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The Crystal Structure of KI.Hg(CN)$_2$*

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Crystals of KI.Hg(CN)$_2$ are orthorhombic:

$$a_0=4\cdot412,\ b_0=16\cdot190,\ c_0=9\cdot690\ \text{Å (all } \pm 0\cdot004\ \text{Å}),\ Z=4\ .$$

Of the possible space groups, $Cmc2_1$, $C2cm$ and $Cmcm$, the centric group $Cmcm$ was selected. The crystal structure was refined to $R=0\cdot097$ using Mo $K\alpha$ radiation with counter data out to 2θ of 50°.

Linear Hg(CN)$_2$ groups are incorporated normal to sheets consisting of iodine atoms weakly bound to the central mercury atom. The sheets are puckered at a 140° dihedral angle about the strings of iodines parallel to a_0. Each mercury atom is coordinated to four iodine atoms and conversely each iodine atom is surrounded by four mercury atoms. Hg–I bond lengths are 3·383 Å, lying between the 2·75 Å predicted for covalent single bond radii and the 3·70 Å from van der Waals contact radii. The Hg–C distance of 2·079 Å is near the 1·986 Å measured in Hg(CN)$_2$ but is shorter than 2·20 Å predicted for single bond covalent radii. Adjacent sheets are held together by the K$^+$ ions.

Introduction

In the system Hg(CN)$_2$.KI.H$_2$O or HgI$_2$.KCN.H$_2$O the only complex solid phase obtained is KI.Hg(CN)$_2$ (Aggarwal & Mehrota, 1958). Infra-red absorption spectra of the solid phase, KI.Hg(CN)$_2$, and of aqueous solutions of this and related mercuric cyanide complexes have been obtained at this laboratory (Penneman & Jones, 1961). The crystal structure analysis of KI.Hg(CN)$_2$ is the first of a series of investigations of the crystal chemistry of complex cyanides and halides.

Experimental

Potassium iododicyanomercurate(II) was prepared by evaporating at room temperature an aqueous solution containing potassium iodide and mercuric cyanide in the molar ratio 1:1. KI.Hg(CN)$_2$ formed from solution as colorless lath-shaped crystals. Recrystallized material kept in a closed container remains stable for long periods of time. However, KI.Hg(CN)$_2$ decomposed on exposure to X-rays in a photochemical process which apparently occurred over a period of four to six weeks rendering the crystals metallic black in color. It was also noticed that some samples, when left in an open dish in laboratory atmosphere, developed a crust of red HgI$_2$ crystals. Thermogravimetric analysis of pure, fresh KI.Hg(CN)$_2$ showed no composition change in the sample until the melting point was approached.

X-ray diffraction data and optical properties are given in Table 1. Partial X-ray powder diffraction data are given in Table 2. The long lath-shaped crystals will give preferred orientation effects unless the sample is very thoroughly ground.

Table 1. KI.Hg(CN)$_2$ *crystallographic data*

X-Ray diffraction data

Diffraction symmetry: Includes space groups $Cmc2_1(C_{2v}^{12})$, $C2cm(C_{2v}^{16})$, $Cmcm(D_{2h}^{17})$. Studies suggest $Cmcm$ to be the correct space group assignment.

Cell dimensions: $a_0=4\cdot412$; $b_0=16\cdot190$; $c_0=9\cdot690$ Å.
(λ Cu $K\alpha=1\cdot5418$ Å).
$a_0:b_0:c_0=0\cdot273:1:0\cdot599$; cell volume $=692\cdot2$ Å^3.
Formula weights per cell: 4.
Formula weight: 422·4.
Density: $3\cdot9_4$ g.cm.$^{-3}$ (X-ray); $4\cdot0_4$ g.cm.$^{-3}$ (pycnometric).

Optical properties

Biaxial negative.
Refractive indices (5893 Å):

$$n_x=1\cdot718\pm0\cdot005,\quad n_y=1\cdot84\pm0\cdot01,\quad n_z=1\cdot88\pm0\cdot01;$$

geometric mean 1·81. Molecular refractivity 45·9 cm.$^{-3}$.
Optic orientation: $X=b$, $Y=a$, $Z=c$.
Optical axial angle: $2V=60°\pm2°$, dispersion moderate $r>v$.
Colorless.

The lath-like crystals could be easily cleaved and the chunky pieces were shaped to ellipsoids in a Bond sphere grinder. Specimens used for the collection of intensity data were ellipsoids with no axial ratio greater than two. An ellipsoid was prepared and the data were collected over a short period of time (four days) using Mo $K\alpha$ radiation and a proportional counter on the G. E. goniostat. Four monitor spots were used throughout the run to insure that no decomposition had occurred. Intensities for a total of 380 unique reflections were obtained by averaging equivalent reflections from a total of 775 measured and of the 380 examined, 306 were above background.

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Table 2. KI.Hg(CN)$_2$. *Partial powder diffraction data*

	I				
hkl	obs.	calc.	d_o	d_c	$\sin^2\theta_c$
020	95	100	8·071	8·095	0·0091
021	25	9	6·166	6·212	0·0154
002	4	2	4·841	4·845	0·0253
110	40	10	4·251	4·257	0·0328
022	50	13	4·145	4·157	0·0344
040	70	22	4·034	4·048	0·0363
111	—	1	—	3·897	0·0391
041	45	10	3·724	3·735	0·0426
130	4	2	3·412	3·416	0·0509
131	100	17	—	3·221	0·0573
112		88	3·196	3·198	0·0581
042	15	4	3·098	3·106	0·0616
023	20	5	2·995	3·000	0·0660
132	80	34	2·787	2·791	0·0763
060	10	2	2·692	2·698	0·0816
150	50	11	2·605	2·610	0·0872
061	—	4	—	2·599	0·0880
113	—	1	—	2·573	0·0898
043	20	2	2·517	2·525	0·0932
151		3		2·521	0·0935
004	35	11	2·418	2·422	0·1013
062	60	13	2·352	2·357	0·1069
133		6		2·347	0·1079
024	45	11	2·319	2·321	0·1103
152	40	8	2·296	2·298	0·1125
200	35	10	2·204	2·206	0·1221

I_o: Relative peak intensities, from diffractometer measurements.

I_c: Final atomic parameters (Table 3), average overall temperature factor, $B=3{\cdot}2$, not absorption corrected.

d_o: Philips 114·6 mm. powder camera, Straumanis mounting $\lambda(\text{Cu } K\alpha)=1{\cdot}5418$ Å.

Prior to averaging the equivalent reflections, an empirical absorption correction was applied. For KI.Hg(CN)$_2$ the $\mu(\text{Mo } K\alpha)=311$ cm.$^{-1}$ and the average 0·04 mm. specimen diameter gave $\mu r=0{\cdot}6$. The absorption correction was made up of a spherical absorption effect modified for the ellipsoidal specimen shape by coefficients from an empirical curve obtained from measurements on the crystal itself. Though this constituted an improvement in the data, the non-spherical absorption effect proved to be the largest source of error in the refinement of the structure. Corrections for the usual Lorentz-polarization factors were applied to the unique reflections.

Structure determination

The systematic absences (*hkl*: $h+k$ odd and *h0l*: (h odd) l odd) were characteristic of three space groups, $Cmc2_1$, $C2cm$ and $Cmcm$. Throughout the experimental phase of this investigation there was no indication of non-centric symmetry. Also, since a Wilson plot indicated a centric space group, $Cmcm$ was chosen as the most probable space group. An *0kl* Patterson projection revealed the y and z parameters of the Hg, I and K$^+$ atoms. Then a full *hkl* Patterson function was computed for x sections at 0, $\frac{1}{8}$, $\frac{1}{4}$, $\frac{3}{8}$ and $\frac{1}{2}$ and from it were deduced approximate x, y, z parameters for the three heavier atoms. Mercury was placed at the origin and a few least-squares cycles were computed in order to obtain better y parameters for I and K$^+$ as well as approximate scale and isotropic temperature factors. Following this, a full $F_o(hkl)$ Fourier was computed using phases from the last least-squares cycle. The C and N peaks appeared near the Hg on a line nearly parallel to the y axis. Polarized infrared spectra from a single crystal confirmed this orientation of the cyanides.

Least-squares refinement with all five atoms and isotropic temperature factors essentially completed the refinement with an R factor of 0·120. Further least-squares runs were made using anisotropic thermal parameters and the additional variables helped bring the R factor to below 0·100, but with little change in position parameters of the atoms. Both an F_o Fourier and a ΔF Fourier were computed using the final parameters. No false or spurious peaks were observed.

All computational work was performed on an IBM 704 using codes prepared at Los Alamos by A. C. Larson, D. T. Cromer, and F. H. Kruse. Scattering factor values were generated within the computer using the exponential expression of Forsyth & Wells (1959). In the final stages of refinement, possible anomalous dispersion effects in mercury were examined by carrying out least-squares calculations using an f_{Hg} expression successively reduced by one electron increments. The resulting R factors and sums of residuals squared indicated no improvement in the structure and thus no anomalous dispersion effects from mercury.

Most least-squares calculations were made with unit weight for the $F_o(hkl)$. When an experimentally determined standard deviation of $I_o(hkl)$ was properly modified and applied to the least-squares calculation, no improvement in the structure was observed. It appears that the main limiting factor in this refinement was the X-ray absorption effect and possibly the chemical stability of the crystal.

Table 3. KI.Hg(CN)$_2$. *Final atomic parameters at* $R=0{\cdot}097$

$(0, 0, 0;\ \frac{1}{2}, \frac{1}{2}, 0)+$

Hg	(a)	$0, 0, 0;\ 0, 0, \frac{1}{2}$
I	(c)	$0, y, \frac{1}{4};\ 0, \bar{y}, \frac{1}{4}$
		$y = 0{\cdot}4480 \pm 0{\cdot}0004$
K$^+$	(c)	$y = 0{\cdot}7641 \pm 0{\cdot}0013$
C	(f)	$0, y, z;\ 0, \bar{y}, z;\ 0, y, \frac{1}{2}-z;\ 0, \bar{y}, \frac{1}{2}+z$
		$y = 0{\cdot}1253 \pm 0{\cdot}0033$
		$z = 0{\cdot}0468 \pm 0{\cdot}0059$
N	(f)	$y = 0{\cdot}1854 \pm 0{\cdot}0030$
		$z = 0{\cdot}0863 \pm 0{\cdot}0068$

The final parameters are given in Table 3. The observed and calculated structure factors are presented in Table 4.

Discussion of the structure

Pertinent bond lengths, contact distances and bond angles are recorded in Table 5. Diagrammatic pictures

Table 4. *Final observed and calculated structure factors for* KI.Hg(CN)$_2$

The column headings are k, F_o and F_c.

If $F_o < 0$ it was unobserved and the minus sign should be interpreted as 'less than'

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H=  0 L=  0   H=  0 L=  1   H=  5 L=  1   H=  5 L=  2   H=  0 L=  4   H=  0 L=  5   H=  1 L=  6   H=  2 L=  7   H=  1 L=  9
 2 270 363     0  28  -0     5  35 -31     3  72  69     2 363 319    10  25   7     7  84  87    12  45  51     7  50 -43
 4 297 349     2 111 101    H=  0 L=  2   H=  0 L=  3    4 321 284    12  51 -55     9  31  36    H=  3 L=  7    9 -30   0
 6 176 177     4 177 176     0 130  90     0  39  -0     6 124 107    14 -23 -17    11  51  55     1 -30   8    11 -30  23
 8 138 130     6 162 165     2 218 182     2 203-161     8 125 119    16  30 -39    13  63  60     3  83  64    H=  2 L=  9
10  85  74     8  49  36     4 155 142     4 117 -96    10  45  46    H=  1 L=  5   15  84  89     5  48  57     0 -30   0
12 103  95    10 -16  19     6 311 339     6 150-141    12  83  79     1  26 -26    H=  2 L=  6    7  48  62     2  54  45
14 100  99    12  78 -82     8 263 282     8  30 -32    14  91  97     3 149-137     0 -26   2     9 -30   5     4  53  60
16 149 148    14  40 -35    10 279 295    10 -19   0    16 102 110     5  70 -68     2  66  80    H=  4 L=  7    6  61  72
18 122 111    16  51 -53    12 177 178    12  69  66    18  94 105     7  82 -83     4  74  83     0 -32  -0     8 -30  30
H=  1 L=  0   18 -23  -7    14 134 130    14  62  64    H=  1 L=  4    9 -23   3     6 142 154     2 -32 -33    H=  3 L=  9
 1 166 154    H=  1 L=  1   16  80  86    16  66  60     1  83  82    11  23  20     8 145 159     4 -32 -41     1 -32  -9
 3 106  94     1  31 -26    18  43  45    18  31  -3     3 134 126    13  70  72    10 147 161    H=  0 L=  8    3 -32 -53
 5 283 285     3 199-194    H=  1 L=  2   H=  1 L=  3    5 198 197    15  53  58    12 102 112     0 260 230    H=  0 L= 10
 7 286 280     5  95 -91     1 395 445     1  45 -39     7 232 228    H=  2 L=  5   14  76  79     2 205 184     0 -30  -4
 9 322 311     7 139-136     3 311 321     3 168 169     9 263 266     0 -25  -0    H=  3 L=  6    4 184 165     2 -31  38
11 230 216     9 -16   9     5 208 197     5 126 125    11 157 171     2  53  55     1 127 160     6  66  65     4  69  67
13 167 159    11 -19  21     7 147 148     7 124 110    13 148 151     4  90  95     3 118 140     8  49  46     6 111 112
15  90  90    13  73  69     9  61  58     9  21  12    15  63  71     6  99 106     5  58  72    10 -26  22     8  99 106
17  76  80    15  58  57    11  88  93    11 -19 -24    17  56  58     8  40  35     7  40  47    12  49  55    H=  1 L= 10
H=  2 L=  0   17 -23  24    13  71  64    13  57 -56    H=  2 L=  4   10 -23   4     9 -26  15    H=  1 L=  8    1 135 144
 0 438 441    H=  2 L=  1   15 129 133    15  28 -26     0 284 311    12  36 -45    11  32  30     1 -28  27     3 113 124
 2 272 257     0 -21  -0    17 105 107    17 -23 -32     2 208 230    14 -23 -16    H=  4 L=  6    3  72  68     5  69  74
 4 263 243     2  82  76    H=  2 L=  2   H=  2 L=  3    4 192 205    H=  3 L=  5    0 -31  -7     5 116 121     7 -30  33
 6 125 118     4 133 120     0  50  50     0 -21  -0     6  77  79     1 -28 -16     2  40  29     7 133 136    H=  2 L= 10
 8 105  92     6 128 120     2 112 121     2 105-104     8  82  82     3  72 -83     4 -30  37     9 149 159     0 -32  -7
10  54  49     8  39  30     4 103 104     4  71 -80    10 -23  31     5  42 -48     6  63  77    11 110 124     2 -32  27
12  69  70    10 -19  12     6 246 239     6 102-104    12  66  59     7  44 -53    H=  0 L=  7   13  91 101     4  40  48
14  82  77    12  66 -64     8 216 212     8  23 -26    14  67  75     9  30  -0     0 -25  -0    H=  2 L=  8    6  72  89
16 119 116    14  31 -30    10 228 224    10 -19  -1    16  85  88    11 -23  15     2  81 -72     0 165 182    H=  0 L= 11
H=  3 L=  0   16  43 -44    12 145 139    12  54  55    H=  3 L=  4   13  56  48     4 102 -90     2 121 145     0 -32   0
 1  58  59    H=  3 L=  1   14 104 102    14  58  51     1 -26  36    H=  4 L=  5    6  85 -74     4 117 129     2  41 -37
 3  62  57     1 -23 -13    16  56  65    16  49  49     3  44  62     0 -30  -0     8 -26 -17     6  40  49     4  64 -54
 5 149 143     3 112-102    H=  3 L=  2   H=  3 L=  3    5  97 112     2  46  32    10 -23  -5     8  46  33    H=  1 L= 11
 7 173 158     5  66 -61     1 214 229     1 -26  -6     7 125 135     4  41  52    12  71  63    10 -30  14     1 -32  14
 9 204 184     7  87 -77     3 168 175     3  86  94     9 164 162     6  59  58    14  51  53    H=  3 L=  8    3  54  60
11 145 130     9 -19   2     5 110 104     5  71  74    11 112 109     8 -26  20    H=  1 L=  7    1 -31  10
13 107 100    11  28  16     7  79  75     7  75  70    13  93  94    H=  0 L=  6    1 -26  10     3  60  37
15  55  54    13  54  47     9  26  26    11 -21 -16    H=  4 L=  4    0  48   6     3 108  97     5  54  75
H=  4 L=  0   15  37  38    11  44  48    13  35 -38     0 131 148     2 143 116     5  82  83     7  61  87
 0 212 182    H=  4 L=  1   13  44  37    H=  4 L=  3    2  99 109     4 128 113     7 101  95    H=  0 L=  9
 2 142 120     0 -28  -0    15  85  83     0 -28  -0     4  84  94     6 229 199     9 -23   6     0  56   0
 4 125 106     2  52  40    H=  4 L=  2    2  52 -48     6  40  34     8 217 204    11  31 -15     2  75  55
 6  48  45     4  70  59     0 -28   8     4  49 -48     8  31  31    10 199 202    13 -26 -30     4  82  71
 8  36  36     6  72  62     2  32  43     6  54 -54    10  31   8    12 140 141    H=  2 L=  7    6  94  88
10 -23  14     8 -21  18     4  46  44     8 -23 -16    H=  0 L=  5   14 101 101     0 -28  -0     8  46  37
12  32  29    10 -23   4     6 118 108    10 -23  -1     0  56  -0    16  45  46     2  48 -58    10 -30   4
H=  5 L=  0   12  41 -34     8 116 105    H=  5 L=  3    2  84  67    H=  1 L=  6    4  61 -73    H=  1 L=  9
 1 -25  11    H=  5 L=  1   10 125 111     1 -32   2     4 154 124     1 267 261     6  58 -61     1  44 -10
 3 -25  17     1 -30  -7    H=  5 L=  2   H=  0 L=  4    6 161 136     3 257 238     8 -26 -15     3  82 -78
 5  65  51     3  52 -45     1  89  91     0 464 433     8  58  43     5 112 121    10  43  -3     5  62 -56
```

Table 5. KI.Hg(CN)$_2$. *Distances and angles*

Bond lengths		Contact distances	
Hg–I	3·383 ± 0·011 Å	N–N	3·172 ± 0·142
Hg–C	2·079 ± 0·096	N–N	3·470 ± 0·142
C–N	1·046 ± 0·139	I–C	3·814 ± 0·097
		I–I	4·412 ± 0·010

K$^+$ coordination

K$^+$–N	3·001 ± 0·107
K$^+$–N	3·360 ± 0·107
K$^+$–I	3·706 ± 0·039

Angles

I–I–I dihedral angle	139·0 ± 1·5°
I–Hg–I (in rectangular plane)	81·4 ± 1·5 98·6 ± 1·5
C–Hg–N (versus 180° expected)	176·5 ± 2·5
Hg–C–N (versus 180° expected)	171·0 ± 8·0
C–Hg–I (versus 90° expected)	85·0 ± 2·5 95·0 ± 2·5

of the structure are presented in Figs. 1 and 2. This structure can be described as consisting of corrugated sheets of I atoms loosely held together by coordination with the mercury atoms of the Hg(CN)$_2$ groups. The Hg(CN)$_2$ portion of the structure is nearly linear and is normal to the plane of I atoms coordinated to it. The 139° dihedral angle in the folds of the sheets comes about from the K$^+$ ion's influence in binding the sheets together. Notice in Fig. 1 that the K$^+$ ion lies between two N atoms in the same *yz* plane and this K$^+$ ion is near the I atoms above and below it. Also, there are at about 3·2 Å two N atoms above and two below the K$^+$ ion. The projection down *z* (Fig. 2) shows the N atoms above and below the K$^+$ ion, actually closer than the two in the *yz* plane of the K$^+$ ion. Thus, the K$^+$ ion can be said to exist in an 8-fold coordination with 6 N atoms and 2 I atoms.

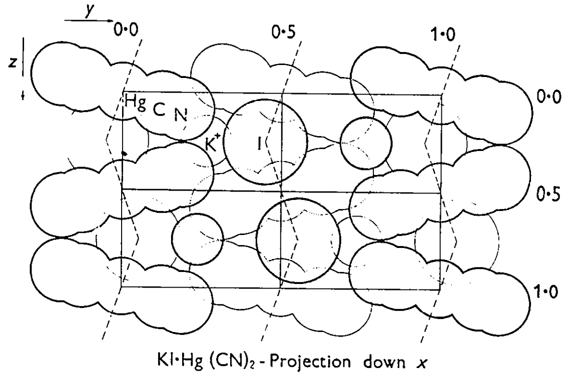

Fig. 1. Structure of KI.Hg(CN)$_2$ viewed down *X* axis. Dashed lines trace corrugated sheets of iodine atoms.

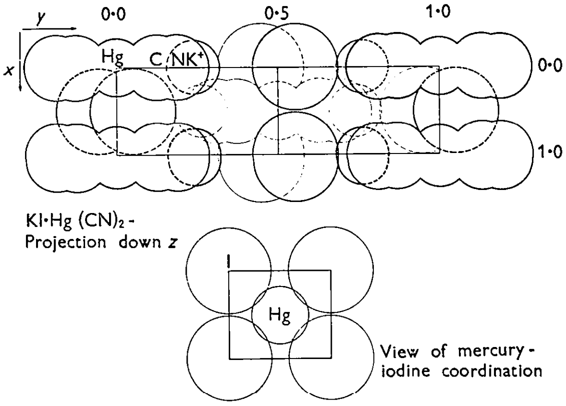

Fig. 2. Structure of KI.Hg(CN)$_2$ viewed down *Z* axis. In the view of Hg–I coordination *X* is vertical and *Z* is the projected horizontal axis.

In the lower portion of Fig. 2 is a view down the Hg(CN)$_2$ axis normal to the rectangular (nearly square) plane of four I atoms nearest the Hg atom. The Hg–I bond length of 3·38 Å lies between the tetrahedral covalent Hg–I single bond length of 2·75 Å and van der Waals contact distance of 3·70 Å. This kind of weak 'equatorial' bonding to mercury has been observed before, as described in review by Wells (1962). Closer approach of iodine to mercury is also prevented by contact between the cyanide carbon and iodine.

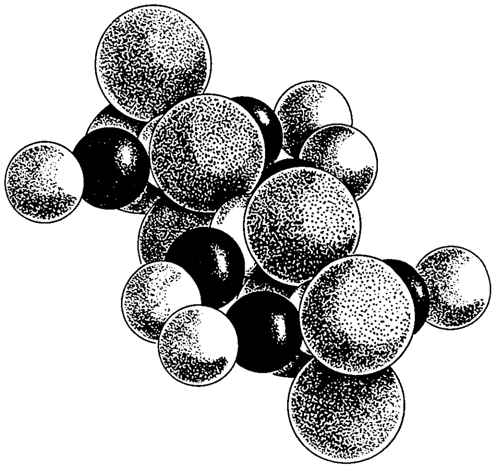

Fig. 3. Sketch of the Hg(CN)$_2$I$^-$ portion of the KI.Hg(CN)$_2$ structure. Large spheres represent iodine atoms; N–C–Hg–C–N groups are apparent.

In KI.Hg(CN)$_2$ the Hg–C bond is 2·079 ± 0·096 Å while in Hg(CN)$_2$ Hvoslef (1958) reports 1·986 ± 0·016 Å and summation of single covalent bond lengths predicts 2·25 Å. Our X-ray diffraction data do not allow resolution of the light atoms as well as in Hvoslef's neutron diffraction experiment. Thus, we found $C \equiv N = 1{\cdot}046 \pm 0{\cdot}139$ Å while Hvoslef obtained 1·186 ± 0·024 Å.

Though the carbon and nitrogen were not located with great precision, the bond angles in the Hg(CN)$_2$ group deviate only slightly from an ideal 180°. In the structure analysis of crystalline Hg(CN)$_2$ Hvoslef (1958) found bond angles which were less than 180° by a number of standard deviations (C–Hg–C = 171 ± 2°, Hg–C–N = 173 ± 2°). Interactions between mercury and nitrogen in Hg(CN)$_2$ account for some

Table 6. KI.Hg(CN)$_2$. *Thermal parameters*

1. Anisotropic thermal parameters, × 10^4 (±5%)

	B_{11}	B_{22}	B_{33}	B_{23}
Hg	491	22	70	−14
I	329	33	38	—
K+	452	29	104	—
C	510	19	58	54
N	812	13	153	−40

2. Magnitudes and direction cosines of the principal axes of the vibration ellipsoids

	Axis	R.m.s. amplitude	B_i	C_{ia}	C_{ib}	C_{ic}
Hg	1	0·22	3·82	1·00	0·0	0·0
	2	0·16	2·01	0·0	0·82	0·58
	3	0·19	2·96	0·0	−0·58	0·82
I	1	0·18	2·56	1·00	0·0	0·0
	2	0·21	3·43	0·0	1·00	0·0
	3	0·13	1·41	0·0	0·0	1·00
K+	1	0·21	3·52	1·00	0·0	0·0
	2	0·20	3·09	0·0	1·00	0·0
	3	0·22	3·91	0·0	0·0	1·00
C	1	0·22	3·97	1·00	0·0	0·0
	2	0·07	0·41	0·0	0·72	−0·69
	3	0·22	3·78	0·0	0·69	0·72
N	1	0·28	6·32	1·00	0·0	0·0
	2	0·11	1·01	0·0	0·97	0·25
	3	0·28	6·08	0·0	−0·25	0·97

of the non-linearity while in KI.Hg(CN)$_2$ the iodine atoms prevent this kind of interaction. Infrared studies of the crystals indicate that the Hg(CN)$_2$ group is linear or nearly linear, ruling out pronounced departure from 180°. Obviously, more precise carbon and nitrogen parameters are needed to resolve this problem conclusively.

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Structure du Di-Nitrosométhane Cis

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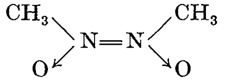
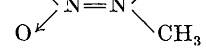


crystallizes in the orthorhombic space group $P2_12_12_1$.

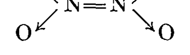
The unit-cell dimensions are: $a = 6·03$, $b = 12·81$, $c = 5·41$ Å; $Z = 4$. The crystal structure was solved by the interpretation of the three-dimensional Patterson function and refined by Fourier and least-squares methods down to a final R value of 0·156 for the 538 observed reflections. The molecule is planar within the experimental errors. The bond lengths and angles are: C–N = 1·47 ± 0·03; N–N = 1·31 ± 0·02; N–O = 1·31 ± 0·02 Å; C–N–O = 120·0 ± 1·5; C–N–N = 121·5 ± 1·5; O–N–N = 119·0 ± 1·5°.

Introduction

Gowenlock & Trotman (1955) ont mis en évidence l'existence de deux isomères géométriques dans le di-nitrosométhane (CH$_3$NO)$_2$:



trans



cis

La structure de l'isomère trans a déjà été déterminée par diffraction des R.X. (Van Meerssche & Germain, 1959). La structure électronique de ce composé a été également étudiée par la méthode des orbitales moléculaires (Van Meerssche & Leroy, 1960). La détermination de la structure de l'isomère cis fait l'objet du présent travail.

Partie expérimentale

Le monomère CH$_3$NO se forme lors de l'irradiation du nitrite de butyle tertiaire par les rayons U.V. (Coe & Doumani, 1948):

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