Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supporting Information

Co-crystallisation through halogen bonding with racemic or enantiopure sulfinamides

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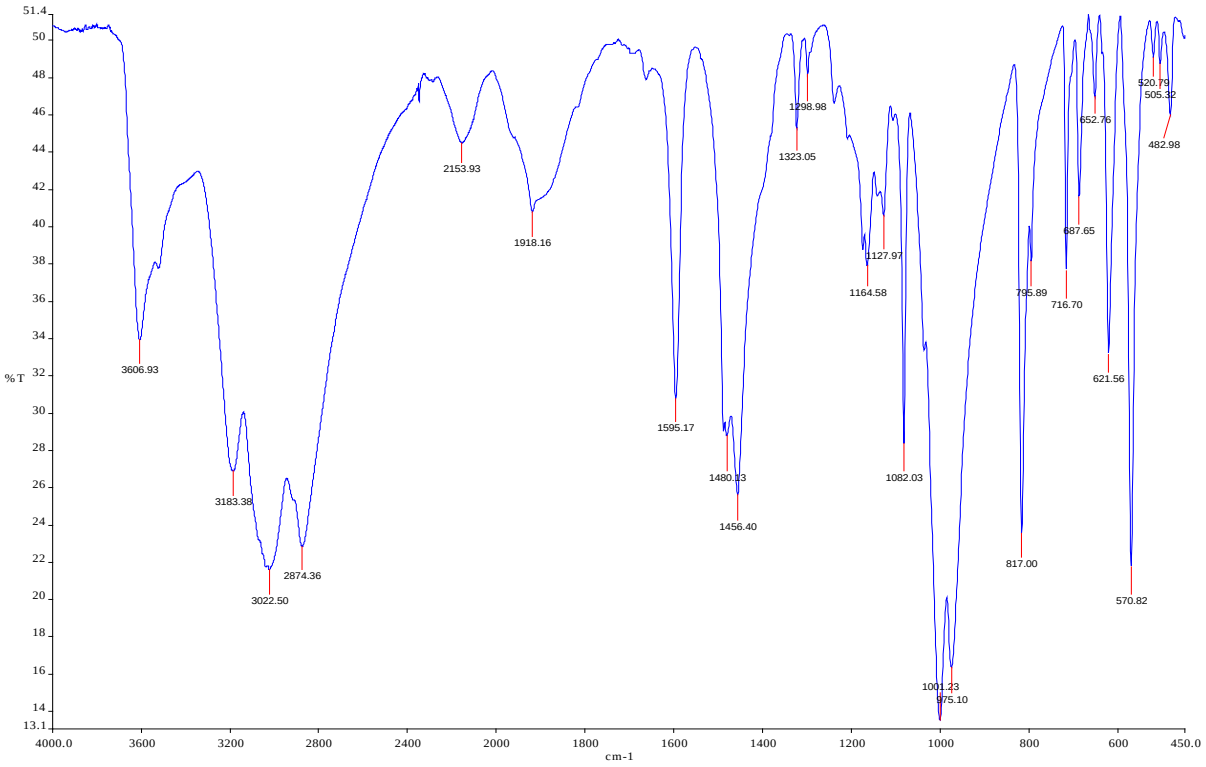
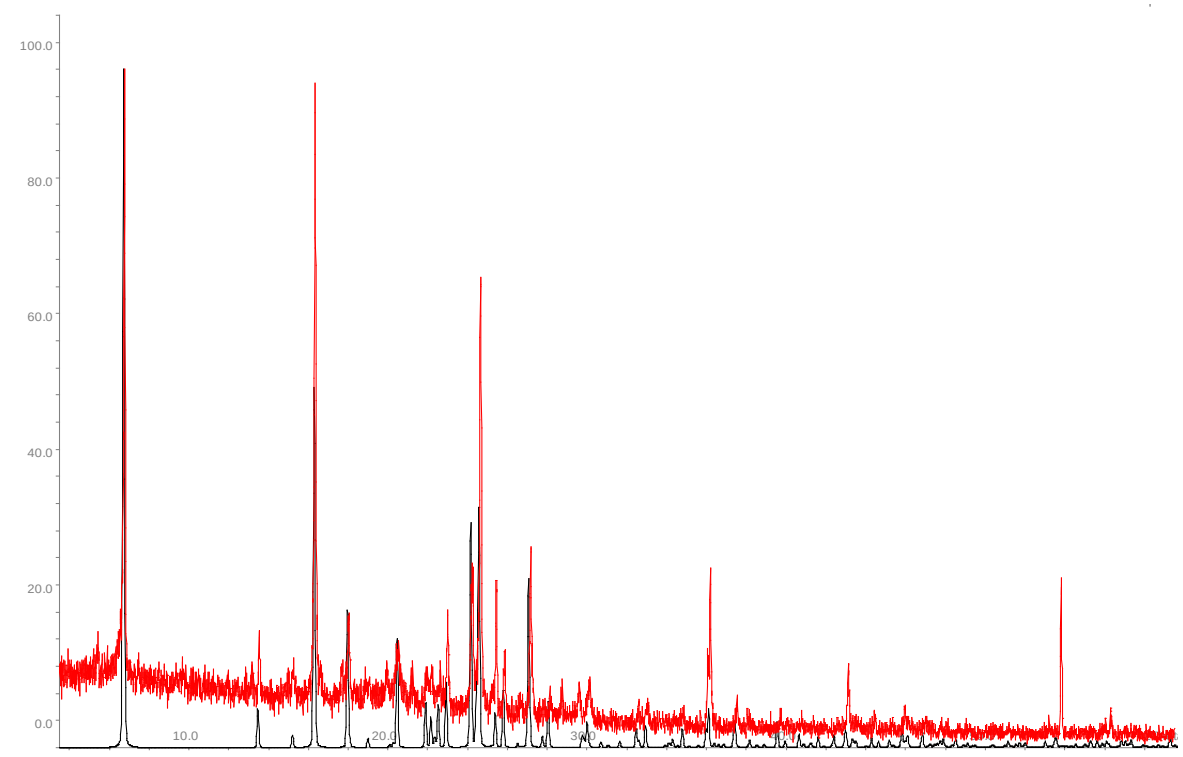
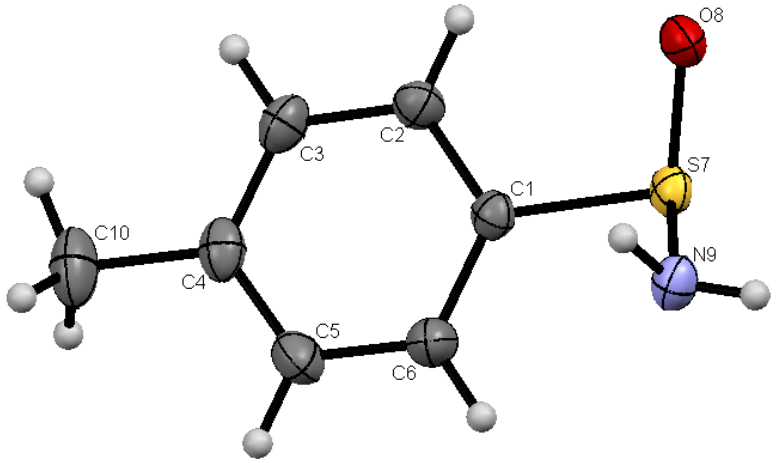
IR spectra for **(±)-2**.



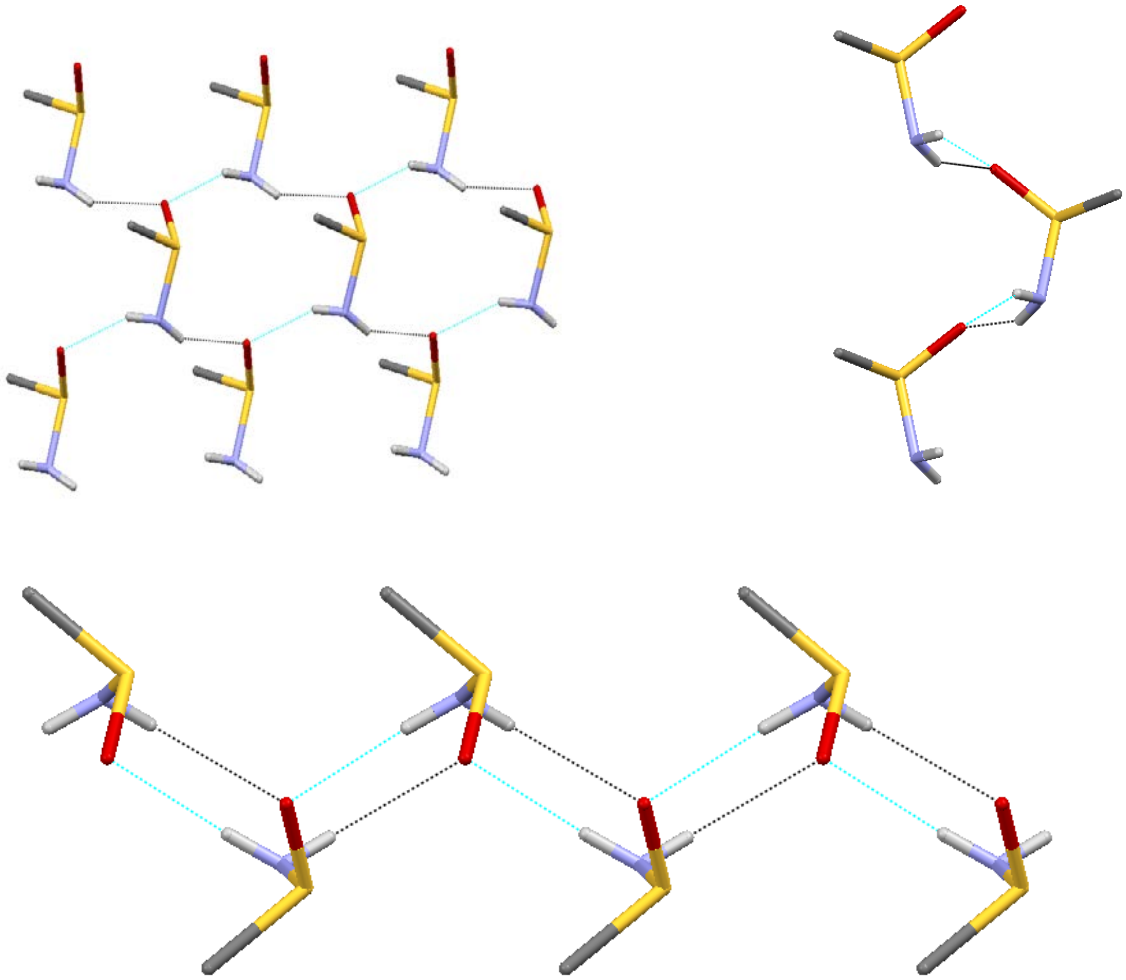
PXRD pattern of **(±)-2** obtained from solution crystallization (red) overlaid with theoretical pattern (black).



ORTEP plot of **(±)-2** (ellipsoids shown at 30% probability).

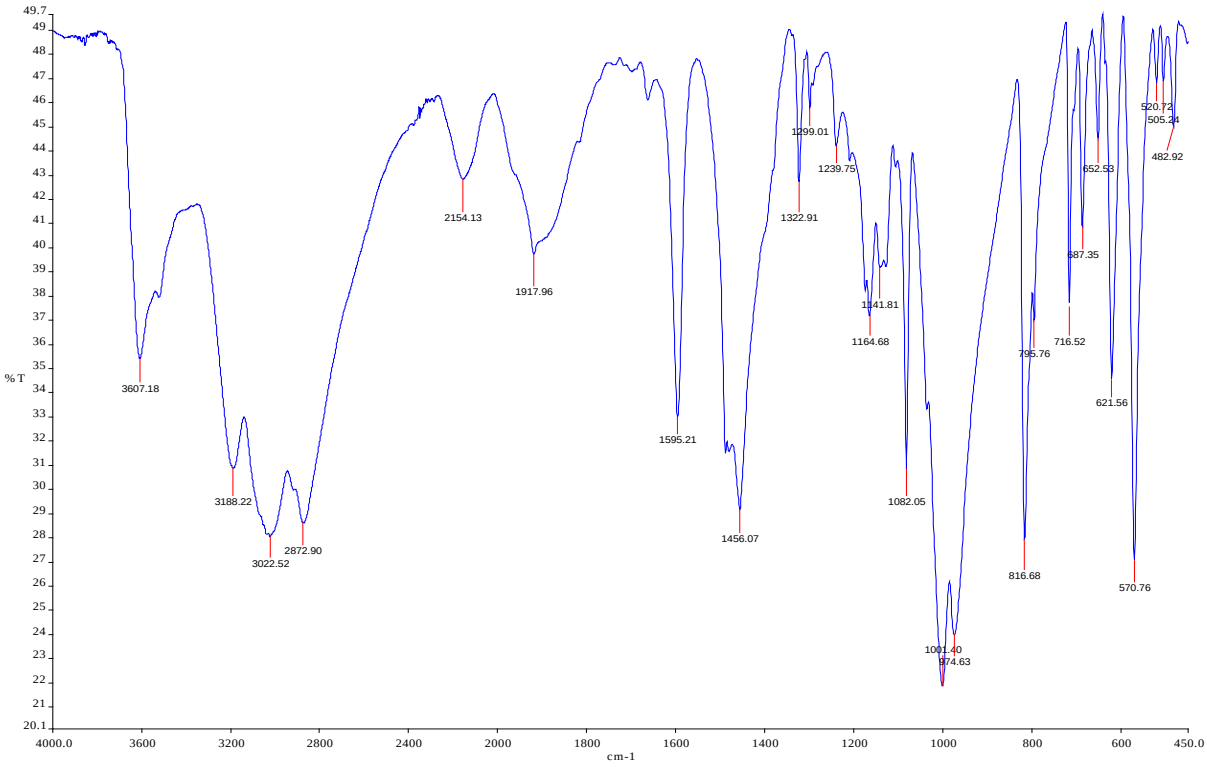


Hydrogen bonding in **(±)-2**. (The *p*-tolyl group is removed for clarity.)

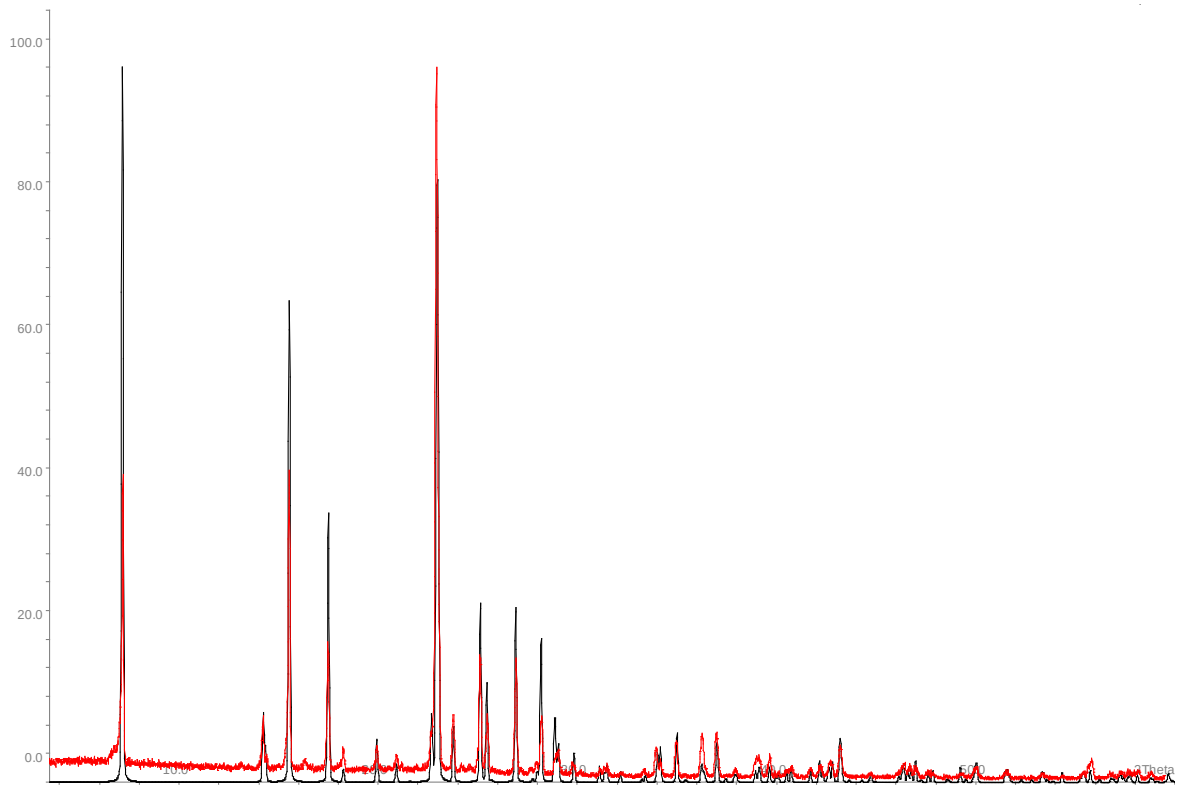


Analytical Data and Figures for (*S*)-*2*

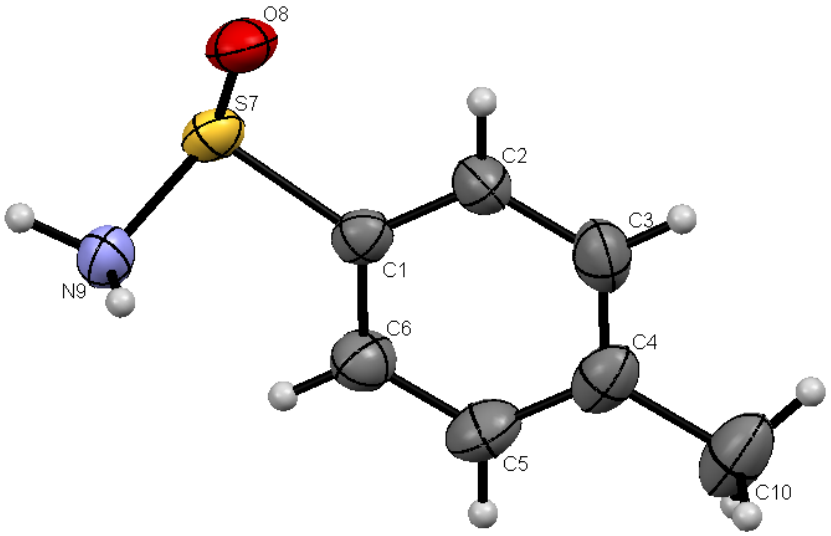
IR spectra for **(*S*)-2**



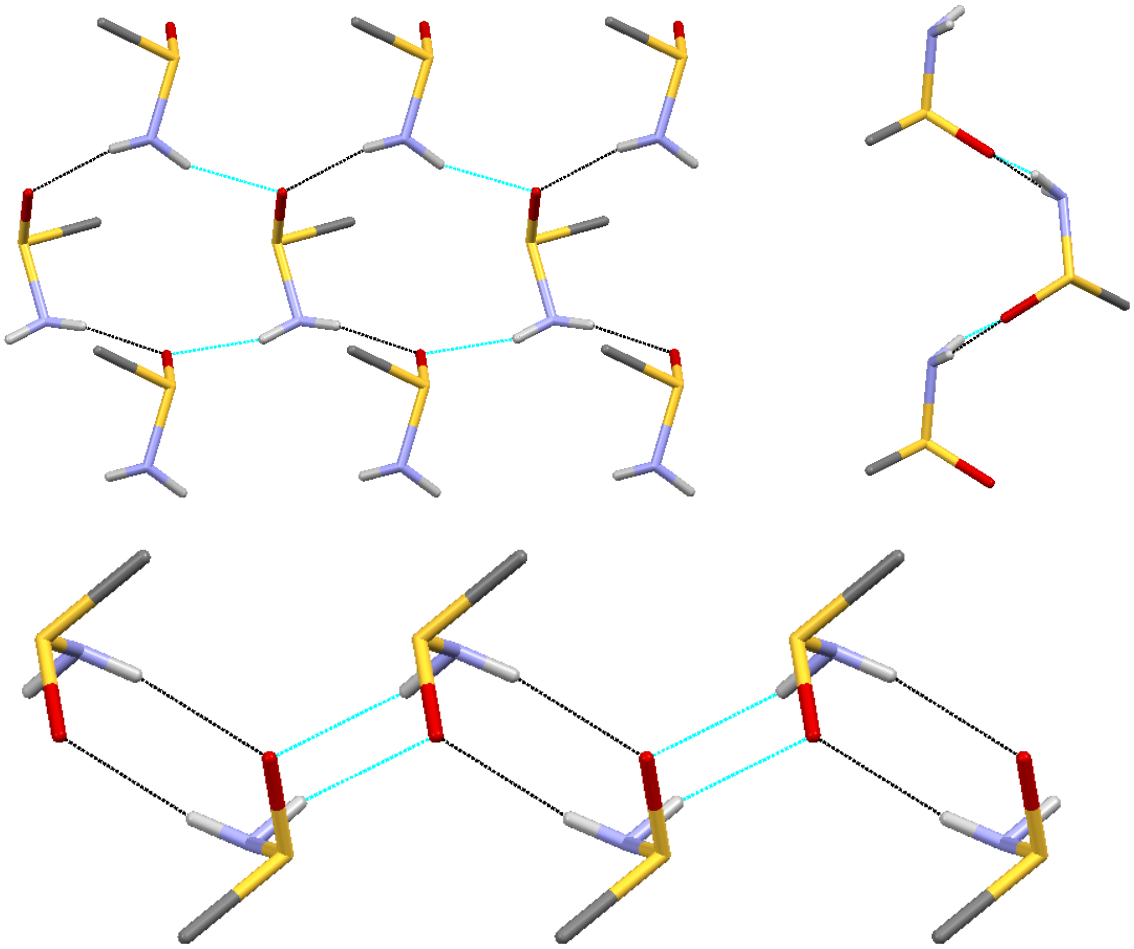
PXRD pattern of **(*S*)-2** obtained from solution crystallization (black).



ORTEP plot of **(*S*)-2** (ellipsoids shown at 30% probability).

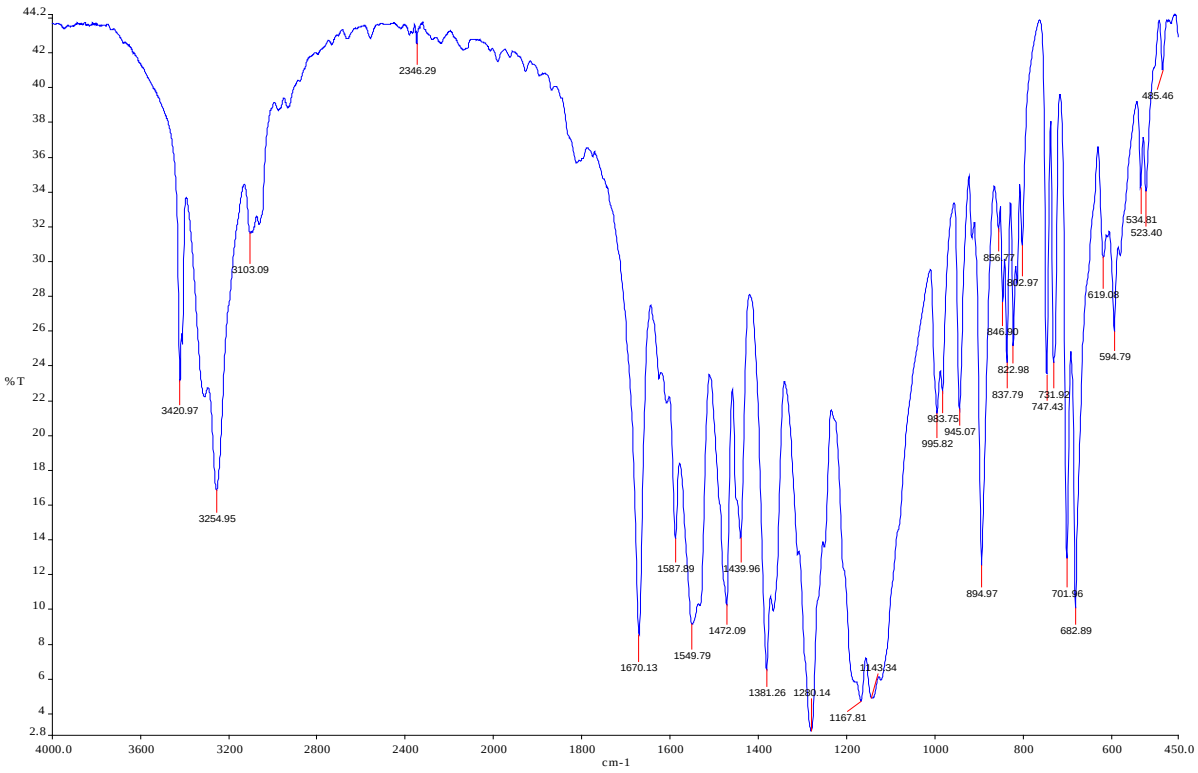


Hydrogen bonding in **(*S*)-2**. (The *p*-tolyl group is removed for clarity.)

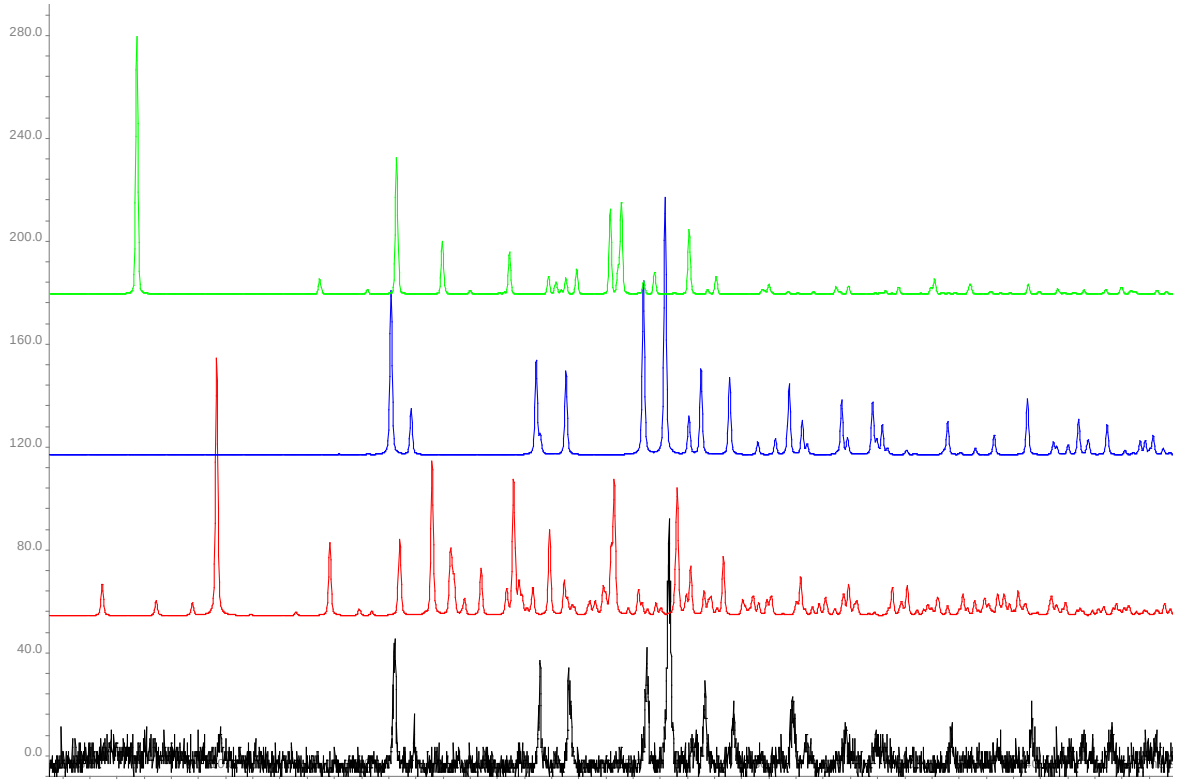


Analytical Data and Figures for 1.(±)-2

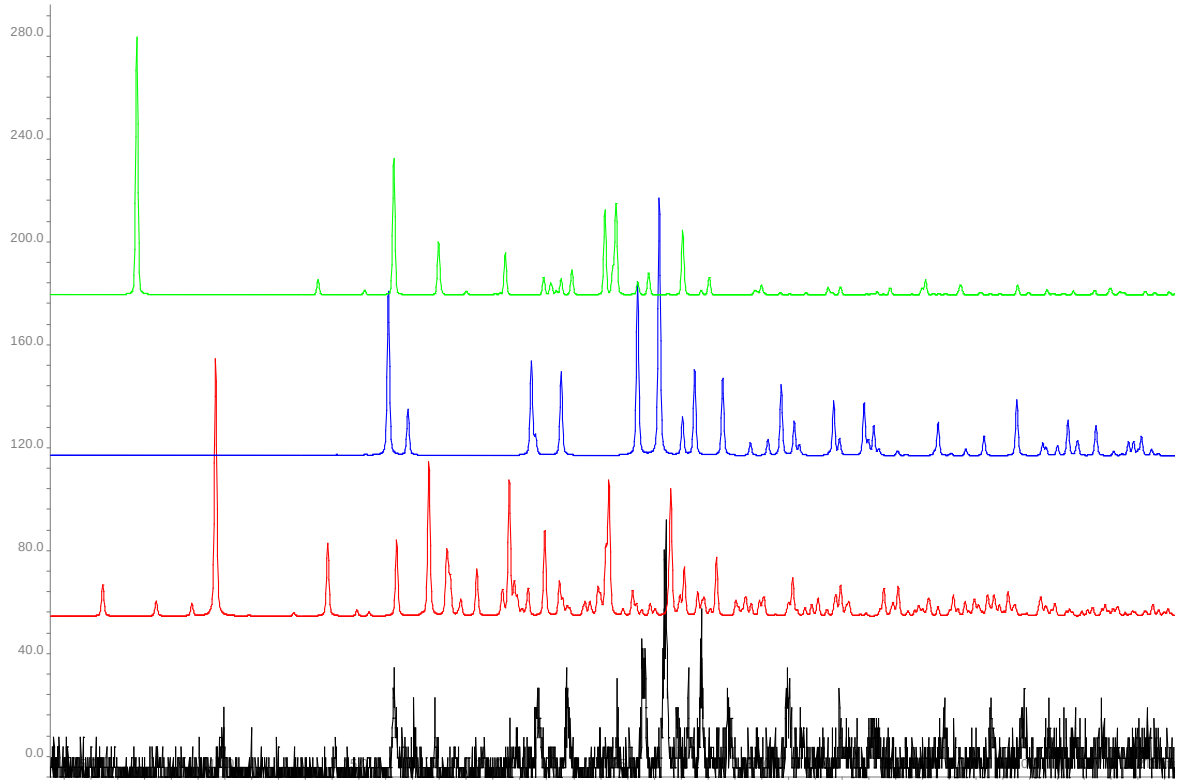
IR spectra for **1.(±)-2**



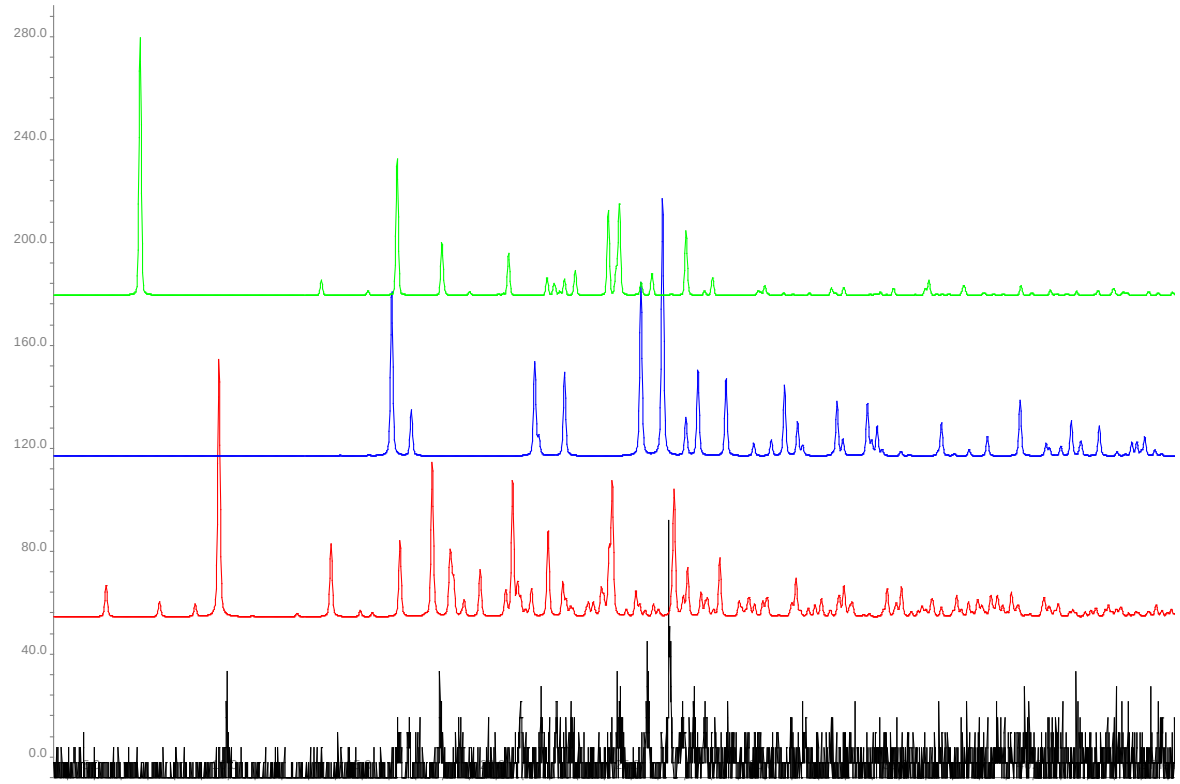
PXRD pattern of neat grind in ratio of 2:1. **1**: **(±)-2** (black), overlaid with theoretical patterns of **1.(±)-2** cocrystal, (red), **1** (blue) and **(±)-2** (green).



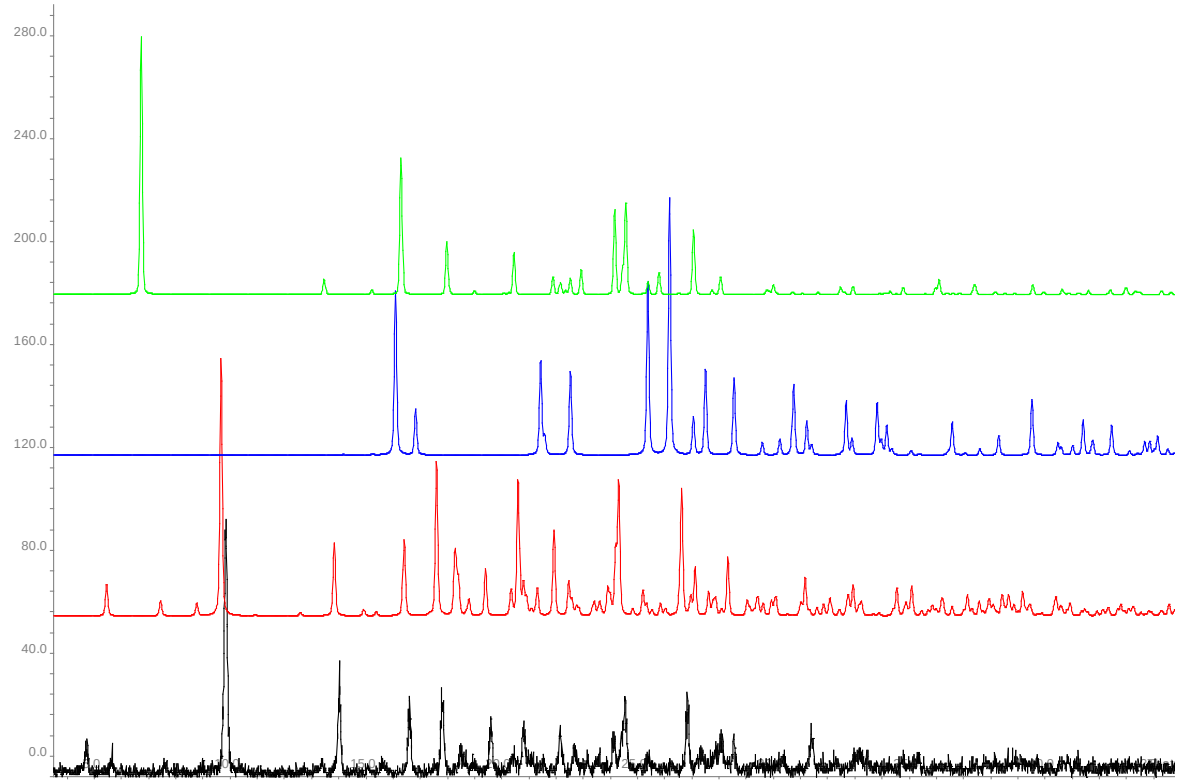
PXRD pattern of neat grind in ratio of 1:1. **1**: **(±)-2** (black), overlaid with theoretical patterns of **1.(±)-2** cocrystal, (red), **1** (blue) and **(±)-2** (green).



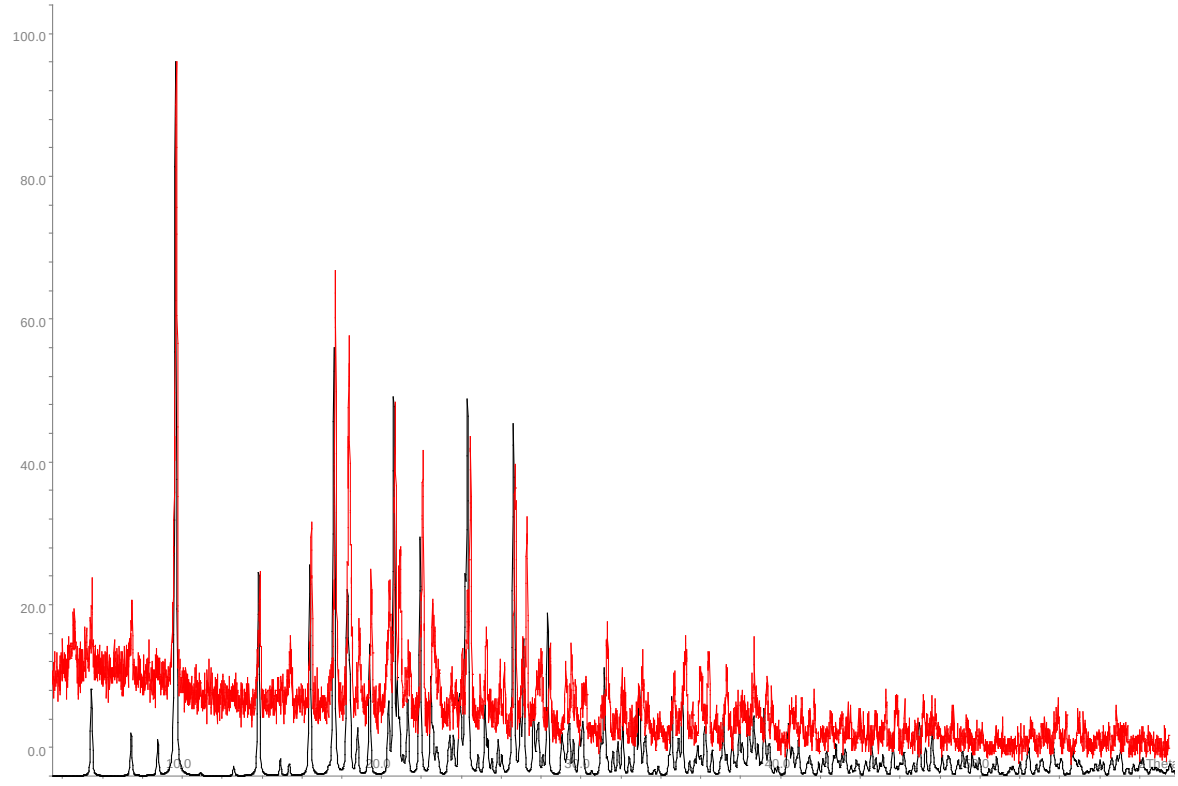
PXRD pattern of neat grind in ratio of 1:2. **1**: **(±)-2** (black), overlaid with theoretical patterns of **1.(±)-2** cocrystal, (red), **1** (blue) and **(±)-2** (green).



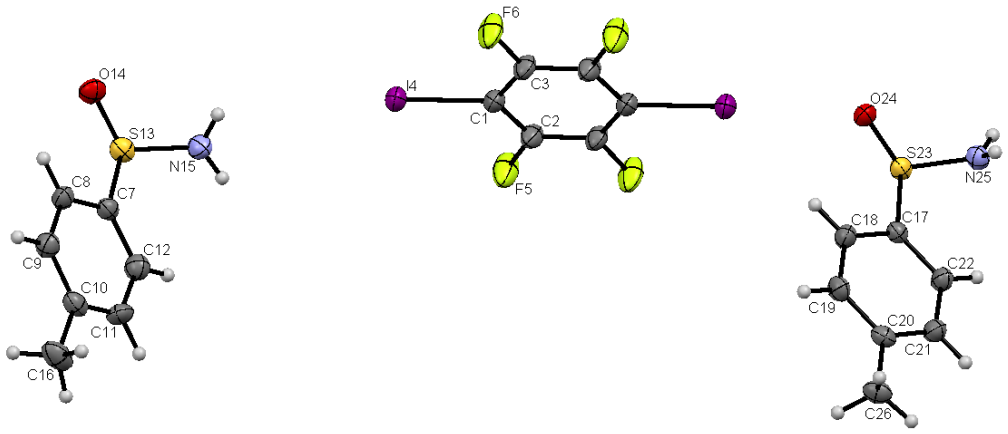
PXRD pattern of neat grind in ratio of 1:4. **1**: **(±)-2** (black), overlaid with theoretical patterns of **1.(±)-2** cocrystal, (red), **1** (blue) and **(±)-2** (green).



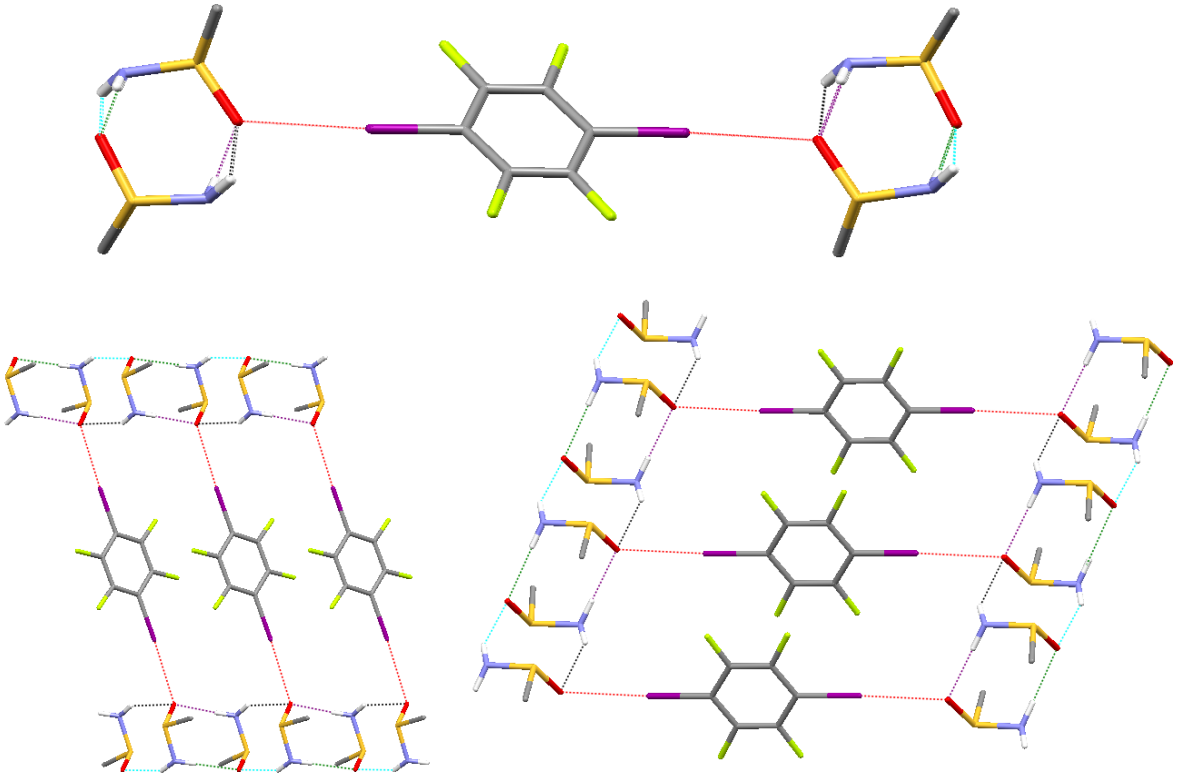
PXRD pattern of **1.(±)-2** obtained from solution crystallization (red) overlaid with theoretical pattern (black).



ORTEP plot of **1.(±)-2** (ellipsoids shown at 30% probability).

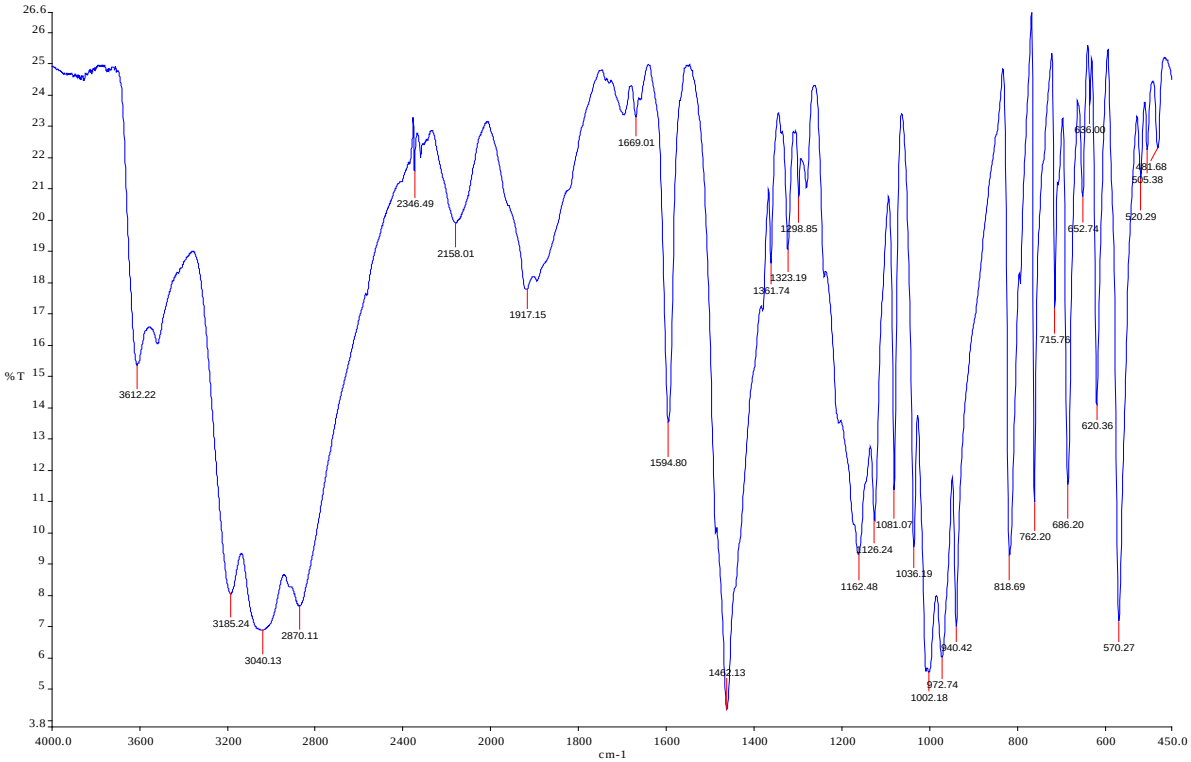


Hydrogen bonding in **1.(±)-2**

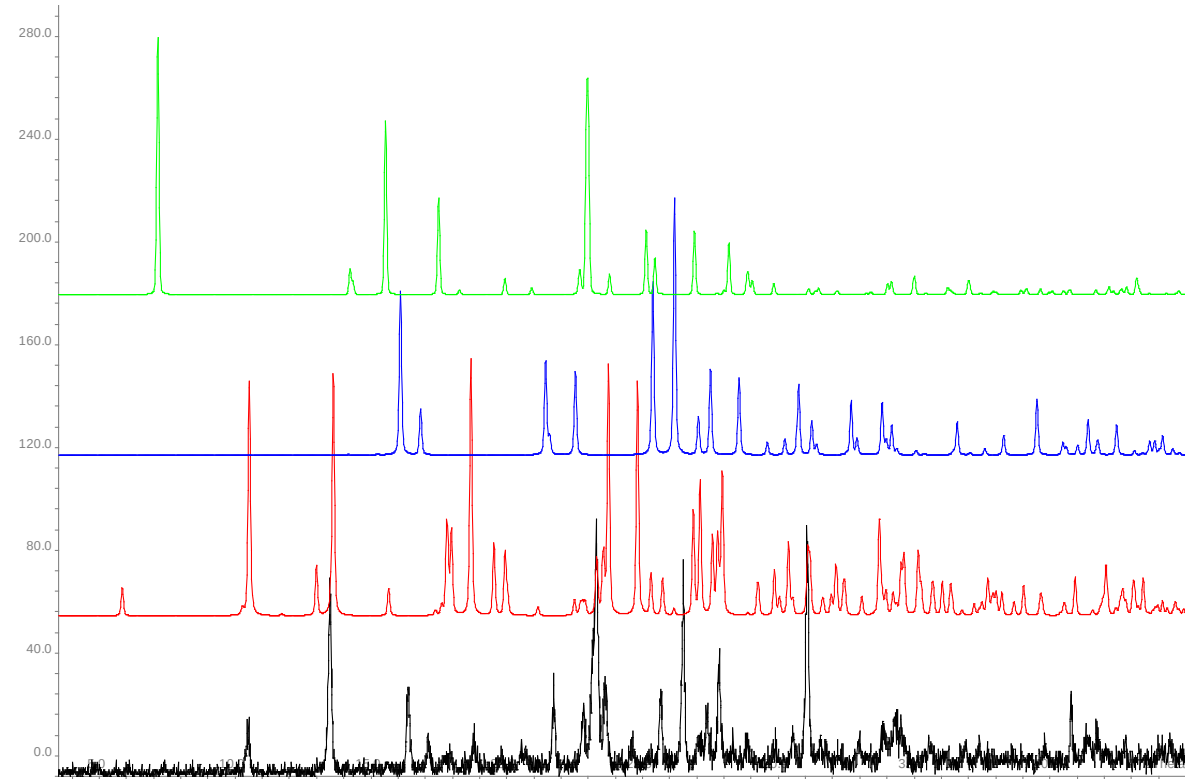


Analytical Data and Figures for 1.(*S*)-2

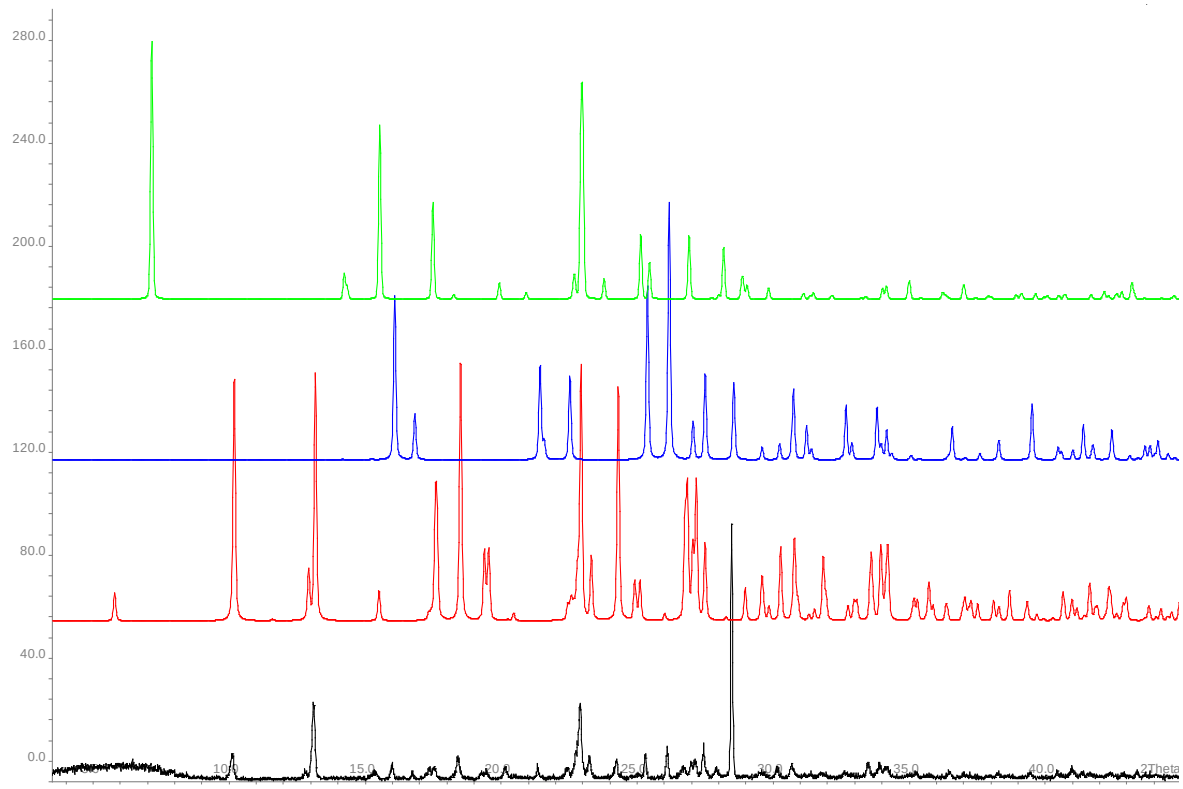
IR spectra for **1.(*S*)-2**



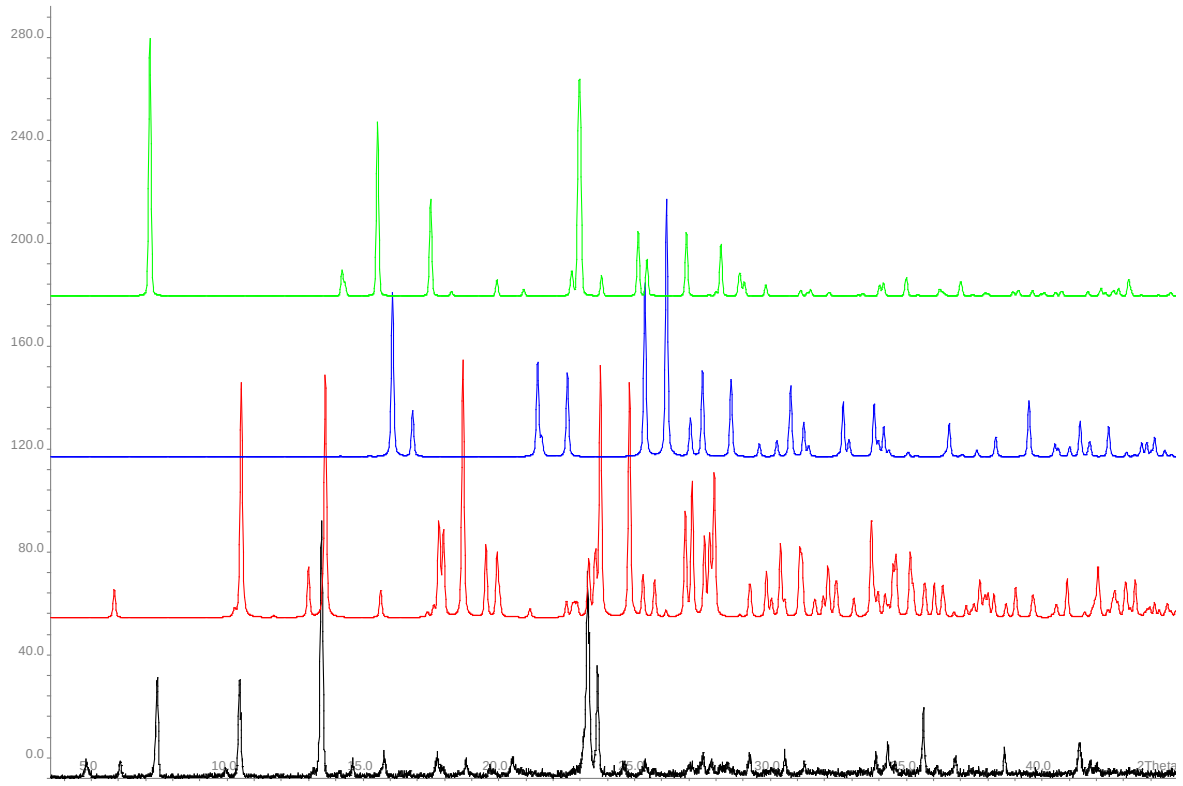
PXRD pattern of neat grind in ratio of 2:1. **1**: **(*S*)-2** (black), overlaid with theoretical patterns of **1.(*S*)-2** cocrystal, (red), **1** (blue) and **(*S*)-2** (green).



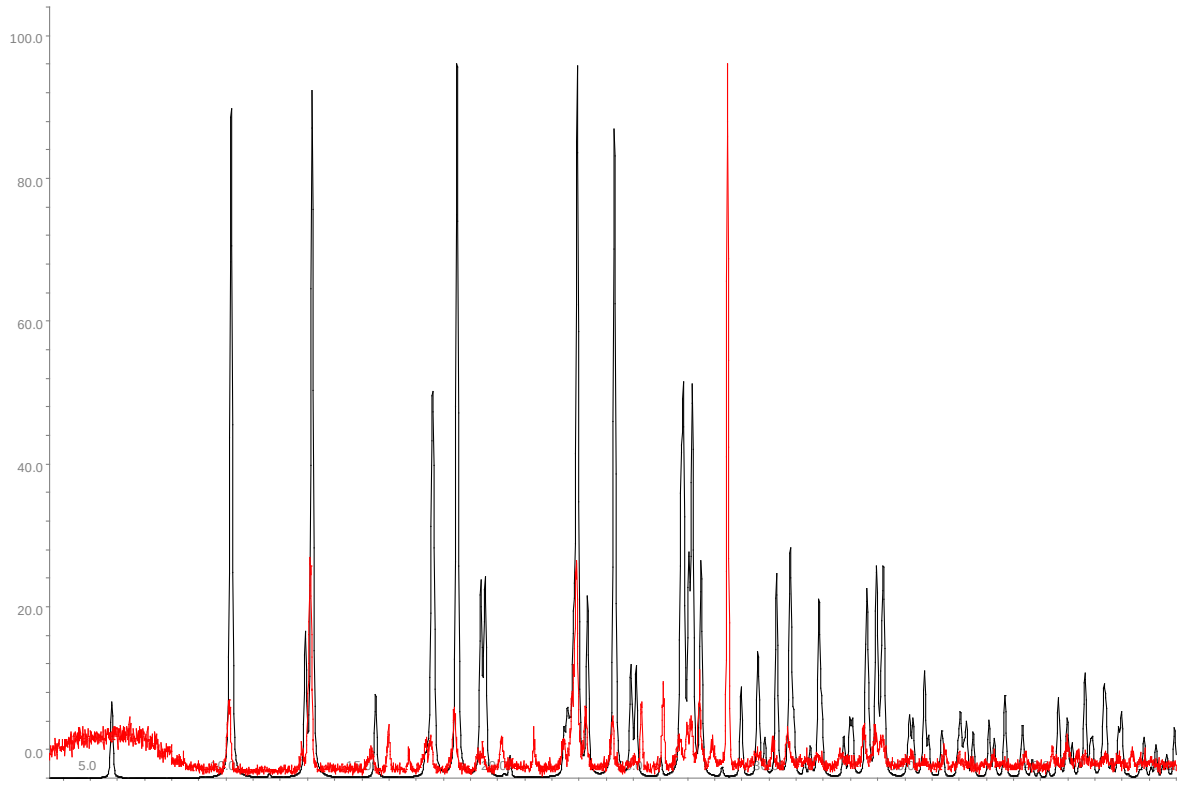
PXRD pattern of neat grind in ratio of 1:1. **1**: **(*S*)-2** (black), overlaid with theoretical patterns of **1.(*S*)-2** cocrystal, (red), **1** (blue) and **(*S*)-2** (green).



PXRD pattern of neat grind in ratio of 1:2. **1**: **(*S*)-2** (black), overlaid with theoretical patterns of **1.(*S*)-2** cocrystal, (red), **1** (blue) and **(*S*)-2** (green).

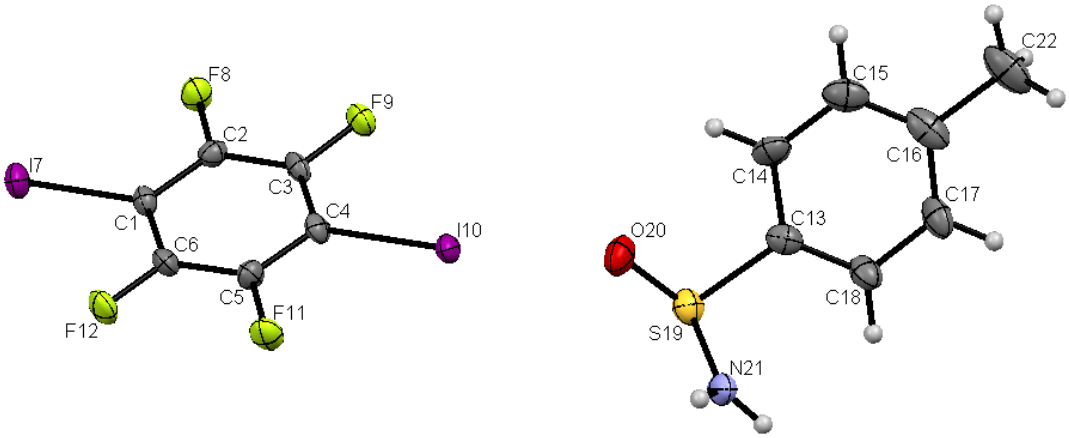


PXRD pattern of **1.(*S*)-2** obtained from solution crystallization (red) overlaid with theoretical pattern (black).

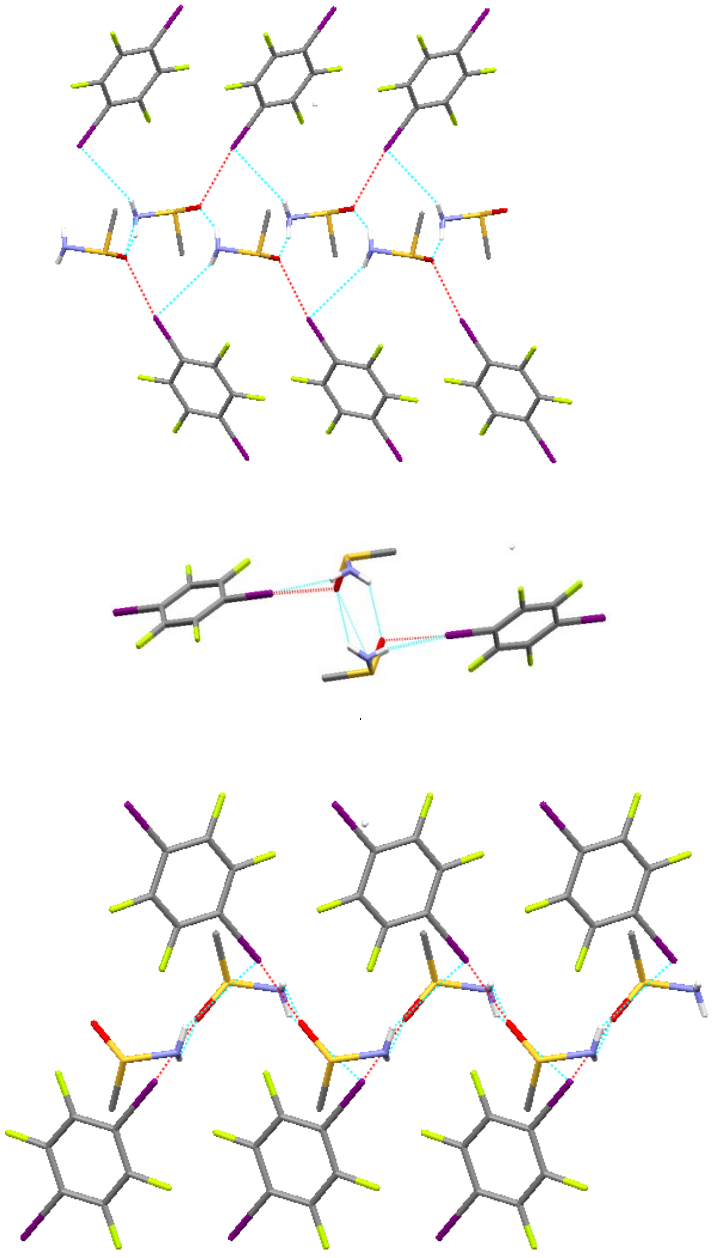


* The PXRD patterns contain minor impurities of 1,4-diiodotetraflurorbenzene

ORTEP plot of **1.(*S*)-2** (ellipsoids shown at 50% probability).

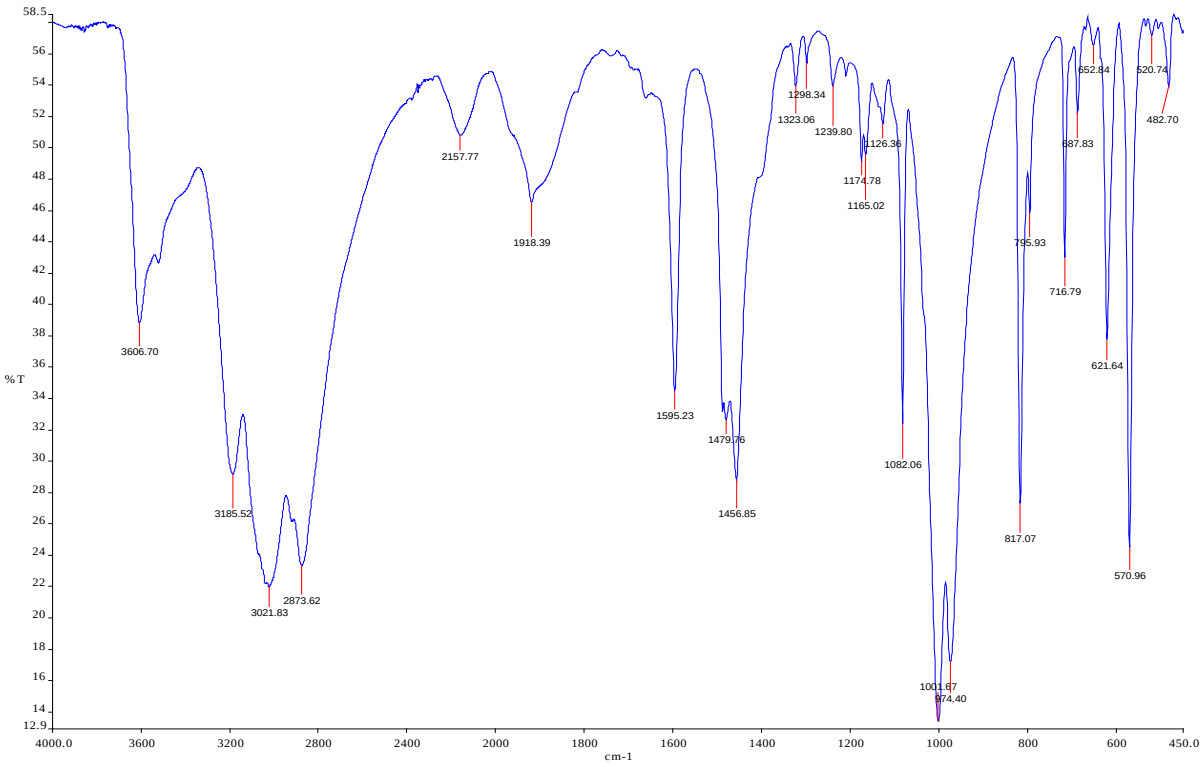


Hydrogen bonding in **1.(*S*)-2**

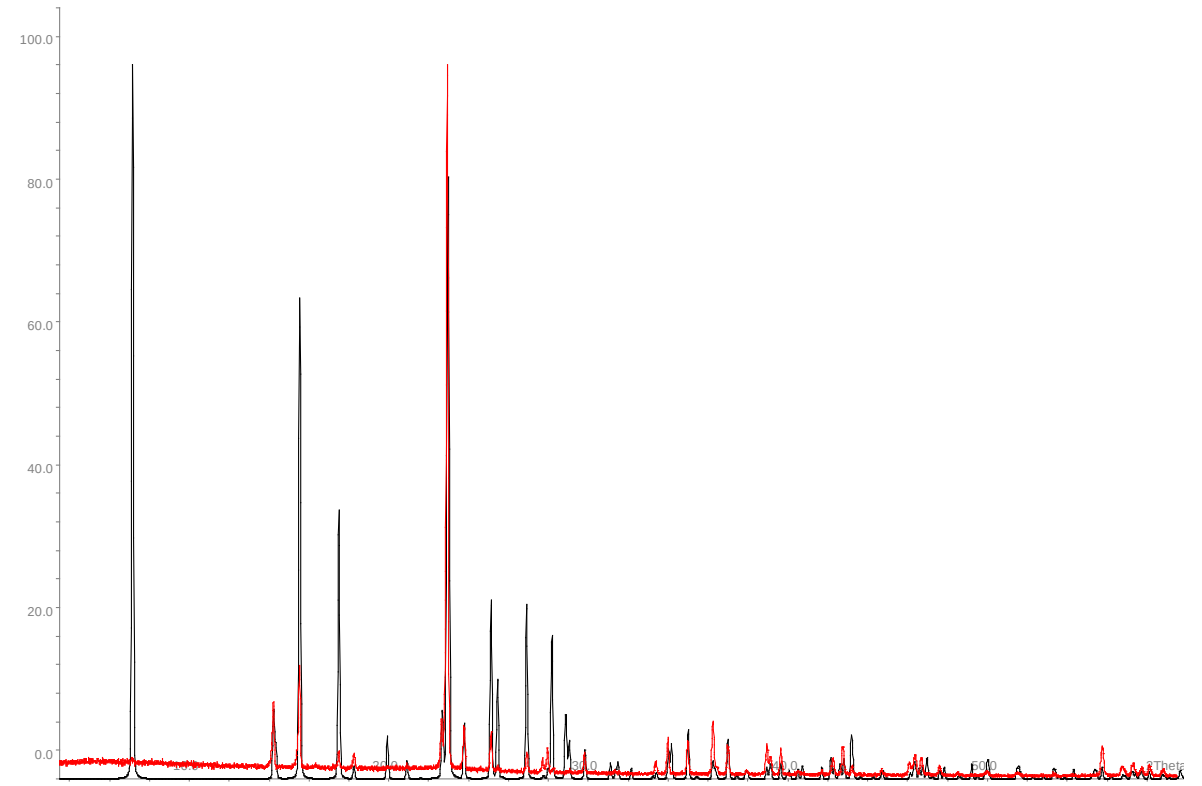


Analytical Data and Figures for (*R*)-*2*

IR spectra for **(*R*)-2**

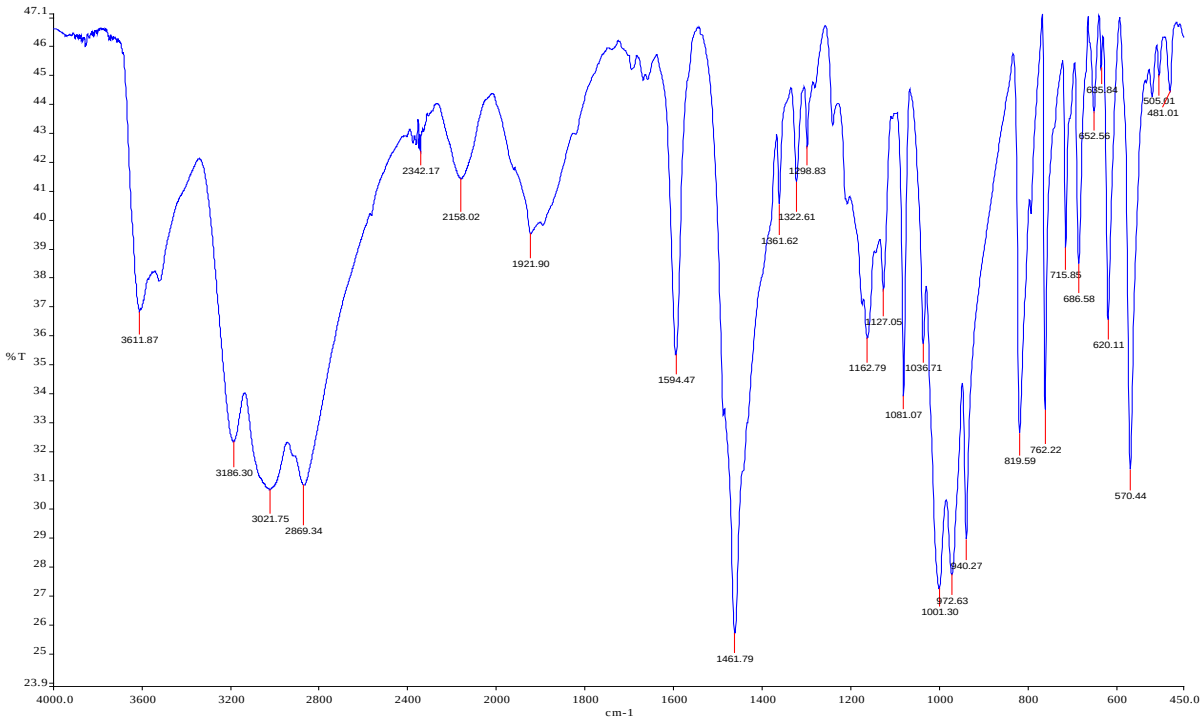


PXRD pattern of **(*R*)-2** obtained from solution crystallization (red) overlaid with theoretical pattern (black).

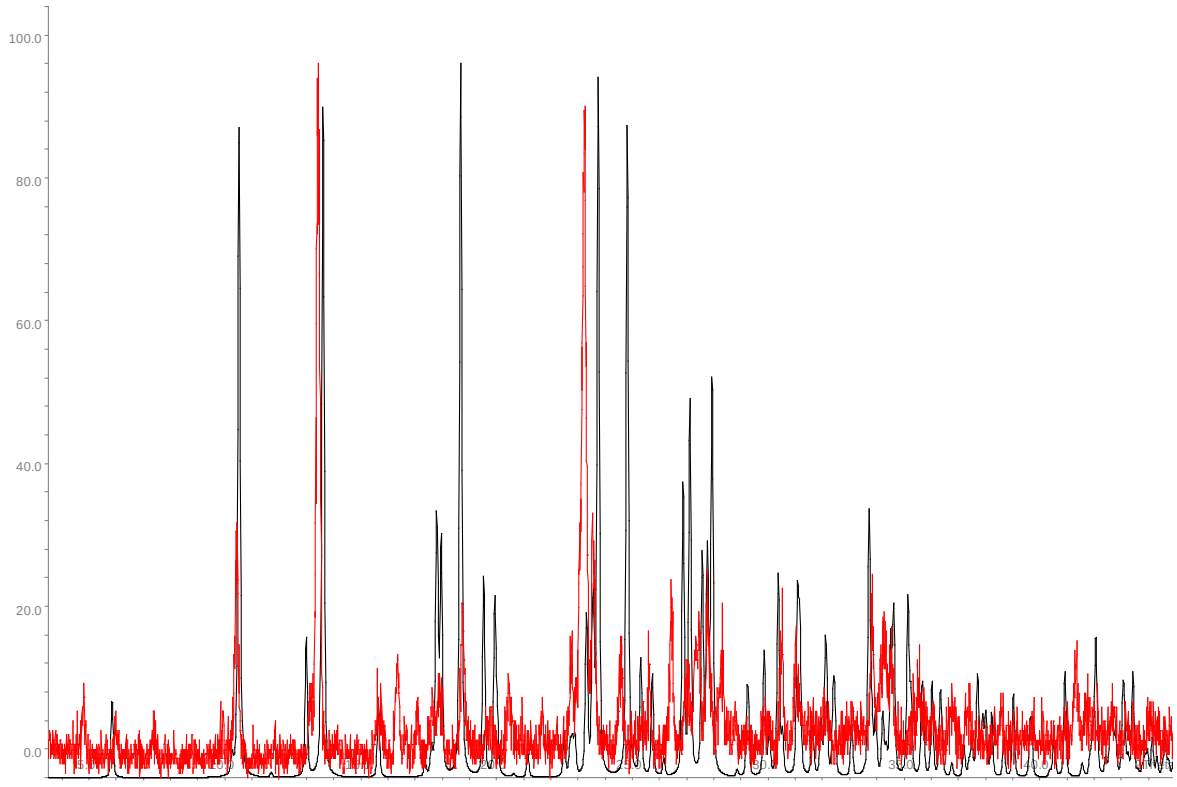


Analytical Data and Figures for 1.(*R*)-*2*

IR spectra for **1.(*R*)-2**



PXRD pattern of **1.(*R*)-2** obtained from solution crystallization (red) overlaid with theoretical pattern (black).



* The PXRD patterns contain minor impurities from both starting co-formers.

Intermolecular Interactions

Table 01. Details of the Hydrogen Bonding Interactions Observed in the Co-crystals

Cocrystal	Stoichiometry	Nature of interaction	Distance [a] (Å)	Angle at I (°)	Angle at O (°)	Number of donors to O
1.(±)-2	1:4	I···O	2.958(2)	176.63(11)	121.88(12)	1
1.(*S*)-*2*	1:1	I···O	2.767(5)	173.4(2)	123.6(3)	1

Table 02. Details of the Moderate Hydrogen Bonding Interactions Observed in the Starting Materials and Co-crystals

Cocrystal	Nature of interaction	Distance D-H (Å)	Distance H···A (Å)	Distance D···A (Å)	Angle (°)
(±)-2	N9–H9B···O8	0.88(3)	2.16(4)	2.981(4)	156.(4)
	N9–H9A···O8	0.82(3)	2.20(3)	2.966(4)	155.(4)
(*S*)-*2*	N9–H9A···O8	0.838(17)	2.198(17)	3.021(3)	168.(3)
	N9–H9B···O8	0.94(3)	2.05(3)	2.947(3)	160.(2)
1.(±)-2	N25–H25B···O14	0.89(4)	2.15(4)	3.024(5)	167.(3)
	N25–H25A···O14	0.85(4)	2.45(4)	3.210(4)	150.(4)
	N15–H15A···O24	0.872(18)	2.14(2)	2.994(4)	168.(3)
	N15–H15B···S23	0.886(19)	2.93(3)	3.580(3)	132.(3)
	N15–H15B···O24	0.886(19)	2.12(3)	2.921(4)	150.(4)
1.(*S*)-*2*	N21–H21A···O20	0.81	2.27	2.905(8)	135.6