Can an entirely negative fluorine in a molecule, viz. perfluorobenzene, interact attractively with the entirely negative site(s) on another molecule(s)? Like liking like!

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Supplementary Information

Fig. S1: RDG vs. Sign(λ₂)×ρ (left) and RDG = 0.6 a.u. isosurface (right) NCI graphical plots for H₃N⋯FC₆F₅. The spikes in the λ₂ < 0 and λ₂ > 0 regions represent to the bonded (attractive) and non-bonded (repulsive) interactions, respectively. The respective s = 0.6 a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer labeling in Fig. 1 is in consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).

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Fig. S2: RDG vs. Sign($\lambda_2$)$\varpi$ plot for H$_2$O···FC$_6$F$_5$ a), H$_2$O···FC$_6$F$_5$ b), H$_3$CF···FC$_6$F$_5$ c), H$_3$CF···FC$_6$F$_5$ d), HF···FC$_6$F$_5$ e) and HF···FC$_6$F$_5$ f) (values in a.u.). The spikes in the $\lambda_2 < 0$ and $\lambda_2 > 0$ regions represent the bonded (attractive) and non-bonded (repulsive) interactions, respectively. The respective $s = 0.6$ a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer labeling in Fig. 1 is consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).
Fig. S3: RDG vs. \text{Sign}(\lambda_2) \times \rho$ plot for $\text{H}_2\text{CO} \cdots \text{FC}_6\text{F}_5$ h), $\text{H}_2\text{CO} \cdots \text{FC}_6\text{F}_5$ i), $\text{C}_5\text{F}_5\text{N} \cdots \text{FC}_6\text{F}_5$ j), $\text{C}_4\text{F}_4\text{N}_2 \cdots \text{FC}_6\text{F}_5$ k), $\text{C}_4\text{F}_4\text{N}_2 \cdots \text{FC}_6\text{F}_5$ l), and (\text{CF})$_4\text{N}_2 \cdots \text{FC}_6\text{F}_5$ m) (values in a.u.). The spikes in the $\lambda_2 < 0$ and $\lambda_2 > 0$ regions represent the bonded (attractive) and non-bonded (repulsive) interactions, respectively. The respective $s = 0.6$ a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer labeling in Fig. 1 is consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).