

Supporting Information

coordinates of complex 1
optimized (basis set A and VWN functional)

Ni	0.000000	0.000000	0.000000
S	1.483637	1.578470	0.000000
C	3.037034	0.684887	0.000000
C	4.216702	1.436130	0.000000
N	5.195074	2.079764	0.000000
S	1.483637	-1.578470	0.000000
C	3.037034	-0.684887	0.000000
C	4.216702	-1.436130	0.000000
N	5.195074	-2.079764	0.000000
S	-1.483637	1.578470	0.000000
C	-3.037034	0.684887	0.000000
C	-4.216702	1.436130	0.000000
N	-5.195074	2.079764	0.000000
S	-1.483637	-1.578470	0.000000
C	-3.037034	-0.684887	0.000000
C	-4.216702	-1.436130	0.000000
N	-5.195074	-2.079764	0.000000

coordinates of complex 2
optimized (basis set A and VWN functional)

Ni	0.000000	0.000000	0.002075
S	-1.514133	0.000000	-1.535141
S	1.514133	0.000000	-1.535141
O	-1.298296	0.000000	1.306913
O	1.298296	0.000000	1.306913
C	-2.928794	0.000000	-0.418954
C	-2.590197	0.000000	0.944956
C	-3.623574	0.000000	1.895267
C	-4.946607	0.000000	1.478626
C	-5.270807	0.000000	0.115847
C	-4.254343	0.000000	-0.833888
C	2.928794	0.000000	-0.418954
C	2.590197	0.000000	0.944956
C	3.623574	0.000000	1.895267
C	4.946607	0.000000	1.478626
C	5.270807	0.000000	0.115847
C	4.254343	0.000000	-0.833888
H	-5.747190	0.000000	2.225115
H	-6.316387	0.000000	-0.204435
H	-3.348716	0.000000	2.953975
H	-4.482293	0.000000	-1.904863
H	5.747190	0.000000	2.225115
H	6.316387	0.000000	-0.204435
H	3.348716	0.000000	2.953975
H	4.482293	0.000000	-1.904863

coordinates of complex 3
optimized (basis set A and VWN functional)

Ni	-0.124840	0.057670	0.000000
Cl	2.186329	0.100159	0.000000
Cl	-0.894467	-2.058276	0.000000
N	-0.332802	0.282116	-1.936858
N	-0.332802	0.282116	1.936858
C	-0.059541	1.876552	0.000000
C	-0.019114	2.545825	-1.213242
C	-0.069624	3.935593	-1.218190
C	-0.122704	4.621584	0.000000
C	-0.069624	3.935593	1.218190
C	-0.019114	2.545825	1.213242
C	0.243934	1.611375	-2.334555
C	0.243934	1.611375	2.334555
C	-1.793305	0.301114	-2.178377
C	0.316229	-0.796544	-2.707376
C	-1.793305	0.301114	2.178377
C	0.316229	-0.796544	2.707376
H	-0.040753	4.492546	-2.161070
H	-0.164894	5.714722	0.000000
H	-0.040753	4.492546	2.161070
H	-0.168256	1.920020	-3.315181
H	1.339043	1.468227	-2.413319
H	1.339043	1.468227	2.413319
H	-0.168256	1.920020	3.315181
H	-1.989724	0.377840	-3.268203
H	-2.229889	1.175249	-1.664770
H	-2.232558	-0.627801	-1.781413
H	0.246768	-0.571212	-3.791718
H	-0.185166	-1.748458	-2.478230
H	1.370563	-0.864869	-2.391593
H	-1.989724	0.377840	3.268203
H	-2.232558	-0.627801	1.781413
H	-2.229889	1.175249	1.664770
H	0.246768	-0.571212	3.791718
H	1.370563	-0.864869	2.391593
H	-0.185166	-1.748458	2.478230

coordinates of complex 4

optimized (basis set A and VWN functional)

Co	1.883421	-0.610245	-0.184423
S	0.536000	-2.206677	-0.689663
S	0.291266	0.790930	0.175910
C	3.598392	-1.705925	-0.124951
C	3.620269	-0.841054	-1.276523
C	3.496052	0.497507	-0.811388
C	3.406497	0.457743	0.627975
C	3.513573	-0.902142	1.056476
H	3.644724	-2.796006	-0.152307
H	3.685443	-1.161196	-2.316827
H	3.441494	1.394170	-1.429927
H	3.274048	1.323474	1.278151
H	3.487157	-1.262653	2.084698
C	-1.226097	-0.197813	-0.078655
C	-1.075816	-1.491558	-0.463121
H	-1.924335	-2.139716	-0.699883
C	-2.503605	0.425172	0.136505
H	-1.771255	2.459338	0.056901
H	-4.025526	3.472314	0.429441
H	-5.803881	-0.263456	0.687257
H	-3.637573	-1.413161	0.358357
C	-2.654680	1.829060	0.189579
C	-3.904045	2.384429	0.394725
N	-5.028674	1.657111	0.563630
C	-4.891953	0.323329	0.529144
C	-3.683561	-0.321515	0.327238