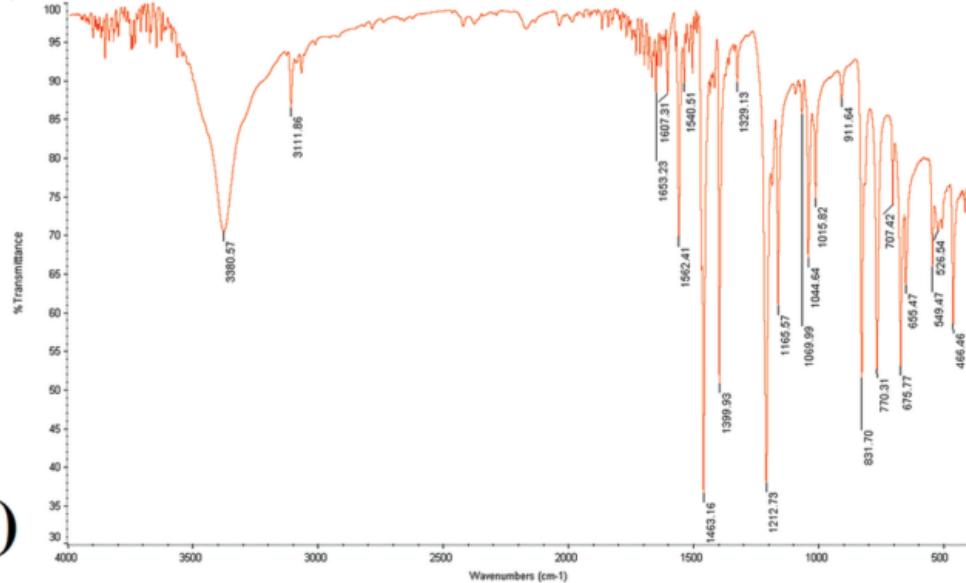
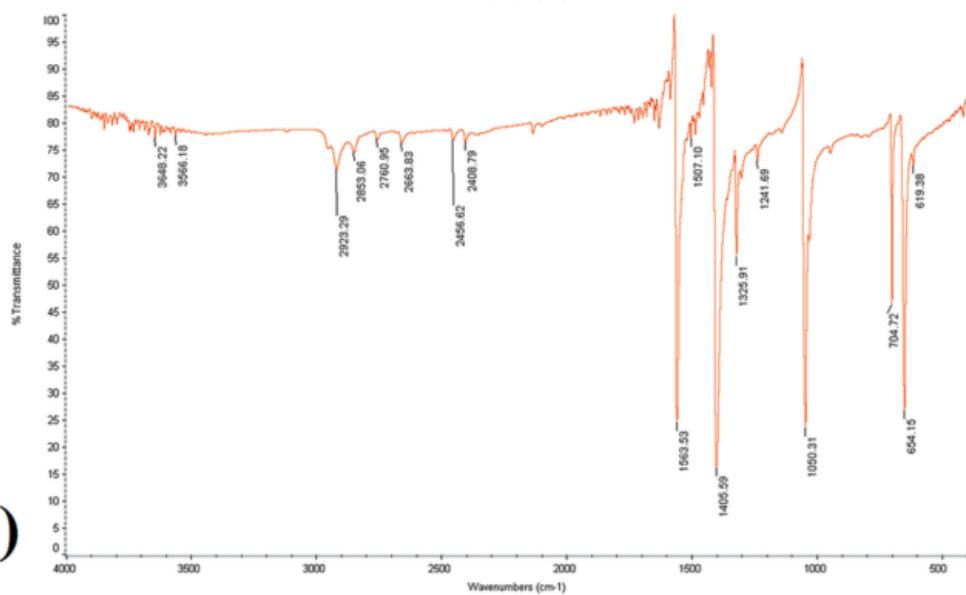


(a)



(b)



(c)

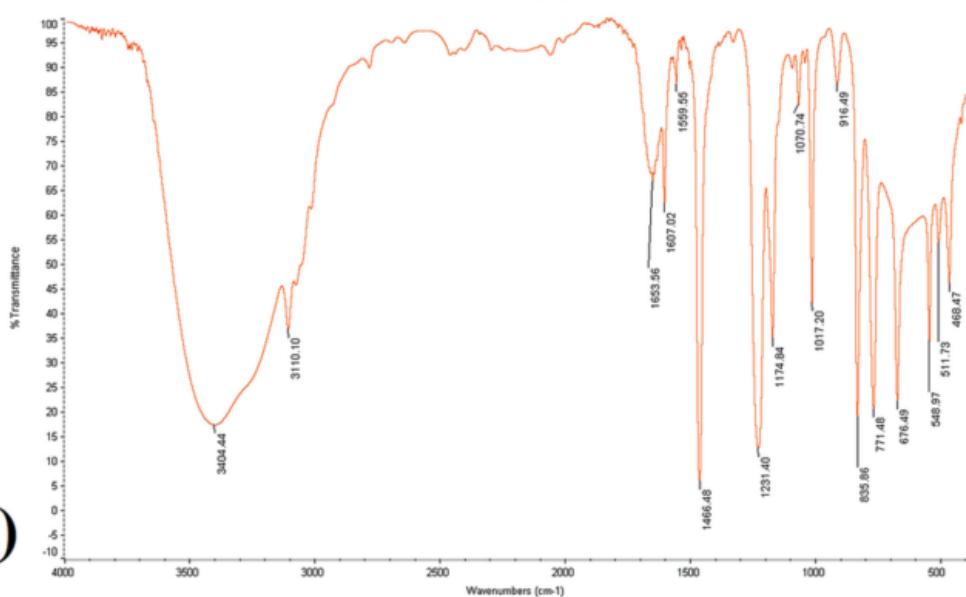


Fig. S1. The IR spectra of (a) (I), (b) $\text{I}_3\text{F}_3\text{Bz}$ and (c) O-Py.

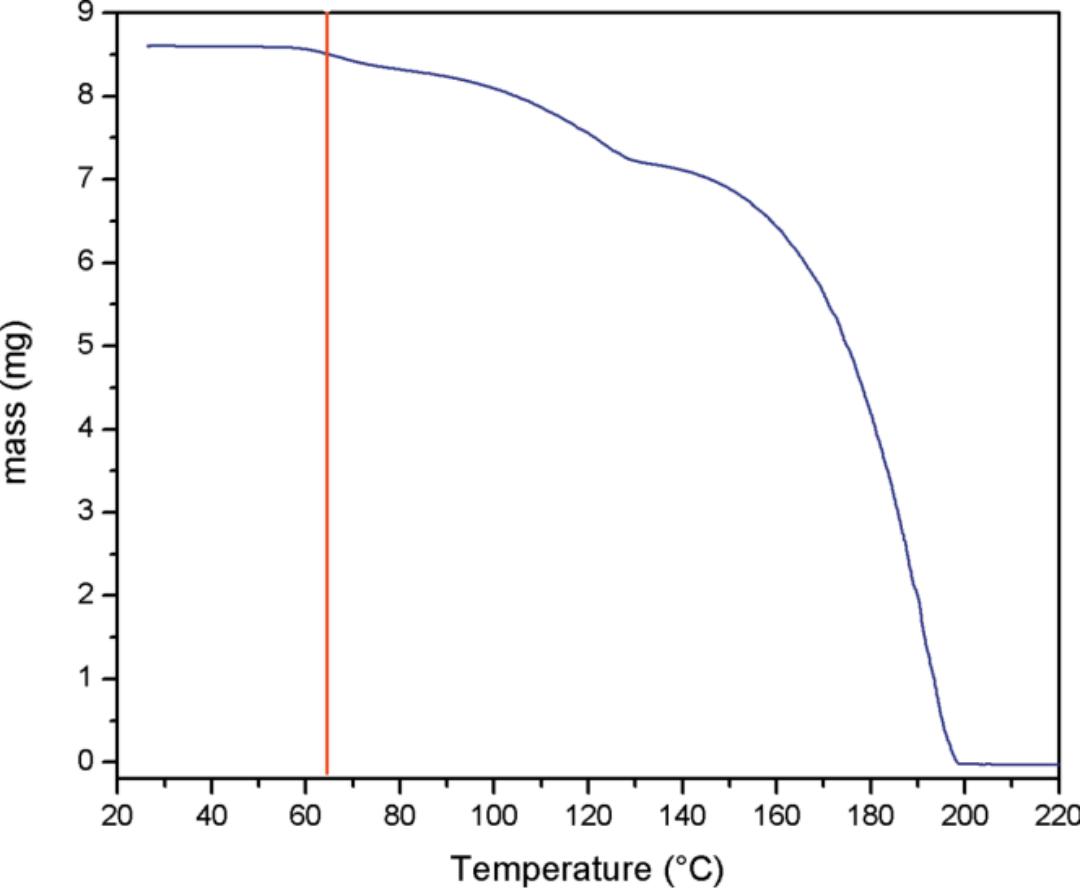


Fig. S2. The TGA diagram for (I).

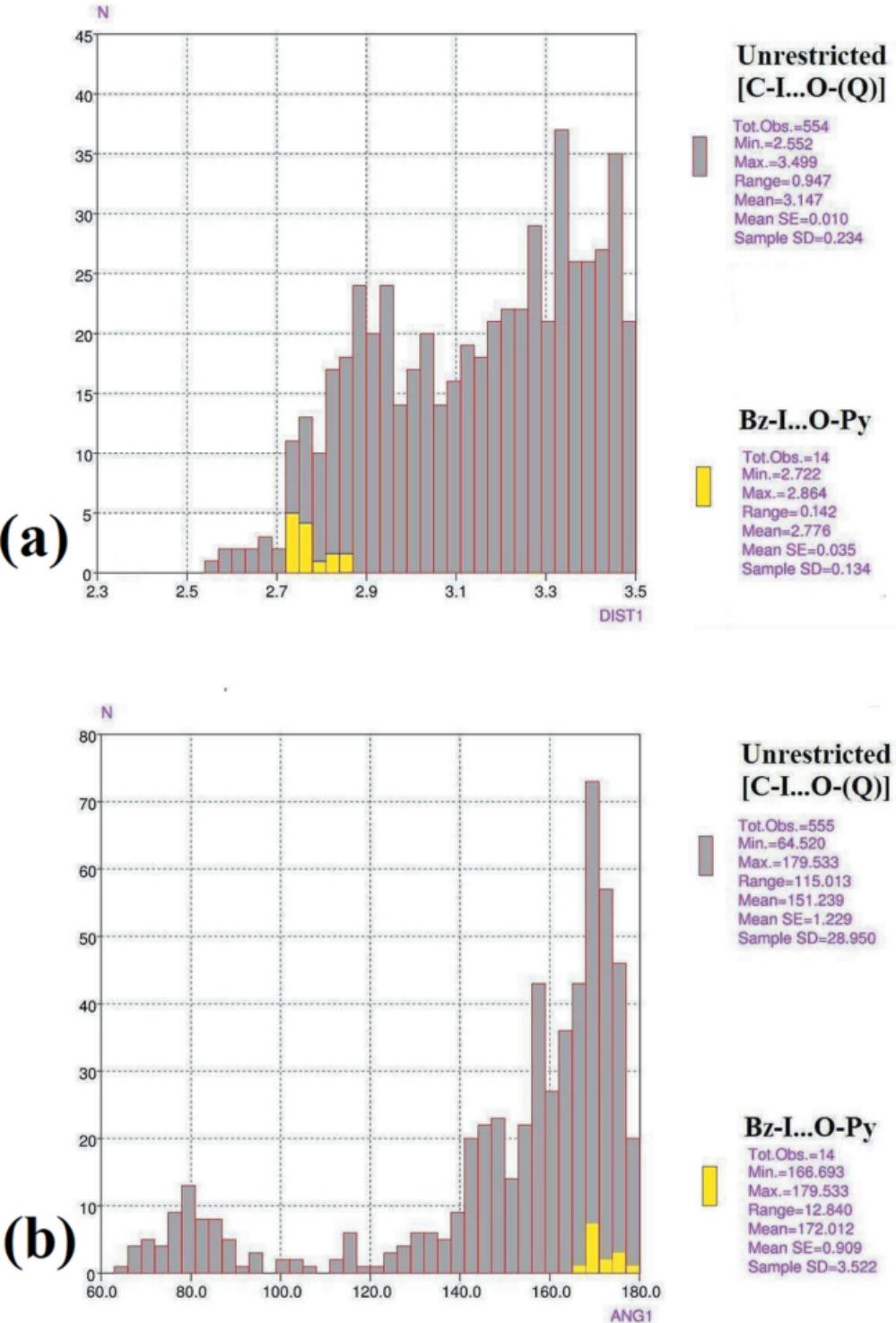


Fig. S3. (a) Distance and (b) angular distributions of C-I…O interactions (\AA , $^{\circ}$) as found in the CSD, searched under different restrictions: (grey) unrestricted (of the C-I…O-Q type; Q is any nonmetal); (yellow) of the Bz-I…O-Py type. Only structures without disorder and errors, with $R < 0.10$ have been considered. Histograms generated by *VISTA*, in the CCDC package.

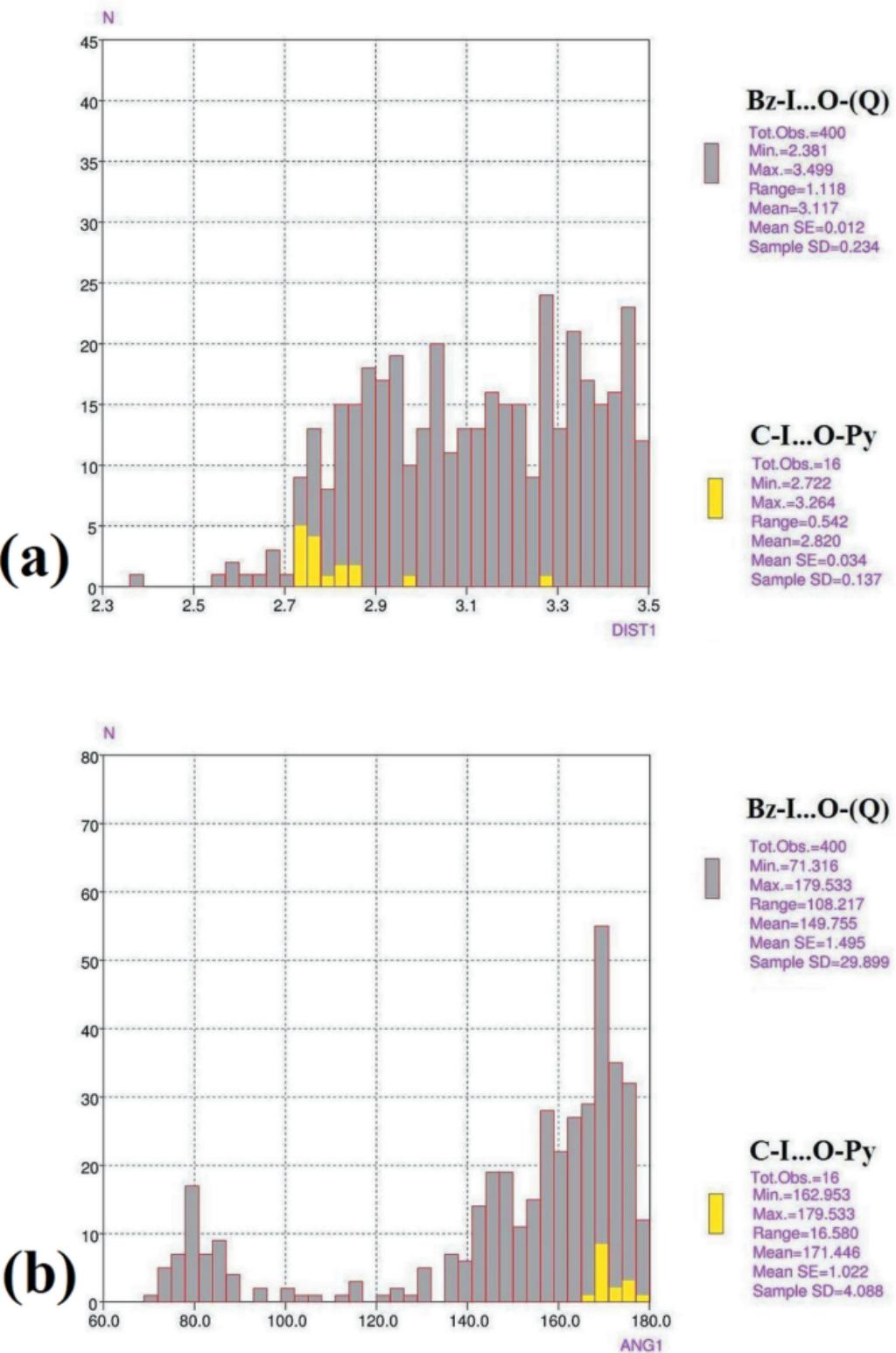


Fig. S4. (a) Distance and (b) angular distributions of C-I...O interactions (\AA , $^\circ$) as found in the CSD, searched under different restrictions: (grey) of the Bz-I...O-Q type (Q is any nonmetal); (yellow) of the C-I...O-Py type. Only structures without disorder and errors, with $R < 0.10$ have been considered. Histograms generated by *VISTA*, in the CCDC package.