Halogen⋯halogen contra C–H⋯halogen interactions†

Marcin Podsiadlo, Anna Olejniczak and Andrzej Katrusiak*

Pressure affects the competition between C–H⋯X hydrogen bonds and X⋯X halogen⋯halogen interactions. In bromomethane, CH3Br, pressure changes the molecular arrangement of the two solid-state phases of this compound: low-pressure phase α is dominated by halogen⋯halogen interactions, whereas above 1.5 GPa the β phase is governed by C–H⋯halogen bonds. The CH3Br phase α is isostructural with solid CH3I of orthorhombic space group Pnma, while CH3Br phase β is polar, isostructural with CH3Cl and CH3CN crystals, of orthorhombic space group Cmca. The crystal structures of CH3Cl (b.p. = 249.1 K) and CH3Br (b.p. = 276.7 K) have been determined by high pressure single-crystal X-ray diffraction up to 4.38 GPa and 2.85 GPa, respectively. In CH3Br, pressure of 1.5 GPa enforces the close packing and opposite electrostatic-potential matching between molecular surfaces in contact. The interwoven C–H⋯X bonded diamondoid networks of β-CH3X are similar to those of acetonitrile, H2O ice VII and solidified X2 halogens. The phase diagrams of CH3Br and CH3Cl have been constructed.

Introduction

The molecular arrangement in crystals is most often associated either with Kitaigorodski’s close packing rule or with specific intermolecular interactions, such as OH⋯O hydrogen bonds in H2O ice. Even weak specific interactions, such as halogen⋯halogen,1–3 halogen⋯O4–5 and CH⋯O contacts,6 can compete between themselves7,8 and with the close packing rule.9 Members of the group of halomethanes (CH3X, X = Cl, Br, I) are the simplest organic polar compounds and ideal models for studying weak halogen⋯halogen and C–H⋯halogen interactions. In many molecular crystals without strong hydrogen bonds the X⋯X and C–H⋯X interactions dominate the molecular arrangement and are the shortest intermolecular contacts in the crystal structure.10 Pressure can considerably modify the intermolecular interactions in crystals. It was evidenced that weak hydrogen bonds CH⋯O11–13 and CH⋯N14 significantly increase their role in high-pressure structures. For example, formamide15 and (+)-sucrose16 transform at high pressure as a result of the increased role of CH⋯O interactions, in sucrose competing with OH⋯O bonds. The competition between halogen⋯halogen and C–H⋯X halogen interactions was studied for a series of six dihalomethanes CH2XY (X, Y = Cl, Br, I). They crystallize in several structural types of space group Pbcn (CH2Cl2, CH2BrCl phase II), C2/c (CH3Br2, CH3I2 phase I, CH2BrCl phase I, CH2BrI), Pnma (CH3ClI phase III), Pna21 (CH3ClI phase IV) and Fmm2 (CH3I2 phase II).17–22 In all of these compounds and their polymorphs, halogen⋯halogen interactions persist despite considerable structural differences. However, the persistence of halogen⋯halogen contacts in dihalomethanes can be due to the geometric effect of at least two-thirds of the molecular surface (for CH3ClI) belonging to the halogen atoms. In these structures, even if other contacts are preferred and formed, the halogen⋯halogen contacts would be formed simply for there is no other molecular surface available. In methyl halides, of general formula CH3X, there is one halogen atom per molecule (hence its molecular surface is smaller than those of CH2X2 and CHCl3) and the competition between C–H⋯X and X⋯X interactions is more apparent. Therefore we have studied the structures of methyl halides in order to determine the effect of pressure on X⋯X and H⋯X interactions. CH3Cl and CH3Br are gases under normal conditions, which required that a special technique be developed and employed for loading these gases into the diamond-anvil cell (DAC).

The low-temperature/ambient-pressure CH3Br and CH3I crystals are isostructural, of the orthorhombic space group Pnma,23,24 while the CH3Cl crystal has a different structure, of the orthorhombic space group Cmca.25 At room temperature the Pnma-symmetric CH3I structure is stable up to at least 2.5 GPa.26 No polymorphs or phase transitions were detected in CH3Cl and CH3I at low temperature, while calorimetric measurements indicated that CH3Br undergoes a first-order phase transition at 173.75 K.27 The Raman and far infrared spectra showed that the deuterated analogue, CD3Br, transforms at 158 K, about 16 K below the transition of CH3Br.28 The crystal structures of CD3Br in both its phases were determined by neutron powder diffraction at 175 K and 146 K.29 We have
presently established that in that study the high- and low-temperature phases were confused. Initially, the sample had been kinetically flash-frozen and cryo-ground in the temperature and atmosphere of liquid nitrogen. In accordance with Ostwald’s rule the sample crystallized in the high-temperature phase $\alpha$ and at 146 K it was metastable throughout data collection. This $\alpha$-phase determined at 146 K was of the orthorhombic space group $Pnma$. Then the sample had transformed to the low-temperature $\beta$ phase before it was warmed to 175 K, i.e. 17 K above the transition temperature of CD$_3$Br at 158 K. Again, the $\beta$ phase remained metastable under these conditions for the duration of powder data collection at least. Thus incidently at higher temperature the crystal structure of low-temperature phase $\beta$ was determined. This $\beta$-phase is of the orthorhombic space group $Cmc2_1$. Consequently, in that previous study the persistence of crystal phases in their metastable regions caused the reversed assignment of high- and low-temperature phases $\alpha$ and $\beta$, respectively.\textsuperscript{29}

The phase diagrams of CH$_3$Br and CH$_3$Cl presently outlined in our study are shown in Fig. 1. These phase diagrams of CH$_3$Cl and CH$_3$Br have similar melting and boiling boundaries, shifting slightly toward lower temperature and higher pressure for CH$_3$Cl. In this respect, the transition of CH$_3$Br between solid phase $\alpha$, isostructural with the crystal of CH$_4$, and phase $\beta$, isostructural with CH$_3$I, is particularly intriguing. The crystal structure of perdeuterated methyl fluoride, CD$_3$F, determined by neutron powder diffraction at 5 K, is of the monoclinic space group $P2_1/n$ and is distinctly different from other methyl halides.\textsuperscript{30} Presently, we have extended the structural relationship and phase diagrams of CH$_3$Cl and CH$_3$Br into the high-pressure region (Fig. 1) and investigated the role of X⋯X and C−H⋯X interactions in the CH$_3$X structures and CH$_3$Br transformations.

**Experimental**

Chloromethane, CH$_3$Cl (m.p. 175.5 K, b.p. 249.1 K), and bromomethane, CH$_3$Br (m.p. 179.5 K, b.p. 276.7 K), of 99.5% purity from Sigma-Aldrich were used. For high-pressure studies they were loaded into a modified Merrill-Bassett\textsuperscript{31} diamond-anvil cell (DAC) by combining compression and cryogenic conditions and in situ crystallized. At 295 K, CH$_3$Cl froze at 0.78 GPa and CH$_3$Br at 0.65 GPa in the form of a polycrystalline mass, filling the whole volume of the high-pressure chamber. The single crystals of CH$_3$Cl and CH$_3$Br (Fig. 2) were obtained under isochoric conditions: the DAC with the polycrystalline mass was heated with a hot-air gun till all but one grain melted. Then the DAC was slowly cooled to room temperature and the single crystal grew and eventually filled the entire volume of the chamber. The experimental details and progress of growing the single crystals of CH$_3$Cl are shown in Fig. S1–S4\textsuperscript{†} and of CH$_3$Br in S5–S9 in the ESI\textsuperscript{†}.

Diffraction data were collected at 295 K using a KUMA KM4-CCD diffractometer with graphite-monochromated MoK$_\alpha$ radiation.\textsuperscript{32} The CrysAlisCCD and CrysAlisRED programs\textsuperscript{33} were used for the data collection and determination of the $UB$ matrix and for the initial data reduction and $Lp$ corrections for both compounds. The intensity of reflections has been accounted for by the absorption of X-rays by the DAC, sample shadowing by the gasket, and absorption of the sample crystal itself.\textsuperscript{34,35} The crystal structures of CH$_3$Cl and CH$_3$Br were solved by direct methods. H atoms were located from molecular geometry, in $\alpha$-CH$_3$Br the disordered model
was applied (Shelxl instruction AFIX 137), and the structures were refined with anisotropic C and X atoms. Details of the experiments, structure refinements and crystal data are given in the ESL†

The program GAUSSIAN03 and a PC were used with the B3LYP/3-21G** level of theory for DFT calculations of the electrostatic potential on the surface of CH₃X molecules. Electrostatic potential was mapped onto the molecular surfaces defined as 0.001 a.u. electron-density envelope.

**Discussion**

Isobaric and isothermal freezing of halomethanes CH₃X leads to the same crystalline phases. At 295 K, CH₃Cl and CH₃I crystallize at 0.78 and 0.41 GPa, respectively, in their low-temperature/0.1 MPa phases of CH₃Cl and CH₃I and they are stable within the investigated pressure range. At 295 K, CH₃Br freezes at 0.65 GPa in phase α (space group Pnma) and at 1.50 GPa it transforms to phase β (space group Cmc2₁). At this transition the unit-cell volume decreases by −4.7 Å³ (−1.9%) (Fig. 3).

Two main molecular-association types conform to the opposite electrostatic-potential matching principle. In CH₃X molecules the negative electrostatic potential (Fig. 4) is on the rim about the C–X bond, the more positive potential region is on the “caps” of the X atom at the extension of the C–X bond and the highest potential is around the H-atoms. The electrostatic potential magnitude and the area at the extension of C–X bonds increase from F to I (Fig. 4).

Fig. 3 The molecular volume (unit cell V) as a function of pressure of CH₃Cl (green), CH₃Br (red) and CH₃I (purple). Symmetry Cmc2₁ is indicated by circles and Pnma by squares. The red dashed vertical line marks the transition between CH₃Br phases α and β. Low temperature/0.1 MPa data from ref. 23–25; 295 K/high pressure data of CH₃I from ref. 26. The dashed lines between the low-temperature/0.1 MPa and 295 K/high-pressure points are for guiding the eye only.

Fig. 4 (a) Molecules CH₃F, CH₃Cl, CH₃Br and CH₃I as well as their surfaces with electrostatic potential colour scale, common for all drawings and ranging from ~0.015 (red) to 0.015 a.u. (blue); (b) the electrostatic potential magnitude on the surface of the methyl H-atoms and at the polar caps of the halogens plotted against the minimum potential in all CH₃X surfaces located on the rim of halogen atoms. Symbols δ₊H and δ₊X denote the maximum electrostatic potential magnitudes on the surface of H and X atoms, respectively.

Based on the electrostatic-potential magnitudes (Fig. 4), the halogen···halogen interactions in CH₃I are stronger than those in CH₃Br and those in CH₃Cl are still weaker. Indeed, the CH₃I structure is governed by I···I contacts, and no Cl···Cl but C–H···Cl contacts are formed in CH₃Cl.

The positive electrostatic potential on the halogen atom polar region of the molecular surface can act like H-donors in hydrogen bonds. Fig. 4 shows that the magnitude of polar electrostatic potential of the iodine atom is approximately twice as high as that of bromine and that no positive polar potential exists in CH₃Cl. This is consistent with the strongest preference for the X···X bonds in CH₃I and in CH₃Br.

The electrostatic potential of the H atoms is higher than that of the I atoms and approximately equal for all CH₃Cl, CH₃Br and CH₃I. A large contribution to the X···X interactions arises
from the polarizability of halogen atoms. This contribution to dispersion forces between Cl⋯Cl, Br⋯Br and I⋯I atoms is equal to −2.5, −3.2 and −4.9 kJ mol⁻¹, respectively. Thus the high positive potential at the polar region of the iodine atom and the strongest dispersion forces of I⋯I interactions favour the halogen⋯halogen bonds in CH₃I. The lower positive potential of Br and the weaker dispersion interactions make the Br⋯Br bonds less competitive. Pressure reverses the balance between the two polymorphs of CH₃Br and it can be argued that it enforces the most efficient involvement of all H-donors in the compressed structure. This pressure effect was observed in sucrose,¹⁶ acetonitrile¹⁴ and formamide.¹⁵

Halomethanes CH₃X crystallize either in space group Cmc2₁ or in space group Pnma. Although the space-group symmetries are different, the CH₃X structures have much in common (Fig. 5): the unit cells are roughly similar (after exchanging axes [x] and [y]; cf. Tables 1 and S1 and S2 in the ESI¹), four molecules in the unit cells are located on the mirror planes, and the molecular arrangements in both these symmetries approximate the prototypical orthorhombic symmetry Cmca of isostructural Cl₂, Br₂ and I₂ crystals.³⁹,⁴⁰ This subgroup–group relationship results from the symmetry of halomethane molecules, C₃v, lower than that of the dihalogen molecules, Dᵥ₄h. Fig. 5 shows that the prototypic Cmca symmetry is broken due to the antiparallel arrangement of molecules in α-CH₃Br and the parallel arrangement of molecules in β-CH₃Br. The encircled molecules in the plane perpendicular to [z] are all antiparallel in α-CH₃Br (Fig. 5a) and parallel in β-CH₃Br (Fig. 5b). Both these phases correspond to the prototypic Br₂ structure of higher space group symmetry Cmca, where the molecules are located on the inversion centres.

In phase α-CH₃Br, of space group symmetry Pnma, the molecular layers are linked by Br⋯Br interactions of type II.¹¹⁻¹³ The positive and negative regions of each bromine atom are electrostatically matched with its two Br neighbours in a zigzag chain (Fig. 5a). The C–Br⋯Br⁻⁻⁻⁻⁻Cl contacts are asymmetric, with the C–Br⋯Br angles close to 120° and 170° (see Table 2). Within the layers the electro-positive methyl groups are also arranged in a zigzag motif between the negative rims of the Br atoms in the neighbouring layers (Fig. 5).

In β-CH₃Br the halogen bonds Br⋯Br are broken and replaced by bonds C–H⋯Br (Fig. 5b, Table 2). Each CH₃Br molecule forms three C–H⋯Br bonds on the H-donor side and accepts three C–H⋯Br bonds around the Br atom. The molecules are arranged head-to-tail into two 3-dimensional interpenetrating (CH⋯Br)-bonded networks (Fig. 5b). Between these two networks the molecular parts of opposite electrostatic potential are closer than those of the same sign. The difference between phases α and β is most apparent in the ratio of Br⋯Br contacts contributin 5.5% to the overall Hirschfeld surface at low pressure and this contribution is reduced five-fold at high pressure to about 1%. This rearrangement causes a massive effect for the H⋯Br Hirschfeld-surface contributions, increasing from 49.6% at 1.11 GPa to 62.1% at 1.55 GPa. These changes in contributing Hirschfeld areas are compensated for in the reduced surface of H⋯H contacts of 44.9% and 36.9%, respectively.

**Table 1** Selected crystal data of CH₃X (X = Cl, Br, I) phases at their lowest pressure stability region at 295 K

|                  | CH₃Clᵇ | α-CH₃Brᵇ | β-CH₃Brᵇ | CH₃Brᵇ |
|------------------|--------|-----------|-----------|--------|
| Pressure (GPa)   | 0.53   | 1.11      | 1.55      | 1.22   |
| Space group      | Pnma   | Pnma      | Cmc2₁     | Cmc2₁  |
| Unit cell (Å)    | 4.4968(9) | 4.372(5) | 4.387(9)  | 4.314(10) |
| a                | 4.375(4) | 4.375(5) | 4.513(5)  | 4.531(5) |
| c                | 9.491(2) | 9.196(9) | 7.749(5)  | 7.334(9) |
| Volume (Å³)      | 305.83(11) | 256.3(4) | 247.1(5)  | 232.9(6) |
| Z                | 4      | 4         | 4         | 4      |

*a Ref. 26. b This work.*
Isobaric,25 isothermal and isochoric crystallization of CH3Cl all lead to the same phase isostructural with β-CH3Br. It is apparent that weaker Cl⋯Cl interactions are overcome by C–H⋯Cl bonds (see Table 3) and no Pnma-symmetric polymorph is formed. The CH3Cl structure is consistent with the chlorophobic rule.44,45

It is remarkable that CH3Br phase β is isostructural with the high-pressure acetonitrile phase β.14 The CH3Br and CH3CN molecules are similar in shape and in the electrostatic potential distribution on the molecular surface (except the polar Br-atom positive region, which is not involved in the C–H⋯Br bonds). Also, the favoured directions of C–H⋯X bonds are similar. Consequently, a similar aggregation of three molecules around each –Br and –CN atoms takes place (Fig. 6). The difference, that in acetonitrile the transition is induced by the transformation between 2-fold C–H⋯N (α-CH3CN) to 3-fold C–H⋯N (β-CH3CN) bonding whereas methyl bromide transforms between 2-fold Br⋯Br (α-CH3Br) to 3-fold C–H⋯Br.

| Table 2 | Selected interatomic distances (Å) and angles (°) of the crystalline CH3Br phase α and β structure at high pressure compared with those observed at low-temperature. Intermolecular distances shorter than the sum of van der Waals radii22 are written in bold |

| CH3Br at: | Phase α | Phase α | Phase α |
|-----------|---------|---------|---------|
| 0.1 MPa/153 K | 1.863 | 1.912(10) | 1.898(9) |
| 1.0 MPa/153 K | 1.919(16) | 1.892(14) | 2.024(25) |
| 1.11 GPa/295 K | 3.285(8) | 3.242 | 3.058 |
| 1.50 GPa/295 K | 3.315 | 3.084 |

| CH3Cl at: | Phase α | Phase α | Phase α |
|-----------|---------|---------|---------|
| 0.1 MPa/148 K | 1.805 | 1.746(7) | 1.792(4) | 1.750(5) | 1.716(7) |
| 1.22 GPa/295 K | 3.906(5) | 3.871(8) | 3.712(5) | 3.670(7) |
| 1.69 GPa/295 K | 64.4 | 63.4(3) | 61.7(2) | 66.3(2) | 64.7(3) |
| 2.91 GPa/295 K | 156.1 | 156.9(3) | 156.5(1) | 151.0(2) | 151.1(2) |
| 4.38 GPa/295 K | 3.507 | 3.454(8) | 3.371(5) | 3.316(6) | 3.285(8) |
| 3.618 | 3.407(5) | 3.409(7) | 3.322(8) |
| 3.734 | 3.650(6) | 3.582(5) | 3.421(3) | 3.391(8) |
| 3.138 | 3.085 | 2.962 | 2.788 | 2.706 |
| 3.125 | 3.011 | 2.926 | 2.855 | 2.823 |

| Reference | 24, 25 | This work. Symmetry codes: (i) −x, y, 0.5 + z; −x, −y, −0.5 + z; (j) −x, 1 − y, 0.5 + z; (k) −x, −y, 0.5 + z; (l) −0.5 + x, 0.5 + y, z; 0.5 + x, 0.5 + y, z; (n) −0.5 − x, 0.5 − y, 0.5 − z; 0.5 − x, 0.5 − y, 0.5 − z. |
(β-CH₃Br) bonding, is meaningful. It indicates that, apart from other factors, the steric hindrance between large halogen atoms can be disadvantageous for their close association.

Conclusions

Phase α-CH₃Br, isostructural with CH₃I and dominated by halogen···halogen bonds, is destabilized by pressure and transforms into phase β-CH₃Br governed by C–H···halogen interactions. Phase β of CH₃Br and the CH₃Cl crystal are isostructural. It can be envisaged that CH₃I may also transform into a C–H···I bonded phase at pressure considerably higher than 2.5 GPa as obtained in our previous study. Due to halogen···halogen and C–H···halogen forces systematically increasing in the CH₃Cl < CH₃Br < CH₃I sequence, only CH₃Cl up to 1.2 GPa and CD₃Br phase β determined at ambient pressure and 175 K are the loose crystals. This indicates that CH₃X molecules are more evenly accommodated in space group Cmc2₁ and that C–H···X interactions are favoured by the close-packing effect. This effect can significantly contribute to the stability of CH₃X at high pressure. However, detailed measurements of the CH₃Br crystal volume as a function of temperature are still needed to evaluate the contribution of close packing to the C–H···X versus X···X competition.

Acknowledgements

This study was supported by the TEAM grant no. 2009-4/6 from the Foundation for Polish Science.

Notes and references

1 F. F. Awwadi, R. D. Willett, K. A. Peterson and B. Twamley, Chem. – Eur. J., 2006, 12, 8952–8960.
2 C. M. Reddy, M. T. Kirchner, R. V. Gundakaram, K. A. Padmanabhan and G. R. Desiraju, Chem. – Eur. J., 2006, 12, 2222–2234.
3 P. Metrangolo, F. Meyer, T. Pilati, G. Resnati and G. Terraneo, Angew. Chem., Int. Ed., 2008, 47, 6114–6127.
4 A. Mukherjee and G. R. Desiraju, IUCrJ, 2014, 1, 49–60.
5 P. Politzer, J. S. Murray and T. Clark, Phys. Chem. Chem. Phys., 2013, 15, 11178–11189.
6 A. R. Jagarlapudi, P. Sarma and G. R. Desiraju, Acc. Chem. Res., 1986, 19, 222–228.
7 P. Metrangolo and G. Resnati, Science, 2008, 321, 918–919.
8 T. J. Mooibroek and P. Gamez, CrystEngComm, 2013, 15, 4565–4570.
9 S. L. Price, A. J. Stone, J. Lucas, R. S. Rowland and A. E. Thornley, J. Am. Chem. Soc., 1994, 116, 4910–4918.
10 M. Kaźmierczak and A. Katrusiak, Cryst. Growth Des., 2014, 14, 2223–2229.
11 H.-C. Chang, J.-C. Jiang, C.-W. Chuang and S. H. Lin, Chem. Phys. Lett., 2004, 397, 205–210.
12 K. F. Dziubek, D. Jęczmiński and A. Katrusiak, J. Phys. Chem. Lett., 2010, 1, 844–849.
13 K. M. Lee, H.-C. Chang, J.-C. Jiang, J. C. C. Chen, H.-E. Kao, S. H. Lin and I. J. B. Lin, J. Am. Chem. Soc., 2003, 125, 12358–12364.
14 A. Olejniczak and A. Katrusiak, J. Phys. Chem. B, 2008, 112, 7183–7190.
15 R. Gajda and A. Katrusiak, Cryst. Growth Des., 2011, 11, 4768–4774.
16 E. Patyk, J. Skumiel, M. Podsiadlo and A. Katrusiak, Angew. Chem., Int. Ed., 2012, 51, 2146–2150.
17 M. Podsiadlo, K. Dziubek and A. Katrusiak, Acta Crystallogr., Sect. B: Struct. Sci., 2005, 61, 595–600.
18 M. Podsiadlo, K. Dziubek, M. Szafrański and A. Katrusiak, Acta Crystallogr., Sect. B: Struct. Sci., 2006, 62, 1090–1098.
19 M. Podsiadlo and A. Katrusiak, Acta Crystallogr., Sect. B: Struct. Sci., 2007, 63, 903–911.
20 M. Podsiadlo and A. Katrusiak, J. Phys. Chem. B, 2008, 112, 5355–5362.
21 M. Podsiadlo and A. Katrusiak, CrystEngComm, 2008, 10, 1436–1442.
22 M. Podsiadlo and A. Katrusiak, CrystEngComm, 2009, 11, 1391–1395.
23 R. M. Ibberson and M. Prager, Z. Kristallogr., 2007, 222, 416–419.
24 T. Kawaguchi, M. Hijikigawa, Y. Hayafuji, M. Ikeda, R. Fukushima and Y. Tomiie, Bull. Chem. Soc. Jpn., 1973, 46, 53–56.
25 R. D. Burbank, J. Am. Chem. Soc., 1953, 75, 1211–1214.
26 M. Podsiadlo and A. Katrusiak, CrystEngComm, 2009, 11, 1951–1957.
27 C. J. Egan and J. D. Kemp, J. Am. Chem. Soc., 1938, 60, 2097–2101.
28 O. S. Binbrek, A. Anderson and B. H. Torrie, J. Chem. Phys., 1985, 82, 1468–1475.
29 P. N. Gerlach, B. H. Torrie and B. M. Powell, Mol. Phys., 1986, 57, 919–930.
30 R. M. Ibberson and M. Prager, Acta Crystallogr., Sect. B: Struct. Sci., 1996, 52, 892–895.
31 W. A. Bassett, High Pressure Res., 2009, 29, 163–186.
32 A. Budzianowski and A. Katrusiak, High-Pressure Crystallography, ed. A. Katrusiak and P. F. McMillan, Kluwer Academic Publisher, Dordrecht, 2004, pp. 101–112.
33 Oxford Diffraction Ltd., Xcalibur CCD system, CrysAlis Software system, Version 1.171, 2004.
34 A. Katrusiak, REDSHABS – Program for Correcting Reflections Intensities for DAC Absorption, Gasket Shadowing and Sample Crystal Absorption, Adam Mickiewicz University, Poznań, Poland, 2003.
35 A. Katrusiak, Z. Kristallogr., 2004, 219, 461–467.
36 G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Crystallogr., 2008, 64, 112–122.
37 M. J. Frisch, et al., GAUSSIAN03, Revision B.04., Gaussian, Inc., Pittsburgh, PA, USA, 2003.
38 R. F. W. Bader, M. T. Carroll, J. R. Cheeseman and C. Chang, J. Am. Chem. Soc., 1987, 109, 7968–7979.
39 R. M. Ibberson, O. Moze and C. Petrillo, Mol. Phys., 1992, 76, 395–403.
40 B. M. Powell, K. M. Heal and B. H. Torrie, Mol. Phys., 1984, 53, 929–939.
41 G. R. Desiraju and R. Parthasarathy, J. Am. Chem. Soc., 1989, 111, 8725–8726.
42 P. Metrangolo and G. Resnati, IUCrJ, 2014, 1, 5–7.
43 T. Sakurai, M. Sundaralingam and G. A. Jeffrey, Acta Crystallogr., 1963, 16, 354–363.
44 O. V. Grineva and P. M. Zorky, Zh. Fiz. Khim., 1998, 72, 714–720 (In Russian).
45 O. V. Grineva and P. M. Zorky, Kristallografiya, 2000, 45, 692–698 (In Russian).
46 M. Bujak, M. Podsiadlo and A. Katrusiak, CrystEngComm, 2011, 13, 396–398.
47 M. Kaźmierczak and A. Katrusiak, J. Phys. Chem. C, 2013, 117, 1441–1446.
48 D. R. Lide, CRC Handbook of Chemistry and Physics, CRC Press Inc., Boca Raton, FL, 90th edn, 2010.
49 A. Katrusiak, J. Mol. Graphics Modell., 2001, 19, 363–367.
50 J. J. McKinnon, M. A. Spackman and A. S. Mitchell, Acta Crystallogr., Sect. B: Struct. Sci., 2004, 60, 627–668.
51 S. K. Wolff, D. J. Grimwood, J. J. McKinnon, D. Jayatilaka and N. A. Spackman, CrystalExplorer 2.0, University of Western Australia, Perth, Australia, 2007.
52 A. Bondi, J. Phys. Chem., 1964, 68, 441–451.