N7	−0.1314 (5)	0.5527 (2)	0.69979 (12)	0.0325 (7)
C8	−0.2937 (6)	0.5135 (3)	0.6576 (2)	0.0322 (8)
N9	−0.4367 (5)	0.6041 (2)	0.63339 (11)	0.0273 (6)
C1′	−0.6362 (6)	0.5932 (3)	0.58475 (15)	0.0271 (7)
C2′	−0.5775 (6)	0.6472 (3)	0.51328 (15)	0.0268 (7)
C3′	−0.4109 (6)	0.5695 (3)	0.47173 (14)	0.0271 (7)
O3′	−0.3880 (5)	0.6204 (2)	0.40286 (11)	0.0391 (6)
C4′	−0.5090 (5)	0.4421 (3)	0.46598 (14)	0.0279 (7)
C41′	−0.3616 (6)	0.3559 (3)	0.4239 (2)	0.0356 (8)
O41′	−0.1237 (4)	0.3582 (2)	0.44553 (13)	0.0439 (6)
O4′	−0.5425 (4)	0.3936 (2)	0.53593 (10)	0.0312 (6)
C5′	−0.7075 (6)	0.4624 (3)	0.5752 (2)	0.0314 (8)

Table 2. *Selected geometric parameters (Å, °)*

N1—C2	1.361 (4)	C8—N9	1.375 (4)
N1—C6	1.389 (4)	N9—C1′	1.479 (4)
C2—N3	1.331 (4)	C1′—C5′	1.513 (5)
C2—N2	1.346 (4)	C1′—C2′	1.519 (4)
N3—C4	1.345 (4)	C2′—C3′	1.509 (5)
C4—C5	1.383 (4)	C3′—O3′	1.429 (4)
C4—N9	1.387 (4)	C3′—C4′	1.521 (4)
C5—N7	1.381 (4)	C4′—O4′	1.444 (4)
C5—C6	1.416 (4)	C4′—C41′	1.505 (5)
C6—O6	1.232 (4)	C41′—O41′	1.431 (5)
N7—C8	1.304 (4)	O4′—C5′	1.427 (4)
C2—N1—C6	125.0 (2)	C8—N9—C4	106.2 (2)
N3—C2—N2	119.8 (3)	C8—N9—C1′	127.9 (2)
N3—C2—N1	124.1 (3)	C4—N9—C1′	125.9 (2)
N2—C2—N1	116.1 (3)	N9—C1′—C5′	111.3 (2)
C2—N3—C4	112.1 (2)	N9—C1′—C2′	110.6 (2)
N3—C4—C5	127.9 (3)	C5′—C1′—C2′	109.2 (2)
N3—C4—N9	127.1 (3)	C3′—C2′—C1′	112.7 (2)
C5—C4—N9	105.0 (3)	O3′—C3′—C2′	108.3 (2)
N7—C5—C4	111.0 (3)	O3′—C3′—C4′	109.5 (2)
N7—C5—C6	129.8 (3)	C2′—C3′—C4′	109.1 (2)
C4—C5—C6	119.2 (3)	O4′—C4′—C41′	109.2 (3)
O6—C6—N1	121.0 (3)	O4′—C4′—C3′	109.1 (2)
O6—C6—C5	127.5 (3)	C41′—C4′—C3′	114.4 (3)
N1—C6—C5	111.5 (3)	O41′—C41′—C4′	112.1 (3)
C8—N7—C5	104.8 (3)	C5′—O4′—C4′	111.8 (2)
N7—C8—N9	113.1 (3)	O4′—C5′—C1′	113.0 (3)

Table 3. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N7^{i}	0.99 (4)	1.83 (4)	2.784 (3)	160 (3)
N2—H2*A*···O6^{i}	1.02 (4)	1.98 (4)	2.978 (4)	164 (3)
N2—H2*B*···O41′^{ii}	0.85 (4)	2.31 (4)	3.132 (4)	161 (3)
O3′—H3′2···N3^{iii}	0.77 (6)	2.10 (6)	2.864 (4)	176 (3)
O41′—H41′···O4′^{iv}	1.12 (4)	1.72 (4)	2.841 (3)	175 (3)

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

Scattering factors, dispersion corrections and absorption coefficients were taken from *International Tables for Crystallography*, (1992, Vol. C, Tables 6.1.1.4, 4.2.6.8 and 4.2.4.2).

Data collection and data reduction: *XSCANS* (Siemens, 1994). Program used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program used to refine structure and to prepare material for publication: *SHELXL*93 (Sheldrick, 1993) and *SHELXTL/PC*.

This work was supported by the Research Council of KU Leuven (Belgium). LVM is a Senior Research Associate of the National Fund for Scientific Research (Belgium).

References

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Eschenmoser, A. (1993). *Proceedings of the R. A. Welch Foundation 37th Conference on Chemical Research: 40 Years of the DNA Double Helix*, October 25–26, Houston, Texas.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Herdewijn, P., De Winter, H., Doboszewski, B., Verheggen, I., Augustyns, A., Hendrix, C., Saison-Behmoaras, T., De Ranter, C. & Van Aerschot, A. (1994). *Carbohydrate Modifications in Antisense Research, Hexopyronosyl-like Oligonucleotides, ACS Symposium Series*, No. 580, pp. 80–99.

Saenger, W. (1984). *Principles of Nucleic Acid Structure*. New York: Springer.

Sheldrick, G. M. (1990). *SHELXTL/PC User's Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Siemens (1994). *XSCANS User's Manual*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Taylor, R. & Kennard, O. (1982). *J. Am. Chem. Soc.* **104**, 3209–3212.

Van Aerschot, A., Verheggen, I., Hendrix, C. & Herdewijn, P. (1995). *Angew. Chem.* **107**, 1483–1485.

Verheggen, I., Van Aerschot, A., Toppet, S., Snoeck, R., Janssen, G., Balzarini, J., De Clercq, E. & Herdewijn, P. (1993). *J. Med. Chem.* **36**, 2033–2040.

Verheggen, I., Van Aerschot, A., Van Meervelt, L., Rozenski, J., Wiebe, L., Snoeck, R., Andrei, G., Balzarini, J., Claes, P., De Clercq, E. & Herdewijn, P. (1995). *J. Med. Chem.* **38**, 826–835.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DE1015). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1996). C**52**, 1215–1218

First Example of a Crystalline Urazole Nucleoside: (1*R*,2*R*)-Urazole-α-D-pyranosyl-2-deoxyriboside

Paul D. Robinson,[a] Cal Y. Meyers,[b] Vera M. Kolb[c] and Patricia A. Colloton[c]

[a]*Department of Geology, Southern Illinois University, Carbondale, IL 62901-4324, USA,* [b]*Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, IL 62901-4409, USA, and* [c]*Department of Chemistry, University of Wisconsin-Parkside, Kenosha, Wisconsin 53141-2000, USA. E-mail: robinson@geo.siu.edu*

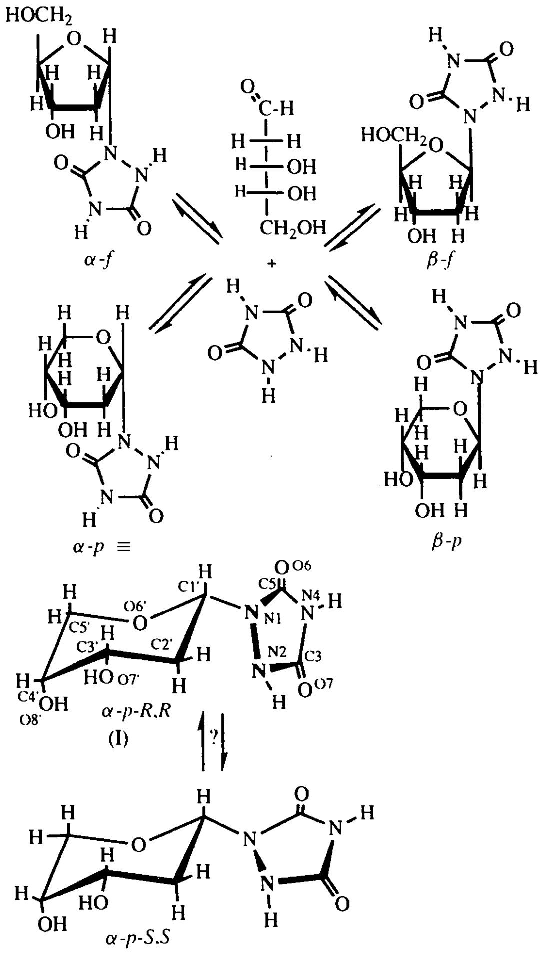
(Received 27 October 1995; accepted 22 November 1995)

Abstract

The first example of a crystalline urazole nucleoside has been synthesized from the reaction of D-deoxyribose with urazole and characterized by X-ray crystallography as a single α-pyranoside diastereomer [IUPAC name: 1-(2-deoxy-α-D-*erythro*-pentopyranosyl)-1(*R*),2(*R*),4-triazolidine-3,5-dione, $C_7H_{11}N_3O_5$]. The pyranosyl group and H atom on the two pyramidal hydrazidic N atoms have an *R*,*R*-*trans* configuration, and the H atom on the trigonal imidic N atom is coplanar with the ring. Intermolecular hydrogen bonding is extensive and involves pyranose–pyranose, pyranose–urazole and urazole–urazole interactions. Each molecule is linked *via* eight hydrogen bonds to six surrounding molecules in which the urazole hydrazidic N(H) atom and imidic N atom are donors and carbonyl O atoms are acceptors, and the pyranose hydroxylic O atoms are donors as well as acceptors. The pyranose ring O atom does not participate in conventional hydrogen bonding but may be involved in a weak intermolecular C—H···O interaction.

Comment

Urazole, a heterocyclic hydrazine-based compound, is a prebiotic mimic of uracil, the hydrogen-bonding moieties of the two being identical (Kolb, Dworkin & Miller, 1994). Urazole has a prebiotic advantage over uracil in making nucleosides with ribose (ribosides); the urazole ribosides form spontaneously upon mixing urazole and ribose in aqueous solution (Kolb *et al.*, 1994). Urazole ribosides are unique in that they exist as a mixture of furanose (*f*) and pyranose (*p*) forms of the ribose component, of which the *β-p* form predominates, as it does in ribose itself (Kolb *et al.*, 1994). Present-day nucleosides, however, are found in the *f* form exclusively, thus leading to the common *f*-ribonucleic acids (RNA). The *p*-nucleosides could have had a greater role in prebiotic RNA; artificially made *p*-RNA exhibits great stability and the ability to form linear duplexes and the latter may be better suited for replication than traditional *f*-RNA under primitive-Earth conditions (Pitsch, Wenderborn, Jaun & Eschenmoser, 1993). No crystal structure of a prebiotically important urazole nucleoside has been reported previously because of their failure to form appropriate crystals. We were ultimately successful in this task. From the reaction of urazole with D-2-deoxyribose in aqueous solution at room temperature, a mixture was obtained which contained four urazole deoxyribosides identified in solution as the α-furanoside (*α-f*), β-furanoside (*β-f*), α-pyranoside (*α-p*) and β-pyranoside (*β-p*), illustrated in the scheme below. After *ca* 50 days, crystals began to separate; ^{1}H and ^{13}C NMR spectra suggested they represented a single compound suitable for X-ray analysis.



The X-ray structure identified the crystals as (1*R*,2*R*)-urazole-α-D-pyranosyl-2-deoxyriboside, (I), the first example of a crystalline urazole nucleoside and a rare example of a pyranose nucleoside. Fig. 1 shows the molecular structure of (I) along with the atom-numbering scheme. Crystalline (I) is a single diastereomer whose urazole ring is essentially planar, the mean deviation from the plane being 0.041 Å. The edge-on view of the urazole moiety, Fig. 2, clearly shows its stereochemistry. The *R*,*R* chirality of the pyramidal hydrazidic N1,N2 atoms arises from the *trans* juxtaposition of C1′ of the D-deoxyribose ring and H2, which imposes torsion angles of −74.6 (19) for C1′—N1—N2—H2, −148.7 (2) for C1′—N1—C5—N4, and −143 (2)° for H2—N2—C3—N4. In contrast, the imidic N4 atom is trigonal planar, the torsion angles being −179 (2) for H4—N4—C3—N2 and −174 (2)° for H4—N4—C5—N1. Full resonance involving imidic N4 with both C=O groups is readily effected by the coplanarity of O6—C5—N4—C3—O7, with torsion angles of −177.9 (2) for O6—C5—N4—C3 and −175.4 (2)° for O7—C3—N4—C5. The overall geometric parameters and chiral aspects of the urazole moiety of crystalline (I) are very similar to those we reported for crystalline (1*R*,2*R*)-1-methylurazole and (1*R*,2*R*)-4-methylurazole in their respective racemic mixtures (Meyers, Lutfi, Kolb & Robinson, 1994; Meyers, Lutfi, Hou & Robinson, 1995; *cf.* Tenon, Carles & Aycard, 1995; Belaj, 1992; Baker, Timberlake, Alender, Majeste & Trefonas, 1982).

The hydrogen-bond data in Table 3 show that intermolecular hydrogen bonding is extensive and involves pyranose–pyranose, pyranose–urazole and urazole–urazole interactions. Each molecule is linked *via* eight hydrogen bonds to six surrounding molecules in which the urazole hydrazidic N2 atom and imidic N4 atom are donors and carbonyl O6 and O7 atoms are accep-

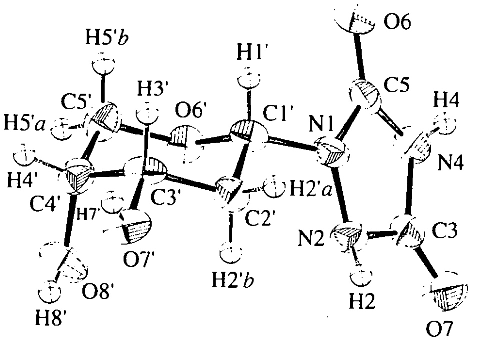


Fig. 1. The molecular structure of (I) showing the atom-numbering scheme Displacement ellipsoids are at the 50% probability level. H atoms are shown as unlabeled isotropic spheres of arbitrary radii.

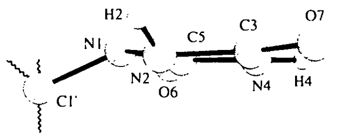


Fig. 2. Edge-on view showing the stereochemistry of the urazole moiety of crystalline (I).

tors, and the pyranose hydroxylic O7′ and O8′ atoms are donors as well as acceptors. These strong intermolecular hydrogen bonds no doubt contribute to the high melting point (475–476 K) of (I). While the pyranose ring O atom (O6′) does not participate in hydrogen bonding with N—H or O—H, a situation also observed in ribofuranosides (Birnbaum, Blonski, & Hruska, 1983), the possibility of a weak C3′—H3′···O6′ intermolecular interaction was noted (*cf.* Glusker, Lewis & Rossi, 1994). The exclusively chiral-selective intermolecular hydrogen bonding we observed in crystalline racemic 1-methylurazole (an *R*,*R* enantiomer hydrogen bonds to two *R*,*R* enantiomers and two *S*,*S* enantiomers, and *vice versa*; Meyers *et al.*, 1994) and crystalline racemic 4-methylurazole (an *R*,*R* enantiomer hydrogen bonds to one *R*,*R* enantiomer and three *S*,*S* enantiomers and *vice versa*; Meyers *et al.*, 1995) cannot be observed with crystalline (I), whose urazole moiety is singularly *R*,*R* configured.

The exclusive formation of the crystalline *R*,*R* diastereomer is a question of concern. Whether it is the exclusive kinetic product of asymmetric induction during its formation, or that both diastereomers are formed and equilibrate in solution and the *R*,*R* diastereomer selectively crystallizes, is a problem now being investigated.

Experimental

After a period of 50 d at room temperature, a 0.1 *M* aqueous solution of urazole and 2-deoxyribose contained a mixture of 40% urazole 2-deoxyribosides in a ratio of α-*p*:β-*p*:α-*f*:β-*f* = 4:2:1:1, and 60% of unreacted 2-deoxyribose in a corresponding ratio of 2:2:1:1 (determined by ^{1}H NMR). The crystals that separated from this solution were isolated and dried and identified as (I); m.p. 475–476 K (corr.) with decomposition. ^{13}C NMR (DMSO-d_6), δ: 31.64 (C2), 66.32 (C5), 67.67 (C3), 68.54 (C4), 80.72 (C1), 154.94 (C=O) and 155.22 p.p.m. (C=O). Detailed experimental data and the surprisingly faster rate of the reaction of 2-deoxyribose compared with ribose are reported elsewhere (Kolb & Colloton, 1996).

Crystal data

$C_7H_{11}N_3O_5$
M_r = 217.18
Monoclinic
$P2_1$
a = 8.539 (2) Å
b = 5.229 (6) Å
c = 10.268 (3) Å
β = 97.20 (2)°
V = 454.9 (8) Å^3
Z = 2
D_x = 1.585 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 9.18–10.43°
μ = 0.13 mm^{-1}
T = 296 K
Bladed fragment
0.47 × 0.31 × 0.12 mm
Colorless

Data collection

Rigaku AFC-5*S* diffractometer
$\omega/2\theta$ (rate 3° min^{-1} in ω, 3 reps. max)
Absorption correction: ψ scans (North, Phillips & Mathews, 1968)
$T_{\min}$ = 0.94, $T_{\max}$ = 1.00
1789 measured reflections
898 independent reflections

821 observed reflections [$I > \sigma(I)$]
$R_{\rm int}$ = 0.022
$\theta_{\max}$ = 25°
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 6$
$l = -12 \rightarrow 12$
3 standard reflections monitored every 100 reflections intensity decay: 0.3%

Refinement

Refinement on F
R = 0.027
wR = 0.029
S = 1.23
821 reflections
147 parameters
Only coordinates of H2, H4, H7′, H8′ refined; others riding (C—H = 0.95 Å)
$w = 4F_o^2/\sigma^2(F_o^2)$
$(\Delta/\sigma)_{\max}$ = 0.0001
$\Delta\rho_{\max}$ = 0.11 e Å^{-3}
$\Delta\rho_{\min}$ = −0.16 e Å^{-3}

Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.3.1)
Absolute configuration: determined from the known absolute chirality of the D-2-deoxyribopyranosyl moiety

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O6	0.34628 (17)	0.5429	0.49037 (13)	0.0432 (5)
O7	0.4127 (2)	1.0390 (6)	0.13312 (15)	0.0519 (6)
N1	0.2318 (2)	0.5448 (6)	0.27431 (16)	0.0325 (5)
N2	0.2373 (2)	0.7213 (7)	0.16998 (18)	0.0340 (6)
N4	0.4115 (2)	0.8333 (6)	0.33455 (17)	0.0383 (7)

C3	0.3607 (2)	0.8832 (7)	0.2034 (2)	0.0352 (7)
C5	0.3328 (2)	0.6316 (7)	0.3790 (2)	0.0329 (7)
O6′	−0.01648 (17)	0.6263 (5)	0.33418 (13)	0.0326 (5)
O7′	−0.2245 (2)	0.0626 (6)	0.08408 (15)	0.0396 (5)
O8′	−0.3053 (2)	0.5707 (5)	0.15080 (16)	0.0440 (6)
C1′	0.0827 (3)	0.4305 (7)	0.29228 (19)	0.0311 (7)
C2′	0.0047 (2)	0.2999 (6)	0.1700 (2)	0.0319 (7)
C3′	−0.1496 (3)	0.1831 (6)	0.1992 (2)	0.0311 (7)
C4′	−0.2542 (3)	0.3869 (7)	0.24896 (19)	0.0348 (8)
C5′	−0.1633 (3)	0.5227 (7)	0.3642 (2)	0.0371 (8)

Table 2. *Selected geometric parameters (Å, °)*

O6—C5	1.226 (3)	O6′—C1′	1.429 (3)
O7—C3	1.209 (3)	O6′—C5′	1.434 (3)
N1—N2	1.419 (3)	O7′—C3′	1.419 (3)
N1—C5	1.369 (3)	O8′—C4′	1.421 (3)
N1—C1′	1.439 (3)	C1′—C2′	1.509 (3)
N2—C3	1.362 (3)	C2′—C3′	1.516 (3)
N4—C3	1.387 (3)	C3′—C4′	1.520 (4)
N4—C5	1.360 (3)	C4′—C5′	1.509 (3)
N2—N1—C5	107.5 (2)	N1—C1′—O6′	107.9 (2)
N2—N1—C1′	118.71 (18)	N1—C1′—C2′	112.7 (2)
C5—N1—C1′	121.17 (17)	O6′—C1′—C2′	111.00 (19)
N1—N2—C3	108.17 (18)	C1′—C2′—C3′	108.73 (17)
C3—N4—C5	111.4 (2)	O7′—C3′—C2′	109.01 (17)
O7—C3—N2	126.8 (2)	O7′—C3′—C4′	111.6 (2)
O7—C3—N4	127.8 (2)	C2′—C3′—C4′	110.3 (2)
N2—C3—N4	105.4 (2)	O8′—C4′—C3′	112.16 (18)
O6—C5—N1	125.7 (2)	O8′—C4′—C5′	108.6 (2)
O6—C5—N4	127.9 (2)	C3′—C4′—C5′	109.1 (2)
N1—C5—N4	106.4 (2)	O6′—C5′—C4′	112.76 (18)
C1′—O6′—C5′	111.1 (2)		

Table 3. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O7′ⁱ	0.87 (2)	1.86 (2)	2.727 (4)	173 (3)
N4—H4···O6ⁱⁱ	0.89 (3)	1.91 (2)	2.789 (4)	169 (2)
O7′—H7′···O8′ⁱⁱⁱ	0.81 (4)	1.97 (4)	2.771 (5)	170 (2)
O8′—H8′···O7ⁱᵛ	0.82 (3)	2.27 (3)	2.949 (4)	140 (3)

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *PROCESS* in *TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *LS* in *TEXSAN*. Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *FINISH* in *TEXSAN*, *PLATON* (Spek, 1990).

Thanks are expressed by PAC for a NASA Undergraduate Research Scholarship, administered through the Wisconsin Space Grant Consortium, and for a University of Wisconsin-Parkside Scholarship. CYM is grateful to Southern Illinois University-Carbondale for supporting this research through Distinguished Professorship research funding.

Lists of structure factors, torsion angles, least-squares-planes data, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1140). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Baker, R. J., Timberlake, J. W., Alender, J. T., Majeste, R. & Trefonas, L. M. (1982). *Cryst. Struct. Commun.* **11**, 763–768.
Belaj, F. (1992). *Acta Cryst.* C**48**, 1088–1090.
Birnbaum, G. I., Blonski, W. J. P. & Hruska, F. E. (1983). *Can. J. Chem.* **61**, 2299–2304.
Glusker, J. P., Lewis, M. & Rossi, M. (1994). *Crystal Structure Analysis for Chemists and Biologists*, pp. 632, 634. New York: VCH.
Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Kolb, V. M. & Colloton, P. A. (1996). American Chemical Society, National Meeting, New Orleans, March 24–29. Accepted.
Kolb, V. M., Dworkin, J. P. & Miller, S. L. (1994). *J. Mol. Evol.* **38**, 549–557.
Meyers, C. Y., Lutfi, H. G., Hou, Y.-Q. & Robinson, P. D. (1995). American Chemical Society, National Meeting, Chicago, August 20–24. Abstract ORGN 296.
Meyers, C. Y., Lutfi, H. G., Kolb, V. M. & Robinson, P. D. (1994). *Acta Cryst.* C**50**, 1925–1928.
Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Pitsch, S., Wenderborn, S., Juan, B. & Eschenmoser, A. (1993). *Helv. Chim. Acta*, **76**, 2161–2183.
Sheldrick, G. M. (1985). *SHELXS*86. *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford University Press.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.
Tenon, J. A., Carles, M. & Aycard, J.-P. (1995). *Acta Cryst.* C**51**, 1440–1442.

Acta Cryst. (1996). C**52**, 1218–1220

1,1-Diamino-2,2-dicyanoethene

Christopher S. Frampton

Roche Research Centre, PO Box 8, Welwyn Garden City, Hertfordshire AL7 3AY, England. E-mail: framptoc@rwep03.dnet.roche.com

(*Received 26 October 1995; accepted 20 November 1995*)

Abstract

The molecule of the title nitrile [1,1-diamino-2,2-ethenedicarbonitrile, $C_4H_4N_4$] is planar and exhibits a high degree of electron delocalization. It is compared with its two structural isomers of the same formula.

Comment

Although the crystal structures of diaminofumaronitrile, (I) (Yamada, Nagashima, Iwashita, Nakamura & Kumashiro, 1968), and its *cis*-isomer diaminomaleonitrile,