range effects by means of a Fourier synthesis with coefficients $(F_o - F_H)\ \lambda^2/\sin^2\theta$ where F_H is the contribution of H_O to the structure factor. Potentials are then added for neutral spherical Hartree–Fock atoms (except for H_O). The electrostatic potential in the O—H—O region is a basin with a minimum of $-1{\cdot}13\ e\ \text{Å}^{-1}$ at the twofold axis. Alternative H_O sites are near the walls, but are located in a flattened region where there would not be a strong electrostatic force directed towards the central minimum.

Related literature. Ammonium dihydrogenphosphate and related isomorphous crystals have been extensively studied because of their piezoelectric properties. The X-ray structure has been determined for tetragonal $NH_4H_2PO_4$ at 153 K and for the antiferroelectric orthorhombic structure at 143 K (Keeling & Pepinsky, 1955). Following these studies of the structure in projection, the structure has been redetermined three-dimensionally at 152 K and 143 K by Fukami, Akahoshi, Hukuda & Yagi (1987) and at room temperature by Khan & Baur (1973). Because of interest in the O—H—O system, the structure was also determined in projection by neutron diffraction for the tetragonal form at ambient temperature (Tenzer, Frazer & Pepinsky, 1958). High-resolution neutron diffraction data for the isomorphous KH_2PO_4 have been used to show that the proton in the O—H—O system is distributed bimodally (Kuhs, Nelmes & Tibballs, 1983), although no details were given.

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Structure of Caesium Dicyanamide

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Abstract. $Cs[(CN)_2N]$, $M_r = 199{\cdot}0$, monoclinic, $C2/c$, $a = 9{\cdot}385\ (5)$, $b = 12{\cdot}702\ (9)$, $c = 8{\cdot}261\ (5)$ Å, $\beta = 110{\cdot}94\ (4)°$, $V = 920\ (2)$ Å^3, $Z = 8$, $D_m = 2{\cdot}86$, $D_x = 2{\cdot}873\ (3)$ Mg m^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu = 8{\cdot}0$ mm^{-1}, $F(000) = 704$, $T = 299\ (1)$ K, $R = 0{\cdot}050$ for 1012 reflections.

Experimental. The crystals of the title compound were prepared as very thin plates by dropping a freshly obtained (through ion exchange) aqueous solution of dicyanamide $[NH(CN)_2]$ into an aqueous solution of Cs_2CO_3, and then allowing water to evaporate at ambient temperature. D_m by flotation in $C_2H_4Br_2/CH_2I_2$. Crystal 0·55 × 0·40 × 0·04 mm was cut from a larger one, and placed in a capillary. Syntex $P2_1$ diffractometer, lattice parameters from 15 reflections with 2θ between 18 and 28° (Mo $K\alpha$), variable $\omega/2\theta$ scan, $4 < 2\theta < 60°$, two standards every 50 reflections, mean relative e.s.d. of the control reflections 2·4%, index range $h\ 0 \rightarrow 13$, $k\ -17 \rightarrow 17$, $l\ -11 \rightarrow 10$. 2890 intensities measured of which 2034 had $I \geq 3\sigma(I)$ and of which 1012 were unique, R_{int} (after absorption corrections) = 0·0335. Absorption corrections with *DIFABS* (Walker & Stuart, 1983) between 0·620 and 1·396. Structure was solved with *SHELX*86 (Sheldrick, 1986) and refined with *SHELX*76 (Sheldrick, 1976). Neutral atom scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV), real and imaginary components of anomalous dispersion included for all atoms. Final full-matrix least-squares refinement based on F with all atoms anisotropic, $R = 0{\cdot}0500$,

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Table 1. *Atomic coordinates and equivalent U factors* (Å^2)

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

	x	y	z	U_{eq}
Cs1	0	−0·0191 (1)	0·25	0·0660 (3)
Cs2	0·5	0·1219 (1)	0·25	0·0668 (3)
N1	0·0969 (13)	0·1733 (10)	0·0696 (13)	0·084 (3)
N2	0·2249 (14)	0·3226 (10)	0·2446 (15)	0·090 (3)
N3	0·1801 (12)	0·4131 (10)	0·4814 (13)	0·082 (3)
C1	0·1511 (12)	0·2464 (9)	0·1577 (12)	0·063 (3)
C2	0·1941 (12)	0·3676 (8)	0·3710 (14)	0·065 (3)

Table 2. *Bonds lengths* (Å) *and angles* (°) *in the dicyanamide anion*

N1—C1	1·18 (2)	N2—C2	1·31 (2)
C1—N2	1·26 (2)	C2—N3	1·13 (2)
N1—C1—N2	172 (2)	N3—C2—N2	173 (2)
C1—N2—C2	124 (2)		

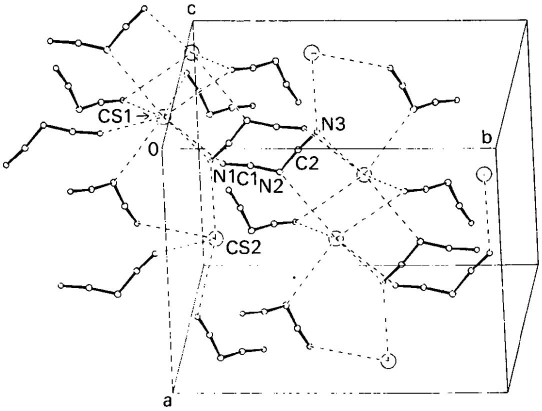

Fig. 1. View of the crystal structure. The dashed lines represent the Cs—N contacts shorter than 3·4 Å.

wR = 0·0496, the maximum shift/e.s.d. was 0·002, $\Delta\rho$ between − 1·09 and 1·27 e Å^{-3} and the highest peaks were around the Cs$^+$ ions, $w = 1/\sigma^2(F)$, 56 parameters refined. Table 1 presents final atomic parameters, the geometry of the dicyanamide anion is shown in Table 2 and the *ORTEP*II (Johnson, 1976) view of the crystal packing is given in Fig. 1.*

Related literature. The theoretically predicted and the observed geometry of the dicyanamide anion was discussed by Jensen, Klewe & Tjelta (1977) and its coordination properties by Kapshuk & Skopenko (1986).

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54108 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of an Fe–S Cluster Complex

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Abstract. Hexacarbonyl-1κ^3C,2κ^3C-μ-methoxymethanethiolato-μ-benzenethiolatodiiron(*Fe–Fe*), [$Fe_2(C_2H_5OS)(C_6H_5S)(CO)_6$], M_r = 466·04, monoclinic, $P2_1/n$, a = 9·023 (3), b = 12·081 (5), c = 16·720 (11) Å, β = 97·04°, V = 1808 (2) Å^3, Z = 4, D_x = 1·71 Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 1·90 mm^{-1}, F(000) = 936, room temperature, R = 0·038 for 1490 reflections with $I > 3\sigma(I)$. The two Fe

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