Electronic Supplementary Data

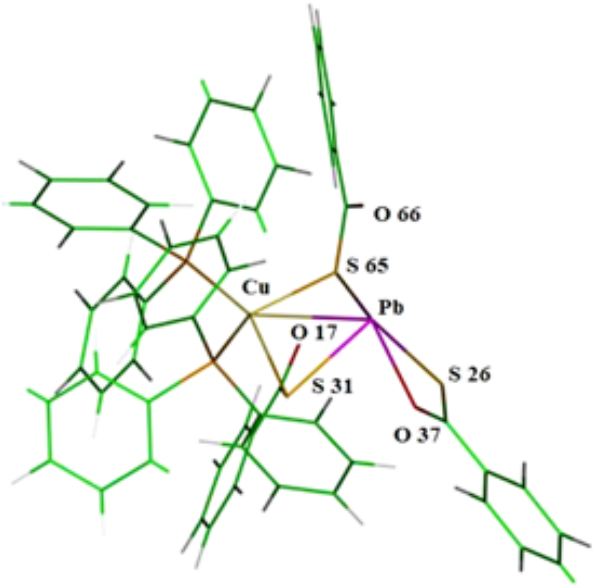

Fig. S1

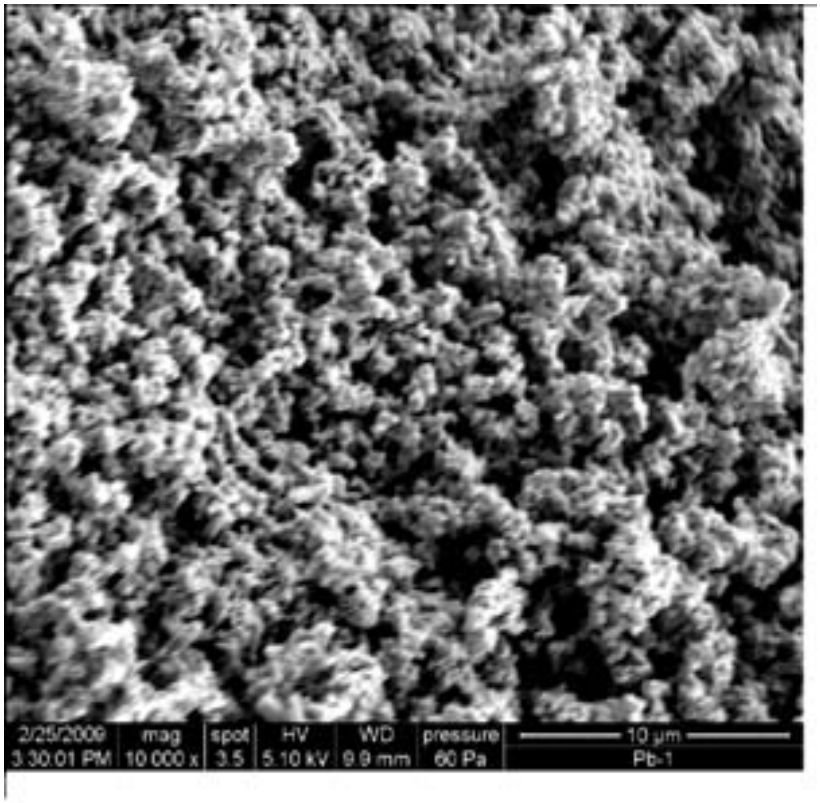

Fig. S2

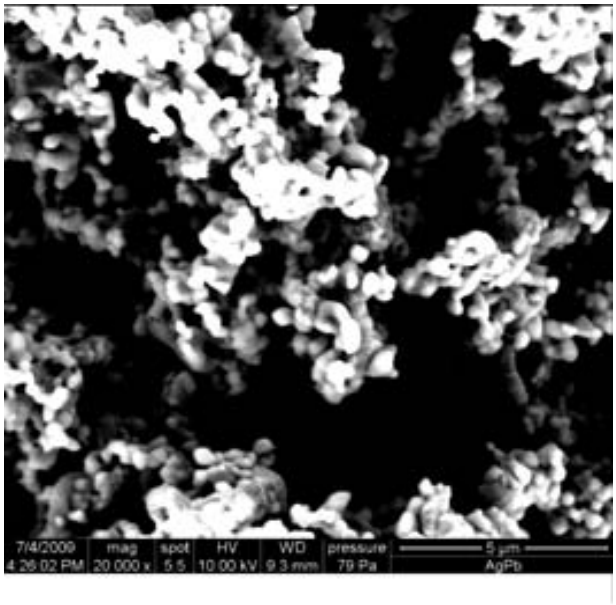

Fig. S3

Table S1- Geometrical parameters of complex 1

Bond length(in Å)

	Optimized	**Crystal structure**	
Pb-S(26)	2.722	Pb-S(3)	2.709
Pb-S(31)	2.808	Pb-S(1)	2.794
Pb-S(65)	2.728	Pb-S(2)	2.794
Pb-O(37)	2.507	Pb-O(3)	2.678
Cu-P(69)	2.370	Cu-P(1)	2.272
Cu-P(63)	2.322	Cu-P(2)	2.290
Cu-S(31)	2.400	Cu-S(1)	2.411
Cu-S(65)	2.439	Cu-S(2)	2.427
Cu-Pb	3.310	Cu-Pb	3.378
S(26)-C(30)	1.758	S(3)-C(15)	1.758
S(31)-C(19)	1.798	S(1)-C(1)	1.779
S(65)-C(74)	1.787	S(2)-C(8)	1.784

O(37)-C(30)	1.259	O(3)-C(15)	1.242
O(17)-C(19)	1.238	O(1)-C(1)	1.227
O(66)-C(74)	1.240	O(2)-C(8)	1.238
Bond Angle(°)			
S(65)-Pb-S(31)	84.77	S(2)-Pb-S(1)	81.12
S(26)-Pb-S(31)	85.66	S(3)-Pb-S(1)	82.94
O(37)-Pb-S(31)	142.31	O(3)-Pb-S(1)	139.09
O(37)-Pb-S(65)	79.46	O(3)-Pb-S(2)	89.64
O(37)-Pb-S(26)	60.45	O(3)-Pb-S(3)	57.83
O(37)-Pb-Cu	125.15	O(3)-Pb-Cu	133.70
P(69)-Cu-P(63)	116.72	P(1)-Cu-P(2)	118.03
P(69)-Cu-S(65)	99.46	P(1)-Cu-S(2)	114.47
P(63)-Cu-S(65)	113.04	P(2)-Cu-S(2)	105.20
P(69)-Cu-S(31)	103.16	P(1)-Cu-S(1)	110.01
P(63)-Cu-S(31)	120.47	P(2)-Cu-S(1)	109.73
S(65)-Cu-S(31)	100.91	S(2)-Cu-S(1)	97.37
Cu-S(65)-Pb	79.45	Cu-S(2)-Pb	80.56
Cu-S(31)-Pb	78.51	Cu-S(1)-Pb	80.28

Table S2. Results of Natural bond orbital (NBO) calculations.

Complex	**1**		**2**	
Method	**HF**	**DFT/PBE1**	**HF**	**DFT/PBE1**
Residual Charge				
Pb	+1.4	+1.2	+1.3	+1.1
M	+0.71	+0.66	+0.67	+0.59
$O_{(terminal)}$	-0.81	-0.69	-0.75	-0.64

$O_{(bridging\ thiobenzoate\ 1)}$	-0.73	-0.66,	-0.69	-0.59,
$O_{(bridging\ thiobenzoate\ 2)}$	-0.76	-0.62	-0.71	-0.61
$S_{(terminal)}$	-0.47	-0.36	-0.48	-0.38
$S_{(bridging\ 1)}$	-0.53	-0.44,	-0.54	-0.44,
$S_{(bridging\ 2)}$	-0.58	-0.49	-0.57	-0.47
P 1	+0.86	+0.83	+0.86	+0.82,
P 2	+0.86	+0.82	+0.86	0.82

Selected Data from Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Orbital	Energy (kcal/mol)			
Donor Accepter				
LpPb- Lp*M	9.16	6.92		
Lp*Pb-Lp*M	7.29	8.05	19.17	11.44
LpPb-Ry*M	9.86	9.30		
Lp*Pb-RY*M	7.90	11.57	80.20	38.91
CR M- Lp*Pb	3.72	3.13		
Wiberg bond index				
Pb-M	0.1	0.04	0.01	0.01
$Pb\text{-}S_{(bridging)}$	0.30	0.35	0.38	0.45
	0.30	0.38	0.29	0. 0.36
$Pb\text{-}S_{(terminal)}$	0.25	0.28	0.39	0.46
$Pb\text{-}O_{(terminal)}$	0.08	0.10	0.05	0.08
$M\text{-}S_{(bridging)}$	0.11	0.13	0.96	0.12
	0.12	0.15	0.11	0.14