Supplementary Material

Making and Breaking - Insight Into the Symmetry of Salen Analogues

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Figure S1. Examples of two-dimensional (2D) Hirshfeld (fingerprint) diagrams of various intermolecular interactions in the crystal structure for the meta compound.

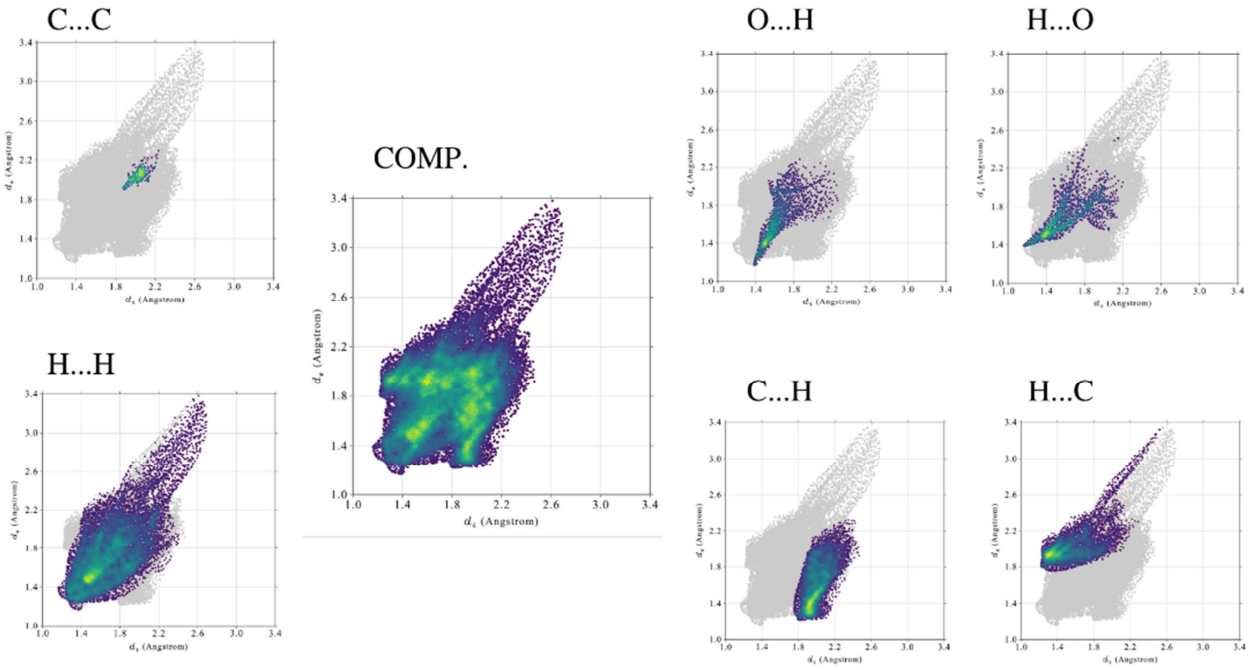

Figure S2. Examples of two-dimensional (2D) Hirshfeld (fingerprint) diagrams of various intermolecular interactions in the crystal structure for the ortho compound.

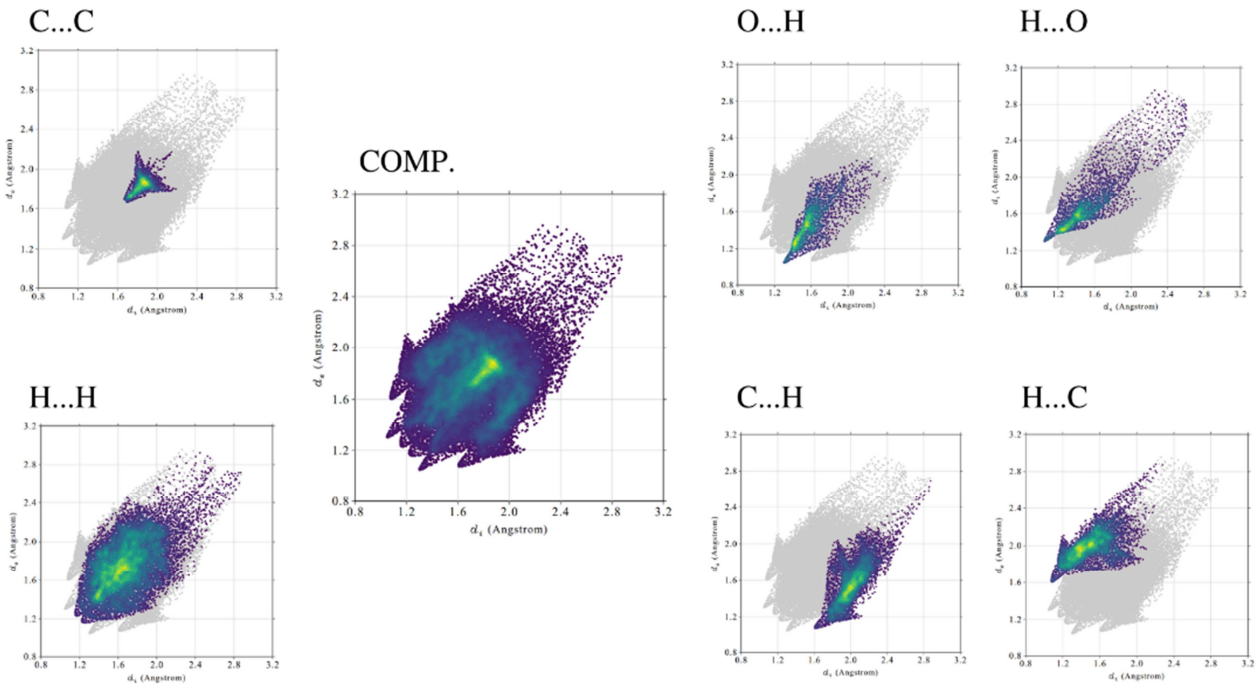

Figure S3. Combined QTAIM and NCI results for all of the studied Schiff bases in PCM: molecular structure with ball and stick visualization (a) and only stick visualization for clarity of BCPs and RCPs as well as other intramolecular interactions identified by NCI index (b).

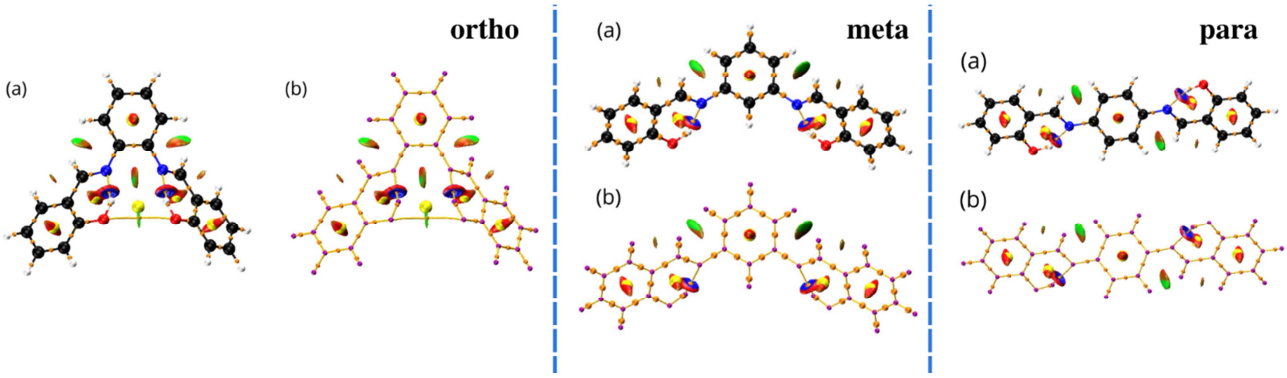

Figure S4. NCI scatter graphs for all of the compounds in PCM: ortho (left), meta (middle) and para (right).

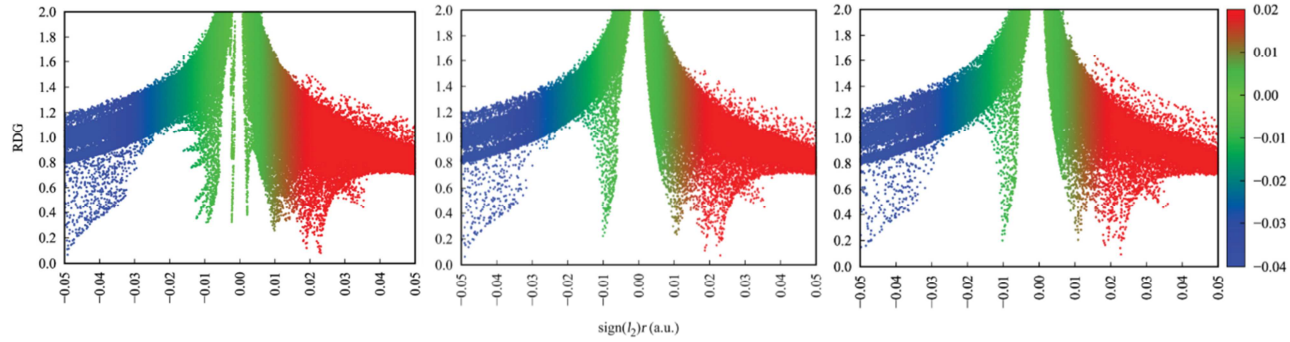

Table S1. Electron density, ρBCP, is given in $e{\cdot}a_0^{-3}$ atomic units and its Laplacian ∇^2ρBCP, is in $e{\cdot}a_0^{-5}$ units at the BCPs. VρBCP stands for BCP potential energy density. They are properties derived from QTAIM. The results were obtained using ωB97XD/6-311+G(2d,2p) level of theory in PCM.

	Ortho	**Meta**	**Para**
O – H			
ρBCP	0.3415	0.3412	0.3406
∇^2ρBCP	-2.5765	-2.5744	-2.5663
VρBCP	-0.7881	-0.7877	-0.7862
H … N			
ρBCP	0.0492	0.0493	0.0499
∇^2ρBCP	0.1106	0.1100	0.1100
VρBCP	-0.0431	-0.0432	-0.0437

Figure S5. ELF plot for the intramolecular hydrogen bond in the ortho compound in vacuo (left) and in PCM (right).

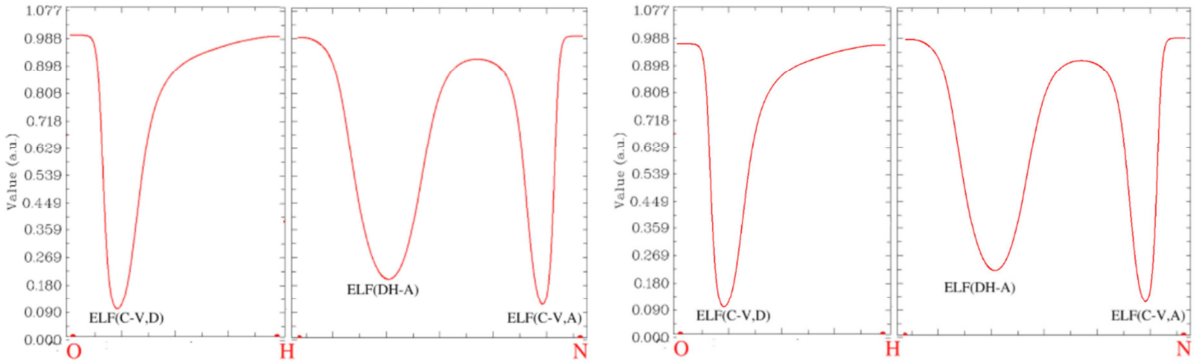

Figure S6. ELF plot for the intramolecular hydrogen bond in the meta compound in vacuo (left) and in PCM (right).

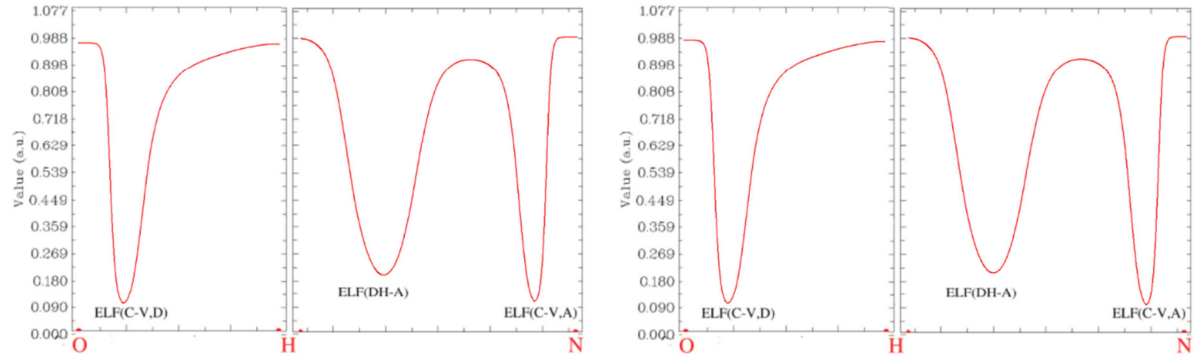

Figure S7. ELF plot for the intramolecular hydrogen bond in the para compound in vacuo (left) and in PCM (right).

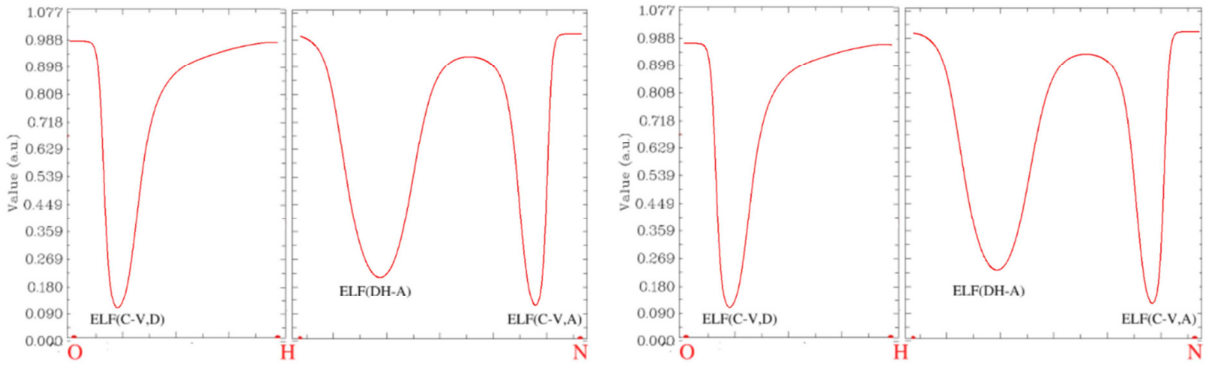

Table S2. Core-valence bifurcation point values and CVB indexes for all of the compounds in PCM.

	Ortho	**Meta**	**Para**
ELF(C-V,D)	0.1027	0.1029	0.1030
ELF(C-V,A)	0.1177	0.1176	0.1178
ELF(DH-A)	0.2224	0.2239	0.2275
CVB index	-0.1197	-0.1210	-0.1245