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Proton-Displacive Ferroelectricity in Neutral Cocrystals of Anilic Acids with Phenazine

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Contents: Hydrogen-Bonded Parameters, Molecular Geometry, and Infrared Absorption Spectra of Phz-H_2xa Cocrystals

Table S1. Hydrogen-bond parameters of co-crystals at room temperature.

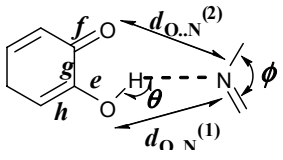
Cocrystal	$d_{O\cdots N}^{(1)}$/Å	$d_{O\cdots N}^{(2)}$/Å	θ(°)	Dihedral angle φ (°)	Ref.
Phz-H_2ca (α)	2.724(2)	3.461(2)	132	44.42(2)	1
Phz-D_2ca (α)	2.732(3)	3.474(3)	138	44.32(3)	1
Phz-H_2ba (α)	2.744(5)	3.421(4)	138	44.57(5)	1
Phz-D_2ba (α)	2.757(4)	3.437(3)	119	44.53(4)	1
Phz-H_2ba (β)	2.670(4)	2.996(5)	155	86.99(5)	†
Phz-H_2fa (α)	2.697(2)	3.410(2)	150	45.63(2)	†
Phz-H_2fa (γ)	2.672(2)	3.136(3)	155	68.73(4)	†
Phz-H_2ia (β)	2.675(4)	2.967(5)	159	88.37(4)	†

Table S2. Molecular geometry at hydrogen bonding sites in co-crystals.

Neutral crystals	C−OH	C=O	C−C	C=C		Ref.
H_2fa	1.334	1.215	1.496	1.332		2
H_2ca	1.322	1.222	1.501	1.346		3
H_2ba	1.323	1.225	1.504	1.347		4
H_2ia	1.327	1.223	1.508	1.345		5
Co-crystals	Geometry for OH···N form					
	e/Å	*f*/Å	*g*/Å	*h*/Å	ϕ/deg	
Phz-H_2ca (α)	1.305(2)	1.229(3)	1.508(3)	1.355(3)	118.3(1)	1
Phz-D_2ca (α)	1.304(3)	1.215(4)	1.514(4)	1.352(4)	118.0(2)	1
Phz-H_2ba (α)	1.313(5)	1.222(7)	1.514(6)	1.348(7)	117.9(4)	1
Phz-D_2ba (α)	1.314(3)	1.212(5)	1.524(5)	1.342(5)	118.4(3)	1
Phz-H_2ba (β)	1.313(6)	1.221(4)	1.507(6)	1.347(5)	118.5(3)	†
Phz-H_2fa (α)	1.315(2)	1.220(2)	1.499(2)	1.346(2)	117.9(1)	†
Phz-H_2fa (γ)	1.330(3)	1.227(3)	1.482(4)	1.341(3)	118.4(2)	†
Phz-H_2ia (β)	1.317(5)	1.217(4)	1.519(5)	1.346(5)	118.1(3)	†

†this work

See right for definition of geometry parameters.



Reference

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