

Supplementary Data

Synthesis and Structural Studies of Complexes of Bis(pentafluorophenyl)mercury with Di(phosphane oxide) Ligands

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Table of contents

1) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of 1Hg .	S2
2) $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of 1Hg .	S2
3) IR spectrum of 1Hg .	S3
4) Intermolecular contacts and interactions in compound 1Hg .	S3 – S5
5) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction mixture (Scheme 1.2) having compound 2a .	S5
6) ^1H NMR spectrum of 2 .	S6
7) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of 2 .	S6
8) ^{13}C NMR spectrum of 2 .	S7
9) IR spectrum of ligand 2 .	S7
10) Intermolecular contacts and interactions in compound 2 .	S8
11) Intermolecular contacts and interactions in compound 2Hg .	S8 – S12
12) $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of 3Hg .	S12
13) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of 3Hg .	S13
14) IR spectrum of 3 .	S13
15) IR spectrum of 3Hg .	S14
16) Intermolecular contacts and interactions in complex 3Hg .	S14 – S15
17) Intramolecular interactions in complexes 1Hg , 2Hg and 3Hg .	S15

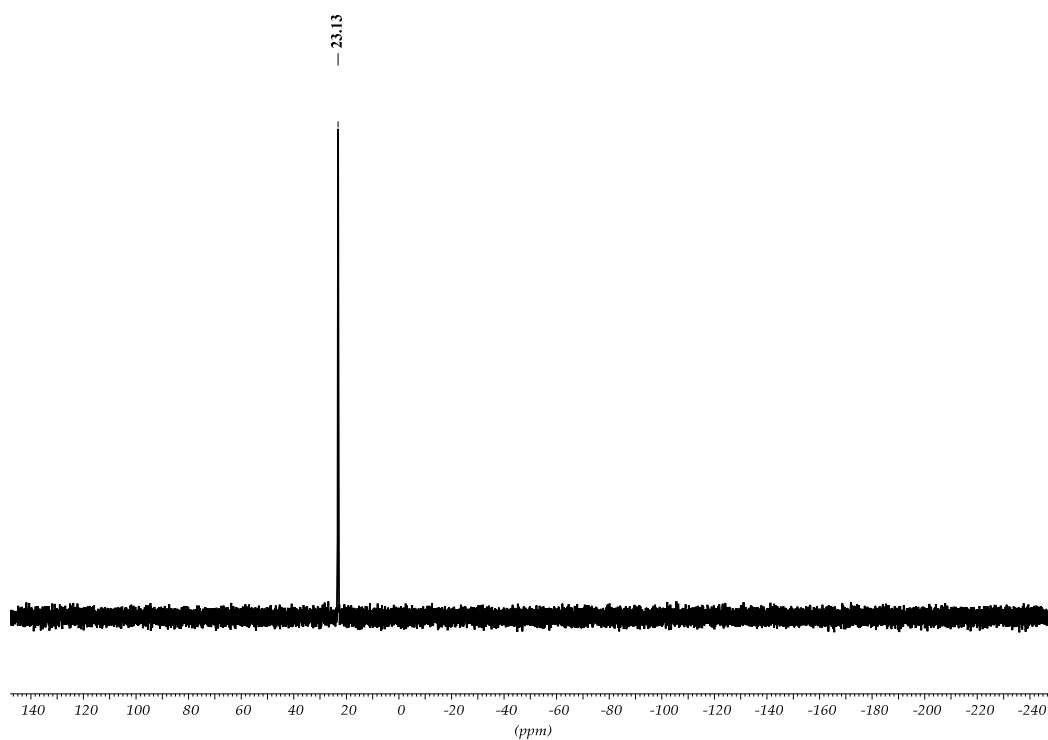


Figure S1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1Hg**.

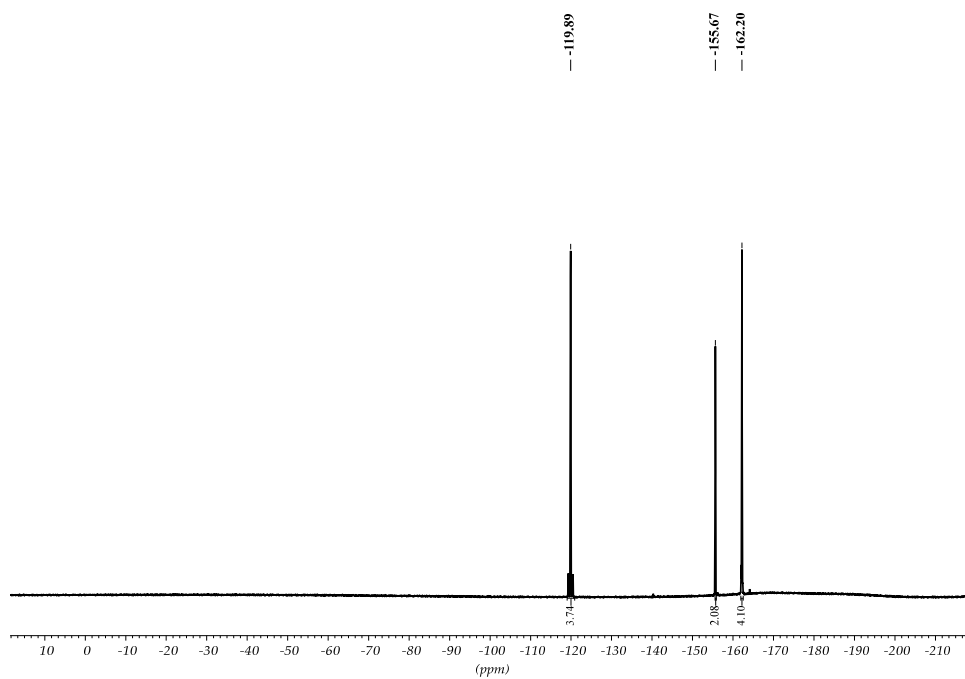


Figure S2. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **1Hg**.

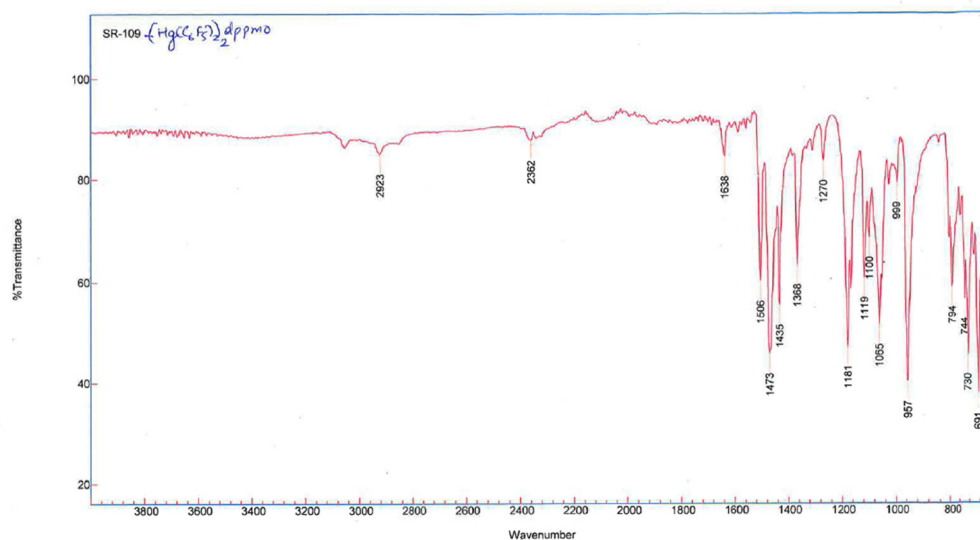


Figure S3. IR spectrum of **1Hg**.

Table S1. Intermolecular contacts and interactions in compound **1Hg**

C...F bond contacts	
C12-F5	3.007
C9-F4	3.153
C15-F6	3.164
C8-F6	3.063
CH...FC interactions	
H13(CH2)-F3	2.471
H15-F6	2.496
$\pi \cdots \pi$ interaction	
C2-C18	3.384

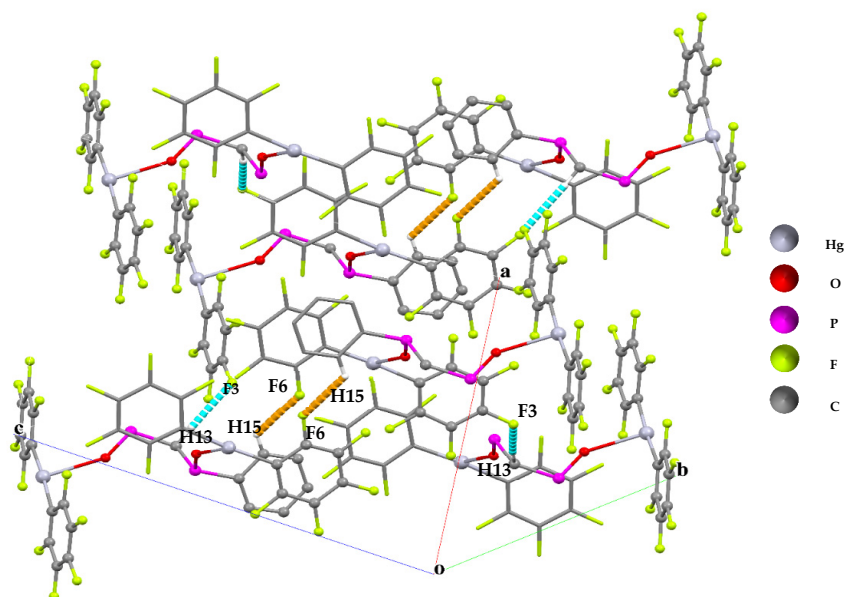


Figure S4. Packing diagrams showing the two-dimensional arrangement of complex **1Hg** involving: intermolecular H...F interactions (greenish-blue and orange dotted lines), which propagate along the *a*- and *b*-axes.

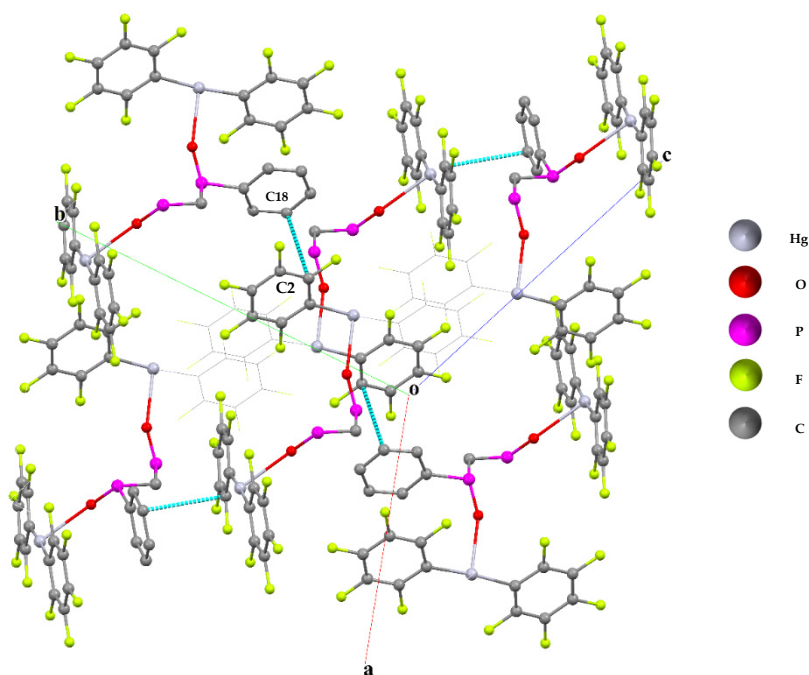
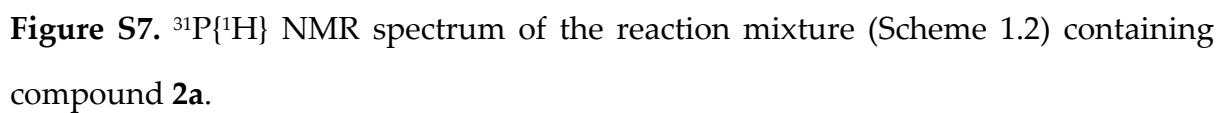
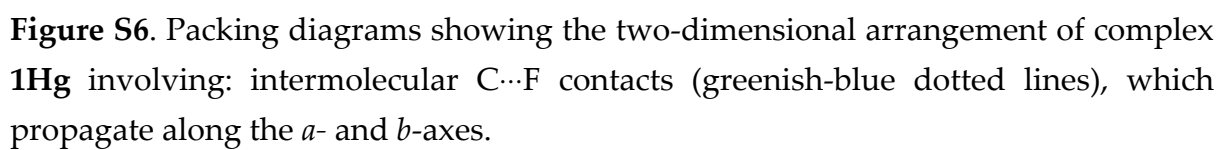


Figure S5. Packing diagrams showing the two-dimensional arrangement of complex **4** involving: intermolecular $\pi \cdots \pi$ interactions (greenish-blue dotted lines), which propagate along the *a*- and *b*-axes.



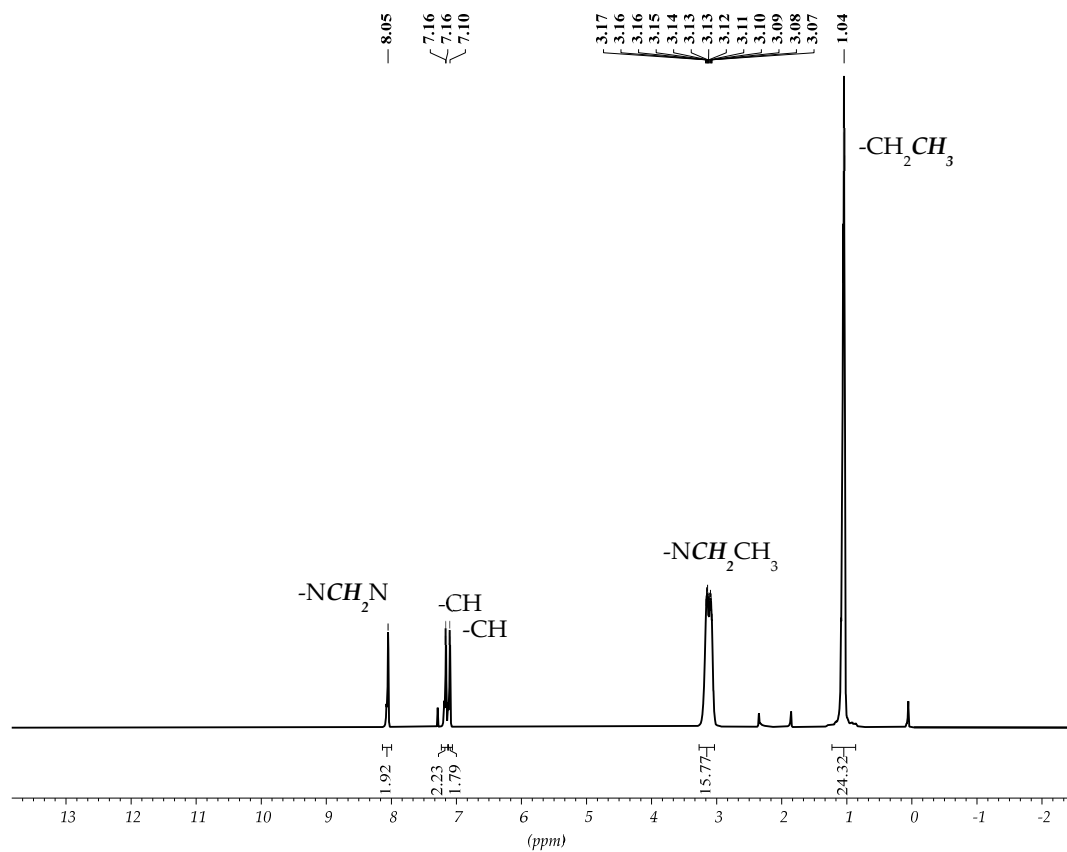


Figure S8. 1H NMR spectrum of **2**.

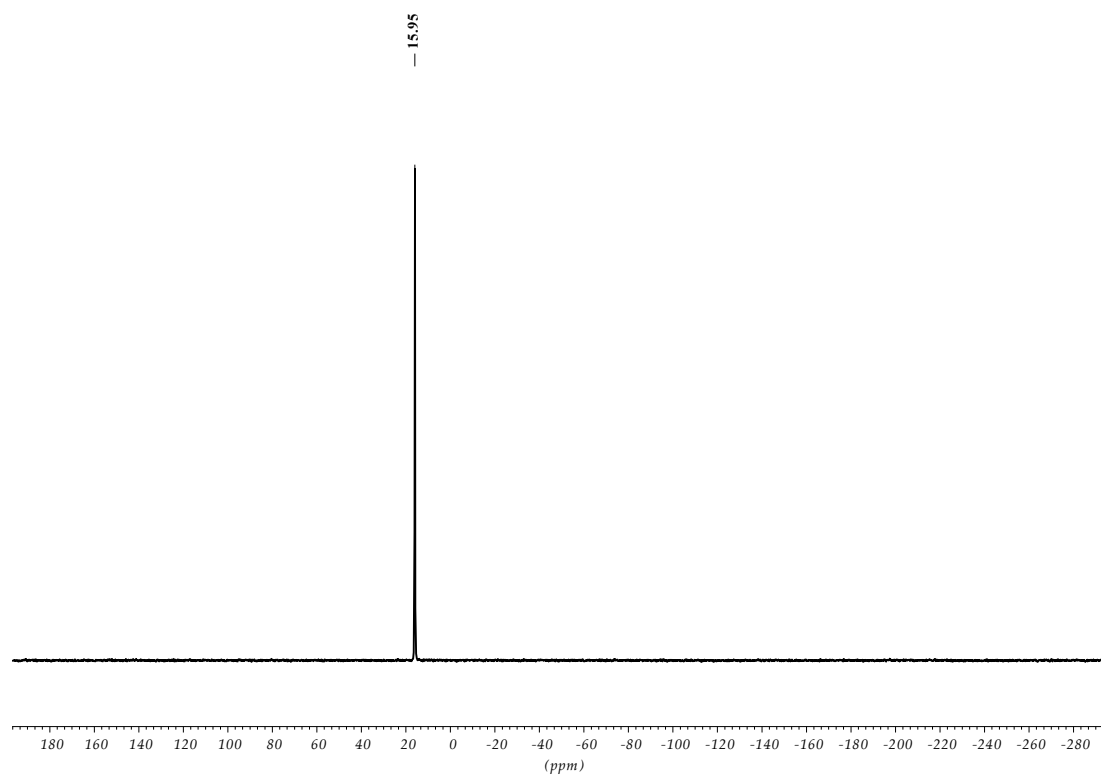


Figure S9. $^{31}P\{^1H\}$ NMR spectrum of **2**.

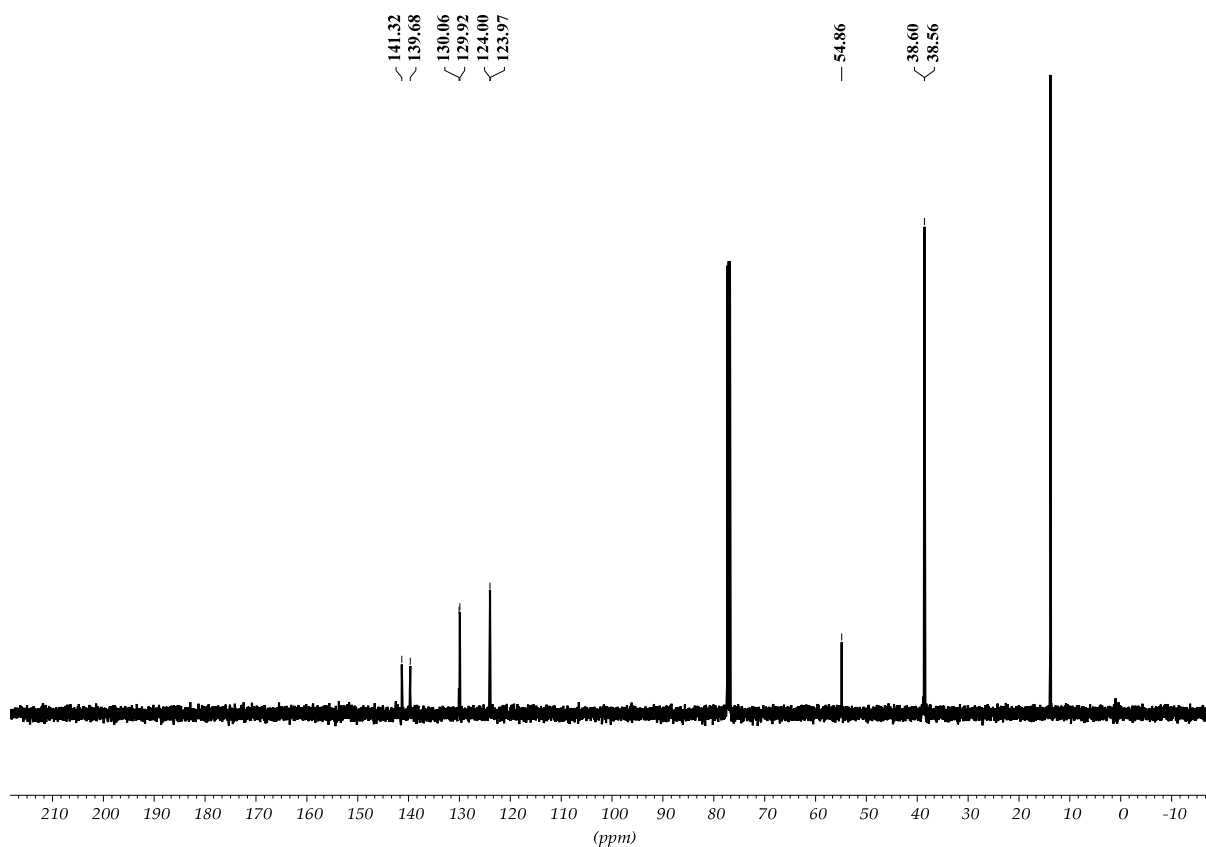


Figure S10. ¹³C NMR spectrum of **2**.

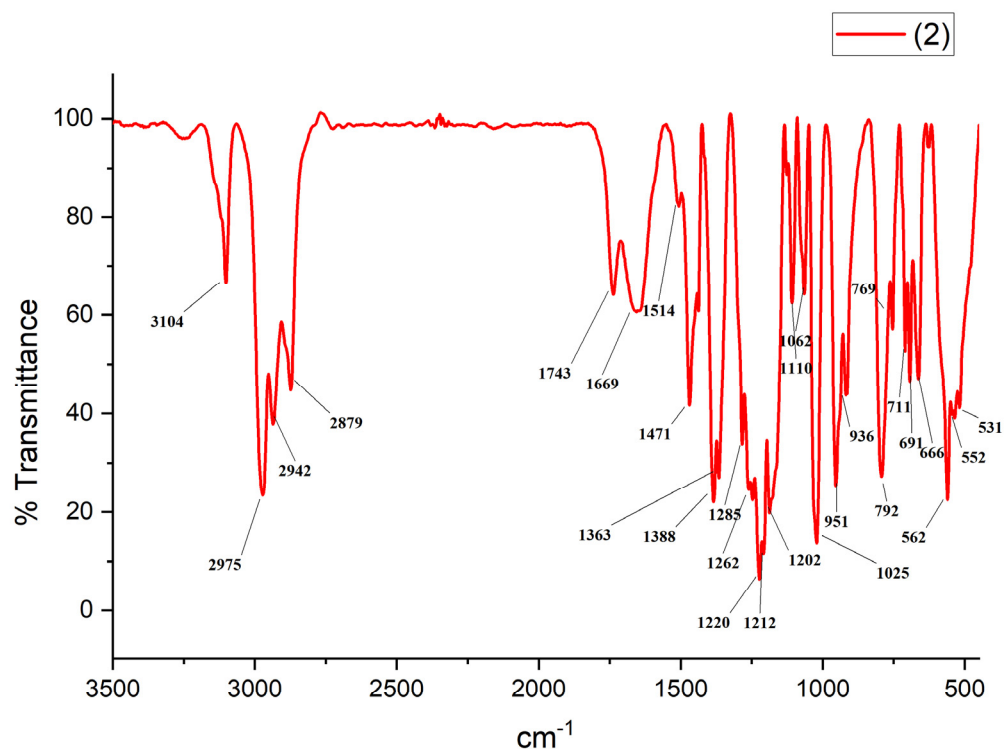


Figure S11. IR spectrum of ligand **2**.

Table S2. Intermolecular contacts and interactions in compounds **2**.

C-H...C-H interactions	
H22B-C3	2.789
H22A-C15	2.785
C-H...O interaction	
H1B-O2	2.642

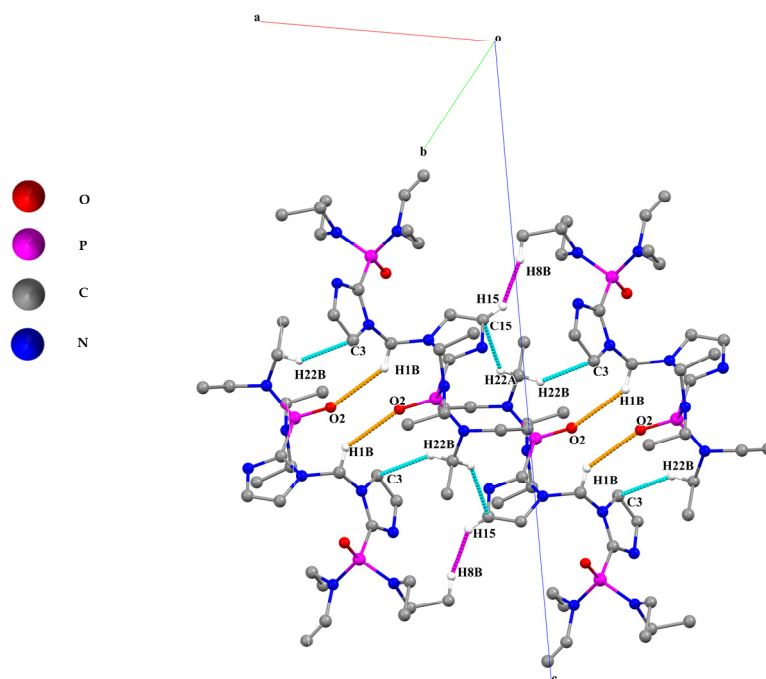


Figure S12. Packing diagrams showing the two-dimensional arrangement of ligand biphosphane **2** involving (i) intermolecular C...H interactions (greenish-blue and orange dotted lines), which propagate along the *a*- and *c*-axes, (ii) intermolecular H...O interactions (orange dotted lines), which propagate along the *a*-axis and (iii) intermolecular H...H contacts (pink dotted lines), which propagate along the *c*-axis.

Table S3. Intermolecular contacts and interactions in complex **2Hg**

C...F bond contacts	
C33-F4	3.017
C33-F5	3.070
C-H ...F-C interactions	
H43A-F1	2.438
H23B-F2	2.373

C-H \cdots C-H contacts	
H10B-C31	3.043
H45C-H8A	2.335
C-H \cdots N interaction	
H22A-N6	2.693

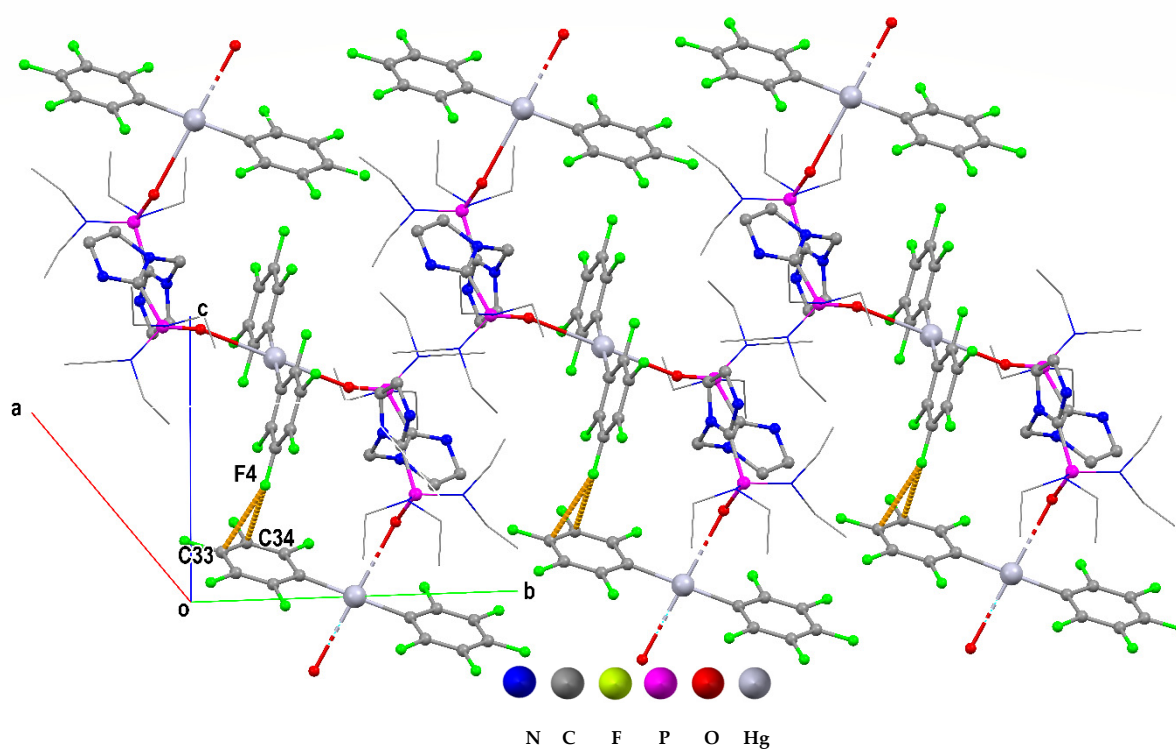


Figure S13. Packing diagrams showing the two-dimensional arrangement of complex **2Hg** involving intermolecular C \cdots F contacts (orange dotted lines), which propagate along the *c*-axis.

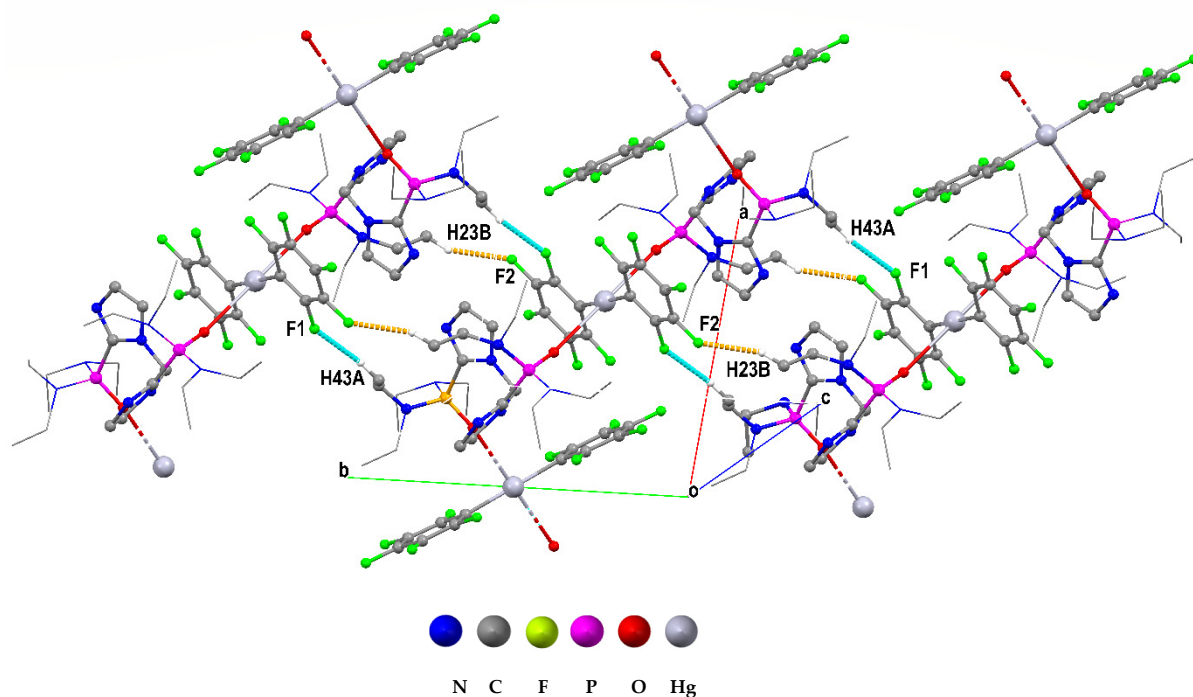


Figure S14. Packing diagrams showing the two-dimensional arrangement of complex **2Hg** involving intermolecular C...F contacts (greenish blue dotted lines) and H...F interactions (orange dotted lines), which propagate along the *b*-axis.

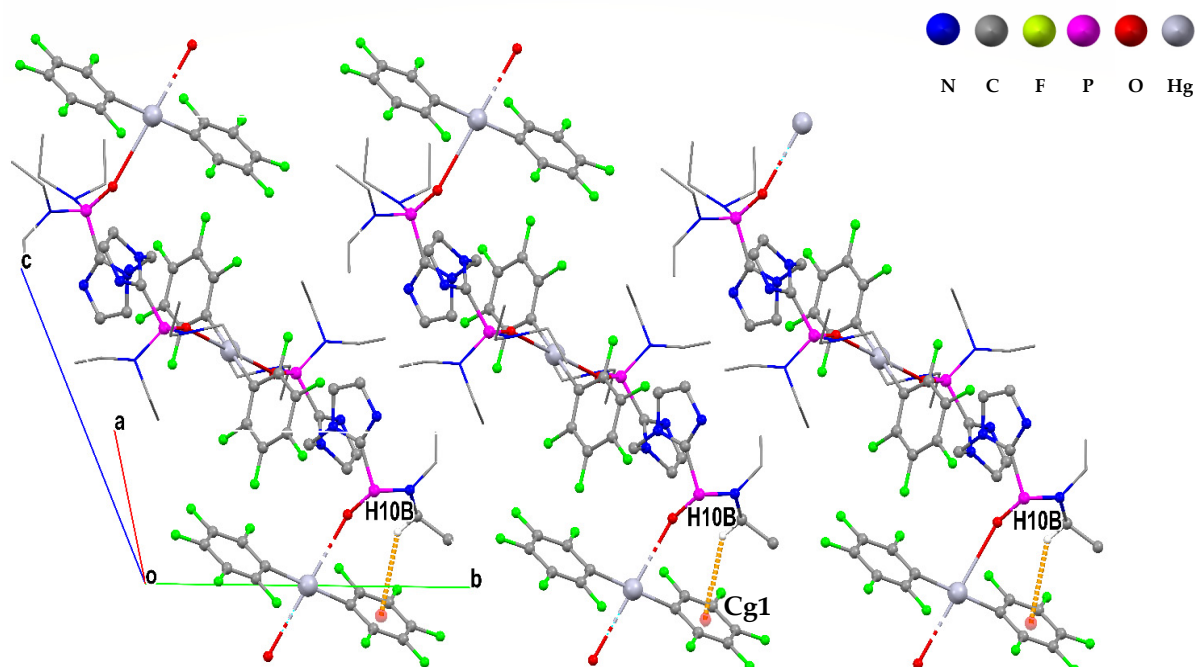


Figure S15. Packing diagrams showing the two-dimensional arrangement of complex **2Hg** involving: Cg1...H interactions (orange dotted lines) along *a*-axis direction.

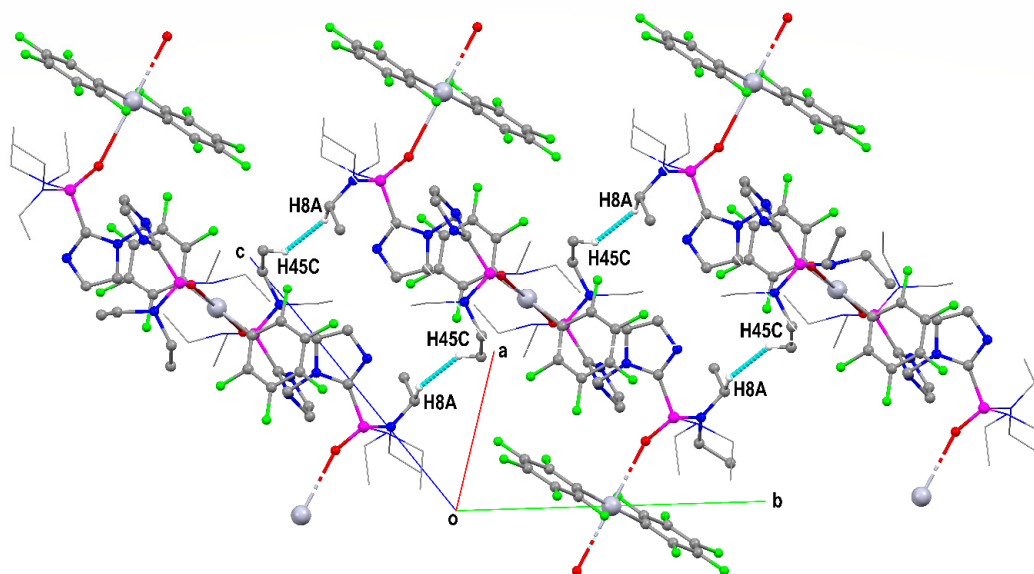


Figure S16. Packing diagrams showing the two-dimensional arrangement of complex **2Hg** involving intermolecular H...H contacts (greenish blue dotted lines), which propagate along the *b*-axis.

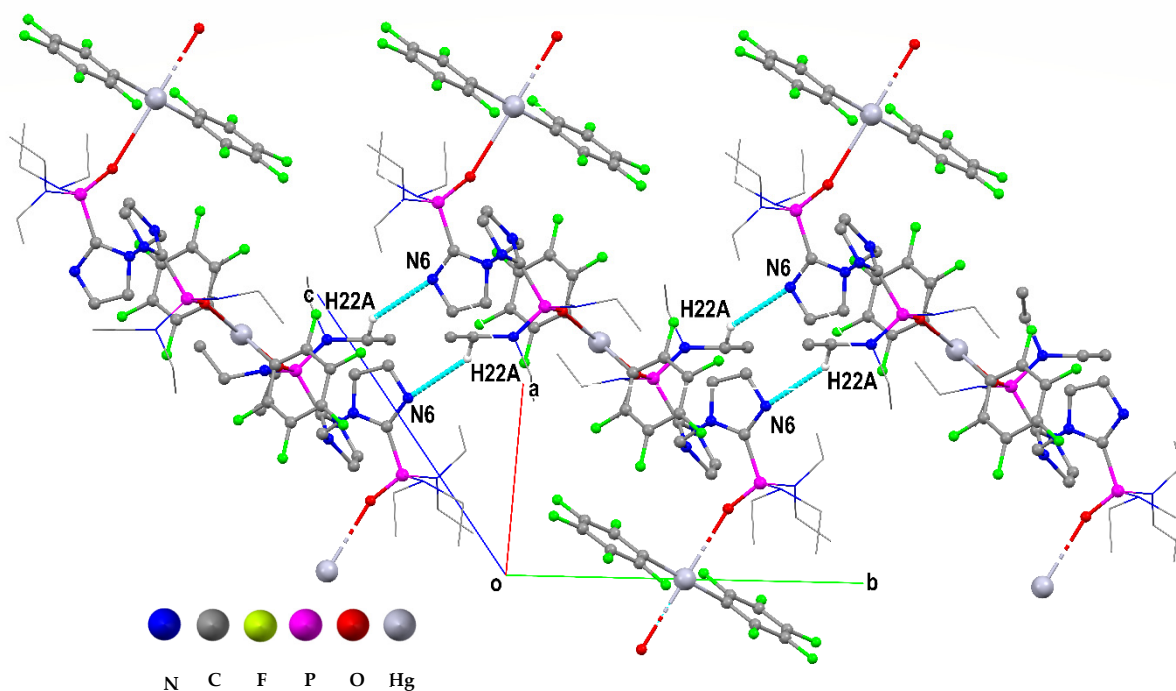


Figure S17. Packing diagrams showing the two-dimensional arrangement of complex **2Hg** involving intermolecular N...H interactions (greenish blue dotted lines), which propagate along the *b*-axis.

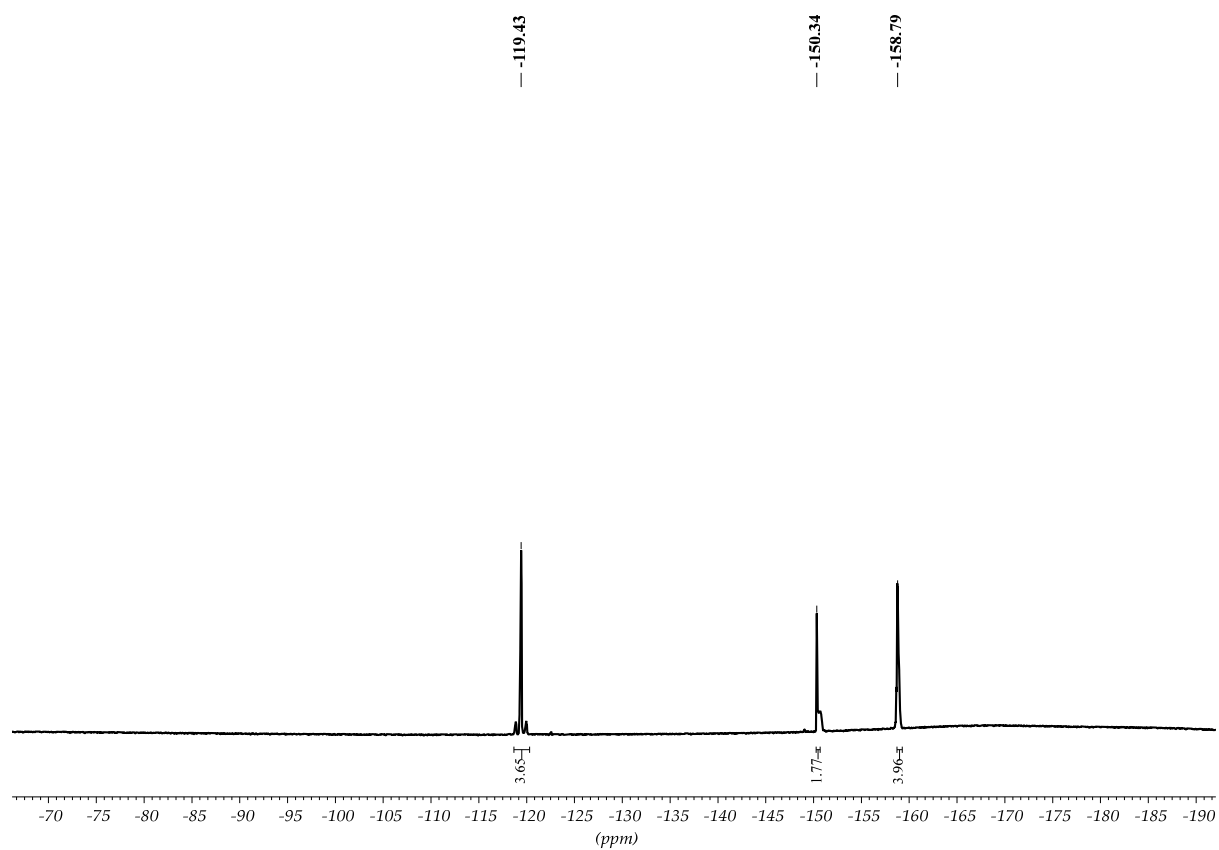


Figure S18. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of 3Hg .

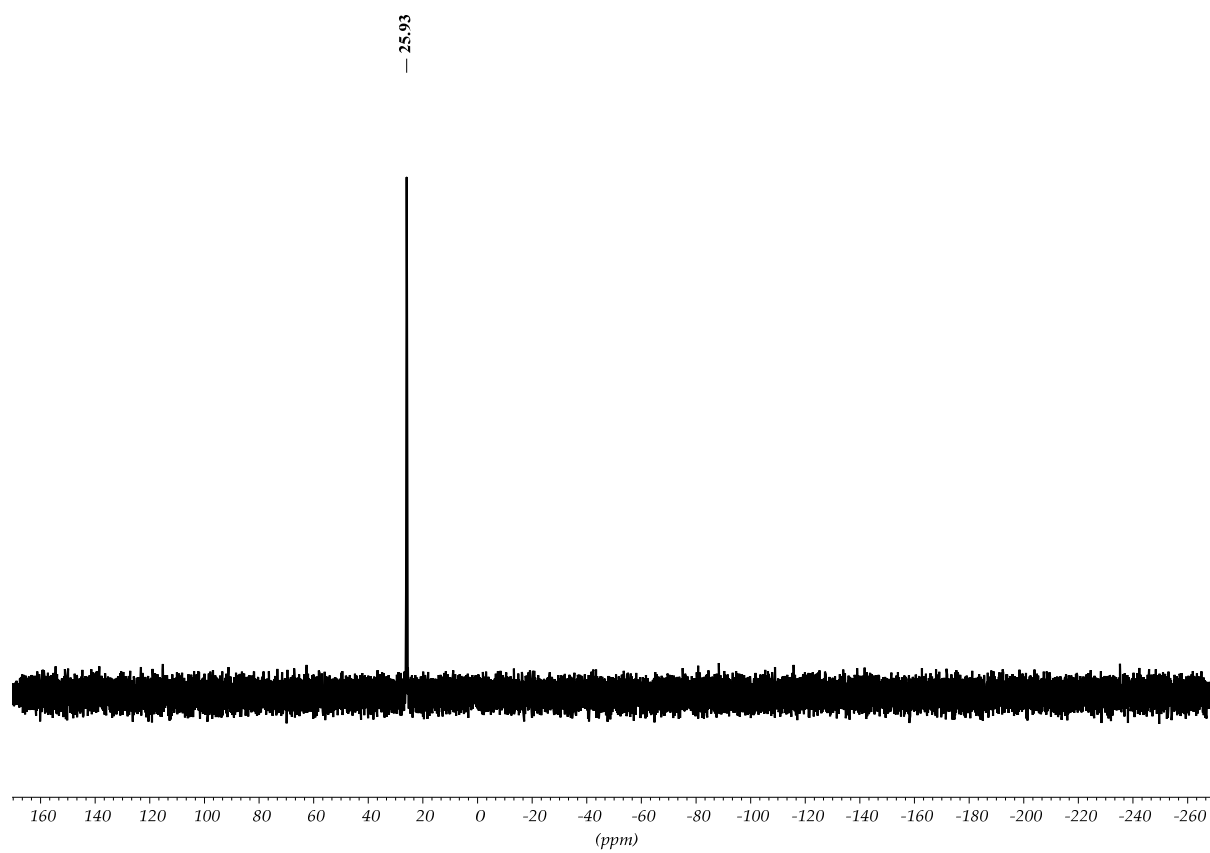


Figure S19. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of 3Hg .

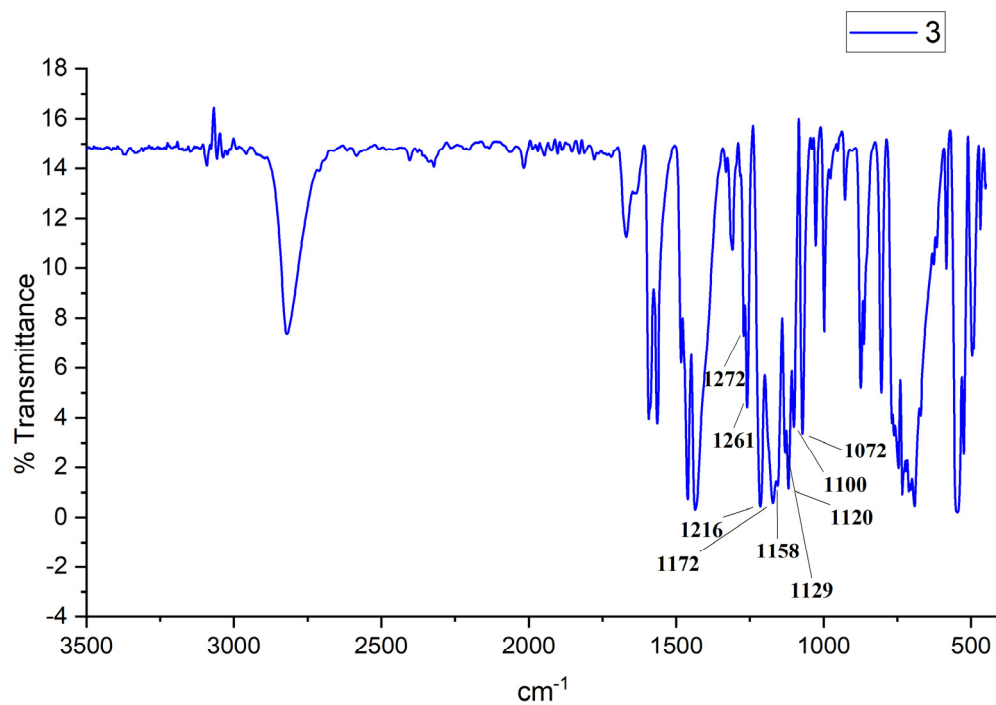


Figure S20. IR spectrum of **3**.

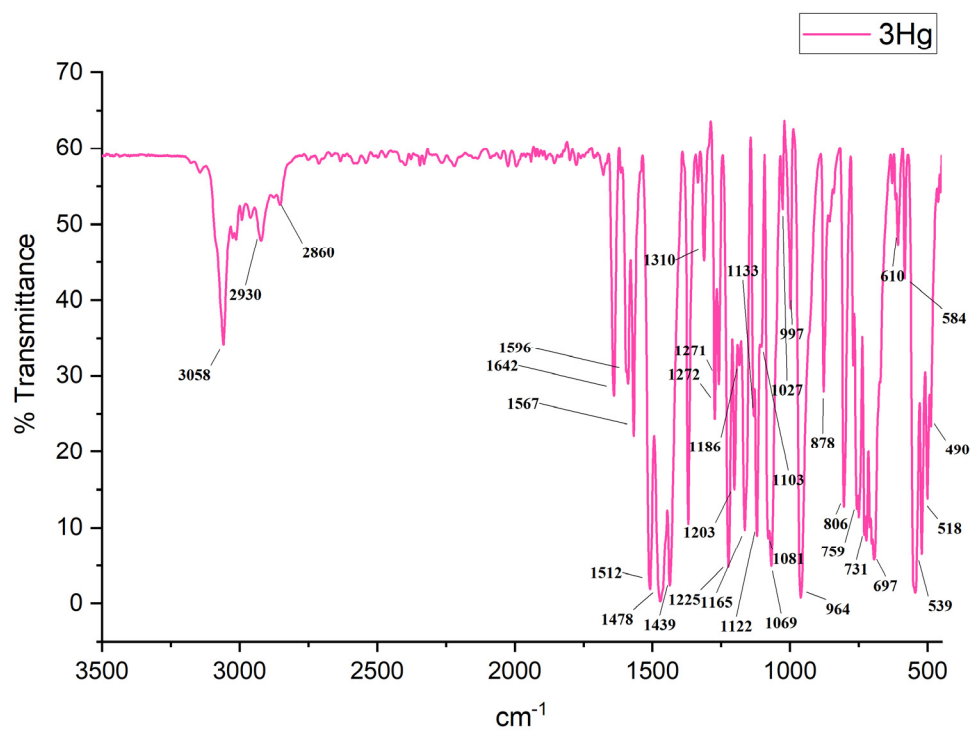


Figure S21. IR spectrum of **3Hg**.

Table S4. Intermolecular contacts and interactions in complex 3Hg

C\cdotsF contacts	
C8-F2	3.153
C45-F9	3.151
CH \cdotsFC interactions	
H24-F4	2.483
H17-F10	2.593
H35-F9	2.407
H-C \cdots O interaction	
C47-O3	3.191

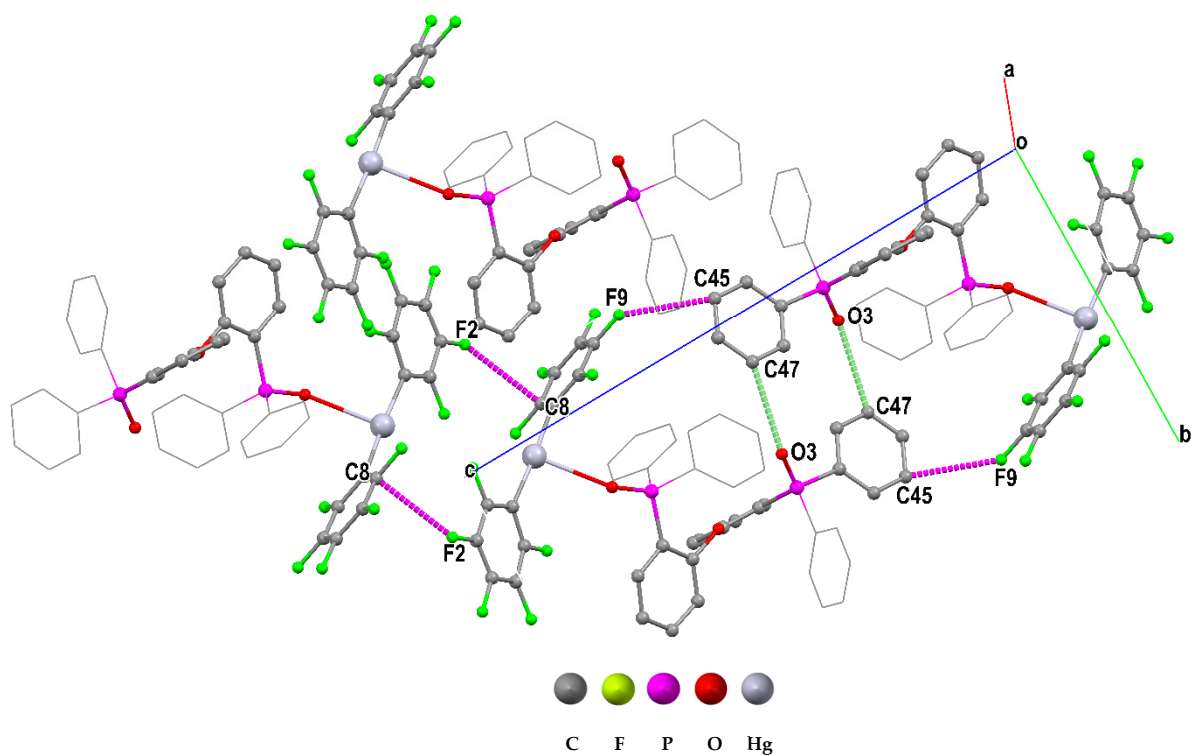


Figure S22. Packing diagrams showing the two-dimensional arrangement of complex **3Hg** involving (i) intermolecular C \cdots F contacts (pink dotted lines), which propagate along the *b*- and *c*-axes and (ii) intermolecular C \cdots O interactions (green dotted lines), which propagate along the *b*-axis.

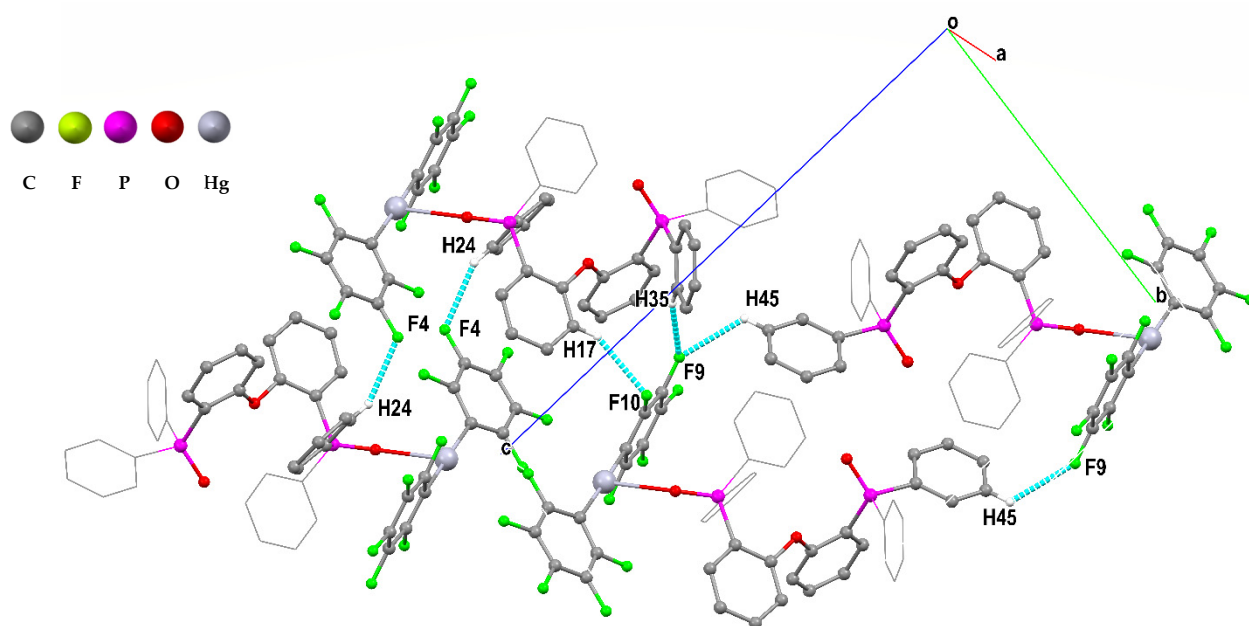


Figure S23. Packing diagrams showing the two-dimensional arrangement of complex **3Hg** involving intermolecular H...F interactions (green blue dotted lines), which propagate along the *a*-, *b*- and *c*-axes.

Table S5. Intramolecular contacts in complexes **1Hg**, **2Hg** and **3Hg**

Compound	Distance (Å)		
	1Hg	2Hg	3Hg
Hg- <i>o</i> -F	3.138 – 3.262	3.177 – 3.242	3.097 – 3.299
Hg- <i>o</i> -C	3.001 – 3.064	3.026 – 3.058	2.987 – 3.090