A Combined X-ray Crystallography and Theoretical Study of PPh2CH2SPh and PPh2C6H4SMe Ligands

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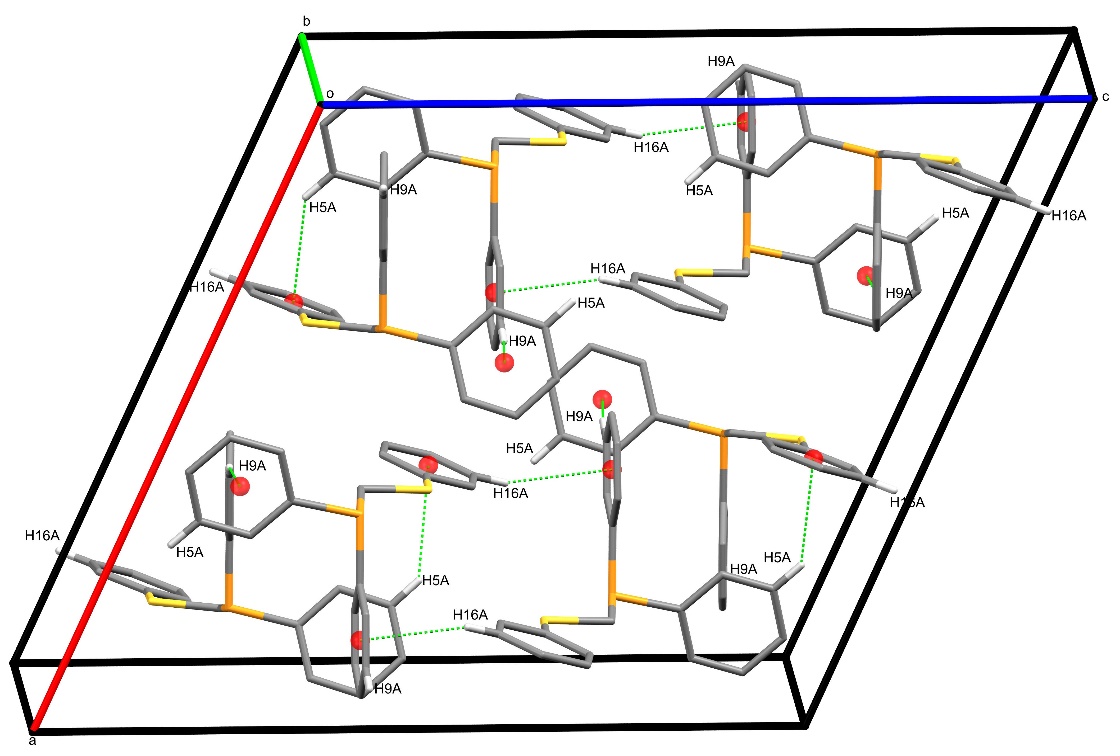
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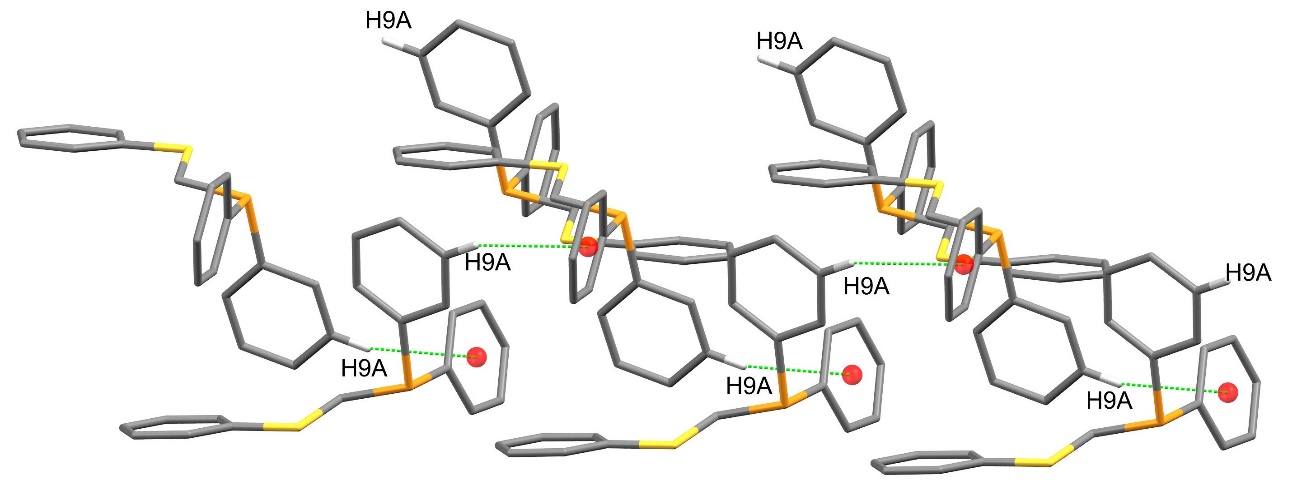
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**Supplemental Materials**



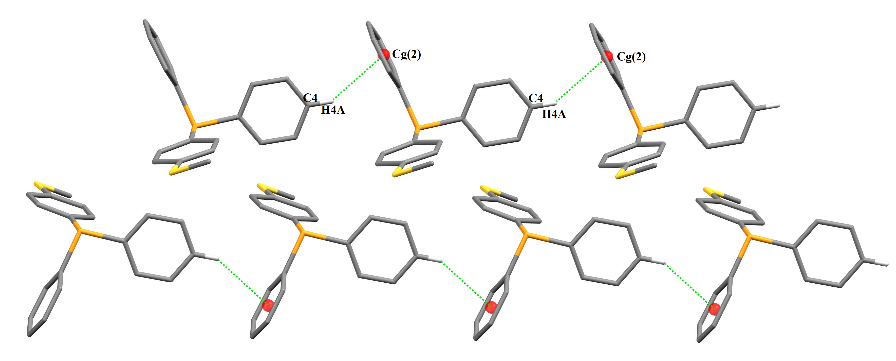
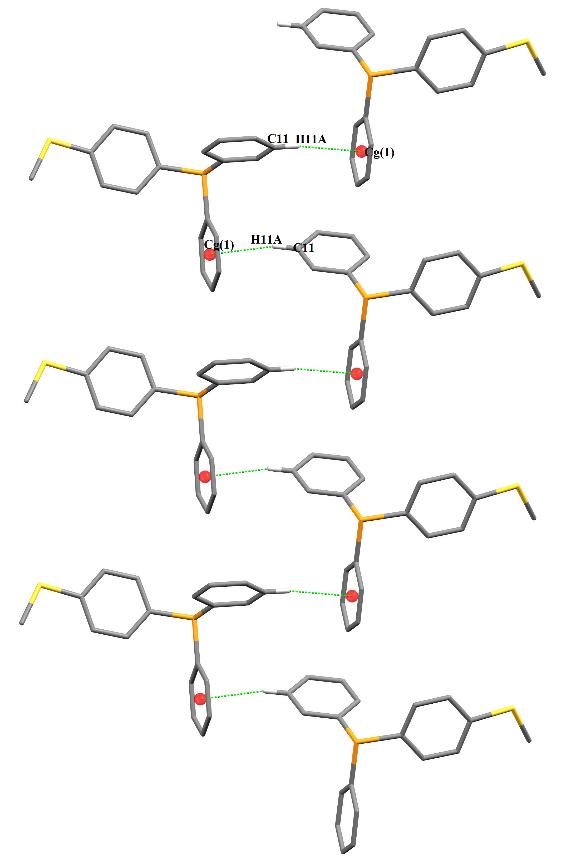
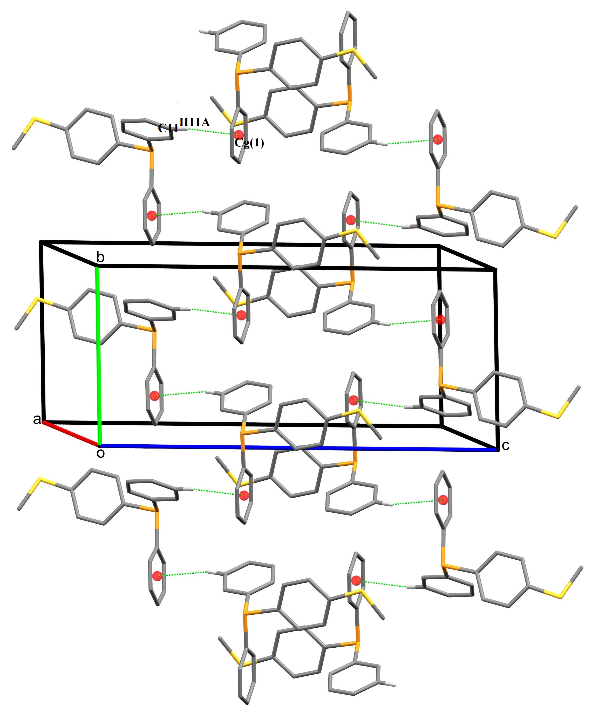
**Figure S 1:** Crystal packing of **1**: C16–H16A···Cg(2) in the *c*-direction and the interaction with C9–H5A···Cg(3) shows 2D sheet in *ac*-plane.



**Figure S 2:** Crystal packing of 1: C9–H9A···Cg(1) in the *b*-direction.

**Table S 1:** C–H···π interaction geometries for **1** and **2**.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Structure | C–H···Cg (Å) | C–H (Å) | H···Cg (Å) | C···Cg (Å) | C–H···Cg (°) |
| **1** | C5–H5A···Cg(3) | 0.95 | 2.96 | 3.7125(17) | 137 |
|  | C16–H16A···Cg(2) | 0.95 | 2.78 | 3.6245(16) | 149 |
|  | C9–H9A···Cg(1) | 0.95 | 2.95 | 3.8464(15) | 158 |
| **2** | C4–H4A···Cg(2) | 0.95 | 2.80 | 3.6428(13) | 148 |
|  | C11–H11A···Cg(1) | 0.95 | 2.68 | 3.5880(14) | 160 |

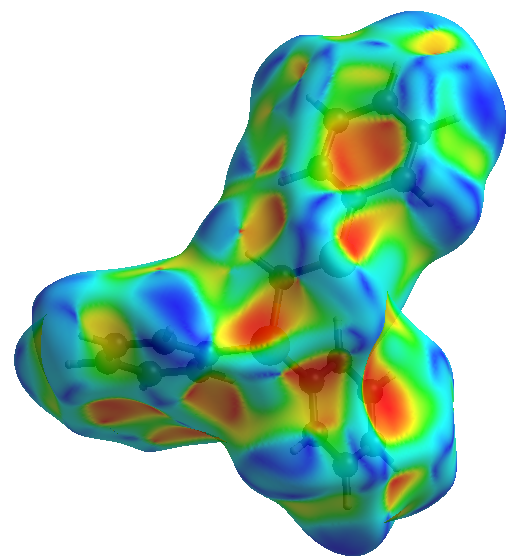
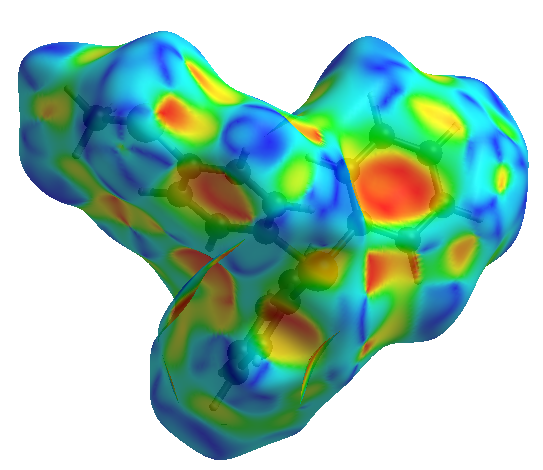


c

a

b

**Figure S 3**:Crystal packing of **2**: [C11–H11A···Cg(1) and C4–H4A···Cg(2)] shows head-to-head arrangement along *b*-direction.



(**1**) (**2**)

**Figure S 4**: Hirshfeld surfaces **1** and **2** mapped over shape-index with a red spot (inside

the black arrows) signifying the involvement of the C–H···π interactions.