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Supplementary Information

Effect of Methyl Groups in a Pyrimidine-based Flexible Ligand on the Formation of Silver(I) Coordination Networks

Fabio Marchetti, Riccardo Pettinari, Corrado di Nicola, Claudio Pettinari, Anup Paul, Alessandra Crispini, Eugenia Giorno, Sonia Stoia, Francesco Lelj, and Mario Amati

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Tests on different computational methods.

The computational method used in this work and presented in the main paper (M06-based DFT computations detailed in "Computational Method") was undergone to some tests to confirm the likelihood of the obtained results. Some relevant results reported in the paper were newly computed by using different methods.

A first test was performed on the interaction energies between couples of molecules (Figures 5 and 6 and Table 3). Couples A-G full interaction energies were computed by using the same basis set and pseudopotential of Table 3 but the B97D3 xc functional was used in place of M06.

Table S1. Computed interaction energies (kcal/mol) of selected couples of molecules shown in Figures 5 and 6. Computations performed at the B97D3 level if theory (see "Computational Details"). Differently to Table 3, only the full interaction energy was computed.

		BSSE Corrected	Not Corrected
	$[(L)AgNO_3]_2$ [a]		
Couple A	Full	-8.57	-10.15
Couple B	Full	-34.25	-42.12
Couple C	Full	-23.78	-30.07
Couple D	Full	-66.49	-83.72
	1		
Couple E	Full	-3.40	-5.50
Couple F	Full	-11.09	-13.90
Couple G	Full	-42.71	-51.94

[a] A. Mizar, C. Pettinari, F. Marchetti, I. Timokhin and A. Crispini, *Inorg. Chem. Commun*., 2012, **24**, 20-23.

Table S1 reports these results. The observed trend of the interaction energies is in line with the M06 results. The B97D3 values are invariably more stabilizing than the M06 ones, but all the conclusions described in the text (which was based on trends rather than absolute values) are confirmed by the B97D3 results.

Table S2. Computed energies (kcal/mol) of the Steps 1-3 for the **1b** minimum and transition structure shown in Figure 4. The cc-pVTZ basis set is centered on all the atoms apart from Ag. Reported in parenthesis are the energy gaps between the transition and minima structures.

1b		
	Minimum Structure	**TS Structure**
Preparation energy (Step 1)	+1.94	+2.52 (+0.58)
Interactions among ligands (Step 2)	-3.97	-6.14 (-2.40)
Ag-ligands interaction (Step 3)	-204.20	-195.58 (+8.63)
Total Energy	-206.01	-199.20 (+6.81)

A second test was performed about the dependence of our results from the used basis set. Steps 1-3 (Table 2) energies was newly computed using the more complete cc-pVTZ basis set in place of the 6-31G(d), which was used for the results in the paper. Table S2 collects our results for **1b** (Figure 4 for a graphical description of the "minimum" and "TS" structures). Single point computations were performed on the same structures optimized for the Table 2 values.

A comparison between Table S2 and Table 2 (for **1b**) allows concluding that no significant changes can be attributed to the use of a smaller basis set centered on the ligands in spite of their importance in determining the preferred arrangement of the inner coordination sphere. The larger aug-cc-pVTZ basis set was further applied for computing Steps 1 and 2 energies. Table S3 collects also these values.

Table S3. Computed energies (kcal/mol) of the Steps 1-2 for the **1b** minimum and transition structure shown in Figure 4. The aug-cc-pVTZ basis set is centered on all the atoms. Reported in parenthesis are the energy gaps between the transition and minima structures.

1b		
	Minimum Structure	**TS Structure**
Preparation energy (Step 1)	+1.82	+2.43 (+0.61)
Interactions among ligands (Step 2)	-3.89	-6.24 (-2.35)

Atomic Charges of L and L^{Me} Hydrogen atoms.

DFT computations were performed on **L** and **L^{Me}** experimental structures with the aim to compute the atomic charges of the hydrogen atoms. The same computational method detailed in "Computational Methods" and used throughout the main paper was applied. The ligands structures were extracted from the $[(L)AgNO_3]_2$ and **1** crystals, respectively.

Table S4. Hydrogen atomic charges (rages for each type oh H atoms) computed for **L** and **L^{Me}**. Mulliken's and NPA (Natural Population Analysis) charges are reported. The values in parenthesis were obtained after structure optimization of the C-H bond distances (and freezing the remaining parameters).

Hydrogen Atoms	**L**		**L^{Me}**	
	Mulliken	**NPA**	**Mulliken**	**NPA**
Phenyl Hydrogens	0.12 (0.15)	0.14 (0.14)	0.12-0.13 (0.14-0.16)	0.14 (0.14)
Ph-CH_2-S	0.22-0.24 (0.20-0.22)	0.23-0.25 (0.26-0.28)	0.22-0.23 (0.20-0.21)	0.23-0.24 (0.26-0.28)
Pyrimidine Hydrogens (*ortho* to N)	0.19-0.21 (0.20-0.22)	0.22-0.23 (0.23-0.25)	----	----
Pyrimidine Hydrogens (*meta* to N)	0.14-0.15 (0.15)	0.15-0.16 (0.14-0.15)	0.13-0.14 (0.13)	0.15 (0.14-0.15)

Table S4 lists the Mulliken's and NPA charges (Natural Charges, atomic charges obtained from the NBO-based Natural Population Analysis, g09 key: population = npa). As the experimental C-H distances

were arbitrary chosen, the same charges were also computed after C-H bond distances optimization, in which all the other parameters were frozen (such charges are in parenthesis).

From the "Ph-CH_2-S" entry, the most protic hydrogen atoms (intended as the H atoms of higher charge) are the ones of the methylene group linked to the phenyl group and the S atom. This finding is common to both **L** and **L^{Me}**. In **L**, the pyrimidine hydrogen atoms in *ortho* to the N heteroatoms are computed as relatively protic in comparison to the *meta* ones.

Energy curves at the B97D3 level.

The energy curves of Figure 4 were computed with the B97D3 xc functional. The basis set and pseudopotential used for M06 computations (see "Computational Methods" for details) were applied also in these computations. Figure S1 shows the obtained results.

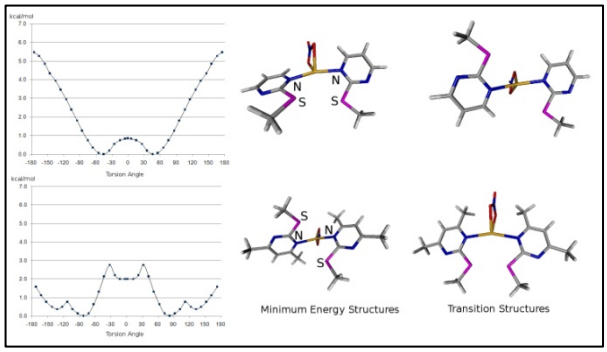

Figure S1. Molecular energy as a function of the relative position of the two pyrimidine rings measured by the dihedral defined by the S-N-N-S atoms showed in the left structure) and (see "Computational Details" for a more extended description) in the case of the model complexes **Dc** (top) and **1b** (bottom). The shown structures correspond to the minimum energy and transition structures associated to the respective energy curves.

In comparison to Figure 4 in the paper, **Dc** (top part of the figure) shows a very similar energy curve. This fact confirms the energy preference for a minimum structure suitable to dinuclear complexes, as obtained from M06 computations. **1b** shows a more different curve (bottom) in comparison to Figure 3 (bottom) in which a smaller barrier around 0 degrees is obtained. However, the general characteristics are preserved, like the absolute minimum around 90 degrees and an energy barrier which hinders the obtainment of torsion angles around 0 degrees, hence hindering dinuclear complexes as described by M06 computations.

Cartesian coordinates (angstrom) of Couples A-G discussed in the paper.

Couple A

Ag	1.780273	10.055614	5.333420
S	9.047450	13.966819	11.473683
S	4.569940	11.765557	5.766321
S	9.642691	8.709133	7.937806
O	-0.749866	10.181254	4.641875
O	0.226480	11.771609	3.819201
O	-1.829101	11.546968	3.434040
N	10.057528	15.591965	13.213888
N	7.672801	15.533328	13.141593
N	2.110519	11.849126	6.595103
N	3.549700	13.480242	7.528713
N	12.209264	8.942720	8.343908
N	10.819214	10.247594	9.761151
N	-0.803697	11.189504	3.921412
C	6.678132	13.139543	8.658020
H	6.331728	13.999849	8.589464
C	6.603798	12.280499	7.578572
C	7.121360	10.990527	7.703219
H	7.063395	10.404765	6.984003
C	7.716241	10.568366	8.872414
C	7.779722	11.439239	9.940643
H	8.171750	11.159082	10.735895
C	7.269490	12.724387	9.847157
C	7.322236	13.669645	11.031309
H	6.891900	14.508567	10.801958
H	6.850799	13.281121	11.784181
C	8.883135	15.166038	12.755185
C	7.658350	16.438554	14.115090
H	6.833218	16.726797	14.434188
C	8.774791	16.964243	14.668525
H	8.730755	17.606949	15.339129
C	9.962424	16.508626	14.194864
H	10.745783	16.844511	14.565068
C	6.000124	12.737314	6.285977
H	5.730730	13.664467	6.378216
H	6.675994	12.694502	5.592936
C	3.298296	12.453565	6.755898
C	2.517208	13.983709	8.198070
H	2.659850	14.703354	8.770203
C	1.258117	13.481884	8.072176
H	0.540039	13.865666	8.520907
C	1.090539	12.404387	7.273185
H	0.241277	12.035354	7.188425
C	8.237141	9.171581	8.999554
H	8.500232	9.032982	9.923192
H	7.506745	8.561227	8.813829
C	13.275545	9.539919	8.887371
H	14.123576	9.292848	8.595696
C	13.167156	10.491025	9.844665
H	13.915770	10.921569	10.188692
C	11.913160	10.788336	10.283424
H	11.818812	11.398314	10.978957
C	11.012585	9.383910	8.793886
Ag	12.474359	7.108636	7.131336
S	5.207182	3.197431	0.991073
S	9.684692	5.398694	6.698435
S	4.611941	8.455117	4.526950
O	15.004498	6.982996	7.822881
O	14.028153	5.392641	8.645555
O	16.083733	5.617282	9.030716
N	4.197104	1.572285	-0.749132
N	6.581831	1.630922	-0.676836
N	12.144113	5.315124	5.869654
N	10.704932	3.684008	4.936043
N	2.045368	8.221530	4.120848
N	3.435418	6.916656	2.703606
N	15.058329	5.974746	8.543344
C	7.576500	4.024707	3.806737
H	7.922904	3.164401	3.875293
C	7.650834	4.883751	4.886184
C	7.133272	6.173723	4.761537
H	7.191237	6.759485	5.480753
C	6.538391	6.595884	3.592343
C	6.474910	5.725011	2.524113
H	6.082882	6.005168	1.728862
C	6.985142	4.439863	2.617599
C	6.932396	3.494605	1.433447
H	7.362732	2.655683	1.662798
H	7.403833	3.883129	0.680576
C	5.371497	1.998212	-0.290429
C	6.596282	0.725696	-1.650334
H	7.421414	0.437453	-1.969431
C	5.479841	0.200007	-2.203769
H	5.523877	-0.442699	-2.874373
C	4.292208	0.655624	-1.730108
H	3.508849	0.319739	-2.100311
C	8.254508	4.426936	6.178780
H	8.523902	3.499783	6.086540
H	7.578638	4.469748	6.871820
C	10.956336	4.710685	5.708858
C	11.737424	3.180542	4.266686
H	11.594782	2.460896	3.694554
C	12.996515	3.682366	4.392580
H	13.714593	3.298584	3.943849
C	13.164093	4.759863	5.191571
H	14.013355	5.128896	5.276331
C	6.017491	7.992670	3.465202
H	5.754400	8.131268	2.541564
H	6.747887	8.603023	3.650927
C	0.979087	7.624331	3.577385
H	0.131056	7.871402	3.869060
C	1.087476	6.673225	2.620092
H	0.338862	6.242681	2.276064
C	2.341472	6.375914	2.181332
H	2.435820	5.765936	1.485799
C	3.242047	7.780340	3.670871
Ag	-12.811880	4.256954	-7.131336
S	-5.544703	8.168159	-0.991073
S	-10.022213	5.966896	-6.698435
S	-4.949463	2.910473	-4.526950
O	-15.342019	4.382594	-7.822881
O	-14.365674	5.972948	-8.645555
O	-16.421255	5.748307	-9.030716
N	-4.534625	9.793304	0.749132
N	-6.919353	9.734668	0.676836
N	-12.481634	6.050465	-5.869654
N	-11.042453	7.681581	-4.936043

N	-2.382889	3.144060	-4.120848
N	-3.772939	4.448933	-2.703606
N	-15.395851	5.390844	-8.543344
C	-7.914022	7.340882	-3.806737
H	-8.260425	8.201188	-3.875293
C	-7.988355	6.481839	-4.886184
C	-7.470794	5.191866	-4.761537
H	-7.528758	4.606104	-5.480753
C	-6.875913	4.769706	-3.592343
C	-6.812432	5.640579	-2.524113
H	-6.420403	5.360421	-1.728862
C	-7.322663	6.925726	-2.617599
C	-7.269917	7.870985	-1.433447
H	-7.700253	8.709907	-1.662798
H	-7.741354	7.482461	-0.680576
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C	-6.933803	10.639894	1.650334
H	-7.758936	10.928136	1.969431
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C	-4.629729	10.709965	1.730108
H	-3.846370	11.045850	2.100311
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H	-8.861423	7.865807	-6.086540
H	-7.916159	6.895842	-6.871820
C	-11.293858	6.654904	-5.708858
C	-12.074946	8.185048	-4.266686
H	-11.932303	8.904693	-3.694554
C	-13.334037	7.683223	-4.392580
H	-14.052114	8.067005	-3.943849
C	-13.501614	6.605726	-5.191571
H	-14.350876	6.236693	-5.276331
C	-6.355013	3.372920	-3.465202
H	-6.091921	3.234321	-2.541564
H	-7.085409	2.762566	-3.650927
C	-1.316609	3.741259	-3.577385
H	-0.468578	3.494187	-3.869060
C	-1.424997	4.692365	-2.620092
H	-0.676384	5.122909	-2.276064
C	-2.678993	4.989675	-2.181332
H	-2.773341	5.599653	-1.485799
C	-3.579568	3.585249	-3.670871
Ag	-2.117795	1.309975	-5.333420
S	-9.384972	-2.601230	-11.473683
S	-4.907461	-0.399967	-5.766321
S	-9.980212	2.656456	-7.937806
O	0.412344	1.184335	-4.641875
O	-0.564001	-0.406020	-3.819201
O	1.491580	-0.181379	-3.434040
N	-10.395050	-4.226376	-13.213888
N	-8.010322	-4.167739	-13.141593
N	-2.448041	-0.483536	-6.595103
N	-3.887222	-2.114653	-7.528713
N	-12.546786	2.422869	-8.343908
N	-11.156736	1.117996	-9.761151
N	0.466176	0.176085	-3.921412
C	-7.015653	-1.773953	-8.658020
H	-6.669250	-2.634259	-8.589464
C	-6.941319	-0.914910	-7.578572
C	-7.458881	0.375063	-7.703219
H	-7.400917	0.960825	-6.984003
C	-8.053762	0.797223	-8.872414
C	-8.117243	-0.073650	-9.940643
H	-8.509272	0.206507	-10.735895
C	-7.607011	-1.358797	-9.847157
C	-7.659758	-2.304056	-11.031309
H	-7.229422	-3.142978	-10.801958
H	-7.188320	-1.915532	-11.784181
C	-9.220656	-3.800448	-12.755185
C	-7.995871	-5.072965	-14.115090
H	-7.170739	-5.361207	-14.434188
C	-9.112313	-5.598653	-14.668525
H	-9.068277	-6.241360	-15.339129
C	-10.299946	-5.143036	-14.194864
H	-11.083304	-5.478921	-14.565068
C	-6.337645	-1.371725	-6.285977
H	-6.068251	-2.298878	-6.378216
H	-7.013515	-1.328913	-5.592936
C	-3.635817	-1.087975	-6.755898
C	-2.854729	-2.618119	-8.198070
H	-2.997371	-3.337765	-8.770203
C	-1.595638	-2.116295	-8.072176
H	-0.877561	-2.500076	-8.520907
C	-1.428061	-1.038797	-7.273185
H	-0.578798	-0.669764	-7.188425
C	-8.574662	2.194009	-8.999554
H	-8.837754	2.332608	-9.923192
H	-7.844266	2.804363	-8.813829
C	-13.613066	1.825670	-8.887371
H	-14.461097	2.072742	-8.595696
C	-13.504677	0.874564	-9.844665
H	-14.253291	0.444020	-10.188692
C	-12.250682	0.577254	-10.283424
H	-12.156333	-0.032725	-10.978957
C	-11.350107	1.981679	-8.793886

Couple B

Ag	1.780273	10.055614	5.333420
S	9.047450	13.966819	11.473683
S	4.569940	11.765557	5.766321
S	9.642691	8.709133	7.937806
O	-0.749866	10.181254	4.641875
O	0.226480	11.771609	3.819201
O	-1.829101	11.546968	3.434040
N	10.057528	15.591965	13.213888
N	7.672801	15.533328	13.141593
N	2.110519	11.849126	6.595103
N	3.549700	13.480242	7.528713
N	12.209264	8.942720	8.343908
N	10.819214	10.247594	9.761151
N	-0.803697	11.189504	3.921412
C	6.678132	13.139543	8.658020
H	6.331728	13.999849	8.589464
C	6.603798	12.280499	7.578572
C	7.121360	10.990527	7.703219
H	7.063395	10.404765	6.984003
C	7.716241	10.568366	8.872414
C	7.779722	11.439239	9.940643
H	8.171750	11.159082	10.735895
C	7.269490	12.724387	9.847157
C	7.322236	13.669645	11.031309
H	6.891900	14.508567	10.801958
H	6.850799	13.281121	11.784181
C	8.883135	15.166038	12.755185
C	7.658350	16.438554	14.115090
H	6.833218	16.726797	14.434188
C	8.774791	16.964243	14.668525
H	8.730755	17.606949	15.339129
C	9.962424	16.508626	14.194864
H	10.745783	16.844511	14.565068
C	6.000124	12.737314	6.285977
H	5.730730	13.664467	6.378216
H	6.675994	12.694502	5.592936
C	3.298296	12.453565	6.755898
C	2.517208	13.983709	8.198070
H	2.659850	14.703354	8.770203
C	1.258117	13.481884	8.072176
H	0.540039	13.865666	8.520907
C	1.090539	12.404387	7.273185
H	0.241277	12.035354	7.188425
C	8.237141	9.171581	8.999554
H	8.500232	9.032982	9.923192
H	7.506745	8.561227	8.813829
C	13.275545	9.539919	8.887371
H	14.123576	9.292848	8.595696
C	13.167156	10.491025	9.844665
H	13.915770	10.921569	10.188692
C	11.913160	10.788336	10.283424
H	11.818812	11.398314	10.978957
C	11.012585	9.383910	8.793886
Ag	12.474359	7.108636	7.131336
S	5.207182	3.197431	0.991073
S	9.684692	5.398694	6.698435
S	4.611941	8.455117	4.526950
O	15.004498	6.982996	7.822881
O	14.028153	5.392641	8.645555
O	16.083733	5.617282	9.030716
N	4.197104	1.572285	-0.749132
N	6.581831	1.630922	-0.676836
N	12.144113	5.315124	5.869654
N	10.704932	3.684008	4.936043
N	2.045368	8.221530	4.120848
N	3.435418	6.916656	2.703606
N	15.058329	5.974746	8.543344
C	7.576500	4.024707	3.806737
H	7.922904	3.164401	3.875293
C	7.650834	4.883751	4.886184
C	7.133272	6.173723	4.761537
H	7.191237	6.759485	5.480753
C	6.538391	6.595884	3.592343
C	6.474910	5.725011	2.524113
H	6.082882	6.005168	1.728862
C	6.985142	4.439863	2.617599
C	6.932396	3.494605	1.433447
H	7.362732	2.655683	1.662798
H	7.403833	3.883129	0.680576
C	5.371497	1.998212	-0.290429
C	6.596282	0.725696	-1.650334
H	7.421414	0.437453	-1.969431
C	5.479841	0.200007	-2.203769
H	5.523877	-0.442699	-2.874373
C	4.292208	0.655624	-1.730108
H	3.508849	0.319739	-2.100311
C	8.254508	4.426936	6.178780
H	8.523902	3.499783	6.086540
H	7.578638	4.469748	6.871820
C	10.956336	4.710685	5.708858
C	11.737424	3.180542	4.266686
H	11.594782	2.460896	3.694554
C	12.996515	3.682366	4.392580
H	13.714593	3.298584	3.943849
C	13.164093	4.759863	5.191571
H	14.013355	5.128896	5.276331
C	6.017491	7.992670	3.465202
H	5.754400	8.131268	2.541564
H	6.747887	8.603023	3.650927
C	0.979087	7.624331	3.577385
H	0.131056	7.871402	3.869060
C	1.087476	6.673225	2.620092
H	0.338862	6.242681	2.276064
C	2.341472	6.375914	2.181332
H	2.435820	5.765936	1.485799
C	3.242047	7.780340	3.670871
Ag	-3.523080	4.256954	-7.131336
S	3.744097	8.168159	-0.991073
S	-0.733413	5.966896	-6.698435
S	4.339337	2.910473	-4.526950
O	-6.053219	4.382594	-7.822881
O	-5.076874	5.972948	-8.645555
O	-7.132455	5.748307	-9.030716
N	4.754175	9.793304	0.749132
N	2.369447	9.734668	0.676836
N	-3.192834	6.050465	-5.869654
N	-1.753653	7.681581	-4.936043

N	6.905911	3.144060	-4.120848
N	5.515861	4.448933	-2.703606
N	-6.107051	5.390844	-8.543344
C	1.374778	7.340882	-3.806737
H	1.028375	8.201188	-3.875293
C	1.300445	6.481839	-4.886184
C	1.818006	5.191866	-4.761537
H	1.760042	4.606104	-5.480753
C	2.412887	4.769706	-3.592343
C	2.476368	5.640579	-2.524113
H	2.868397	5.360421	-1.728862
C	1.966137	6.925726	-2.617599
C	2.018883	7.870985	-1.433447
H	1.588547	8.709907	-1.662798
H	1.547446	7.482461	-0.680576
C	3.579782	9.367377	0.290429
C	2.354997	10.639894	1.650334
H	1.529864	10.928136	1.969431
C	3.471438	11.165582	2.203769
H	3.427402	11.808289	2.874373
C	4.659071	10.709965	1.730108
H	5.442430	11.045850	2.100311
C	0.696771	6.938654	-6.178780
H	0.427377	7.865807	-6.086540
H	1.372641	6.895842	-6.871820
C	-2.005058	6.654904	-5.708858
C	-2.786146	8.185048	-4.266686
H	-2.643503	8.904693	-3.694554
C	-4.045237	7.683223	-4.392580
H	-4.763314	8.067005	-3.943849
C	-4.212814	6.605726	-5.191571
H	-5.062076	6.236693	-5.276331
C	2.933787	3.372920	-3.465202
H	3.196879	3.234321	-2.541564
H	2.203391	2.762566	-3.650927
C	7.972191	3.741259	-3.577385
H	8.820222	3.494187	-3.869060
C	7.863803	4.692365	-2.620092
H	8.612416	5.122909	-2.276064
C	6.609807	4.989675	-2.181332
H	6.515459	5.599653	-1.485799
C	5.709232	3.585249	-3.670871
Ag	7.171005	1.309975	-5.333420
S	-0.096172	-2.601230	-11.473683
S	4.381339	-0.399967	-5.766321
S	-0.691412	2.656456	-7.937806
O	9.701144	1.184335	-4.641875
O	8.724799	-0.406020	-3.819201
O	10.780380	-0.181379	-3.434040
N	-1.106250	-4.226376	-13.213888
N	1.278478	-4.167739	-13.141593
N	6.840759	-0.483536	-6.595103
N	5.401578	-2.114653	-7.528713
N	-3.257986	2.422869	-8.343908
N	-1.867936	1.117996	-9.761151
N	9.754976	0.176085	-3.921412
C	2.273147	-1.773953	-8.658020
H	2.619550	-2.634259	-8.589464
C	2.347481	-0.914910	-7.578572
C	1.829919	0.375063	-7.703219
H	1.887883	0.960825	-6.984003
C	1.235038	0.797223	-8.872414
C	1.171557	-0.073650	-9.940643
H	0.779528	0.206507	-10.735895
C	1.681789	-1.358797	-9.847157
C	1.629042	-2.304056	-11.031309
H	2.059378	-3.142978	-10.801958
H	2.100480	-1.915532	-11.784181
C	0.068144	-3.800448	-12.755185
C	1.292929	-5.072965	-14.115090
H	2.118061	-5.361207	-14.434188
C	0.176487	-5.598653	-14.668525
H	0.220523	-6.241360	-15.339129
C	-1.011146	-5.143036	-14.194864
H	-1.794504	-5.478921	-14.565068
C	2.951155	-1.371725	-6.285977
H	3.220549	-2.298878	-6.378216
H	2.275285	-1.328913	-5.592936
C	5.652983	-1.087975	-6.755898
C	6.434071	-2.618119	-8.198070
H	6.291429	-3.337765	-8.770203
C	7.693162	-2.116295	-8.072176
H	8.411239	-2.500076	-8.520907
C	7.860739	-1.038797	-7.273185
H	8.710002	-0.669764	-7.188425
C	0.714138	2.194009	-8.999554
H	0.451046	2.332608	-9.923192
H	1.444534	2.804363	-8.813829
C	-4.324266	1.825670	-8.887371
H	-5.172297	2.072742	-8.595696
C	-4.215877	0.874564	-9.844665
H	-4.964491	0.444020	-10.188692
C	-2.961882	0.577254	-10.283424
H	-2.867533	-0.032725	-10.978957
C	-2.061307	1.981679	-8.793886

Couple C

Ag	3.185559	7.108636	7.131336
S	-4.081618	3.197431	0.991073
S	0.395892	5.398694	6.698435
S	-4.676859	8.455117	4.526950
O	5.715698	6.982996	7.822881
O	4.739353	5.392641	8.645555
O	6.794933	5.617282	9.030716
N	-5.091696	1.572285	-0.749132
N	-2.706969	1.630922	-0.676836
N	2.855313	5.315124	5.869654
N	1.416132	3.684008	4.936043
N	-7.243432	8.221530	4.120848
N	-5.853382	6.916656	2.703606
N	5.769529	5.974746	8.543344
C	-1.712300	4.024707	3.806737
H	-1.365896	3.164401	3.875293
C	-1.637966	4.883751	4.886184
C	-2.155528	6.173723	4.761537
H	-2.097563	6.759485	5.480753
C	-2.750409	6.595884	3.592343
C	-2.813890	5.725011	2.524113
H	-3.205918	6.005168	1.728862
C	-2.303658	4.439863	2.617599
C	-2.356404	3.494605	1.433447
H	-1.926068	2.655683	1.662798
H	-1.884967	3.883129	0.680576
C	-3.917303	1.998212	-0.290429
C	-2.692518	0.725696	-1.650334
H	-1.867386	0.437453	-1.969431
C	-3.808959	0.200007	-2.203769
H	-3.764923	-0.442699	-2.874373
C	-4.996592	0.655624	-1.730108
H	-5.779951	0.319739	-2.100311
C	-1.034292	4.426936	6.178780
H	-0.764898	3.499783	6.086540
H	-1.710162	4.469748	6.871820
C	1.667536	4.710685	5.708858
C	2.448624	3.180542	4.266686
H	2.305982	2.460896	3.694554
C	3.707715	3.682366	4.392580
H	4.425793	3.298584	3.943849
C	3.875293	4.759863	5.191571
H	4.724555	5.128896	5.276331
C	-3.271309	7.992670	3.465202
H	-3.534400	8.131268	2.541564
H	-2.540913	8.603023	3.650927
C	-8.309713	7.624331	3.577385
H	-9.157744	7.871402	3.869060
C	-8.201324	6.673225	2.620092
H	-8.949938	6.242681	2.276064
C	-6.947328	6.375914	2.181332
H	-6.852980	5.765936	1.485799
C	-6.046753	7.780340	3.670871
Ag	-7.508527	10.055614	5.333420
S	-0.241350	13.966819	11.473683
S	-4.718860	11.765557	5.766321
S	0.353891	8.709133	7.937806
O	-10.038666	10.181254	4.641875
O	-9.062320	11.771609	3.819201
O	-11.117901	11.546968	3.434040
N	0.768728	15.591965	13.213888
N	-1.615999	15.533328	13.141593
N	-7.178281	11.849126	6.595103
N	-5.739100	13.480242	7.528713
N	2.920464	8.942720	8.343908
N	1.530414	10.247594	9.761151
N	-10.092497	11.189504	3.921412
C	-2.610668	13.139543	8.658020
H	-2.957072	13.999849	8.589464
C	-2.685002	12.280499	7.578572
C	-2.167440	10.990527	7.703219
H	-2.225405	10.404765	6.984003
C	-1.572559	10.568366	8.872414
C	-1.509078	11.439239	9.940643
H	-1.117050	11.159082	10.735895
C	-2.019310	12.724387	9.847157
C	-1.966564	13.669645	11.031309
H	-2.396900	14.508567	10.801958
H	-2.438001	13.281121	11.784181
C	-0.405665	15.166038	12.755185
C	-1.630450	16.438554	14.115090
H	-2.455582	16.726797	14.434188
C	-0.514009	16.964243	14.668525
H	-0.558045	17.606949	15.339129
C	0.673624	16.508626	14.194864
H	1.456983	16.844511	14.565068
C	-3.288676	12.737314	6.285977
H	-3.558070	13.664467	6.378216
H	-2.612806	12.694502	5.592936
C	-5.990504	12.453565	6.755898
C	-6.771592	13.983709	8.198070
H	-6.628950	14.703354	8.770203
C	-8.030683	13.481884	8.072176
H	-8.748761	13.865666	8.520907
C	-8.198261	12.404387	7.273185
H	-9.047523	12.035354	7.188425
C	-1.051659	9.171581	8.999554
H	-0.788568	9.032982	9.923192
H	-1.782055	8.561227	8.813829
C	3.986745	9.539919	8.887371
H	4.834776	9.292848	8.595696
C	3.878356	10.491025	9.844665
H	4.626970	10.921569	10.188692
C	2.624360	10.788336	10.283424
H	2.530012	11.398314	10.978957
C	1.723785	9.383910	8.793886
Ag	-6.440763	18.474225	7.131336
S	-13.707940	14.563020	0.991073
S	-9.230429	16.764283	6.698435
S	-14.303180	19.820706	4.526950
O	-3.910624	18.348585	7.822881
O	-4.886969	16.758231	8.645555
O	-2.831388	16.982872	9.030716
N	-14.718018	12.937875	-0.749132
N	-12.333290	12.996511	-0.676836
N	-6.771009	16.680714	5.869654
N	-8.210190	15.049598	4.936043

N	-16.869754	19.587119	4.120848
N	-15.479704	18.282246	2.703606
N	-3.856792	17.340335	8.543344
C	-11.338621	15.390297	3.806737
H	-10.992218	14.529991	3.875293
C	-11.264287	16.249340	4.886184
C	-11.781849	17.539313	4.761537
H	-11.723885	18.125075	5.480753
C	-12.376730	17.961473	3.592343
C	-12.440211	17.090600	2.524113
H	-12.832240	17.370757	1.728862
C	-11.929979	15.805453	2.617599
C	-11.982726	14.860194	1.433447
H	-11.552390	14.021272	1.662798
H	-11.511288	15.248718	0.680576
C	-13.543624	13.363802	-0.290429
C	-12.318839	12.091285	-1.650334
H	-11.493707	11.803043	-1.969431
C	-13.435281	11.565597	-2.203769
H	-13.391245	10.922890	-2.874373
C	-14.622914	12.021214	-1.730108
H	-15.406272	11.685329	-2.100311
C	-10.660613	15.792525	6.178780
H	-10.391219	14.865372	6.086540
H	-11.336483	15.835337	6.871820
C	-7.958785	16.076275	5.708858
C	-7.177697	14.546131	4.266686
H	-7.320339	13.826485	3.694554
C	-5.918606	15.047955	4.392580
H	-5.200529	14.664174	3.943849
C	-5.751029	16.125453	5.191571
H	-4.901766	16.494486	5.276331
C	-12.897630	19.358259	3.465202
H	-13.160722	19.496858	2.541564
H	-12.167234	19.968613	3.650927
C	-17.936034	18.989920	3.577385
H	-18.784065	19.236992	3.869060
C	-17.827645	18.038814	2.620092
H	-18.576259	17.608270	2.276064
C	-16.573650	17.741504	2.181332
H	-16.479301	17.131525	1.485799
C	-15.673075	19.145929	3.670871
Ag	-17.134848	21.421204	5.333420
S	-9.867671	25.332409	11.473683
S	-14.345181	23.131146	5.766321
S	-9.272431	20.074723	7.937806
O	-19.664987	21.546844	4.641875
O	-18.688642	23.137198	3.819201
O	-20.744223	22.912557	3.434040
N	-8.857593	26.957554	13.213888
N	-11.242321	26.898918	13.141593
N	-16.804602	23.214715	6.595103
N	-15.365421	24.845831	7.528713
N	-6.705857	20.308310	8.343908
N	-8.095907	21.613183	9.761151
N	-19.718819	22.555094	3.921412
C	-12.236990	24.505132	8.658020
H	-12.583393	25.365438	8.589464
C	-12.311323	23.646089	7.578572
C	-11.793762	22.356116	7.703219
H	-11.851726	21.770354	6.984003
C	-11.198881	21.933956	8.872414
C	-11.135400	22.804829	9.940643
H	-10.743371	22.524672	10.735895
C	-11.645631	24.089976	9.847157
C	-11.592885	25.035235	11.031309
H	-12.023221	25.874157	10.801958
H	-12.064322	24.646711	11.784181
C	-10.031986	26.531627	12.755185
C	-11.256771	27.804144	14.115090
H	-12.081904	28.092386	14.434188
C	-10.140330	28.329832	14.668525
H	-10.184366	28.972539	15.339129
C	-8.952697	27.874215	14.194864
H	-8.169338	28.210100	14.565068
C	-12.914997	24.102904	6.285977
H	-13.184391	25.030057	6.378216
H	-12.239127	24.060092	5.592936
C	-15.616826	23.819154	6.755898
C	-16.397914	25.349298	8.198070
H	-16.255271	26.068944	8.770203
C	-17.657005	24.847474	8.072176
H	-18.375082	25.231255	8.520907
C	-17.824582	23.769976	7.273185
H	-18.673844	23.400943	7.188425
C	-10.677981	20.537170	8.999554
H	-10.414889	20.398571	9.923192
H	-11.408377	19.926816	8.813829
C	-5.639577	20.905509	8.887371
H	-4.791546	20.658437	8.595696
C	-5.747965	21.856615	9.844665
H	-4.999352	22.287159	10.188692
C	-7.001961	22.153925	10.283424
H	-7.096309	22.763904	10.978957
C	-7.902536	20.749500	8.793886

Couple D

Ag	10.021949	-1.525140	0.206653
S	1.843154	-7.714983	0.984714
S	7.278669	-2.845676	-1.067766
S	1.745599	-1.379960	1.583022
O	12.642519	-1.427865	0.069623
O	11.921304	-2.037231	-1.738080
O	14.000694	-1.818589	-1.508820
N	0.574526	-9.967428	1.066806
N	2.920194	-10.105788	1.484282
N	9.522180	-3.669995	-0.052990
N	7.996264	-5.376088	-0.656510
N	-0.837667	-1.569615	1.270692
N	0.293614	-3.602286	1.752314
N	12.883725	-1.753143	-1.102787
C	4.692819	-5.527121	-0.163630
H	5.082719	-6.178696	-0.700518
C	4.945790	-4.191484	-0.410137
C	4.358570	-3.228475	0.411583
H	4.534798	-2.329072	0.257420
C	3.522861	-3.585507	1.447554
C	3.283279	-4.924196	1.680098
H	2.727477	-5.173618	2.382574
C	3.856844	-5.902480	0.883443
C	3.607641	-7.372662	1.157261
H	4.111121	-7.914245	0.528949
H	3.900666	-7.594932	2.054341
C	1.797723	-9.462845	1.208954
C	2.777425	-11.418520	1.638207
H	3.533085	-11.921122	1.843438
C	1.596173	-12.065256	1.513889
H	1.532003	-12.987534	1.613926
C	0.509671	-11.301429	1.233719
H	-0.316938	-11.718413	1.153955
C	5.816439	-3.783967	-1.558965
H	6.101495	-4.581163	-2.032162
H	5.292708	-3.248147	-2.173408
C	8.353556	-4.122318	-0.534380
C	8.893621	-6.285474	-0.288638
H	8.669912	-7.186755	-0.345356
C	10.129433	-5.940973	0.166416
H	10.758357	-6.588683	0.388247
C	10.407770	-4.623524	0.286103
H	11.239981	-4.367761	0.612638
C	2.927264	-2.541609	2.338652
H	2.477901	-2.993417	3.070414
H	3.653068	-2.025035	2.721881
C	-1.964740	-2.269864	1.102439
H	-2.746551	-1.814052	0.887307
C	-2.010342	-3.616666	1.232079
H	-2.793597	-4.093244	1.078684
C	-0.858702	-4.243069	1.599169
H	-0.880069	-5.160764	1.747896
C	0.261833	-2.308248	1.543985
Ag	-0.932122	0.632613	1.484572
S	7.246673	6.822455	0.706510
S	1.811158	1.953149	2.758990
S	7.344228	0.487433	0.108202
O	-3.552691	0.535338	1.621601
O	-2.831476	1.144704	3.429305
O	-4.910866	0.926063	3.200045
N	8.515302	9.074901	0.624419
N	6.169633	9.213261	0.206941
N	-0.432352	2.777468	1.744214
N	1.093563	4.483562	2.347735
N	9.927495	0.677088	0.420532
N	8.796213	2.709759	-0.061090
N	-3.793897	0.860616	2.794012
C	4.397008	4.634594	1.854853
H	4.007109	5.286170	2.391742
C	4.144037	3.298957	2.101361
C	4.731257	2.335948	1.279641
H	4.555029	1.436545	1.433805
C	5.566966	2.692980	0.243669
C	5.806549	4.031668	0.011126
H	6.362350	4.281092	-0.691350
C	5.232982	5.009953	0.807781
C	5.482186	6.480135	0.533963
H	4.978706	7.021718	1.162275
H	5.189161	6.702405	-0.363117
C	7.292104	8.570318	0.482271
C	6.312401	10.525993	0.053017
H	5.556743	11.028596	-0.152214
C	7.493654	11.172729	0.177335
H	7.557825	12.095006	0.077299
C	8.580157	10.408902	0.457505
H	9.406765	10.825886	0.537268
C	3.273388	2.891440	3.250189
H	2.988331	3.688636	3.723386
H	3.797119	2.355619	3.864632
C	0.736271	3.229791	2.225604
C	0.196207	5.392946	1.979863
H	0.419915	6.294229	2.036580
C	-1.039606	5.048446	1.524809
H	-1.668529	5.696156	1.302977
C	-1.317942	3.730996	1.405122
H	-2.150154	3.475234	1.078586
C	6.162563	1.649082	-0.647428
H	6.611927	2.100890	-1.379190
H	5.436759	1.132508	-1.030656
C	11.054568	1.377337	0.588786
H	11.836379	0.921525	0.803918
C	11.100169	2.724139	0.459144
H	11.883424	3.200717	0.612541
C	9.948530	3.350542	0.092055
H	9.969895	4.268238	-0.056671
C	8.827995	1.415723	0.147239
Ag	0.932122	-0.632613	-1.484572
S	-7.246673	-6.822456	-0.706510
S	-1.811159	-1.953149	-2.758990
S	-7.344228	-0.487433	-0.108202
O	3.552691	-0.535338	-1.621601
O	2.831476	-1.144704	-3.429304
O	4.910866	-0.926062	-3.200044
N	-8.515302	-9.074901	-0.624419
N	-6.169633	-9.213261	-0.206942
N	0.432353	-2.777468	-1.744215
N	-1.093563	-4.483561	-2.347734

N	-9.927494	-0.677088	-0.420532
N	-8.796213	-2.709759	0.061090
N	3.793898	-0.860616	-2.794012
C	-4.397008	-4.634594	-1.854854
H	-4.007109	-5.286169	-2.391742
C	-4.144038	-3.298957	-2.101361
C	-4.731257	-2.335948	-1.279641
H	-4.555029	-1.436545	-1.433805
C	-5.566966	-2.692980	-0.243670
C	-5.806548	-4.031669	-0.011126
H	-6.362350	-4.281091	0.691350
C	-5.232983	-5.009953	-0.807782
C	-5.482186	-6.480135	-0.533963
H	-4.978706	-7.021718	-1.162275
H	-5.189162	-6.702405	0.363117
C	-7.292104	-8.570318	-0.482271
C	-6.312402	-10.525993	-0.053017
H	-5.556742	-11.028595	0.152214
C	-7.493654	-11.172729	-0.177335
H	-7.557825	-12.095007	-0.077299
C	-8.580156	-10.408902	-0.457505
H	-9.406766	-10.825886	-0.537269
C	-3.273388	-2.891440	-3.250190
H	-2.988332	-3.688636	-3.723386
H	-3.797120	-2.355620	-3.864632
C	-0.736271	-3.229791	-2.225604
C	-0.196207	-5.392947	-1.979863
H	-0.419916	-6.294228	-2.036581
C	1.039606	-5.048446	-1.524808
H	1.668530	-5.696156	-1.302977
C	1.317942	-3.730997	-1.405122
H	2.150153	-3.475234	-1.078586
C	-6.162563	-1.649082	0.647428
H	-6.611926	-2.100890	1.379190
H	-5.436759	-1.132508	1.030656
C	-11.054567	-1.377337	-0.588786
H	-11.836379	-0.921525	-0.803918
C	-11.100169	-2.724139	-0.459145
H	-11.883424	-3.200717	-0.612541
C	-9.948530	-3.350542	-0.092055
H	-9.969896	-4.268237	0.056672
C	-8.827995	-1.415721	-0.147239
Ag	-10.021949	1.525140	-0.206653
S	-1.843154	7.714982	-0.984714
S	-7.278670	2.845676	1.067766
S	-1.745599	1.379960	-1.583022
O	-12.642518	1.427865	-0.069623
O	-11.921304	2.037231	1.738081
O	-14.000693	1.818590	1.508821
N	-0.574526	9.967428	-1.066805
N	-2.920194	10.105788	-1.484283
N	-9.522180	3.669995	0.052990
N	-7.996264	5.376089	0.656511
N	0.837667	1.569615	-1.270692
N	-0.293614	3.602286	-1.752315
N	-12.883725	1.753143	1.102788
C	-4.692819	5.527121	0.163629
H	-5.082718	6.178697	0.700517
C	-4.945790	4.191484	0.410137
C	-4.358570	3.228475	-0.411583
H	-4.534798	2.329072	-0.257420
C	-3.522861	3.585507	-1.447555
C	-3.283279	4.924196	-1.680098
H	-2.727477	5.173619	-2.382574
C	-3.856845	5.902480	-0.883443
C	-3.607641	7.372662	-1.157261
H	-4.111121	7.914245	-0.528949
H	-3.900666	7.594932	-2.054342
C	-1.797724	9.462845	-1.208954
C	-2.777426	11.418520	-1.638207
H	-3.533085	11.921123	-1.843439
C	-1.596173	12.065256	-1.513889
H	-1.532003	12.987533	-1.613926
C	-0.509671	11.301429	-1.233719
H	0.316938	11.718413	-1.153956
C	-5.816440	3.783967	1.558964
H	-6.101496	4.581163	2.032162
H	-5.292709	3.248146	2.173408
C	-8.353556	4.122318	0.534380
C	-8.893621	6.285473	0.288639
H	-8.669912	7.186756	0.345356
C	-10.129433	5.940973	-0.166416
H	-10.758357	6.588683	-0.388247
C	-10.407770	4.623523	-0.286102
H	-11.239982	4.367761	-0.612639
C	-2.927264	2.541609	-2.338652
H	-2.477901	2.993417	-3.070414
H	-3.653068	2.025035	-2.721880
C	1.964740	2.269864	-1.102439
H	2.746551	1.814052	-0.887307
C	2.010341	3.616666	-1.232080
H	2.793597	4.093244	-1.078684
C	0.858703	4.243069	-1.599169
H	0.880068	5.160765	-1.747896
C	-0.261832	2.308250	-1.543985

Couple E

Ag	0.000000	0.000000	0.000000
N	0.000000	0.000000	2.261811
C	1.203371	0.000000	2.890971
N	1.425489	-0.128854	4.194055
C	0.334855	-0.252251	4.984858
C	0.582982	-0.388926	6.460408
H	1.113519	-1.172182	6.623682
H	1.049903	0.387406	6.779461
H	-0.256863	-0.468738	6.919573
C	-0.949509	-0.232321	4.436757
H	-1.695097	-0.299910	4.988071
C	-1.100059	-0.108866	3.060972
C	-2.454912	-0.114611	2.399459
H	-2.577176	0.704860	1.913504
H	-2.510759	-0.857010	1.791742
H	-3.137116	-0.195496	3.068781
N	0.403876	1.024291	-1.961468
O	-1.784082	-1.736385	-0.283035
N	-1.146235	-2.678355	-0.778107
O	0.045110	-2.486162	-1.025698
O	-1.684148	-3.761573	-1.000653
C	1.251075	0.539972	-2.903650
C	2.249305	-0.504614	-2.480599
H	2.816289	-0.146085	-1.794743
H	1.784983	-1.272284	-2.142812
H	2.783904	-0.760815	-3.236769
C	1.152469	0.985961	-4.212886
H	1.726430	0.653682	-4.863222
C	0.189948	1.933748	-4.546996
C	-0.000587	2.436170	-5.948103
H	0.150925	3.383330	-5.971742
H	-0.895884	2.246889	-6.236975
H	0.622841	1.998772	-6.533171
N	-0.623960	2.461580	-3.594529
C	-0.474397	1.975767	-2.366714
S	-1.473381	2.592752	-1.043110
C	-2.661628	3.669549	-1.918709
H	-3.223218	3.139513	-2.504729
H	-2.186826	4.323661	-2.456827
C	-3.507086	4.368241	-0.876385
C	-4.601272	3.705571	-0.295489
H	-4.811215	2.839468	-0.562927
C	-5.378889	4.341667	0.686900
H	-6.109104	3.909669	1.067774
C	-5.054658	5.647387	1.068722
H	-5.570777	6.073134	1.714636
C	-3.971611	6.328817	0.501497
H	-3.754470	7.196185	0.757276
C	-3.207147	5.674072	-0.468736
H	-2.483449	6.116040	-0.852107
S	2.557749	0.241134	1.777535
C	4.027975	-0.098754	2.823825
H	4.192706	-1.052428	2.868516
H	3.879894	0.231452	3.723465
C	5.220827	0.606992	2.201602
C	5.545032	1.912726	2.583399
H	5.028908	2.338473	3.229310
H	6.845192	3.461544	2.271929
C	6.628060	2.594172	2.016155
C	7.392531	1.939427	1.045928
H	8.116216	2.381404	0.662544
C	7.092619	0.633595	0.638295
H	7.612255	0.204162	-0.002381
C	5.998455	-0.029091	1.219214
H	5.788540	-0.895205	0.951791
H	-0.567867	-5.990380	-1.148388
C	-0.328115	-6.802738	-1.619910
H	-0.510346	-7.559938	-1.039985
C	-1.130398	-6.920930	-2.897720
C	-1.608466	-8.163977	-3.330834
H	-1.435451	-8.921923	-2.819333
C	-2.340686	-8.291333	-4.514933
H	-2.648901	-9.126661	-4.783503
C	-2.588918	-7.140797	-5.272382
H	-3.075512	-7.213215	-6.061575
C	-1.395085	-5.779428	-3.672789
H	-1.085475	-4.948450	-3.391097
C	-2.122615	-5.885140	-4.870255
C	-2.424238	-4.652791	-5.706004
H	-1.702791	-4.011367	-5.624049
H	-2.513589	-4.899327	-6.639576
S	-3.993567	-3.921689	-5.094030
C	-4.579321	-2.996912	-6.484681
N	-5.635788	-2.200659	-6.178397
C	-6.191394	-1.508388	-7.214111
C	-7.323665	-0.634128	-6.977188
H	-7.041939	0.139689	-6.264616
H	-8.152294	-1.214485	-6.574099
H	-7.627138	-0.170988	-7.914913
C	-5.659379	-1.625454	-8.492352
C	-4.550342	-2.448838	-8.698495
C	-3.912345	-2.624396	-10.047432
H	-4.376249	-2.085202	-10.692881
H	-3.961705	-3.547857	-10.306822
H	-2.992816	-2.352078	-10.003518
N	-4.008635	-3.147417	-7.674473
S	1.441570	-6.768106	-2.072797
C	2.237538	-6.783727	-0.492682
N	3.580964	-6.614856	-0.580478
C	4.277123	-6.674405	0.582206
C	3.601989	-6.848019	1.780863
C	2.215609	-6.968018	1.779341
N	1.520086	-6.963895	0.611227
C	5.771930	-6.508033	0.515382
H	6.140460	-6.570113	1.400570
H	6.146271	-7.198075	-0.036088
H	5.981764	-5.650655	0.141372
H	4.073184	-6.884047	2.580523
C	1.414060	-7.120725	3.038721
H	0.938086	-7.953527	3.016039
H	2.003254	-7.110690	3.797029
H	0.789477	-6.395752	3.110424
H	-6.037364	-1.161967	-9.204197

Couple F

Ag	0.000000	0.000000	0.000000
S	0.000000	0.000000	3.124068
S	5.124642	0.000000	7.652072
S	-0.409620	4.875223	6.349300
N	-1.713525	-0.723504	1.286922
N	-2.337869	-1.271613	3.543460
N	7.398824	-0.926024	8.545437
N	7.576194	0.806810	6.885621
N	2.076239	5.680002	5.695593
N	0.219827	6.506743	4.408672
N	0.854954	-2.416725	-1.587877
O	-0.194710	-1.776979	-1.755712
O	1.642750	-1.997743	-0.738541
O	1.089414	-3.433562	-2.238499
C	-2.896380	-1.228535	0.832566
C	-3.812855	-1.764227	1.729088
H	-4.623984	-2.103787	1.427118
C	-3.504225	-1.786322	3.090947
C	-1.518246	-0.763665	2.630128
C	-4.437347	-2.353293	4.123092
H	-5.227159	-2.687465	3.690579
H	-4.000022	-3.069154	4.589903
H	-4.680801	-1.664680	4.746824
C	-3.149762	-1.203716	-0.653516
H	-4.010401	-1.585023	-0.837476
H	-3.126912	-0.296014	-0.966868
H	-2.469556	-1.713129	-1.102305
C	0.143187	-0.456661	4.896853
H	-0.732681	-0.454552	5.312988
H	0.523720	-1.343402	4.983534
C	1.042035	0.564029	5.573905
C	0.492390	1.710014	6.157367
H	-0.429062	1.833629	6.135184
C	1.296478	2.675622	6.773910
C	2.679713	2.474211	6.797210
H	3.224824	3.108288	7.205682
C	3.262529	1.339651	6.218931
C	2.435520	0.385774	5.602499
H	2.813712	-0.369156	5.211622
C	4.760458	1.130963	6.264127
H	5.212109	1.980191	6.397145
H	5.070022	0.746071	5.430000
C	6.893768	-0.021527	7.669238
C	8.749387	-0.965470	8.665607
C	9.535414	-0.141539	7.874389
H	10.460913	-0.168320	7.948639
C	8.930672	0.725392	6.969342
C	9.339407	-1.946930	9.642955
H	10.297386	-1.873767	9.630633
H	9.015177	-1.754145	10.525066
H	9.083780	-2.837182	9.395732
C	9.715896	1.619260	6.054871
H	10.655105	1.479641	6.198659
H	9.498846	1.414195	5.142911
H	9.498183	2.535507	6.238501
C	0.662559	3.891304	7.448382
H	1.368264	4.461421	7.788579
H	0.137299	3.588289	8.207217
C	0.777927	5.767752	5.381015
C	2.919829	6.414559	4.939362
C	1.078538	7.242267	3.666484
C	2.439598	7.205686	3.911296
H	3.024851	7.707007	3.390829
C	4.386991	6.346328	5.310463
H	4.893546	6.900577	4.712853
H	4.503305	6.655978	6.211603
H	4.692933	5.438207	5.240979
C	0.456574	8.105971	2.598027
H	1.145911	8.585371	2.132865
H	-0.024518	7.553221	1.979983
H	-0.147984	8.730697	3.004409
N	1.365211	1.642241	-0.706322
S	-6.033616	2.568247	-6.127729
S	-0.908970	2.568279	-1.599677
S	-6.443273	7.443492	-2.902534
N	-7.747139	1.844731	-7.964873
N	-8.371482	1.296630	-5.708333
N	1.542602	3.375079	-2.366132
N	-3.957419	8.248283	-3.556246
N	-5.813836	9.075002	-4.843174
C	-8.929992	1.339695	-8.419227
C	-9.846466	0.804004	-7.522703
H	-10.657594	0.464440	-7.824671
C	-9.537836	0.781915	-6.160843
C	-7.551860	1.804576	-6.621666
C	-10.470956	0.214945	-5.128697
H	-11.260768	-0.119230	-5.561208
H	-10.033630	-0.500912	-4.661883
H	-10.714413	0.903561	-4.504968
C	-9.183374	1.364507	-9.905309
H	-10.044012	0.983196	-10.089267
H	-9.160526	2.272207	-10.218665
H	-8.503166	0.855093	-10.354095
C	-5.890428	2.111594	-4.354942
H	-6.766297	2.113703	-3.938808
H	-5.509892	1.224855	-4.268257
C	-4.991583	3.132290	-3.677894
C	-5.541232	4.278276	-3.094438
H	-6.462685	4.401888	-3.116621
C	-4.737147	5.243889	-2.477899
C	-3.353911	5.042482	-2.454597
H	-2.808802	5.676562	-2.046128
C	-2.771092	3.907921	-3.032871
C	-3.598098	2.954039	-3.649299
H	-3.219904	2.199108	-4.040173
C	-1.273177	3.699246	-2.987612
H	-0.821530	4.548476	-2.854596
H	-0.963607	3.314366	-3.821743
C	0.860154	2.546725	-1.582542
C	2.715775	1.602780	-0.586175
C	3.501799	2.426692	-1.377416
H	4.427299	2.399901	-1.303182
C	2.897078	3.293644	-2.282394
C	3.305800	0.621325	0.391175
H	4.263780	0.694476	0.378836
H	2.981588	0.814124	1.273290
H	3.050159	-0.268926	0.143967
C	3.682324	4.187527	-3.196832
H	4.621530	4.047894	-3.053034
H	3.465286	3.982487	-4.108800
H	3.464619	5.103771	-3.013181
C	-5.371093	6.459587	-1.803441
H	-4.665392	7.029709	-1.463246
H	-5.896354	6.156574	-1.044606
C	-5.255727	8.336025	-3.870816
C	-3.113838	8.982847	-4.312480
C	-4.955133	9.810532	-5.585366
C	-3.594078	9.773972	-5.340542
H	-3.008830	10.275297	-5.861012
C	-1.646673	8.914625	-3.941385
H	-1.140125	9.468878	-4.538998
H	-1.530357	9.224274	-3.040246
H	-1.340726	8.006506	-4.010872
C	-5.577105	10.674215	-6.653834
H	-4.887774	11.153621	-7.118997
H	-6.058186	10.121452	-7.271874
H	-6.181675	11.298936	-6.247461
S	-5.757594	11.345289	3.078578
S	-4.049500	8.436916	9.027437
S	-3.954536	5.877221	1.989422
N	-6.434866	13.086472	1.249825
N	-4.072857	12.894995	1.657802
N	-4.037326	8.389629	11.639935
N	-5.972866	7.405184	10.603729
N	-5.794397	4.797442	3.633651
N	-6.305600	4.978515	1.290187
C	-6.194486	13.992705	0.259066
C	-4.889475	14.363062	-0.041643
H	-4.717932	14.974889	-0.720362
C	-3.835703	13.805257	0.685555
C	-5.343758	12.579092	1.879119
C	-2.398189	14.157579	0.426874
H	-2.350527	14.807670	-0.278570
H	-2.010134	14.522089	1.225728
H	-1.916996	13.367805	0.167624
C	-7.380731	14.580654	-0.462322
H	-7.075196	15.198272	-1.129506
H	-7.881415	13.876355	-0.881740
H	-7.942695	15.039689	0.167817
C	-4.170577	11.065500	3.958865
H	-3.429836	11.120953	3.335530
H	-4.046732	11.737519	4.645655
C	-4.218667	9.682672	4.586251
C	-3.749814	8.571131	3.878809
H	-3.399114	8.690501	3.025812
C	-3.796054	7.282937	4.424244
C	-4.327368	7.121662	5.707266
H	-4.362014	6.270298	6.081471
C	-4.808866	8.213039	6.440999
C	-4.755412	9.496190	5.871367
H	-5.076918	10.226955	6.349226
C	-5.369023	8.022661	7.833559
H	-5.654113	7.102531	7.955859
H	-6.134749	8.601674	7.968262
C	-4.796921	8.023521	10.576966
C	-4.509415	8.055120	12.866822
C	-5.735929	7.418745	12.982644
H	-6.066529	7.192285	13.820618
C	-6.468187	7.120882	11.837453
C	-3.680317	8.432430	14.065500
H	-4.124243	8.140459	14.866069
H	-2.820326	8.011528	14.004942
H	-3.569439	9.384314	14.090706
C	-7.818122	6.467306	11.885896
H	-8.067114	6.313126	12.800508
H	-8.466305	7.040590	11.471123
H	-7.784983	5.629649	11.419143
C	-3.228302	6.095641	3.647891
H	-3.376474	5.288210	4.162562
H	-2.268612	6.213732	3.555179
C	-5.525300	5.147564	2.369879
C	-6.993813	4.214141	3.844030
C	-7.499638	4.385553	1.517988
C	-7.868440	3.999327	2.794123
H	-8.694930	3.600550	2.944525
C	-7.291810	3.784939	5.265974
H	-8.163868	3.386097	5.302932
H	-6.634437	3.146254	5.551294
H	-7.266298	4.552003	5.843965
C	-8.365710	4.155541	0.304961
H	-9.184051	3.730901	0.572138
H	-8.560504	4.996058	-0.112826
H	-7.901214	3.590703	-0.316425

Couple G

Ag	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.505612
N	1.214265	0.000000	2.760148
O	1.619828	-0.069952	3.918967
O	1.991793	0.061878	1.806648
N	-0.868635	-2.072677	-0.255495
C	-1.848951	-2.628635	0.512963
C	-2.505180	-1.760343	1.556368
H	-3.171412	-2.268991	2.022574
H	-1.841392	-1.452137	2.179257
H	-2.917676	-1.004665	1.130421

C	-2.197929	-3.961866	0.335891
H	-2.869989	-4.345365	0.851333
C	-1.529496	-4.721494	-0.626678
C	-1.842623	-6.169818	-0.875276
H	-2.535170	-6.454769	-0.273842
H	-1.053634	-6.696715	-0.728649
H	-2.139632	-6.281807	-1.781777
N	-0.567897	-4.166289	-1.399417
C	-0.298532	-2.883802	-1.183384
S	0.890657	-2.043185	-2.189072
C	1.694858	-3.407424	-3.118546
H	2.390070	-3.813940	-2.579981
H	1.041278	-4.087512	-3.343564
C	2.293520	-2.823003	-4.386692
C	3.596385	-2.296761	-4.388605
H	4.103532	-2.313590	-3.608702
C	4.139769	-1.745997	-5.561298
H	5.007082	-1.410336	-5.561314
C	1.542381	-2.779530	-5.565556
H	0.677742	-3.121941	-5.566074
C	3.362269	-1.721436	-6.725845
H	3.719035	-1.356657	-7.504115
C	2.061179	-2.232582	-6.744870
C	1.235411	-2.246467	-8.030395
H	1.103719	-3.168428	-8.306428
H	1.738351	-1.800033	-8.727914
S	-0.394315	-1.443103	-7.874757
C	0.038011	0.275907	-7.921445
N	-1.010269	1.090749	-7.720871
C	-0.743776	2.414964	-7.789144
C	-1.922857	3.337014	-7.604714
H	-2.313766	3.187552	-6.742268
H	-1.629682	4.248534	-7.672302
H	-2.575681	3.160484	-8.285579
C	0.538602	2.868981	-8.040422
H	0.716045	3.781080	-8.076727
C	1.553841	1.950328	-8.237173
C	2.977594	2.352533	-8.562894
H	3.570728	2.000574	-7.893994
H	3.043718	3.309805	-8.576535
H	3.219802	2.001811	-9.423008
N	1.304304	0.624565	-8.180591
N	0.379928	2.076868	-0.775835
C	1.618593	2.605816	-0.937005
C	2.788079	1.658348	-0.971686
H	2.681106	1.044696	-1.701341
H	2.829157	1.170888	-0.147241
H	3.600611	2.157520	-1.089369
C	1.773695	3.980730	-1.027932
H	2.620109	4.348629	-1.132878
C	0.655164	4.805895	-0.961623
C	0.747961	6.302654	-1.015799
H	1.668951	6.564344	-1.090498
H	0.262069	6.625990	-1.777369
H	0.374330	6.675668	-0.214491
N	-0.592426	4.276275	-0.855455
C	-0.656770	2.952114	-0.764063
S	-2.227932	2.149612	-0.629871
C	-3.372113	3.560086	-0.431090
H	-3.191731	4.021237	0.402301
H	-3.257582	4.189384	-1.161664
C	-4.783207	3.013964	-0.431058
C	-5.560721	3.038519	-1.595608
H	-5.203967	3.403308	-2.373880
C	-6.861799	2.527359	-1.614632
H	-7.364410	2.518897	-2.397070
C	-7.380585	1.980405	-0.435316
H	-8.245218	1.637980	-0.435830
C	-6.629441	1.936945	0.743545
H	-6.995907	1.579194	1.519829
C	-5.326577	2.463201	0.741627
H	-4.819421	2.446360	1.521525
Ag	3.218563	5.483193	-4.685294
O	5.002410	4.531575	-3.205293
N	4.894281	5.237012	-2.190456
O	5.576443	5.019500	-1.190665
O	4.071046	6.152831	-2.223607
N	3.947587	7.373835	-5.661840
C	3.887084	8.595802	-5.076047
C	2.957869	8.767869	-3.904062
H	2.058522	8.576901	-4.178136
H	3.213062	8.166191	-3.202726
H	3.010199	9.672563	-3.584660
C	4.693589	9.623223	-5.541538
H	4.660212	10.460450	-5.140644
C	5.552400	9.393567	-6.612102
C	6.480415	10.444773	-7.146504
H	6.380623	11.251002	-6.634331
H	7.386340	10.135221	-7.080859
H	6.267575	10.622437	-8.065069
N	5.575427	8.186133	-7.236458
C	4.781166	7.251359	-6.725352
S	4.720988	5.642836	-7.459897
C	6.066843	5.724970	-8.692789
H	6.921811	5.826290	-8.247253
H	5.935100	6.485623	-9.281788
C	6.042372	4.439132	-9.489945
C	6.642942	3.278153	-8.974914
H	7.066229	3.306093	-8.146795
C	6.607149	2.075964	-9.701449
H	7.010848	1.307397	-9.367934
C	5.975561	2.055609	-10.949048
H	5.955044	1.262883	-11.434857
C	5.373598	3.200386	-11.484034
H	4.930723	3.160035	-12.300816
C	5.414731	4.383664	-10.740651
H	5.016581	5.151129	-11.084921
N	1.874491	3.664142	-4.667452
C	2.287932	2.364671	-4.700328
C	3.760717	2.097224	-4.880981
H	4.249598	2.498730	-4.157529
H	4.054942	2.475899	-5.713248
H	3.915382	1.150661	-4.886747
C	1.364307	1.337993	-4.547006
H	1.638069	0.449923	-4.575366
C	0.017942	1.653174	-4.351208
C	-1.041163	0.602794	-4.170946
H	-1.472858	0.727069	-3.322526
H	-1.689713	0.678363	-4.875341
H	-0.636182	-0.267642	-4.200511
N	-0.394590	2.941428	-4.333920
C	0.542234	3.867861	-4.501589
S	0.098178	5.579759	-4.568268
C	-1.656361	5.580524	-4.026602
H	-1.707122	5.571969	-3.059143
H	-2.110079	4.793813	-4.366521
C	-2.315800	6.836090	-4.571421
C	-2.947405	6.815780	-5.819027
H	-2.967966	6.023060	-6.304846
C	-3.549315	7.960591	-6.353994
C	-3.508118	9.143854	-5.610598
H	-3.906235	9.911344	-5.954853
C	-2.880503	9.199262	-4.359863
H	-2.865437	9.989574	-3.869881
C	-2.279980	8.038265	-3.844864
H	-1.856716	8.066173	-3.016733
C	-4.276938	7.894351	-7.695940
H	-5.051099	7.315124	-7.602570
H	-4.598480	8.780598	-7.919465
S	-3.247130	7.278887	-9.069382
C	-2.247778	8.695516	-9.442082
N	-2.503697	9.856205	-8.826020
C	-1.727645	10.901097	-9.185249
C	-0.738800	10.750651	-10.140746
H	-0.204398	11.472335	-10.382232
C	-0.554297	9.514100	-10.732913
N	-1.316951	8.454580	-10.379418
C	0.467020	9.262321	-11.813627
H	1.075431	8.579724	-11.525778
H	0.021207	8.975392	-12.613527
H	0.951190	10.071955	-11.990990
C	-2.033116	12.225759	-8.516749
H	-1.930743	12.135575	-7.565698
H	-2.934854	12.485297	-8.719166
H	-1.426225	12.894562	-8.841272

Table S5. Selected bond length (Å) and angles (°) of **1** and **5** complexes.

	1	**5**
Ag-N(1)	2.261(3)	2.206(5)
Ag-N(3)	2.250(3)	2.239(5)
Ag-O(1)	2.506(3)	2.318(14)
N(3)-Ag-N(1)	150.68(10)	153.1(2)
N(3)-Ag-O(1)	110.17(13)	92.0(4)
N(1)-Ag-O(1)	96.50(12)	114.3(4)