Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2017

Electronic Supplementary Information

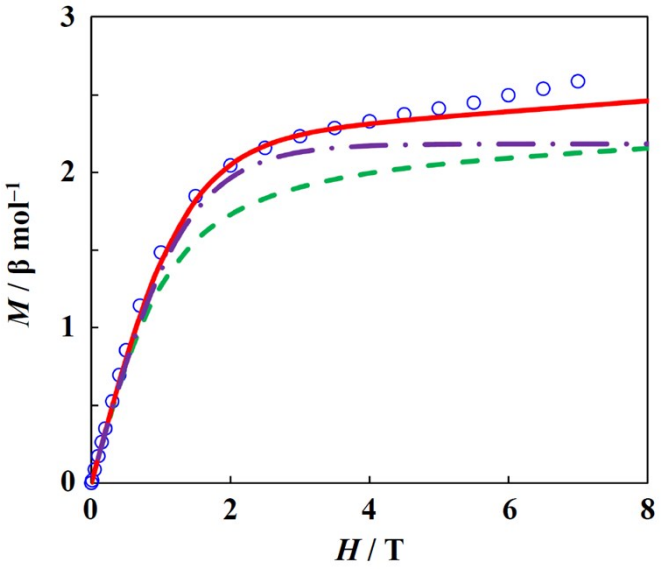


Fig. S1 The *M versus H* plot. The observed data (○) and the theoretical curves by the average magnetization method (---), the average *g*-factor method (- · -), and the average Zeeman coefficients method (–), with the best-fitting parameter set (λ, κ, Δ) = (–110 cm^{-1}, 0.86, –530 cm^{-1}).

DFT calculation results

(a) Cartesian coordinates for all atoms

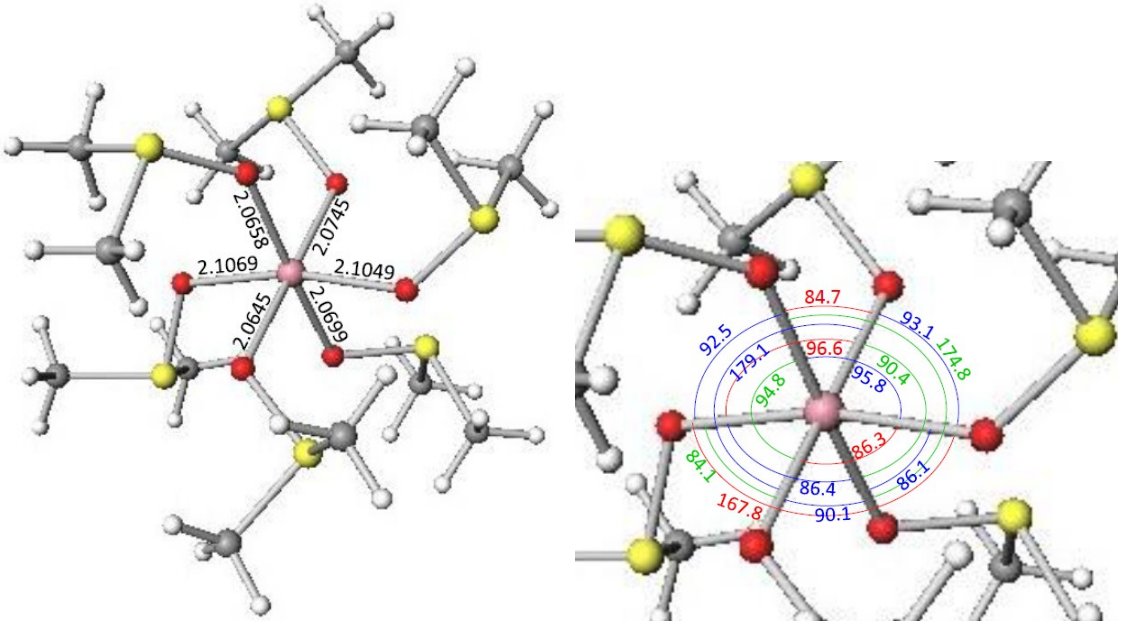
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
CO	27.0	0.0861378863	0.0301084582	-0.0678512552
S	16.0	2.9827619623	-1.3096225939	1.3314342483
S	16.0	-0.1503595035	1.5871922094	2.7565777216
S	16.0	1.6223636978	2.3632623337	-2.1312674724
S	16.0	-2.8695671762	1.1627940098	-0.2516891884
S	16.0	0.4373445274	-1.5341357528	-2.8980267583
S	16.0	-0.8696677720	-2.4526844225	1.6982313799
O	8.0	1.4565876149	-0.5740585507	1.4111825076
O	8.0	-0.1980179736	1.7259340908	1.0763368167
O	8.0	1.4899627797	0.8948944743	-1.3124626237
O	8.0	-1.5208826862	0.7877805705	-1.2003423693
O	8.0	0.4019865837	-1.6707888813	-1.2127856465
O	8.0	-1.3425771025	-0.9686025127	1.0483813698
C	6.0	2.6594734320	-2.9145886817	0.5045183987
H	1.0	2.2477171881	-3.5903972118	1.2490886793
H	1.0	3.6055353128	-3.3082767268	0.1372021092
H	1.0	1.9354653501	-2.7299603628	-0.2914079326
C	6.0	3.8891512279	-0.4030924680	0.0154379056
H	1.0	4.3500435039	0.4656061468	0.4790906009
H	1.0	3.1685508286	-0.0839030897	-0.7425981622
H	1.0	4.6622096067	-1.0599158109	-0.3791091034
C	6.0	1.5177402590	2.2118854063	3.1738968511
H	1.0	2.2108419035	1.4687985822	2.7932218259
H	1.0	1.6037219447	2.3021338955	4.2551983671
H	1.0	1.6738118647	3.1722756926	2.6877102483
C	6.0	-1.1823659151	3.0137638811	3.2586867099
H	1.0	-2.2077015730	2.7876069619	2.9790548678
H	1.0	-0.8380286989	3.9032685952	2.7356758798
H	1.0	-1.1106142190	3.1436160259	4.3369608739
C	6.0	1.1196046839	3.6490538341	-0.9189058737
H	1.0	2.0131679213	3.9379719257	-0.3709020248

H	1.0	0.3875464332	3.2121940471	-0.2367189702
H	1.0	0.7342169304	4.5064016155	-1.4678282362
C	6.0	0.1834235197	2.3603085924	-3.2683758203
H	1.0	0.4212480030	1.6791265594	-4.0814631166
H	1.0	0.0509951389	3.3662271120	-3.6628458126
H	1.0	-0.6829390603	2.0085446167	-2.7061837672
C	6.0	-3.6143134502	2.5307384777	-1.2159351412
H	1.0	-2.9657385090	3.3964346561	-1.1110426395
H	1.0	-4.5993954042	2.7558228044	-0.8108058917
H	1.0	-3.6835059985	2.2363457914	-2.2610228006
C	6.0	-4.0279390782	-0.1955949723	-0.6494421032
H	1.0	-3.5550317153	-1.0954190061	-0.2683449357
H	1.0	-4.1739423174	-0.2546126512	-1.7257586853
H	1.0	-4.9726372756	-0.0135797800	-0.1402464729
C	6.0	-1.3413264352	-1.5725978726	-3.3317408794
H	1.0	-1.7674186678	-0.6913600012	-2.8540551540
H	1.0	-1.7865659338	-2.4797511196	-2.9283427542
H	1.0	-1.4432963898	-1.5328677317	-4.4146888188
C	6.0	0.9457918578	-3.2241640755	-3.3882775971
H	1.0	2.0049246994	-3.3322546807	-3.1700477797
H	1.0	0.7764487743	-3.3473379265	-4.4564734452
H	1.0	0.3650421274	-3.9419146685	-2.8128516193
C	6.0	-2.4666666450	-3.3418080553	1.7968971495
H	1.0	-2.7621942796	-3.6069500886	0.7852021501
H	1.0	-3.2080244996	-2.6876778668	2.2510848917
H	1.0	-2.3331405049	-4.2457109540	2.3885669510
C	6.0	-0.6003712387	-2.0646875463	3.4660586740
H	1.0	0.2826802195	-1.4336200255	3.4976460353
H	1.0	-0.4385209558	-2.9930046937	4.0110722747
H	1.0	-1.4669892225	-1.5304484956	3.8492288657

DFT calculation

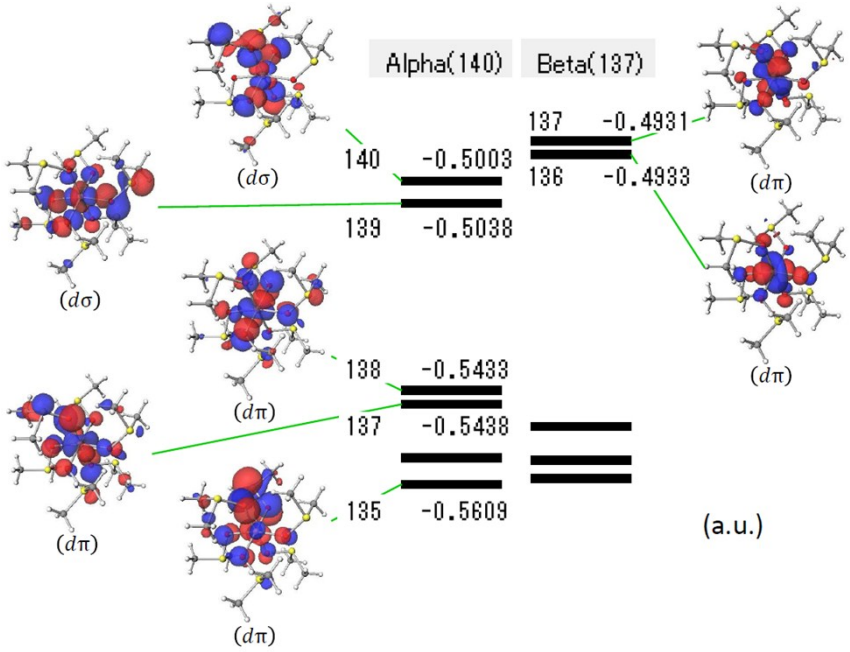
(b) main bond distances (Å) and angles (°) for the optimized structure



DFT calculation

(c) MO diagram

Main occupied orbitals



DFT calculation

(d) total energy value

TOTAL ENERGY = -4696.2220026946 (a.u.)

DFT calculation

(e) Mulliken spin density values of main atoms

ATOMIC SPIN DENSITY AT THE NUCLEUS (A.U.)

			SPIN DENS	ALPHA DENS	BETA DENS
1	CO	27.0	0.2596146	6286.81624	6286.55663
2	S	16.0	-0.0096664	1252.95342	1252.96308
3	S	16.0	0.0105806	1252.99790	1252.98732
4	S	16.0	-0.0096265	1252.97230	1252.98193
5	S	16.0	0.0093417	1253.01849	1253.00915
6	S	16.0	0.0081904	1252.98671	1252.97852
7	S	16.0	0.0060780	1252.98040	1252.97433
8	O	8.0	0.0665230	145.58224	145.51572
9	O	8.0	0.0648887	145.60038	145.53549
10	O	8.0	0.0765293	145.58205	145.50552
11	O	8.0	0.0649015	145.59394	145.52904
12	O	8.0	0.0617908	145.59444	145.53264
13	O	8.0	0.0583217	145.59246	145.53414