The Iodine-Oxygen Halogen Bond: Solid-state Structures of 3-Iodopropiolamides

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− Electronic Supporting Information −

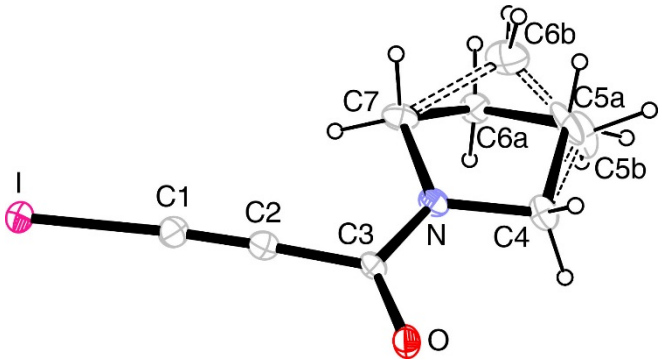

Fig. S1 Structure of 3-iodopropiolamide **3a** (PK248) in the crystal. Displacement ellipsoids represent a 30% probability. The pyrrolidine ring is conformationally disordered. The positions of C5a/C5b and C6a/C6b and could be resolved; site occupation factors were refined at 0.565/0.435.

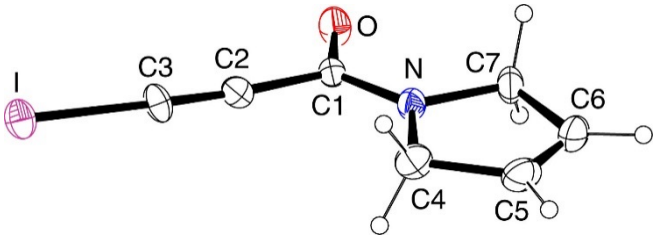

Fig. S2 Structure of 3-iodopropiolamide **3b** (PK276) in the crystal. Displacement ellipsoids represent a 30% probability.

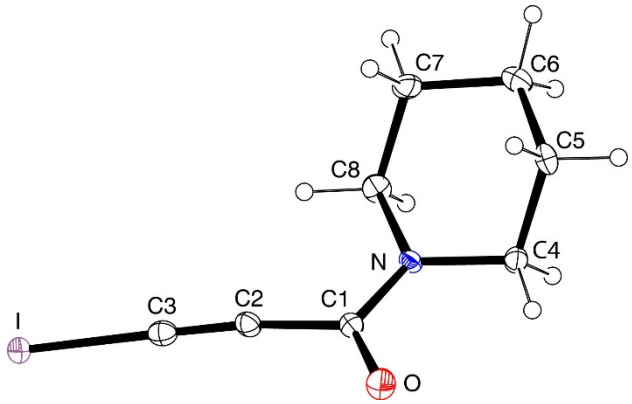

Fig. S3 Structure of 3-iodopropiolamide **3c** (PK257) in the crystal. Displacement ellipsoids represent a 30% probability.

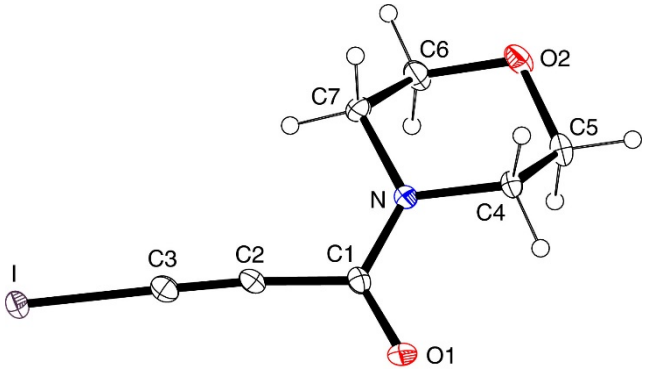

Fig. S4 Structure of 3-iodopropiolamide **3d** (PK254) in the crystal. Displacement ellipsoids represent a 30% probability.

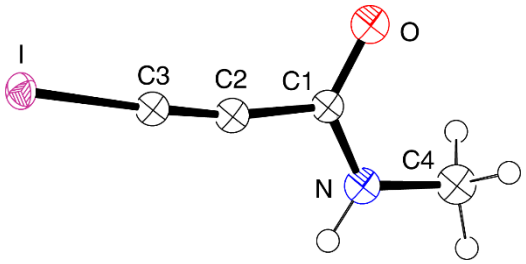

Fig. S5 Structure of 3-iodopropiolamide **3e** (PK281) in the crystal. Displacement ellipsoids represent a 50% probability.

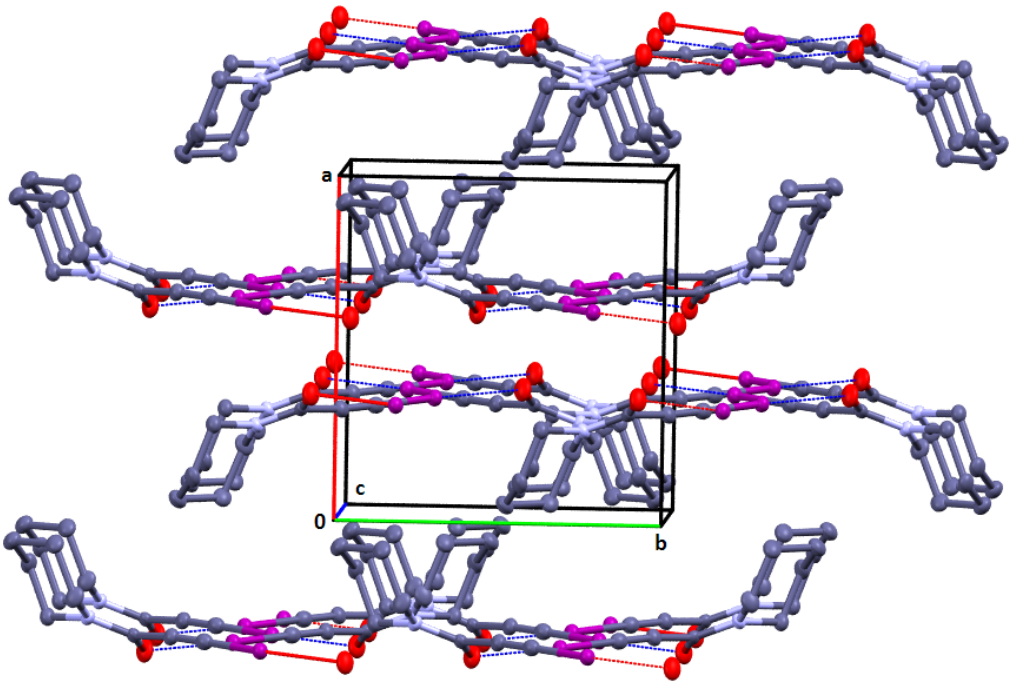

Fig. S6 Packing diagram of **3c** (PK257) (PK257_Abs_packing_view on ba plane.png). Hanging contacts are shown with red dashed bonds.

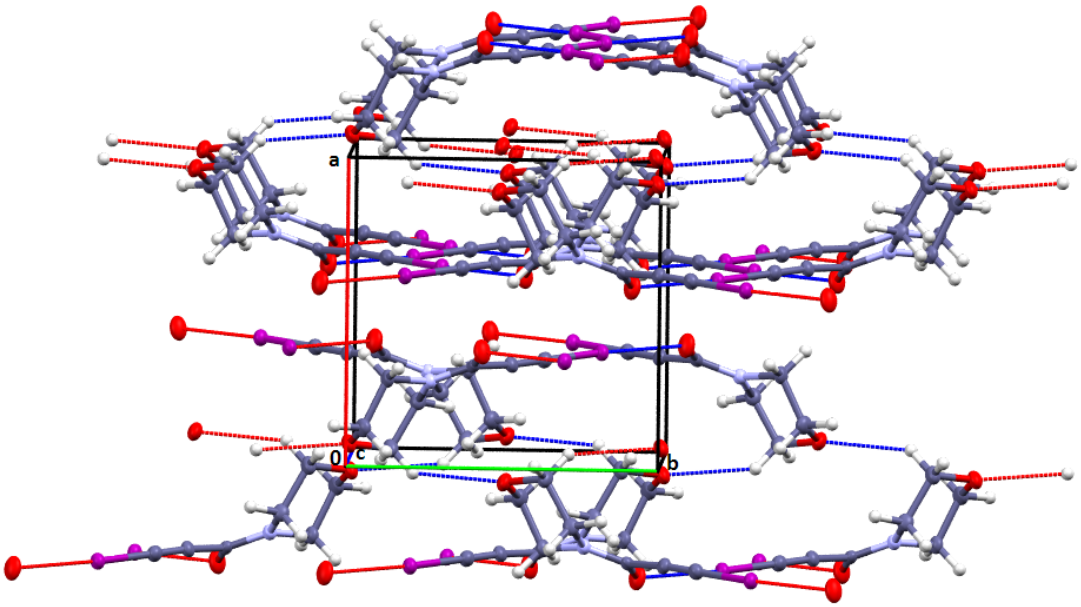

Fig. S7 Packing diagram of **3d** (PK257) (PK254_Abs_Packing_view approx down c_Jan15.png). Hanging contacts are shown with a red dashed bond. For the sake of clarity, the packing within the given dimensions has not been completed.

Table S1. Selected bond lengths and angles in **3a**−**f**.

Compound	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**
Bond lengths (Å)						
C1−O	1.237(5)	1.233(6)	1.239(3)	1.236(3)	1.248(7)	1.245(4)
C1−N	1.337(5)	1.331(6)	1.336(4)	1.333(5)	1.330(8)	1.313(4)
C1−C2	1.451(7)	1.458(7)	1.450(5)	1.453(5)	1.445(9)	1.466(4)
C2−C3	1.184(7)	1.192(7)	1.199(5)	1.191(5)	1.211(8)	1.192(4)
C3−I	2.007(5)	1.999(5)	2.016(4)	2.010(4)	1.993(6)	2.001(3)
Bond angles (°)						
C1−C2−C3	175.6(5)	175.8(6)	173.5(3)	173.5(4)	170.2(6)	178.0(3)
C2−C3−I	177.0(4)	175.7(5)	179.1(3)	179.0(3)	176.7(5)	176.9(3)