Electronic Supplementary Material (ESI) for Dalton Transactions

Towards a Low-Spin Configuration in Extended Metal Atom Chains. Theoretical Study of Trimetallic Systems with 22 Metal Electrons

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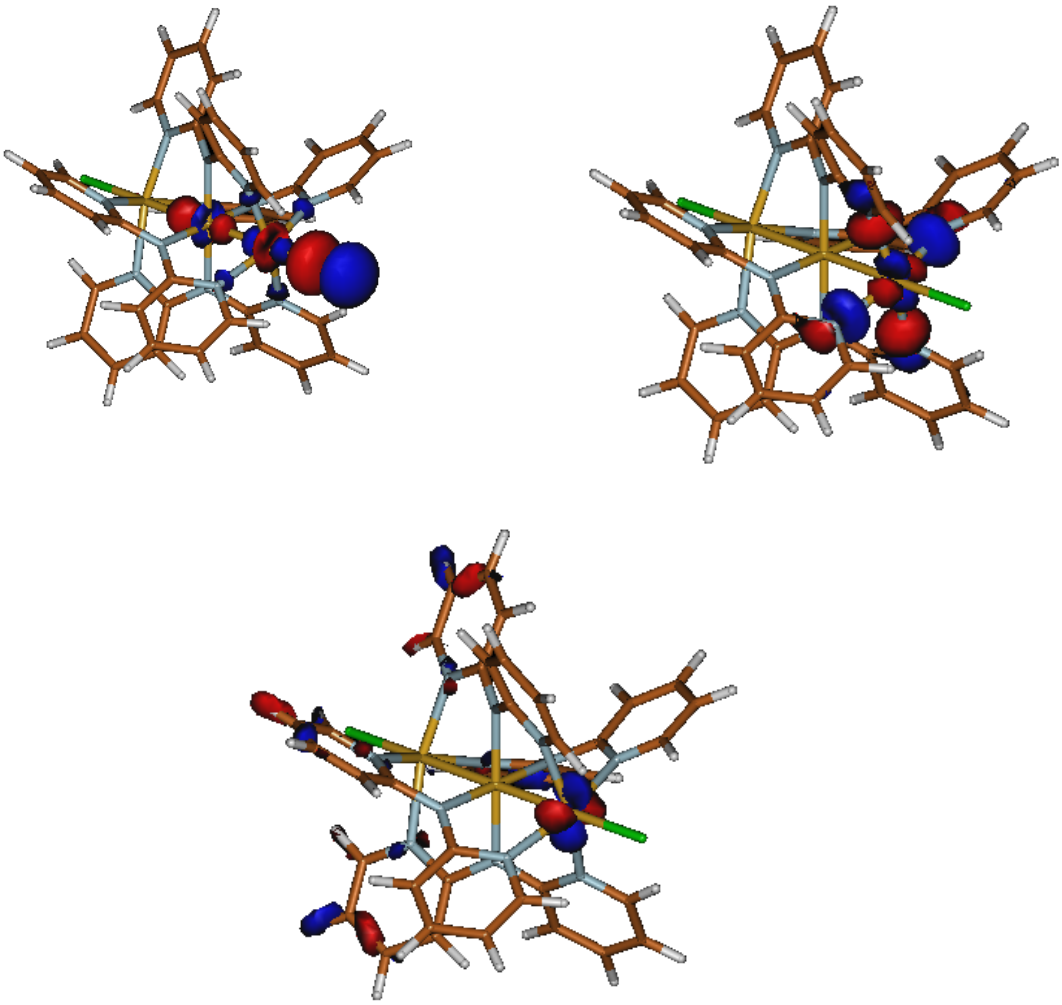
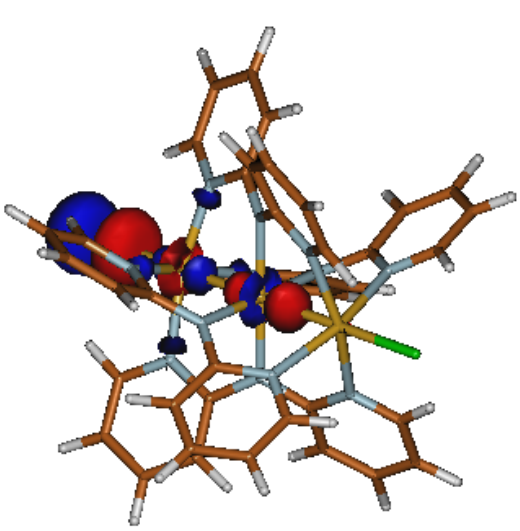
Supporting Information

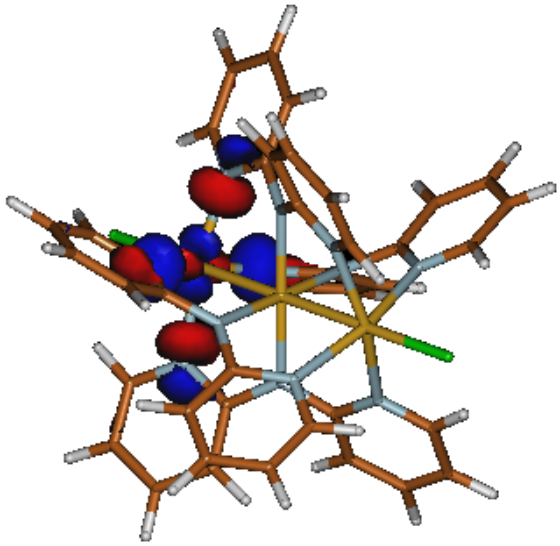
Figure S1. Singly-occupied molecular orbitals (alpha and beta spatial parts) obtained from a DFT broken-symmetry calculation for $CoPdCo(dpa)_4Cl_2$.

Alpha orbitals



Beta orbitals





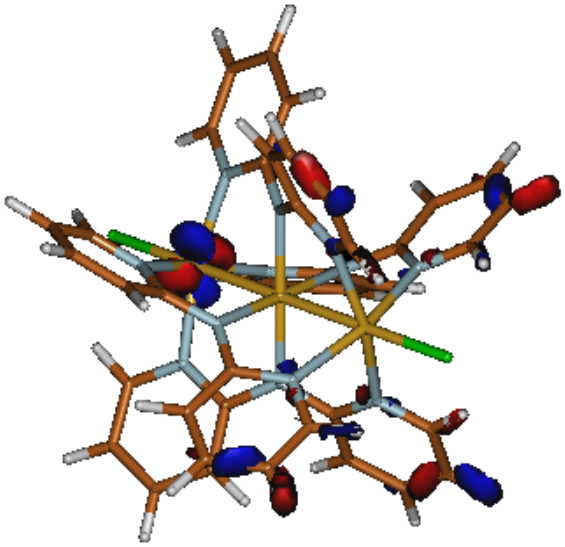


Table S1. DFT-optimized cartesian coordinates for compounds **2**-**8**.

Complex **2**: $CoPdCo(dpa)_4(NCS)_2$

Energy of the ground state: E(BS1)= -2823.4711833 a.u.

Coordinates (Angstroms)

	x	y	z
Pd	0.000000	0.000000	0.000000
Co	0.000000	0.000000	2.524164
Co	0.000000	0.000000	-2.524164
N	0.000000	0.000000	4.606365
C	0.000000	0.000000	5.795804
S	0.000000	0.000000	7.474622
N	0.000000	0.000000	-4.606365
C	0.000000	0.000000	-5.795804
S	0.000000	0.000000	-7.474622
N	0.000000	2.047473	0.000000
N	0.000000	-2.047473	0.000000
N	-2.047473	0.000000	0.000000
N	2.047473	0.000000	0.000000
N	0.683001	-2.036743	2.249142
N	-2.036743	-0.683001	2.249142
N	2.036743	0.683001	2.249142
N	-0.683001	2.036743	2.249142
N	-0.683001	-2.036743	-2.249142
N	2.036743	-0.683001	-2.249142
N	-2.036743	0.683001	-2.249142
N	0.683001	2.036743	-2.249142
C	0.605951	-2.708294	1.057050
C	-2.708294	-0.605951	1.057050
C	2.708294	0.605951	1.057050
C	-0.605951	2.708294	1.057050
C	-0.605951	-2.708294	-1.057050
C	2.708294	-0.605951	-1.057050
C	-2.708294	0.605951	-1.057050
C	0.605951	2.708294	-1.057050
C	1.208834	-3.997061	0.928057
C	-3.997061	-1.208834	0.928057
C	3.997061	1.208834	0.928057
C	-1.208834	3.997061	0.928057
C	-1.208834	-3.997061	-0.928057
C	3.997061	-1.208834	-0.928057
C	-3.997061	1.208834	-0.928057
C	1.208834	3.997061	-0.928057
C	1.840327	-4.584907	2.022672
C	-4.584907	-1.840327	2.022672
C	4.584907	1.840327	2.022672
C	-1.840327	4.584907	2.022672
C	-1.840327	-4.584907	-2.022672
C	4.584907	-1.840327	-2.022672
C	-4.584907	1.840327	-2.022672
C	1.840327	4.584907	-2.022672
C	1.884868	-3.891522	3.252193

C	-3.891522	-1.884868	3.252193
C	3.891522	1.884868	3.252193
C	-1.884868	3.891522	3.252193
C	-1.884868	-3.891522	-3.252193
C	3.891522	-1.884868	-3.252193
C	-3.891522	1.884868	-3.252193
C	1.884868	3.891522	-3.252193
C	1.306695	-2.621495	3.301232
C	-2.621495	-1.306695	3.301232
C	2.621495	1.306695	3.301232
C	-1.306695	2.621495	3.301232
C	-1.306695	-2.621495	-3.301232
C	2.621495	-1.306695	-3.301232
C	-2.621495	1.306695	-3.301232
C	1.306695	2.621495	-3.301232
H	1.203974	-4.492190	-0.035593
H	-4.492190	-1.203974	-0.035593
H	4.492190	1.203974	-0.035593
H	-1.203974	4.492190	-0.035593
H	-1.203974	-4.492190	0.035593
H	4.492190	-1.203974	0.035593
H	-4.492190	1.203974	0.035593
H	1.203974	4.492190	0.035593
H	2.309417	-5.560273	1.918168
H	-5.560273	-2.309417	1.918168
H	5.560273	2.309417	1.918168
H	-2.309417	5.560273	1.918168
H	-2.309417	-5.560273	-1.918168
H	5.560273	-2.309417	-1.918168
H	-5.560273	2.309417	-1.918168
H	2.309417	5.560273	-1.918168
H	2.360366	-4.308905	4.132850
H	-4.308905	-2.360366	4.132850
H	4.308905	2.360366	4.132850
H	-2.360366	4.308905	4.132850
H	-2.360366	-4.308905	-4.132850
H	4.308905	-2.360366	-4.132850
H	-4.308905	2.360366	-4.132850
H	2.360366	4.308905	-4.132850
H	1.325146	-2.034497	4.214200
H	-2.034497	-1.325146	4.214200
H	2.034497	1.325146	4.214200
H	-1.325146	2.034497	4.214200
H	-1.325146	-2.034497	-4.214200
H	2.034497	-1.325146	-4.214200
H	-2.034497	1.325146	-4.214200
H	1.325146	2.034497	-4.214200

Complex **3**: $CoNiCo(dpa)_4Cl_2$

Energy of the ground state: E(BS2)= -2690.0979266 a.u.

Coordinates (Angstroms)

	x	y	z
Ni	0.000000	0.000000	0.000000
Co	0.000000	0.000000	2.414129
Co	0.000000	0.000000	-2.414129
Cl	0.000000	0.000000	4.982498
Cl	0.000000	0.000000	-4.982498
N	0.000000	1.905398	0.000000
N	0.000000	-1.905398	0.000000
N	-1.905398	0.000000	0.000000
N	1.905398	0.000000	0.000000
N	0.739009	-1.868658	2.224084
N	-1.868658	-0.739009	2.224084
N	1.868658	0.739009	2.224084
N	-0.739009	1.868658	2.224084
N	-0.739009	-1.868658	-2.224084
N	1.868658	-0.739009	-2.224084
N	-1.868658	0.739009	-2.224084
N	0.739009	1.868658	-2.224084
C	0.631027	-2.557786	1.040690
C	-2.557786	-0.631027	1.040690
C	2.557786	0.631027	1.040690
C	-0.631027	2.557786	1.040690
C	-0.631027	-2.557786	-1.040690
C	2.557786	-0.631027	-1.040690
C	-2.557786	0.631027	-1.040690
C	0.631027	2.557786	-1.040690
C	1.237041	-3.843085	0.910728
C	-3.843085	-1.237041	0.910728
C	3.843085	1.237041	0.910728
C	-1.237041	3.843085	0.910728
C	-1.237041	-3.843085	-0.910728
C	3.843085	-1.237041	-0.910728
C	-3.843085	1.237041	-0.910728
C	1.237041	3.843085	-0.910728
C	1.919034	-4.407809	1.986917
C	-4.407809	-1.919034	1.986917
C	4.407809	1.919034	1.986917
C	-1.919034	4.407809	1.986917
C	-1.919034	-4.407809	-1.986917
C	4.407809	-1.919034	-1.986917
C	-4.407809	1.919034	-1.986917
C	1.919034	4.407809	-1.986917
C	2.010154	-3.689368	3.197973
C	-3.689368	-2.010154	3.197973
C	3.689368	2.010154	3.197973
C	-2.010154	3.689368	3.197973
C	-2.010154	-3.689368	-3.197973
C	3.689368	-2.010154	-3.197973
C	-3.689368	2.010154	-3.197973
C	2.010154	3.689368	-3.197973
C	1.418376	-2.425379	3.257551

C	-2.425379	-1.418376	3.257551
C	2.425379	1.418376	3.257551
C	-1.418376	2.425379	3.257551
C	-1.418376	-2.425379	-3.257551
C	2.425379	-1.418376	-3.257551
C	-2.425379	1.418376	-3.257551
C	1.418376	2.425379	-3.257551
H	1.196418	-4.351335	-0.045208
H	-4.351335	-1.196418	-0.045208
H	4.351335	1.196418	-0.045208
H	-1.196418	4.351335	-0.045208
H	-1.196418	-4.351335	0.045208
H	4.351335	-1.196418	0.045208
H	-4.351335	1.196418	0.045208
H	1.196418	4.351335	0.045208
H	2.390693	-5.381806	1.880241
H	-5.381806	-2.390693	1.880241
H	5.381806	2.390693	1.880241
H	-2.390693	5.381806	1.880241
H	-2.390693	-5.381806	-1.880241
H	5.381806	-2.390693	-1.880241
H	-5.381806	2.390693	-1.880241
H	2.390693	5.381806	-1.880241
H	2.527288	-4.084869	4.065323
H	-4.084869	-2.527288	4.065323
H	4.084869	2.527288	4.065323
H	-2.527288	4.084869	4.065323
H	-2.527288	-4.084869	-4.065323
H	4.084869	-2.527288	-4.065323
H	-4.084869	2.527288	-4.065323
H	2.527288	4.084869	-4.065323
H	1.450115	-1.824048	4.160273
H	-1.824048	-1.450115	4.160273
H	1.824048	1.450115	4.160273
H	-1.450115	1.824048	4.160273
H	-1.450115	-1.824048	-4.160273
H	1.824048	-1.450115	-4.160273
H	-1.824048	1.450115	-4.160273
H	1.450115	1.824048	-4.160273

Complex **4**: $CoNiCo(dpa)_4(NCS)_2$

Energy of the ground state: E(BS2)= -2866.0578544 a.u.

Coordinates (Angstroms)

	x	y	z
Ni	0.000000	0.000000	0.000000
Co	0.000000	0.000000	2.410454
Co	0.000000	0.000000	-2.410454
N	0.000000	0.000000	4.558862
C	0.000000	0.000000	5.747889
S	0.000000	0.000000	7.430584
N	0.000000	0.000000	-4.558862
C	0.000000	0.000000	-5.747889
S	0.000000	0.000000	-7.430584
N	0.000000	1.907966	0.000000
N	0.000000	-1.907966	0.000000
N	-1.907966	0.000000	0.000000
N	1.907966	0.000000	0.000000
N	0.726012	-1.868149	2.226694
N	-1.868149	-0.726012	2.226694
N	1.868149	0.726012	2.226694
N	-0.726012	1.868149	2.226694
N	-0.726012	-1.868149	-2.226694
N	1.868149	-0.726012	-2.226694
N	-1.868149	0.726012	-2.226694
N	0.726012	1.868149	-2.226694
C	0.623005	-2.560759	1.045677
C	-2.560759	-0.623005	1.045677
C	2.560759	0.623005	1.045677
C	-0.623005	2.560759	1.045677
C	-0.623005	-2.560759	-1.045677
C	2.560759	-0.623005	-1.045677
C	-2.560759	0.623005	-1.045677
C	0.623005	2.560759	-1.045677
C	1.223885	-3.849666	0.927448
C	-3.849666	-1.223885	0.927448
C	3.849666	1.223885	0.927448
C	-1.223885	3.849666	0.927448
C	-1.223885	-3.849666	-0.927448
C	3.849666	-1.223885	-0.927448
C	-3.849666	1.223885	-0.927448
C	1.223885	3.849666	-0.927448
C	1.890118	-4.414484	2.013423
C	-4.414484	-1.890118	2.013423
C	4.414484	1.890118	2.013423
C	-1.890118	4.414484	2.013423
C	-1.890118	-4.414484	-2.013423
C	4.414484	-1.890118	-2.013423
C	-4.414484	1.890118	-2.013423
C	1.890118	4.414484	-2.013423
C	1.973928	-3.692335	3.223271
C	-3.692335	-1.973928	3.223271
C	3.692335	1.973928	3.223271
C	-1.973928	3.692335	3.223271
C	-1.973928	-3.692335	-3.223271

C	3.692335	-1.973928	-3.223271
C	-3.692335	1.973928	-3.223271
C	1.973928	3.692335	-3.223271
C	1.391664	-2.424375	3.268807
C	-2.424375	-1.391664	3.268807
C	2.424375	1.391664	3.268807
C	-1.391664	2.424375	3.268807
C	-1.391664	-2.424375	-3.268807
C	2.424375	-1.391664	-3.268807
C	-2.424375	1.391664	-3.268807
C	1.391664	2.424375	-3.268807
H	1.190798	-4.362736	-0.026112
H	-4.362736	-1.190798	-0.026112
H	4.362736	1.190798	-0.026112
H	-1.190798	4.362736	-0.026112
H	-1.190798	-4.362736	0.026112
H	4.362736	-1.190798	0.026112
H	-4.362736	1.190798	0.026112
H	1.190798	4.362736	0.026112
H	2.355905	-5.392030	1.916085
H	-5.392030	-2.355905	1.916085
H	5.392030	2.355905	1.916085
H	-2.355905	5.392030	1.916085
H	-2.355905	-5.392030	-1.916085
H	5.392030	-2.355905	-1.916085
H	-5.392030	2.355905	-1.916085
H	2.355905	5.392030	-1.916085
H	2.479499	-4.087307	4.097377
H	-4.087307	-2.479499	4.097377
H	4.087307	2.479499	4.097377
H	-2.479499	4.087307	4.097377
H	-2.479499	-4.087307	-4.097377
H	4.087307	-2.479499	-4.097377
H	-4.087307	2.479499	-4.097377
H	2.479499	4.087307	-4.097377
H	1.431763	-1.820158	4.167426
H	-1.820158	-1.431763	4.167426
H	1.820158	1.431763	4.167426
H	-1.431763	1.820158	4.167426
H	-1.431763	-1.820158	-4.167426
H	1.820158	-1.431763	-4.167426
H	-1.820158	1.431763	-4.167426
H	1.431763	1.820158	-4.167426

Complex **5**: $RhNiRh(dpa)_4Cl_2$

Energy of the ground state: E(BS2)= -2618.9448599 a.u.

Coordinates (Angstroms)

	x	y	z
Ni	0.000000	0.000000	0.000000
Rh	0.000000	0.000000	2.413148
Rh	0.000000	0.000000	-2.413148
Cl	0.000000	0.000000	5.123833
Cl	0.000000	0.000000	-5.123833
N	0.000000	1.931359	0.000000
N	0.000000	-1.931359	0.000000
N	-1.931359	0.000000	0.000000
N	1.931359	0.000000	0.000000
N	0.710671	-1.954663	2.244610
N	-1.954663	-0.710671	2.244610
N	1.954663	0.710671	2.244610
N	-0.710671	1.954663	2.244610
N	-0.710671	-1.954663	-2.244610
N	1.954663	-0.710671	-2.244610
N	-1.954663	0.710671	-2.244610
N	0.710671	1.954663	-2.244610
C	0.628769	-2.601500	1.034950
C	-2.601500	-0.628769	1.034950
C	2.601500	0.628769	1.034950
C	-0.628769	2.601500	1.034950
C	-0.628769	-2.601500	-1.034950
C	2.601500	-0.628769	-1.034950
C	-2.601500	0.628769	-1.034950
C	0.628769	2.601500	-1.034950
C	1.251818	-3.875636	0.878707
C	-3.875636	-1.251818	0.878707
C	3.875636	1.251818	0.878707
C	-1.251818	3.875636	0.878707
C	-1.251818	-3.875636	-0.878707
C	3.875636	-1.251818	-0.878707
C	-3.875636	1.251818	-0.878707
C	1.251818	3.875636	-0.878707
C	1.900342	-4.477563	1.955855
C	-4.477563	-1.900342	1.955855
C	4.477563	1.900342	1.955855
C	-1.900342	4.477563	1.955855
C	-1.900342	-4.477563	-1.955855
C	4.477563	-1.900342	-1.955855
C	-4.477563	1.900342	-1.955855
C	1.900342	4.477563	-1.955855
C	1.946224	-3.807008	3.197229
C	-3.807008	-1.946224	3.197229
C	3.807008	1.946224	3.197229
C	-1.946224	3.807008	3.197229
C	-1.946224	-3.807008	-3.197229
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C	-3.807008	1.946224	-3.197229
C	1.946224	3.807008	-3.197229
C	1.353969	-2.545377	3.283326

C	-2.545377	-1.353969	3.283326
C	2.545377	1.353969	3.283326
C	-1.353969	2.545377	3.283326
C	-1.353969	-2.545377	-3.283326
C	2.545377	-1.353969	-3.283326
C	-2.545377	1.353969	-3.283326
C	1.353969	2.545377	-3.283326
H	1.240765	-4.351579	-0.094737
H	-4.351579	-1.240765	-0.094737
H	4.351579	1.240765	-0.094737
H	-1.240765	4.351579	-0.094737
H	-1.240765	-4.351579	0.094737
H	4.351579	-1.240765	0.094737
H	-4.351579	1.240765	0.094737
H	1.240765	4.351579	0.094737
H	2.379775	-5.445106	1.828293
H	-5.445106	-2.379775	1.828293
H	5.445106	2.379775	1.828293
H	-2.379775	5.445106	1.828293
H	-2.379775	-5.445106	-1.828293
H	5.445106	-2.379775	-1.828293
H	-5.445106	2.379775	-1.828293
H	2.379775	5.445106	-1.828293
H	2.433304	-4.235759	4.066158
H	-4.235759	-2.433304	4.066158
H	4.235759	2.433304	4.066158
H	-2.433304	4.235759	4.066158
H	-2.433304	-4.235759	-4.066158
H	4.235759	-2.433304	-4.066158
H	-4.235759	2.433304	-4.066158
H	2.433304	4.235759	-4.066158
H	1.358979	-1.969373	4.204009
H	-1.969373	-1.358979	4.204009
H	1.969373	1.358979	4.204009
H	-1.358979	1.969373	4.204009
H	-1.358979	-1.969373	-4.204009
H	1.969373	-1.358979	-4.204009
H	-1.969373	1.358979	-4.204009
H	1.358979	1.969373	-4.204009

Complex **6**: $RhNiRh(dpa)_4(NCS)_2$

Energy of the ground state: E(BS2)= -2794.8924797 a.u.

Coordinates (Angstroms)

	x	y	z
Ni	0.000000	0.000000	0.000000
Rh	0.000000	0.000000	2.411667
Rh	0.000000	0.000000	-2.411667
N	0.000000	0.000000	4.716989
C	0.000000	0.000000	5.906272
S	0.000000	0.000000	7.591465
N	0.000000	0.000000	-4.716989
C	0.000000	0.000000	-5.906272
S	0.000000	0.000000	-7.591465
N	0.000000	1.932320	0.000000
N	0.000000	-1.932320	0.000000
N	-1.932320	0.000000	0.000000
N	1.932320	0.000000	0.000000
N	0.703569	-1.955296	2.245787
N	-1.955296	-0.703569	2.245787
N	1.955296	0.703569	2.245787
N	-0.703569	1.955296	2.245787
N	-0.703569	-1.955296	-2.245787
N	1.955296	-0.703569	-2.245787
N	-1.955296	0.703569	-2.245787
N	0.703569	1.955296	-2.245787
C	0.624790	-2.603163	1.037403
C	-2.603163	-0.624790	1.037403
C	2.603163	0.624790	1.037403
C	-0.624790	2.603163	1.037403
C	-0.624790	-2.603163	-1.037403
C	2.603163	-0.624790	-1.037403
C	-2.603163	0.624790	-1.037403
C	0.624790	2.603163	-1.037403
C	1.244490	-3.879503	0.887350
C	-3.879503	-1.244490	0.887350
C	3.879503	1.244490	0.887350
C	-1.244490	3.879503	0.887350
C	-1.244490	-3.879503	-0.887350
C	3.879503	-1.244490	-0.887350
C	-3.879503	1.244490	-0.887350
C	1.244490	3.879503	-0.887350
C	1.883048	-4.482535	1.969816
C	-4.482535	-1.883048	1.969816
C	4.482535	1.883048	1.969816
C	-1.883048	4.482535	1.969816
C	-1.883048	-4.482535	-1.969816
C	4.482535	-1.883048	-1.969816
C	-4.482535	1.883048	-1.969816
C	1.883048	4.482535	-1.969816
C	1.924073	-3.810879	3.211109
C	-3.810879	-1.924073	3.211109
C	3.810879	1.924073	3.211109
C	-1.924073	3.810879	3.211109
C	-1.924073	-3.810879	-3.211109

C	3.810879	-1.924073	-3.211109
C	-3.810879	1.924073	-3.211109
C	1.924073	3.810879	-3.211109
C	1.337845	-2.546898	3.289346
C	-2.546898	-1.337845	3.289346
C	2.546898	1.337845	3.289346
C	-1.337845	2.546898	3.289346
C	-1.337845	-2.546898	-3.289346
C	2.546898	-1.337845	-3.289346
C	-2.546898	1.337845	-3.289346
C	1.337845	2.546898	-3.289346
H	1.237919	-4.358131	-0.084734
H	-4.358131	-1.237919	-0.084734
H	4.358131	1.237919	-0.084734
H	-1.237919	4.358131	-0.084734
H	-1.237919	-4.358131	0.084734
H	4.358131	-1.237919	0.084734
H	-4.358131	1.237919	0.084734
H	1.237919	4.358131	0.084734
H	2.358583	-5.452409	1.847366
H	-5.452409	-2.358583	1.847366
H	5.452409	2.358583	1.847366
H	-2.358583	5.452409	1.847366
H	-2.358583	-5.452409	-1.847366
H	5.452409	-2.358583	-1.847366
H	-5.452409	2.358583	-1.847366
H	2.358583	5.452409	-1.847366
H	2.403373	-4.240284	4.083755
H	-4.240284	-2.403373	4.083755
H	4.240284	2.403373	4.083755
H	-2.403373	4.240284	4.083755
H	-2.403373	-4.240284	-4.083755
H	4.240284	-2.403373	-4.083755
H	-4.240284	2.403373	-4.083755
H	2.403373	4.240284	-4.083755
H	1.348056	-1.971174	4.208534
H	-1.971174	-1.348056	4.208534
H	1.971174	1.348056	4.208534
H	-1.348056	1.971174	4.208534
H	-1.348056	-1.971174	-4.208534
H	1.971174	-1.348056	-4.208534
H	-1.971174	1.348056	-4.208534
H	1.348056	1.971174	-4.208534

Complex **7**: $RhPdRh(dpa)_4Cl_2$

Energy of the ground state: E(BS2)= -2576.3499926 a.u.

Coordinates (Angstroms)

	x	y	z
Pd	0.000000	0.000000	0.000000
Rh	0.000000	0.000000	2.463653
Rh	0.000000	0.000000	-2.463653
Cl	0.000000	0.000000	5.206638
Cl	0.000000	0.000000	-5.206638
N	0.000000	2.030584	0.000000
N	0.000000	-2.030584	0.000000
N	-2.030584	0.000000	0.000000
N	2.030584	0.000000	0.000000
N	0.616272	-2.007679	2.282621
N	-2.007679	-0.616272	2.282621
N	2.007679	0.616272	2.282621
N	-0.616272	2.007679	2.282621
N	-0.616272	-2.007679	-2.282621
N	2.007679	-0.616272	-2.282621
N	-2.007679	0.616272	-2.282621
N	0.616272	2.007679	-2.282621
C	0.570388	-2.681869	1.081743
C	-2.681869	-0.570388	1.081743
C	2.681869	0.570388	1.081743
C	-0.570388	2.681869	1.081743
C	-0.570388	-2.681869	-1.081743
C	2.681869	-0.570388	-1.081743
C	-2.681869	0.570388	-1.081743
C	0.570388	2.681869	-1.081743
C	1.176835	-3.969403	0.975026
C	-3.969403	-1.176835	0.975026
C	3.969403	1.176835	0.975026
C	-1.176835	3.969403	0.975026
C	-1.176835	-3.969403	-0.975026
C	3.969403	-1.176835	-0.975026
C	-3.969403	1.176835	-0.975026
C	1.176835	3.969403	-0.975026
C	1.764723	-4.566592	2.088562
C	-4.566592	-1.764723	2.088562
C	4.566592	1.764723	2.088562
C	-1.764723	4.566592	2.088562
C	-1.764723	-4.566592	-2.088562
C	4.566592	-1.764723	-2.088562
C	-4.566592	1.764723	-2.088562
C	1.764723	4.566592	-2.088562
C	1.765617	-3.876727	3.319240
C	-3.876727	-1.765617	3.319240
C	3.876727	1.765617	3.319240
C	-1.765617	3.876727	3.319240
C	-1.765617	-3.876727	-3.319240
C	3.876727	-1.765617	-3.319240
C	-3.876727	1.765617	-3.319240
C	1.765617	3.876727	-3.319240
C	1.199497	-2.601014	3.356583

C	-2.601014	-1.199497	3.356583
C	2.601014	1.199497	3.356583
C	-1.199497	2.601014	3.356583
C	-1.199497	-2.601014	-3.356583
C	2.601014	-1.199497	-3.356583
C	-2.601014	1.199497	-3.356583
C	1.199497	2.601014	-3.356583
H	1.204052	-4.458575	0.008748
H	-4.458575	-1.204052	0.008748
H	4.458575	1.204052	0.008748
H	-1.204052	4.458575	0.008748
H	-1.204052	-4.458575	-0.008748
H	4.458575	-1.204052	-0.008748
H	-4.458575	1.204052	-0.008748
H	1.204052	4.458575	-0.008748
H	2.231506	-5.544311	1.997005
H	-5.544311	-2.231506	1.997005
H	5.544311	2.231506	1.997005
H	-2.231506	5.544311	1.997005
H	-2.231506	-5.544311	-1.997005
H	5.544311	-2.231506	-1.997005
H	-5.544311	2.231506	-1.997005
H	2.231506	5.544311	-1.997005
H	2.202803	-4.299176	4.217259
H	-4.299176	-2.202803	4.217259
H	4.299176	2.202803	4.217259
H	-2.202803	4.299176	4.217259
H	-2.202803	-4.299176	-4.217259
H	4.299176	-2.202803	-4.217259
H	-4.299176	2.202803	-4.217259
H	2.202803	4.299176	-4.217259
H	1.182704	-2.009514	4.267736
H	-2.009514	-1.182704	4.267736
H	2.009514	1.182704	4.267736
H	-1.182704	2.009514	4.267736
H	-1.182704	-2.009514	-4.267736
H	2.009514	-1.182704	-4.267736
H	-2.009514	1.182704	-4.267736
H	1.182704	2.009514	-4.267736

Complex **8**: $RhPdRh(dpa)_4(NCS)_2$

Energy of the ground state: E(BS2)= -2752.2991733 a.u.

Coordinates (Angstroms)

	x	y	z
Pd	0.000000	0.000000	0.000000
Rh	0.000000	0.000000	2.463020
Rh	0.000000	0.000000	-2.463020
N	0.000000	0.000000	4.800475
C	0.000000	0.000000	5.990405
S	0.000000	0.000000	7.675622
N	0.000000	0.000000	-4.800475
C	0.000000	0.000000	-5.990405
S	0.000000	0.000000	-7.675622
N	0.000000	2.032069	0.000000
N	0.000000	-2.032069	0.000000
N	-2.032069	0.000000	0.000000
N	2.032069	0.000000	0.000000
N	0.599290	-2.010118	2.286251
N	-2.010118	-0.599290	2.286251
N	2.010118	0.599290	2.286251
N	-0.599290	2.010118	2.286251
N	-0.599290	-2.010118	-2.286251
N	2.010118	-0.599290	-2.286251
N	-2.010118	0.599290	-2.286251
N	0.599290	2.010118	-2.286251
C	0.561273	-2.684438	1.086196
C	-2.684438	-0.561273	1.086196
C	2.684438	0.561273	1.086196
C	-0.561273	2.684438	1.086196
C	-0.561273	-2.684438	-1.086196
C	2.684438	-0.561273	-1.086196
C	-2.684438	0.561273	-1.086196
C	0.561273	2.684438	-1.086196
C	1.163833	-3.974502	0.987336
C	-3.974502	-1.163833	0.987336
C	3.974502	1.163833	0.987336
C	-1.163833	3.974502	0.987336
C	-1.163833	-3.974502	-0.987336
C	3.974502	-1.163833	-0.987336
C	-3.974502	1.163833	-0.987336
C	1.163833	3.974502	-0.987336
C	1.735059	-4.574450	2.107899
C	-4.574450	-1.735059	2.107899
C	4.574450	1.735059	2.107899
C	-1.735059	4.574450	2.107899
C	-1.735059	-4.574450	-2.107899
C	4.574450	-1.735059	-2.107899
C	-4.574450	1.735059	-2.107899
C	1.735059	4.574450	-2.107899
C	1.724403	-3.885077	3.339264
C	-3.885077	-1.724403	3.339264
C	3.885077	1.724403	3.339264
C	-1.724403	3.885077	3.339264
C	-1.724403	-3.885077	-3.339264

C	3.885077	-1.724403	-3.339264
C	-3.885077	1.724403	-3.339264
C	1.724403	3.885077	-3.339264
C	1.166038	-2.606842	3.367037
C	-2.606842	-1.166038	3.367037
C	2.606842	1.166038	3.367037
C	-1.166038	2.606842	3.367037
C	-1.166038	-2.606842	-3.367037
C	2.606842	-1.166038	-3.367037
C	-2.606842	1.166038	-3.367037
C	1.166038	2.606842	-3.367037
H	1.200291	-4.465075	0.022170
H	-4.465075	-1.200291	0.022170
H	4.465075	1.200291	0.022170
H	-1.200291	4.465075	0.022170
H	-1.200291	-4.465075	-0.022170
H	4.465075	-1.200291	-0.022170
H	-4.465075	1.200291	-0.022170
H	1.200291	4.465075	-0.022170
H	2.197745	-5.554418	2.022497
H	-5.554418	-2.197745	2.022497
H	5.554418	2.197745	2.022497
H	-2.197745	5.554418	2.022497
H	-2.197745	-5.554418	-2.022497
H	5.554418	-2.197745	-2.022497
H	-5.554418	2.197745	-2.022497
H	2.197745	5.554418	-2.022497
H	2.147864	-4.309523	4.242642
H	-4.309523	-2.147864	4.242642
H	4.309523	2.147864	4.242642
H	-2.147864	4.309523	4.242642
H	-2.147864	-4.309523	-4.242642
H	4.309523	-2.147864	-4.242642
H	-4.309523	2.147864	-4.242642
H	2.147864	4.309523	-4.242642
H	1.149225	-2.017071	4.277097
H	-2.017071	-1.149225	4.277097
H	2.017071	1.149225	4.277097
H	-1.149225	2.017071	4.277097
H	-1.149225	-2.017071	-4.277097
H	2.017071	-1.149225	-4.277097
H	-2.017071	1.149225	-4.277097
H	1.149225	2.017071	-4.277097