Electronic Supplementary Material for CrystEngComm

Supplementary Information: Isostructural relations in dihalomethanes and disproportionation of bromoiodomethane

Marcin Podsiadło[a] and Andrzej Katrusiak[a]*

[a]*Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland.*

*E-mail: katran@amu.edu.pl

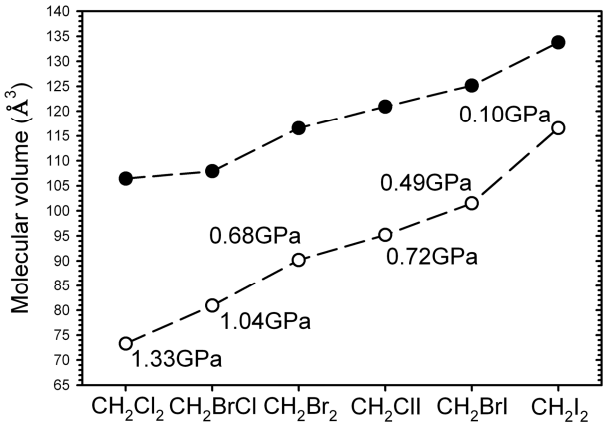

Figure S1. Molecular volume as a function of pressure for dihalomethanes. Full circles represent data calculated at 295 K/0.10 MPa, while open ones those measured at freezing pressures.

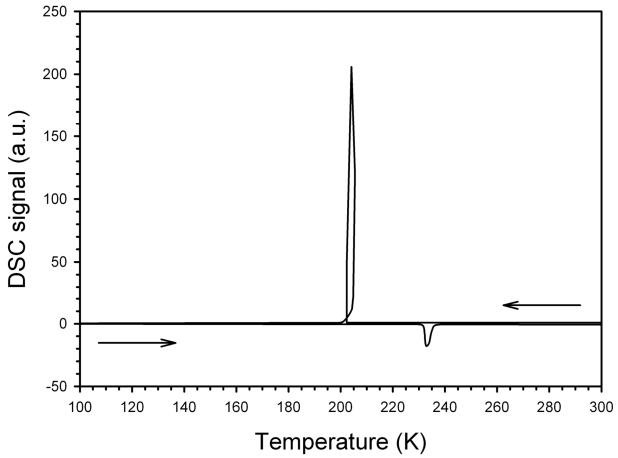

Figure S2. Differential scanning calorimetry thermograph for 6.78mg of CH_2BrI performed in the 300–100 K range with a rate of 10 K·min^{-1}. The arrows indicate the direction of the temperature changes.

Table S1. Atomic coordinates ($\cdot 10^4$), U_{eq} and U_{iso} ($Å^2 \cdot 10^3$) for CH_2BrI and CH_2I_2 phase II.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}/U_{iso}
CH_2BrI at 220 K				
I1/Br1	945(1)	6690(2)	1319(1)	52(1)
I2/Br2	3547(1)	6451(2)	1290(1)	52(1)
C1	2111(8)	4279(2)	1069(2)	52(3)
H1	1753(2)	3501(9)	407(3)	63
H2	2305(2)	2403(2)	1460(3)	63
CH_2BrI at 100 K				
I1/Br1	925(1)	6803(1)	1311(1)	23(1)
I2/Br2	3559(1)	6587(2)	1289(1)	24(1)
C1	2132(5)	4241(2)	1072(2)	30(2)
H1	1757(2)	3625(10)	381(3)	36
H2	2352(2)	2537(3)	1548(3)	36
CH_2BrI at 0.54 GPa				
I1/Br1	880(1)	6780(1)	1295(1)	53(1)
I2/Br2	3541(1)	6561(1)	1304(1)	53(1)
C1	2082(5)	4280(1)	1069(2)	63(10)
H1	1772(2)	3478(10)	389(4)	75
H2	2280(2)	2409(2)	1491(3)	75
CH_2I_2 at 0.80 GPa				
I1	0	1376(1)	2665(1)	45(3)
C1	0	0	-288(2)	64(93)
H1	1328(1)	0	-1138(2)	84