Electronic Supplementary Information

Thallium(I)phosphorodithioates containing intra- and intermolecular π-hole triel bonds

Tahira Firdoos,[a] Pretam Kumar,[a] Nipunn Sharma,[a] Rosa M. Gomila,[b] Antonio Frontera,[b] Puneet Sood[c] and Sushil K. Pandey*[a]

[a]*Post Graduate Department of Chemistry, University of Jammu, Baba Saheb Ambedkar Road, Jammu Tawi-180006, J&K, India*

[b]*Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain*

[c]*Advanced Materials Research Center, Block-A2 Building, Kamand Campus, Indian Institute of Technology, Mandi, Himachal Pradesh-175005, India.*

**Email: kpsushil@rediffmail.com*

Table S1 Selected bond lengths of compounds **1** and **2** (Å)

Compound 1		**Compound 2**	
Tl1—S1	3.123 (14)	Tl1—S2	3.114 (3)
Tl1—S2	3.044 (13)	Tl1—S1	3.158 (3)
S1—P1	1.966 (18)	S2—P1	1.967 (4
S2—P1	1.967 (19)	S1—P1	1.966 (4)
P1—O2	1.617 (4)	P1—O2	1.613 (7)
P1—O1	1.600 (3)	P1—O1	1.618 (7)
O2—C9	1.408 (5)	O2—C9	1.415 (11)
O1—C1	1.416 (5)	O1—C1	1.396 (11)

Symmetry code(s): (i) $-x$, $-y+1$, $-z+1$.

Table S2 Selected bond angles of compounds **1** and **2** (º)

Compound 1		**Compound 2**	
S2—Tl1—S1	65.76 (3)	S2—Tl1—S1	64.89 (7)
P1—S1—Tl1	86.37 (6)	P1—S2—Tl1	89.33 (12)
S1—P1—S2	116.73 (9)	P1—S1—Tl1	88.08 (12)
O2—P1—S1	111.16 (15)	S1—P1—S2	117.65 (18)
O2—P1—S2	110.65 (15)	O2—P1—S2	110.7 (3)
O1—P1—S1	112.58 (14)	O2—P1—S1	111.9 (3)
O1—P1—S2	105.97 (14)	O2—P1—O1	92.0 (4)
O1—P1—O2	98.09 (19)	O1—P1—S2	110.8 (3)
P1—S2—Tl1	88.60 (6)	S2—Tl1—S1	64.89 (7)
C9—O2—P1	122.7 (3)	P1—S2—Tl1	89.33 (12)
C1—O1—P1	123.0 (3)	P1—S1—Tl1	88.08 (12)
C10—C9—O2	119.3 (4)	S1—P1—S2	117.65 (18)
C14—C9—O2	117.6 (4)	O2—P1—S2	110.7 (3)
C2—C1—O1	119.8 (4)	O2—P1—S1	111.9 (3)
C2—C1—C6	122.8 (5)	O2—P1—O1	92.0 (4)

Symmetry code(s): (i) $-x$, $-y+1$, $-z+1$.

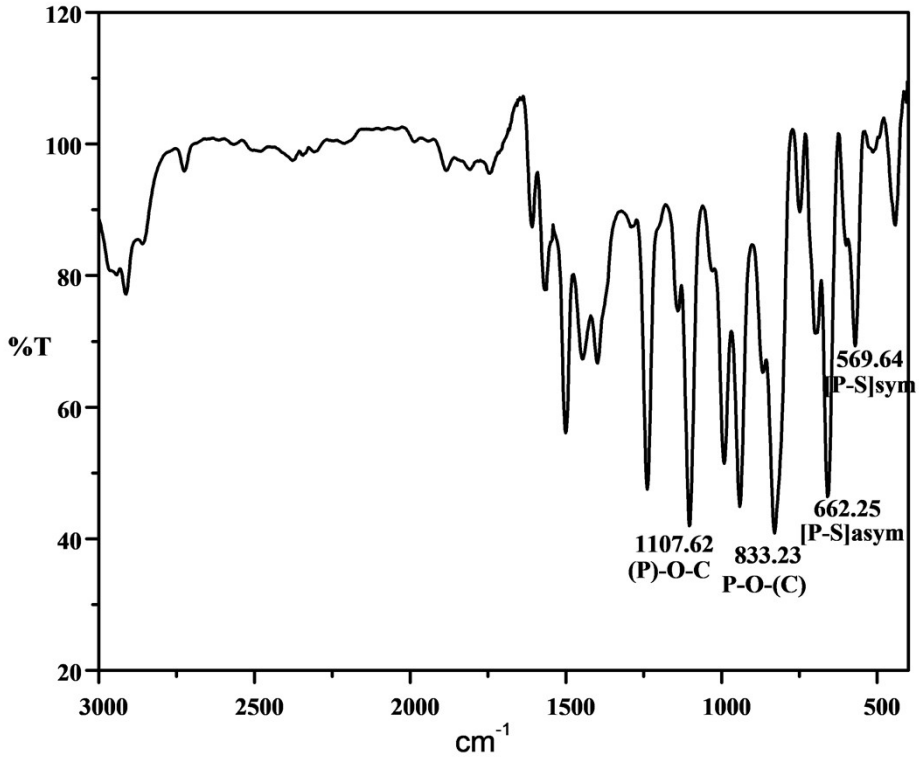

Fig. S1 FTIR spectra of Compound **1**

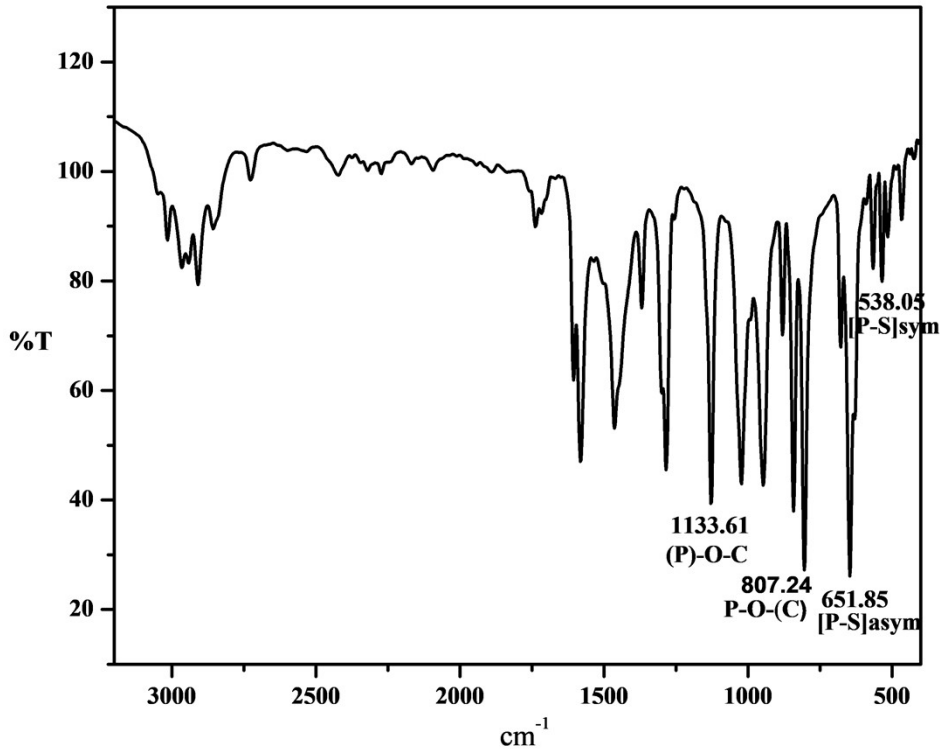

Fig. S2 FTIR spectra of Compound **2**

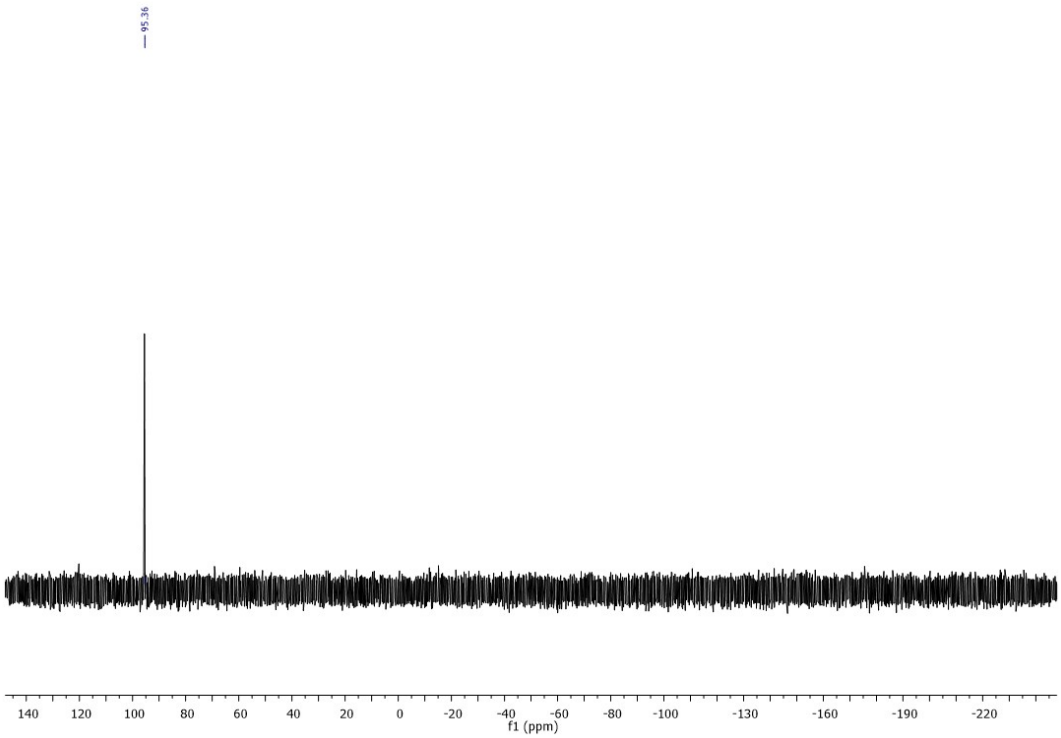

Fig. S3 ^{31}P NMR spectra of Compound **1** ($CDCl_3$)

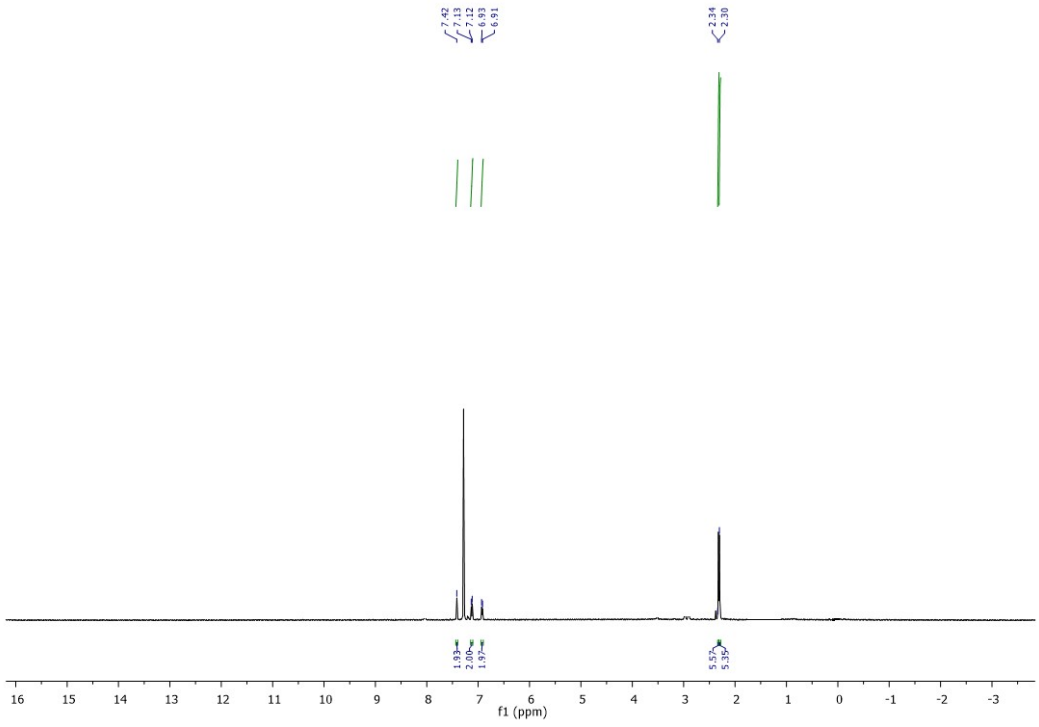

Fig. S4 ^{1}H NMR spectra of Compound **1** ($CDCl_3$)

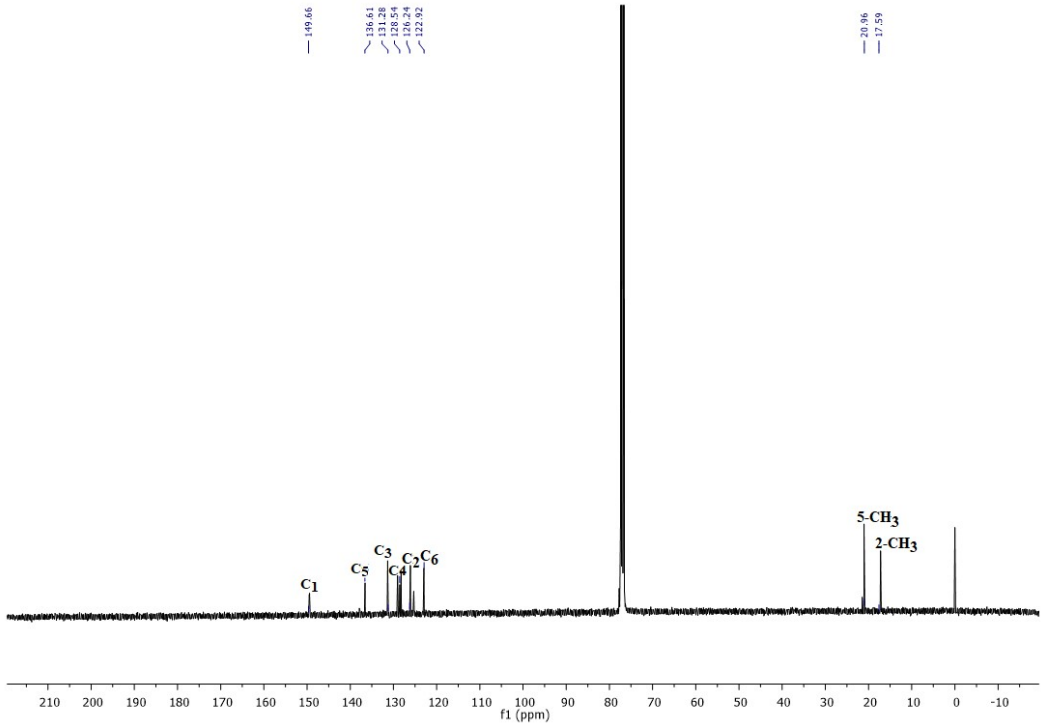

Fig. S5 ^{13}C NMR spectra of Compound **1** ($CDCl_3$)

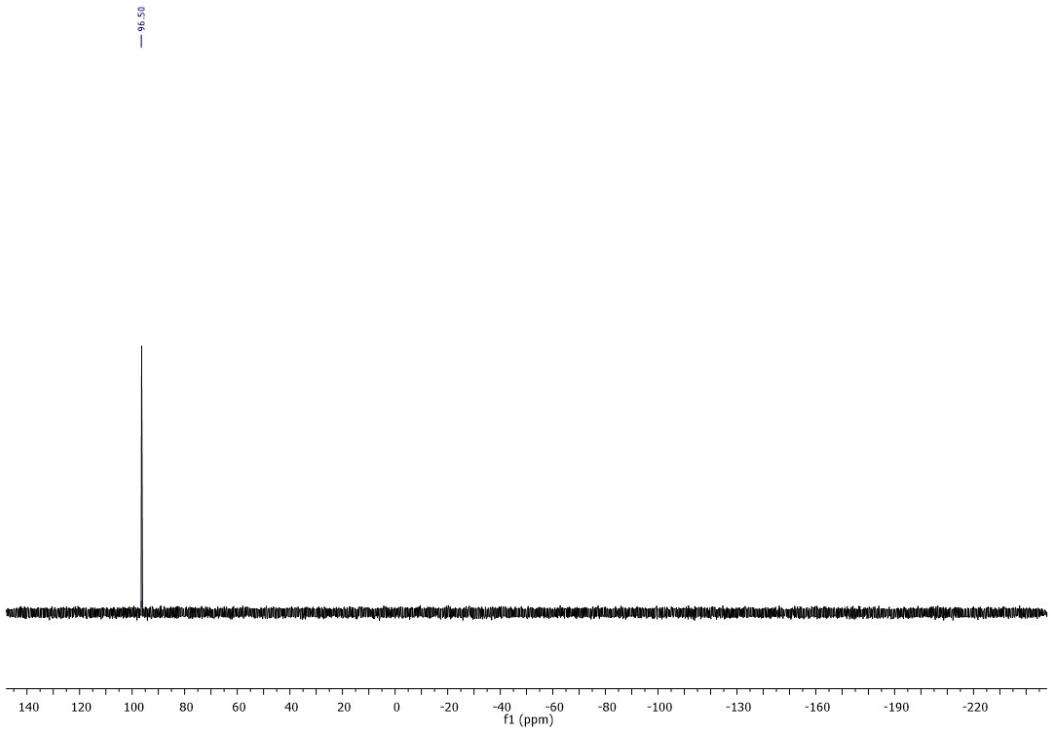

Fig. S6 ^{31}P NMR spectra of Compound **2** ($CDCl_3$)

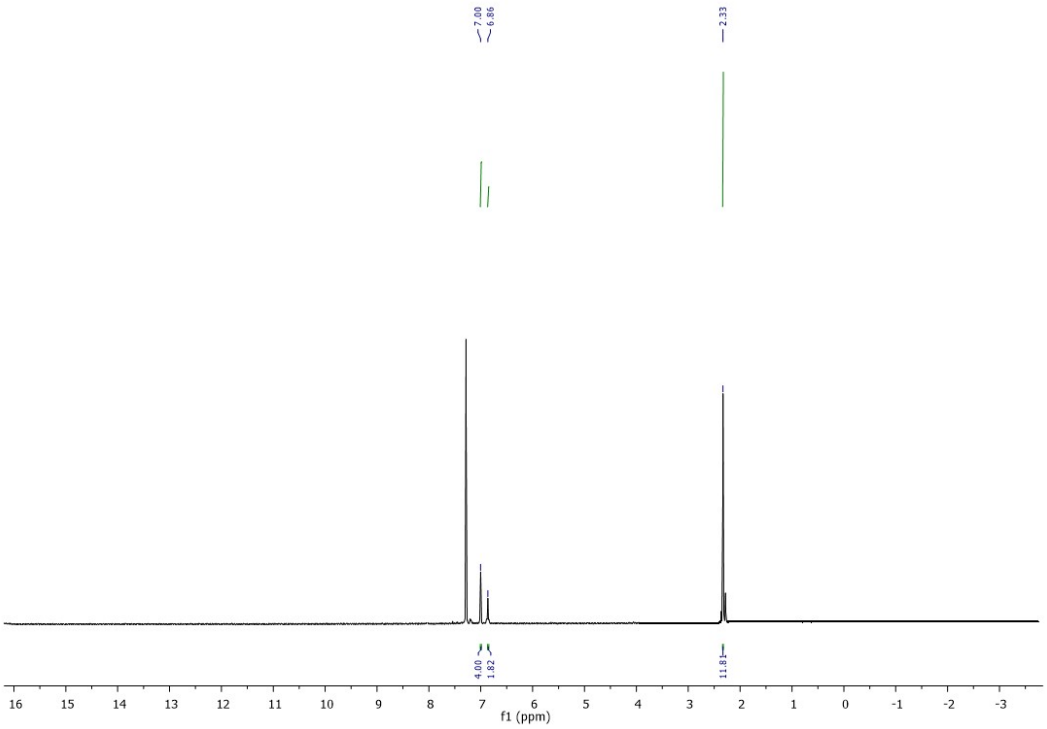

Fig. S7 ^{1}H NMR spectra of Compound **2** ($CDCl_3$)

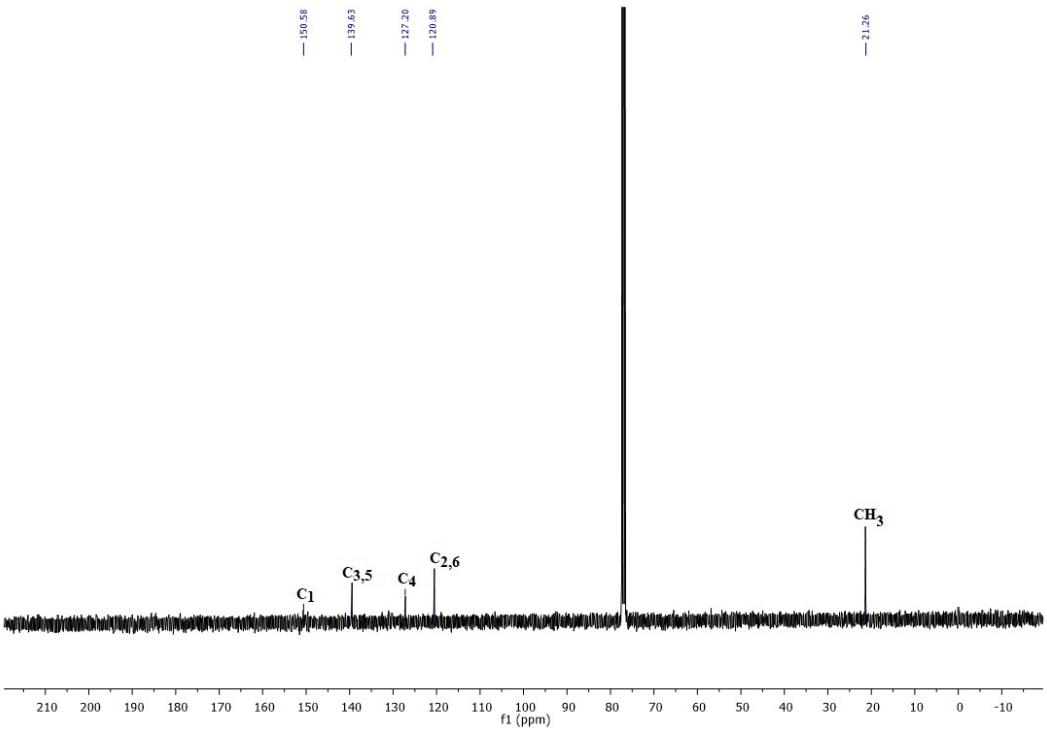

Fig. S8 ^{13}C NMR spectra of Compound **2** ($CDCl_3$)

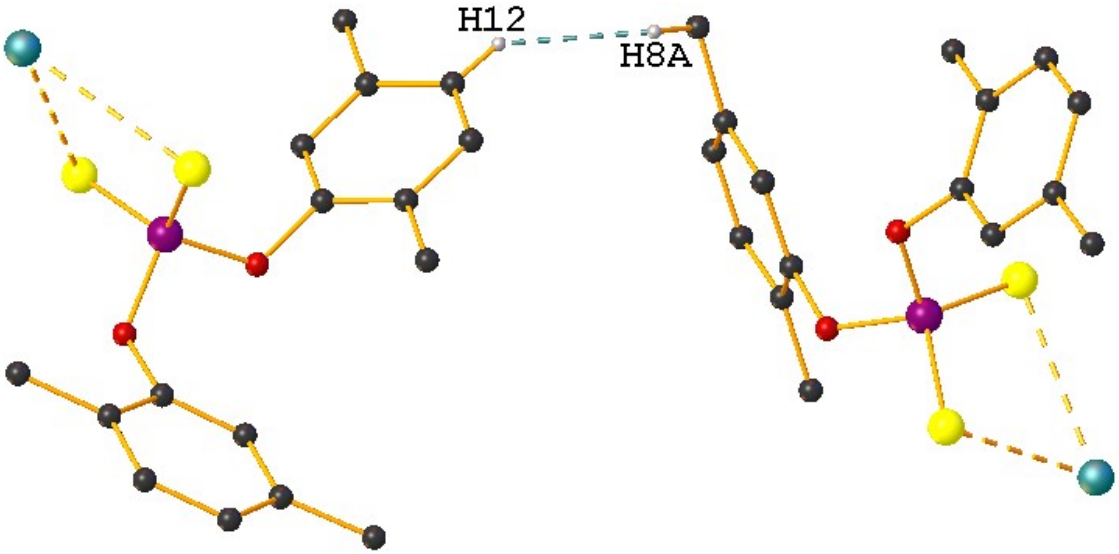

Fig. S9 Supramolecular motif of compound **1** generated through H···H interactions.

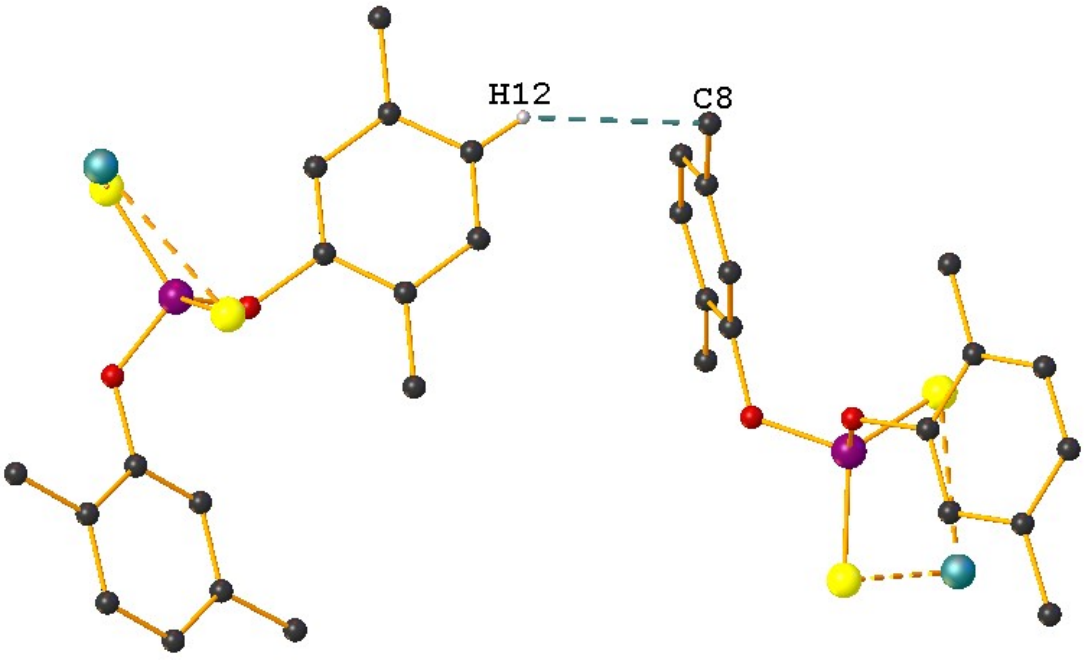

Fig. S10 Supramolecular dimer of compound **1** generated through C···H interactions.

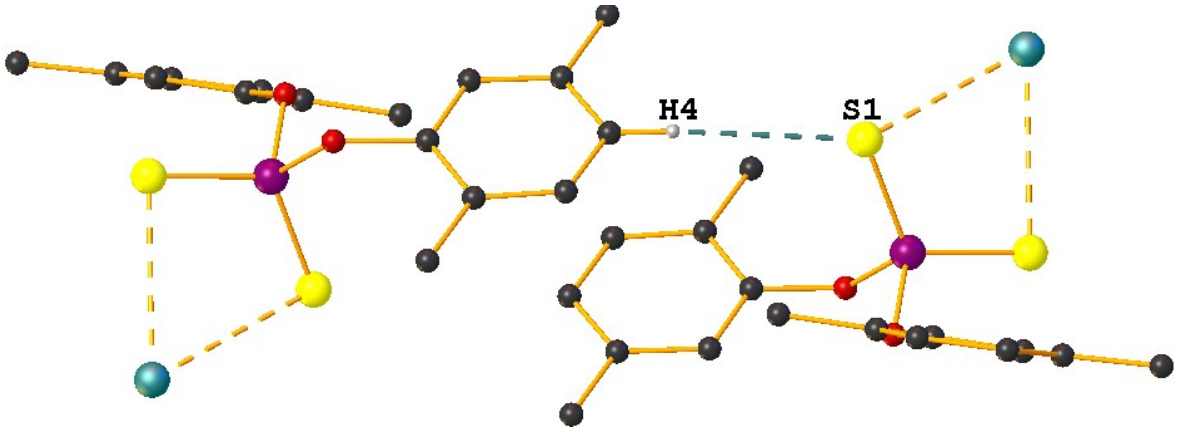

Fig. S10 Supramolecular dimeric assembly of compound **1** generated through S···H interactions.

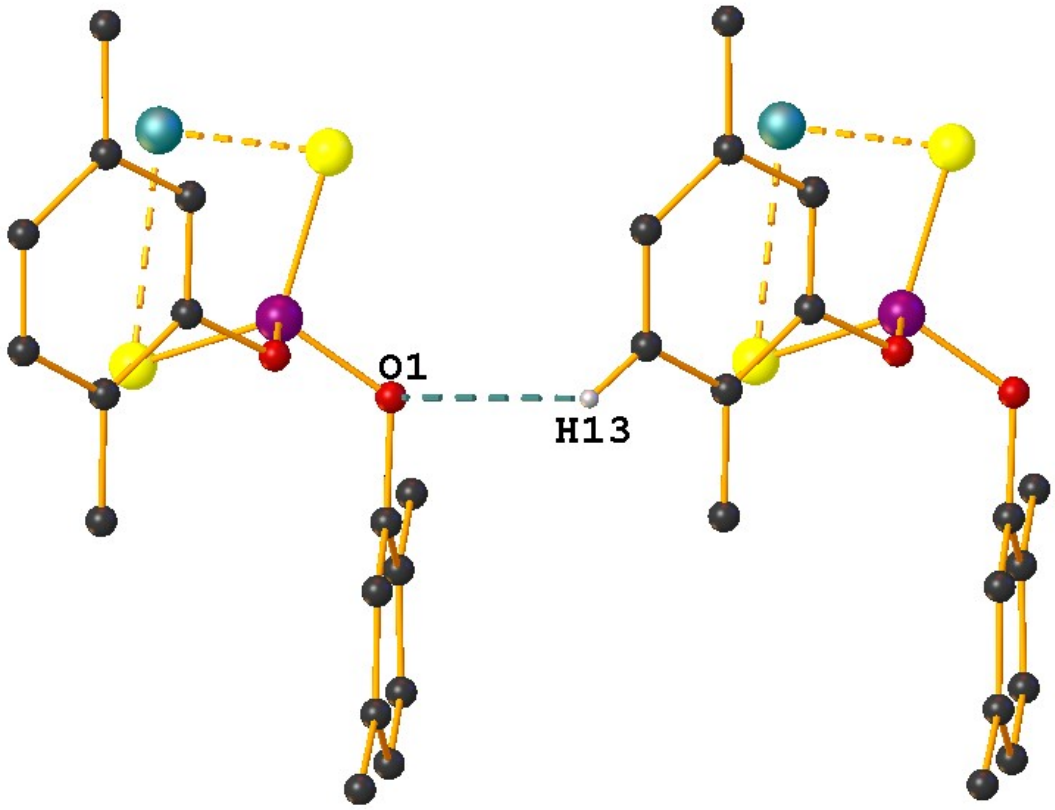

Fig. S12 Supramolecular dimer of compound **1** generated through O···H interactions.

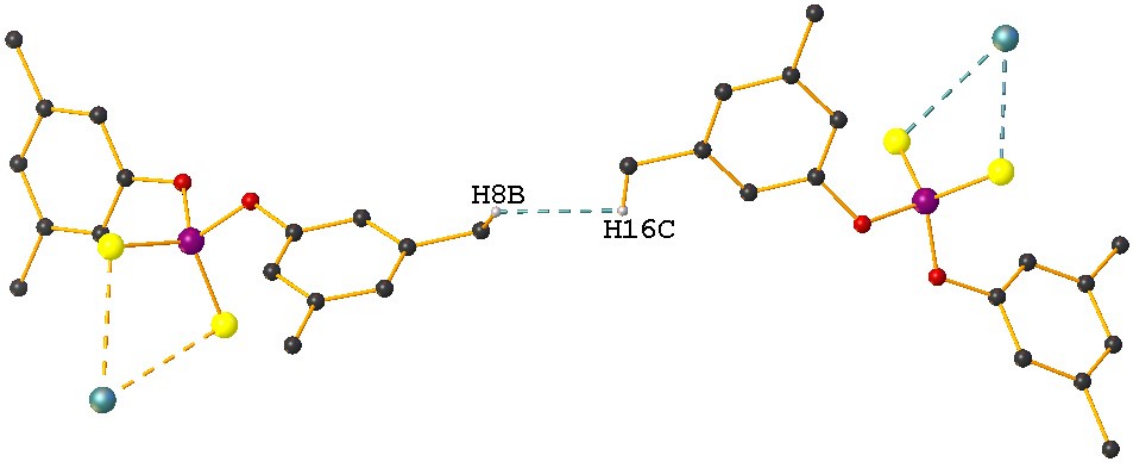

Fig. S13 Supramolecular motif of compound **2** generated through H···H interactions.

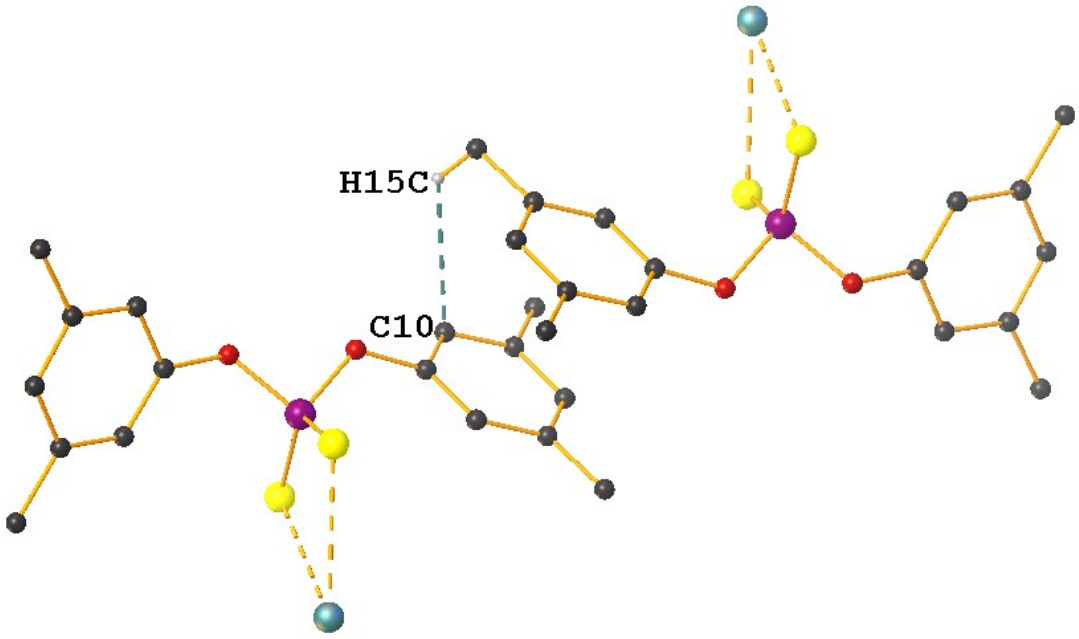

Fig. S14 Supramolecular dimer of compound **2** formed through C···H interactions.