Table 1. *Fractional coordinates* ($\times 10^4$; *for* $H\times 10^3$) *and equivalent isotropic thermal parameters* ($Å^2\times 10^3$) *for 2-chloro-1-(2,4-dihydroxyphenyl)ethanone*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a}_i.\mathbf{a}_j).$$

	x	y	z	U_{eq}
C(1)	5424 (8)	−2169 (4)	1567 (8)	29 (1)
C(2)	4654 (9)	−1996 (4)	−320 (9)	33 (2)
C(3)	4086 (8)	−2634 (4)	−1607 (9)	34 (2)
C(4)	4206 (8)	−3499 (4)	−1004 (9)	34 (1)
C(5)	4993 (9)	−3705 (4)	830 (9)	35 (2)
C(6)	5562 (8)	−3073 (4)	2107 (9)	33 (1)
C(7)	6038 (8)	−1514 (4)	2911 (9)	30 (1)
C(8)	5813 (10)	−572 (4)	2213 (10)	40 (2)
O(9)	3551 (6)	−4145 (3)	−2122 (7)	45 (1)
O(10)	6297 (6)	−3293 (3)	3872 (6)	46 (1)
O(11)	6695 (6)	−1667 (3)	4576 (6)	39 (1)
Cl	7092 (3)	157 (1)	3742 (3)	48 (1)
H(2)	462 (9)	−149 (5)	−110 (10)	92 (10)*
H(3)	366 (9)	−252 (5)	−315 (10)	92 (10)*
H(5)	519 (10)	−430 (4)	111 (10)	92 (10)*
H(8*A*)	636 (9)	−22 (4)	77 (10)	92 (10)*
H(8*B*)	443 (10)	−22 (4)	195 (10)	92 (10)*
H(9)	298 (9)	−373 (5)	−324 (10)	92 (10)*
H(10)	606 (9)	−267 (5)	485 (10)	92 (10)*

* Isotropic temperature factor.

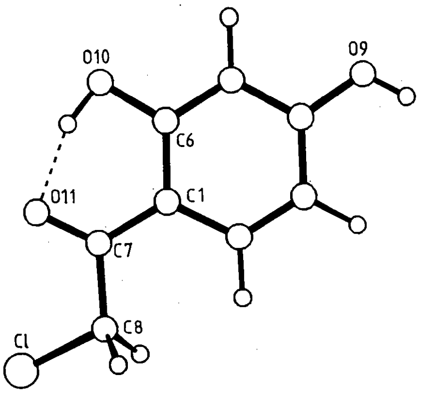

Fig. 1. Drawing of a molecule of 2-chloro-1-(2,4-dihydroxyphenyl)ethanone with the atom numbering.

Related literature. ω-Chlororesacetophenone showed a strong inhibition of the growth of the gram-positive micro organisms *Staphylococcus aureus, Bacillus licheniformis, B. cereus* and *Micrococcus luteus*, the gram-negative organisms *Escherichia coli* and *Pseudomonas aeruginosa*, the yeast *Candida albicans* and certain *Aspergillus* moulds when tested by the direct plate method (van der Vyver & Lötter, 1971). It did not seem to possess any phototoxic activity (Weimarck & Nilsson, 1980). The molecule is planar; the distance of the Cl atom from the least-squares plane of all non-H atoms is 0·21 (9) Å. The packing is unexceptional. Related structures: 2-hydroxy-4-ω,ω-dichloroacetophenone (Chattopadhyay & Mazumdar, 1984) and 2,2-dichloro-2′-hydroxy-4′-methoxyacetophenone (Chattopadhyay, Banerjee, Mazumdar & Podder, 1985).

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Acta Cryst. (1988). C**44**, 1144–1147

The Structure of the Ethylenediammonium Salt of 3-Nitro-1,2,4-triazol-5-one, $C_2H_4(NH_3)_2.2C_2N_4O_3H$*

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(*Received* 22 *September* 1987; *accepted* 5 *February* 1988)

Abstract. $C_6H_{12}N_{10}O_6$, $M_r = 320·22$, triclinic, $P\bar{1}$, $a = 6·528$ (3), $b = 10·780$ (2), $c = 14·236$ (3) Å, $\alpha = 81·11$ (2), $\beta = 87·13$ (3), $\gamma = 74·05$ (3)°, $V = 951·73$ Å^3, $Z = 3$, $D_x = 1·676$ Mg m^{-3}, λ(Mo $K\alpha_1$) = 0·70926 Å, $\mu = 0·14$ mm^{-1}, $F(000) = 498$, room temperature, final $R = 0·030$ for 1693 observed reflections [$I > 2\sigma(I)$] out of 2469 independent reflections. There are 1·5 formula units in the asymmetric unit.

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* This work was performed under the auspices of the US Department of Energy.

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0108-2701/88/061144-04$03.00

Table 1. *Final least-squares parameters for the ethylenediammonium salt of* 3-*nitro*-1,2,4-*triazol*-5-*one* (*positional parameters for* C,N,O × 10^4)

Equivalent isotropic $U \times 10^2 = \frac{1}{3}\sum_i U_{ii}$.

	x	y	z	U_{eq}(Å^2)
Anion 1				
C(1)	−2618 (3)	4992 (2)	−0467 (2)	2·8 (2)
C(2)	−1640 (4)	2953 (3)	−0337 (2)	2·8 (3)
N(1)	−2168 (3)	3498 (2)	−1251 (2)	3·3 (2)
N(2)	−2809 (3)	4825 (2)	−1345 (1)	3·3 (2)
N(3)	−1953 (3)	3937 (2)	0187 (1)	3·1 (2)
N(4)	−3155 (3)	6301 (2)	−0224 (2)	3·9 (2)
O(1)	−0969 (3)	1746 (2)	−0058 (1)	3·9 (2)
O(2)	−2986 (3)	6406 (2)	0609 (1)	5·7 (2)
O(3)	−3779 (3)	7213 (2)	−0858 (1)	5·9 (2)
Anion 2				
C(3)	2307 (3)	1582 (3)	6407 (2)	3·2 (3)
C(4)	3495 (4)	−0450 (3)	6624 (2)	3·4 (3)
N(5)	2913 (3)	0007 (2)	5701 (2)	3·7 (3)
N(6)	2141 (3)	1327 (2)	5551 (1)	3·5 (2)
N(7)	3089 (3)	0597 (2)	7094 (1)	3·5 (2)
N(8)	1688 (3)	2933 (2)	6564 (2)	4·4 (3)
O(4)	4286 (3)	−1631 (2)	6946 (1)	4·6 (2)
O(5)	1855 (3)	3162 (2)	7362 (2)	7·0 (3)
O(6)	1026 (3)	3773 (2)	5872 (2)	5·8 (2)
Anion 3				
C(5)	7219 (3)	1849 (3)	6481 (2)	3·0 (3)
C(6)	3808 (4)	6126 (3)	3777 (2)	3·2 (3)
N(9)	3973 (3)	6635 (2)	4575 (1)	3·4 (2)
N(10)	6697 (3)	2031 (2)	5588 (1)	3·5 (2)
N(11)	6997 (3)	2881 (2)	6928 (1)	3·3 (2)
N(12)	8051 (3)	0531 (2)	6969 (2)	3·8 (3)
O(7)	4345 (3)	4909 (2)	3720 (1)	4·2 (2)
O(8)	8524 (3)	0390 (2)	7804 (1)	5·4 (2)
O(9)	8226 (3)	−0366 (2)	6507 (1)	5·7 (2)
Ethylenediammonium cation 1				
C(7)	4878 (4)	0217 (3)	9472 (2)	3·3 (3)
N(13)	2736 (4)	0215 (3)	9165 (2)	3·5 (2)
Ethylenediammonium cation 2				
C(8)	−0592 (4)	3524 (3)	2439 (2)	4·0 (3)
C(9)	−0363 (4)	3277 (3)	3496 (2)	3·3 (3)
N(14)	−2813 (4)	3686 (3)	2168 (2)	3·7 (2)
N(15)	1895 (4)	3103 (3)	3747 (2)	4·0 (3)

Thus one en cation lies on a center of symmetry. The bond distances and angles in the three anions are very similar. Rings are planar within 0·01 Å and the entire anions are planar within 0·04 Å. The nitro groups are rotated less than 1° out of the ring planes. All H atoms except those on the C atoms are involved in hydrogen bonds. The remaining H on each of the anions is clearly in the 1 position of the 1,2,4-triazole ring.

Experimental. Title compound (ENTO) prepared by adding ethylenediamine to 3-nitro-1,2,4-triazole-5-one (NTO) dissolved in methanol (Lee & Coburn, 1985). Pale yellow crystals for X-ray diffraction crystallized from methanol. Selected crystal *ca* 0·13 × 0·13 × 0·51 mm. CAD-4 diffractometer, θ–2θ scan. Scan range $(0\cdot8 + 0\cdot34\tan\theta)^\circ$. Scan speed 0·4 to 5·5° min^{-1}. Background first and last 1/6 of scan. Graphite-monochromated Mo $K\alpha$ radiation. Unit cell, 25 reflections $7 < \theta < 21^\circ$, no absorption corrections, $(\sin\theta)/\lambda_{\max} = 0\cdot540$ Å^{-1}, index range $-7 \leq h \leq 7$, $-11 \leq k \leq 11$, $-15 \leq l \leq 15$, 4417 reflections measured and averaged to yield 2469 unique reflections of which 1693 were observed with $I > 2\sigma(I)$, $R_F = 0\cdot018$. Standard reflections $\bar{1}09$ and 060 showed no significant variation. Least squares minimized $\sum w(\Delta F)^2$ with $w = [\sigma_c^2(F) + 0\cdot03F^2]^{-1}$, $\sigma_c^2(F)$ based on counting statistics. Structure could not be solved by *MULTAN* (Germain, Main & Woolfson, 1971). Structure was solved by *RANTAN* (Jia-Xing, 1983) which is part of the *TEXRAY* structure analysis codes.* Scale factor, positional parameters, anisotropic thermal parameters for C, N, O, and isotropic thermal parameters for H were refined. Final $R = 0\cdot030$, $wR = 0\cdot037$, $S = 1\cdot5$. Max. $\Delta/\sigma = 5 \times 10^{-4}$. Final ΔF Fourier synthesis $-0\cdot17 < \Delta\rho < 0\cdot20$ e Å^{-3}. Scattering factors f (RHF for C, N, O and SDS for H), f', f'' from *International Tables for X-ray Crystallography* (1974). Calculations on CRAY-1 using the Los Alamos Crystal Structure System developed primarily by A. C. Larson.†

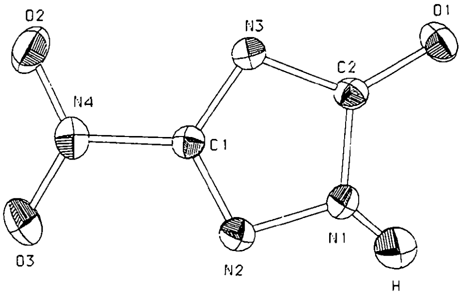

Fig. 1. *ORTEP* (Johnson, 1965) drawing of anion 1 to show atom-numbering scheme. Thermal ellipsoids are 30% probability.

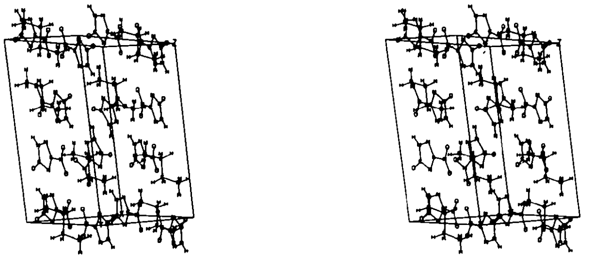

Fig. 2. Stereo drawing of the structure. The origin is at the lower right. Hydrogen bonds are dotted.

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* Molecular Structure Corporation, 3304 Longmire Drive, College Station, TX 77840, USA.

† Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bonds and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44757 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and angles* (°)

Anion 1		Anion 2		Anion 3	
C(1)–N(2)	1·307 (3)	C(3)–N(6)	1·307 (3)	C(5)–N(10)	1·304 (3)
C(1)–N(3)	1·338 (3)	C(3)–N(7)	1·333 (3)	C(5)–N(11)	1·336 (3)
C(1)–N(4)	1·449 (3)	C(3)–N(8)	1·450 (3)	C(5)–N(12)	1·451 (3)
C(2)–N(1)	1·363 (3)	C(4)–N(5)	1·364 (3)	C(6)–N(9)	1·358 (3)
C(2)–N(3)	1·354 (3)	C(4)–N(7)	1·357 (3)	C(6)–N(11)	1·356 (3)
C(2)–O(1)	1·260 (3)	C(4)–O(4)	1·257 (3)	C(6)–O(7)	1·276 (3)
N(1)–N(2)	1·363 (3)	N(5)–N(6)	1·359 (3)	N(9)–N(10)	1·370 (3)
N(4)–O(2)	1·222 (3)	N(8)–O(5)	1·216 (3)	N(12)–O(8)	1·219 (3)
N(4)–O(3)	1·220 (3)	N(8)–O(6)	1·236 (3)	N(12)–O(9)	1·228 (3)
N(2)–C(1)–N(3)	118·5 (2)	N(6)–C(3)–N(7)	118·8 (2)	N(10)–C(5)–N(11)	119·4 (2)
N(2)–C(1)–N(4)	119·6 (2)	N(6)–C(3)–N(8)	118·5 (2)	N(10)–C(5)–N(12)	119·5 (2)
N(3)–C(1)–N(4)	121·9 (2)	N(7)–C(3)–N(8)	122·7 (2)	N(11)–C(5)–N(12)	121·2 (2)
N(1)–C(2)–O(1)	124·6 (2)	N(5)–C(4)–O(4)	124·6 (3)	N(9)–C(6)–O(7)	124·4 (2)
N(3)–C(2)–O(1)	127·8 (2)	N(7)–C(4)–O(4)	128·2 (2)	N(11)–C(6)–O(7)	126·9 (2)
C(2)–N(1)–N(2)	111·6 (2)	C(4)–N(5)–N(6)	111·8 (2)	C(6)–N(9)–N(10)	110·8 (2)
C(1)–N(2)–N(1)	100·1 (2)	C(3)–N(6)–N(5)	100·0 (2)	C(5)–N(10)–N(9)	100·0 (2)
C(1)–N(3)–C(2)	102·2 (2)	C(3)–N(7)–C(4)	102·1 (2)	C(5)–N(11)–C(6)	101·1 (2)
C(1)–N(4)–O(2)	117·2 (2)	C(3)–N(8)–O(5)	118·0 (2)	C(5)–N(12)–O(8)	118·0 (2)
C(1)–N(4)–O(3)	118·0 (2)	C(3)–N(8)–O(6)	117·4 (2)	C(5)–N(12)–O(9)	117·3 (2)
O(2)–N(4)–O(3)	124·8 (2)	O(5)–N(8)–O(6)	124·6 (3)	O(8)–N(12)–O(9)	124·7 (2)

Ethylenediammonium cation 1		Ethylenediammonium cation 2	
C(7)–C(7)	1·5069 (4)	C(8)–C(9)	1·495 (3)
C(7)–N(13)	1·487 (3)	C(8)–N(14)	1·475 (4)
		C(9)–N(15)	1·489 (3)
C(7)–C(7)–N(13)	110·3 (1)	C(9)–C(8)–N(14)	110·9 (2)
		C(8)–C(9)–N(15)	109·7 (2)

X–H···*Y*	Symmetry operation on *Y*	*d*(*X*–*Y*) (Å)	*d*(H···*Y*) (Å)	*X*–H···*Y* (°)
N(1)–H(3)···O(1)	−*x* *y* 1−*z*	2·789 (3)	1·93 (3)	155 (2)
N(1)–H(4)···N(8)	*x* *y* *z*	2·919 (3)	2·00 (3)	164 (2)
N(1)–H(5)···O(1)	*x* *y* 1+*z*	2·811 (3)	1·87 (3)	159 (2)
N(2)–H(10)···O(4)	1−*x* −*y* 1−*z*	2·758 (3)	1·83 (3)	164 (3)
N(2)–H(11)···O(7)	−1+*x* *y* *z*	3·034 (3)	2·20 (3)	143 (3)
N(2)–H(12)···N(4)	*x* *y* *z*	2·834 (3)	1·90 (4)	159 (3)
N(3)–H(13)···N(9)	*x* *y* *z*	2·939 (3)	2·07 (4)	156 (3)
N(3)–H(14)···O(7)	*x* *y* *z*	2·834 (3)	1·97 (3)	154 (3)
N(3)–H(15)···O(4)	1−*x* −*y* 1−*z*	2·787 (3)	1·90 (3)	150 (2)
N(6)–H(1)···N(12)	−1+*x* *y* −1+z	2·886 (3)	2·07 (3)	158 (2)
N(10)–H(2)···N(13)	1−*x* −*y* 1−*z*	3·025 (3)	2·24 (3)	164 (2)
N(14)–H(3)···O(7)	1−*x* 1−*y* 1−*z*	2·807 (3)	1·80 (3)	160 (2)

Fig. 1 is a drawing of anion 1 and shows the atom-numbering scheme. Final parameters are given in Table 1. Bond lengths and angles are given in Table 2. A stereo drawing of the structure is shown in Fig. 2.

Related literature. No structures of 1,2,4-triazole anions were found in the literature. The nitro-group parameters are nearly identical to those found in bis-(3-nitro-1,2,4-triazolyl-5) dihydrate (Nikitina, Starova, Frank-Kramenetskaya & Pevzner, 1982). Structures are known for numerous substituted 1,2,4-triazole rings; see *e.g.* Reck & Just (1982), Valkonen, Pitkanen & Pajunen (1985), and Dupont, Dideberg & Jamoulle (1984). The structure of 1,2,4-triazole itself is given by Jeffrey, Ruble & Yates (1983). The reported bond lengths in the ring vary considerably and the present dimensions are within the reported range.

NTO is a good insensitive explosive (Lee & Coburn, 1985). ENTO is even more insensitive having an ERL Type 12 (Federov & Sheffield, 1975) drop-weight impact sensitivity greater than 320 cm. It is thought that extensive hydrogen bonding leads to impact insensitivity, although an interesting counter example of that view is given by Oyumi, Rheingold & Brill (1987) for trinitroethylnitroguanidine.

Structures of other small explosive molecules are given by Cromer, Coburn, Ryan & Wasserman (1986) (1-methyl-2,3,4,5-tetranitropyrrole) and by Cromer, Ryan & Coburn (1987) (3,5-dinitroisoxazole).

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Acta Cryst. (1988). C**44**, 1147–1148

trans-1,2,5-Triphenylsilacyclopentane

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(*Received* 16 *November* 1987; *accepted* 23 *February* 1988)

Abstract. $C_{22}H_{22}Si$, $M_r = 314{\cdot}5$, monoclinic, $P2_1/c$, $a = 17{\cdot}446$ (3), $b = 5{\cdot}8572$ (12), $c = 18{\cdot}348$ (3) Å, $\beta = 111{\cdot}41$ (2)°, $V = 1746$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}195$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) = 0·71073 Å, $\mu = 1{\cdot}3$ cm^{-1}, $F(000) = 672$, $T = 297$ K, $R = 0{\cdot}045$ for 1972 observations (of 3618 unique data). Si—C distances are 1·891 (3) and 1·889 (4) Å within the silacyclopentane ring, and 1·863 (2) Å to the phenyl group. The five-membered ring assumes a nearly perfect twist or half-chair conformation, with the twist axis through the Si atom.

Experimental. Clear prism, dimensions 0·22 × 0·30 × 0·35 mm, mounted on a glass fiber, space group from systematic absences: $h0l$, $l = 2n$; $0k0$, $k = 2n$, cell dimensions from setting angles for 24 reflections having $10 \leq \theta \leq 15°$. Data collection on Enraf–Nonius CAD-4 diffractometer, Mo $K\alpha$ radiation, graphite mono-

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters*

	x	y	z	B_{eq}(Å^2)
Si	0·80471 (4)	0·0961 (1)	0·82533 (4)	2·99 (1)
C2	0·8800 (1)	0·3391 (4)	0·8638 (1)	3·18 (6)
C3	0·8790 (2)	0·3755 (5)	0·9466 (2)	4·58 (7)
C4	0·7913 (2)	0·3455 (6)	0·9430 (2)	4·81 (7)
C5	0·7591 (1)	0·1136 (5)	0·9041 (1)	3·65 (6)
C6	0·9652 (1)	0·3224 (4)	0·8613 (1)	3·12 (6)
C7	0·9965 (2)	0·4995 (5)	0·8301 (2)	3·86 (6)
C8	1·0757 (2)	0·4912 (6)	0·8309 (2)	4·79 (7)
C9	1·1254 (2)	0·3069 (6)	0·8625 (2)	4·64 (7)
C10	1·0954 (2)	0·1277 (5)	0·8932 (2)	4·31 (7)
C11	1·0161 (1)	0·1358 (5)	0·8922 (2)	3·74 (6)
C12	0·6677 (1)	0·0760 (5)	0·8835 (1)	3·27 (6)
C13	0·6401 (2)	−0·1173 (5)	0·9104 (2)	4·11 (7)
C14	0·5571 (2)	−0·1508 (5)	0·8943 (2)	4·65 (7)
C15	0·5007 (2)	0·0072 (6)	0·8516 (2)	4·70 (7)
C16	0·5273 (2)	0·1977 (6)	0·8246 (2)	4·63 (7)
C17	0·6095 (2)	0·2305 (5)	0·8398 (2)	4·11 (7)
C18	0·7342 (1)	0·1351 (4)	0·7216 (1)	2·95 (5)
C19	0·6776 (2)	−0·0324 (5)	0·6835 (2)	4·19 (7)
C20	0·6284 (2)	−0·0136 (6)	0·6050 (2)	5·04 (8)
C21	0·6351 (2)	0·1743 (6)	0·5630 (2)	5·05 (8)
C22	0·6900 (2)	0·3427 (6)	0·5993 (2)	5·06 (8)
C23	0·7393 (2)	0·3233 (5)	0·6775 (2)	4·12 (7)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Bond lengths* (Å), *angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

Si—C2	1·891 (2)	C10—C11	1·379 (4)
Si—C5	1·892 (3)	C12—C13	1·390 (4)
Si—C18	1·865 (2)	C12—C17	1·377 (3)
C2—C3	1·541 (4)	C13—C14	1·383 (4)
C2—C6	1·508 (4)	C14—C15	1·371 (4)
C3—C4	1·520 (4)	C15—C16	1·370 (5)
C4—C5	1·542 (4)	C16—C17	1·372 (4)
C5—C12	1·516 (3)	C18—C19	1·387 (3)
C6—C7	1·390 (4)	C18—C23	1·390 (4)
C6—C11	1·393 (3)	C19—C20	1·386 (4)
C7—C8	1·379 (4)	C20—C21	1·373 (5)
C8—C9	1·374 (4)	C21—C22	1·367 (4)
C9—C10	1·382 (5)	C22—C23	1·382 (3)
C2—Si—C5	96·0 (1)	C6—C11—C10	121·4 (3)
C2—Si—C18	113·5 (1)	C5—C12—C13	119·9 (2)
C5—Si—C18	117·9 (1)	C5—C12—C17	122·4 (2)
Si—C2—C3	102·5 (2)	C13—C12—C17	117·7 (2)
Si—C2—C6	120·0 (2)	C12—C13—C14	120·8 (2)
C3—C2—C6	113·9 (2)	C13—C14—C15	120·3 (3)
C2—C3—C4	108·4 (2)	C14—C15—C16	119·2 (3)
C3—C4—C5	108·3 (3)	C15—C16—C17	120·6 (3)
Si—C5—C4	102·5 (2)	C12—C17—C16	121·4 (3)
Si—C5—C12	120·0 (2)	Si—C18—C19	120·8 (2)
C4—C5—C12	114·7 (2)	Si—C18—C23	122·2 (2)
C2—C6—C7	120·3 (2)	C19—C18—C23	116·9 (2)
C2—C6—C11	122·0 (2)	C18—C19—C20	121·7 (3)
C7—C6—C11	117·7 (2)	C19—C20—C21	119·9 (3)
C6—C7—C8	120·9 (3)	C20—C21—C22	119·5 (2)
C7—C8—C9	120·6 (3)	C21—C22—C23	120·4 (3)
C8—C9—C10	119·6 (3)	C18—C23—C22	121·5 (3)
C9—C10—C11	119·8 (3)		
C5—Si—C2—C3	13·8 (2)	C2—C3—C4—C5	52·9 (3)
C2—Si—C5—C4	13·3 (2)	C3—C4—C5—Si	−38·2 (2)
Si—C2—C3—C4	−38·6 (3)		

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0108-2701/88/061147-02$03.00