

Figure S1. The displacement of the arylamino N1 from the Fe/Ct2/C6 plane bisecting the Cp2 ring plane, in polymorph (I), left and (II) right. Different orientation of the arylamino with regard to the same plane (below).

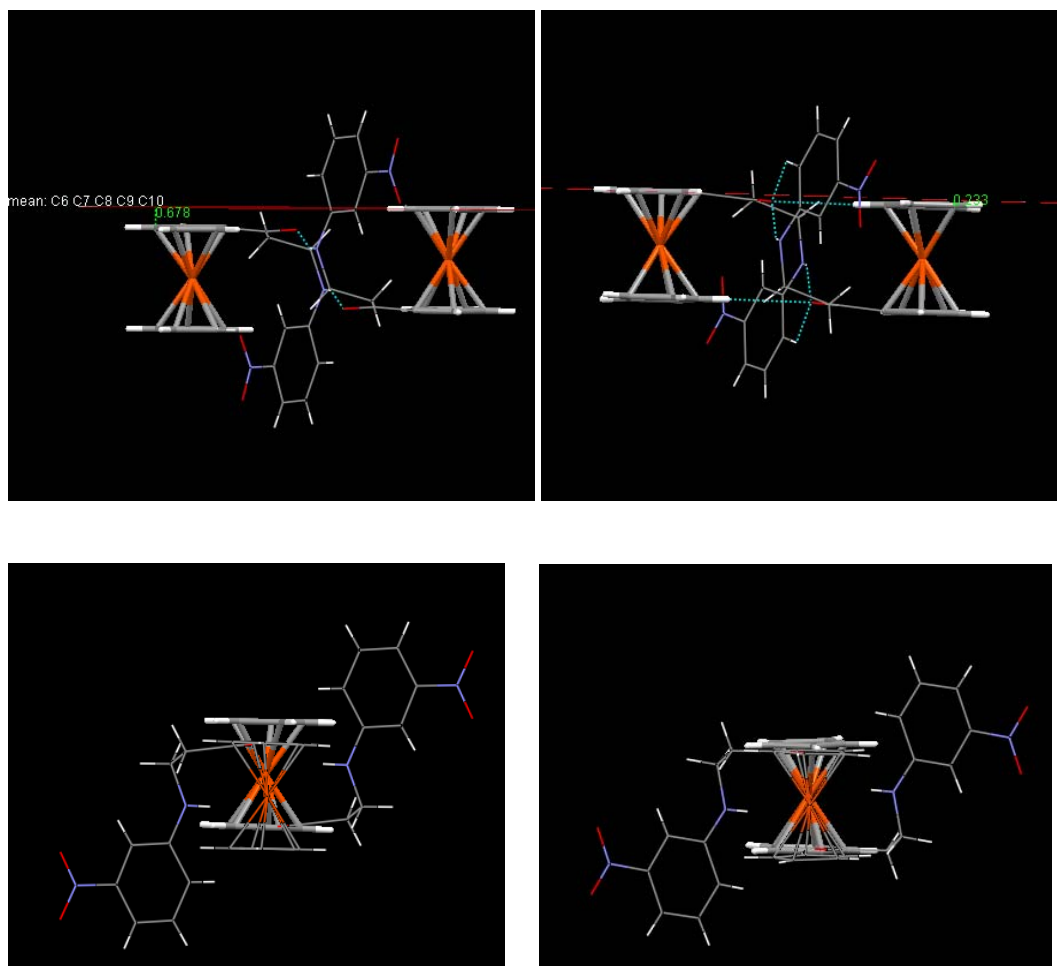


Figure S2. The mutual position of the Fc units within the N-H...O dimer of (I) left and (II) right. The mean deviation of the C atoms constituting the neighboring Cp2 from the level of Cp1 plane is 0.67(2) in (I) and 0.20(5) in II (distances indicated on the figures concern the displacement of atom C4).

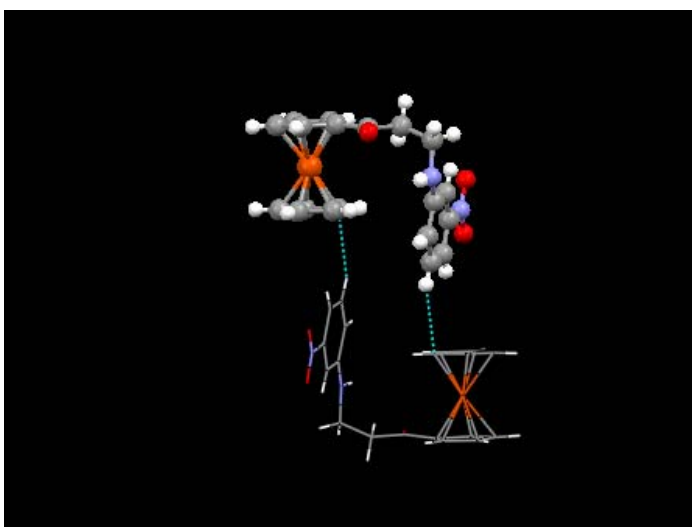
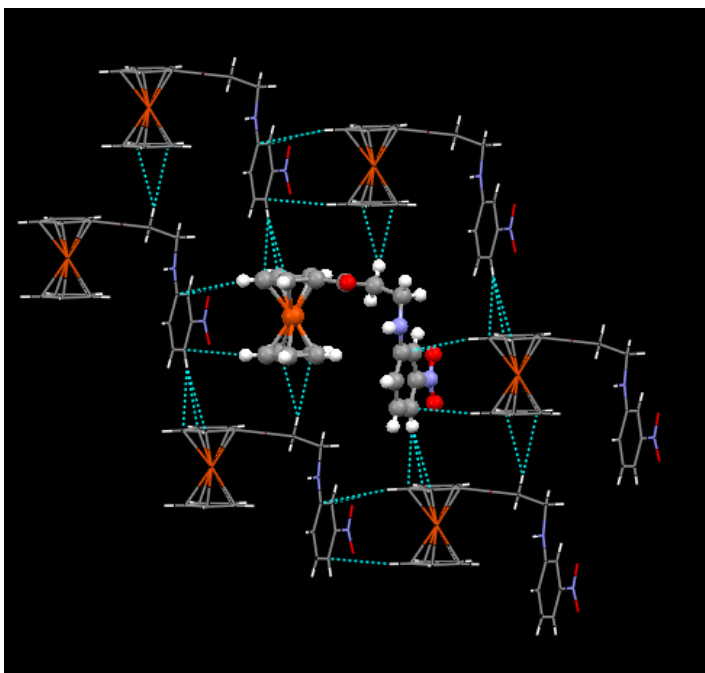


Figure S3. C–H... $\pi$  interactions in polymorph (I), above, connect the reference molecule with the six surrounding molecules. Only one C–H... $\pi$  is present in the crystal packing of polymorph (II) (indicated H...C contacts are all shorter than 3.1 Å).

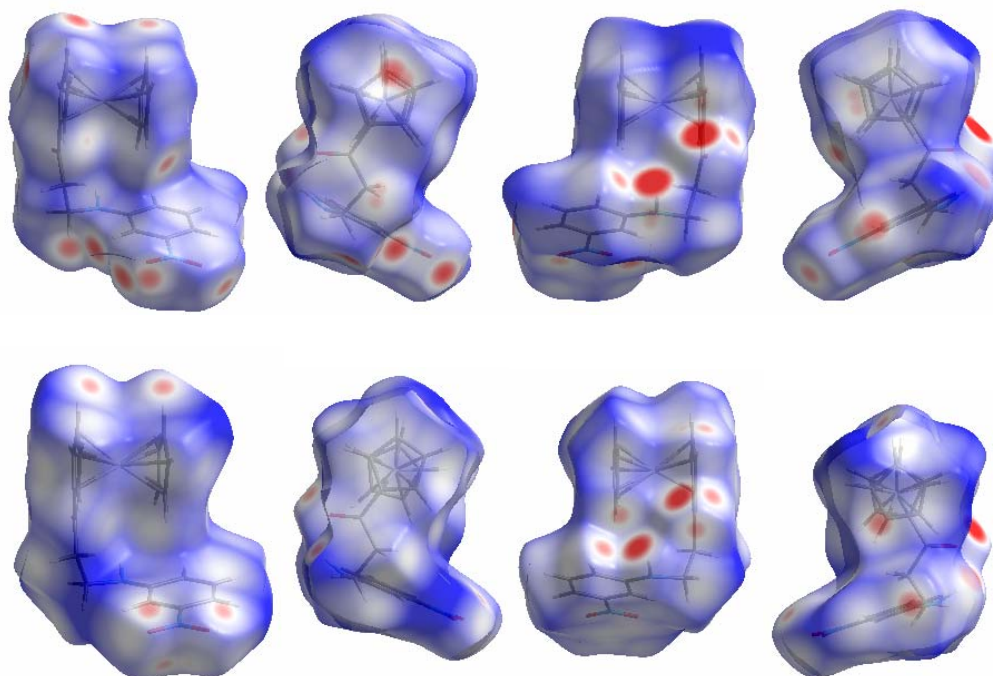


Figure S4. Hirshfeld surfaces of (I), above and (II) below, mapped with  $d_{\text{norm}}$  (normalized contact distance,  $d_i$  and  $d_e$  are normalized by the van der Waals radius of the atom involved). Where atoms make intermolecular contacts closer than the sum of their van der Waals radii, these contacts are highlighted in red on  $d_{\text{norm}}$  surface. Longer contacts are blue, and contacts around the sum of van der Waals radii are white.