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Differences between Carbon Suboxide and its Heavier Congeners as Ligands in Transition Metal Complexes: A Theoretical Study

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Supplementary Material

Tables S1-S23: The theoretical Cartesian coordinates for local minima structures (23 structures);

Complete Gaussian 09 reference (Reference 45)

Table S1. The theoretical Cartesian coordinates (in Å) for the structure **Ir1O-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.279120	1.898802	0.041580
2	15	0	-2.049084	1.038601	-0.494049
3	15	0	-0.954613	-0.648535	1.968828
4	15	0	2.088821	-1.125783	0.176569
5	6	0	3.240181	0.107773	0.893486
6	1	0	2.980707	0.220131	1.954984
7	1	0	4.275523	-0.248280	0.847624
8	6	0	3.061808	1.423071	0.149717
9	1	0	3.424543	1.326053	-0.881945
10	1	0	3.637078	2.233772	0.610117
11	6	0	-2.899223	1.166804	1.129690
12	1	0	-2.444117	2.007397	1.670702
13	1	0	-3.957056	1.415583	0.985725
14	6	0	-2.727489	-0.131289	1.905228
15	1	0	-3.277183	-0.943172	1.411678
16	1	0	-3.135234	-0.049984	2.919182
17	77	0	0.022161	-0.041409	-0.151673
18	6	0	0.135045	-0.420572	-2.194988
19	6	0	-0.459783	-1.546377	-1.603673
20	6	0	-1.110521	-2.639744	-1.851313
21	6	0	-2.142059	2.722278	-1.171936
22	1	0	-1.607509	3.427939	-0.528466
23	1	0	-1.692982	2.748656	-2.168863
24	1	0	-3.183539	3.048636	-1.248851
25	6	0	-3.211737	0.116331	-1.543828
26	1	0	-3.365666	-0.891346	-1.148966
27	1	0	-4.174134	0.633433	-1.602912
28	1	0	-2.802402	0.012728	-2.552206
29	6	0	-1.122772	-2.416703	2.389065
30	1	0	-1.842201	-2.561600	3.201542
31	1	0	-1.464216	-2.972272	1.510549
32	1	0	-0.165793	-2.839032	2.703973
33	6	0	-0.372651	0.078302	3.541891
34	1	0	0.687414	-0.146128	3.699024
35	1	0	-0.480389	1.166390	3.507406

36	1	0	-0.937371	-0.301390	4.399669
37	6	0	1.070418	3.040097	1.452418
38	1	0	0.037247	3.395833	1.516567
39	1	0	1.305644	2.523470	2.387934
40	1	0	1.728179	3.910322	1.358826
41	6	0	1.294087	3.004586	-1.404788
42	1	0	0.418252	3.656053	-1.418794
43	1	0	2.185679	3.639314	-1.392501
44	1	0	1.289190	2.400872	-2.317962
45	6	0	2.881821	-1.674488	-1.362993
46	1	0	2.972618	-0.842089	-2.065978
47	1	0	3.871025	-2.099789	-1.170136
48	1	0	2.254955	-2.432674	-1.840175
49	6	0	2.234511	-2.578245	1.256369
50	1	0	3.255161	-2.971800	1.236678
51	1	0	1.987343	-2.317098	2.289312
52	1	0	1.552945	-3.364322	0.919934
53	8	0	-1.703495	-3.645789	-2.012816
54	8	0	0.486794	0.076497	-3.239037

Table S2. The theoretical Cartesian coordinates (in Å) for the structure **Ir1O-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.461996	0.422691	0.014056
2	15	0	-0.582690	2.274688	-0.523331
3	15	0	-0.951200	0.188933	1.787611
4	15	0	0.723867	-2.236332	-0.087112
5	6	0	2.438991	-2.319552	0.566115
6	1	0	2.383874	-2.188165	1.655338
7	1	0	2.863942	-3.314173	0.388901
8	6	0	3.288879	-1.228530	-0.071995
9	1	0	3.444975	-1.447847	-1.136249
10	1	0	4.283665	-1.176343	0.384759
11	6	0	-1.189431	2.872973	1.100519
12	1	0	-0.310397	3.175537	1.685165
13	1	0	-1.816300	3.762860	0.977814
14	6	0	-1.937691	1.746555	1.798179
15	1	0	-2.875799	1.522782	1.272407
16	1	0	-2.206434	2.011900	2.826907
17	77	0	0.090997	0.033199	-0.235977
18	6	0	-1.362626	-0.575182	-1.612625
19	6	0	-2.614681	-1.059358	-1.731657
20	6	0	-3.612677	-1.319407	-0.950187
21	6	0	3.158233	1.157007	1.536260
22	1	0	2.910528	0.533906	2.400208
23	1	0	4.247254	1.249670	1.473090
24	1	0	2.736191	2.152221	1.710730
25	6	0	3.345160	1.329631	-1.300354
26	1	0	2.993249	0.994201	-2.279990
27	1	0	3.161101	2.403984	-1.224540
28	1	0	4.425501	1.164277	-1.234621
29	6	0	-2.206424	-1.036247	2.271441
30	1	0	-1.746839	-1.968390	2.605175
31	1	0	-2.802200	-0.639488	3.099926
32	1	0	-2.875287	-1.258056	1.436319
33	6	0	0.071947	0.312144	3.292372
34	1	0	-0.549251	0.393421	4.190039
35	1	0	0.702591	-0.577694	3.389582
36	1	0	0.728437	1.185229	3.238283

37	6	0	-0.194167	-3.454493	0.897468
38	1	0	-0.141093	-3.208221	1.961601
39	1	0	-1.243341	-3.468068	0.590259
40	1	0	0.225610	-4.454450	0.754759
41	6	0	0.592076	3.549162	-1.066097
42	1	0	1.422473	3.633806	-0.358956
43	1	0	0.993716	3.290521	-2.049348
44	1	0	0.099093	4.523148	-1.139428
45	6	0	-1.971757	2.468184	-1.675476
46	1	0	-1.685120	2.083880	-2.657926
47	1	0	-2.827896	1.878421	-1.337332
48	1	0	-2.263689	3.518232	-1.769058
49	6	0	0.803751	-2.995198	-1.735145
50	1	0	1.253821	-3.991196	-1.681936
51	1	0	-0.205780	-3.078973	-2.146226
52	1	0	1.375982	-2.364424	-2.419530
53	8	0	-4.611538	-1.604481	-0.378654
54	8	0	-0.406770	-0.312352	-2.398490

Table S3. The theoretical Cartesian coordinates (in Å) for the structure **Ir1S-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.279806	0.663855	0.347521
2	15	0	-0.775026	2.162565	-0.509298
3	15	0	-1.181030	0.232474	1.985531
4	15	0	0.905668	-2.167652	0.384473
5	6	0	2.576294	-1.992281	1.122671
6	1	0	2.442801	-1.767457	2.189631
7	1	0	3.128273	-2.936640	1.060210
8	6	0	3.313964	-0.860478	0.422422
9	1	0	3.541350	-1.132891	-0.616786
10	1	0	4.271481	-0.637418	0.906720
11	6	0	-1.515446	2.830862	1.032940
12	1	0	-0.699744	3.233502	1.649012
13	1	0	-2.180318	3.670140	0.798987
14	6	0	-2.251762	1.720123	1.767734
15	1	0	-3.126975	1.395833	1.188799
16	1	0	-2.626242	2.059598	2.740197
17	77	0	0.087582	0.007200	-0.041661
18	6	0	0.116354	-0.344583	-2.105320
19	6	0	-1.107389	-0.815304	-1.694465
20	6	0	-2.300694	-1.265682	-1.533199
21	6	0	0.276446	3.514199	-1.115242
22	1	0	1.047386	3.766123	-0.381153
23	1	0	0.760469	3.224343	-2.051793
24	1	0	-0.327079	4.408375	-1.298129
25	6	0	-2.143825	2.143048	-1.703392
26	1	0	-2.923533	1.444623	-1.387857
27	1	0	-2.572016	3.143946	-1.811427
28	1	0	-1.778904	1.804428	-2.676790
29	6	0	-2.425468	-1.023594	2.436085
30	1	0	-3.142227	-0.608390	3.151718
31	1	0	-2.969018	-1.356005	1.545288
32	1	0	-1.957712	-1.896788	2.895999
33	6	0	-0.364592	0.550298	3.591239
34	1	0	0.313126	-0.272076	3.842919
35	1	0	0.228175	1.468603	3.544992

36	1	0	-1.098541	0.649251	4.397720
37	6	0	2.697701	1.553240	1.885937
38	1	0	2.122325	2.482892	1.948723
39	1	0	2.448059	0.944420	2.759930
40	1	0	3.762838	1.803588	1.922924
41	6	0	3.134727	1.620580	-0.937748
42	1	0	2.890786	2.682585	-0.873329
43	1	0	4.218324	1.512672	-0.828377
44	1	0	2.830813	1.247221	-1.923672
45	6	0	1.145138	-3.180422	-1.102497
46	1	0	1.779900	-2.657030	-1.822166
47	1	0	1.594932	-4.144897	-0.849142
48	1	0	0.180723	-3.354283	-1.587436
49	6	0	0.030917	-3.289542	1.513554
50	1	0	0.545510	-4.253116	1.575153
51	1	0	-0.018956	-2.858473	2.517826
52	1	0	-0.988796	-3.462433	1.157320
53	16	0	1.014802	-0.121080	-3.438558
54	16	0	-3.763331	-1.784548	-1.254307

Table S4. The theoretical Cartesian coordinates (in Å) for the structure **Ir1S-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.657244	-0.120931	-0.018082
2	15	0	0.140060	2.368891	-0.444255
3	15	0	-0.563763	0.413330	1.912550
4	15	0	0.374769	-2.337737	0.009217
5	6	0	2.046897	-2.765272	0.640575
6	1	0	2.053878	-2.569835	1.721700
7	1	0	2.242600	-3.835896	0.510783
8	6	0	3.093988	-1.916016	-0.067191
9	1	0	3.155993	-2.196279	-1.126665
10	1	0	4.092508	-2.072151	0.355987
11	6	0	-0.035901	3.064794	1.242770
12	1	0	0.954972	3.052456	1.717309
13	1	0	-0.362218	4.109892	1.202669
14	6	0	-1.019623	2.198032	2.014874
15	1	0	-2.026441	2.288428	1.585248
16	1	0	-1.096142	2.500863	3.065113
17	77	0	0.276051	0.018484	-0.210914
18	6	0	-1.460474	-0.197677	-1.349532
19	6	0	-2.764044	-0.329241	-1.159947
20	6	0	-3.946872	-0.407295	-0.688318
21	6	0	3.575251	0.488661	1.440545
22	1	0	3.263805	-0.053041	2.338289
23	1	0	4.654552	0.357521	1.313855
24	1	0	3.375005	1.552698	1.603140
25	6	0	3.660997	0.518991	-1.400334
26	1	0	3.206139	0.230335	-2.351872
27	1	0	3.723414	1.609008	-1.371812
28	1	0	4.679501	0.119508	-1.356230
29	6	0	-2.124222	-0.376711	2.412968
30	1	0	-1.964330	-1.400700	2.754723
31	1	0	-2.574598	0.188576	3.234992
32	1	0	-2.823888	-0.395928	1.571105
33	6	0	0.510030	0.172452	3.366986
34	1	0	-0.037336	0.367235	4.294626
35	1	0	0.889766	-0.853745	3.400067
36	1	0	1.368201	0.848966	3.319045

37	6	0	-0.765078	-3.216062	1.117741
38	1	0	-0.588125	-2.931733	2.158939
39	1	0	-1.798894	-2.972462	0.857502
40	1	0	-0.627181	-4.297578	1.029955
41	6	0	1.502029	3.300534	-1.200240
42	1	0	2.412506	3.200869	-0.601647
43	1	0	1.700668	2.917588	-2.205051
44	1	0	1.251816	4.362822	-1.273869
45	6	0	-1.327287	2.954212	-1.335467
46	1	0	-1.295583	2.598208	-2.368535
47	1	0	-2.233765	2.546155	-0.880508
48	1	0	-1.373020	4.046916	-1.331515
49	6	0	0.213953	-3.266494	-1.541341
50	1	0	0.356033	-4.335655	-1.357155
51	1	0	-0.780301	-3.105633	-1.965649
52	1	0	0.939527	-2.919539	-2.280216
53	16	0	-0.325339	-0.153046	-2.611292
54	16	0	-5.429507	-0.507696	-0.149954

Table S5. The theoretical Cartesian coordinates (in Å) for the structure **Ir1Se-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.594970	-0.440251	0.193385
2	15	0	-0.183972	-0.231148	-2.356970
3	15	0	0.695523	-2.401348	-0.201346
4	15	0	-0.329103	-0.156821	2.368001
5	6	0	-1.992897	-0.718509	2.902607
6	1	0	-1.999826	-1.816237	2.868984
7	1	0	-2.183340	-0.428691	3.941910
8	6	0	-3.037738	-0.140517	1.958504
9	1	0	-3.102788	0.948864	2.080288
10	1	0	-4.036924	-0.541492	2.163360
11	6	0	0.146283	-1.953235	-2.895672
12	1	0	-0.803207	-2.504139	-2.842175
13	1	0	0.470719	-1.973370	-3.942226
14	6	0	1.183179	-2.578945	-1.972813
15	1	0	2.151646	-2.072405	-2.084742
16	1	0	1.351273	-3.635055	-2.212905
17	77	0	-0.289034	-0.213870	0.009276
18	6	0	-0.061201	1.863282	-0.088783
19	6	0	1.219319	1.396725	0.057708
20	6	0	2.479083	1.165762	0.174231
21	6	0	-1.596461	0.305466	-3.362205
22	1	0	-2.458702	-0.345506	-3.190407
23	1	0	-1.872308	1.329960	-3.095597
24	1	0	-1.345677	0.274738	-4.426473
25	6	0	1.198147	0.741232	-3.020093
26	1	0	2.146079	0.403889	-2.591790
27	1	0	1.240471	0.660385	-4.110248
28	1	0	1.070774	1.791824	-2.743109
29	6	0	2.272624	-2.769900	0.634866
30	1	0	2.780921	-3.606313	0.144635
31	1	0	2.926262	-1.891094	0.603417
32	1	0	2.111414	-3.039090	1.680855
33	6	0	-0.267827	-3.924322	0.108066
34	1	0	-0.616925	-3.950275	1.145472
35	1	0	-1.146723	-3.957680	-0.541913
36	1	0	0.335736	-4.819646	-0.073455

37	6	0	-3.379618	-2.044762	-0.181179
38	1	0	-3.201342	-2.319766	-1.226258
39	1	0	-2.952827	-2.828492	0.450729
40	1	0	-4.461199	-2.006164	-0.015530
41	6	0	-3.662772	0.754204	-0.662763
42	1	0	-3.829346	0.463112	-1.701914
43	1	0	-4.636294	0.810528	-0.165485
44	1	0	-3.188301	1.744360	-0.644953
45	6	0	-0.133075	1.497256	3.088336
46	1	0	-0.891081	2.179083	2.694220
47	1	0	-0.208113	1.457055	4.178914
48	1	0	0.843662	1.903899	2.811559
49	6	0	0.835404	-1.162251	3.332688
50	1	0	0.701197	-0.989323	4.404569
51	1	0	0.682338	-2.226719	3.132228
52	1	0	1.861695	-0.897707	3.062037
53	34	0	4.151511	0.796832	0.316729
54	34	0	-0.931230	3.385639	-0.344826

Table S6. The theoretical Cartesian coordinates (in Å) for the structure **Ir1Se-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.985192	-0.182884	0.112132
2	15	0	0.553798	2.367290	-0.341108
3	15	0	-0.176451	0.483214	2.065481
4	15	0	0.640255	-2.333090	0.216398
5	6	0	2.311717	-2.790367	0.830124
6	1	0	2.344438	-2.564736	1.905083
7	1	0	2.475617	-3.869159	0.727721
8	6	0	3.366552	-1.989699	0.079275
9	1	0	3.386331	-2.287104	-0.977358
10	1	0	4.371513	-2.171026	0.476893
11	6	0	0.517104	3.093327	1.343389
12	1	0	1.530246	3.027909	1.762626
13	1	0	0.252060	4.155842	1.303930
14	6	0	-0.474742	2.302156	2.184141
15	1	0	-1.497882	2.474365	1.825181
16	1	0	-0.456659	2.610178	3.235432
17	77	0	0.610282	0.017461	-0.073566
18	6	0	-1.176969	-0.145365	-1.133300
19	6	0	-2.475220	-0.200071	-0.894420
20	6	0	-3.681244	-0.209797	-0.480022
21	6	0	3.903079	0.401932	1.581493
22	1	0	3.584223	-0.150354	2.470310
23	1	0	4.982288	0.266787	1.459091
24	1	0	3.705911	1.464426	1.758186
25	6	0	4.037100	0.415470	-1.254139
26	1	0	3.596939	0.139279	-2.216194
27	1	0	4.141956	1.502166	-1.228554
28	1	0	5.038278	-0.021873	-1.183234
29	6	0	-1.795498	-0.169572	2.575215
30	1	0	-1.729845	-1.213458	2.886264
31	1	0	-2.176936	0.412764	3.420132
32	1	0	-2.504584	-0.100622	1.743966
33	6	0	0.882097	0.136618	3.511094
34	1	0	0.348526	0.341439	4.444578
35	1	0	1.196308	-0.912408	3.516926
36	1	0	1.781480	0.758484	3.480754

37	6	0	-0.496978	-3.113713	1.398188
38	1	0	-0.296742	-2.761578	2.414628
39	1	0	-1.529577	-2.864507	1.137923
40	1	0	-0.382807	-4.201335	1.383363
41	6	0	1.907821	3.225733	-1.192184
42	1	0	2.838929	3.119517	-0.627541
43	1	0	2.051382	2.796433	-2.187373
44	1	0	1.687360	4.291966	-1.296816
45	6	0	-0.938489	3.024644	-1.138225
46	1	0	-0.988631	2.672856	-2.171895
47	1	0	-1.836478	2.665276	-0.628560
48	1	0	-0.925509	4.118669	-1.130493
49	6	0	0.406100	-3.338150	-1.276071
50	1	0	0.501229	-4.401151	-1.033987
51	1	0	-0.587804	-3.152276	-1.691535
52	1	0	1.131802	-3.068559	-2.047017
53	34	0	-5.306973	-0.218296	0.088442
54	34	0	-0.011309	-0.172867	-2.584583

Table S7. The theoretical Cartesian coordinates (in Å) for the structure **Ir2O-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.023773	-0.143400	2.387930
2	15	0	-0.023773	-0.143400	-2.387930
3	6	0	-1.535103	-0.919547	-3.036467
4	6	0	-2.091571	-0.506148	-4.255404
5	6	0	-2.119565	-1.987805	-2.344633
6	6	0	-3.210613	-1.156799	-4.774779
7	1	0	-1.659611	0.338325	-4.791942
8	6	0	-3.232132	-2.641025	-2.869086
9	1	0	-1.722033	-2.286526	-1.376797
10	6	0	-3.779896	-2.228312	-4.085095
11	1	0	-3.637946	-0.822624	-5.717082
12	1	0	-3.681491	-3.463438	-2.318464
13	1	0	-4.654480	-2.732695	-4.488415
14	6	0	-0.023773	1.532696	-3.070634
15	6	0	1.119971	2.078632	-3.665506
16	6	0	-1.167239	2.326965	-2.889411
17	6	0	1.111484	3.405169	-4.100192
18	1	0	2.015583	1.470876	-3.790603
19	6	0	-1.169830	3.646672	-3.333414
20	1	0	-2.036618	1.908257	-2.381033
21	6	0	-0.032456	4.187595	-3.939992
22	1	0	2.001651	3.826093	-4.561189
23	1	0	-2.056302	4.259505	-3.191154
24	1	0	-0.035928	5.221208	-4.277737
25	6	0	-0.023773	1.532696	3.070634
26	6	0	1.119971	2.078632	3.665506
27	6	0	-1.167239	2.326965	2.889411
28	6	0	1.111484	3.405169	4.100192
29	1	0	2.015583	1.470876	3.790603
30	6	0	-1.169830	3.646672	3.333414
31	1	0	-2.036618	1.908257	2.381033
32	6	0	-0.032456	4.187595	3.939992
33	1	0	2.001651	3.826093	4.561189
34	1	0	-2.056302	4.259505	3.191154
35	1	0	-0.035928	5.221208	4.277737
36	6	0	-1.535103	-0.919547	3.036467

37	6	0	-2.091571	-0.506148	4.255404
38	6	0	-2.119565	-1.987805	2.344633
39	6	0	-3.210613	-1.156799	4.774779
40	1	0	-1.659611	0.338325	4.791942
41	6	0	-3.232132	-2.641025	2.869086
42	1	0	-1.722033	-2.286526	1.376797
43	6	0	-3.779896	-2.228312	4.085095
44	1	0	-3.637946	-0.822624	5.717082
45	1	0	-3.681491	-3.463438	2.318464
46	1	0	-4.654480	-2.732695	4.488415
47	6	0	1.334868	-1.003450	-3.246974
48	6	0	1.219719	-1.303788	-4.613865
49	6	0	2.512879	-1.339172	-2.567805
50	6	0	2.264485	-1.929928	-5.288029
51	1	0	0.305536	-1.054735	-5.151396
52	6	0	3.558985	-1.965377	-3.247858
53	1	0	2.619875	-1.099618	-1.511492
54	6	0	3.437552	-2.262358	-4.604977
55	1	0	2.162617	-2.162582	-6.345065
56	1	0	4.469421	-2.219367	-2.711029
57	1	0	4.252538	-2.753682	-5.131279
58	6	0	1.334868	-1.003450	3.246974
59	6	0	1.219719	-1.303788	4.613865
60	6	0	2.512879	-1.339172	2.567805
61	6	0	2.264485	-1.929928	5.288029
62	1	0	0.305536	-1.054735	5.151396
63	6	0	3.558985	-1.965377	3.247858
64	1	0	2.619875	-1.099618	1.511492
65	6	0	3.437552	-2.262358	4.604977
66	1	0	2.162617	-2.162582	6.345065
67	1	0	4.469421	-2.219367	2.711029
68	1	0	4.252538	-2.753682	5.131279
69	77	0	0.123138	-0.170217	0.000000
70	6	0	0.890115	1.842796	0.000000
71	6	0	0.639732	3.113190	0.000000
72	6	0	1.906493	0.901041	0.000000
73	17	0	-2.387406	0.441294	0.000000
74	6	0	0.443500	-1.998606	0.000000
75	8	0	0.730015	-3.132597	0.000000
76	8	0	3.101201	0.712836	0.000000
77	8	0	0.353752	4.255980	0.000000

Table S8. The theoretical Cartesian coordinates (in Å) for the structure **Ir2S-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.390982	-0.216620	-0.074201
2	15	0	2.384281	-0.228712	-0.063179
3	6	0	3.029982	-1.278615	-1.404731
4	6	0	4.318459	-1.059458	-1.916234
5	6	0	2.285388	-2.365002	-1.877068
6	6	0	4.853638	-1.922666	-2.870491
7	1	0	4.897163	-0.197756	-1.584875
8	6	0	2.825452	-3.232377	-2.824544
9	1	0	1.267214	-2.513770	-1.526232
10	6	0	4.111679	-3.016898	-3.319848
11	1	0	5.850249	-1.738274	-3.263896
12	1	0	2.234063	-4.070499	-3.184351
13	1	0	4.530857	-3.691080	-4.062775
14	6	0	3.005532	1.432973	-0.415310
15	6	0	3.363061	2.281963	0.642589
16	6	0	3.021661	1.915135	-1.732805
17	6	0	3.778593	3.585439	0.380319
18	1	0	3.314660	1.919922	1.669452
19	6	0	3.448084	3.216850	-1.987872
20	1	0	2.685442	1.275696	-2.547401
21	6	0	3.831588	4.051082	-0.935519
22	1	0	4.055011	4.237964	1.204456
23	1	0	3.465139	3.584164	-3.010768
24	1	0	4.157740	5.068381	-1.138854
25	6	0	-2.998999	1.456174	-0.393286
26	6	0	-3.336296	2.285026	0.687027
27	6	0	-3.013202	1.970526	-1.698500
28	6	0	-3.726388	3.602814	0.459831
29	1	0	-3.289437	1.896921	1.704444
30	6	0	-3.416021	3.286387	-1.918600
31	1	0	-2.694584	1.345065	-2.530974
32	6	0	-3.775995	4.102044	-0.843636
33	1	0	-3.985573	4.239847	1.301373
34	1	0	-3.431713	3.679493	-2.931945
35	1	0	-4.081782	5.130606	-1.020271
36	6	0	-3.032954	-1.241582	-1.435783

37	6	0	-4.309884	-1.001042	-1.965927
38	6	0	-2.296212	-2.335647	-1.903209
39	6	0	-4.841162	-1.850424	-2.934950
40	1	0	-4.882454	-0.134290	-1.637088
41	6	0	-2.832505	-3.188941	-2.865138
42	1	0	-1.286452	-2.501558	-1.535995
43	6	0	-4.107273	-2.951771	-3.380009
44	1	0	-5.828755	-1.649765	-3.342921
45	1	0	-2.247183	-4.033045	-3.220815
46	1	0	-4.523694	-3.614868	-4.134461
47	6	0	3.313057	-0.763960	1.410642
48	6	0	4.708380	-0.603213	1.457026
49	6	0	2.659882	-1.373604	2.487561
50	6	0	5.432873	-1.048825	2.558066
51	1	0	5.227656	-0.114743	0.633097
52	6	0	3.388764	-1.817496	3.592420
53	1	0	1.576761	-1.474296	2.484593
54	6	0	4.773058	-1.661179	3.628241
55	1	0	6.511763	-0.917505	2.583389
56	1	0	2.866674	-2.279110	4.426481
57	1	0	5.339349	-2.006250	4.490068
58	6	0	-3.331290	-0.772991	1.384281
59	6	0	-4.727584	-0.618201	1.415383
60	6	0	-2.688020	-1.388802	2.463476
61	6	0	-5.463366	-1.076977	2.503369
62	1	0	-5.238801	-0.124692	0.589414
63	6	0	-3.428293	-1.846162	3.555277
64	1	0	-1.604456	-1.483717	2.472875
65	6	0	-4.813614	-1.696474	3.575664
66	1	0	-6.543050	-0.950609	2.516891
67	1	0	-2.914287	-2.313127	4.391369
68	1	0	-5.388623	-2.052377	4.427295
69	77	0	-0.004214	-0.294027	0.147985
70	6	0	0.005570	1.782014	0.880293
71	6	0	0.021878	2.906907	0.254893
72	6	0	-0.008455	0.848748	1.880560
73	16	0	-0.025895	0.702941	3.495949
74	16	0	0.044162	4.219226	-0.604298
75	17	0	0.004578	0.155537	-2.370517
76	6	0	-0.010108	-2.094290	0.582031
77	8	0	-0.012217	-3.212546	0.927967

Table S9. The theoretical Cartesian coordinates (in Å) for the structure **Ir2S-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.387712	-0.326161	0.002573
2	15	0	-2.387719	-0.326160	0.002566
3	6	0	-3.105701	-0.855113	1.590179
4	6	0	-4.361614	-0.383517	2.002668
5	6	0	-2.434896	-1.791854	2.385469
6	6	0	-4.938087	-0.854878	3.181044
7	1	0	-4.877887	0.374366	1.413706
8	6	0	-3.016192	-2.267806	3.558052
9	1	0	-1.437922	-2.122704	2.105508
10	6	0	-4.270407	-1.803787	3.957319
11	1	0	-5.907591	-0.475590	3.494523
12	1	0	-2.480521	-2.990262	4.168591
13	1	0	-4.719654	-2.168358	4.878022
14	6	0	-3.023662	1.343707	-0.262052
15	6	0	-3.462440	1.758446	-1.525640
16	6	0	-2.924505	2.272755	0.785600
17	6	0	-3.822174	3.090314	-1.733142
18	1	0	-3.513636	1.044320	-2.346571
19	6	0	-3.289055	3.599031	0.571806
20	1	0	-2.532119	1.955422	1.751510
21	6	0	-3.737404	4.009401	-0.686719
22	1	0	-4.159224	3.410261	-2.715944
23	1	0	-3.193902	4.319588	1.379816
24	1	0	-4.006249	5.049647	-0.853830
25	6	0	3.023662	1.343703	-0.262044
26	6	0	3.462442	1.758442	-1.525633
27	6	0	2.924507	2.272752	0.785606
28	6	0	3.822181	3.090307	-1.733134
29	1	0	3.513639	1.044315	-2.346563
30	6	0	3.289064	3.599026	0.571813
31	1	0	2.532115	1.955423	1.751516
32	6	0	3.737415	4.009395	-0.686711
33	1	0	4.159233	3.410253	-2.715936
34	1	0	3.193913	4.319583	1.379824
35	1	0	4.006265	5.049639	-0.853822
36	6	0	3.105694	-0.855114	1.590186

37	6	0	4.361609	-0.383523	2.002673
38	6	0	2.434881	-1.791844	2.385483
39	6	0	4.938078	-0.854879	3.181053
40	1	0	4.877889	0.374352	1.413707
41	6	0	3.016172	-2.267790	3.558071
42	1	0	1.437906	-2.122688	2.105525
43	6	0	4.270390	-1.803777	3.957335
44	1	0	5.907584	-0.475595	3.494531
45	1	0	2.480494	-2.990237	4.168615
46	1	0	4.719633	-2.168343	4.878043
47	6	0	-3.240766	-1.354889	-1.238759
48	6	0	-4.644349	-1.359506	-1.283019
49	6	0	-2.528193	-2.161860	-2.132964
50	6	0	-5.319411	-2.159865	-2.199739
51	1	0	-5.211382	-0.732224	-0.595870
52	6	0	-3.206318	-2.967128	-3.049420
53	1	0	-1.439705	-2.149642	-2.117937
54	6	0	-4.600066	-2.969829	-3.083349
55	1	0	-6.406225	-2.154737	-2.223755
56	1	0	-2.641869	-3.591448	-3.737404
57	1	0	-5.127082	-3.598705	-3.796981
58	6	0	3.240757	-1.354890	-1.238756
59	6	0	4.644340	-1.359500	-1.283014
60	6	0	2.528190	-2.161858	-2.132967
61	6	0	5.319408	-2.159845	-2.199741
62	1	0	5.211368	-0.732224	-0.595856
63	6	0	3.206320	-2.967111	-3.049432
64	1	0	1.439702	-2.149654	-2.117939
65	6	0	4.600068	-2.969802	-3.083362
66	1	0	6.406222	-2.154710	-2.223755
67	1	0	2.641876	-3.591429	-3.737421
68	1	0	5.127088	-3.598666	-3.797004
69	77	0	0.000000	-0.427795	-0.082065
70	6	0	0.000000	1.468203	-1.059628
71	6	0	0.000000	2.753728	-0.761346
72	16	0	0.000000	0.418099	-2.378309
73	6	0	0.000000	3.912363	-0.235024
74	16	0	0.000000	5.384487	0.354219
75	17	0	0.000000	0.514498	2.218296
76	6	0	0.000000	-2.313940	0.115473
77	8	0	0.000000	-3.481091	0.113004

Table S10. The theoretical Cartesian coordinates (in Å) for the structure **Ir2Se-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.355965	0.215518	-2.392476
2	15	0	0.355965	0.215518	2.392476
3	6	0	1.213533	1.671646	3.075525
4	6	0	1.125441	1.928931	4.453094
5	6	0	1.987246	2.515316	2.271958
6	6	0	1.800969	3.009176	5.013810
7	1	0	0.517498	1.287798	5.090562
8	6	0	2.668571	3.593967	2.836545
9	1	0	2.024227	2.349046	1.198070
10	6	0	2.579285	3.842314	4.205544
11	1	0	1.721083	3.199644	6.081168
12	1	0	3.262026	4.245564	2.200200
13	1	0	3.108197	4.685835	4.642834
14	6	0	-1.338403	0.347454	3.011377
15	6	0	-2.093577	-0.810869	3.254214
16	6	0	-1.932786	1.608978	3.154680
17	6	0	-3.416392	-0.703876	3.676710
18	1	0	-1.646780	-1.794430	3.108914
19	6	0	-3.256137	1.708489	3.581335
20	1	0	-1.360766	2.505197	2.921456
21	6	0	-3.997212	0.555328	3.846795
22	1	0	-3.996124	-1.604309	3.862792
23	1	0	-3.711359	2.689089	3.694717
24	1	0	-5.030748	0.636190	4.175686
25	6	0	-1.338403	0.347454	-3.011377
26	6	0	-2.093577	-0.810869	-3.254214
27	6	0	-1.932786	1.608978	-3.154680
28	6	0	-3.416392	-0.703876	-3.676710
29	1	0	-1.646780	-1.794430	-3.108914
30	6	0	-3.256137	1.708489	-3.581335
31	1	0	-1.360766	2.505197	-2.921456
32	6	0	-3.997212	0.555328	-3.846795
33	1	0	-3.996124	-1.604309	-3.862792
34	1	0	-3.711359	2.689089	-3.694717
35	1	0	-5.030748	0.636190	-4.175686
36	6	0	1.213533	1.671646	-3.075525

37	6	0	1.125441	1.928931	-4.453094
38	6	0	1.987246	2.515316	-2.271958
39	6	0	1.800969	3.009176	-5.013810
40	1	0	0.517498	1.287798	-5.090562
41	6	0	2.668571	3.593967	-2.836545
42	1	0	2.024227	2.349046	-1.198070
43	6	0	2.579285	3.842314	-4.205544
44	1	0	1.721083	3.199644	-6.081168
45	1	0	3.262026	4.245564	-2.200200
46	1	0	3.108197	4.685835	-4.642834
47	6	0	1.073669	-1.191150	3.301417
48	6	0	0.705261	-1.454852	4.631400
49	6	0	2.056636	-1.984726	2.697768
50	6	0	1.316206	-2.484244	5.341875
51	1	0	-0.080655	-0.867377	5.105014
52	6	0	2.668583	-3.015053	3.411919
53	1	0	2.327670	-1.819589	1.657305
54	6	0	2.303976	-3.264343	4.734431
55	1	0	1.018417	-2.680331	6.368835
56	1	0	3.420875	-3.629916	2.924552
57	1	0	2.778245	-4.070735	5.288833
58	6	0	1.073669	-1.191150	-3.301417
59	6	0	0.705261	-1.454852	-4.631400
60	6	0	2.056636	-1.984726	-2.697768
61	6	0	1.316206	-2.484244	-5.341875
62	1	0	-0.080655	-0.867377	-5.105014
63	6	0	2.668583	-3.015053	-3.411919
64	1	0	2.327670	-1.819589	-1.657305
65	6	0	2.303976	-3.264343	-4.734431
66	1	0	1.018417	-2.680331	-6.368835
67	1	0	3.420875	-3.629916	-2.924552
68	1	0	2.778245	-4.070735	-5.288833
69	77	0	0.464220	0.058647	0.000000
70	6	0	-1.416167	-1.154917	0.000000
71	6	0	-2.573967	-0.595434	0.000000
72	6	0	-0.271954	-1.890533	0.000000
73	17	0	-0.544956	2.411976	0.000000
74	6	0	2.311748	0.073634	0.000000
75	8	0	3.481564	0.029299	0.000000
76	34	0	0.281417	-3.572749	0.000000
77	34	0	-4.034155	0.291916	0.000000

Table S11. The theoretical Cartesian coordinates (in Å) for the structure **Ir2Se-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.569256	-0.060319	-2.391617
2	15	0	-0.569256	-0.060319	2.391617
3	6	0	-1.181873	-1.620343	3.105848
4	6	0	-0.736937	-2.056255	4.363597
5	6	0	-2.156082	-2.366553	2.432209
6	6	0	-1.268874	-3.209622	4.937783
7	1	0	0.047549	-1.506496	4.883294
8	6	0	-2.692282	-3.514177	3.011014
9	1	0	-2.470075	-2.069950	1.434741
10	6	0	-2.252916	-3.937310	4.266209
11	1	0	-0.909203	-3.541955	5.908513
12	1	0	-3.442679	-4.087244	2.472358
13	1	0	-2.664478	-4.839014	4.713400
14	6	0	1.111326	0.112042	3.031084
15	6	0	1.597494	1.353026	3.461604
16	6	0	1.979341	-0.987267	2.938104
17	6	0	2.939753	1.486880	3.818276
18	1	0	0.930943	2.213574	3.509174
19	6	0	3.315676	-0.847254	3.302033
20	1	0	1.607615	-1.935914	2.551242
21	6	0	3.797536	0.389142	3.740400
22	1	0	3.315525	2.452256	4.148090
23	1	0	3.988730	-1.696557	3.216807
24	1	0	4.846750	0.498462	4.004213
25	6	0	1.111326	0.112042	-3.031084
26	6	0	1.597494	1.353026	-3.461604
27	6	0	1.979341	-0.987267	-2.938104
28	6	0	2.939753	1.486880	-3.818276
29	1	0	0.930943	2.213574	-3.509174
30	6	0	3.315676	-0.847254	-3.302033
31	1	0	1.607615	-1.935914	-2.551242
32	6	0	3.797536	0.389142	-3.740400
33	1	0	3.315525	2.452256	-4.148090
34	1	0	3.988730	-1.696557	-3.216807
35	1	0	4.846750	0.498462	-4.004213
36	6	0	-1.181873	-1.620343	-3.105848

37	6	0	-0.736937	-2.056255	-4.363597
38	6	0	-2.156082	-2.366553	-2.432209
39	6	0	-1.268874	-3.209622	-4.937783
40	1	0	0.047549	-1.506496	-4.883294
41	6	0	-2.692282	-3.514177	-3.011014
42	1	0	-2.470075	-2.069950	-1.434741
43	6	0	-2.252916	-3.937310	-4.266209
44	1	0	-0.909203	-3.541955	-5.908513
45	1	0	-3.442679	-4.087244	-2.472358
46	1	0	-2.664478	-4.839014	-4.713400
47	6	0	-1.534665	1.225425	3.254889
48	6	0	-1.497775	1.285683	4.657463
49	6	0	-2.340091	2.131689	2.555973
50	6	0	-2.252916	2.231745	5.344527
51	1	0	-0.872231	0.588847	5.214605
52	6	0	-3.100603	3.077036	3.245970
53	1	0	-2.362227	2.104418	1.467882
54	6	0	-3.059518	3.128874	4.638582
55	1	0	-2.214217	2.268251	6.430282
56	1	0	-3.723764	3.774161	2.691489
57	1	0	-3.652400	3.866018	5.174859
58	6	0	-1.534665	1.225425	-3.254889
59	6	0	-1.497775	1.285683	-4.657463
60	6	0	-2.340091	2.131689	-2.555973
61	6	0	-2.252916	2.231745	-5.344527
62	1	0	-0.872231	0.588847	-5.214605
63	6	0	-3.100603	3.077036	-3.245970
64	1	0	-2.362227	2.104418	-1.467882
65	6	0	-3.059518	3.128874	-4.638582
66	1	0	-2.214217	2.268251	-6.430282
67	1	0	-3.723764	3.774161	-2.691489
68	1	0	-3.652400	3.866018	-5.174859
69	77	0	-0.661549	0.029599	0.000000
70	6	0	1.296185	0.848299	0.000000
71	6	0	2.559949	0.473844	0.000000
72	6	0	3.740776	0.002073	0.000000
73	17	0	0.146078	-2.325963	0.000000
74	6	0	-2.555138	-0.073218	0.000000
75	8	0	-3.721153	-0.020156	0.000000
76	34	0	5.357234	-0.608366	0.000000
77	34	0	0.295727	2.401177	0.000000

Table S12. The theoretical Cartesian coordinates (in Å) for the structure **NiO-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.699851	0.105679	-0.022924
2	15	0	-1.900956	-0.250277	-0.075444
3	6	0	2.338191	0.161706	1.689116
4	6	0	3.056063	1.248273	2.209662
5	6	0	2.112741	-0.958660	2.503875
6	6	0	3.528041	1.217933	3.522491
7	1	0	3.240334	2.123794	1.588106
8	6	0	2.593569	-0.992026	3.811802
9	1	0	1.553035	-1.804704	2.099882
10	6	0	3.298464	0.098721	4.326121
11	1	0	4.080718	2.068014	3.916067
12	1	0	2.413200	-1.867956	4.430277
13	1	0	3.667322	0.077345	5.349006
14	6	0	1.616945	1.867962	-0.510828
15	6	0	2.112739	2.310507	-1.746857
16	6	0	0.924609	2.780793	0.302995
17	6	0	1.918309	3.629527	-2.159539
18	1	0	2.662556	1.623227	-2.389002
19	6	0	0.734783	4.097510	-0.110307
20	1	0	0.540707	2.463083	1.273148
21	6	0	1.224165	4.526608	-1.346401
22	1	0	2.314863	3.956121	-3.118257
23	1	0	0.201273	4.789608	0.538171
24	1	0	1.071805	5.553859	-1.669180
25	6	0	3.114283	-0.503411	-1.006351
26	6	0	4.444985	-0.382916	-0.589060
27	6	0	2.836446	-1.095387	-2.247035
28	6	0	5.480365	-0.851827	-1.398916
29	1	0	4.671998	0.062212	0.379237
30	6	0	3.871319	-1.546268	-3.064302
31	1	0	1.796625	-1.220805	-2.556394
32	6	0	5.196352	-1.428472	-2.638347
33	1	0	6.510309	-0.769537	-1.059757
34	1	0	3.643586	-2.005549	-4.023106
35	1	0	6.005046	-1.795865	-3.265667
36	6	0	-1.802318	1.008494	1.248080

37	6	0	-2.373620	2.283062	1.152526
38	6	0	-1.093164	0.662993	2.408462
39	6	0	-2.222326	3.200989	2.193700
40	1	0	-2.920154	2.567582	0.254100
41	6	0	-0.943761	1.576761	3.450453
42	1	0	-0.642568	-0.328899	2.481474
43	6	0	-1.504092	2.853246	3.340520
44	1	0	-2.660822	4.192501	2.105516
45	1	0	-0.381650	1.297369	4.338843
46	1	0	-1.381337	3.573696	4.145777
47	6	0	-2.355865	0.712195	-1.562689
48	6	0	-3.680623	1.070167	-1.854544
49	6	0	-1.333103	1.124635	-2.427605
50	6	0	-3.971878	1.833142	-2.985615
51	1	0	-4.486649	0.741588	-1.198367
52	6	0	-1.623399	1.894043	-3.553441
53	1	0	-0.303619	0.832312	-2.214762
54	6	0	-2.943945	2.249693	-3.834789
55	1	0	-5.002686	2.101221	-3.204825
56	1	0	-0.819359	2.207454	-4.215524
57	1	0	-3.173485	2.842987	-4.716749
58	6	0	-3.453142	-1.125470	0.320362
59	6	0	-4.232070	-0.808347	1.440946
60	6	0	-3.868247	-2.161228	-0.530567
61	6	0	-5.408441	-1.511627	1.704804
62	1	0	-3.923082	-0.007740	2.111078
63	6	0	-5.046246	-2.857181	-0.268812
64	1	0	-3.262098	-2.426770	-1.394450
65	6	0	-5.818707	-2.535583	0.850538
66	1	0	-6.004472	-1.255933	2.577630
67	1	0	-5.354368	-3.660430	-0.933503
68	1	0	-6.733836	-3.085668	1.057686
69	28	0	-0.036660	-1.354529	-0.202573
70	6	0	0.864518	-3.015789	-0.261422
71	6	0	1.970068	-3.686535	-0.320571
72	6	0	-0.523804	-3.153729	-0.313278
73	8	0	-1.443459	-3.933047	-0.389209
74	8	0	3.004788	-4.256372	-0.362035

Table S13. The theoretical Cartesian coordinates (in Å) for the structure **NiO-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.886635	-0.282713	-0.181083
2	15	0	-1.631645	0.225545	-0.048287
3	6	0	2.495725	-0.979076	1.394737
4	6	0	3.286862	-0.272719	2.309954
5	6	0	2.159818	-2.315250	1.667240
6	6	0	3.729309	-0.889888	3.481167
7	1	0	3.554875	0.763750	2.108110
8	6	0	2.614045	-2.933660	2.830671
9	1	0	1.545091	-2.869453	0.955097
10	6	0	3.396206	-2.220351	3.743047
11	1	0	4.340447	-0.331365	4.186480
12	1	0	2.353347	-3.970661	3.027246
13	1	0	3.745055	-2.700074	4.654624
14	6	0	2.134029	1.516301	-0.013336
15	6	0	2.721946	2.270929	-1.039165
16	6	0	1.562363	2.189823	1.078947
17	6	0	2.729282	3.664873	-0.978100
18	1	0	3.169945	1.767442	-1.895338
19	6	0	1.566795	3.581865	1.135548
20	1	0	1.112061	1.618604	1.890895
21	6	0	2.143864	4.325628	0.103032
22	1	0	3.189661	4.235013	-1.781916
23	1	0	1.113659	4.084195	1.987654
24	1	0	2.141207	5.412155	0.144213
25	6	0	3.182613	-0.766974	-1.373145
26	6	0	4.545824	-0.610304	-1.081763
27	6	0	2.799803	-1.288408	-2.614853
28	6	0	5.510154	-0.965605	-2.021657
29	1	0	4.849984	-0.211747	-0.113442
30	6	0	3.766929	-1.640074	-3.558690
31	1	0	1.740479	-1.433610	-2.829884
32	6	0	5.120611	-1.478168	-3.263662
33	1	0	6.565467	-0.845425	-1.788213
34	1	0	3.461448	-2.046913	-4.519445
35	1	0	5.874459	-1.756985	-3.996452
36	6	0	-1.393750	0.662788	1.713221

37	6	0	-1.734768	1.900439	2.273487
38	6	0	-0.803831	-0.313214	2.531539
39	6	0	-1.479329	2.159197	3.620688
40	1	0	-2.175407	2.677875	1.651788
41	6	0	-0.552482	-0.058288	3.879462
42	1	0	-0.529018	-1.276831	2.096331
43	6	0	-0.886111	1.183005	4.425849
44	1	0	-1.740123	3.127615	4.041967
45	1	0	-0.086303	-0.823842	4.495888
46	1	0	-0.682331	1.390978	5.473502
47	6	0	-1.638224	1.812499	-0.958445
48	6	0	-2.676091	2.748102	-0.817052
49	6	0	-0.591244	2.092716	-1.844739
50	6	0	-2.641335	3.952739	-1.516431
51	1	0	-3.526841	2.515629	-0.175936
52	6	0	-0.556648	3.296389	-2.548161
53	1	0	0.192946	1.348951	-1.993301
54	6	0	-1.575914	4.233293	-2.377315
55	1	0	-3.449973	4.669993	-1.397282
56	1	0	0.266627	3.498319	-3.230155
57	1	0	-1.552503	5.172045	-2.925984
58	6	0	-3.392935	-0.234640	-0.134126
59	6	0	-4.172062	-0.497241	0.998569
60	6	0	-3.967515	-0.368029	-1.408341
61	6	0	-5.512484	-0.863709	0.858085
62	1	0	-3.737550	-0.408450	1.993450
63	6	0	-5.305712	-0.724387	-1.544514
64	1	0	-3.358984	-0.187054	-2.295054
65	6	0	-6.081775	-0.974081	-0.409705
66	1	0	-6.109742	-1.068068	1.743405
67	1	0	-5.739024	-0.828638	-2.535858
68	1	0	-7.122683	-1.268958	-0.515864
69	28	0	-0.127797	-1.191490	-0.657509
70	6	0	-0.974044	-2.805669	-1.135059
71	6	0	-2.099980	-3.520087	-1.250175
72	6	0	-3.367217	-3.555398	-1.022489
73	8	0	-4.522735	-3.787840	-0.873322
74	8	0	0.269086	-2.953091	-1.303131

Table S14. The theoretical Cartesian coordinates (in Å) for the structure **NiS-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.623083	0.307149	-0.027268
2	15	0	-1.928039	-0.079960	-0.057968
3	6	0	2.350051	0.227449	1.646750
4	6	0	3.019593	1.301534	2.251041
5	6	0	2.238374	-0.984468	2.344304
6	6	0	3.559781	1.165391	3.530779
7	1	0	3.110738	2.249881	1.722302
8	6	0	2.786544	-1.122528	3.618199
9	1	0	1.716793	-1.822999	1.879041
10	6	0	3.444712	-0.045682	4.216655
11	1	0	4.073960	2.006056	3.990721
12	1	0	2.697169	-2.070463	4.143057
13	1	0	3.868237	-0.149646	5.212838
14	6	0	1.380064	2.096536	-0.314539
15	6	0	1.775818	2.702666	-1.516121
16	6	0	0.662957	2.858665	0.621929
17	6	0	1.454576	4.035068	-1.778162
18	1	0	2.339622	2.130654	-2.252685
19	6	0	0.341714	4.188958	0.357242
20	1	0	0.366994	2.411783	1.571808
21	6	0	0.730751	4.781117	-0.846979
22	1	0	1.772175	4.489744	-2.713990
23	1	0	-0.213450	4.761974	1.097329
24	1	0	0.477463	5.818062	-1.054022
25	6	0	3.006046	-0.080898	-1.152450
26	6	0	4.342083	0.192204	-0.836341
27	6	0	2.695981	-0.643535	-2.397957
28	6	0	5.353080	-0.098529	-1.752434
29	1	0	4.593571	0.615669	0.135768
30	6	0	3.704711	-0.920419	-3.319557
31	1	0	1.657103	-0.886068	-2.632388
32	6	0	5.035868	-0.649678	-2.996177
33	1	0	6.389870	0.103422	-1.494329
34	1	0	3.453827	-1.361758	-4.280940
35	1	0	5.826310	-0.877714	-3.707378
36	6	0	-1.839326	0.851308	1.516339

37	6	0	-2.440420	2.096770	1.735505
38	6	0	-1.069437	0.279180	2.540991
39	6	0	-2.260627	2.761285	2.949354
40	1	0	-3.020228	2.569089	0.944763
41	6	0	-0.888706	0.940227	3.754943
42	1	0	-0.592189	-0.688579	2.368224
43	6	0	-1.481126	2.189261	3.958476
44	1	0	-2.722341	3.733896	3.103909
45	1	0	-0.274871	0.487277	4.530285
46	1	0	-1.334824	2.716018	4.898529
47	6	0	-2.282878	1.156494	-1.352174
48	6	0	-3.510168	1.835289	-1.435541
49	6	0	-1.301648	1.410621	-2.317855
50	6	0	-3.733190	2.767623	-2.447013
51	1	0	-4.300287	1.611924	-0.718447
52	6	0	-1.524180	2.341512	-3.332326
53	1	0	-0.361045	0.857840	-2.276200
54	6	0	-2.738327	3.025511	-3.394858
55	1	0	-4.687239	3.286632	-2.502459
56	1	0	-0.750176	2.527960	-4.073491
57	1	0	-2.916321	3.749543	-4.186464
58	6	0	-3.502620	-0.983064	0.087419
59	6	0	-3.960420	-1.426747	1.334533
60	6	0	-4.188752	-1.378160	-1.070758
61	6	0	-5.097837	-2.228416	1.424172
62	1	0	-3.429278	-1.141868	2.241992
63	6	0	-5.329762	-2.172792	-0.978440
64	1	0	-3.825477	-1.065978	-2.049495
65	6	0	-5.787764	-2.600466	0.269177
66	1	0	-5.444908	-2.563782	2.398635
67	1	0	-5.853760	-2.469890	-1.883671
68	1	0	-6.673840	-3.226756	0.339965
69	28	0	-0.063075	-1.198724	-0.288854
70	6	0	0.787443	-2.922790	-0.456391
71	6	0	2.023952	-3.283923	-0.443739
72	6	0	-0.581358	-2.984251	-0.492186
73	16	0	-1.851879	-3.975380	-0.621246
74	16	0	3.560851	-3.631835	-0.412606

Table S15. The theoretical Cartesian coordinates (in Å) for the structure **NiS-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.910145	-0.481481	-0.092779
2	15	0	-1.446993	0.635339	-0.019856
3	6	0	2.497736	-0.938238	1.578237
4	6	0	3.539648	-0.267511	2.234480
5	6	0	1.893887	-2.037660	2.207050
6	6	0	3.964482	-0.685567	3.496185
7	1	0	4.017099	0.588033	1.758050
8	6	0	2.323366	-2.458869	3.464562
9	1	0	1.085543	-2.566694	1.699454
10	6	0	3.358136	-1.781600	4.114164
11	1	0	4.772969	-0.156281	3.994539
12	1	0	1.847385	-3.314391	3.937396
13	1	0	3.691696	-2.107017	5.096769
14	6	0	2.447453	1.256956	-0.289086
15	6	0	3.047132	1.695225	-1.479702
16	6	0	2.148810	2.205055	0.703116
17	6	0	3.334028	3.045956	-1.676199
18	1	0	3.294598	0.977045	-2.260940
19	6	0	2.438493	3.554078	0.504894
20	1	0	1.703068	1.886586	1.645865
21	6	0	3.026392	3.981883	-0.687581
22	1	0	3.801270	3.366063	-2.604854
23	1	0	2.203737	4.270967	1.289060
24	1	0	3.250310	5.034795	-0.841151
25	6	0	3.063342	-1.355171	-1.211385
26	6	0	4.386956	-1.638915	-0.849839
27	6	0	2.619427	-1.690934	-2.497486
28	6	0	5.250379	-2.247008	-1.760498
29	1	0	4.741727	-1.393920	0.150724
30	6	0	3.486880	-2.287089	-3.413012
31	1	0	1.582221	-1.495187	-2.773449
32	6	0	4.804607	-2.566549	-3.044941
33	1	0	6.272963	-2.472028	-1.467122
34	1	0	3.130226	-2.542889	-4.407671
35	1	0	5.480007	-3.039903	-3.753613
36	6	0	-0.942944	1.388839	1.567957

37	6	0	-1.003269	2.759980	1.844963
38	6	0	-0.436515	0.518553	2.544294
39	6	0	-0.539363	3.251153	3.065878
40	1	0	-1.383723	3.452327	1.096032
41	6	0	0.029903	1.006671	3.764387
42	1	0	-0.390672	-0.551116	2.328376
43	6	0	-0.013891	2.378690	4.023581
44	1	0	-0.579579	4.319310	3.267356
45	1	0	0.440161	0.317330	4.498800
46	1	0	0.358539	2.767553	4.968176
47	6	0	-1.257146	1.943650	-1.281294
48	6	0	-2.100517	3.065887	-1.326680
49	6	0	-0.259734	1.807189	-2.254117
50	6	0	-1.926659	4.040851	-2.306883
51	1	0	-2.914344	3.157158	-0.607304
52	6	0	-0.083655	2.782307	-3.235580
53	1	0	0.371441	0.916921	-2.246073
54	6	0	-0.912582	3.903875	-3.259795
55	1	0	-2.586688	4.904488	-2.332568
56	1	0	0.697580	2.661070	-3.982678
57	1	0	-0.780161	4.663806	-4.026076
58	6	0	-3.254419	0.516110	0.141596
59	6	0	-3.883176	0.490351	1.392084
60	6	0	-4.028750	0.351272	-1.018555
61	6	0	-5.267400	0.333871	1.479596
62	1	0	-3.293509	0.602760	2.301233
63	6	0	-5.409340	0.201654	-0.928236
64	1	0	-3.544428	0.339567	-1.995242
65	6	0	-6.032938	0.193772	0.322395
66	1	0	-5.746174	0.318736	2.455889
67	1	0	-5.998580	0.069738	-1.832370
68	1	0	-7.110034	0.063803	0.391715
69	16	0	-0.033747	-3.269089	-0.858702
70	28	0	-0.241591	-1.148808	-0.399841
71	6	0	-1.515530	-2.514308	-0.607862
72	6	0	-2.809920	-2.778810	-0.553133
73	6	0	-4.055314	-3.004033	-0.444571
74	16	0	-5.601586	-3.337740	-0.316371

Table S16. The theoretical Cartesian coordinates (in Å) for the structure **NiSe-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.474058	0.751485	-0.086413
2	15	0	-2.024905	0.115773	0.019616
3	6	0	2.275237	0.873257	1.552197
4	6	0	2.861528	2.056323	2.025752
5	6	0	2.318759	-0.276797	2.354621
6	6	0	3.472895	2.089314	3.278933
7	1	0	2.829867	2.958233	1.415727
8	6	0	2.943601	-0.247092	3.600474
9	1	0	1.860452	-1.199379	1.993793
10	6	0	3.517307	0.937473	4.068047
11	1	0	3.917666	3.014677	3.637463
12	1	0	2.977843	-1.149258	4.206051
13	1	0	3.997784	0.963512	5.043552
14	6	0	1.069905	2.490764	-0.480538
15	6	0	1.383417	3.050522	-1.727369
16	6	0	0.327436	3.254985	0.434418
17	6	0	0.962805	4.340864	-2.052420
18	1	0	1.962470	2.476701	-2.450551
19	6	0	-0.096238	4.541355	0.105975
20	1	0	0.093190	2.846796	1.418100
21	6	0	0.216696	5.088887	-1.140842
22	1	0	1.219400	4.760581	-3.022744
23	1	0	-0.670713	5.115117	0.830631
24	1	0	-0.113819	6.092870	-1.396551
25	6	0	2.841104	0.404690	-1.245550
26	6	0	4.131988	0.914410	-1.057685
27	6	0	2.563330	-0.361670	-2.384613
28	6	0	5.132449	0.652707	-1.993074
29	1	0	4.357026	1.504943	-0.169883
30	6	0	3.560911	-0.614589	-3.325904
31	1	0	1.563469	-0.780983	-2.516399
32	6	0	4.847462	-0.109431	-3.129345
33	1	0	6.135537	1.041716	-1.834916
34	1	0	3.337828	-1.219434	-4.201020
35	1	0	5.630206	-0.315626	-3.855562
36	6	0	-1.939470	1.105459	1.559640

37	6	0	-2.619977	2.310397	1.777516
38	6	0	-1.081051	0.622186	2.559197
39	6	0	-2.429427	3.021561	2.962987
40	1	0	-3.271582	2.717960	1.006665
41	6	0	-0.889590	1.329659	3.744669
42	1	0	-0.543161	-0.313927	2.389500
43	6	0	-1.560648	2.538101	3.945471
44	1	0	-2.953809	3.962298	3.116027
45	1	0	-0.204779	0.945827	4.497424
46	1	0	-1.406902	3.102538	4.862210
47	6	0	-2.474344	1.274330	-1.317273
48	6	0	-3.717166	1.927741	-1.373117
49	6	0	-1.550678	1.489424	-2.347004
50	6	0	-4.009240	2.800306	-2.419600
51	1	0	-4.467411	1.727170	-0.608324
52	6	0	-1.843760	2.357838	-3.398378
53	1	0	-0.597633	0.956259	-2.324514
54	6	0	-3.070323	3.020788	-3.431955
55	1	0	-4.974267	3.300726	-2.452089
56	1	0	-1.112604	2.515500	-4.188166
57	1	0	-3.302401	3.698065	-4.250606
58	6	0	-3.552459	-0.849448	0.242745
59	6	0	-3.936265	-1.286446	1.517244
60	6	0	-4.278820	-1.284757	-0.875624
61	6	0	-5.044667	-2.117272	1.673979
62	1	0	-3.370158	-0.970214	2.392709
63	6	0	-5.390571	-2.109998	-0.716111
64	1	0	-3.972996	-0.976576	-1.874963
65	6	0	-5.778436	-2.526465	0.558694
66	1	0	-5.336045	-2.444813	2.669146
67	1	0	-5.948835	-2.435623	-1.590503
68	1	0	-6.644143	-3.173072	0.681645
69	28	0	-0.093172	-0.899356	-0.188013
70	6	0	0.868190	-2.594936	-0.217034
71	6	0	2.135070	-2.797987	-0.116895
72	6	0	-0.487978	-2.721448	-0.307827
73	34	0	-1.783422	-3.907922	-0.471952
74	34	0	3.836543	-2.977946	0.043013

Table S17. The theoretical Cartesian coordinates (in Å) for the structure **NiSe-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.104858	-0.585776	-0.036412
2	15	0	-0.975400	1.145418	-0.018858
3	6	0	2.696882	-0.860523	1.673479
4	6	0	3.877900	-0.292192	2.173643
5	6	0	1.951814	-1.714510	2.500039
6	6	0	4.299609	-0.568013	3.474645
7	1	0	4.470104	0.370593	1.544159
8	6	0	2.377540	-1.995850	3.797288
9	1	0	1.033740	-2.162758	2.115381
10	6	0	3.551446	-1.420617	4.289536
11	1	0	5.217564	-0.120837	3.848767
12	1	0	1.790189	-2.662569	4.423742
13	1	0	3.882982	-1.636748	5.302532
14	6	0	2.915158	0.980808	-0.528435
15	6	0	3.504169	1.119316	-1.794430
16	6	0	2.840321	2.108208	0.305208
17	6	0	3.995511	2.353208	-2.219835
18	1	0	3.582250	0.257099	-2.455841
19	6	0	3.329724	3.341364	-0.123187
20	1	0	2.409345	2.020759	1.302565
21	6	0	3.904147	3.471082	-1.389555
22	1	0	4.449742	2.439778	-3.204256
23	1	0	3.262607	4.201498	0.539898
24	1	0	4.283034	4.433919	-1.723450
25	6	0	3.054957	-1.805093	-1.018118
26	6	0	4.319319	-2.251566	-0.613196
27	6	0	2.536459	-2.244593	-2.244298
28	6	0	5.052418	-3.121838	-1.419317
29	1	0	4.729500	-1.926658	0.341842
30	6	0	3.275721	-3.104919	-3.057138
31	1	0	1.541944	-1.919700	-2.554138
32	6	0	4.535084	-3.545830	-2.644952
33	1	0	6.028805	-3.468972	-1.089814
34	1	0	2.862925	-3.438002	-4.006069
35	1	0	5.108059	-4.223121	-3.273757
36	6	0	-0.250562	1.996669	1.428514

37	6	0	-0.009136	3.374158	1.495505
38	6	0	0.100579	1.190606	2.520983
39	6	0	0.592526	3.928156	2.625772
40	1	0	-0.257545	4.013118	0.650056
41	6	0	0.703420	1.741197	3.651411
42	1	0	-0.087856	0.116140	2.468901
43	6	0	0.956778	3.113815	3.702120
44	1	0	0.786627	4.997834	2.662826
45	1	0	0.986718	1.095579	4.479871
46	1	0	1.436249	3.548602	4.576054
47	6	0	-0.620380	2.201060	-1.465912
48	6	0	-1.203958	3.467617	-1.637752
49	6	0	0.241949	1.714422	-2.455600
50	6	0	-0.899037	4.238647	-2.757479
51	1	0	-1.920793	3.835492	-0.903914
52	6	0	0.545852	2.483359	-3.578368
53	1	0	0.662907	0.713169	-2.345082
54	6	0	-0.017544	3.750682	-3.726869
55	1	0	-1.356878	5.217200	-2.879555
56	1	0	1.220974	2.090480	-4.335418
57	1	0	0.215818	4.352838	-4.601699
58	6	0	-2.760043	1.403357	0.220311
59	6	0	-3.311382	1.583391	1.494532
60	6	0	-3.613247	1.325282	-0.891871
61	6	0	-4.692482	1.713823	1.650084
62	1	0	-2.661764	1.634454	2.367455
63	6	0	-4.989285	1.462533	-0.734196
64	1	0	-3.195105	1.157515	-1.884188
65	6	0	-5.532445	1.657976	0.538113
66	1	0	-5.110832	1.856450	2.643435
67	1	0	-5.642005	1.393755	-1.600646
68	1	0	-6.608775	1.749983	0.660961
69	28	0	-0.147931	-0.878888	-0.177639
70	6	0	-1.693003	-1.943325	-0.209187
71	6	0	-3.015073	-1.929356	-0.176468
72	6	0	-4.284372	-1.935391	-0.133245
73	34	0	-0.326963	-3.168721	-0.317444
74	34	0	-6.011988	-1.997320	-0.082507

Table S18. The theoretical Cartesian coordinates (in Å) for the structure **PtO-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.729198	0.343355	-0.012196
2	15	0	-1.954538	-0.020213	-0.015504
3	6	0	2.310781	0.608186	1.696450
4	6	0	2.963366	1.773851	2.122530
5	6	0	2.122839	-0.440303	2.610376
6	6	0	3.408775	1.891889	3.439761
7	1	0	3.123424	2.592286	1.421887
8	6	0	2.576296	-0.324872	3.923450
9	1	0	1.611315	-1.347455	2.281480
10	6	0	3.216416	0.844238	4.342860
11	1	0	3.913618	2.801146	3.757984
12	1	0	2.426750	-1.146326	4.619819
13	1	0	3.566386	0.937057	5.368385
14	6	0	1.610156	2.021205	-0.720554
15	6	0	2.108622	2.293047	-2.003914
16	6	0	0.906627	3.030212	-0.041298
17	6	0	1.917954	3.545140	-2.589505
18	1	0	2.660965	1.526163	-2.545259
19	6	0	0.721454	4.281252	-0.628290
20	1	0	0.516385	2.845248	0.960884
21	6	0	1.224403	4.544240	-1.904711
22	1	0	2.319867	3.740263	-3.581223
23	1	0	0.180907	5.051652	-0.082304
24	1	0	1.078661	5.520712	-2.359992
25	6	0	3.191431	-0.342806	-0.866492
26	6	0	4.500146	-0.076722	-0.443854
27	6	0	2.986933	-1.132206	-2.007513
28	6	0	5.585987	-0.599267	-1.146459
29	1	0	4.670794	0.528495	0.445937
30	6	0	4.073453	-1.641390	-2.718017
31	1	0	1.967269	-1.359819	-2.323038
32	6	0	5.374982	-1.378776	-2.285876
33	1	0	6.598033	-0.399495	-0.802273
34	1	0	3.902350	-2.256919	-3.597698
35	1	0	6.222528	-1.789595	-2.829477
36	6	0	-1.786470	1.326474	1.206124

37	6	0	-2.331240	2.605178	1.032584
38	6	0	-1.024366	1.057653	2.352850
39	6	0	-2.102451	3.601718	1.983884
40	1	0	-2.911216	2.832227	0.138638
41	6	0	-0.792564	2.052614	3.301540
42	1	0	-0.589736	0.064600	2.480074
43	6	0	-1.328150	3.330473	3.114743
44	1	0	-2.521705	4.594293	1.835517
45	1	0	-0.180909	1.832705	4.173873
46	1	0	-1.141012	4.112316	3.847003
47	6	0	-2.429478	0.835344	-1.555300
48	6	0	-3.757430	1.193247	-1.830790
49	6	0	-1.425017	1.170402	-2.473356
50	6	0	-4.070463	1.887817	-2.999254
51	1	0	-4.548465	0.917464	-1.133084
52	6	0	-1.737636	1.874730	-3.635352
53	1	0	-0.396998	0.864298	-2.271536
54	6	0	-3.060521	2.235467	-3.899722
55	1	0	-5.103447	2.155954	-3.207799
56	1	0	-0.949066	2.132590	-4.338768
57	1	0	-3.306657	2.777798	-4.809702
58	6	0	-3.485555	-0.874759	0.476340
59	6	0	-4.372506	-0.368948	1.436425
60	6	0	-3.777197	-2.089026	-0.160831
61	6	0	-5.538111	-1.070271	1.751097
62	1	0	-4.150359	0.568979	1.944721
63	6	0	-4.945243	-2.781526	0.149310
64	1	0	-3.073686	-2.505990	-0.879017
65	6	0	-5.828036	-2.273847	1.105938
66	1	0	-6.219110	-0.674593	2.500980
67	1	0	-5.155404	-3.727000	-0.344337
68	1	0	-6.734261	-2.820568	1.356244
69	78	0	-0.057798	-1.305849	-0.116143
70	6	0	0.901138	-3.138715	-0.130618
71	6	0	2.022770	-3.785955	-0.127260
72	6	0	-0.492153	-3.307647	-0.172660
73	8	0	-1.384475	-4.117721	-0.228800
74	8	0	3.068406	-4.335202	-0.118833

Table S19. The theoretical Cartesian coordinates (in Å) for the structure **PtO-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.081526	-0.210641	-0.120862
2	15	0	-1.628602	0.416733	-0.013302
3	6	0	2.058856	0.772287	1.415156
4	6	0	2.713373	1.999835	1.574538
5	6	0	1.296707	0.259651	2.477452
6	6	0	2.591092	2.710772	2.770531
7	1	0	3.301438	2.412127	0.754699
8	6	0	1.181888	0.964759	3.672978
9	1	0	0.775505	-0.691785	2.350154
10	6	0	1.822825	2.199941	3.818828
11	1	0	3.096453	3.667838	2.881102
12	1	0	0.583179	0.558627	4.485441
13	1	0	1.725937	2.758892	4.746597
14	6	0	2.901749	0.872428	-1.332611
15	6	0	4.164477	0.604533	-1.877928
16	6	0	2.196027	2.006422	-1.766270
17	6	0	4.713162	1.463544	-2.833109
18	1	0	4.720704	-0.275969	-1.559159
19	6	0	2.751681	2.867838	-2.708369
20	1	0	1.203862	2.211843	-1.362261
21	6	0	4.012794	2.597381	-3.246909
22	1	0	5.692136	1.244065	-3.252878
23	1	0	2.194595	3.745416	-3.029468
24	1	0	4.444141	3.263453	-3.990319
25	6	0	3.324814	-1.492815	0.249427
26	6	0	4.440746	-1.218379	1.054936
27	6	0	3.168388	-2.773308	-0.297560
28	6	0	5.386920	-2.210212	1.306120
29	1	0	4.560900	-0.226914	1.491683
30	6	0	4.121546	-3.762853	-0.050273
31	1	0	2.289510	-2.999621	-0.900945
32	6	0	5.229928	-3.483509	0.750516
33	1	0	6.245846	-1.991331	1.936045
34	1	0	3.988989	-4.754747	-0.474382
35	1	0	5.966881	-4.257886	0.950246
36	6	0	-1.148496	2.163892	-0.226480

37	6	0	-1.377075	2.802038	-1.456618
38	6	0	-0.435911	2.847914	0.770661
39	6	0	-0.901267	4.092732	-1.683986
40	1	0	-1.927878	2.282578	-2.239623
41	6	0	0.036654	4.139381	0.540602
42	1	0	-0.244507	2.374241	1.734144
43	6	0	-0.189931	4.765130	-0.686998
44	1	0	-1.087040	4.572835	-2.641936
45	1	0	0.589107	4.651325	1.325556
46	1	0	0.182640	5.771161	-0.865258
47	6	0	-3.131363	0.293892	-1.041316
48	6	0	-4.348909	0.848949	-0.624541
49	6	0	-3.054686	-0.336297	-2.289745
50	6	0	-5.471936	0.774410	-1.445129
51	1	0	-4.426899	1.324240	0.352266
52	6	0	-4.178253	-0.404722	-3.113282
53	1	0	-2.110946	-0.784371	-2.603467
54	6	0	-5.388132	0.147651	-2.690766
55	1	0	-6.415833	1.194861	-1.107397
56	1	0	-4.110969	-0.905216	-4.075885
57	1	0	-6.268247	0.080604	-3.325678
58	6	0	-2.226504	0.303366	1.704497
59	6	0	-2.797830	1.390617	2.382909
60	6	0	-2.159725	-0.942511	2.343977
61	6	0	-3.284470	1.234113	3.680456
62	1	0	-2.852118	2.364975	1.897726
63	6	0	-2.654434	-1.099395	3.637638
64	1	0	-1.715689	-1.788087	1.816081
65	6	0	-3.214838	-0.010913	4.309465
66	1	0	-3.721950	2.084570	4.198034
67	1	0	-2.602195	-2.072293	4.119637
68	1	0	-3.598087	-0.131660	5.319945
69	78	0	-0.095455	-1.160476	-0.517113
70	6	0	-1.205773	-2.873285	-0.805737
71	6	0	-2.471524	-3.330563	-0.709076
72	6	0	-3.645306	-2.888060	-0.399018
73	8	0	-0.066446	-3.334333	-1.068152
74	8	0	-4.782484	-2.670413	-0.136001

Table S20. The theoretical Cartesian coordinates (in Å) for the structure **PtS-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.692683	0.553888	-0.021267
2	15	0	-1.959852	0.081859	-0.009722
3	6	0	2.372939	0.693309	1.664566
4	6	0	2.905433	1.882428	2.181658
5	6	0	2.386071	-0.465061	2.458037
6	6	0	3.432072	1.915336	3.473009
7	1	0	2.901799	2.786246	1.573842
8	6	0	2.925180	-0.433286	3.743049
9	1	0	1.969694	-1.392045	2.058296
10	6	0	3.444235	0.758578	4.255565
11	1	0	3.837799	2.844583	3.865819
12	1	0	2.935267	-1.338333	4.344921
13	1	0	3.857148	0.785482	5.261376
14	6	0	1.385837	2.277236	-0.533631
15	6	0	1.801474	2.747584	-1.788284
16	6	0	0.591320	3.110074	0.272245
17	6	0	1.425478	4.017235	-2.228056
18	1	0	2.421352	2.117640	-2.425059
19	6	0	0.215445	4.376295	-0.170683
20	1	0	0.273721	2.768670	1.257951
21	6	0	0.626417	4.833134	-1.425226
22	1	0	1.759353	4.368885	-3.201714
23	1	0	-0.399304	5.005711	0.469053
24	1	0	0.330005	5.820140	-1.772151
25	6	0	3.127309	0.077909	-1.042469
26	6	0	4.418430	0.553168	-0.772655
27	6	0	2.919563	-0.761840	-2.143857
28	6	0	5.485331	0.188956	-1.592476
29	1	0	4.588217	1.199125	0.088871
30	6	0	3.986188	-1.117648	-2.969669
31	1	0	1.918832	-1.154288	-2.335204
32	6	0	5.269497	-0.643875	-2.694209
33	1	0	6.486256	0.551659	-1.370692
34	1	0	3.816601	-1.779264	-3.815272
35	1	0	6.104253	-0.931859	-3.328731
36	6	0	-1.913957	1.206334	1.430249

37	6	0	-2.587752	2.433335	1.465707
38	6	0	-1.134456	0.825098	2.533541
39	6	0	-2.473055	3.269704	2.576578
40	1	0	-3.177447	2.756912	0.610257
41	6	0	-1.022355	1.659422	3.646206
42	1	0	-0.597646	-0.125173	2.503137
43	6	0	-1.687911	2.887521	3.667178
44	1	0	-2.993065	4.225090	2.587331
45	1	0	-0.404386	1.354125	4.487586
46	1	0	-1.593427	3.544796	4.528322
47	6	0	-2.348112	1.132894	-1.447532
48	6	0	-3.621962	1.698405	-1.624124
49	6	0	-1.352918	1.386397	-2.398774
50	6	0	-3.880605	2.526348	-2.714455
51	1	0	-4.416420	1.468278	-0.913931
52	6	0	-1.611397	2.216338	-3.489949
53	1	0	-0.377556	0.911958	-2.282658
54	6	0	-2.871795	2.794261	-3.644535
55	1	0	-4.870185	2.958137	-2.842354
56	1	0	-0.827242	2.406731	-4.219343
57	1	0	-3.075257	3.439479	-4.496001
58	6	0	-3.493247	-0.862548	0.228236
59	6	0	-4.052634	-1.051673	1.498467
60	6	0	-4.072518	-1.501530	-0.878370
61	6	0	-5.190901	-1.842741	1.653932
62	1	0	-3.604668	-0.570358	2.367155
63	6	0	-5.215243	-2.282055	-0.721683
64	1	0	-3.625255	-1.385928	-1.865337
65	6	0	-5.778668	-2.453256	0.544603
66	1	0	-5.620936	-1.978082	2.643300
67	1	0	-5.658187	-2.768074	-1.587485
68	1	0	-6.667937	-3.067024	0.667046
69	78	0	-0.017066	-1.136652	-0.144944
70	6	0	0.847194	-3.080256	-0.188301
71	6	0	2.084274	-3.435884	-0.157757
72	6	0	-0.531303	-3.112582	-0.207690
73	16	0	-1.798555	-4.114281	-0.246785
74	16	0	3.623176	-3.775650	-0.118125

Table S21. The theoretical Cartesian coordinates (in Å) for the structure **PtS-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.122736	-0.292946	-0.035691
2	15	0	-1.426447	0.683914	-0.033046
3	6	0	2.247452	0.694635	1.492079
4	6	0	3.087258	1.806519	1.625830
5	6	0	1.425009	0.322828	2.566844
6	6	0	3.093721	2.544732	2.810558
7	1	0	3.713719	2.116019	0.790275
8	6	0	1.434026	1.058204	3.751609
9	1	0	0.757109	-0.534048	2.456143
10	6	0	2.265737	2.175257	3.873242
11	1	0	3.741376	3.414014	2.900624
12	1	0	0.781396	0.766793	4.571518
13	1	0	2.265574	2.757458	4.791497
14	6	0	2.855358	0.741017	-1.345126
15	6	0	4.241126	0.945109	-1.442504
16	6	0	2.007756	1.337759	-2.286378
17	6	0	4.763898	1.751799	-2.451547
18	1	0	4.910027	0.454660	-0.734422
19	6	0	2.531883	2.147908	-3.294095
20	1	0	0.934483	1.151171	-2.231132
21	6	0	3.908679	2.359185	-3.375833
22	1	0	5.838626	1.901592	-2.521777
23	1	0	1.863012	2.605584	-4.019552
24	1	0	4.318246	2.985193	-4.165306
25	6	0	3.396925	-1.577590	0.206514
26	6	0	4.251858	-1.590062	1.315838
27	6	0	3.525212	-2.580782	-0.767642
28	6	0	5.223136	-2.584026	1.447340
29	1	0	4.160386	-0.822819	2.082878
30	6	0	4.502551	-3.565093	-0.639587
31	1	0	2.852585	-2.588150	-1.625995
32	6	0	5.353943	-3.570023	0.469527
33	1	0	5.877883	-2.585079	2.315442
34	1	0	4.594487	-4.334813	-1.401712
35	1	0	6.110314	-4.344203	0.572270
36	6	0	-0.764545	2.340726	-0.411639

37	6	0	-1.023390	2.953692	-1.647768
38	6	0	0.121572	2.963765	0.481027
39	6	0	-0.397024	4.152882	-1.986680
40	1	0	-1.717733	2.490670	-2.347820
41	6	0	0.746264	4.161257	0.139101
42	1	0	0.312805	2.516975	1.455899
43	6	0	0.496464	4.755976	-1.099314
44	1	0	-0.608831	4.616628	-2.947499
45	1	0	1.428660	4.629098	0.845664
46	1	0	0.987960	5.688193	-1.367502
47	6	0	-2.921981	0.611057	-1.071385
48	6	0	-4.069265	1.341477	-0.734910
49	6	0	-2.898696	-0.128692	-2.259798
50	6	0	-5.177840	1.333496	-1.578742
51	1	0	-4.099987	1.907761	0.195550
52	6	0	-4.008388	-0.134519	-3.104353
53	1	0	-2.012967	-0.717670	-2.503110
54	6	0	-5.147958	0.597384	-2.765318
55	1	0	-6.068319	1.893353	-1.304753
56	1	0	-3.988511	-0.723888	-4.017370
57	1	0	-6.018365	0.581554	-3.416605
58	6	0	-2.050187	0.809595	1.675189
59	6	0	-2.393901	2.032917	2.268915
60	6	0	-2.249882	-0.380025	2.392237
61	6	0	-2.917110	2.065798	3.561424
62	1	0	-2.248739	2.962891	1.720160
63	6	0	-2.786786	-0.345163	3.677491
64	1	0	-1.990952	-1.334178	1.931304
65	6	0	-3.116813	0.877491	4.267036
66	1	0	-3.176339	3.020341	4.013537
67	1	0	-2.948315	-1.275019	4.216949
68	1	0	-3.530643	0.904160	5.272449
69	16	0	-0.057731	-3.546756	-0.658220
70	78	0	-0.069986	-1.150146	-0.331585
71	6	0	-1.464050	-2.646987	-0.441507
72	6	0	-2.779231	-2.771468	-0.304486
73	6	0	-4.010345	-2.518478	-0.104545
74	16	0	-5.557206	-2.277913	0.152921

Table S22. The theoretical Cartesian coordinates (in Å) for the structure **PtSe-I** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.529873	0.978820	-0.038134
2	15	0	-2.062615	0.253442	0.019869
3	6	0	2.265660	1.137081	1.621280
4	6	0	2.768800	2.345446	2.123694
5	6	0	2.357022	-0.023268	2.406071
6	6	0	3.347281	2.393805	3.392295
7	1	0	2.700497	3.251537	1.522356
8	6	0	2.947717	0.024621	3.667781
9	1	0	1.964200	-0.965601	2.017894
10	6	0	3.439435	1.234021	4.165364
11	1	0	3.730389	3.336768	3.774802
12	1	0	3.019984	-0.882651	4.262269
13	1	0	3.893590	1.272806	5.152882
14	6	0	1.092076	2.687550	-0.504984
15	6	0	1.456949	3.208838	-1.754784
16	6	0	0.270761	3.457982	0.335506
17	6	0	1.009376	4.467927	-2.156281
18	1	0	2.096093	2.628742	-2.419372
19	6	0	-0.174453	4.715833	-0.068071
20	1	0	-0.010643	3.076982	1.317817
21	6	0	0.189404	5.224237	-1.317587
22	1	0	1.305634	4.858665	-3.127291
23	1	0	-0.807337	5.296888	0.599559
24	1	0	-0.160188	6.204706	-1.632108
25	6	0	2.943600	0.615424	-1.131690
26	6	0	4.218238	1.153515	-0.908756
27	6	0	2.728125	-0.204440	-2.246562
28	6	0	5.262053	0.870008	-1.788699
29	1	0	4.395561	1.784704	-0.037913
30	6	0	3.769928	-0.478253	-3.132864
31	1	0	1.740839	-0.644385	-2.401570
32	6	0	5.038052	0.057781	-2.903766
33	1	0	6.251385	1.281832	-1.604082
34	1	0	3.594483	-1.123234	-3.990016
35	1	0	5.854851	-0.164813	-3.586384
36	6	0	-2.064790	1.329369	1.499117

37	6	0	-2.845573	2.487323	1.600546
38	6	0	-1.223935	0.979325	2.567013
39	6	0	-2.777723	3.286758	2.741830
40	1	0	-3.487728	2.786119	0.774609
41	6	0	-1.159652	1.775533	3.711245
42	1	0	-0.602681	0.085131	2.482456
43	6	0	-1.934058	2.934621	3.798491
44	1	0	-3.381587	4.189112	2.803595
45	1	0	-0.495249	1.494236	4.525478
46	1	0	-1.878825	3.562241	4.684635
47	6	0	-2.518115	1.318782	-1.387610
48	6	0	-3.806113	1.863588	-1.526189
49	6	0	-1.557143	1.591483	-2.367974
50	6	0	-4.109095	2.691773	-2.605078
51	1	0	-4.579136	1.615506	-0.798718
52	6	0	-1.860643	2.419075	-3.449188
53	1	0	-0.570918	1.132913	-2.283235
54	6	0	-3.133290	2.978458	-3.564000
55	1	0	-5.109061	3.107585	-2.702010
56	1	0	-1.101042	2.623876	-4.200268
57	1	0	-3.372427	3.623051	-4.406514
58	6	0	-3.528706	-0.792236	0.250579
59	6	0	-3.931564	-1.182855	1.534761
60	6	0	-4.188567	-1.327874	-0.865453
61	6	0	-5.000280	-2.062287	1.699979
62	1	0	-3.412871	-0.790766	2.409286
63	6	0	-5.264651	-2.197074	-0.696687
64	1	0	-3.862473	-1.059876	-1.869974
65	6	0	-5.675698	-2.564447	0.585723
66	1	0	-5.306769	-2.354086	2.701607
67	1	0	-5.773977	-2.597957	-1.569797
68	1	0	-6.512167	-3.246879	0.716171
69	78	0	-0.046205	-0.826368	-0.143970
70	6	0	0.943406	-2.748607	-0.166543
71	6	0	2.219821	-2.872992	-0.083825
72	6	0	-0.423888	-2.834824	-0.215308
73	34	0	-1.730265	-4.019029	-0.295605
74	34	0	3.934208	-2.956747	0.037700

Table S23. The theoretical Cartesian coordinates (in Å) for the structure **PtSe-II** using the M06L/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.196451	-0.549917	-0.043303
2	15	0	0.861064	1.378568	0.003353
3	6	0	-3.055348	-1.851361	-0.996158
4	6	0	-4.388136	-2.188100	-0.718811
5	6	0	-2.391534	-2.492583	-2.050018
6	6	0	-5.041711	-3.158321	-1.475296
7	1	0	-4.912840	-1.695990	0.099401
8	6	0	-3.049291	-3.460301	-2.811674
9	1	0	-1.351085	-2.242890	-2.260299
10	6	0	-4.372574	-3.796887	-2.523468
11	1	0	-6.071941	-3.419264	-1.245925
12	1	0	-2.522664	-3.956444	-3.622831
13	1	0	-4.881112	-4.558760	-3.109574
14	6	0	-3.027202	0.964590	-0.633610
15	6	0	-3.029362	2.127132	0.154230
16	6	0	-3.555816	1.028692	-1.932248
17	6	0	-3.541426	3.322421	-0.348141
18	1	0	-2.646032	2.097007	1.174263
19	6	0	-4.070365	2.225336	-2.430573
20	1	0	-3.564725	0.137347	-2.558812
21	6	0	-4.060907	3.377969	-1.642621
22	1	0	-3.537654	4.210789	0.279700
23	1	0	-4.477966	2.256061	-3.438577
24	1	0	-4.458761	4.311202	-2.033366
25	6	0	-2.819142	-0.777969	1.659124
26	6	0	-4.012764	-0.208247	2.126287
27	6	0	-2.077285	-1.603251	2.518166
28	6	0	-4.448615	-0.450636	3.429283
29	1	0	-4.602644	0.431998	1.471647
30	6	0	-2.518740	-1.851661	3.816845
31	1	0	-1.147817	-2.050197	2.159813
32	6	0	-3.703451	-1.272309	4.277672
33	1	0	-5.375044	-0.001101	3.778924
34	1	0	-1.934425	-2.495737	4.469132
35	1	0	-4.045959	-1.461687	5.292372
36	6	0	0.545717	2.364019	-1.496208

37	6	0	1.125507	3.630625	-1.680073
38	6	0	-0.277188	1.839942	-2.500158
39	6	0	0.857055	4.367297	-2.831633
40	1	0	1.809299	4.025446	-0.928680
41	6	0	-0.544323	2.577074	-3.653673
42	1	0	-0.689221	0.836933	-2.378205
43	6	0	0.015132	3.844455	-3.817672
44	1	0	1.312200	5.345556	-2.964873
45	1	0	-1.185608	2.156813	-4.425365
46	1	0	-0.189515	4.419117	-4.717952
47	6	0	0.019088	2.238860	1.375789
48	6	0	-0.290802	3.604673	1.363178
49	6	0	-0.356163	1.464433	2.483669
50	6	0	-0.986055	4.177624	2.428561
51	1	0	-0.025374	4.217367	0.503750
52	6	0	-1.053724	2.035518	3.547969
53	1	0	-0.116998	0.399681	2.491657
54	6	0	-1.376912	3.394343	3.518008
55	1	0	-1.234152	5.236237	2.402221
56	1	0	-1.355683	1.414957	4.388636
57	1	0	-1.931363	3.842115	4.339353
58	6	0	2.620238	1.678549	0.329917
59	6	0	3.536645	1.500389	-0.718766
60	6	0	3.093131	1.992370	1.609991
61	6	0	4.899750	1.670396	-0.496149
62	1	0	3.179107	1.223126	-1.710580
63	6	0	4.462111	2.152765	1.830728
64	1	0	2.394438	2.121158	2.435321
65	6	0	5.365825	1.995534	0.780145
66	1	0	5.604244	1.513354	-1.308463
67	1	0	4.820086	2.398842	2.827691
68	1	0	6.432923	2.107823	0.954692
69	78	0	0.182707	-0.814046	-0.115961
70	6	0	1.905615	-1.907478	-0.098788
71	6	0	3.223873	-1.787702	-0.093116
72	6	0	4.492075	-1.723334	-0.082855
73	34	0	6.221839	-1.666488	-0.074189
74	34	0	0.654879	-3.275400	-0.103103

Complete Gaussian 09 reference (Reference 45)

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