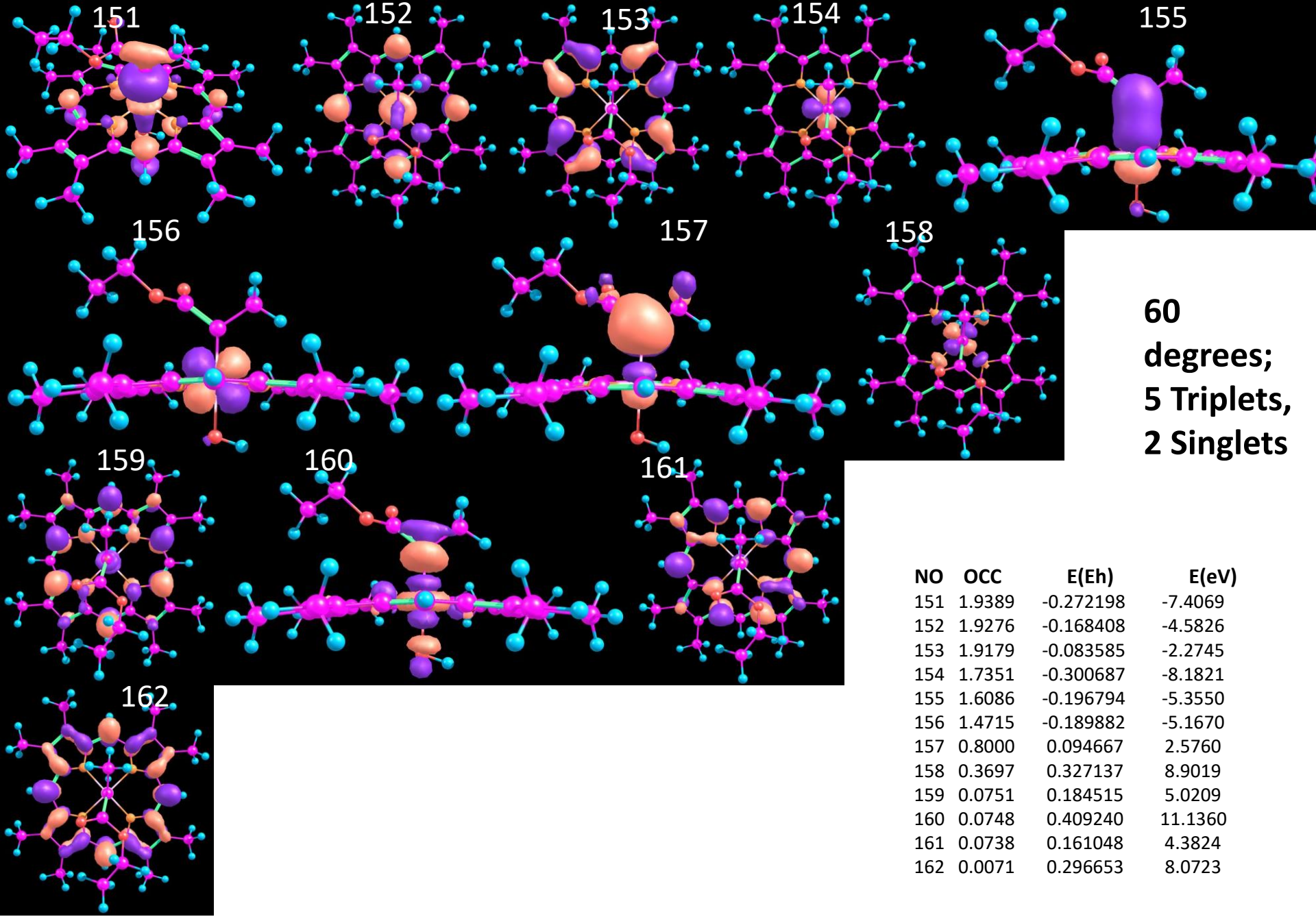
40 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9394	-0.281074	-7.6484
152	1.9281	-0.160199	-4.3592
153	1.9177	-0.084116	-2.2889
154	1.7413	-0.305358	-8.3092
155	1.6019	-0.198099	-5.3905
156	1.4646	-0.189538	-5.1576
157	0.8135	0.081367	2.2141
158	0.3630	0.327796	8.9198
159	0.0751	0.158412	4.3106
160	0.0743	0.389708	10.6045
161	0.0739	0.201413	5.4807
162	0.0071	0.295598	8.0436



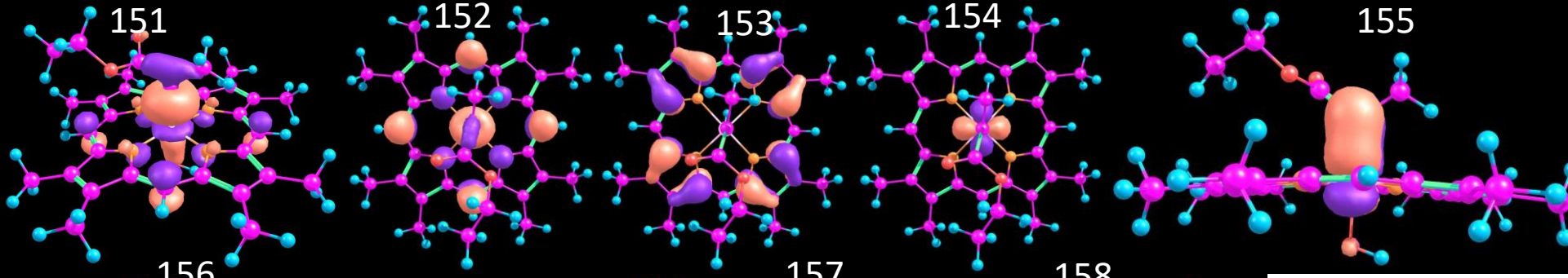
50 degrees; 5 Triplets, 2 Singlets

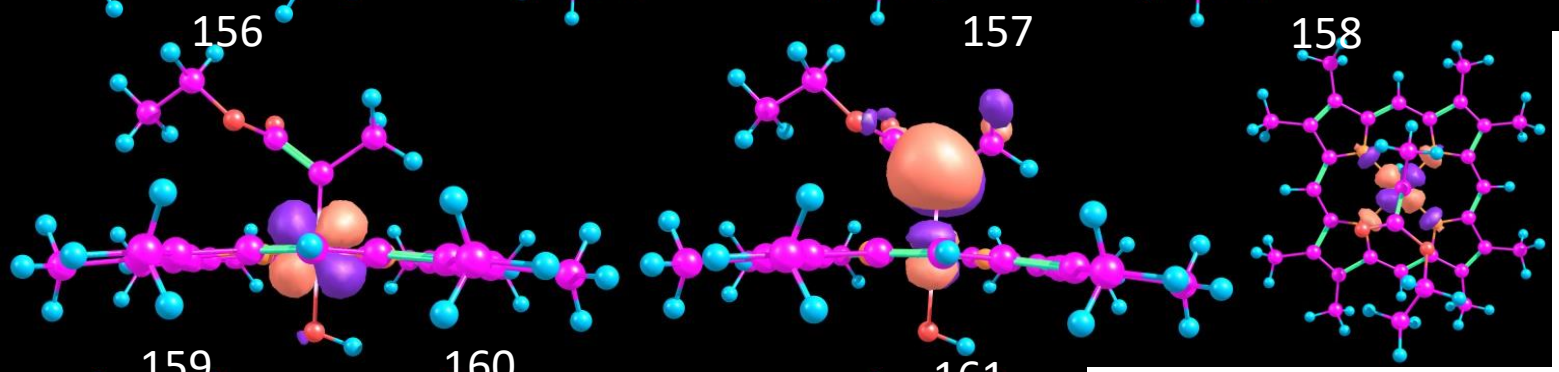
NO	OCC	E(Eh)	E(eV)
151	1.9390	-0.274696	-7.4749
152	1.9277	-0.166071	-4.5190
153	1.9178	-0.083821	-2.2809
154	1.7382	-0.302693	-8.2367
155	1.6058	-0.197352	-5.3702
156	1.4681	-0.189402	-5.1539
157	0.8062	0.088677	2.4130
158	0.3664	0.327747	8.9185
159	0.0752	0.168968	4.5979
160	0.0747	0.416448	11.3321
161	0.0738	0.167495	4.5578
162	0.0071	0.297040	8.0829

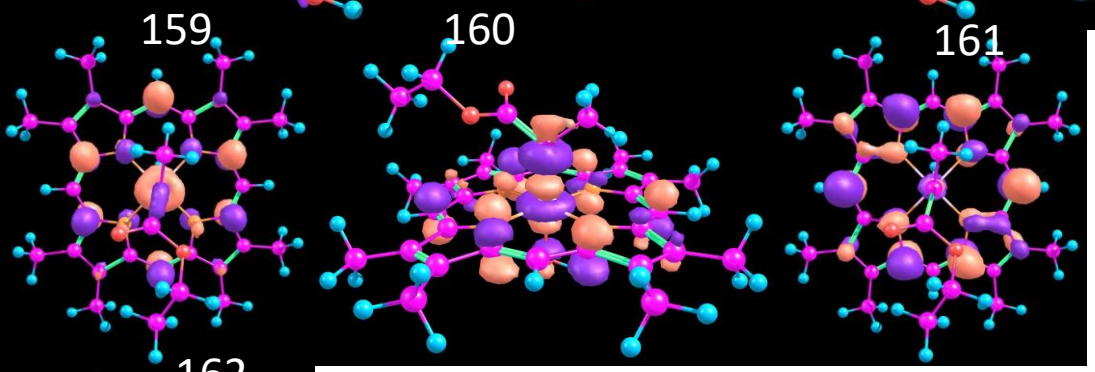


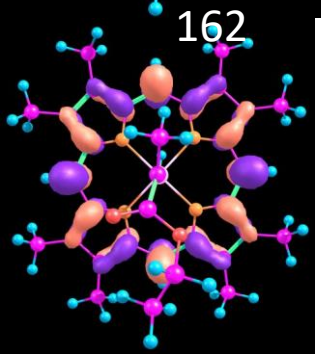
60 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9389	-0.272198	-7.4069
152	1.9276	-0.168408	-4.5826
153	1.9179	-0.083585	-2.2745
154	1.7351	-0.300687	-8.1821
155	1.6086	-0.196794	-5.3550
156	1.4715	-0.189882	-5.1670
157	0.8000	0.094667	2.5760
158	0.3697	0.327137	8.9019
159	0.0751	0.184515	5.0209
160	0.0748	0.409240	11.1360
161	0.0738	0.161048	4.3824
162	0.0071	0.296653	8.0723



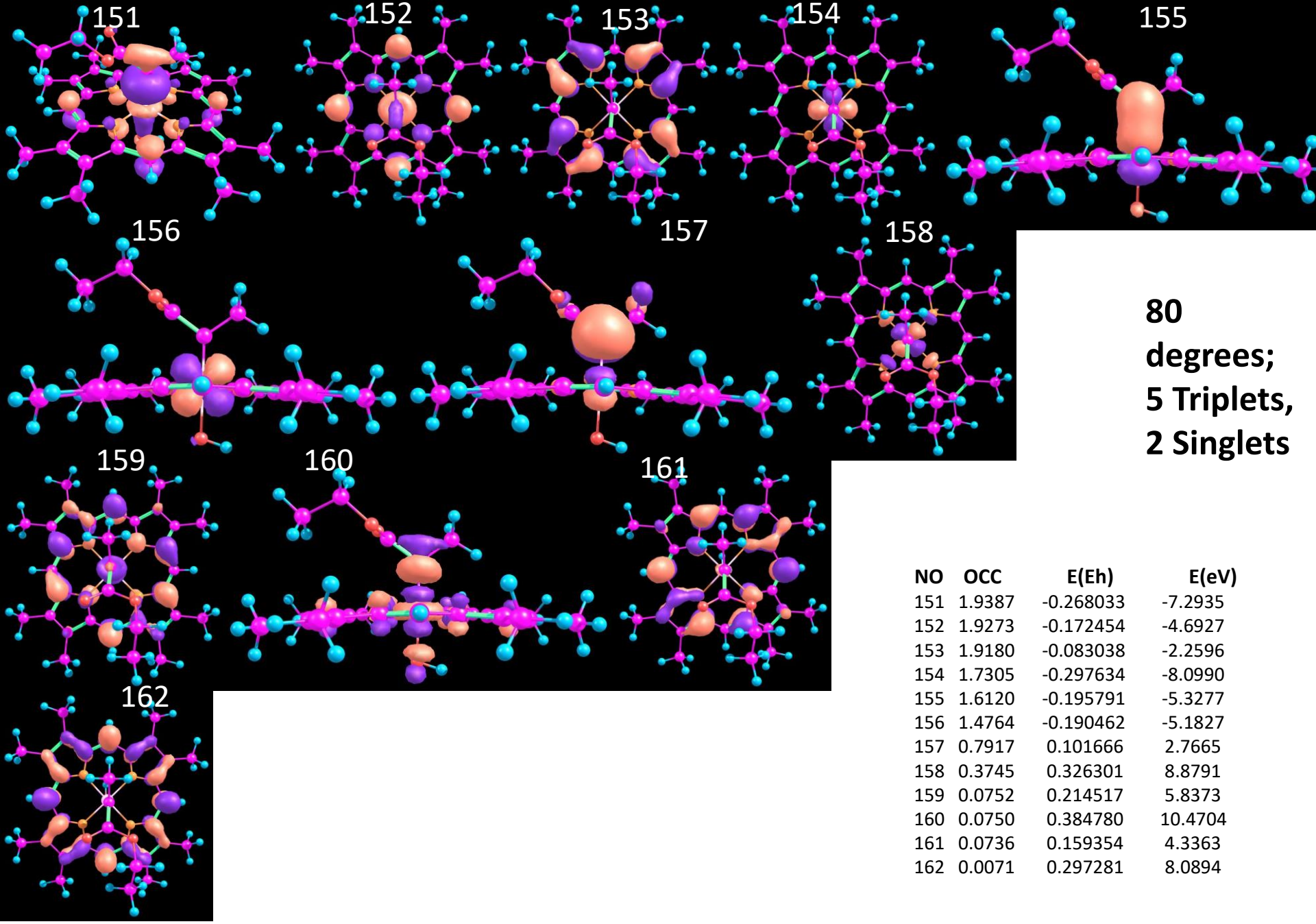






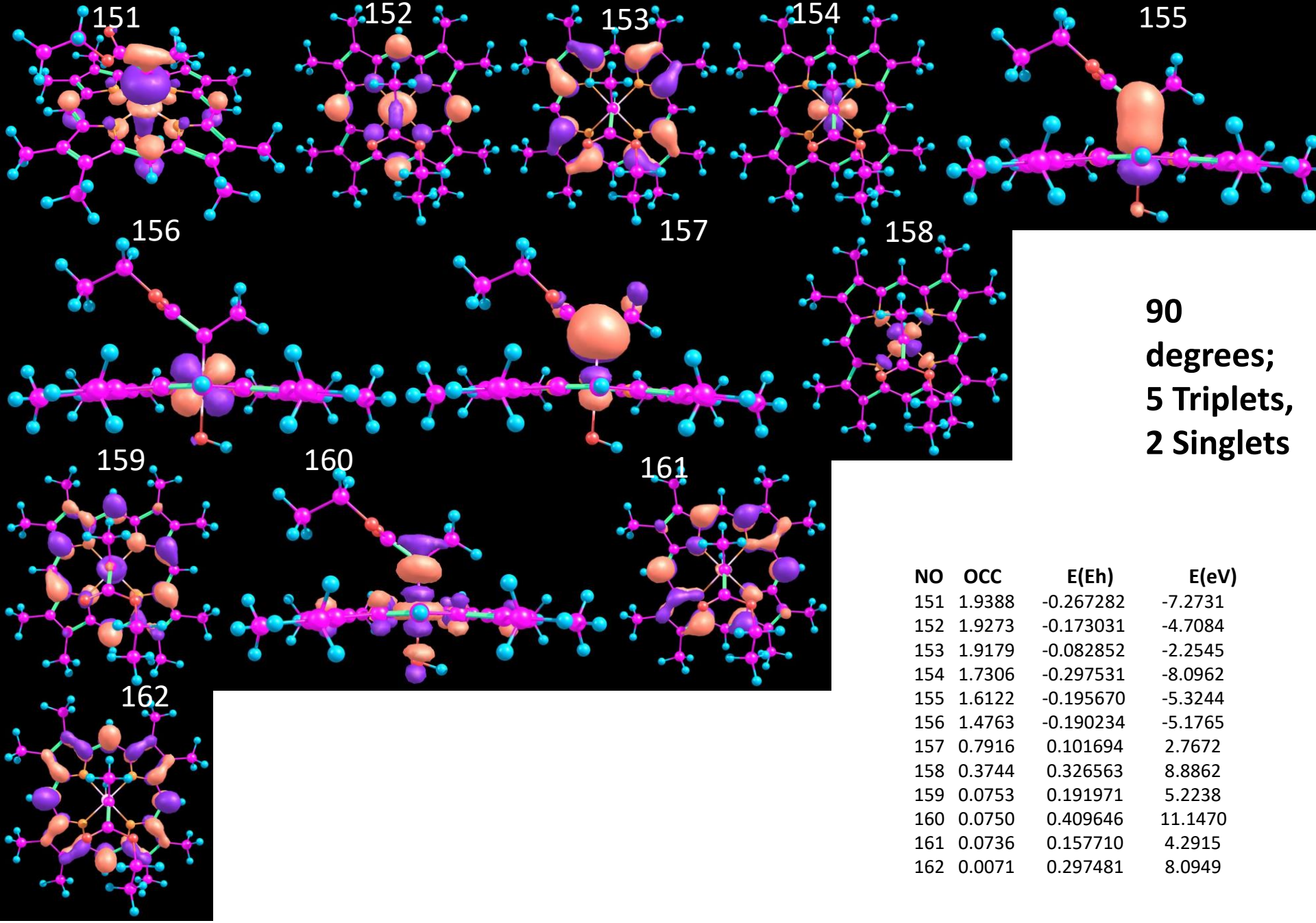
70 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9386	-0.269645	-7.3374
152	1.9273	-0.170508	-4.6398
153	1.9181	-0.083321	-2.2673
154	1.7328	-0.298785	-8.1304
155	1.6107	-0.196360	-5.3432
156	1.4739	-0.189777	-5.1641
157	0.7952	0.099275	2.7014
158	0.3723	0.326798	8.8926
159	0.0751	0.282710	7.6929
160	0.0750	0.309903	8.4329
161	0.0737	0.164630	4.4798
162	0.0071	0.297043	8.0829



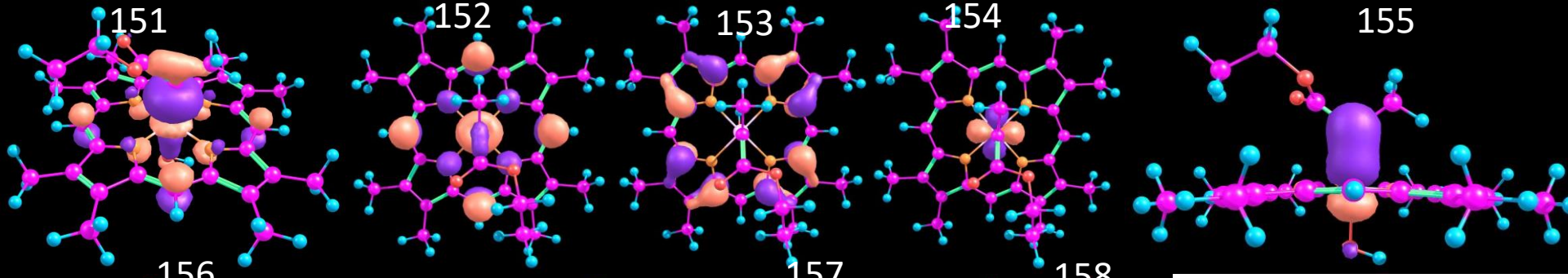
80 degrees; 5 Triplets, 2 Singlets

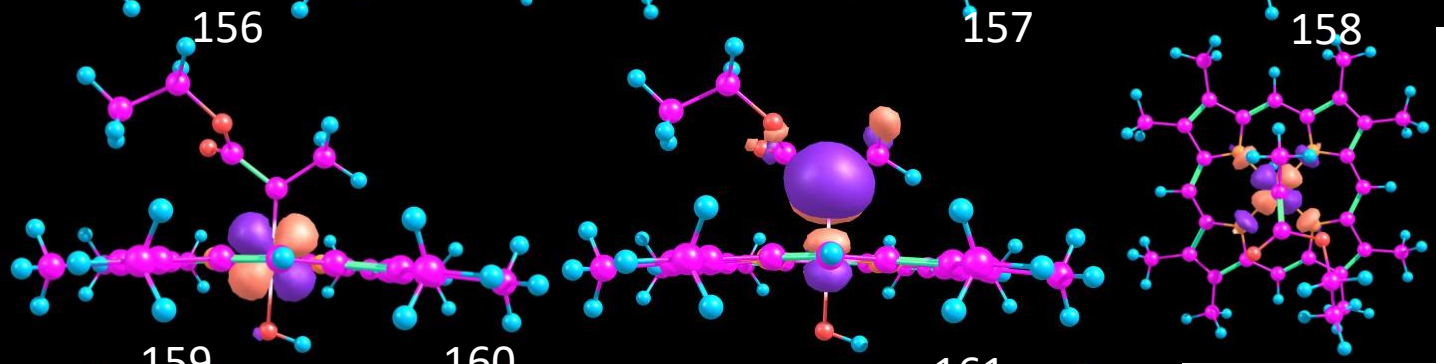
NO	OCC	E(Eh)	E(eV)
151	1.9387	-0.268033	-7.2935
152	1.9273	-0.172454	-4.6927
153	1.9180	-0.083038	-2.2596
154	1.7305	-0.297634	-8.0990
155	1.6120	-0.195791	-5.3277
156	1.4764	-0.190462	-5.1827
157	0.7917	0.101666	2.7665
158	0.3745	0.326301	8.8791
159	0.0752	0.214517	5.8373
160	0.0750	0.384780	10.4704
161	0.0736	0.159354	4.3363
162	0.0071	0.297281	8.0894

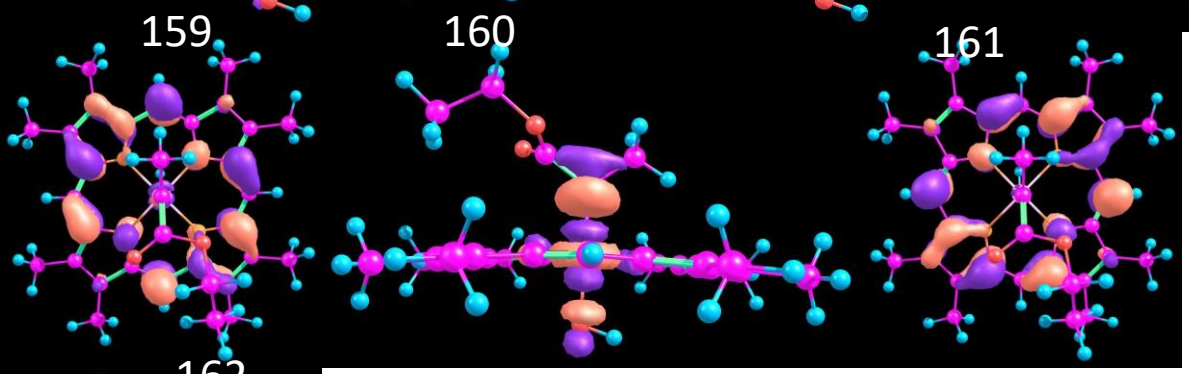


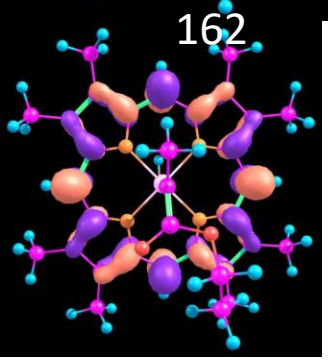
90 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9388	-0.267282	-7.2731
152	1.9273	-0.173031	-4.7084
153	1.9179	-0.082852	-2.2545
154	1.7306	-0.297531	-8.0962
155	1.6122	-0.195670	-5.3244
156	1.4763	-0.190234	-5.1765
157	0.7916	0.101694	2.7672
158	0.3744	0.326563	8.8862
159	0.0753	0.191971	5.2238
160	0.0750	0.409646	11.1470
161	0.0736	0.157710	4.2915
162	0.0071	0.297481	8.0949



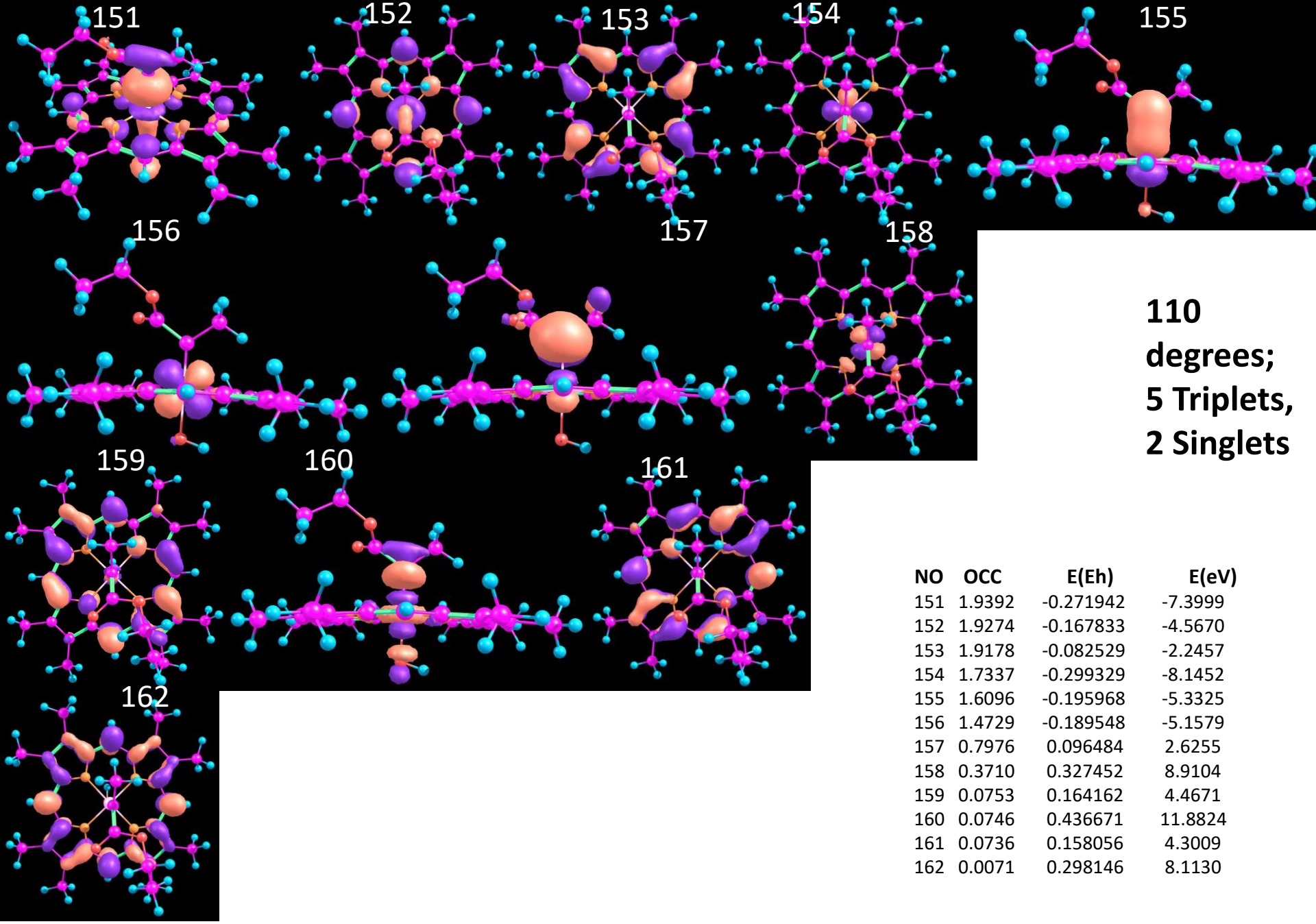






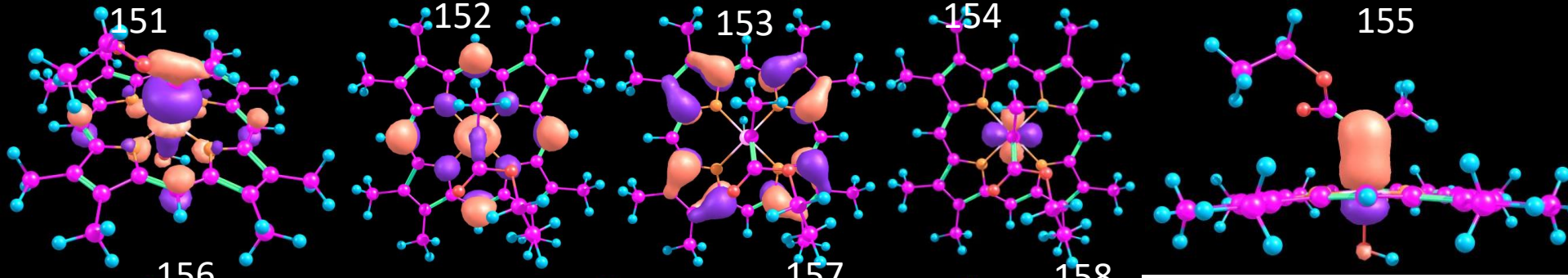
100 degrees; 5 Triplets, 2 Singlets

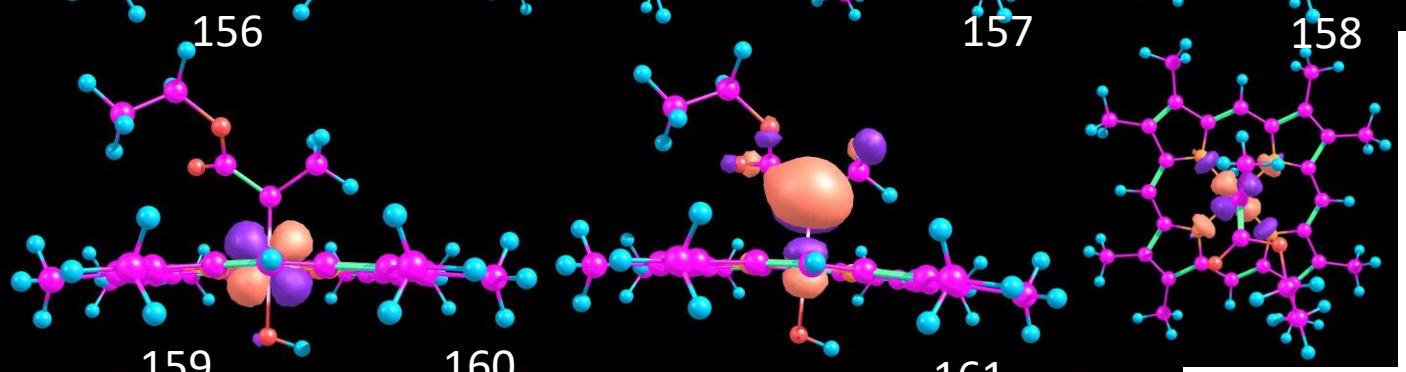
NO	OCC	E(Eh)	E(eV)
151	1.9389	-0.269246	-7.3265
152	1.9273	-0.170968	-4.6523
153	1.9179	-0.082752	-2.2518
154	1.7316	-0.298135	-8.1127
155	1.6113	-0.195786	-5.3276
156	1.4752	-0.190053	-5.1716
157	0.7936	0.100037	2.7221
158	0.3733	0.326810	8.8930
159	0.0753	0.165913	4.5147
160	0.0749	0.435687	11.8557
161	0.0736	0.157562	4.2875
162	0.0071	0.297797	8.1035

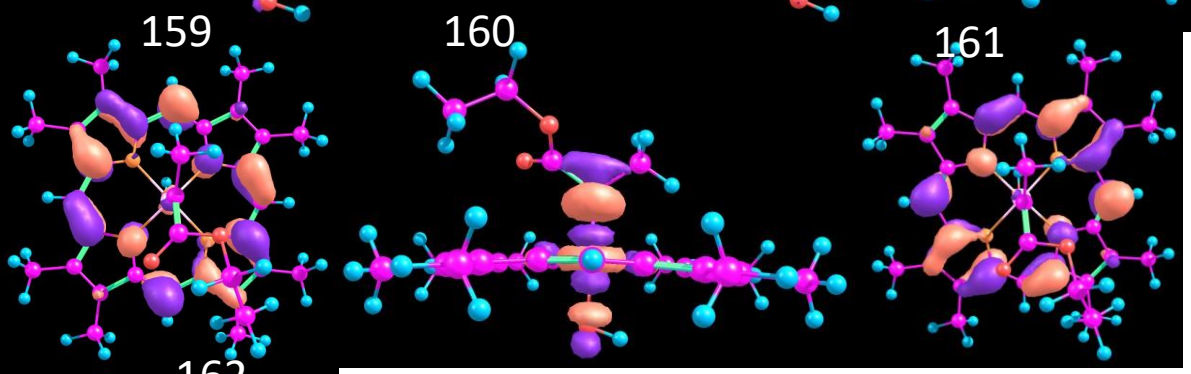


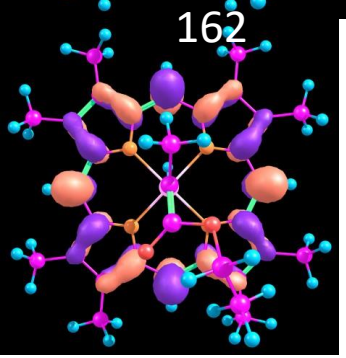
110 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9392	-0.271942	-7.3999
152	1.9274	-0.167833	-4.5670
153	1.9178	-0.082529	-2.2457
154	1.7337	-0.299329	-8.1452
155	1.6096	-0.195968	-5.3325
156	1.4729	-0.189548	-5.1579
157	0.7976	0.096484	2.6255
158	0.3710	0.327452	8.9104
159	0.0753	0.164162	4.4671
160	0.0746	0.436671	11.8824
161	0.0736	0.158056	4.3009
162	0.0071	0.298146	8.1130



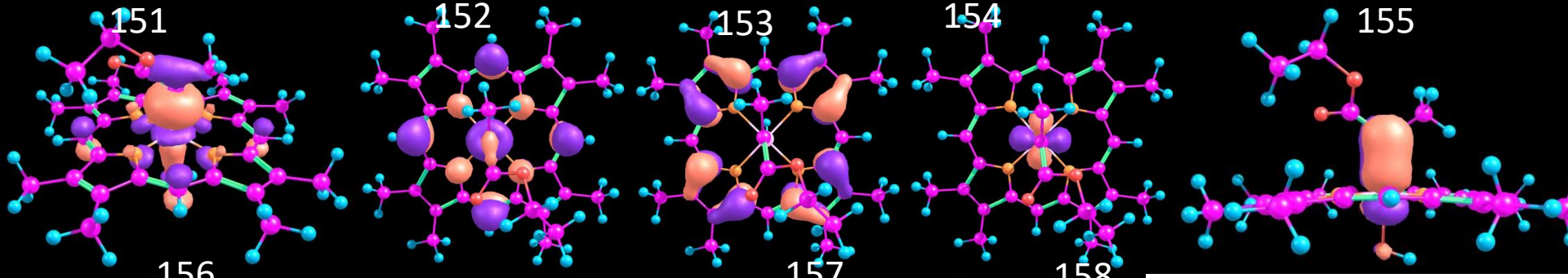


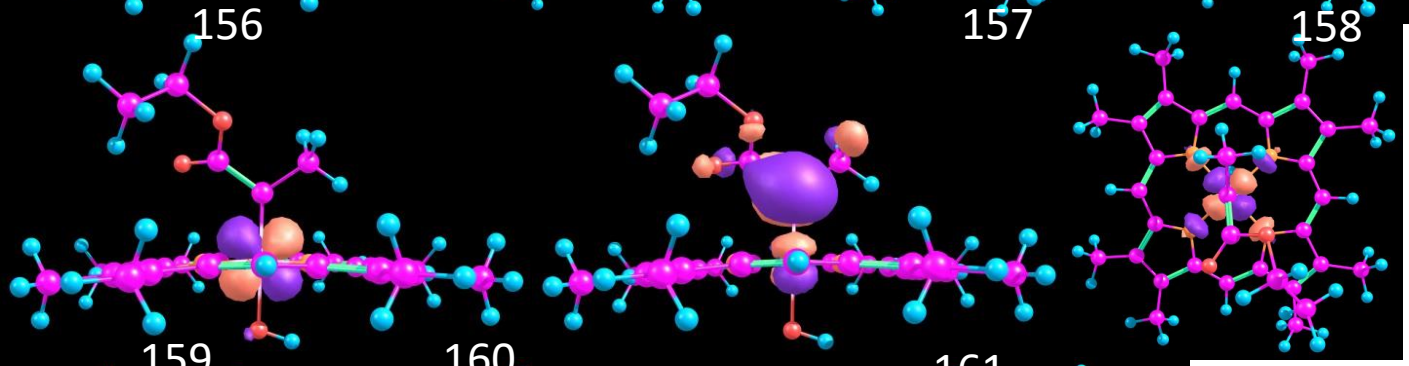


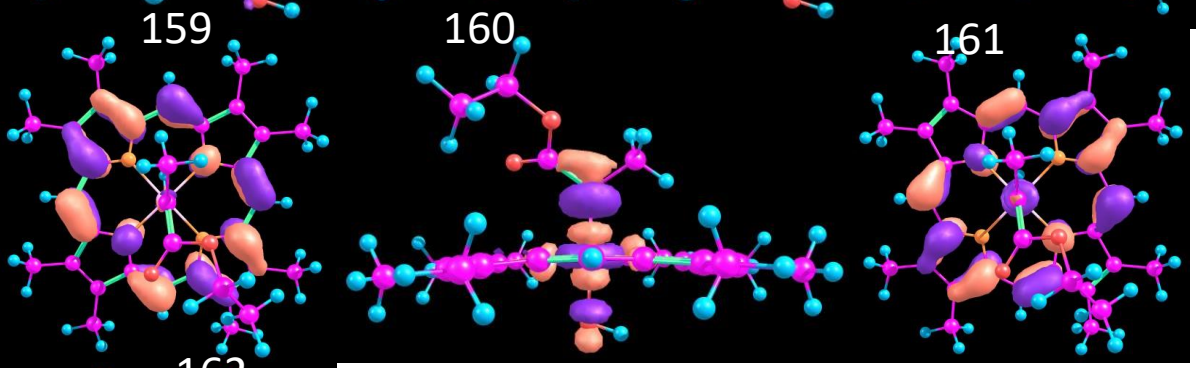


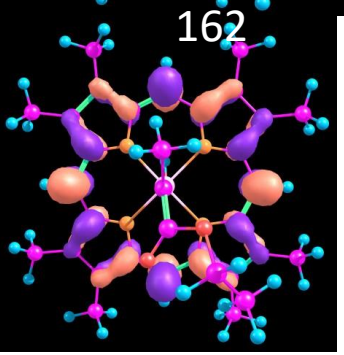
120 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9395	-0.276256	-7.5173
152	1.9276	-0.163532	-4.4499
153	1.9178	-0.082406	-2.2424
154	1.7358	-0.300829	-8.1860
155	1.6076	-0.196430	-5.3451
156	1.4706	-0.189343	-5.1523
157	0.8020	0.091858	2.4996
158	0.3688	0.327733	8.9181
159	0.0753	0.159896	4.3510
160	0.0744	0.440920	11.9981
161	0.0737	0.157442	4.2842
162	0.0071	0.298060	8.1106



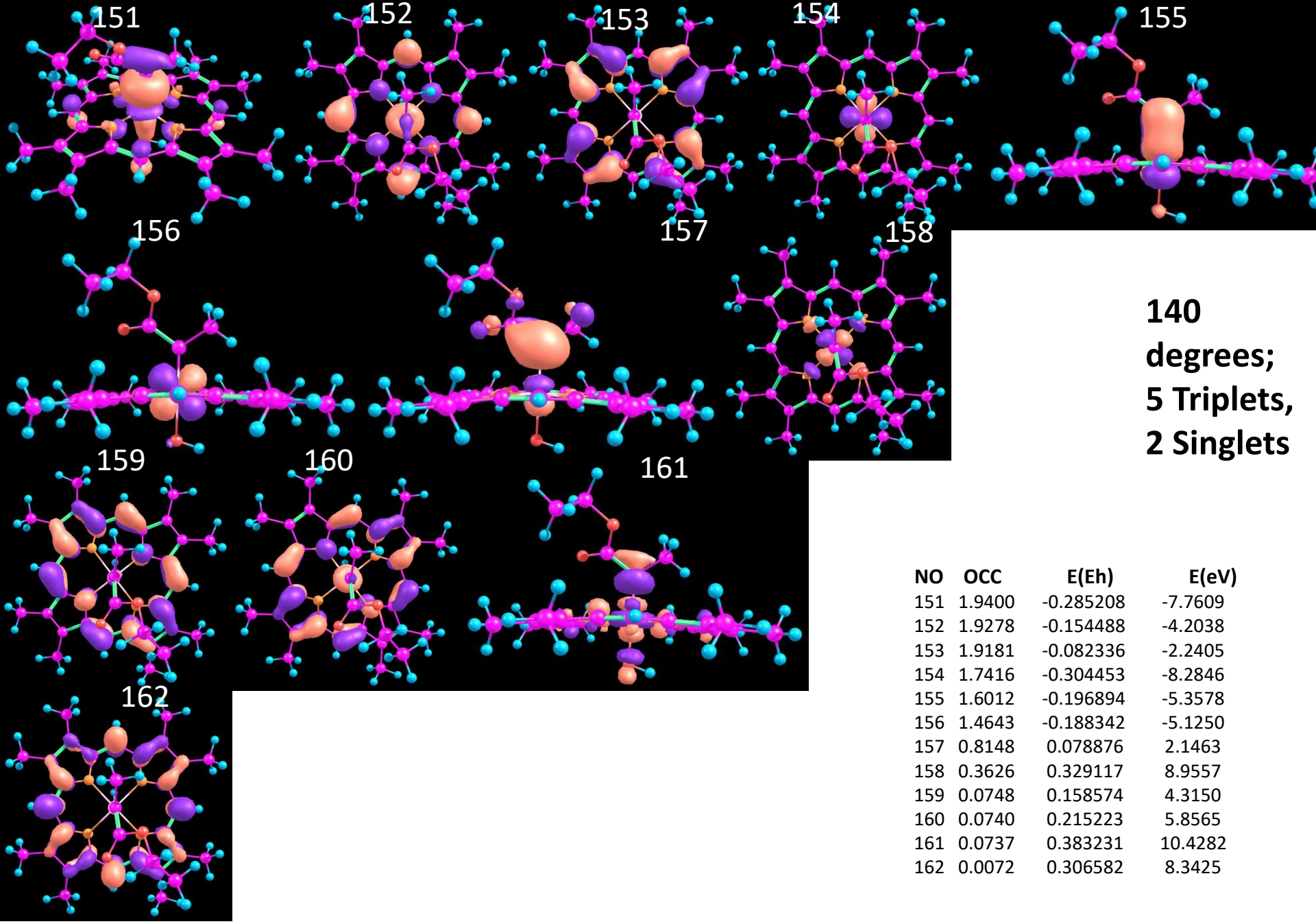






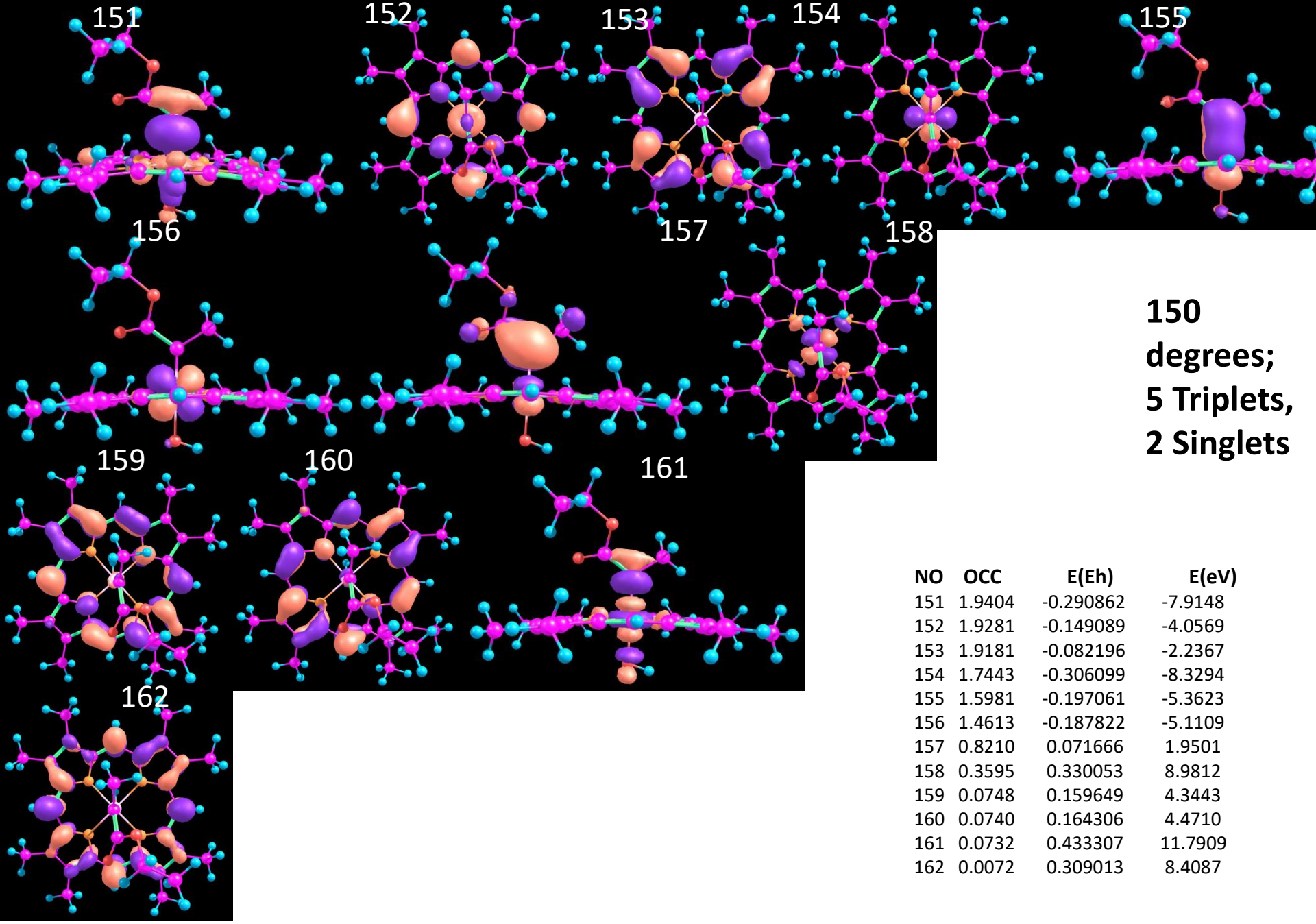
130 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9397	-0.281124	-7.6498
152	1.9276	-0.158359	-4.3092
153	1.9180	-0.082360	-2.2411
154	1.7385	-0.302620	-8.2347
155	1.6047	-0.196782	-5.3547
156	1.4676	-0.188971	-5.1422
157	0.8079	0.085743	2.3332
158	0.3659	0.328211	8.9311
159	0.0750	0.156503	4.2587
160	0.0741	0.415185	11.2978
161	0.0738	0.185826	5.0566
162	0.0071	0.301134	8.1943



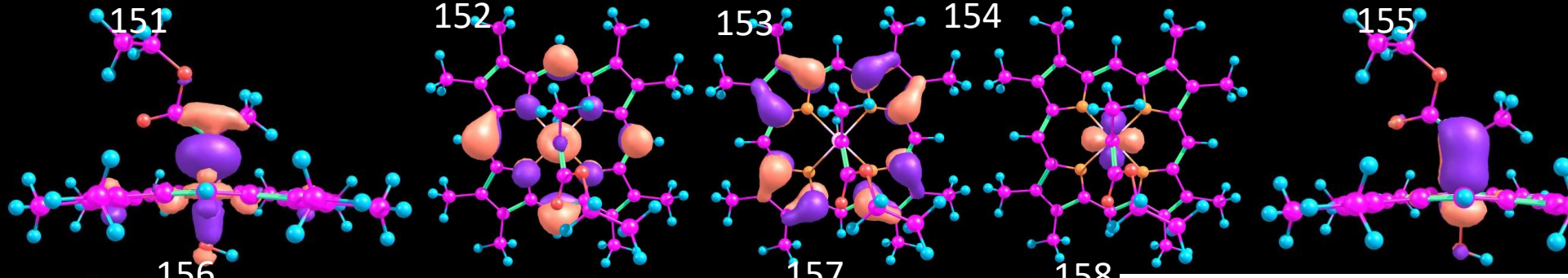
140 degrees; 5 Triplets, 2 Singlets

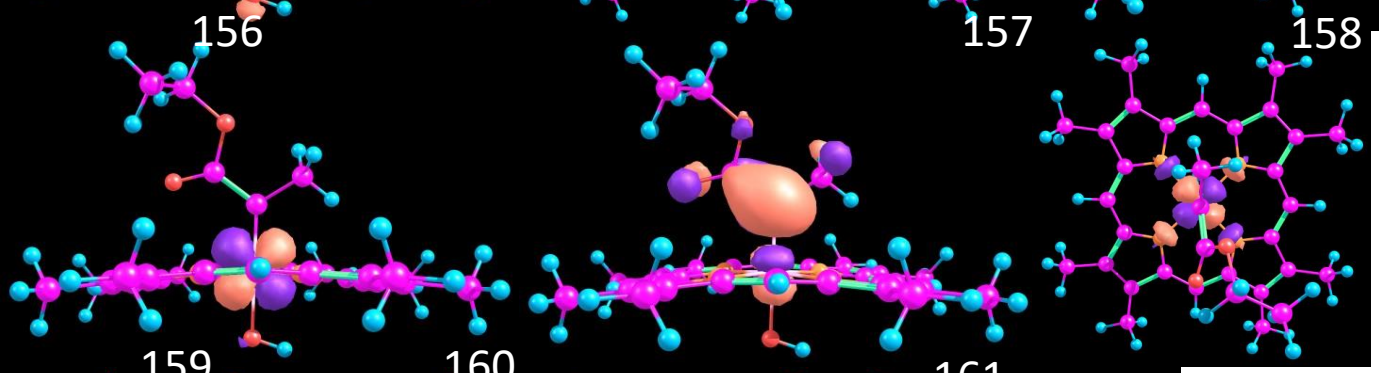
NO	OCC	E(Eh)	E(eV)
151	1.9400	-0.285208	-7.7609
152	1.9278	-0.154488	-4.2038
153	1.9181	-0.082336	-2.2405
154	1.7416	-0.304453	-8.2846
155	1.6012	-0.196894	-5.3578
156	1.4643	-0.188342	-5.1250
157	0.8148	0.078876	2.1463
158	0.3626	0.329117	8.9557
159	0.0748	0.158574	4.3150
160	0.0740	0.215223	5.8565
161	0.0737	0.383231	10.4282
162	0.0072	0.306582	8.3425

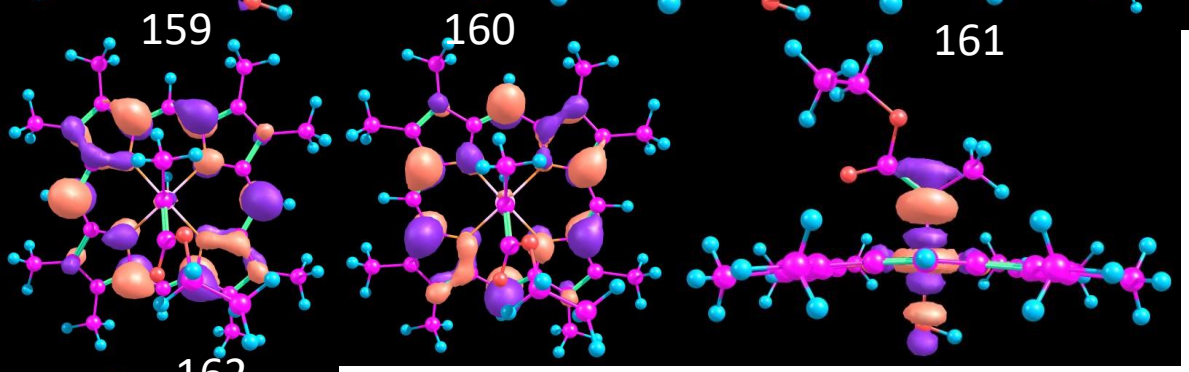


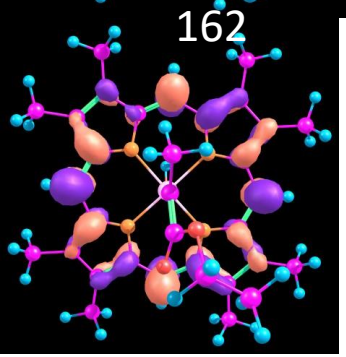
150 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9404	-0.290862	-7.9148
152	1.9281	-0.149089	-4.0569
153	1.9181	-0.082196	-2.2367
154	1.7443	-0.306099	-8.3294
155	1.5981	-0.197061	-5.3623
156	1.4613	-0.187822	-5.1109
157	0.8210	0.071666	1.9501
158	0.3595	0.330053	8.9812
159	0.0748	0.159649	4.3443
160	0.0740	0.164306	4.4710
161	0.0732	0.433307	11.7909
162	0.0072	0.309013	8.4087



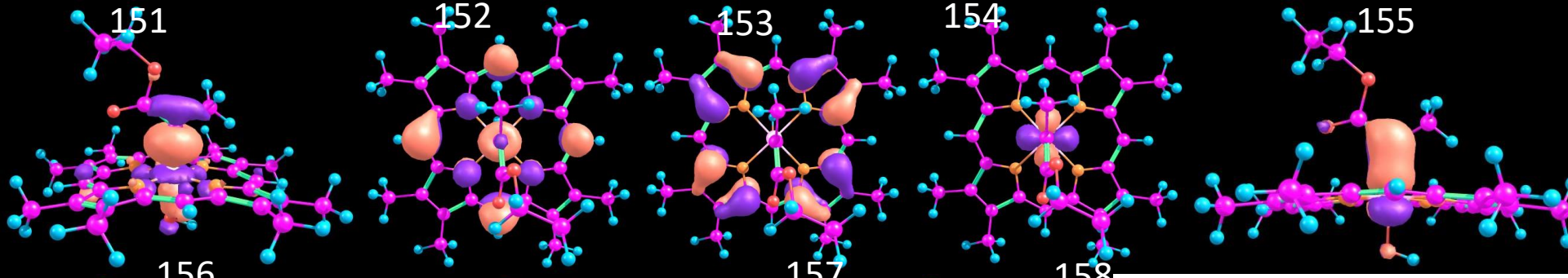


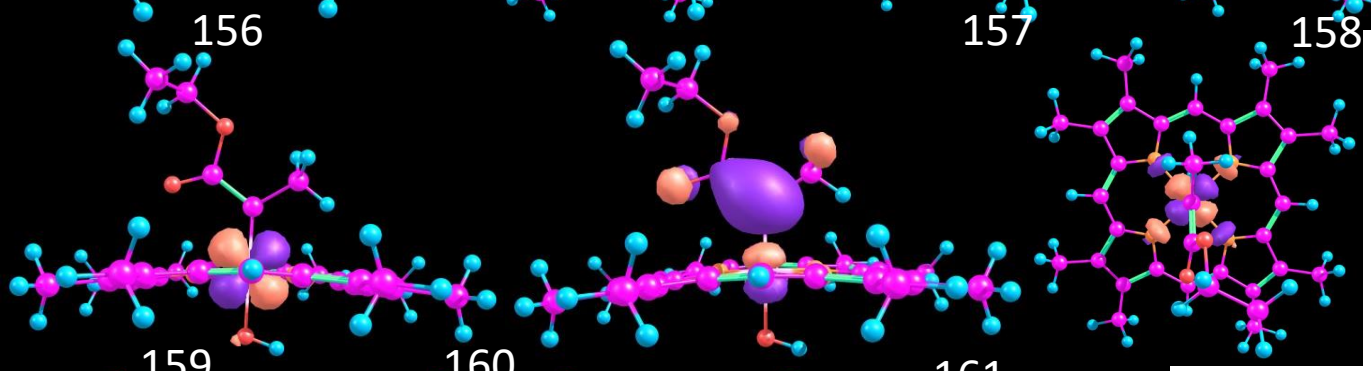


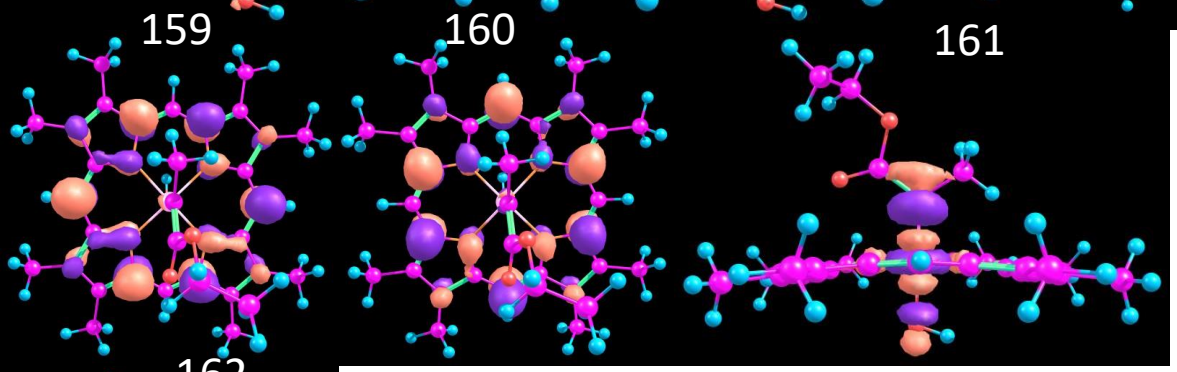


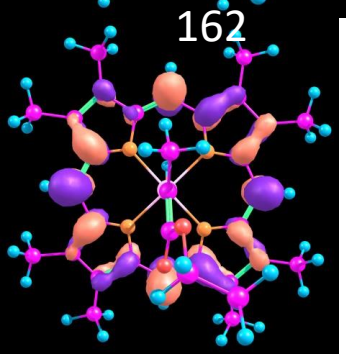
160 degrees; 5 Triplets, 2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9409	-0.297401	-8.0927
152	1.9286	-0.142800	-3.8858
153	1.9179	-0.081762	-2.2249
154	1.7462	-0.307762	-8.3746
155	1.5943	-0.197098	-5.3633
156	1.4590	-0.187953	-5.1145
157	0.8273	0.064377	1.7518
158	0.3571	0.330366	8.9897
159	0.0747	0.158090	4.3018
160	0.0740	0.160194	4.3591
161	0.0726	0.438316	11.9272
162	0.0073	0.311416	8.4740



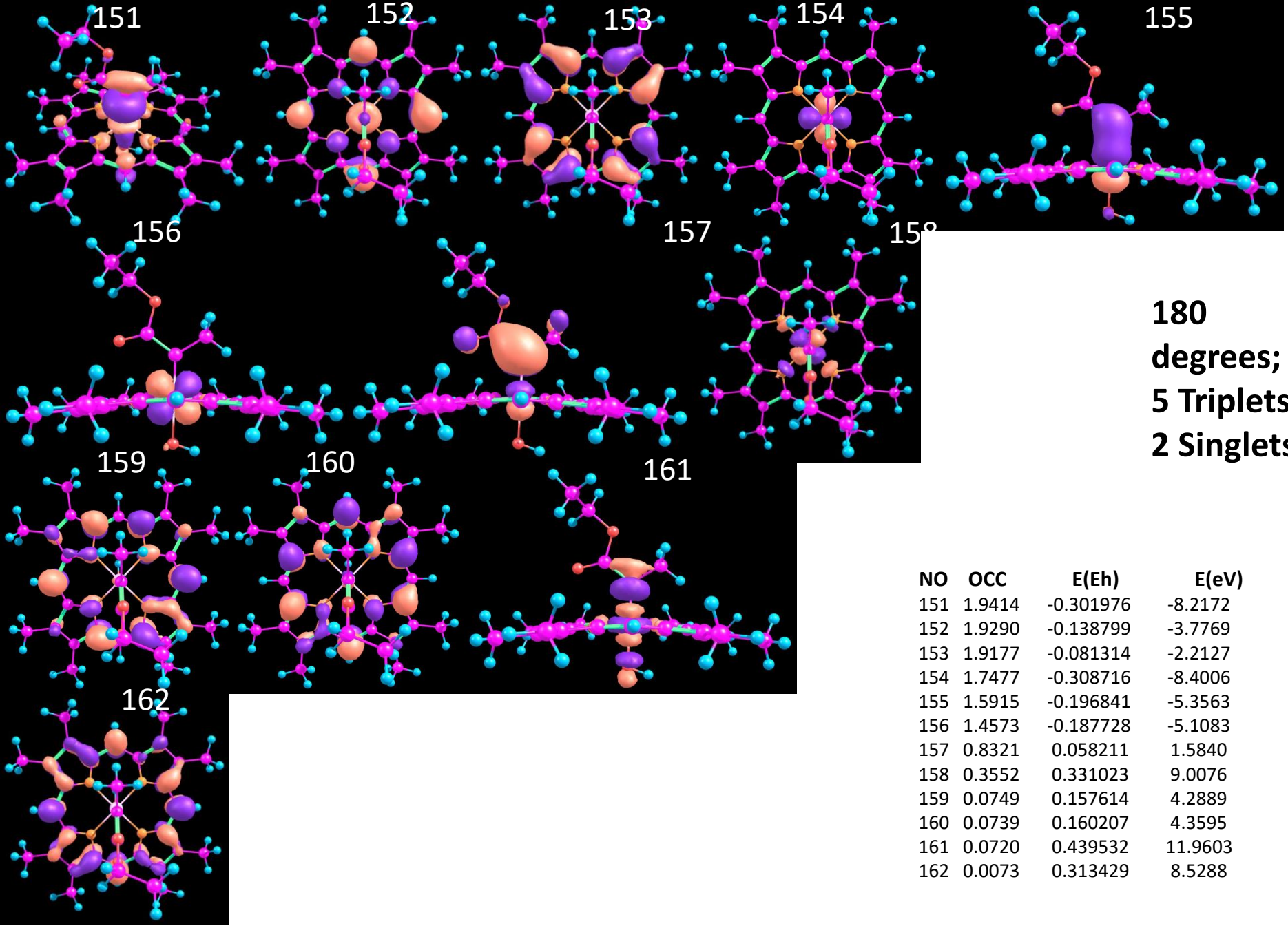






170 degrees; 5 Triplets, 2 Singlets

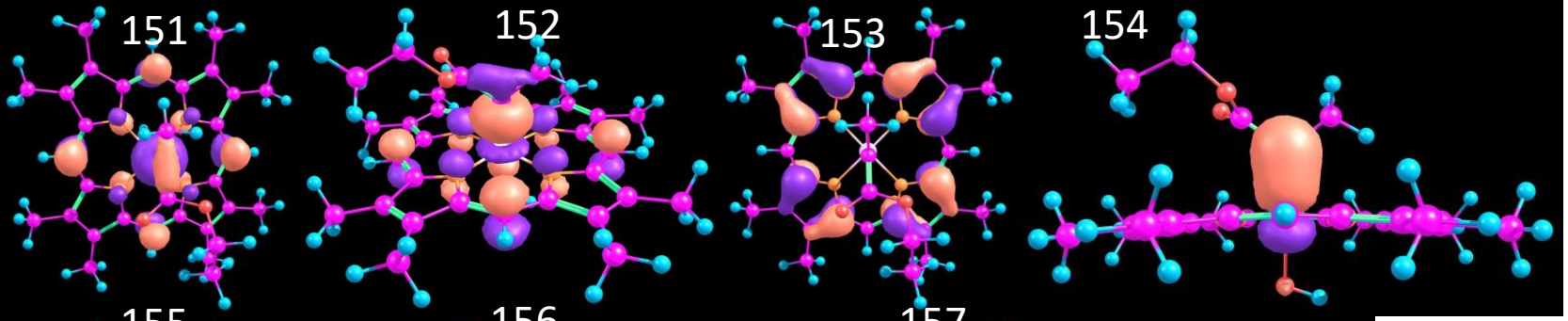
NO	OCC	E(Eh)	E(eV)
151	1.9409	-0.297401	-8.0927
152	1.9286	-0.142800	-3.8858
153	1.9179	-0.081762	-2.2249
154	1.7462	-0.307762	-8.3746
155	1.5943	-0.197098	-5.3633
156	1.4590	-0.187953	-5.1145
157	0.8273	0.064377	1.7518
158	0.3571	0.330366	8.9897
159	0.0747	0.158090	4.3018
160	0.0740	0.160194	4.3591
161	0.0726	0.438316	11.9272
162	0.0073	0.311416	8.4740

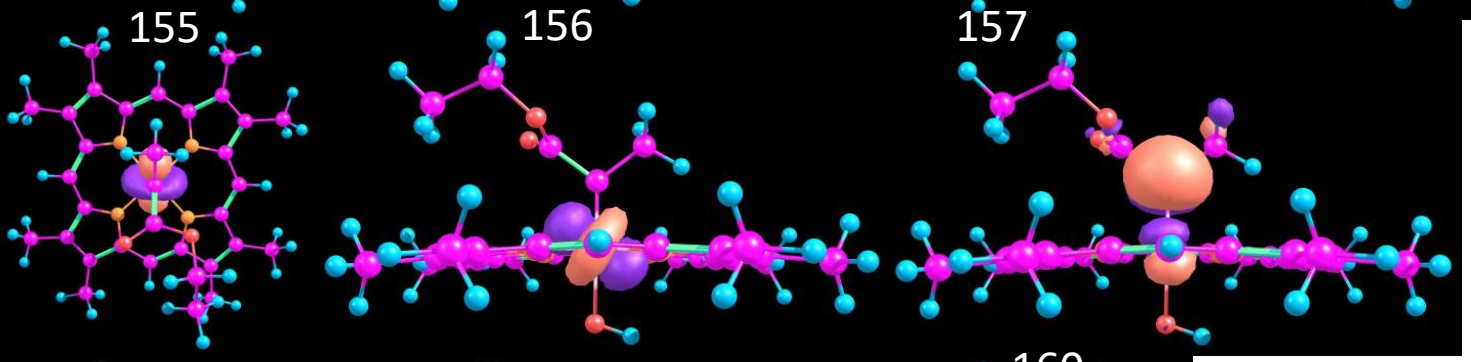


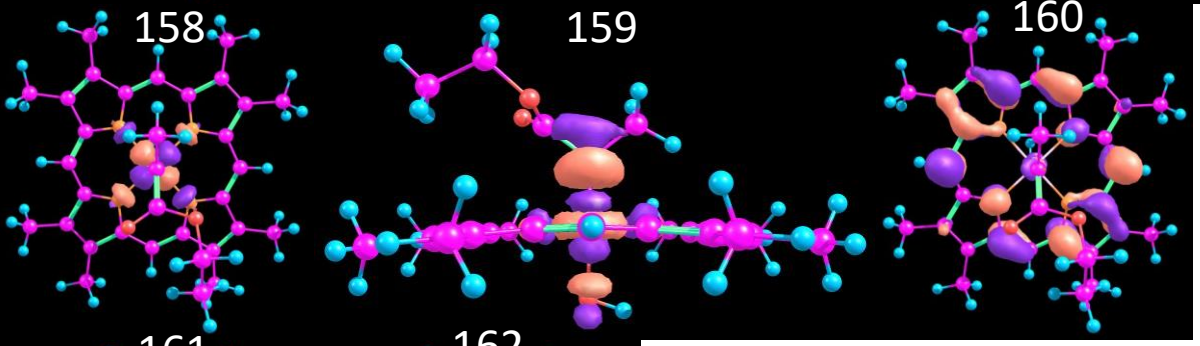
180 degrees; 5 Triplets, 2 Singlets

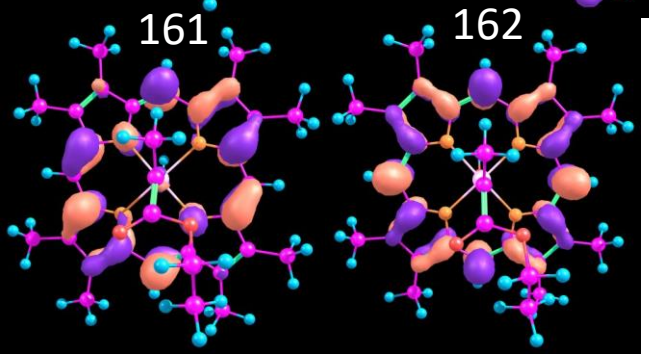
NO	OCC	E(Eh)	E(eV)
151	1.9414	-0.301976	-8.2172
152	1.9290	-0.138799	-3.7769
153	1.9177	-0.081314	-2.2127
154	1.7477	-0.308716	-8.4006
155	1.5915	-0.196841	-5.3563
156	1.4573	-0.187728	-5.1083
157	0.8321	0.058211	1.5840
158	0.3552	0.331023	9.0076
159	0.0749	0.157614	4.2889
160	0.0739	0.160207	4.3595
161	0.0720	0.439532	11.9603
162	0.0073	0.313429	8.5288

Active Space for QD-NEVPT2 on RKS DFT Geometries;Relaxed Scan of Fe-C: Thiolate



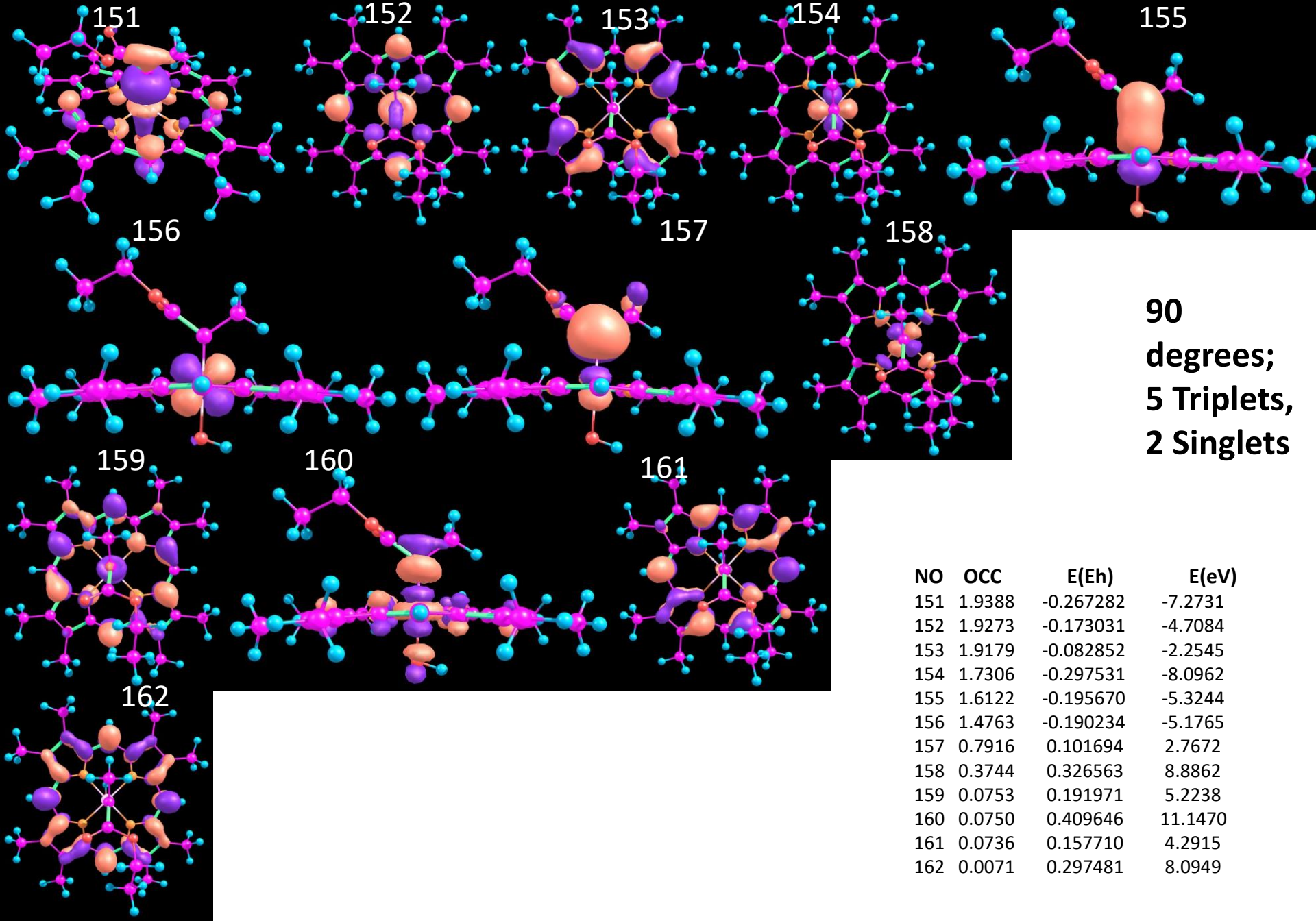






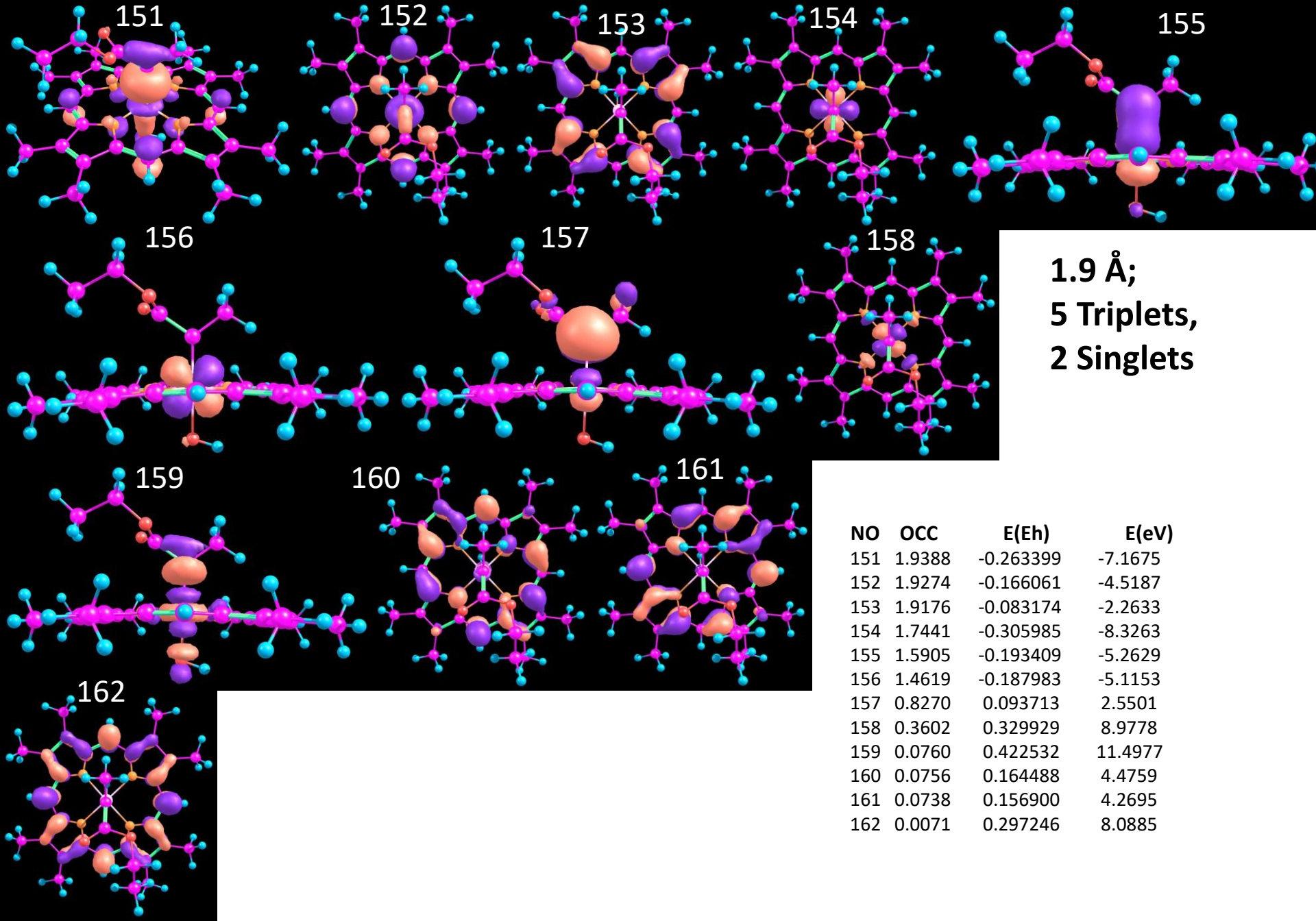
1.7 Å;
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9383	-0.241656	-6.5758
152	1.9271	-0.223805	-6.0900
153	1.9211	-0.082340	-2.2406
154	1.6574	-0.192027	-5.2253
155	1.6153	-0.239851	-6.5267
156	1.5928	-0.229517	-6.2455
157	0.6241	0.143416	3.9026
158	0.4976	0.279530	7.6064
159	0.0741	0.470441	12.8014
160	0.0733	0.165504	4.5036
161	0.0716	0.165066	4.4917
162	0.0072	0.298508	8.1228



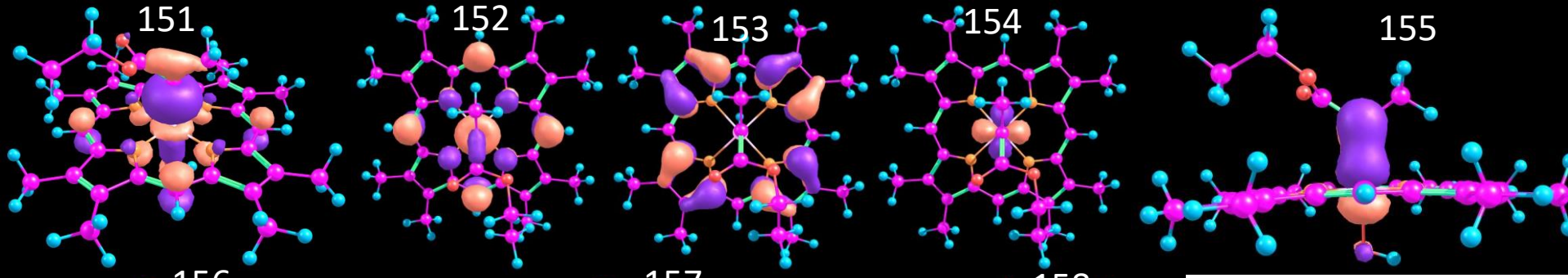
90 degrees; 5 Triplets, 2 Singlets

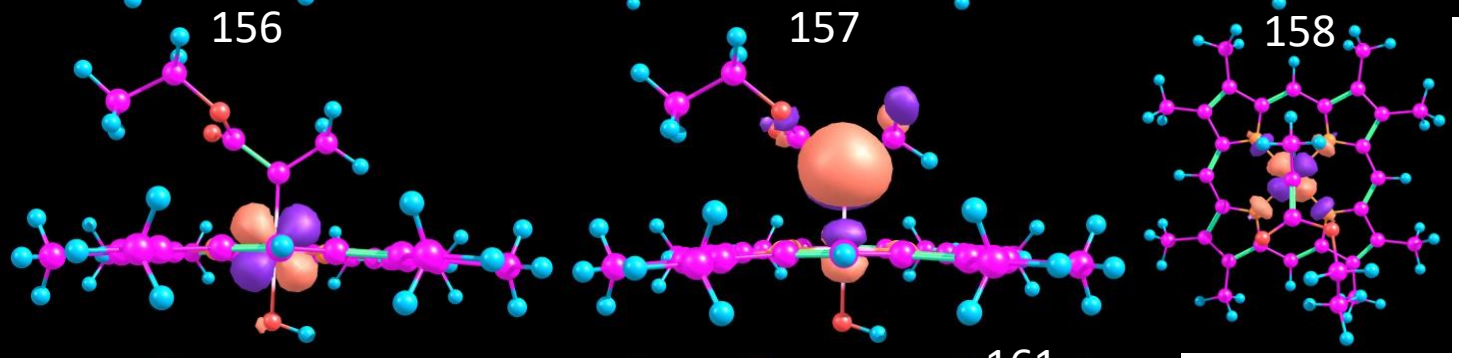
NO	OCC	E(Eh)	E(eV)
151	1.9388	-0.267282	-7.2731
152	1.9273	-0.173031	-4.7084
153	1.9179	-0.082852	-2.2545
154	1.7306	-0.297531	-8.0962
155	1.6122	-0.195670	-5.3244
156	1.4763	-0.190234	-5.1765
157	0.7916	0.101694	2.7672
158	0.3744	0.326563	8.8862
159	0.0753	0.191971	5.2238
160	0.0750	0.409646	11.1470
161	0.0736	0.157710	4.2915
162	0.0071	0.297481	8.0949

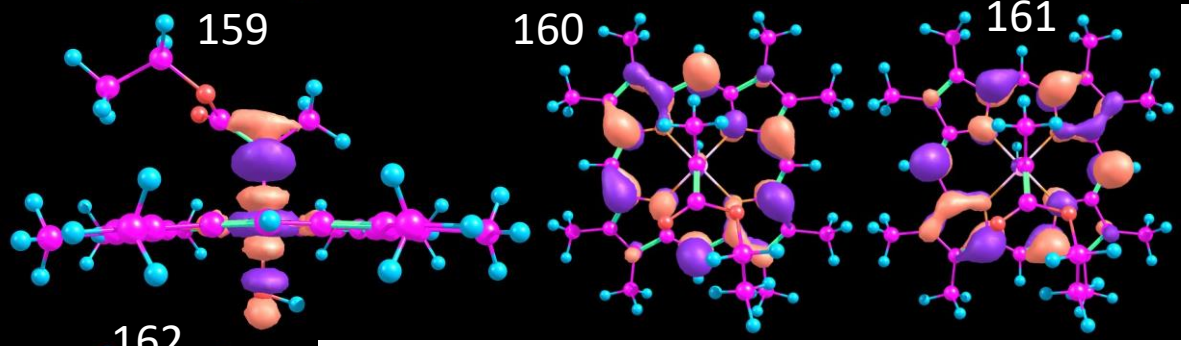


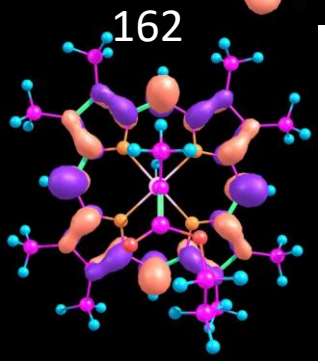
1.9 Å;
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9388	-0.263399	-7.1675
152	1.9274	-0.166061	-4.5187
153	1.9176	-0.083174	-2.2633
154	1.7441	-0.305985	-8.3263
155	1.5905	-0.193409	-5.2629
156	1.4619	-0.187983	-5.1153
157	0.8270	0.093713	2.5501
158	0.3602	0.329929	8.9778
159	0.0760	0.422532	11.4977
160	0.0756	0.164488	4.4759
161	0.0738	0.156900	4.2695
162	0.0071	0.297246	8.0885



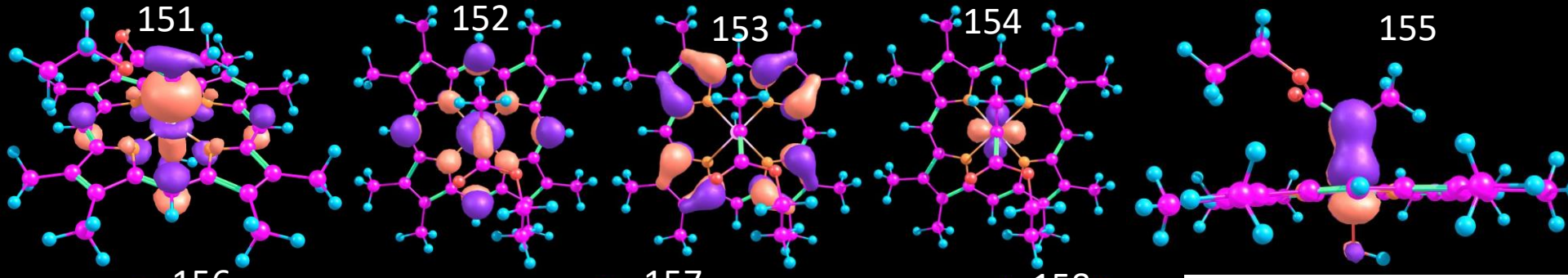


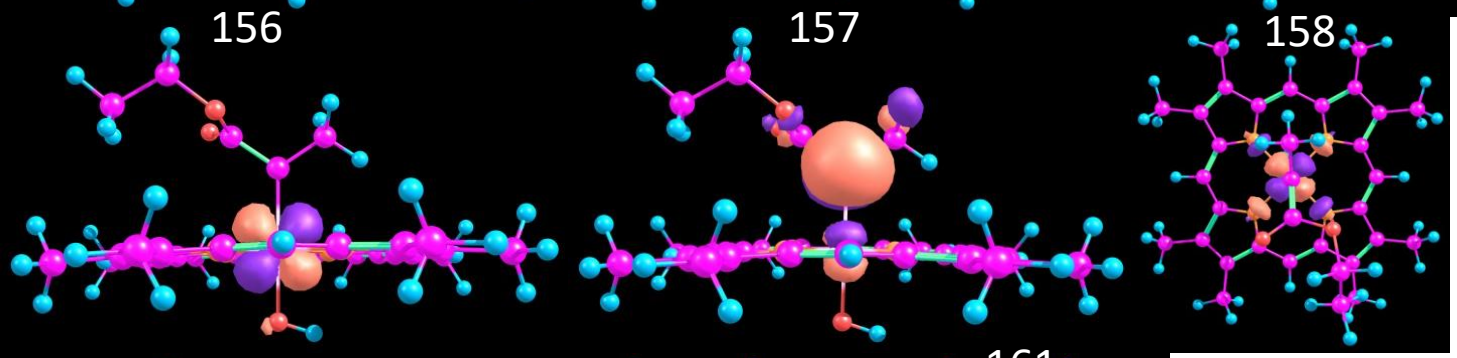


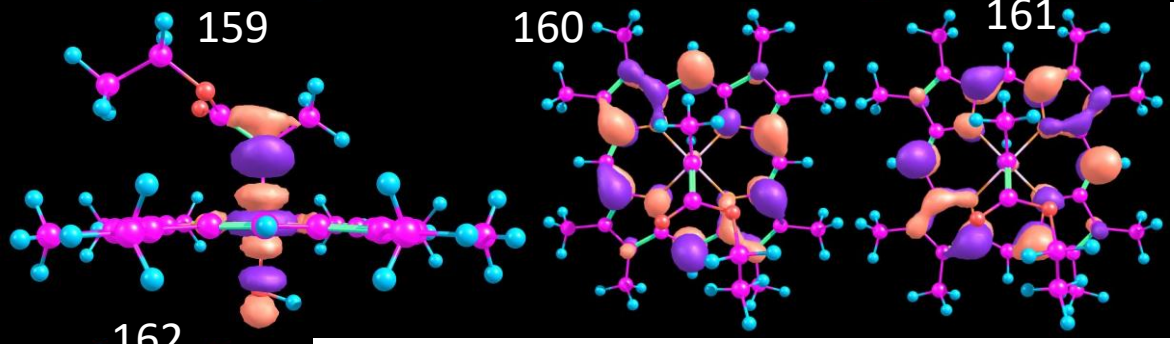


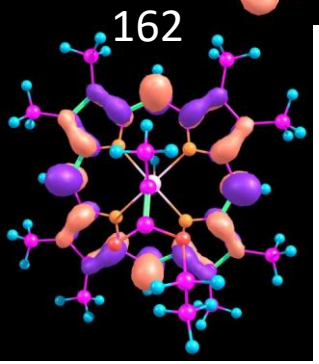
2.0 Å;
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9383	-0.250549	-6.8178
152	1.9273	-0.162491	-4.4216
153	1.9170	-0.083707	-2.2778
154	1.7521	-0.313853	-8.5404
155	1.5575	-0.189790	-5.1644
156	1.4525	-0.189283	-5.1506
157	0.8686	0.086636	2.3575
158	0.3510	0.329772	8.9736
159	0.0781	0.409324	11.1383
160	0.0762	0.154324	4.1994
161	0.0741	0.156072	4.2469
162	0.0071	0.296473	8.0674



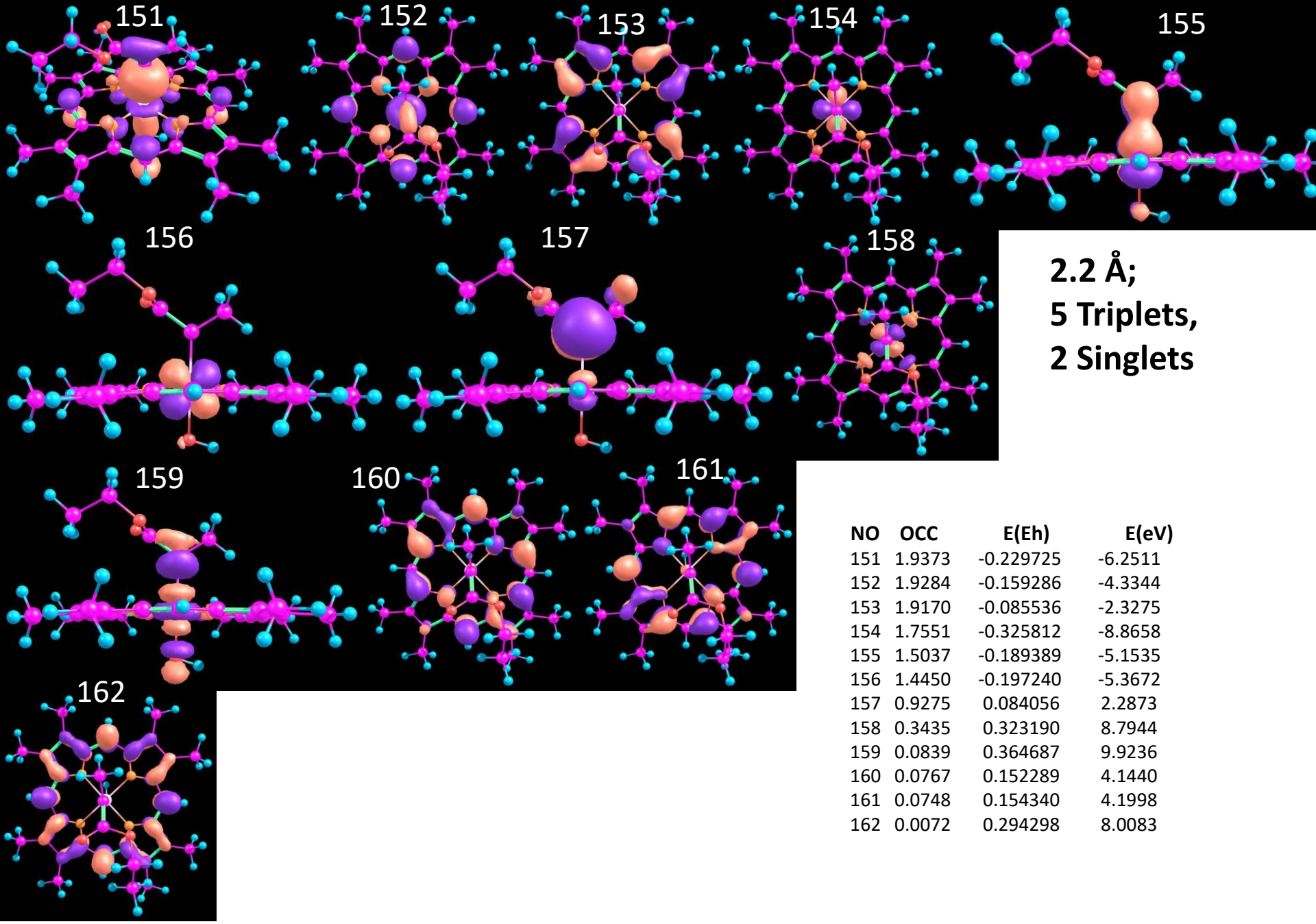






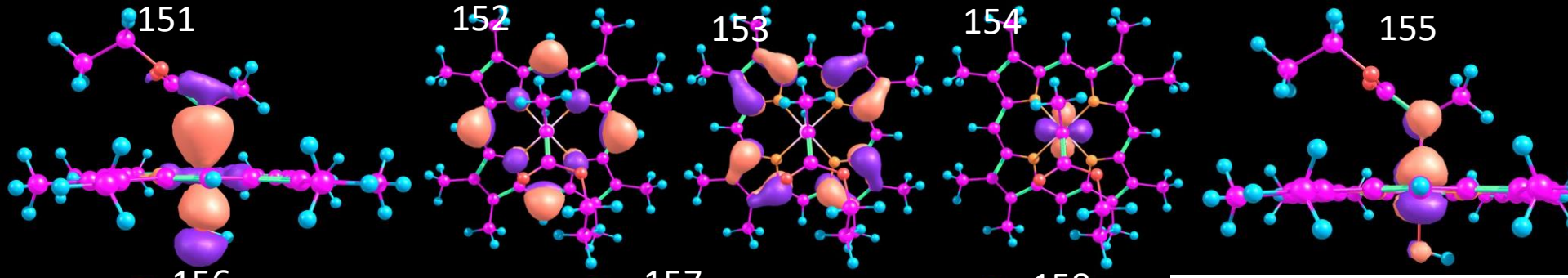
2.1 Å;
5 Triplets,
2 Singlets

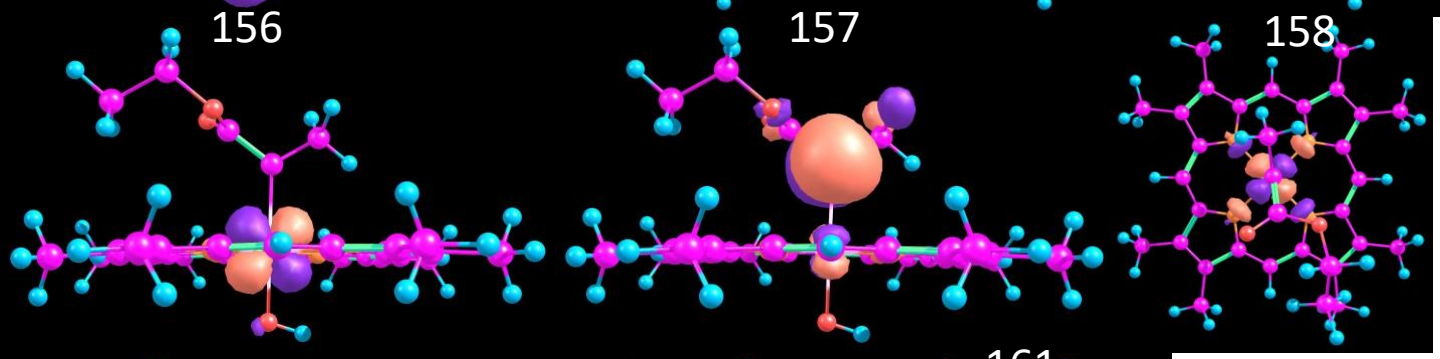
NO	OCC	E(Eh)	E(eV)
151	1.9375	-0.234746	-6.3878
152	1.9273	-0.163978	-4.4621
153	1.9168	-0.084385	-2.2962
154	1.7547	-0.319658	-8.6983
155	1.5285	-0.188068	-5.1176
156	1.4482	-0.192501	-5.2382
157	0.9012	0.083541	2.2733
158	0.3469	0.327286	8.9059
159	0.0808	0.388038	10.5590
160	0.0765	0.153154	4.1675
161	0.0744	0.155303	4.2260
162	0.0071	0.295781	8.0486

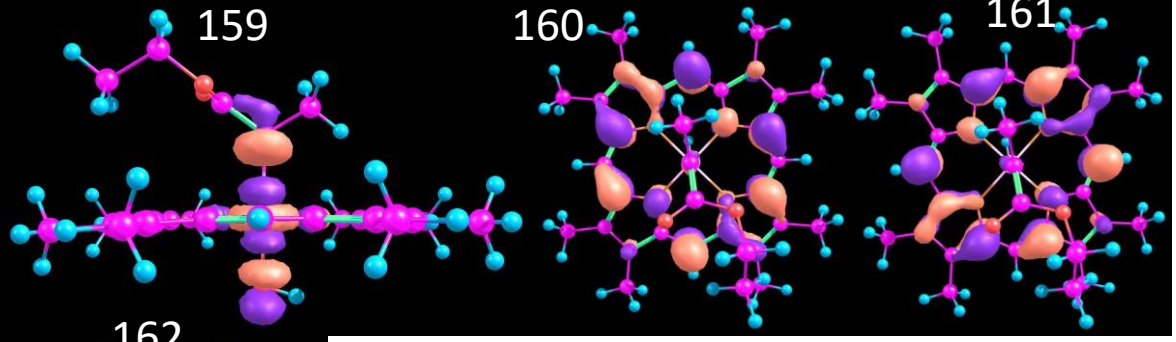


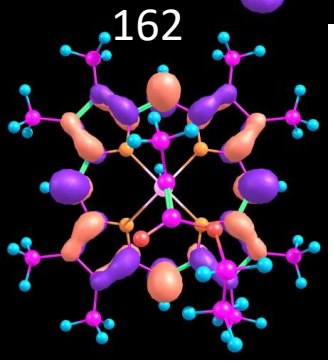
2.2 Å;
5 Triplets,
2 Singlets

NO	OCC	E(Eh)	E(eV)
151	1.9373	-0.229725	-6.2511
152	1.9284	-0.159286	-4.3344
153	1.9170	-0.085536	-2.3275
154	1.7551	-0.325812	-8.8658
155	1.5037	-0.189389	-5.1535
156	1.4450	-0.197240	-5.3672
157	0.9275	0.084056	2.2873
158	0.3435	0.323190	8.7944
159	0.0839	0.364687	9.9236
160	0.0767	0.152289	4.1440
161	0.0748	0.154340	4.1998
162	0.0072	0.294298	8.0083





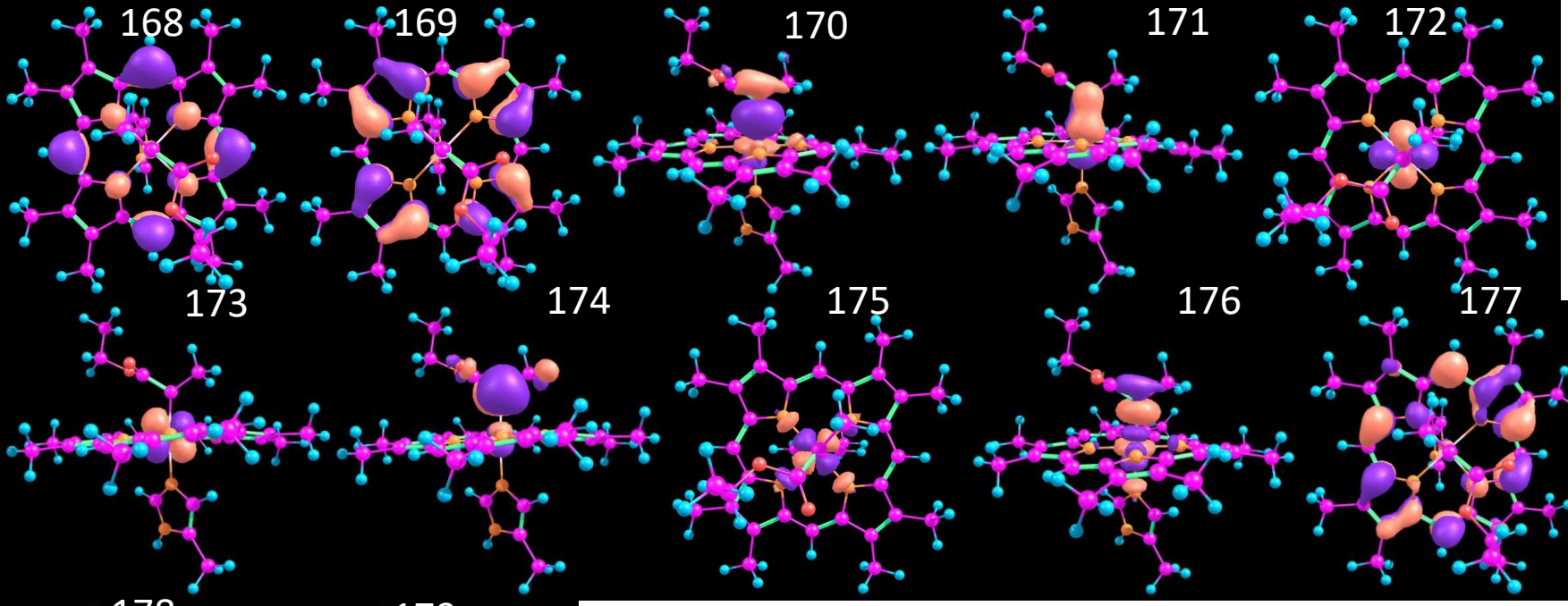




2.3 Å;
5 Triplets,
2 Singlets

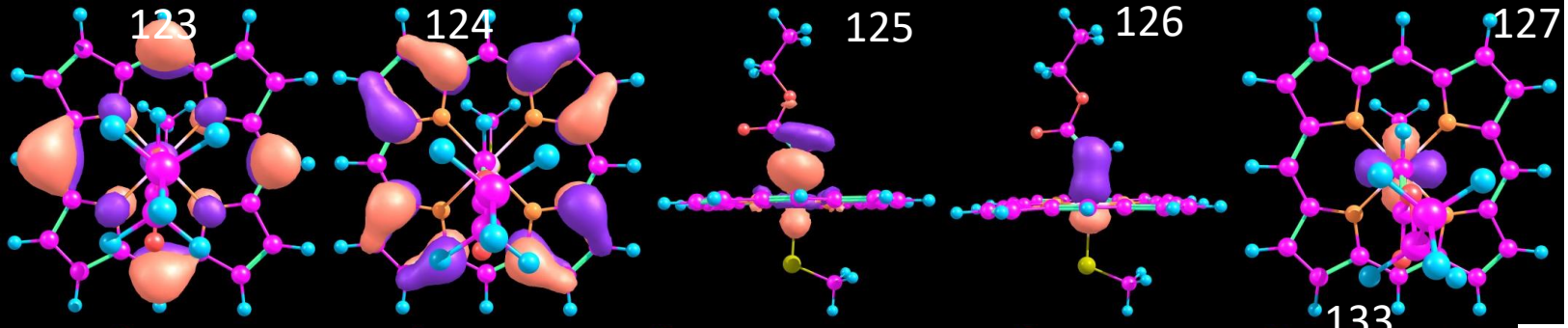
NO	OCC	E(Eh)	E(eV)
151	1.9467	-0.296052	-8.0560
152	1.9332	-0.114214	-3.1079
153	1.9179	-0.087386	-2.3779
154	1.7511	-0.337148	-9.1743
155	1.4748	-0.198536	-5.4024
156	1.4405	-0.208327	-5.6689
157	0.9556	0.095694	2.6040
158	0.3364	0.314025	8.5451
159	0.0849	0.342405	9.3173
160	0.0766	0.151888	4.1331
161	0.0749	0.153781	4.1846
162	0.0073	0.292101	7.9485

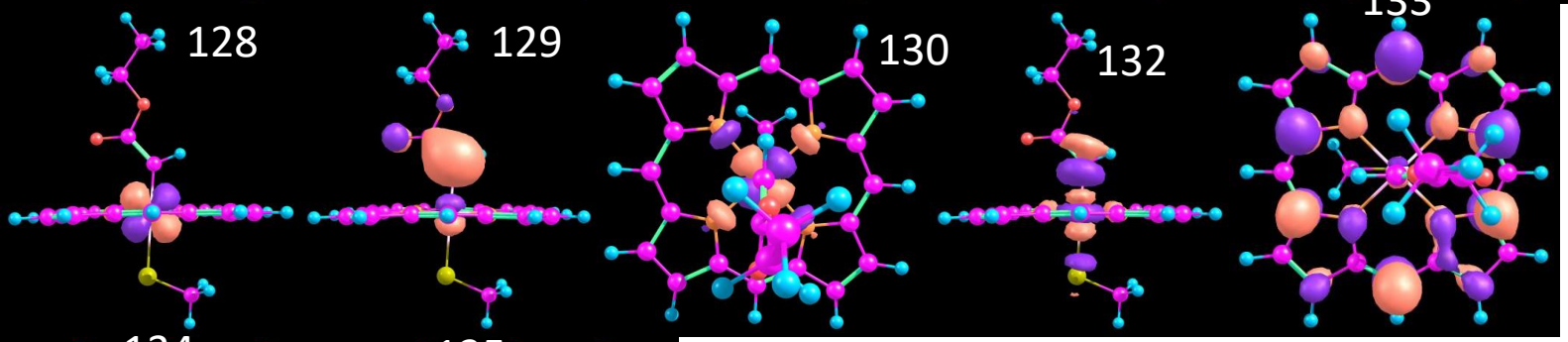
Active Space for QD-NEVPT2 on H-Opt of PDB:6CUN, Sharon et. al OSS, & Crystal of TPP Model

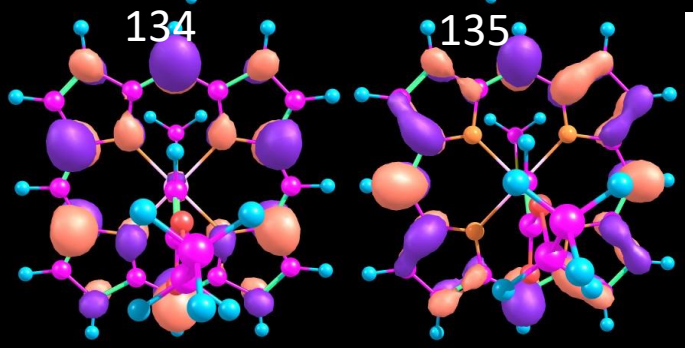


NO	OCC	E(Eh)	E(eV)
168	1.9414	-0.238322	-6.4851
169	1.9144	-0.187243	-5.0951
170	1.8561	-0.375231	-10.2106
171	1.7221	-0.357741	-9.7346
172	1.5025	-0.305789	-8.3209
173	1.2973	-0.223226	-6.0743
174	0.9009	-0.028262	-0.7690
175	0.5587	0.159223	4.3327
176	0.1515	0.255377	6.9492
177	0.0784	0.048548	1.3211
178	0.0704	0.059145	1.6094
179	0.0065	0.205071	5.5803

PDB: 6CUN H-Opt Only;
1 Quintet,
5 Triplets,
2 Singlets

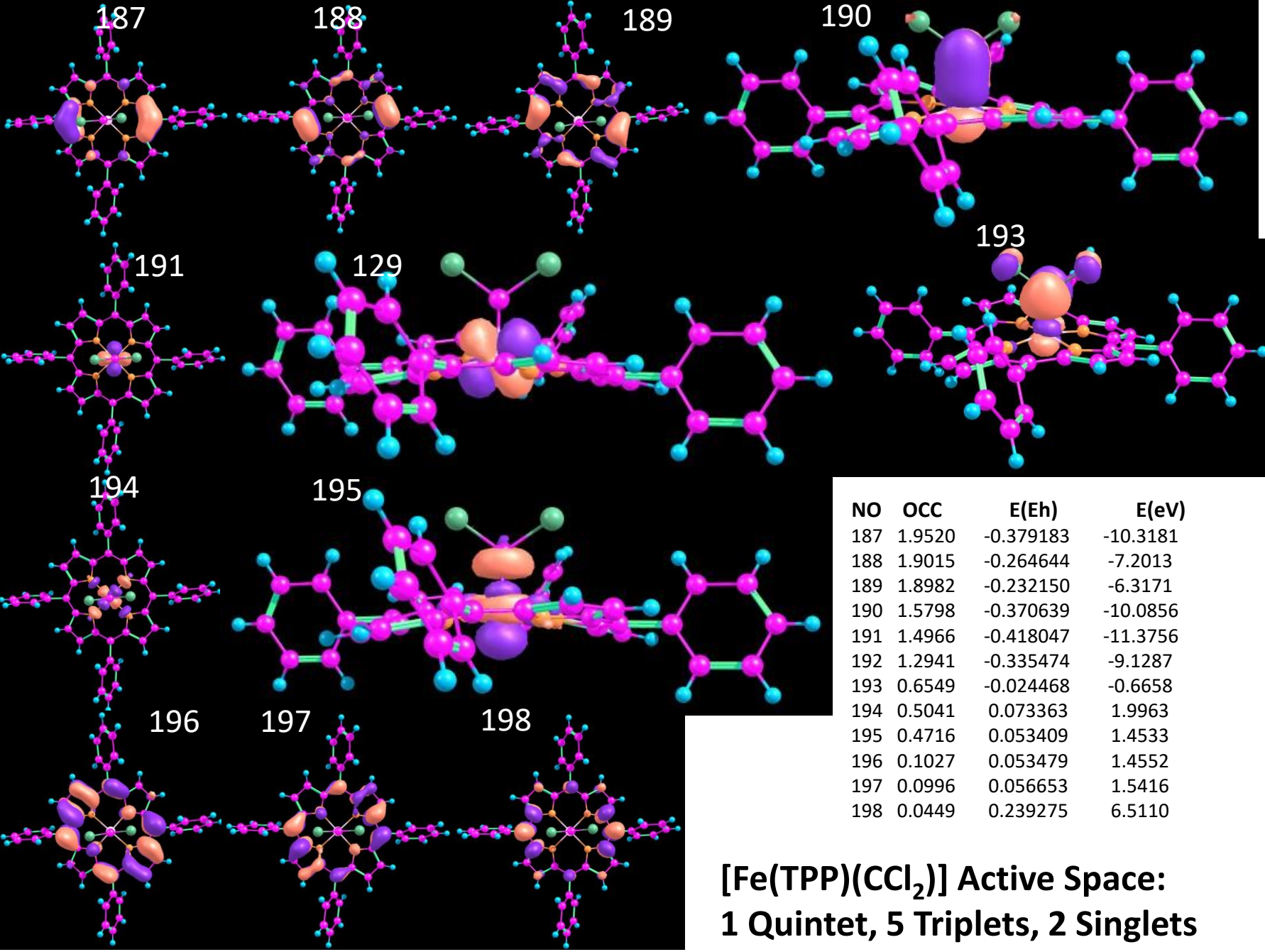






NO	OCC	E(Eh)	E(eV)
123	1.9307	-0.136450	-3.7130
124	1.9226	-0.099476	-2.7069
125	1.8833	-0.302189	-8.2230
126	1.6942	-0.261191	-7.1074
127	1.5037	-0.229484	-6.2446
128	1.2992	-0.148621	-4.0442
129	0.9221	0.007656	0.2083
130	0.5622	0.229953	6.2573
131	0.1264	0.339099	9.2273
132	0.0743	0.146733	3.9928
133	0.0734	0.143788	3.9127
134	0.0078	0.295830	8.0499

Sharon et al. BSS;
1 Quintet,
5 Triplets,
2 Singlets



NO	OCC	E(Eh)	E(eV)
187	1.9520	-0.379183	-10.3181
188	1.9015	-0.264644	-7.2013
189	1.8982	-0.232150	-6.3171
190	1.5798	-0.370639	-10.0856
191	1.4966	-0.418047	-11.3756
192	1.2941	-0.335474	-9.1287
193	0.6549	-0.024468	-0.6658
194	0.5041	0.073363	1.9963
195	0.4716	0.053409	1.4533
196	0.1027	0.053479	1.4552
197	0.0996	0.056653	1.5416
198	0.0449	0.239275	6.5110

[Fe(TPP)(CCl_2)] Active Space:
1 Quintet, 5 Triplets, 2 Singlets