

Polymorphism in cocrystals of urea : 4,4'-bipyridine and salicylic acid : 4,4'- bipyridine

Srinu Tothadi

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India.

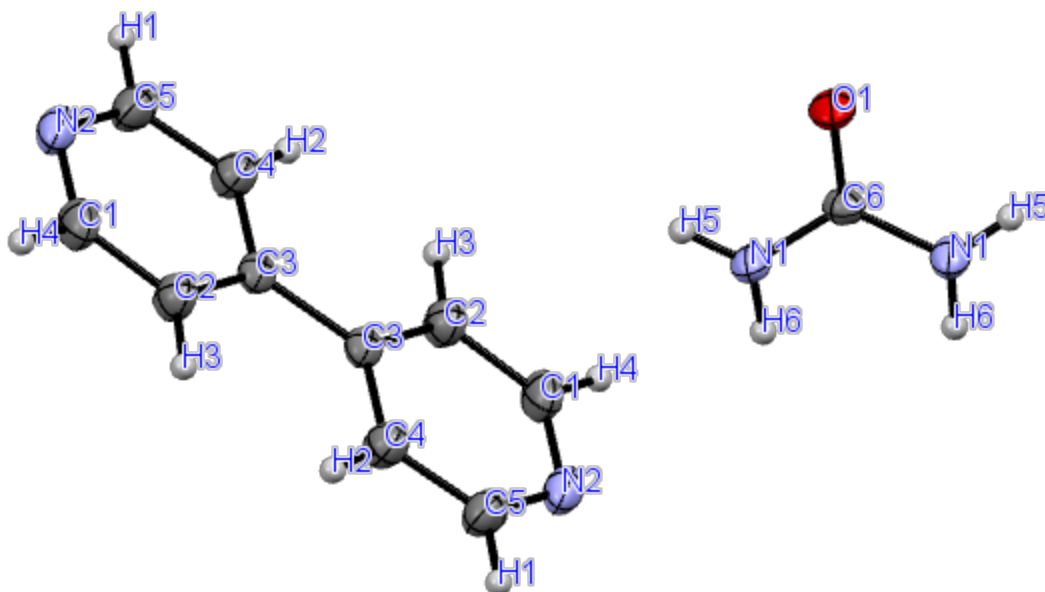
Supporting Information

Content

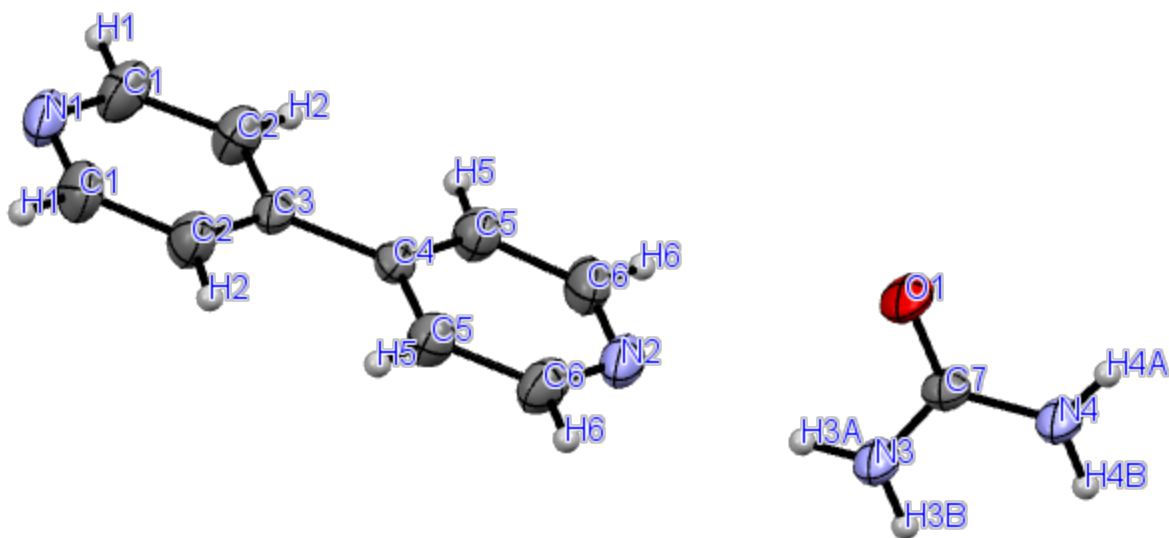
1	ORTEP diagrams (All atoms in molecular structure showing 50% probability displacement ellipsoids)	Page S2
2	Packing polymorphs of Form IB and form IIB	Page S4
3	Cocrystal polymorphs with 4,4-bipyridine	Page S5

1. ORTEP diagrams (All atoms in molecular structure showing 50% probability displacement ellipsoids)

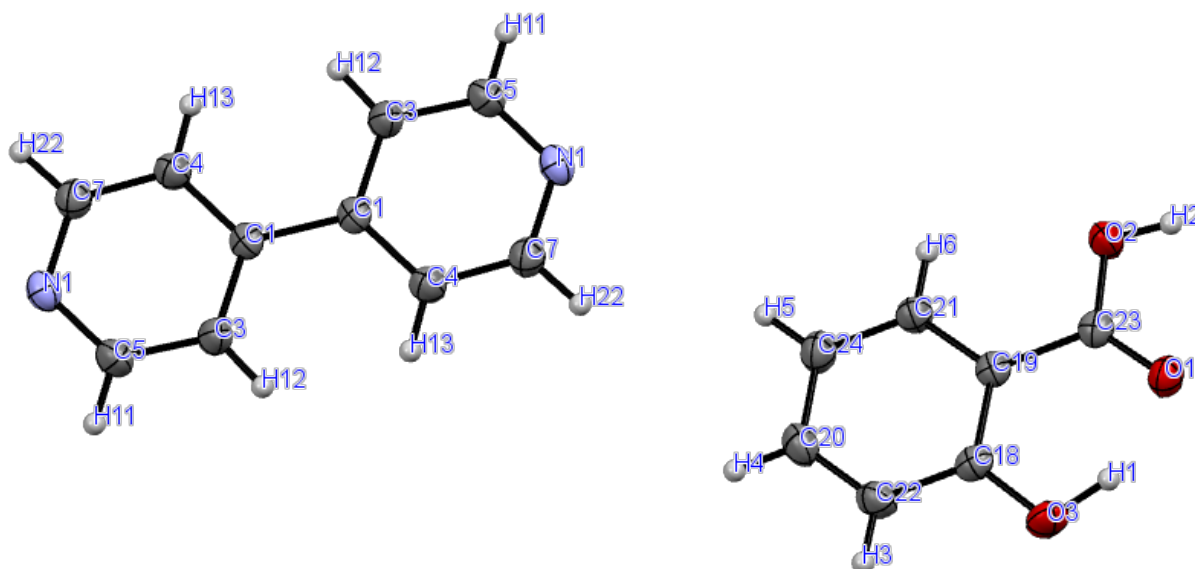
1. Urea : 4,4'-bipyridine polymorphic cocrystals Form IA (1)



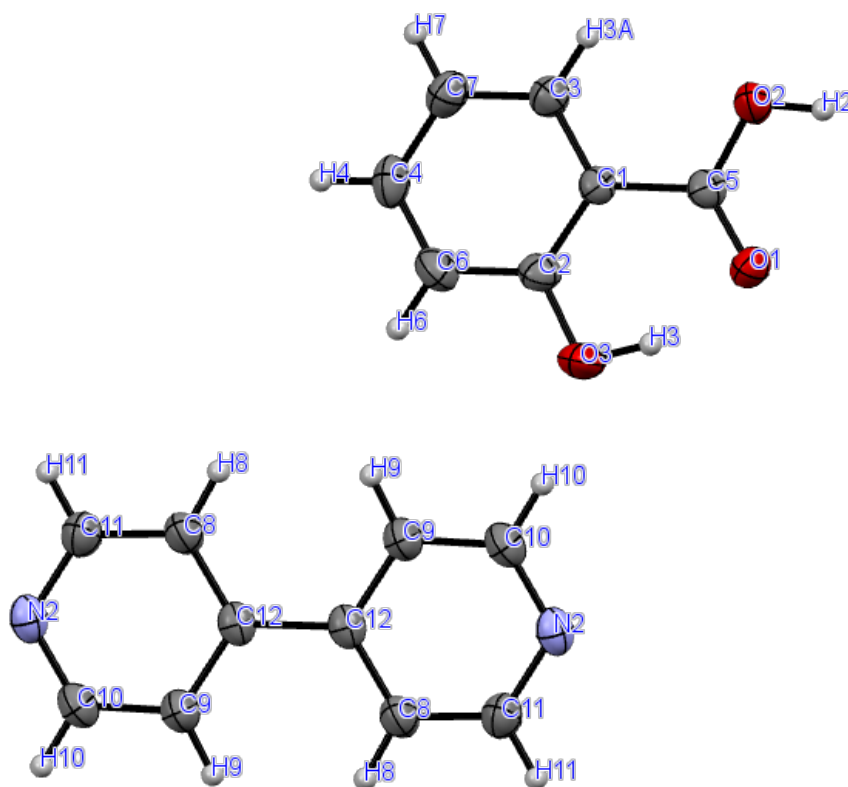
2. Urea : 4,4'-bipyridine polymorphic cocrystals Form II A (2)



3. Salicylic acid and 4,4'-bipyridine cocrystal Form I B (3)



4. Salicylic acid : 4,4'-bipyridine cocrystal Form II B (4)



2. Packing polymorphs of Form IB and form IIB

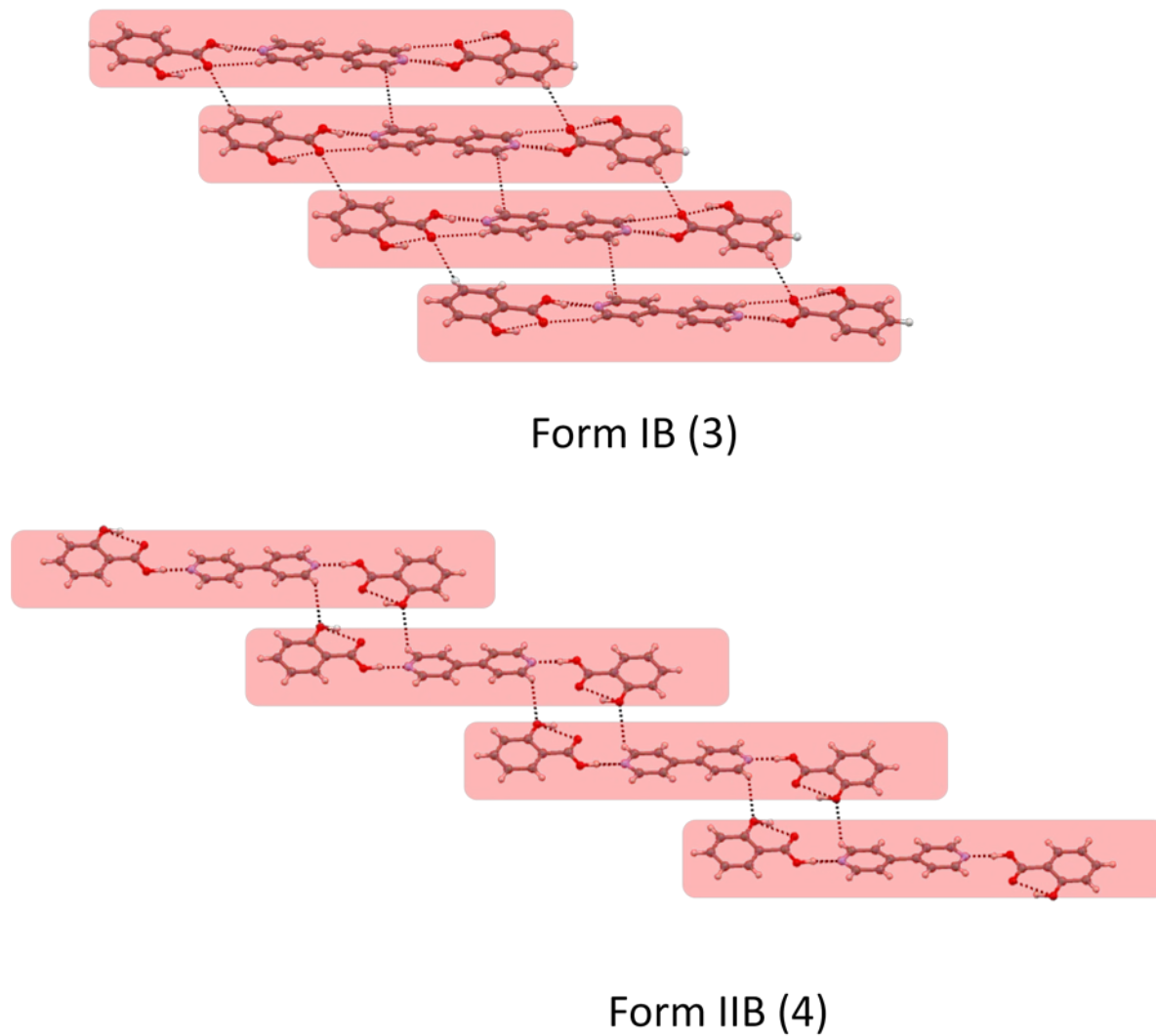


Figure S1. Trimers are obtained with two of salicylic acid and one of 4,4'-bipyridine. Notice Form IIB slides more compare form IB.

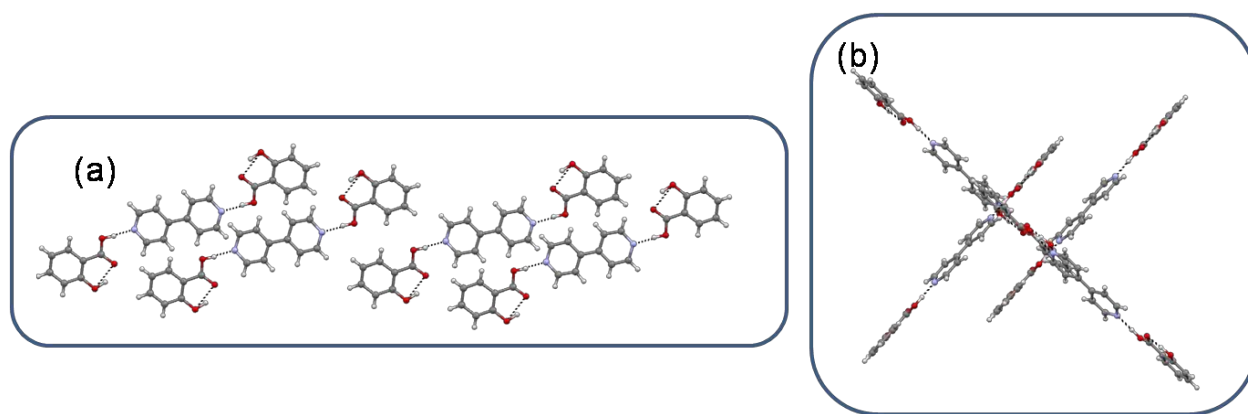


Figure S2. Trimers (a) Parallel in Form IB (b) perpendicular in Form IIB along the c-axis

Table S1. Cocrystal polymorphs with 4,4'-bipyridine

Cocrystal Dimorphs	Cocrystal Trimorphs	Cocrystal quartermorphs
EPUPUB	MACCID	UBUJIM
EPUPUB01	MACCID01	UBUJIM01
ELEGUY	MACCID02	UBUJIM02
ELEGUY01	XOLHUC	UBUJIM03
	XOLHUC01	UBUJIM04
	XOLHUC02	

Polymorphic cocrystal structures with 4,4'-bipyridine are obtained when CSD analysis was carried out with some constrains (must have 4,4'-bipyridine and minimum two different chemical components in the unit cell. 3D coordinates determined, no errors, no ions and only organic structures). Considering Refcodes and cell parameters, manually separated above listed polymorphs from a total of 299 structures.