Hirshfeld surface and supramolecular analyses

Hirshfeld surfaces [1 - 6] for the repeating units of **(1) - (4)** mapped with d_{norm} and shape index are depicted in Figure S4. These maps were constructed from the CIF files using CrystalExplorer (Version 3.1) [7]. Contributions from specific pairs of atom-types are shown in Figure S5. According to our analysis, H···H, C···C, H···C/C···H, and H···O/O···H close contacts contribute 2.9, 1.2, 4.6, and 1.8% to the Hirshfeld surface for **(1)**, respectively (Figure S5). As already mentioned, the two-dimensional polymeric architecture of **(1)** grows parallel to the [001] direction and along the diagonal of the [100] direction. Adjacent polymeric chains are interconnected by Sn(1)···O(2) (3.626 and 3.893 Å) interactions along the [010] direction (Figure S6). In fact, contribution of O···Sn/Sn···O close contacts to the Hirshfeld surface area for **(1)** is larger than that observed for **(2) - (4)** (Figure S5).

Hirshfeld surface analysis for **(2)** indicated that H···H (1.1%) and H···C/C···H (4.6%) contacts do not significantly contribute to its crystal packing (Figure S5). On the other hand, π-π stacking interactions (Cg···Cg, 3.760 Å), represented by complementary blue and orange patches on the shape index surface (Figure S4), connect adjacent phenyl rings along the [001] direction (Figure S7). Moreover, the crystal structure of **(2)** also favours C-H···Sn^{II} close contacts (C-H, 0.93 Å; H···Sn, 3.21 Å; C···Sn, 4.134 Å; C-H···Sn, 173^o) (Figure S5).

In **(3)**, one-dimensional polymeric chains propagate along the diagonal of the [011] plane (Figure 5). Neighbouring zigzag chains are interconnected by classical O(5)-H(5)···O(9) hydrogen bonds (O-H, 0.82 Å; H···O, 1.89 Å; O···O, 2.699 Å; O-H···O, 167^o) along the [010] direction (Figure S8). Furthermore, analysis of the Hirshfeld surface for **(3)** revealed that H···H (3.8%), C···C (1.8%), H···C/C···H (3.2%), and Sn···Sn (0%) close contacts exhibit negligible contributions to its crystal arrangement (Figure S5).

Unlike **(1) - (3)**, our Hirshfeld surface analysis showed that isotropic H···H contacts considerably contribute (17.9%) to the Hirshfeld surface area for **(4)** (Figure S5), a three-dimensional coordination network (Figures 6 and 7). Moreover, contribution of Sn···Sn interactions to **(4)** is larger than that observed for **(1) - (3)** (Figure S5).

References

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[2] M. A. Spackman and J. J. McKinnon, *Cryst. Eng. Comm.*, 2002, **4**, 378–392.

[3] J. J. McKinnon, M. A. Spackman and A. S. Mitchell, *Acta Crystallogr., Sect. B: Struct. Sci*., 2004, **60**, 627–668.

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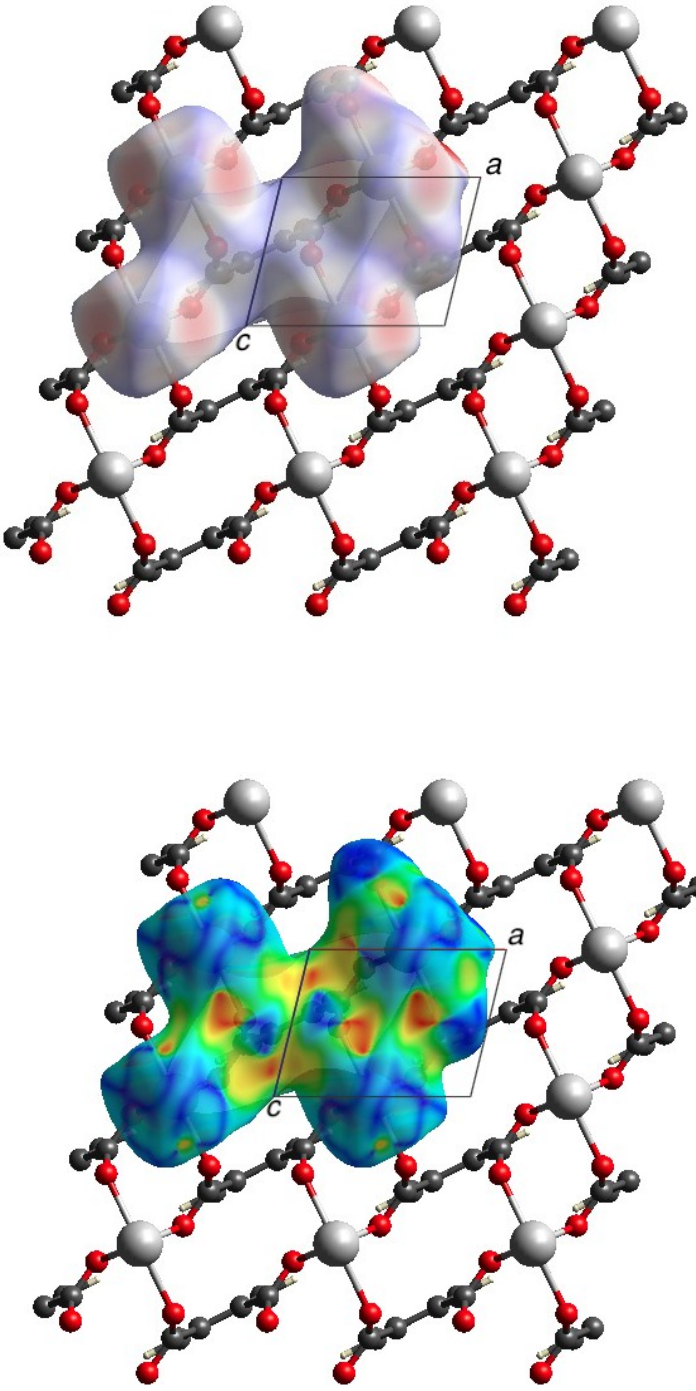
[7] S. K. Wolff, D. J. Grimwood, J. J. McKinnon, M. J. Turner, D. Jayatilaka and M. A. Spackman, CrystalExplorer (Version 3.1), University of Western Australia, 2012.

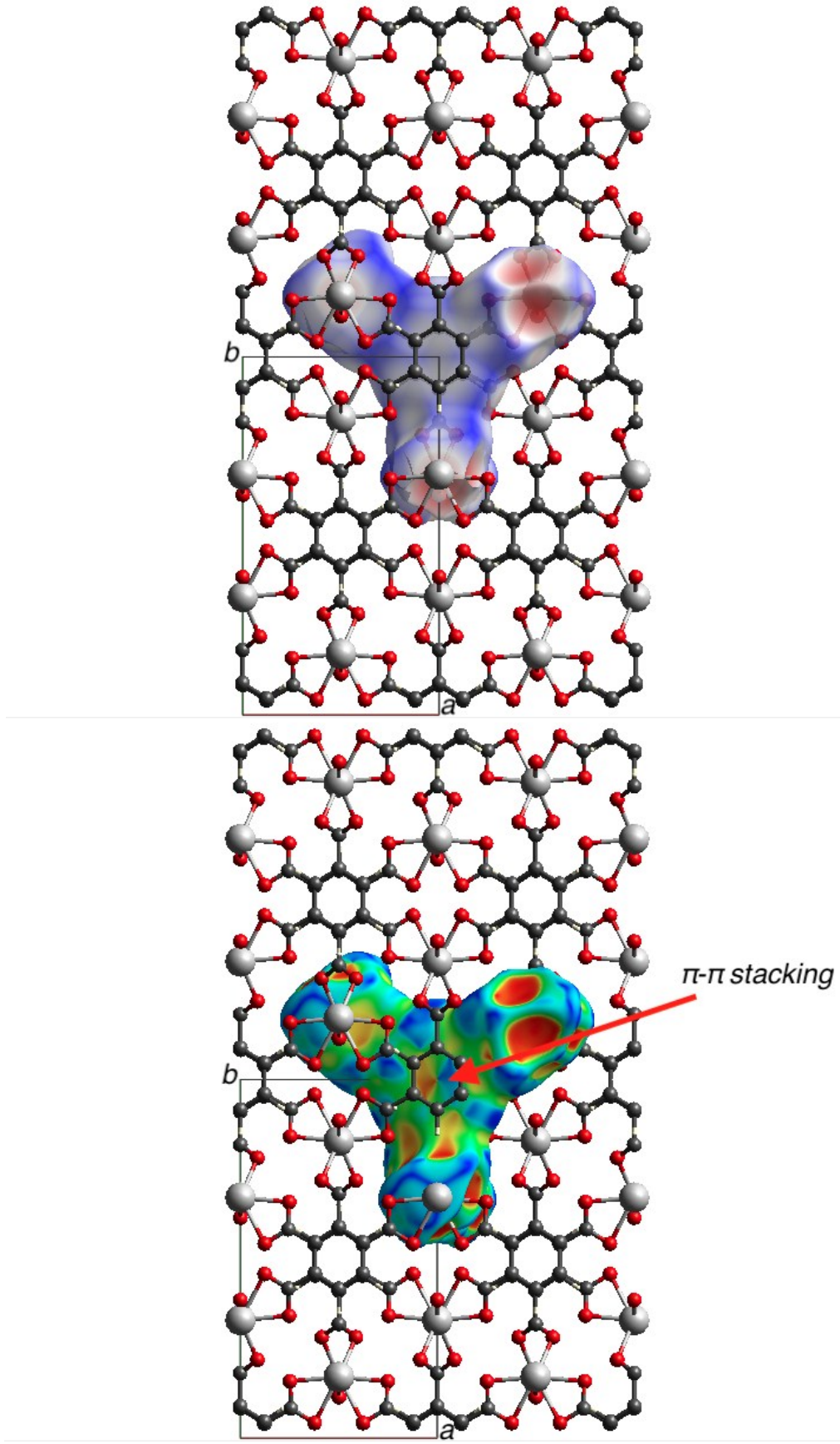
Supplementary Figures

Figure S4. Hirshfeld surfaces for the repeating units of **(1)** - **(4)** mapped with d_{norm} (top) and shape index (bottom).



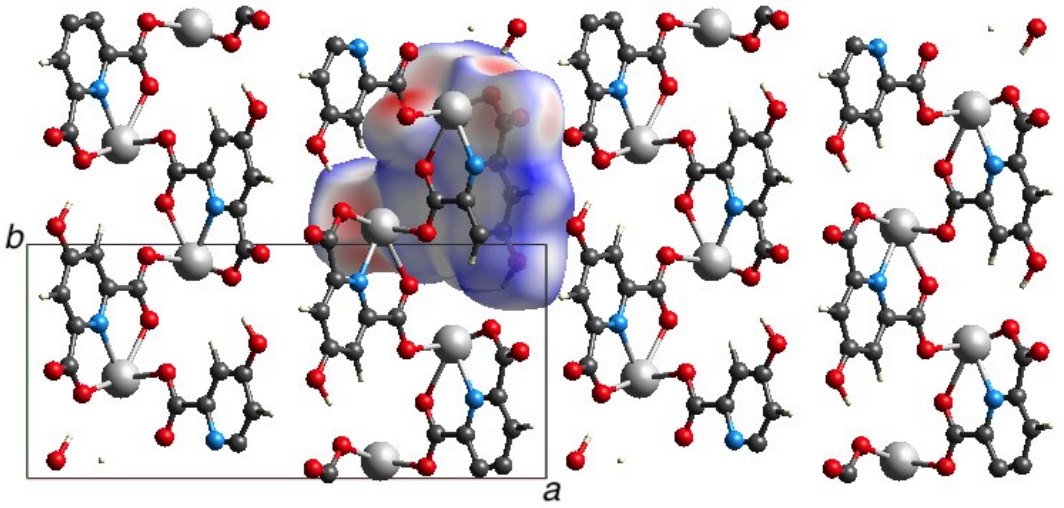
(views down *b*)

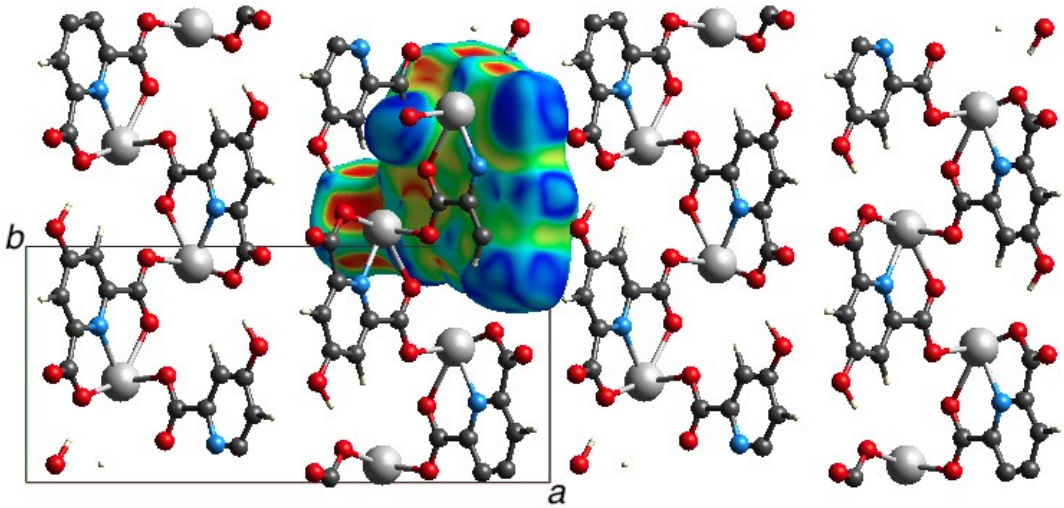
(1)



(views down *c*)

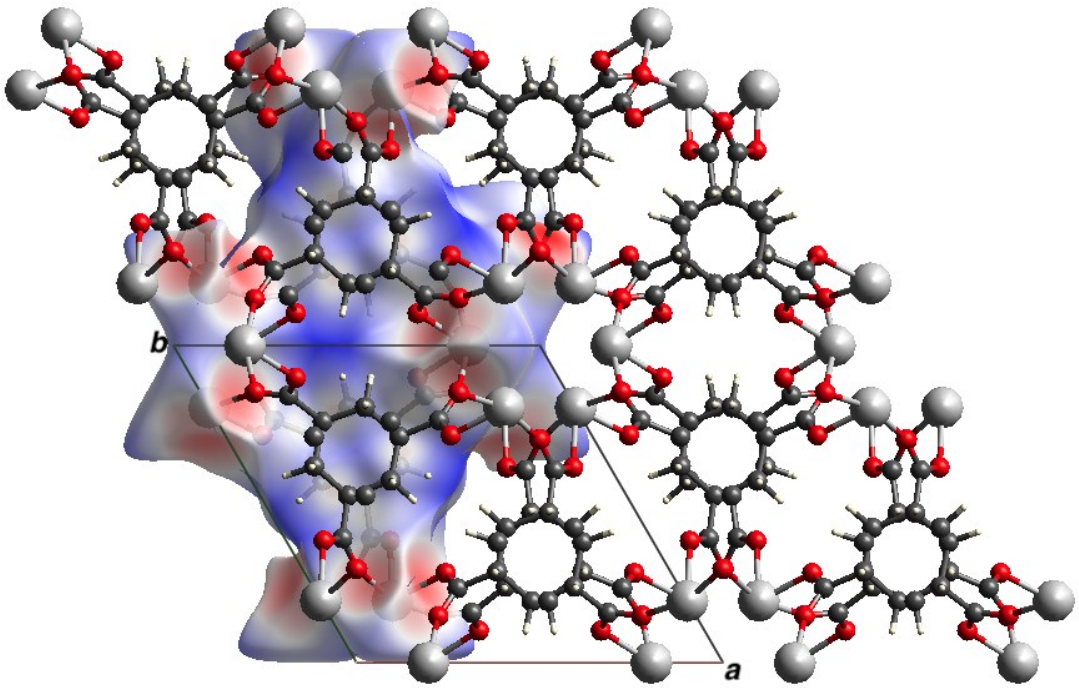
(2)

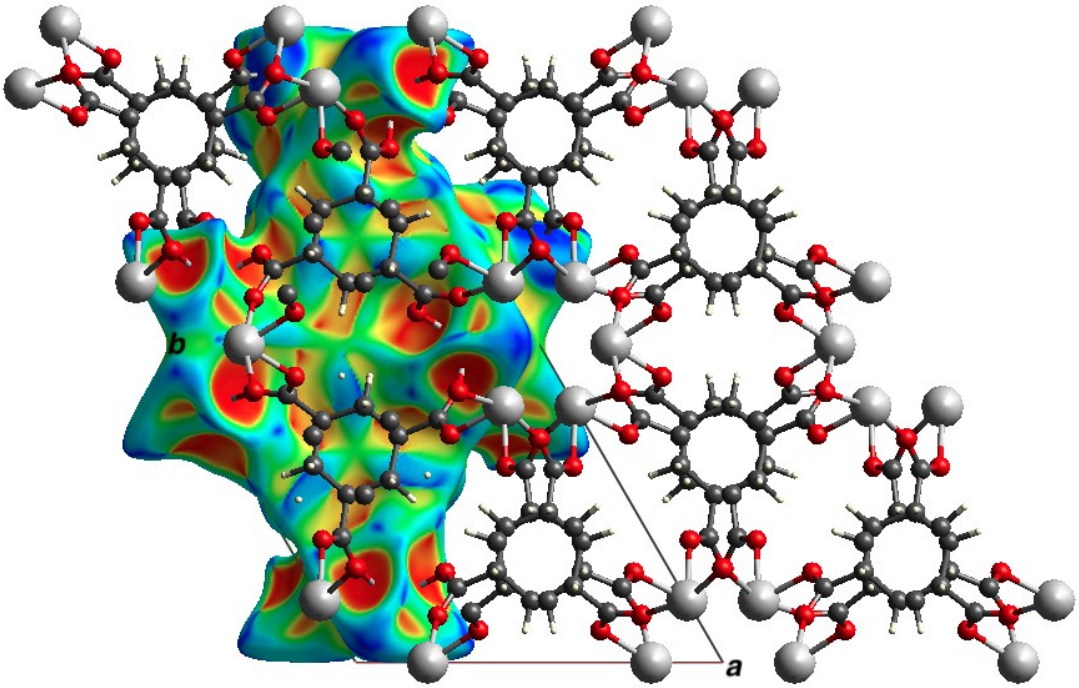




(views down *c*)

(3)





(views down *c*)

(4)

Figure S5. Contributions from specific pairs of atom-types to the Hirshfeld surfaces for the repeating units of **(1)** - **(4)**.

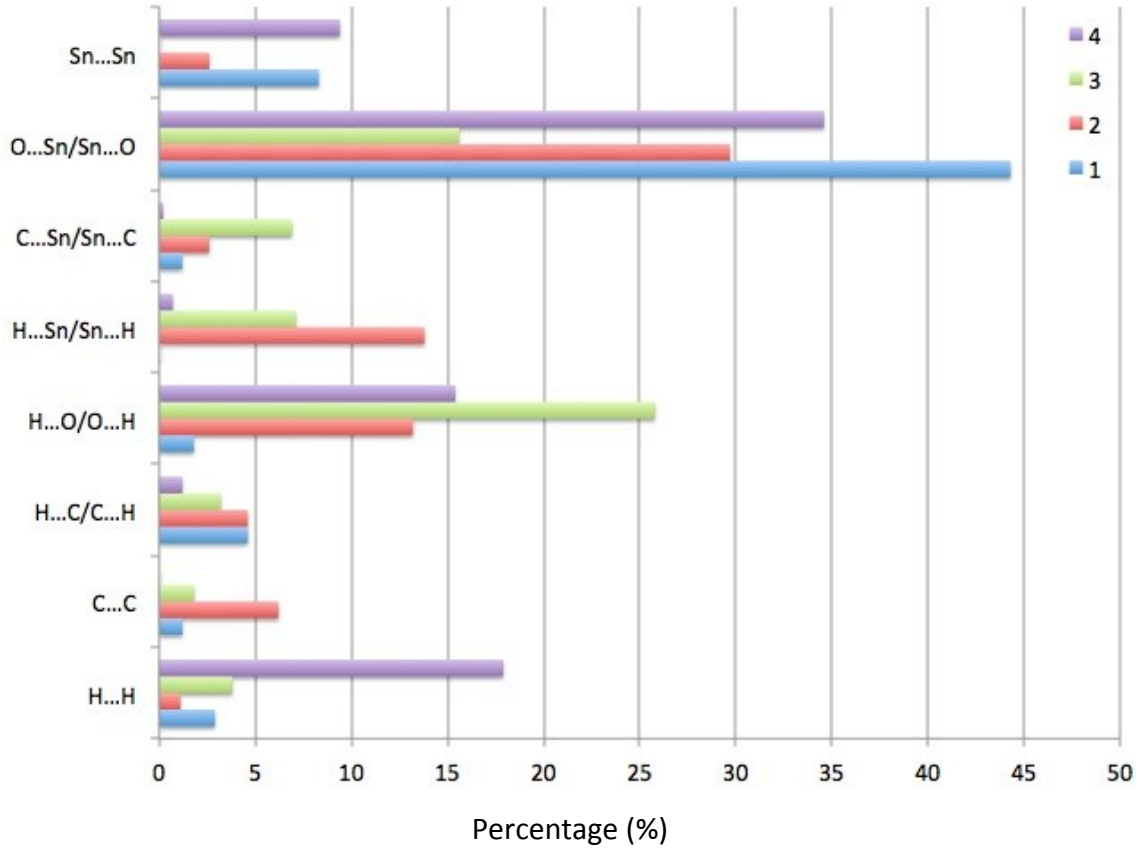
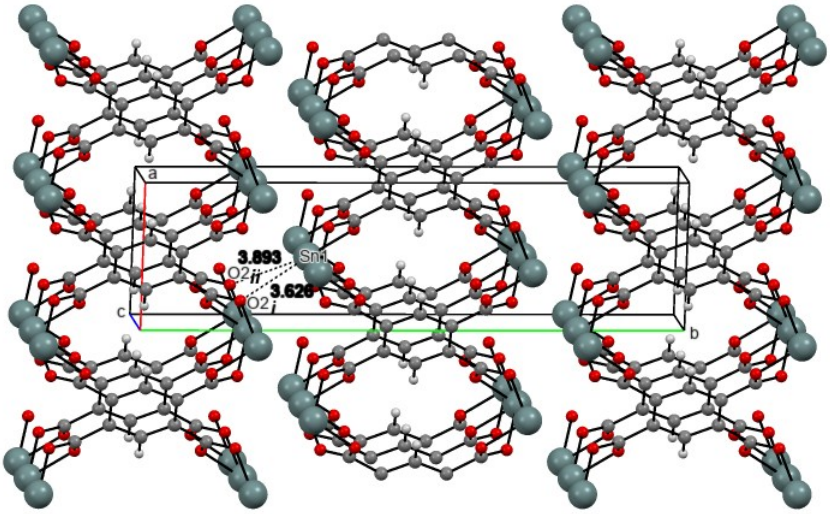
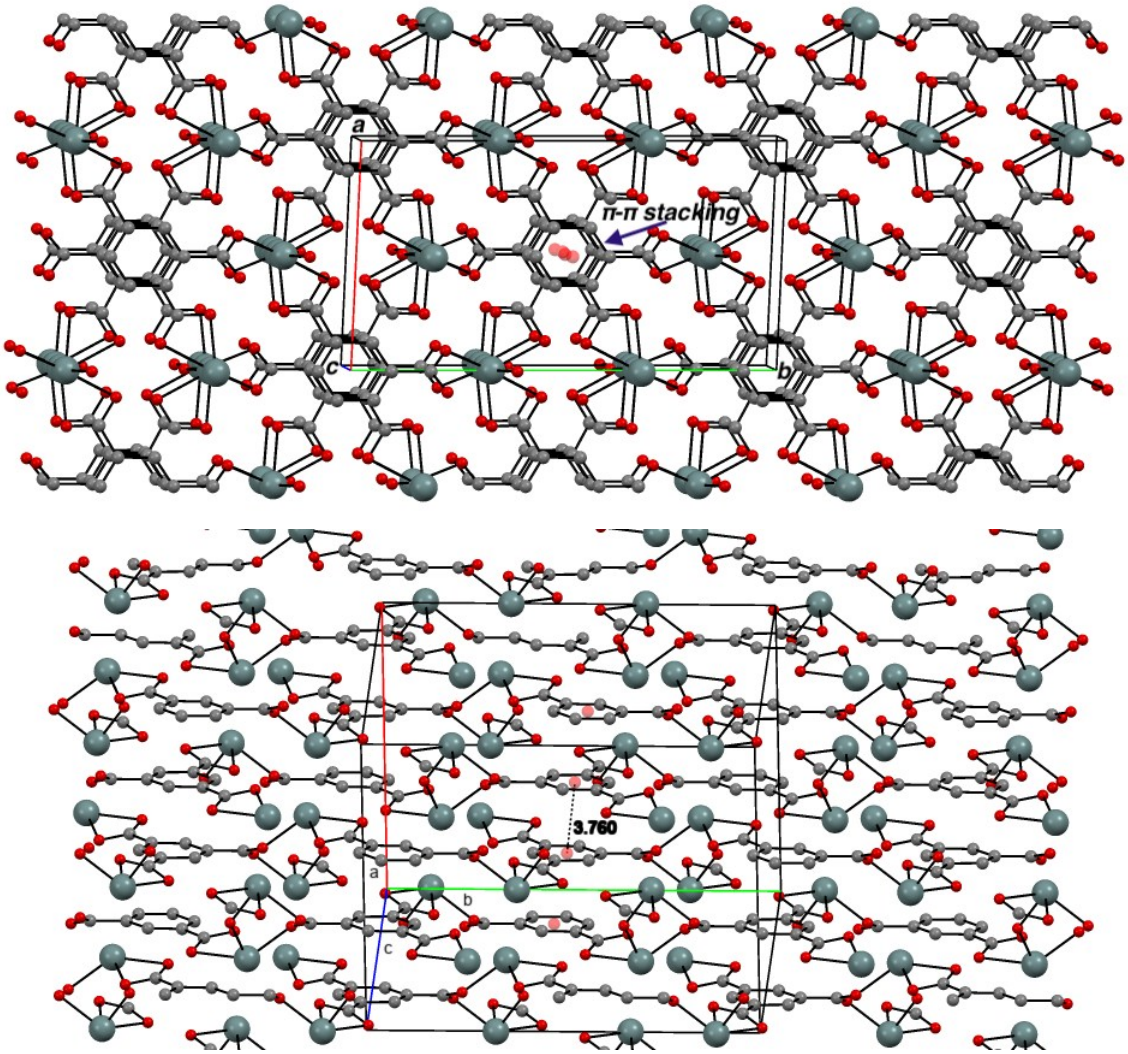


Figure S6. Packing diagram of **(1)** showing secondary Sn···O interactions along the [001] direction.[a]



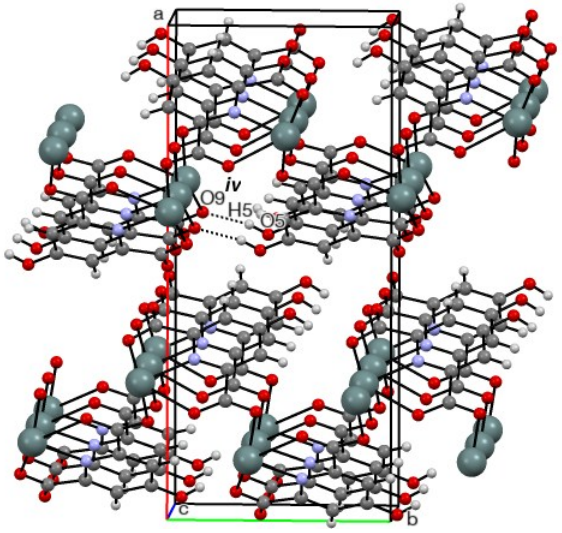
[a] Symmetry codes: (i) 0.5-x,0.5-y,-z; (ii) 0.5-x,0.5-y,1-z.

Figure S7. Packing diagrams of **(2)** showing π-π stacking (Cg···Cg^{iii}, 3.760 Å) interactions along the [001] direction. H atoms are omitted for clarity.[a]



[a] Symmetry code: (iii) x,1-y,-0.5+z.

Figure S8. Packing diagram of **(3)** highlighting O-H···O hydrogen bonds along the [010] direction.[a]



[a] Symmetry code: (iv) x,-1+y,z.