Electronic Supplementary Material (ESI) for CrystEngComm

Diiodoacetylene: compact, strong ditopic halogen bond donor

Catherine Perkins,† Stefano Libri, Harry Adams and Lee Brammer*

Department of Chemistry, University of Sheffield, Brook Hill, Sheffield S3 7HF, UK. Email: lee.brammer@sheffield.ac.uk

Supporting Information

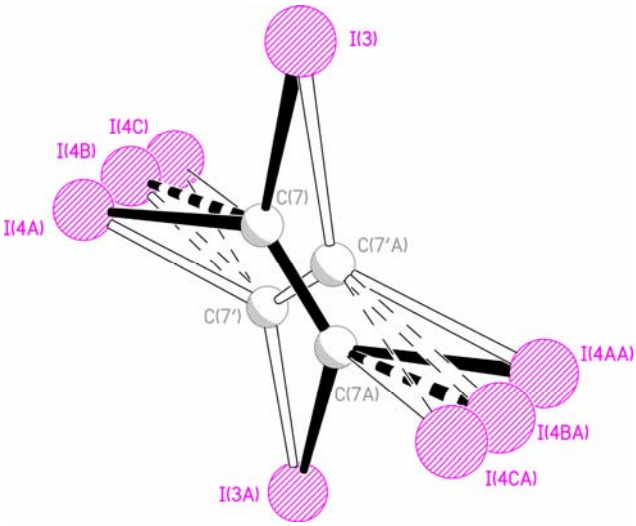

Figure S1. Disorder in one of the two indepenent C_2I_4 molecules of C_2I_4·hmta (**4**). The molecule is situated on a crystallographic inversion centre. Atoms I3 and I3a are involved in C–I···N halogen bonds as depicted in Figure 4.

The C_2I_4 groups shown in Figure S1 lies on an inversion centre and is rotationally disordered about two non-crystallographic axes. Disorder about the normal to the plane of the alkene leads to two orientations rotated by approximately 90 °, in which the four iodine atoms involved remain fixed in an approximate square arrangement (here C7, C7a, I3, I4a, I3a, I4aa in one orientation and C7', C7'a, I3, I4a, I3a, I4aa in the other). The molecule is also rotationally disordered about the I3···I3a axis. Three orientations represented by pairs of iodine atoms I4a/I4aa (58.8(5) % occupancy), I4b/I4ba (11.5(5) %) and I4c/I4ca (27.4(5) %) have been identified and the unique atoms are included in the model. The contribution from the carbon atoms is modelled simply by the atoms C7 and C7' (C7a, C7'a). This model is similar, but not identical to that described by Walsh et al., who report the same adduct with very similar unit cell dimensions, but in space group *C*2/*m*.[S1]

Table S1 Halogen bonding interactions for adducts formed by C_2I_4

CSD REFCODE	**1st independent C_2I_4 molecule**		**2nd independent C_2I_4 molecule**	
	Interactions with other molecules	Interactions with C_2I_4 molecules	Interactions with other molecules	Interactions with C_2I_4 molecules
BERZED	2 C–I···N	2 C–I···I–C		
IETPYA10	2 C–I···N	2 C–I···I–C		
IHUNEE	2 C–I···N	2 C–I···I–C		
QIHBIS	2 C–I···N	2 C–I···I–C		
QIHCEP	2 C–I···N	2 C–I···I–C		
WOJQAN	2 C–I···N	2 C–I···I–C		
WOJQER	2 C–I···N	2 C–I···I–C		
WOJQIV	2 C–I···N	2 C–I···I–C		
WOJQOB	2 C–I···N	2 C–I···I–C		
WOJQUH	2 C–I···N	2 C–I···I–C		
QOJKIJ	2 C–I···O	2 C–I···I–C		
EDAGOF	2 C–I···S	2 C–I···I–C		
EHOGUR	3 C–I···Br^-	1 C–I···I–C		
EHOGUD	2 C–I···S 1 C–I···N	1 C–I···I–C		
NUSCEK	4 C–I···S	none	2 C–I···S	2 C–I···I–C
EHOGOX	4 C–I···I^-	none	2 C–I···I^- 2 non-interacting	none
4 (current work) / QIHCUF (ref. S1)	4 C–I···N	none	2 C–I···N	2 C–I···I–C
XOZBUJ	3 C–I···S 1 C–I···S (v. long)	none	2 C–I···N	2 C–I···π(C_2I_4)
IHUMON	2 C–I···N 2	none		

	C–I···π(arene)			
DARZOM	4 C–I···N	none		
SIVXUR	4 C–I···Cl^-	none		
PAVZUH	4 C–I···Cl^-	none		
PAWBAQ	4 C–I···Br^-	none		
PAWBOE	4 C–I···Br^-	none		
PAWBUK/PAWBUK01	4 C–I···I^-	none	2 C–I···I^- 2 C–I···Br^-	none
SIVXOL	4 C–I···I^-	none	2 C–I···I^- 2 C–I···Br^-	none
SIVXIF	4 C–I···I^-	none		
RAMPAW	4 C–I···I(Pb)	none		

References

S1. R. B. Walsh, C. W. Padgett, P. Metrangolo, G. Resnati, T. W. Hanks and W. T. Pennington, *Cryst. Growth Des.*, 2001, **1**, 165.