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Tris(2-cyanoethyl) isocyanurate

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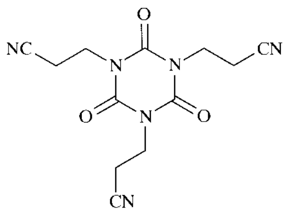
The title compound, 1,3,5-tris(2-cyanoethyl)-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione, $C_{12}H_{12}N_6O_3$, forms a layered structure stabilized by C—H···O and C—H···N hydrogen bonds.

Comment

The importance of C—H···O and C—H···N hydrogen bonds in the crystal structures of organic compounds is well known (Desiraju & Steiner, 1999). In this context, the title compound, (I), is of interest because it contains activated C—H donors and carbonyl and cyano acceptors. Furthermore, the molecule has trigonal symmetry and so its crystal structure could be relevant in the context of octupolar nonlinear optical effects (Thalladi *et al.*, 1997).



(I)

The molecular geometry of (I) is shown in Fig. 1. Two of the cyanoethyl groups are oriented on one side of the heterocyclic ring, whilst the third points in the other direction. The crystal is centrosymmetric and the molecules form a layered structure (Fig. 2). In the (011) plane, each molecule is connected to four inversion-related molecules *via* C—H···O hydrogen bonds [C5—H5*A*···O3^{i}, C7—H7*B*···O1^{ii}, C8—H8*B*···O2^{iii} and C11—H11*A*···O3^{v}; see Table 1]. These interactions will be referred to hereinafter as *i*, *j*, *k* and *l*, respectively. Translation-related molecules are linked *via* C—H···N hydrogen bonds [C8—H8*A*···N6^{iii} and C10—H10*B*···N4^{iv}; see Table 1]. These interactions interactions will be referred to hereinafter as *m* and *n*, respectively.

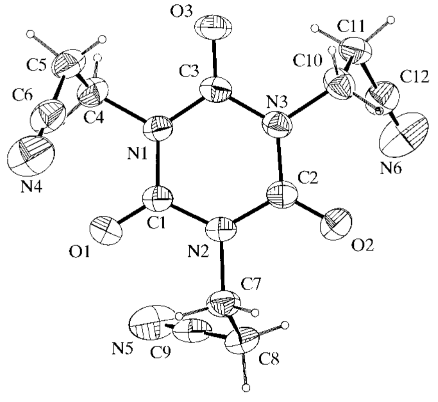


Figure 1
An *ORTEP*II view (Johnson, 1976) and the atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radii.

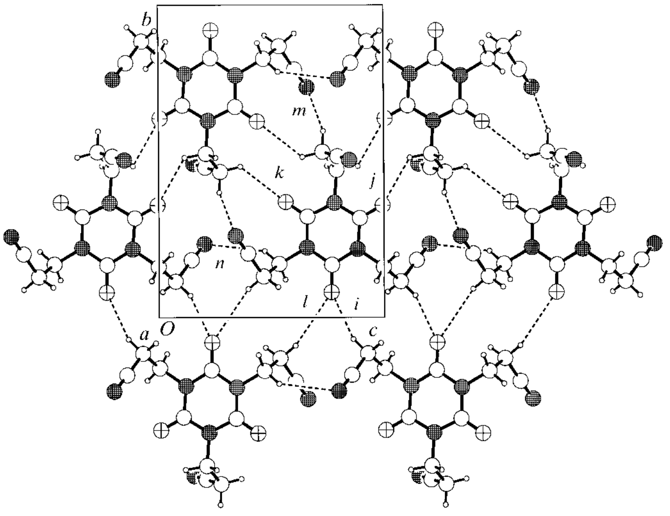


Figure 2
The layer structure of (I) viewed down [100]. O and N atoms are shaded. C—H···O hydrogen bonds are indicated as *i*, *j*, *k* and *l*, and C—H···N hydrogen bonds are indicated as *m* and *n*.

In order to analyse the C—H···N≡C hydrogen bond directionality (φ angle) at the acceptor atom, the Cambridge Structural Database (CSD version 5.17, 197 481 entries; Allen & Kennard, 1993) was searched for C—H···N≡C geometries. Ordered crystal structures of non-metal-atom-containing compounds with $R < 0.075$ were considered. Structures containing charged residues were excluded. In order that acceptor directionality not be biased by steric factors, only those geometries where a single C—H group approaches a cyano group were considered. In other words, geometries with bifurcated acceptors were not selected. The H-atom positions were normalized to standard neutron values, with the H···N distance allowed to lie between 1.5 and 3.0 Å and the H···N≡C angle between 40 and 180°. The mean H···N distance was found to be 2.67 Å for 249 fragments and the mean H···N≡C angle was 132.0°. The angular distribution is shown in Fig. 3. However, after cone-correction (Kroon & Kanters, 1974) it was observed that the distribution of φ angles tends strongly towards a linear geometry at the acceptor N atom. This shows that in C—H···N≡C hydrogen bonds, the main acceptor centre is the lone pair on the N atom rather than the C≡N triple bond.

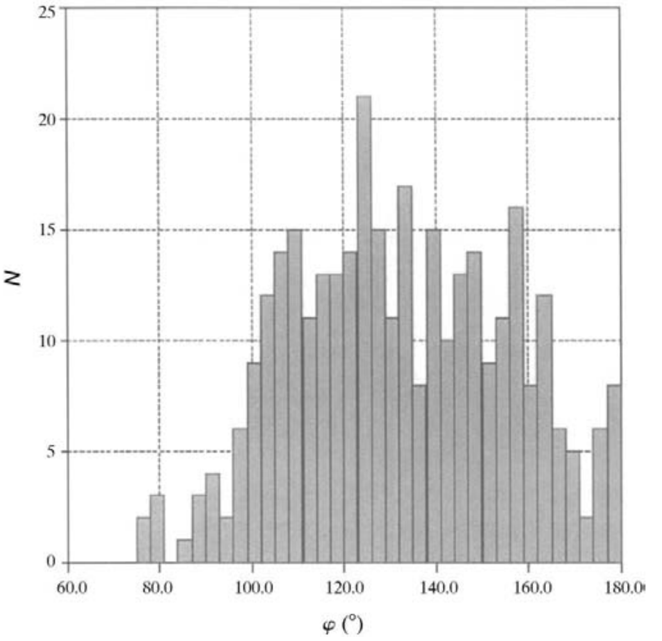


Figure 3
The distribution of φ angles for C—H···N≡C hydrogen bonds. The distribution is not cone-corrected and displays data from 329 non-bifurcated geometries taken from the Cambridge Structural Database (Allen & Kennard, 1993).

Experimental

Colourless crystals (m.p. 502 K) of (I), which was prepared according to the method of Frazier *et al.* (1960), were obtained by crystallization from dimethylformamide.

Crystal data

$C_{12}H_{12}N_6O_3$
$M_r = 288.28$
Monoclinic, $P2_1/n$
$a = 9.727$ (2) Å
$b = 13.781$ (2) Å
$c = 9.956$ (2) Å
$\beta = 90.46$ (2)°
$V = 1334.6$ (4) Å^3
$Z = 4$
$D_x = 1.435$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 9$–11°
$\mu = 0.108$ mm^{-1}
$T = 293$ (2) K
Needle, colourless
0.60 × 0.48 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
4071 measured reflections
3877 independent reflections
2466 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.009$
$\theta_{\rm max} = 29.96°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 19$
$l = -13 \rightarrow 13$
3 standard reflections every 100 reflections intensity decay: <2%

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O3$^{\rm i}$	0.96 (2)	2.59 (2)	3.504 (2)	160 (2)
C7—H7B···O1$^{\rm ii}$	0.97 (2)	2.59 (2)	3.238 (2)	124 (1)
C8—H8A···N6$^{\rm iii}$	0.95 (3)	2.53 (3)	3.382 (3)	150 (2)
C8—H8B···O2$^{\rm iii}$	0.92 (2)	2.73 (2)	3.353 (2)	126 (2)
C10—H10B···N4$^{\rm iv}$	0.99 (2)	2.79 (2)	3.647 (3)	146 (2)
C11—H11A···O3$^{\rm v}$	0.93 (2)	2.98 (2)	3.750 (2)	141 (2)

Symmetry codes: (i) $1-x, -y, 2-z$; (ii) $1-x, 1-y, 2-z$; (iii) $1-x, 1-y, 1-z$; (iv) $x, y, z-1$; (v) $1-x, -y, 1-z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.190$
$S = 1.067$
3877 reflections
239 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1131P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.42$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.35$ e Å^{-3}

The C—H distances range from 0.91 (2)–0.99 (2) Å.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *Xtal* 3.5 (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLUTON*-(*C*) (Spek, 1979–1997); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1500). Services for accessing these data are described at the back of the journal.

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