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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1224). Services for accessing these data are described at the back of the journal.

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Methylxanthines. II.† Anhydrous Theobromine

Kimberly A. Ford, Yukiko Ebisuzaki and Paul D. Boyle

Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, USA. E-mail: boyle@laue.chem.ncsu.edu

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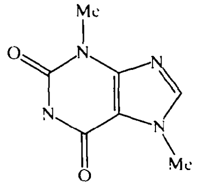
Abstract

Clear crystals of anhydrous theobromine (3,7-dihydro-3,7-dimethyl-1*H*-purine-2,6-dione, $C_7H_8N_4O_2$) were grown by vacuum sublimation and the structure determined. The melting point of anhydrous theobromine has been determined as 620 (1) K. Two molecules in the asymmetric unit form a pseudo-centrosymmetric dimer and pack to form a layered structure of two-dimensional hydrogen-bonded networks.

Comment

Theobromine (3,7-dimethylxanthine) is the principal alkaloid in the cocoa bean and is known to contribute to the stimulating effect of chocolate. The structure of theobromine has, until now, been determined only when the molecule has been used as a ligand for a metal complex (Crowston *et al.*, 1986), as a theobrominium counter-ion (Herbstein & Kapon, 1975, 1979), or as part of a molecular complex (Shefter *et al.*, 1971). As part of our research on methylxanthines (Ebisuzaki *et al.*, 1997), we report the crystal structure of pure anhydrous theobromine, (I).



(I)

Anhydrous theobromine crystallizes with two molecules in the asymmetric unit. The two molecules form a nearly planar pseudo-centrosymmetric hydrogen-bonded dimer. The asymmetric unit and labeling scheme are shown in Fig. 1. In this paper, the molecule which has the unprimed atom labels is referred to as molecule *A*; the primed atom labels belong to molecule *B*. The intramolecular bond lengths and angles are given in Table 1, and are unremarkable. Individual bond lengths and angles agree well with expected values (Allen *et al.*, 1987) as well as with the values obtained from the previously determined structure of the 2:1

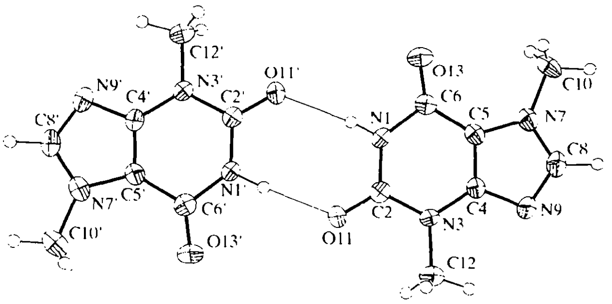


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the title molecule, showing the asymmetric unit and the labelling scheme. Non-H-atom displacements ellipsoids are drawn at the 50% probability level. H atoms are drawn as circles with a small arbitrary radius, for clariy.

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† Part I: Ebisuzaki *et al.* (1997).

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5-chlorosalicylic acid–theobromine complex (Shefter *et al.*, 1971). The dihedral angle between the molecular planes of *A* and *B* is 4.65 (5)°, where the ring of each molecule has been defined by the endocyclic atoms of the molecule.

The centroid of the asymmetric unit (excluding H-atom positions) is located at (0.737, 0.345, 0.517). Performing an inversion through this position and examining the distances between the corresponding pairs of atoms reveals the magnitude of the deviation from a quantitative centrosymmetric relationship. For the non-H-atom pairs the magnitudes are: N1–N1′ 0.107 (3), C2–C2′ 0.163 (4), N3–N3′ 0.137 (3), C4–C4′ 0.042 (4), C5–C5′ 0.047 (4), C6–C6′ 0.024 (4), N7–N7′ 0.149 (3), C8–C8′ 0.110 (4), N9–N9′ 0.011 (3), C10–C10′ 0.321 (6), O11–O11′ 0.232 (3), C12–C12′ 0.073 (6) and O13–O13′ 0.114 (3) Å. It should be noted that the least-squares refinement converged smoothly and exhibited only two correlations with a correlation coefficient above 0.5: a correlation of 0.53 was found between the *x* parameter of C10′ and the *U* parameter of H10*a*′, and a correlation of 0.54 was found between the extinction and scale parameters for the structure refined using full-matrix least squares on F^2, using all the available data. Such behavior is atypical in structure refinements where a crystallographic center of symmetry has been overlooked (Marsh, 1995). In addition, the bond lengths and angles correspond closely to accepted values (see above), and this is often not the case in structures in which a center of symmetry has been overlooked (Baur & Tillmans, 1986).

The crystal structure consists of two-dimensional hydrogen-bonded layers which lie approximately parallel to ($\bar{1}01$), as shown in Fig. 2. The hydrogen-bonding environments for molecules *A* and *B* are topologically identical. Due to the non-zero dihedral angle between the molecular planes, these hydrogen-bonded layers are not flat, however, but display a gentle sinusoidal undulation which propagates along the *b* axis. The mean distance between layers is 3.28 (18) Å, which corresponds closely to the *d* spacing for the $\bar{2}02$ reflection, the most intense peak in the data set.

The hydrogen bonding has been characterized for contacts in which the H-atom-to-acceptor distance is less than 3.0 Å. The hydrogen bonds found may be divided into three categories: short intralayer, long intralayer and interlayer hydrogen-bonding contacts. These contacts are listed in Table 2 in order of increasing H···acceptor distance. The short intralayer contacts are formed by N—H···O and C—H···O contacts and are characterized by H···O distances of less than 2.3 Å. The long intralayer contacts are all C—H···O or C—H···N interactions with H···acceptor distances of 2.65–2.79 Å and the H atom lying within 9° of the plane containing the lone pair of the acceptor atom. Interlayer hydrogen-bond contacts are all methyl C—H···O or methyl C—H···N interactions. For the interlayer group, the H···acceptor distances vary between 2.74 and 2.94 Å, with the H atom deviating by over 50° from the plane containing the lone pair of the acceptor. Analysis of the intermolecular contacts was performed using *PLATON* (Spek, 1990) as well as geometry routines available in the *NRCVAX* package (Gabe *et al.*, 1989).

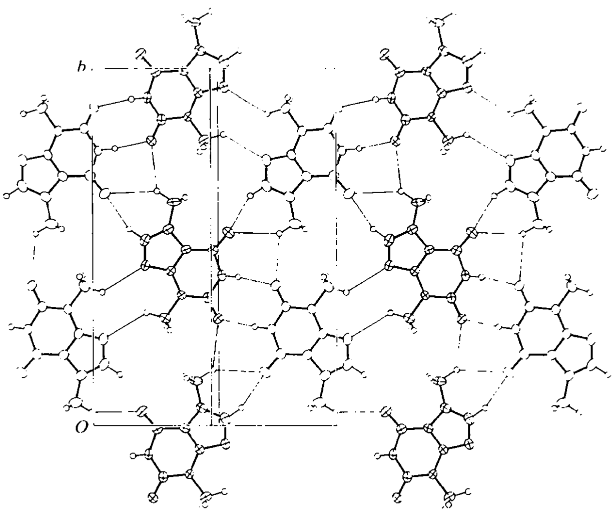

Fig. 2. *ORTEP*II (Johnson, 1976) drawing showing one layer in the two-dimensional hydrogen-bonding pattern. Non-H-atom displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as circles with a small arbitrary radius, for clarity. The molecules with principal ellipses drawn on the ellipsoids denote molecule *A* and the hollow ellipsoids represent the *B* molecules, as noted in the text. The view is approximately down [$\bar{1}01$]. The origin and *b* axis are labeled for reference.

The short intralayer hydrogen bonds occur between the following sets of atoms: N1—H1···O11′, N1′—H1′···O11, C8—H8···O13′ and C8′—H8′···O13. The short intralayer hydrogen bonds are always between *A* and *B* molecules. It is worth noting that the H···O distances of 2.26 (3) and 2.27 (3) Å in the C—H···O interactions are in the short end of the range of H···O distances for C—H···O interactions (Taylor & Kennard, 1982). Without taking into account the longer hydrogen-bond interactions (see below), the structure can be thought of as an *AB* pseudo-centrosymmetric dimer joined *via* N—H···O hydrogen bonds. These dimers are then joined to form the two-dimensional network *via* a total of four short C—H···O hydrogen bonds.

The long intralayer hydrogen bonds involve methyl-H atoms and O or N acceptor atoms. This class of contacts involves the following sets of atoms, with the deviation of the H atom from the plane containing the lone pair of the acceptor atom being given in parentheses: C10—H10*c*···O11 [−0.41 (3) Å], C10′—H10*c*′···O11′ [0.34 (3) Å], C10—H10*c*···O13′ [0.26 (3) Å], C10′—H10*c*′···O13 [−0.04 (3) Å], C12—H12*b*···N9′ [−0.11 (3) Å] and C12′—H12*b*′···N9 [0.09 (4) Å]. For the carbonyl-O atoms in this group of hydrogen bonds, the C—O···H angles vary from 127.5

to 148.8°. Although a little larger than the ideal angle of 120° (Taylor & Kennard, 1984; Murray-Rust & Glusker, 1984), the H atoms for these longer C—H···O interactions point in the vicinity of the sp^2-hybridized lone pairs of the O atoms. The C—H···O angles vary from 126 to 147°. Of particular note, both H10*c* and H10*c*′ participate in bifurcated hydrogen bonding: atom H10*c* is involved in a bifurcated hydrogen bond with O11 and O13′, whereas atom H10*c*′ is involved in a bifurcated hydrogen bond with O11′ and O13. Unlike the short intralayer contacts, these are hydrogen bonds which join *AA* and *BB* pairs of molecules.

A search of the Cambridge Structural Database (CSD; Allen & Kennard, 1993) was performed for intermolecular *N*-methylimidazole···H—C(any)—N contacts between 0.0 and 3.1 Å, to establish a set of parameters with which the C—H···N bonding in theobromine could be compared. The 40 N···H contacts obtained from the CSD ranged between 2.376 and 3.086 Å, with a mean value of 2.85 (19) Å. The donor···acceptor distances varied between 3.206 and 4.038 Å, with a mean of 3.59 (20) Å. The C—H···N angle varied between 90.51 and 169.02°, with a mean of 137 (20)°. The H···N and donor···acceptor contact distances observed in theobromine are roughly 1σ shorter than the mean values obtained from the CSD for these quantities. The C—H···N angles for theobromine are well within 1σ of the mean value obtained from the CSD search.

The long interlayer hydrogen bonds again involve only methyl C—H donors and O and N acceptors. The deviation of the H-atom positions from the plane containing the lone pairs of the acceptors varies from 2.22 to 2.71 Å. The hydrogen bonds in the interlayer class consist of the following sets of atoms: C12—H12*c*···O11, C12′—H12*a*′···O13, C12′—H12*c*′···O13′, C12—H12*a*···N9′ and C10′—H10*b*′···N9.

It is interesting to note that although theobromine and theophylline are isomeric, the melting points of the two compounds differ by a substantial amount: the melting point of theobromine is 620 (1) K, while that of theophylline is 548.8 (5) K (Ebisuzaki *et al.*, 1997), a difference of over 71 K. Although it is difficult to use melting points as a quantitative measure of lattice stability, it appears that the more extensive hydrogen bonding in theobromine may play an important role in this difference in melting point.

Experimental

Commercial theobromine was purified several times by recrystallization from hot water. The dried powder was placed in a sublimation tube and sealed under vacuum. Clear crystals grew when the furnace temperature was 498 (5) K. The melting point was determined as 620 (1) K, using a sealed melting-point capillary.

Crystal data

$C_7H_8N_4O_2$
M_r = 180.16
Monoclinic
$P2_1/c$
a = 9.2990 (14) Å
b = 18.698 (1) Å
c = 9.0381 (16) Å
β = 91.75 (3)°
V = 1570.7 (4) Å^3
Z = 8
D_x = 1.524 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 24 reflections
θ = 18–20°
μ = 0.11 mm^{-1}
T = 293 K
Parallelepiped
0.24 × 0.22 × 0.18 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
2737 measured reflections
2737 independent reflections
$\theta_{\max}$ = 25°

$h = -10 \rightarrow 11$
$k = 0 \rightarrow 22$
$l = 0 \rightarrow 10$
3 standard reflections
frequency: 80 min
intensity decay: 1.3%

Refinement

Refinement on F^2
$R(F)$ = 0.067
$wR(F^2)$ = 0.074
S = 1.58
2737 reflections
300 parameters
All H atoms refined
$w = 1/[\sigma^2(F) + 0.001F^2]$
$(\Delta/\sigma)_{\max}$ = 0.001

$\Delta\rho_{\max}$ = 0.28 e Å^{-3}
$\Delta\rho_{\min}$ = −0.24 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 61 (4)
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Selected geometric parameters (Å, °)*

N1—C2	1.381 (3)	N1′—C2′	1.378 (3)
N1—C6	1.397 (3)	N1′—C6′	1.398 (3)
N1—H1	0.85 (3)	N1′—H1′	0.90 (3)
C2—N3	1.377 (3)	C2′—N3′	1.377 (3)
C2—O11	1.231 (3)	C2′—O11′	1.236 (3)
N3—C4	1.377 (3)	N3′—C4′	1.384 (3)
N3—C12	1.473 (3)	N3′—C12′	1.472 (3)
C4—C5	1.364 (3)	C4′—C5′	1.365 (4)
C4—N9	1.363 (3)	C4′—N9′	1.357 (3)
C5—C6	1.426 (4)	C5′—C6′	1.431 (4)
C5—N7	1.388 (3)	C5′—N7′	1.391 (3)
C6—O13	1.225 (3)	C6′—O13′	1.228 (3)
N7—C8	1.343 (4)	N7′—C8′	1.340 (4)
N7—C10	1.469 (4)	N7′—C10′	1.466 (4)
C8—N9	1.339 (4)	C8′—N9′	1.342 (4)
C8—H8	1.03 (3)	C8′—H8′	0.98 (3)
C2—N1—C6	129.1 (2)	C2′—N1′—C6′	129.2 (2)
C2—N1—H1	116.7 (17)	C2′—N1′—H1′	114.6 (17)
C6—N1—H1	114.2 (17)	C6′—N1′—H1′	116.1 (17)
N1—C2—N3	116.4 (2)	N1′—C2′—N3′	116.7 (2)
N1—C2—O11	121.5 (2)	N1′—C2′—O11′	122.1 (2)
N3—C2—O11	122.1 (2)	N3′—C2′—O11′	121.3 (2)
C2—N3—C4	118.9 (2)	C2′—N3′—C4′	118.8 (2)
C2—N3—C12	119.2 (2)	C2′—N3′—C12′	119.5 (2)
C4—N3—C12	121.8 (2)	C4′—N3′—C12′	121.7 (2)
N3—C4—C5	122.4 (2)	N3′—C4′—C5′	122.2 (2)
N3—C4—N9	124.9 (2)	N3′—C4′—N9′	125.1 (2)
C5—C4—N9	112.7 (2)	C5′—C4′—N9′	112.6 (2)
C4—C5—C6	122.9 (2)	C4′—C5′—C6′	123.0 (2)
C4—C5—N7	105.1 (2)	C4′—C5′—N7′	104.9 (2)
C6—C5—N7	132.0 (2)	C6′—C5′—N7′	132.1 (2)
N1—C6—C5	110.3 (2)	N1′—C6′—C5′	110.1 (2)

N1—C6—O13	121.1 (2)	N1′—C6′—O13′	121.2 (2)
C5—C6—O13	128.6 (2)	C5′—C6′—O13′	128.7 (2)
C5—N7—C8	105.6 (2)	C5′—N7′—C8′	106.0 (2)
C5—N7—C10	127.6 (2)	C5′—N7′—C10′	127.7 (2)
C8—N7—C10	126.8 (2)	C8′—N7′—C10′	126.4 (2)
N7—C8—N9	114.3 (2)	N7′—C8′—N9′	113.8 (2)
N7—C8—H8	121.1 (14)	N7′—C8′—H8′	123.4 (15)
N9—C8—H8	124.4 (14)	N9′—C8′—H8′	122.8 (15)
C4—N9—C8	102.3 (2)	C4′—N9′—C8′	102.8 (2)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1′—H1′···O11	0.90 (3)	1.96 (3)	2.850 (3)	173 (3)
N1—H1···O11′	0.85 (3)	2.00 (3)	2.849 (3)	173 (2)
C8—H8···O13′^{i}	1.03 (3)	2.26 (3)	3.229 (3)	158 (2)
C8′—H8′···O13^{ii}	0.98 (3)	2.27 (3)	3.164 (3)	153 (2)
C12—H12*b*···N9′^{iii}	1.04 (3)	2.65 (3)	3.412 (4)	130 (2)
C12′—H12*b*′···N9^{iv}	1.01 (4)	2.67 (3)	3.420 (4)	131 (2)
C10′—H10*c*′···O13^{ii}	0.99 (4)	2.67 (3)	3.544 (4)	147 (2)
C10—H10*c*···O11^{i}	1.06 (3)	2.69 (3)	3.446 (3)	127 (2)
C12—H12*a*···N9′^{v}	0.97 (3)	2.74 (3)	3.504 (5)	136 (2)
C10—H10*c*···O13′^{i}	1.06 (3)	2.75 (3)	3.658 (4)	143 (2)
C10′—H10*c*′···O11′^{ii}	0.99 (4)	2.76 (3)	3.434 (4)	126 (2)
C12′—H12*a*′···O13^{vi}	0.98 (4)	2.77 (3)	3.710 (5)	161 (3)
C12—H12*c*···O11^{vii}	0.90 (3)	2.79 (3)	3.679 (4)	167 (3)
C12′—H12*c*′···O13′^{viii}	0.97 (4)	2.87 (3)	3.473 (5)	121 (2)
C10′—H10*b*′···N9^{ix}	0.99 (4)	2.94 (4)	3.555 (5)	121 (3)

Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $2 - x, y - \frac{1}{2}, \frac{3}{2} - z$; (iii) $x - 1, y, z - 1$; (iv) $1 + x, y, 1 + z$; (v) $x - 1, \frac{1}{2} - y, z - \frac{1}{2}$; (vi) $2 - x, 1 - y, 1 - z$; (vii) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (viii) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ix) $1 + x, \frac{1}{2} - y, \frac{1}{2} + z$.

H-atom positional and isotropic displacement parameters were allowed to refine. The resulting C—H and N—H bond lengths were in the range 0.90 (3)–1.06 (3) and 0.85 (3)–0.90 (3) Å, respectively. U_{iso} values for the H atoms varied from 0.048 (9) (for H1) to 0.111 (15) Å^2 (for H12*a*′), with an average value of 0.08 Å^2.

Data collection: locally modified *CAD*-4-*ARGUS* (Enraf–Nonius, 1994). Cell refinement: locally modified *CAD*-4-*ARGUS*. Data reduction: *DATRD*2 (*NRCVAX*; Gabe *et al.*, 1989). Program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994). Program(s) used to refine structure: *LSTSQ* (*NRCVAX*). Molecular graphics: *ORTEP*II (Johnson, 1976) as implemented in *NRCVAX*. Software used to prepare material for publication: *TABLES* (*NRCVAX*).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1140). Services for accessing these data are described at the back of the journal.

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Complexe de Tétracyanoquinodiméthane† et 4-Amino-3,5-bis(2-pyridyle)-1,2,4-triazole (TCNQ:abpt)

B. MERNARI,[a] M. EL AZHAR,[a] H. EL ATTARI,[a] M. LAGRENÉE[b] ET M. PIERROT[c]

[a]*Laboratoire de chimie de coordination, Département de chimie, Faculté des Sciences, Université Chouaib Doukkali, B.P. 20, El Jadida, Maroc,* [b]*Laboratoire de cristallochimie et de physicochimie du solide, URA 452, CNRS, ENSCL, Université de Lille 1, BP108, 59655 Villeneuve d'Ascq, France, et* [c]*LBS-UMR 6517, Centre Scientifique Saint-Jérôme, 13397 Marseille, CEDEX 20, France. E-mail: marcel.pierrot@lbs.u-3mrs.fr*

(Reçu le 18 mars 1998, accepté le 16 juin 1998)

Abstract

The title complex, $C_{12}H_4N_4.C_{12}H_{10}N_6$, is the association of a molecule of abpt with TCNQ, where the abpt molecule is slightly twisted and presents two intramolecular N—H···N bonds. The TCNQ:abpt molecules are parallel to the *c* axis and form molecular planes parallel to the (001) planes.

Commentaire

La préparation et l'étude structurale de nouveaux conducteurs électroniques est un domaine en pleine expan-

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† Nom alternatif: 2,2′-(2,5-cyclohexadiène-1,4-diylidène)bis(1,3-propanedinitrile).