Electronic Supplementary Material for CrystEngComm

Supplementary Information: Halogen···oxygen aggregation and disorder modes in pressure frozen XCF_2CF_2X:1,4-dioxane (X=Br,I) complexes

Anna Olejniczak[a], Andrzej Katrusiak[a]* and Ashwani Vij[b]

[a]*Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland. E-mail: katran@amu.edu.pl*

[b]*AFRL/RZSP, Edwards Air Force Base, 10 E. Saturn Blvd, Bldg. 8451. CA, 93524, USA. E-mail: ashwani.vij@edwards.af.mil*

Table S1. Selected crystal data and details of structure refinement for the $ICF_2CF_2I:C_4H_8O_2$ and $BrCF_2CF_2I:C_4H_8O_2$ cocrystals, and for $C_4H_8O_2$.

Compound		$ICF_2CF_2I:C_4H_8O_2$	$BrCF_2CF_2I:C_4H_8O_2$	$C_4H_8O_2$
Pressure (GPa)		0.30(5)	0.62(5)	0.42(5)
Temperature (K)		296(2)	296(2)	296(2)
Formula weight		441.92	394.93	88.10
Wavelength (Å)		0.71073	0.71073	0.71073
Crystal system		Trigonal	Monoclinic	Monoclinic
Space group		$R\bar{3}$	$P2_1/c$	$P2_1/n$
Unit cell dimensions (Å,°)	a	8.838(1)	9.5983(19)	5.6590(10)
	b	8.838(1)	5.9716(12)	6.4100(10)
	c	13.532(3)	9.784(2)	5.8920(10)
	β		107.41(3)	98.36(3)
Volume ($Å^3$)		915.4(3)	535.13(19)	211.46(6)
Z		3	2	2
Calculated density (g/cm^3)		2.405	2.451	1.384
Absorption coefficient (mm^{-1})		5.180	6.755	0.110
F(000)		606	368	96
Crystal size (mm)		0.43/0.43/0.09	0.47/0.47/0.08	0.30/0.30/0.09
θ-range for data collection (°)		3.06 to 29.53	4.05 to 29.31	4.83 to 29.59
Min/max indices: h, k, l		-11/12, -11/12, -8/8	-5/5, -8/8, -13/13	-6/6, -8/8, -4/4
Reflect. coll./ unique (Rint)		1688/237 (0.1380)	3961/455 (0.0663)	1696/180 (0.1265)
Completeness (to θmax) (%,°)		40.7 (to 29.53)	31.0 (to 29.31)	30.4 (to 29.59)
Refinement method		Full-matrix least-squares on F^2		
Data/restrains/ parameters		237/0/39	455/0/64	180/0/29
Goodness-of-fit on F^2		1.440	1.196	1.416
Final R_1/wR_2 ($I>2\sigma_1$)		0.1335/0.3502	0.0700/0.1584	0.1784/0.3250
R_1/wR_2 (all data)		0.1451/0.3668	0.0814/0.1651	0.2073/0.3400
Weighting scheme		$w=1/(\sigma_2(Fo^2)+(0.2000*P)^2+0.00*P)$, where $P=(Max$	$w=1/(\sigma_2(Fo^2)+(0.0643*P)^2+4.19*P)$, where $P=(Max(Fo^2,0)+2*Fc^2$	$w=1/(\sigma_2(Fo^2)+(0.0757*P)^2+1.15*P)$, where $P=(Max(Fo^2,0)+2*Fc^2$

	$(Fo^2,0)+2*Fc^2)/3$	)/3	)/3
Largest diff. peak and hole ($e.Å^{-3}$)	0.380/-1.017	0.504/-0.357	0.180/-0.264

Table S2. The shortest contacts in the structure of phase II of 1,4-dioxane at 0.42 GPa/296 K.

	C4H8O2
p (GPa)/T (K)	0.42/296
O···Hi (Å)	2.655
O···Hii	2.672
C-O···Hi (°)	88.35
C-O···Hii	86.06

Symmetry codes: i: 0.5+x, 1.5-y, 0.5+z; ii: 1.5-x, 0.5+y, 0.5-z