Electronic Supplementary Information

Role of non-covalent interactions in the supramolecular architectures of mercury(II) diphenyldithiophosphates: An experimental and theoretical investigation

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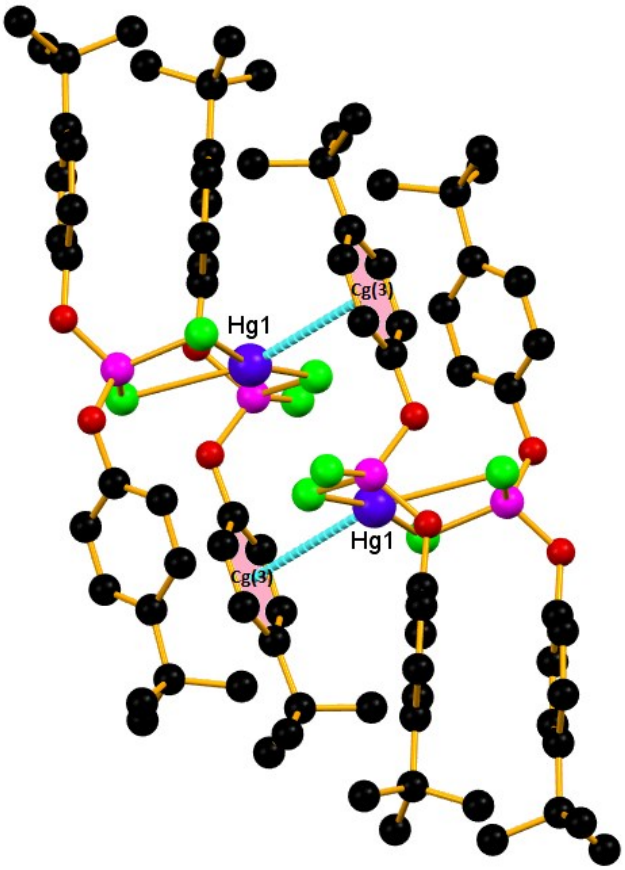

Fig. S1. A dimer unit of complex **1** generated through intermolecular Hg···π SpB interactions. Hydrogen atoms are omitted for clarity. Symmetry transformation = 1 - x, 1 - y, 1 - z, where Hg1···Cg(3) = 3.521 Å [Cg(3) = center of mass of the ring C(21)-C(26)].

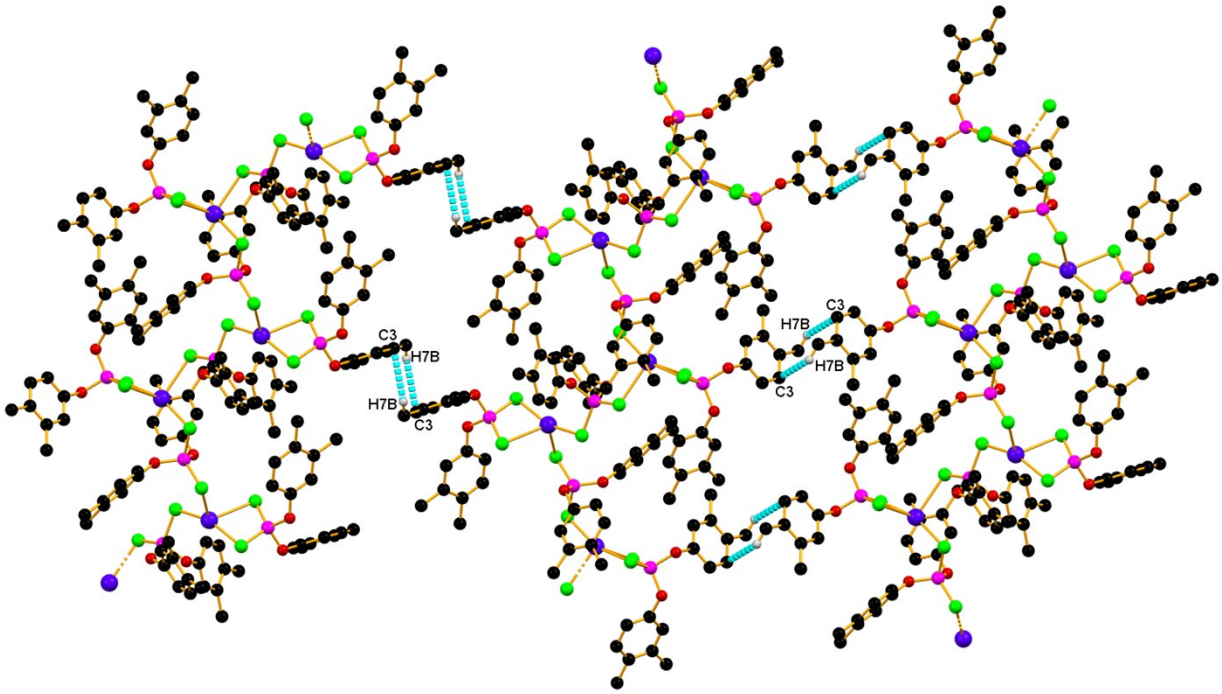

Fig. S2. Supramolecular network of the complex **2** generated through C···H interactions. Only the relevant hydrogen atoms are shown for clarity. Symmetry transformation = - *x*, 1 - y, 1 - z, where H7B···C3 = 2.898 Å.

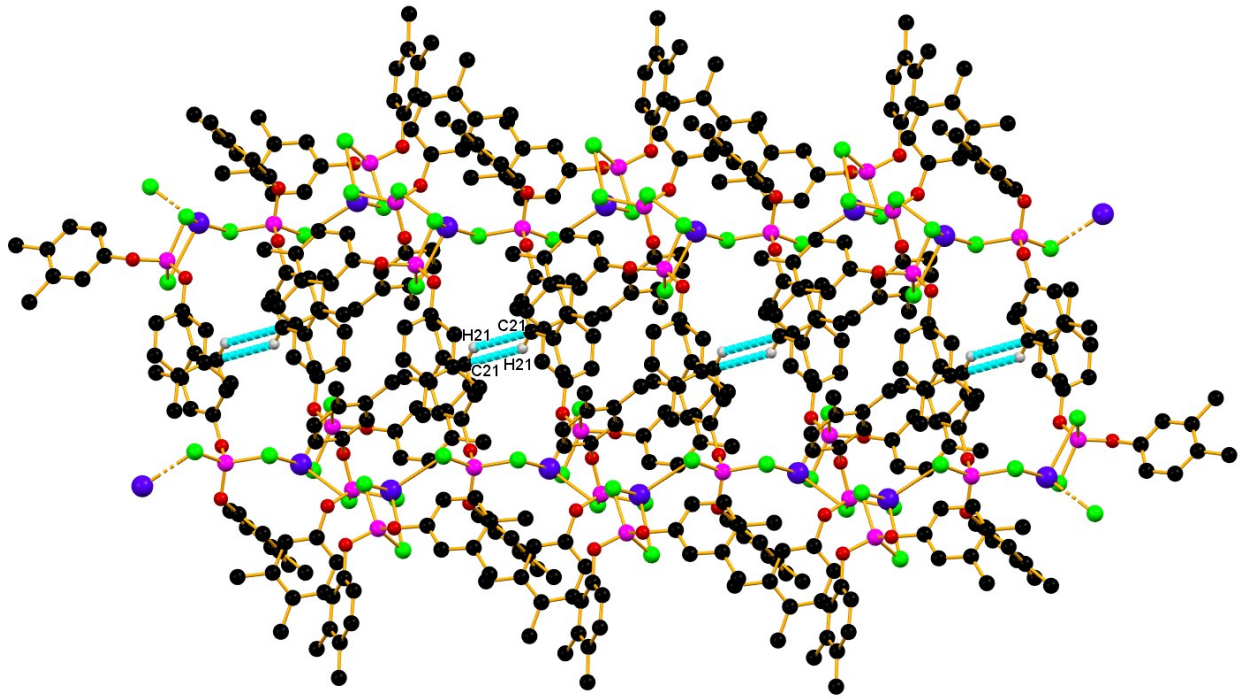

Fig. S3. Supramolecular network of complex **2** generated through C···H interactions. Only the relevant hydrogen atoms are shown for clarity. Symmetry transformation = x, 1.5 - y, - 1/2 + z, where H21···C21= 2.820 Å.

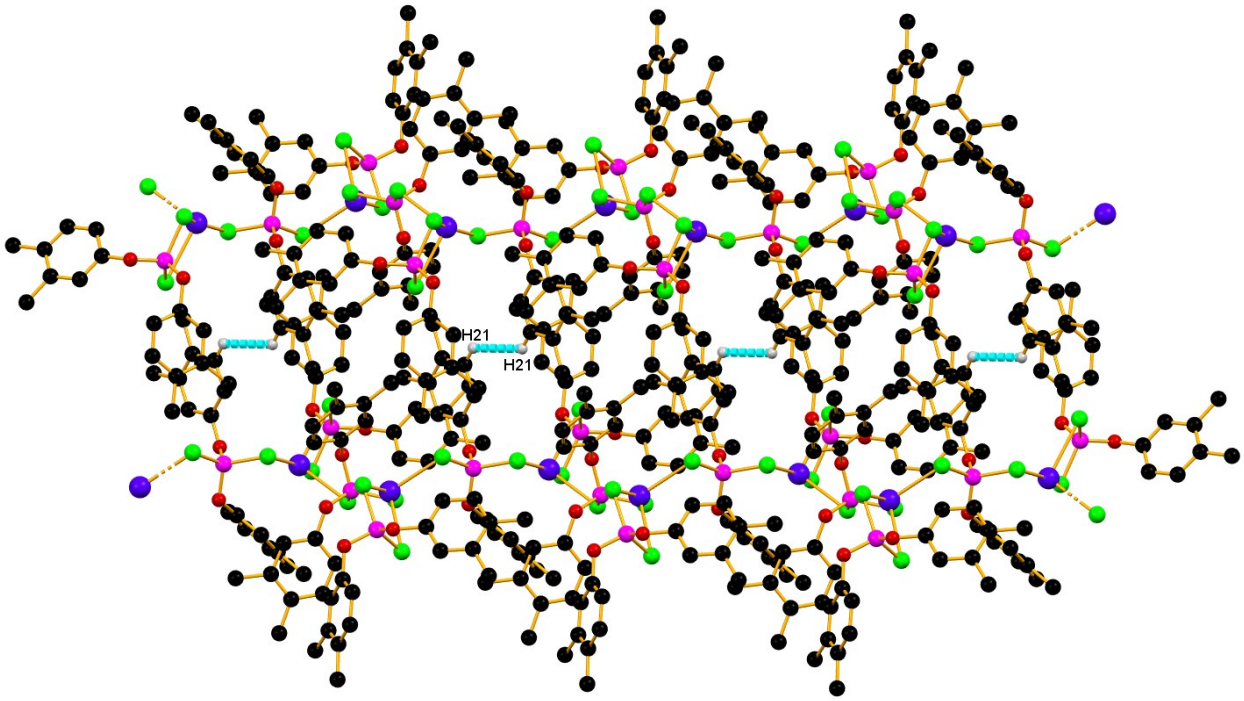

Fig. S4. Supramolecular polymer chain of complex **2** generated through H···H interactions. Only

the relevant hydrogen atoms are shown for clarity. Symmetry transformation = x, 1.5 - y, - 1/2 + z, where H21···H21= 2.203 Å.

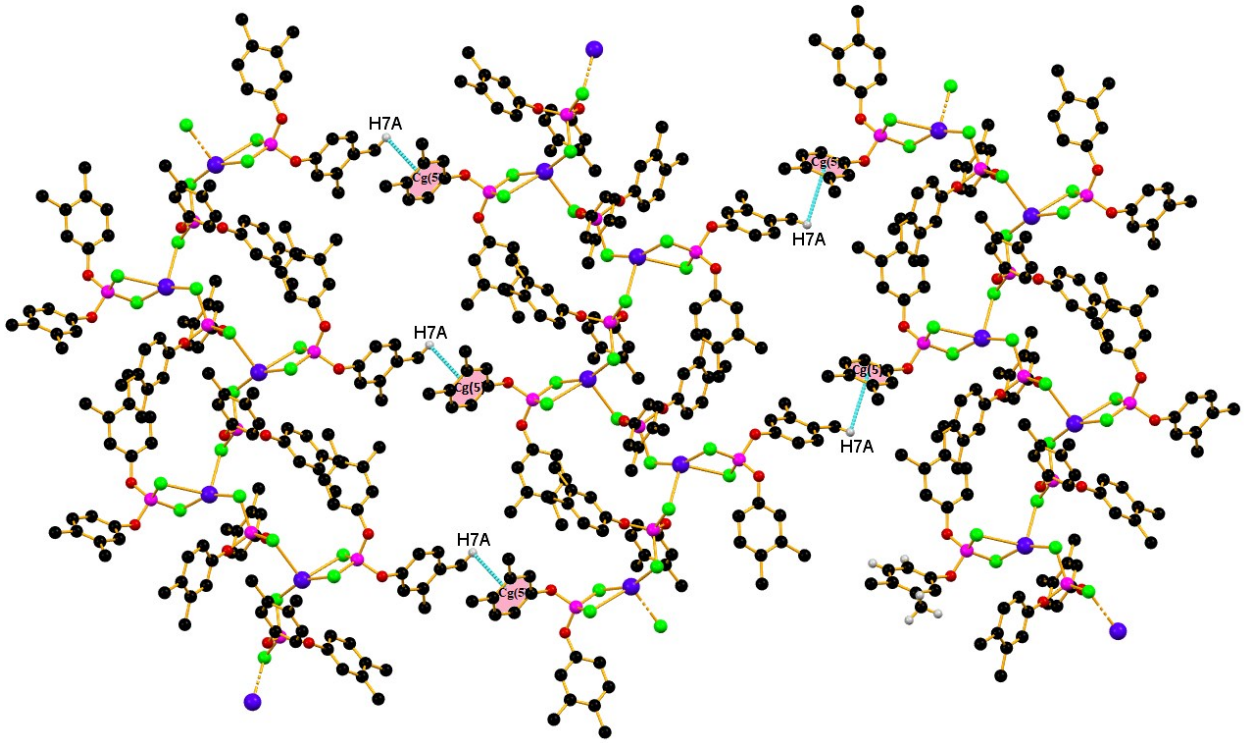

Fig. S5. Supramolecular polymer chain of complex **2** generated through C-H···π interactions. Only the relevant hydrogen atoms are shown for clarity. Symmetry transformation = - *x*, 1 – y, 1 - z, where H7A···Cg5 = 3.429 Å [Cg(5) = center of mass of the ring C(1)-C(6)].

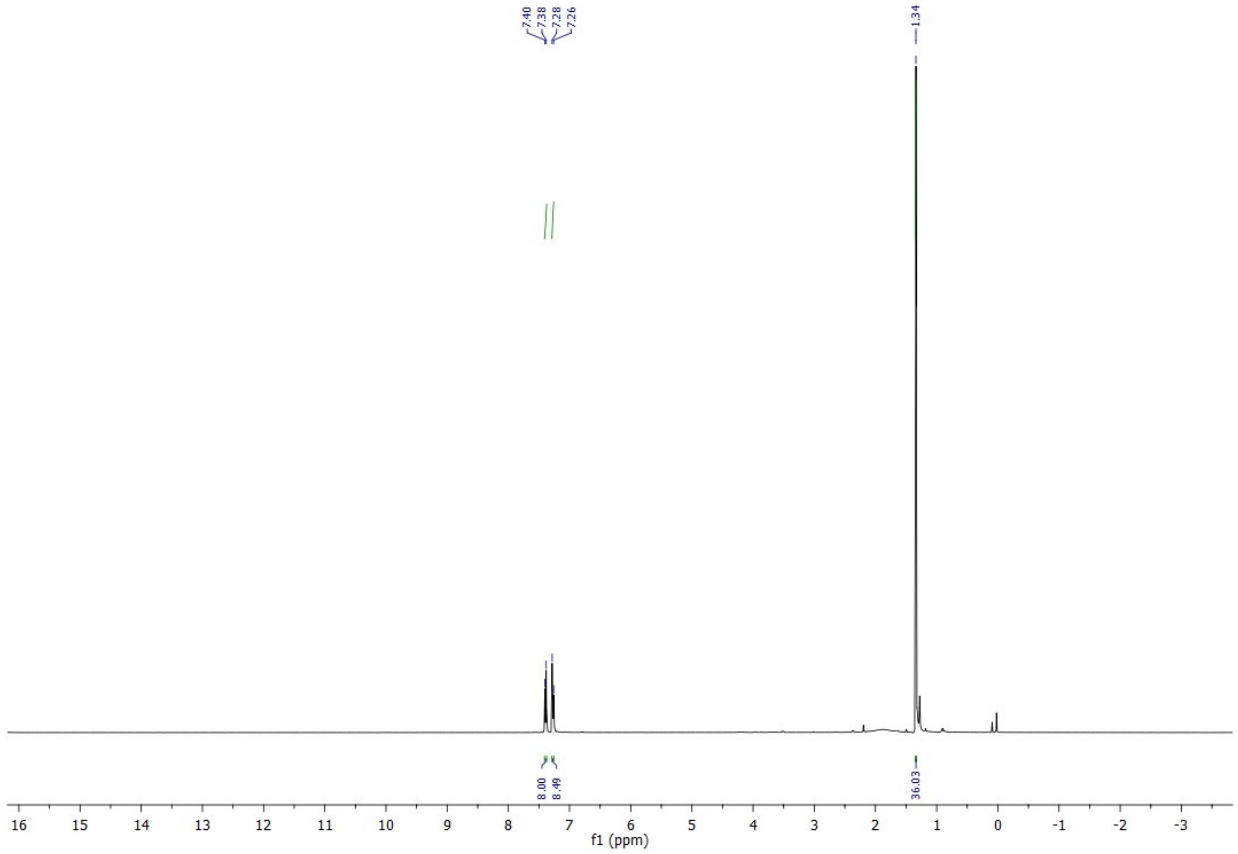

Fig. S6. ^{1}H NMR spectra of complex **1**

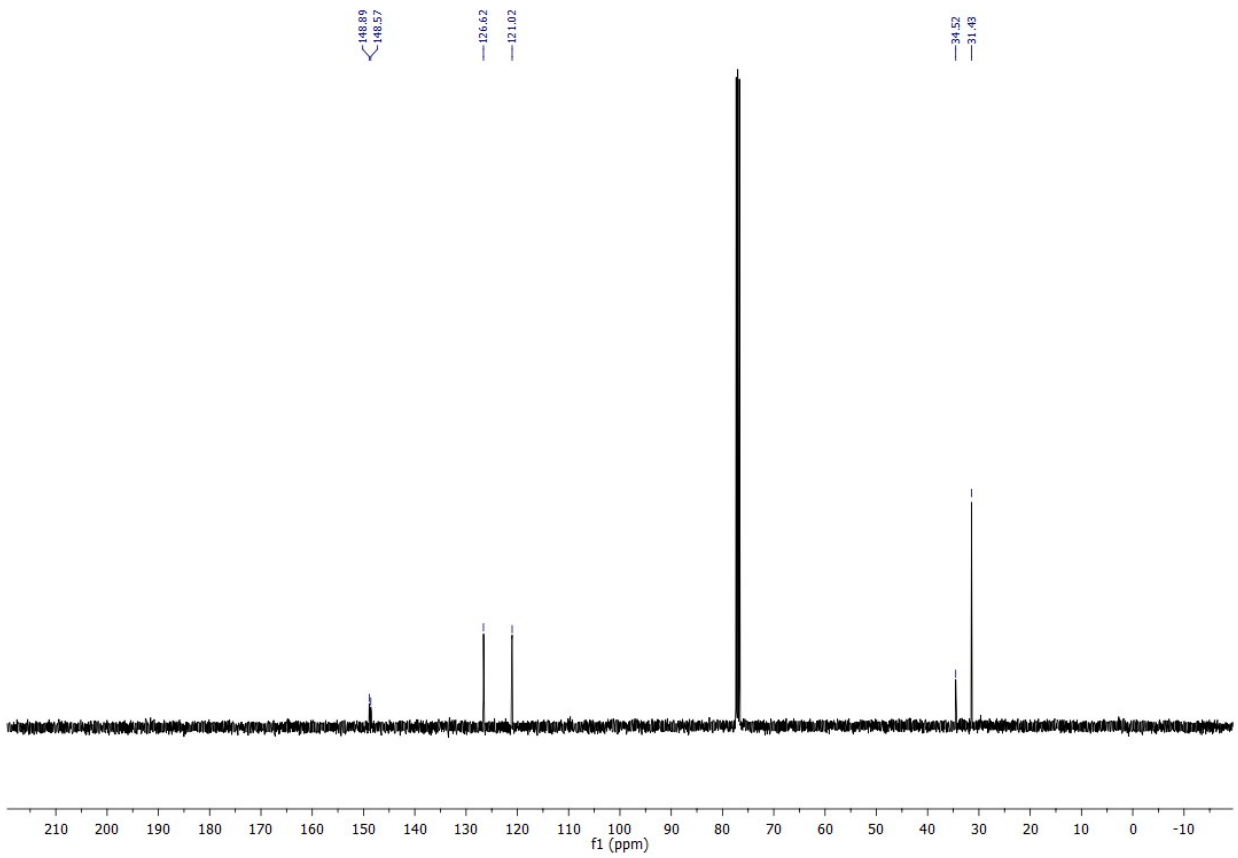

Fig. S7. ^{13}C NMR spectra of complex **1**

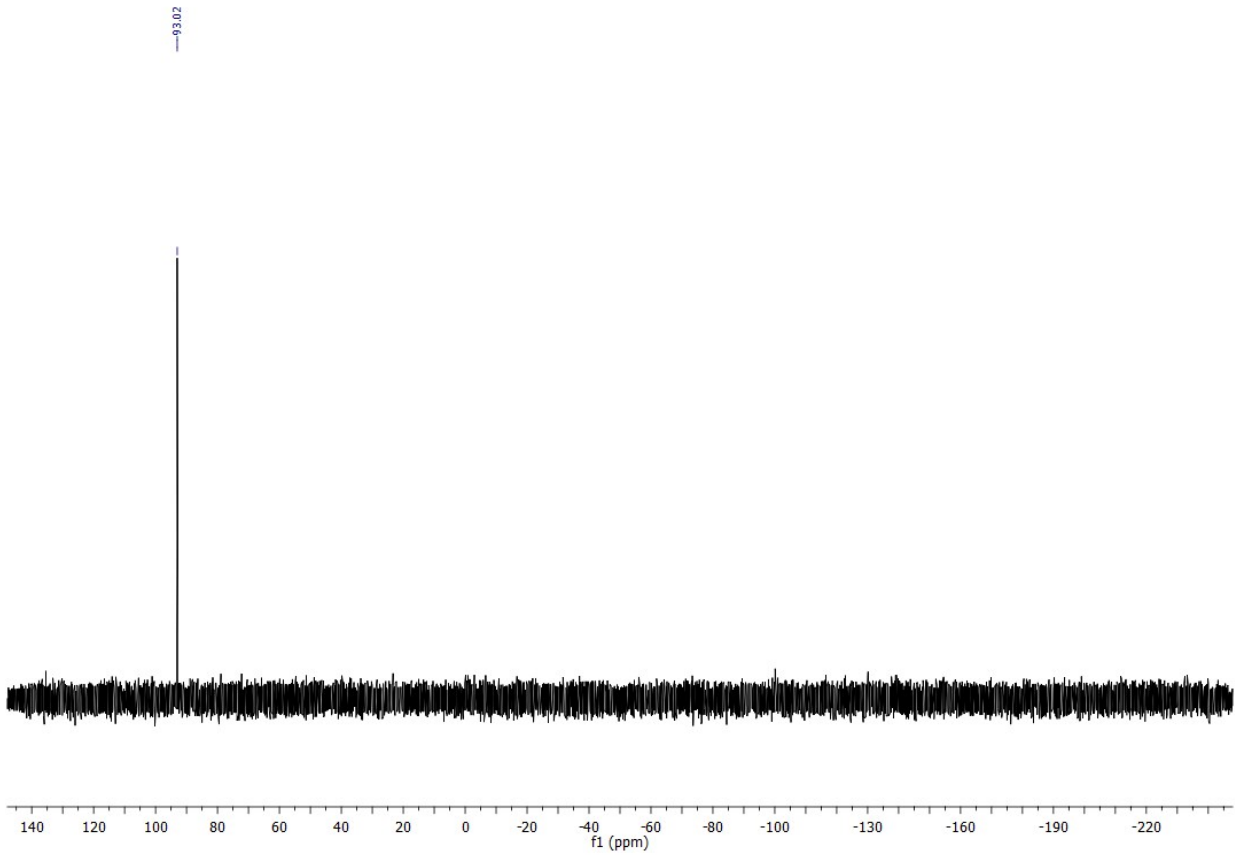

Fig. S8. ^{31}P NMR spectra of complex **1**

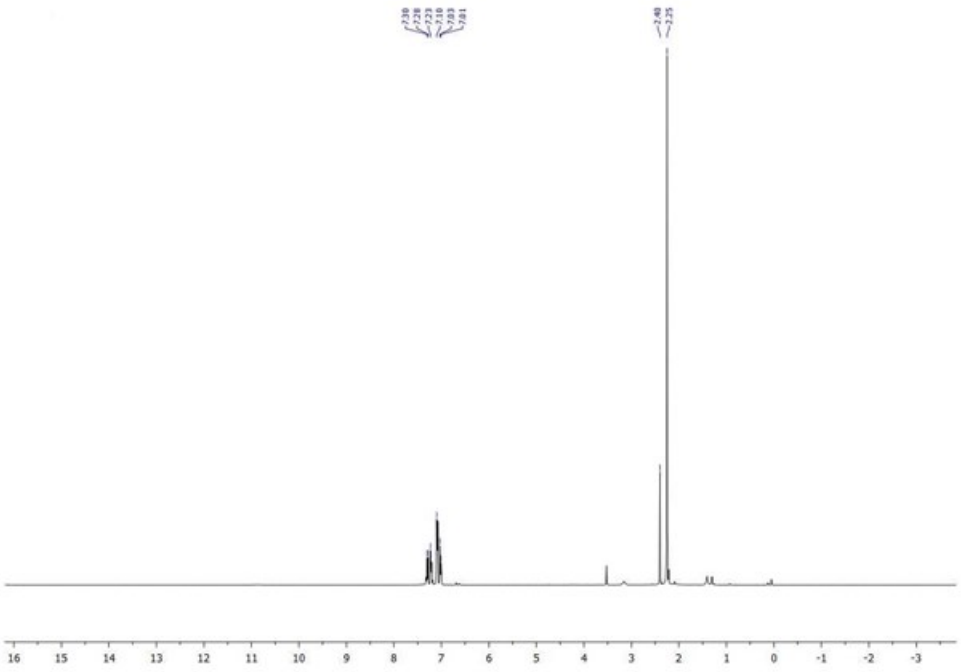

Fig. S9. ^{1}H NMR spectra of complex **2**

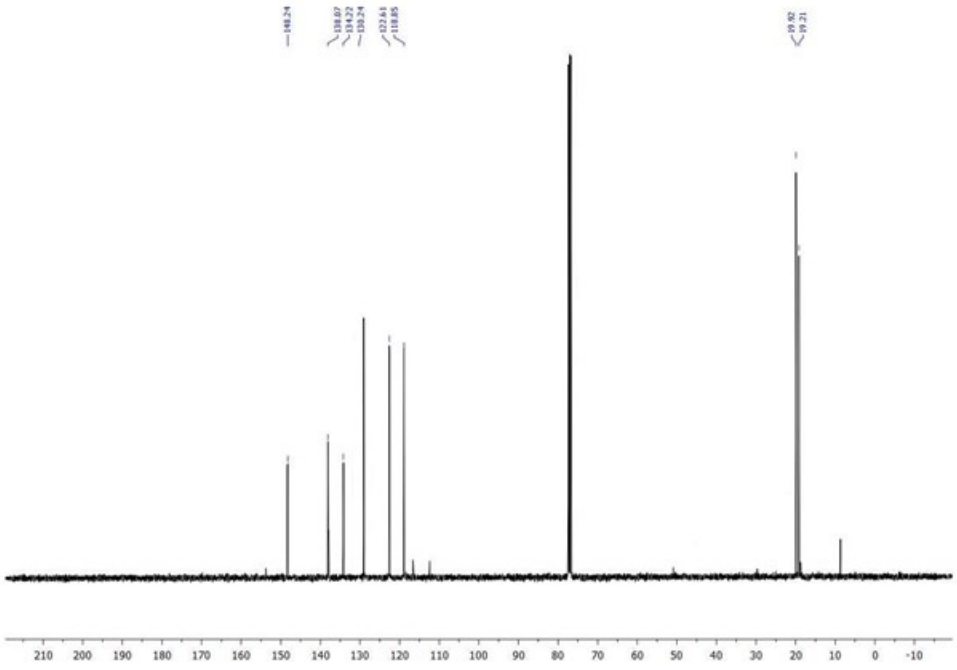

Fig. S10. ^{13}C NMR spectra of complex **2**

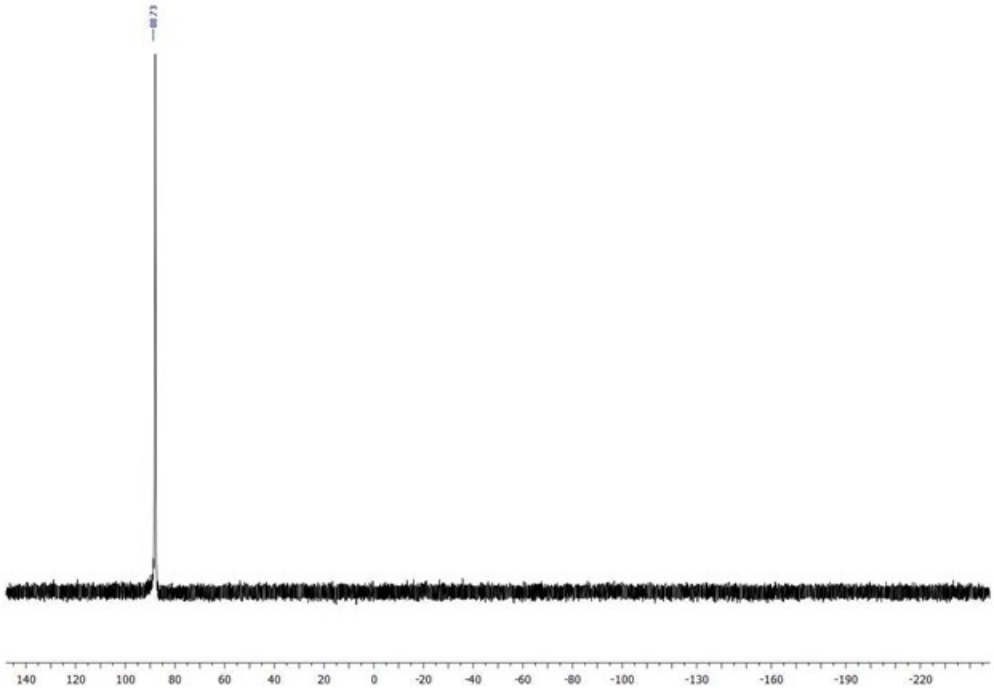

Fig. S11. ^{31}P NMR spectra of complex **2**

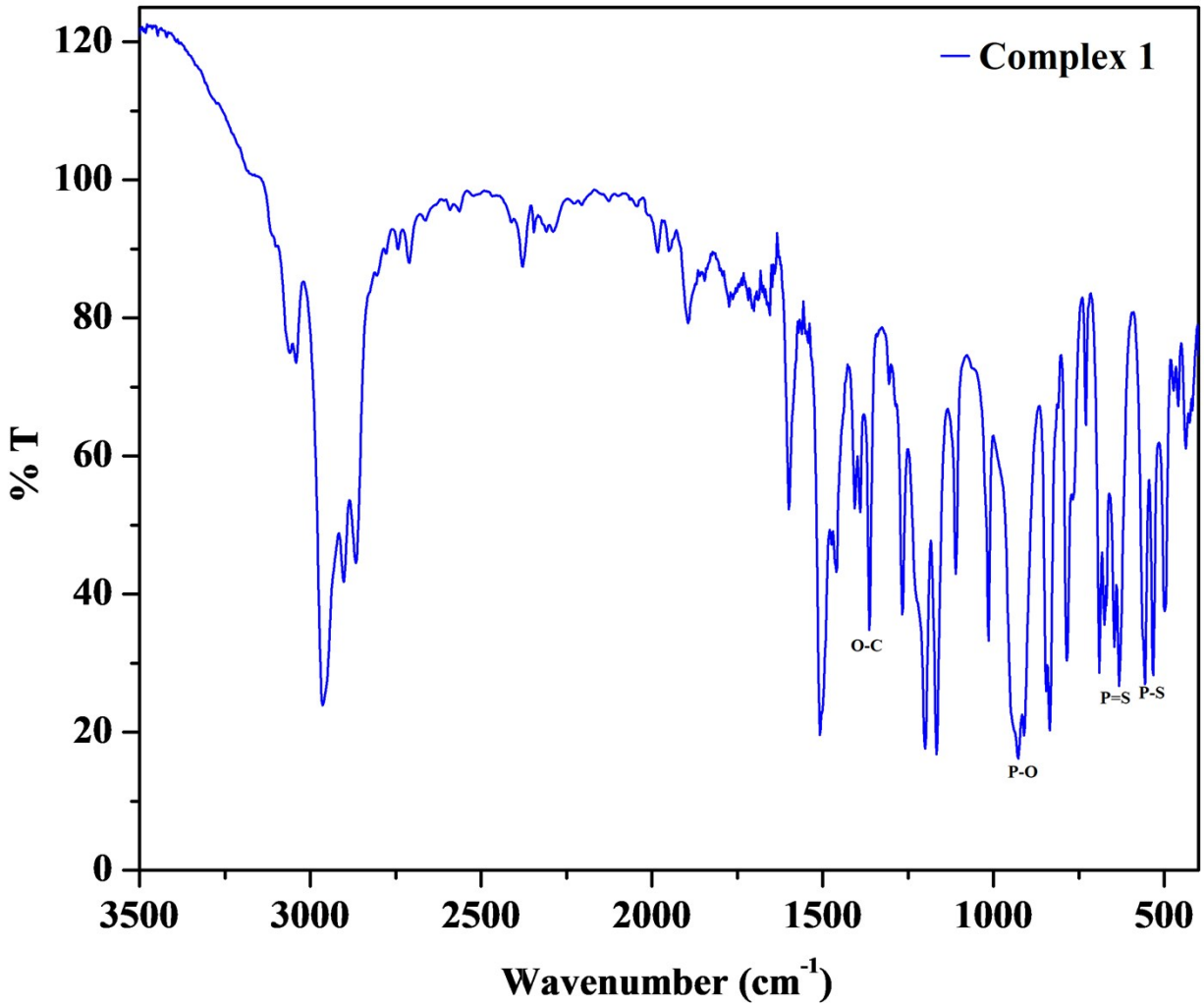

Fig. S12. IR spectra of complex **1**

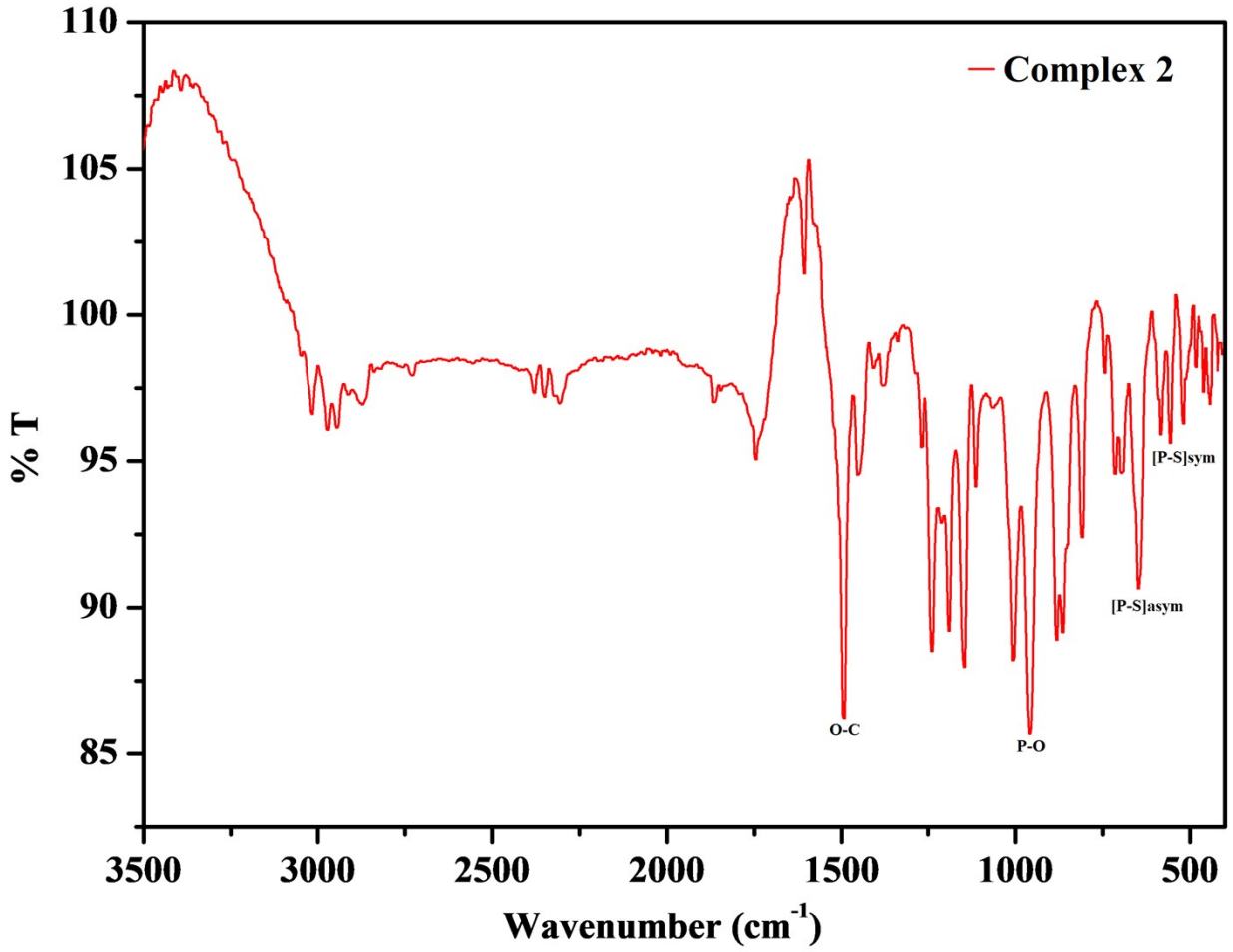

Fig. S13. IR spectra of complex **2**

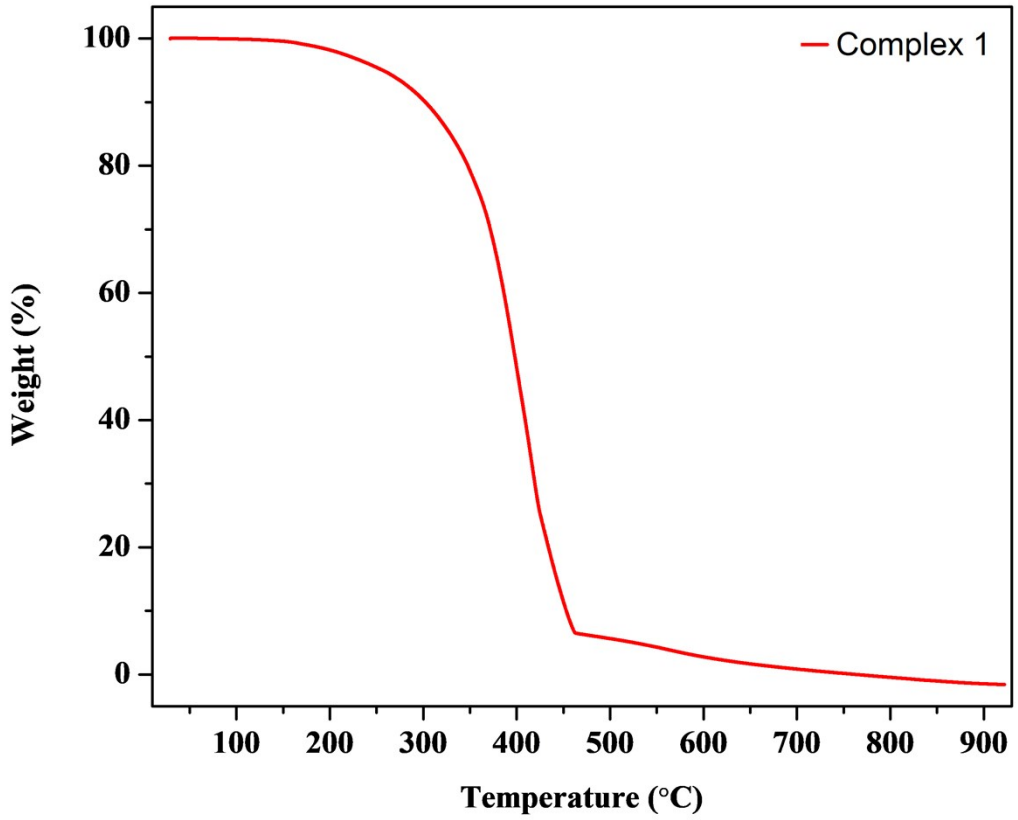

Fig. S14. TGA of complex **1**

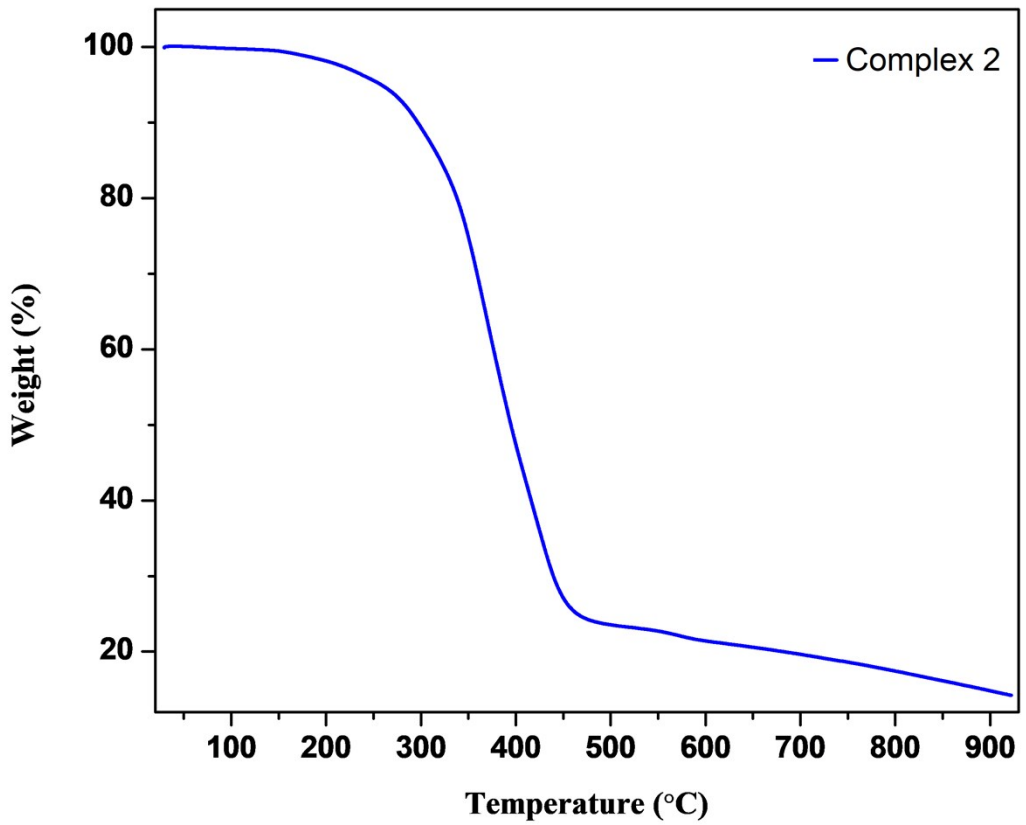

Fig. S15. TGA of complex **2**

Table S1. Selected bond lengths (angstroms) of complexes **1** and **2**

Complex 1		**Complex 2**	
S2—P1	2.0408 (14)	Hg1—S3	2.3907 (11)
S3—P2	2.0590 (14)	Hg1—S2	2.4267 (12)
P1—S1	1.9471 (14)	Hg1—S4^{i}	2.7283 (11)
P1—O1	1.588 (3)	Hg1—S1	2.8868 (12)
P1—O2	1.587 (2)	P2—S3	2.0139 (14)
P2—S4	1.9106 (14)	P2—S4	1.9379 (15)

P2—O3	1.590 (3)	P2—O4	1.585 (3)
P2—O4	1.595 (2)	P2—O3	1.586 (3)
O1—C1	1.414 (4)	P1—S2	2.0254 (15)
O2—C11	1.409 (4)	P1—S1	1.9441 (16)
O3—C21	1.413 (4)	P1—O2	1.595 (3)
O4—C31	1.400 (4)	P1—O1	1.589 (3)
Hg1—S1	2.8347 (10)	O4—C25	1.413 (4)
Hg1—S2	2.3875 (9)	O2—C9	1.421 (5)
Hg1—S3	2.3591 (9)	O3—C17	1.404 (5)
		O1—C1	1.423 (5)

Symmetry code(s): (i) −*x*+1, *y*−1/2, −*z*+1/2.

Table S2. Selected bond angles (degrees) of complexes **1** and **2**

Complex 1		**Complex 2**	
S3—Hg1—S2	166.15 (3)	S3—Hg1—S2	157.98 (4)
S3—Hg1—S1	113.75 (3)	S3—Hg1—S4^{i}	102.62 (4)
S2—Hg1—S1	78.46 (3)	S3—Hg1—S1	107.05 (4)
P2—S3—Hg1	104.06 (5)	S2—Hg1—S4^{i}	97.01 (4)
S4—P2—S3	110.35 (6)	S2—Hg1—S1	77.74 (4)
O3—P2—S3	109.94 (11)	S4^{i}—Hg1—S1	102.89 (4)
O3—P2—S4	117.60 (10)	S4—P2—S3	109.94 (7)
O3—P2—O4	93.28 (13)	O4—P2—S3	111.27 (11)
O4—P2—S3	107.26 (10)	O4—P2—S4	109.75 (11)

O4—P2—S4	117.02 (11)	O4—P2—O3	100.20 (14)
P1—S2—Hg1	89.36 (4)	O3—P2—S3	109.65 (12)
S1—P1—S2	112.73 (6)	O3—P2—S4	115.71 (12)
O2—P1—S2	108.32 (11)	P2—S3—Hg1	101.83 (5)
O2—P1—S1	115.95 (12)	S1—P1—S2	115.30 (7)
O2—P1—O1	94.37 (13)	O2—P1—S2	109.66 (13)
O1—P1—S2	108.97 (12)	O2—P1—S1	113.10 (12)
O1—P1—S1	114.94 (11)	O1—P1—S2	102.50 (12)
P1—S1—Hg1	79.19 (4)	O1—P1—S1	115.66 (13)
C21—O3—P2	123.9 (2)	O1—P1—O2	99.01 (16)
C11—O2—P1	122.4 (2)	P1—S2—Hg1	88.87 (5)
C31—O4—P2	123.2 (2)	P2—S4—Hg1^{ii}	105.18 (5)
C1—O1—P1	121.5 (2)	P1—S1—Hg1	78.09 (5)
		C25—O4—P2	124.1 (2)
		C9—O2—P1	124.2 (3)
		C17—O3—P2	125.8 (3)
		C1—O1—P1	120.3 (2)

Symmetry code(s): (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.