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The Crystal Structure of Cyclotrimethylene-trinitramine

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The structure of cyclotrimethylene-trinitramine (RDX), $C_3H_6N_6O_6$, has been refined from single-crystal neutron-diffraction data. The final weighted R index for 836 independent reflections is 0·021. The compound crystallizes in the orthorhombic space group $Pbca$, $a=13{\cdot}182$ (2), $b=11{\cdot}574$ (2), $c=10{\cdot}709$ (2) Å, $Z=8$. The molecule consists of alternate CH_2 and N–NO_2 groups in a puckered ring. The environment of the carbon atoms is essentially tetrahedral, and the N–NO_2 groups are planar. The molecule possesses a plane of approximate mirror symmetry perpendicular to the plane defined by the three carbon atoms. The thermal motion may be described by rigid-body motion of the ring and separate rigid-body motion of the nitro groups.

Introduction

The compound cyclotrimethylene-trinitramine, $C_3H_6N_6O_6$, also known as Cyclonite, or by the code designation RDX, is a well known explosive. There are two known polymorphic forms, designated RDX(I) and RDX(II) (McCrone, 1950). The structure of RDX(II) has not been determined because of the difficulty of obtaining and preserving well formed crystals, even for short periods, owing to its extreme instability. This paper describes the refinement of the structure of RDX(I); it will be referred to hereafter simply as RDX.

The crystal structure of RDX was first investigated by Hultgren (1936). He reported that it possesses orthorhombic symmetry, with eight molecules per unit cell and most probable space group $V_h^{15}(Pbca)$. A complete crystal morphology has been reported by McCrone (1950). The crystal structure of RDX was reinvestigated by Harris & Reed (1959) using three-dimensional X-ray photographic data. They determined the complete crystal structure except for the hydrogen positions. The present study was undertaken to complete the crystal structure by determining the hydrogen positions and refining overall structural details.

Experimental

The unit-cell dimensions were determined by a least-squares fit to scattering angles measured by X-ray diffraction. For this, the scattering angles (2θ) of the 30 most intense reflections having scattering angles in the range 35 to 60° were measured on an automated Picker 4-circle diffractometer with Mo $K\alpha$ radiation monochromated by a pyrolytic graphite plate. The unit-cell dimensions thus obtained are, $a=13{\cdot}182$ (2), $b=11{\cdot}574$ (2), $c=10{\cdot}709$ (2) Å, and $D_x=1{\cdot}806$. The observed density is reported as $D_m=1{\cdot}816$ (Federoff & Sheffield, 1966) and the melting point is 205 °C (McCrone, 1950).

A crystal, approximately $1{\cdot}4\times1{\cdot}2\times0{\cdot}9$ mm, was used for this experiment. The crystal was mounted on a four-circle neutron diffractometer controlled by a computer (Alperin & Prince, 1970). The crystal was oriented with its a axis nearly, but not exactly, parallel to the φ axis, in order to avoid systematic effects due to multiple diffraction. The diffraction intensities were measured by the procedure described by Prince (1972). With a neutron wavelength of 1·232 Å and a limiting 2θ angle of 100° there are 1590 independent reflections. The intensity at the peak position of each reflection was compared with the intensities at background positions on either side, and if the peak intensity (I_p) did not exceed background (I_b) by 2σ, where σ is given by $\sigma=(I_p+I_b)^{1/2}$, the reflection was considered to be unobserved. 836 of the 1590 independent reflections had observable intensities. The intensities of all observed reflections were converted to relative structure factors and each was assigned a standard deviation, σ_F, based on counting statistics. The calculated linear absorption coefficient is 1·2 cm^{-1}, assuming an effective incoherent scattering cross-section for hydrogen of 42×10^{-24} cm^2 (Rush, Taylor & Havens, 1962). The maximum variation in F due to absorption is less than ±0·8%. This was considered to be negligible, and no absorption corrections were made.

The positional parameters for the heavy atoms, as determined by Harris & Reed (1959), were used to compute signs for F_o and (F_o-F_c) Fourier syntheses. All hydrogen atom positions were determined from the difference synthesis. Three cycles of least-squares refinement with the program *RFINE* (Finger, 1968) with isotropic temperature factors, gave a weighted R index $\{wR=[\sum w(s|F_o|-|F_c|)^2/\sum wF_c^2]^{1/2}$ where s is the scale factor and $w=1/\sigma_F^2\}$ of 0·093. The refinement was continued

with anisotropic temperature factors for all atoms. An isotropic secondary extinction parameter, S, was included in the refinement, using the formula (Zachariasen, 1968) $F_{cor}=|F_c|(1+S\beta F_c^2)^{-1/4}$, where β is a parameter proportional to the Lorentz factor. The final value of S was $0{\cdot}484\times10^{-3}$ for $\beta=1/\sin 2\theta$. The two strongest reflections, 102 and 200, with calculated extinction factors of 0·7282 and 0·7275 respectively, were omitted from the final stage of refinement because of severe extinction. The final discrepancy indices were $wR=0{\cdot}021$ and $R=0{\cdot}039$ for all observed reflections except the two strongest reflections. The largest parameter shift in the last cycle was less than 0·01 of the standard deviation. The final least-squares parameters are given in Table 1, and the observed and calculated structure factors are listed in Table 2. There was no observable trend in the values of the function $1/s\sum_s w(|F_o|-|F_c|)^2$, where s is the number of reflections in a subset, for subsets of the observed reflections divided according to ranges of F and $\sin\theta/\lambda$. The difference Fourier map obtained after final least-squares refinement was featureless.

Discussion

The heavy atom positions obtained in the present work all agree well with those reported in the previous X-ray study of Harris & Reed (1959), with differences of less than 0·02 Å in bond length and 0·8° in bond angle. The interatomic distances and angles in the RDX molecule, as obtained in the present study, are given in Table 3. The molecule of RDX consists of three N–NO_2 groups linked to three methylene groups alternately to form a puckered, six-membered C–N ring (see Figs. 1 and 2). The N(1)–NO_2 group is essentially

Table 1. *Final least-squares parameters for the structure of RDX*

Thermal parameters are the coefficients, B_{ij} (Å^2), in the form $\exp[-\frac{1}{4}(B_{11}a^{*2}h^2+B_{22}b^{*2}k^2+B_{33}c^{*2}l^2+2B_{12}a^*b^*hk+2B_{13}a^*c^*hl+2B_{23}b^*c^*kl)]$. The estimated standard deviations are in parentheses.

	x/a ($\times10^4$)	y/b ($\times10^4$)	z/c ($\times10^4$)	B_{11} ($\times10^2$)	B_{22} ($\times10^2$)	B_{33} ($\times10^2$)	B_{12} ($\times10^2$)	B_{13} ($\times10^2$)	B_{23} ($\times10^2$)
C(1)	1839 (3)	3578 (3)	4400 (3)	322 (15)	297 (13)	206 (14)	−70 (13)	−69 (11)	7 (12)
C(2)	503 (2)	2440 (2)	3395 (3)	233 (15)	145 (11)	344 (13)	8 (13)	−1 (13)	−17 (11)
C(3)	1487 (2)	3813 (3)	2159 (3)	252 (14)	332 (16)	175 (14)	−34 (13)	34 (11)	−31 (12)
N(1)	1761 (2)	4360 (2)	3330 (2)	267 (8)	266 (8)	251 (9)	−109 (8)	1 (8)	0 (8)
N(2)	877 (2)	2996 (2)	4537 (2)	295 (9)	210 (8)	250 (9)	14 (8)	33 (8)	9 (7)
N(3)	536 (1)	3222 (2)	2329 (2)	211 (9)	228 (8)	274 (9)	15 (8)	−35 (7)	−37 (7)
N(4)	2260 (2)	5379 (2)	3346 (2)	217 (8)	241 (9)	348 (10)	−55 (8)	79 (9)	−26 (9)
N(5)	155 (2)	3525 (2)	5294 (2)	455 (14)	322 (10)	256 (10)	157 (10)	104 (9)	77 (9)
N(6)	−333 (2)	3875 (2)	2078 (2)	284 (11)	306 (10)	316 (10)	72 (9)	−72 (9)	−53 (8)
O(1)	2270 (3)	5932 (3)	2388 (4)	566 (23)	330 (17)	407 (19)	−122 (18)	82 (17)	68 (16)
O(2)	2649 (3)	5687 (3)	4338 (4)	342 (16)	330 (17)	417 (19)	−86 (15)	−13 (16)	−131 (14)
O(3)	−693 (3)	3142 (4)	5262 (4)	333 (21)	718 (26)	426 (20)	138 (21)	153 (17)	156 (19)
O(4)	454 (4)	4271 (3)	5990 (3)	894 (32)	381 (21)	258 (16)	251 (22)	57 (20)	−53 (15)
O(5)	−1121 (3)	3534 (4)	2504 (4)	246 (16)	572 (25)	584 (25)	44 (17)	−62 (16)	22 (21)
O(6)	−236 (4)	4691 (4)	1390 (4)	644 (27)	441 (23)	415 (20)	185 (21)	−91 (20)	62 (18)
H(1)	2401 (6)	2944 (7)	4226 (7)	372 (33)	532 (36)	564 (37)	−14 (30)	−128 (31)	141 (32)
H(2)	2013 (6)	4068 (6)	5244 (6)	762 (43)	560 (37)	270 (29)	−201 (34)	−127 (29)	−59 (28)
H(3)	−261 (5)	2117 (6)	3540 (6)	371 (34)	433 (33)	597 (35)	−146 (29)	−18 (31)	16 (27)
H(4)	1015 (5)	1728 (5)	3192 (7)	464 (30)	263 (26)	594 (37)	89 (27)	−16 (27)	−114 (27)
H(5)	2052 (5)	3166 (6)	1917 (6)	314 (28)	602 (37)	524 (37)	46 (30)	80 (25)	−225 (30)
H(6)	1440 (6)	4432 (7)	1413 (7)	637 (44)	602 (39)	363 (35)	−170 (35)	17 (28)	108 (31)

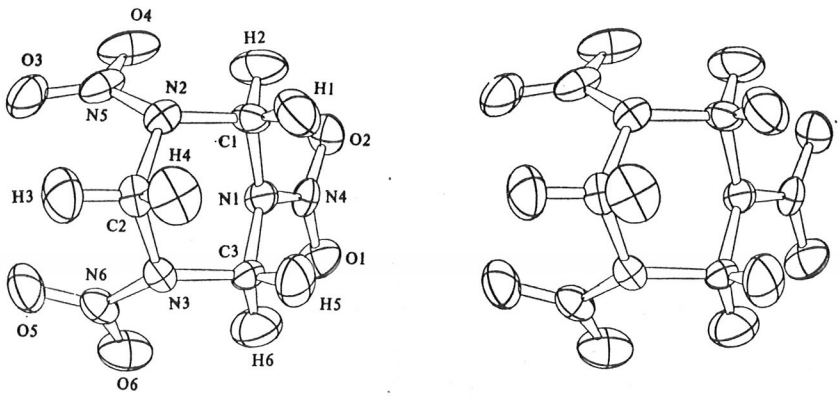

Fig. 1. RDX molecule showing a stereoscopic pair viewed from top of the molecular ring.

coplanar but the N(2)–NO_2 and N(3)–NO_2 groups are slightly bent. The distances of atoms from the best fit mean plane of each N–NO_2 group are given in Table 4. The bond lengths and bond angles of the N(2)–NO_2 and N(3)–NO_2 groups are very similar but the configuration of the N(1)–NO_2 group is quite different. For the N(1)–NO_2 group, the N–N distance is shorter by approximately 0·04 Å, and the C–N–N angles are

Table 2. *Observed and calculated structure factors for RDX*

Unobserved reflections are indicated by an asterisk.

larger by more than 3°. The mean plane of the N(1)–NO_2 group is inclined to the plane defined by the three carbon atoms by only 18°, but the N(2)–NO_2 and N(3)–NO_2 planes are both inclined by 62°. Thus the trigonal molecular symmetry, which might be expected in the free RDX molecule, is not observed in the crystalline state, but there is a pseudo mirror plane passing through the atoms N(4), N(1), C(2), H(3), and H(4). These atoms are essentially coplanar with the plane defined by $0{\cdot}1869x-0{\cdot}1101y+0{\cdot}9762z=3{\cdot}3648$. The atomic distances from the pseudo mirror plane and the inclination angles of the interatomic vectors between the two pseudo mirror symmetric atoms are summarized in Table 5. Only oxygen atoms show significant departures from the mirror symmetric positions. All the pseudosymmetry-related bond lengths and angles in a molecule agree within two standard deviations, with the exception of the N–N–C angles, which disagree by at most 1·5°.

Table 3. *Interatomic distances and angles in RDX*

(*a*) Distances

C(1)–N(1)	1·464 (4) Å	N(1)–N(4)	1·351 (3) Å
C(1)–N(2)	1·443 (4)	N(2)–N(5)	1·392 (3)
C(2)–N(3)	1·468 (4)	N(3)–N(6)	1·398 (3)
C(2)–N(3)	1·458 (4)		
C(3)–N(3)	1·440 (4)	N(4)–O(1)	1·209 (5)
C(3)–N(1)	1·450 (4)	N(4)–O(2)	1·233 (4)
		N(5)–O(3)	1·203 (5)
C(1)–H(1)	1·058 (10)	N(5)–O(4)	1·207 (5)
C(1)–H(2)	1·092 (8)	N(6)–O(5)	1·201 (5)
C(2)–H(3)	1·085 (8)	N(6)–O(6)	1·205 (5)
C(2)–H(4)	1·087 (7)		
C(3)–H(5)	1·088 (8)		
C(3)–H(6)	1·075 (9)		

(*b*) Angles

N(1)–C(1)–N(2)	107·8 (2)°	C(3)–N(1)–C(1)	115·1 (2)°
N(1)–C(1)–H(1)	109·9 (4)	C(3) N(1)–N(4)	120·9 (2)
N(1)–C(1)–H(2)	110·0 (4)	C(1)–N(1)–N(4)	119·7 (2)
N(2)–C(1)–H(1)	108·0 (4)	N(1)–N(4)–O(1)	117·2 (3)
N(2)–C(1)–H(2)	110·0 (5)	N(1)–N(4)–O(2)	117·8 (3)
H(1)–C(1)–H(2)	111·0 (6)	O(1) N(4)–O(2)	125·0 (3)
N(2)–C(2)–N(3)	111·7 (2)	C(1)–N(2)–C(2)	114·6 (2)
N(2)–C(2)–H(3)	110·1 (4)	C(1)–N(2)–N(5)	117·1 (2)
N(2)–C(2)–H(4)	106·9 (4)	C(2)–N(2)–N(5)	116·6 (2)
N(3)–C(2)–H(3)	110·7 (4)	N(2)–N(5)–O(3)	117·2 (3)
N(3)–C(2)–H(4)	107·2 (4)	N(2)–N(5)–O(4)	116·8 (3)
H(3)–C(2)–H(4)	110·1 (6)	O(3)–N(5)–O(4)	125·7 (4)
N(3)–C(3)–N(1)	108·4 (2)	C(2)–N(3)–C(3)	114·8 (2)
N(3)–C(3)–H(5)	107·4 (4)	C(2)–N(3)–N(6)	117·5 (2)
N(3)–C(3)–H(6)	111·1 (4)	C(3)–N(3)–N(6)	115·6 (2)
N(1)–C(3)–H(5)	109·6 (4)	N(3)–N(6)–O(5)	117·3 (3)
N(1)–C(3)–H(6)	111·3 (5)	N(3)–N(6)–O(6)	117·0 (3)
H(5)–C(3)–H(6)	108·8 (6)	O(5)–N(6)–O(6)	125·5 (4)

The methylene groups have essentially tetrahedral configurations, with the bond angles in the range of $109{\cdot}5\pm2°$, and the H–C–H planes perpendicular to the N–C–N planes. The C–H bonds range from 1·06 to 1·09 Å. When corrections for the thermal vibrations are applied by the riding model, they increase to between 1·09 and 1·13 Å.

Table 4. *The atomic distances from the best-fit mean planes of* N–NO_2 *groups*

The mean planes are:

$0{\cdot}8473x-0{\cdot}4601y-0{\cdot}2654z=-1{\cdot}2993$ for N(1)–NO_2
$0{\cdot}2116x-0{\cdot}6696y+0{\cdot}7120z=1{\cdot}3744$ for N(2)–NO_2
$-0{\cdot}1646x-0{\cdot}5725y-0{\cdot}8032z=-4{\cdot}2606$ for N(3)–NO_2.

	N(1)–NO_2	N(2)–NO_2	N(3)–NO_2
N(1)	−0·002		
N(4)	0·008		
O(1)	−0·003		
O(2)	−0·003		
N(2)		0·007	
N(5)		−0·026	
O(3)		0·010	
O(4)		0·009	
N(3)			0·006
N(6)			−0·022
O(5)			0·008
O(6)			0·008
C(1)	0·198	−0·280	
C(2)		−0·536	−0·386
C(3)	0·316		−0·446

Table 5. *Atomic distances from the pseudo mirror plane*

Atoms in plane	Distances	Symmetry-related atom pair	Distances		Angle
N(4)	−0·005 Å	C(1)···C(3)	−1·23 Å	1·23 Å	90°
N(1)	0·006	N(2)···N(3)	−1·21	1·21	90
C(2)	0·003	N(5)···N(6)	−1·76	1·77	89
H(3)	−0·002	O(2)···O(1)	−1·10	1·07	87
H(4)	−0·002	O(3)···O(5)	−1·56	1·47	88
		O(4)···O(6)	−2·46	2·57	89
		H(1)···H(5)	−1·27	1·26	90
		H(2)···H(6)	−2·09	2·10	90

One hydrogen atom in each methylene group is always located very close to oxygen atoms of adjacent nitro groups on both sides, with the distances ranging from 2·22 to 2·30 Å. The C···O intramolecular distances are also short, ranging from 2·63 to 2·68 Å. Although the C–H···O angles, $99\pm1°$, are much smaller than those in conventional hydrogen bonds, the oxygen atoms of the nitro-groups are bound tightly to the molecular ring by strong O···H as well as O···C inter-

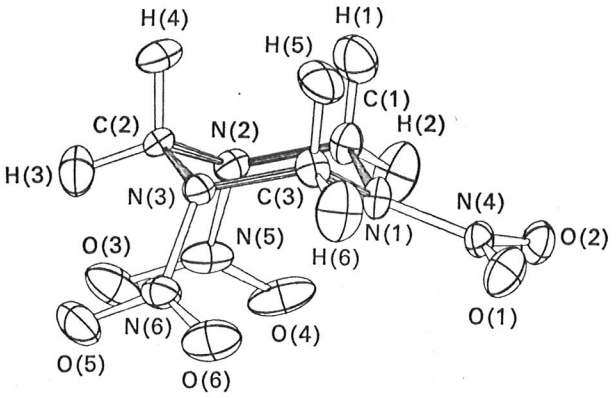

Fig. 2. Side view of the RDX molecule.

actions and tend to form approximately planar C_2N–NO_2 groups. Consequently, we may expect to find some degree of rigidity in the RDX molecule. The rigid body motion analysis by the method of Schomaker & Trueblood (1968) was applied to all the heavy atoms of the molecule, as shown in Table 6. The r.m.s. DELTA $U(I,J)$ was 0·008 Å^2 and the e.s.d. of the DELTA $U(I,J)$ was 0·009. The disagreement with rigid-body molecular motion was greatest for the nitro group atoms. When the rigid-body analysis was applied to the ring atoms alone, the agreement was excellent; the r.m.s. DELTA $U(I,J)$ was 0·0013 Å^2 and the e.s.d. of the DELTA $U(I,J)$ was 0·0019. These facts may suggest that each nitro group possesses an independent libration superimposed upon the molecular libration, as is observed in the other nitro compounds, cyclotetramethylene tetranitramine (Choi & Boutin, 1970) and *s*-trinitrobenzene (Choi & Abel; 1972). The principal axis of the largest molecular libration lies almost exactly on the pseudo mirror plane, and has inclination angles of 34° with the N(1)–N(4) bond and 56° with both the other N–N bonds. Rigid body motion analysis of the nitro group alone is not possible because of the indeterminacy which occurs in the case of planar groups with five or fewer atoms. However, an investigation of the thermal ellipsoids of the nitro-group atoms shows clear evidence of rigid body motion, as shown in Table 7. We define Cartesian coordinate axes (radial, normal, and tangent) to which we refer the directions of the largest root-mean-square displacements, R_3, separately for each atom. For each atom of a nitro group, the radial axis is directed from the ring nitrogen to which the nitro group is attached toward that atom, and the normal axis is perpendicular to both the radial axis and the O···O vector of the nitro group. The normal axis, as defined above, is approximately normal to the best fit mean plane of the N–NO_2 group, with angular deviations of less than 1·5° for all three groups. The largest thermal vibration amplitudes occur in the directions of tangential axes for all atoms except O(1) and O(5), where they are in the normal direction. The direction of the least vibration amplitude is always along the radial axis. This is consistent with rigid-body motion of the nitro group with two dominant modes, one about the normal axis passing through the ring nitrogen atom and the other about a radial axis somewhere near the N–N bond.

Table 6. *Rigid-body motion analysis*

(*a*) Rigid-body motion applied for all heavy atoms

$$\mathbf{T}=\begin{pmatrix}0{\cdot}028 & 0{\cdot}0009 & 0{\cdot}0030\\ & 0{\cdot}0284 & -0{\cdot}0005\\ & & 0{\cdot}0226\end{pmatrix}\quad \mathbf{L}=\begin{pmatrix}0{\cdot}0031 & -0{\cdot}0004 & 0{\cdot}0010\\ & 0{\cdot}0064 & 0{\cdot}0004\\ & & 0{\cdot}0039\end{pmatrix}$$

Principal axes of **L** (°) and their direction cosines

4·6	−0·0700	0·9883	0·1352
3·8	−0·5736	0·0711	−0·8160
2·8	−0·8161	0·1347	0·5620

Displacements of libration axes from the center of mass (Å)

$L_{1,2}=$ 0·057	$L_{1,3}=-0{\cdot}261$
$L_{2,1}=-0{\cdot}424$	$L_{2,3}=-0{\cdot}490$
$L_{3,1}=-0{\cdot}505$	$L_{3,2}=-0{\cdot}705$

(*b*) Rigid-body motion applied for ring atoms alone

$$\mathbf{T}=\begin{pmatrix}0{\cdot}0216 & 0{\cdot}0015 & 0{\cdot}0020\\ & 0{\cdot}0206 & -0{\cdot}0042\\ & & 0{\cdot}0248\end{pmatrix}\quad \mathbf{L}=\begin{pmatrix}0{\cdot}0068 & 0{\cdot}0013 & 0{\cdot}0009\\ & 0{\cdot}0086 & -0{\cdot}0023\\ & & 0{\cdot}0083\end{pmatrix}$$

Principal axes of **L** (°) and their direction cosines

6·0	0·0988	0·7505	−0·6535
5·1	0·7722	0·3563	0·5260
4·0	0·6276	−0·5566	−0·5443

Displacements of libration axes from the center of mass (Å)

$L_{1,2}=-0{\cdot}289$	$L_{1,3}=$ 0·163
$L_{2,1}=-0{\cdot}088$	$L_{2,3}=-0{\cdot}512$
$L_{3,1}=$ 0·229	$L_{3,2}=-0{\cdot}025$

There are several short intermolecular distances in RDX. Those considered to be the most significant are shown in Fig. 3.

It may be interesting to compare the crystal structure of RDX with those of both α- and β-HMX (cyclotetramethylene–tetranitramine) (Cady, Larson & Cromer, 1963; Choi & Boutin, 1970), in view of the close similarity in chemical composition and explosive nature. The bond lengths and angles of RDX agree well with those of α- and β-HMX, except for the C–N–C angles, which are approximately 8° smaller in RDX than in HMX. In both compounds, the N–NO_2 group planes are bound tightly to the molecular ring by strong O···H as well as O···C interactions. The conformation of the N–NO_2 group attachment to the molecular ring in RDX is very similar to that of α-HMX. Very short intermolecular distances occur in both compounds.

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Table 7. *Principal axes of the thermal ellipsoids and orientations of the longest axes*

	R_1	R_2	R_3	Radial	Normal	Tangent	B
N(4)	0·142 (4) Å	0·177 (3) Å	0·225 (3) Å	91°	73°	163°	2·69 Å^2
O(1)	0·170 (6)	0·238 (5)	0·282 (6)	95	31	120	4·34
O(2)	0·156 (7)	0·218 (6)	0·257 (5)	86	73	163	3·63
N(5)	0·161 (4)	0·167 (4)	0·277 (4)	96	87	7	3·44
O(3)	0·167 (6)	0·226 (6)	0·329 (6)	96	100	12	4·93
O(4)	0·158 (7)	0·207 (6)	0·356 (6)	87	91	3	5·11
N(6)	0·164 (4)	0·181 (3)	0·234 (3)	92	86	176	3·02
O(5)	0·170 (6)	0·269 (6)	0·276 (6)	76	164	82	4·67
O(6)	0·183 (7)	0·246 (6)	0·310 (6)	88	107	163	5·00

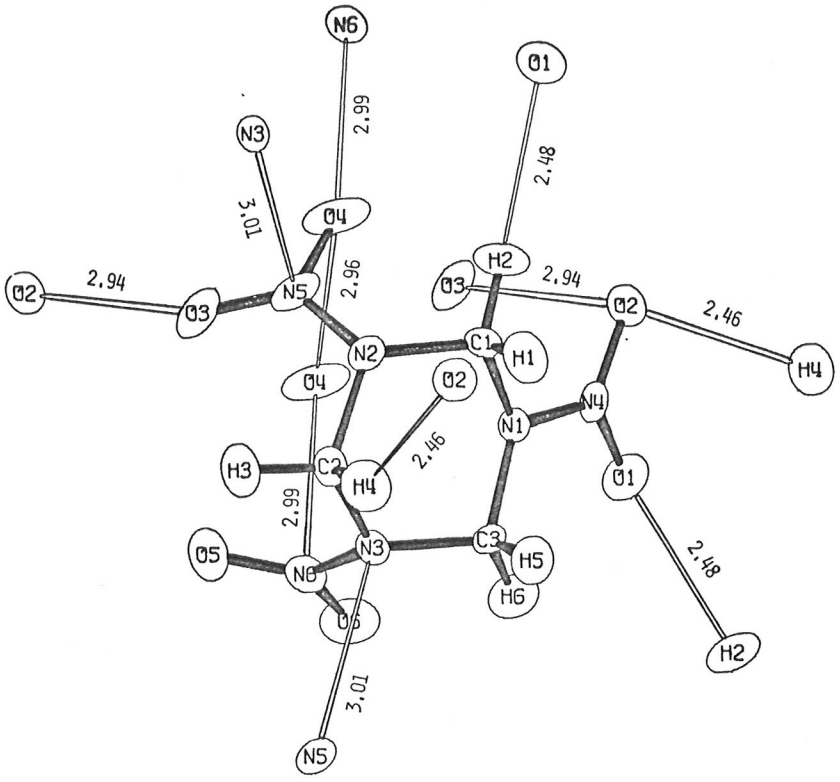

Fig. 3. A diagram of the RDX molecule and some atoms of neighboring molecules showing short intermolecular distances.

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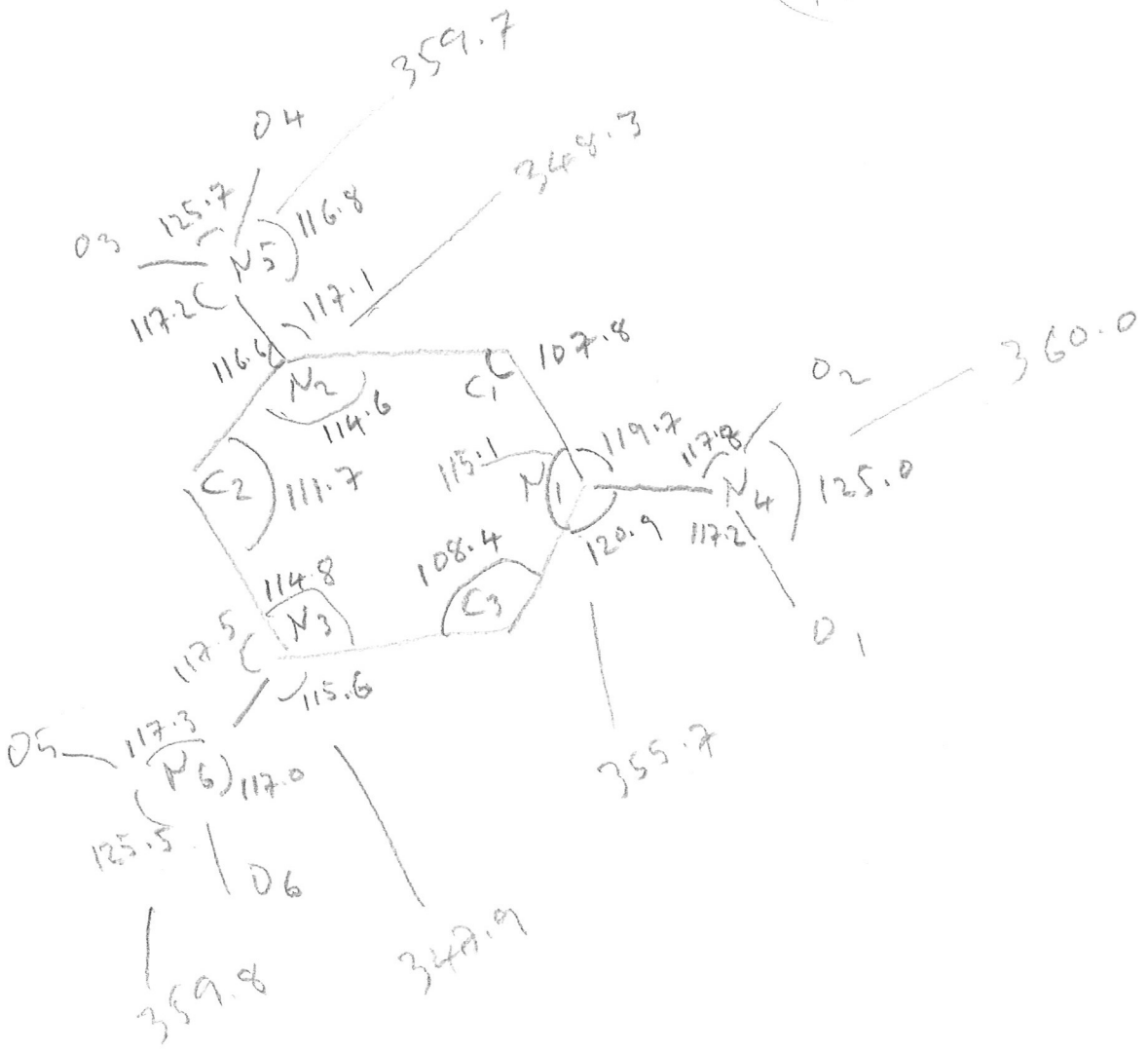
CH01 (1972)

(Tetroxy 328.5)



Bond lengths.

1.46 ✓
1.45 ✓
.95 ✓
.97 ✓
1.46 ✓
1.46 ✓
.93 ✓
.89 ✓
1.46 ✓
1.45 ✓
.95 ✓
.91 ✓
1.36 ✓
1.40 ✓
1.41 ✓
1.22 ✓
1.22 ✓
1.21 ✓
1.21 ✓
1.21 ✓
1.21 ✓

/ Mol

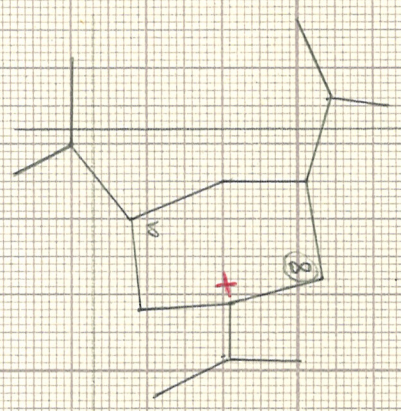
C-N	(1.47)	6
N-N	(1.34)	1
	(1.39)	2
O-N	(1.20)	6
C-H)	(1.00)	6

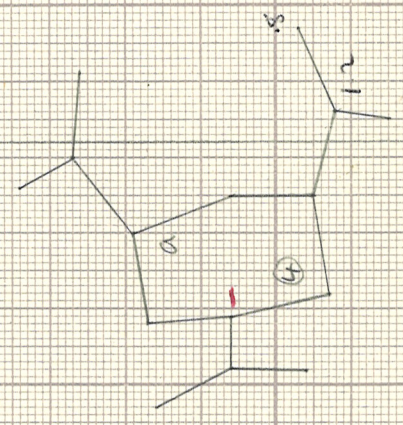
For 1 RDX Molecule.

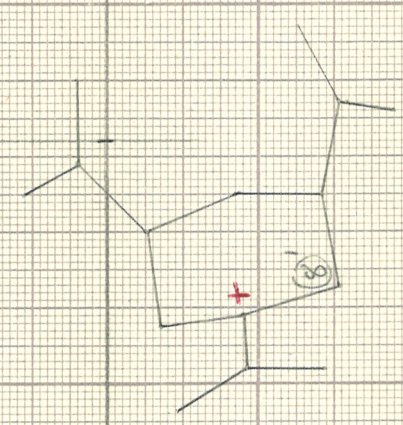
H	White	4·9 nm	1 hole	G off	?
O	Red	6·9 nm	1 hole	6 off.	?

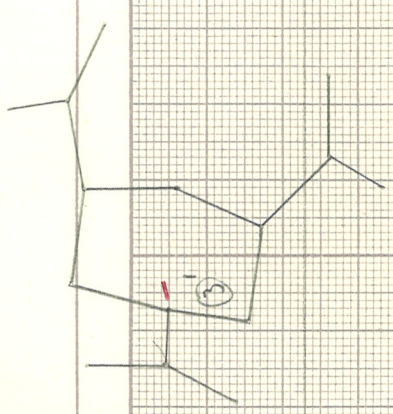
$N_{11, 21, 31}$ 3 holes Planar 117°, 117°, 126°

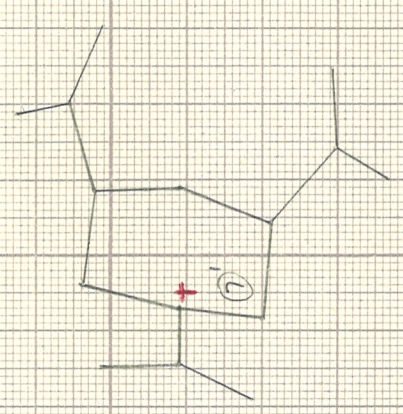
C TBT. ? 6.

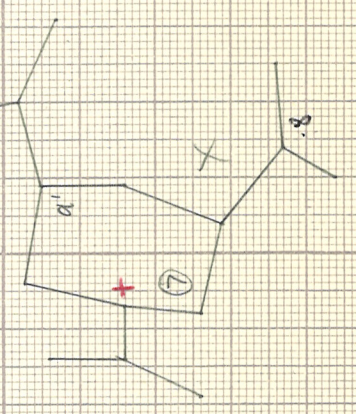


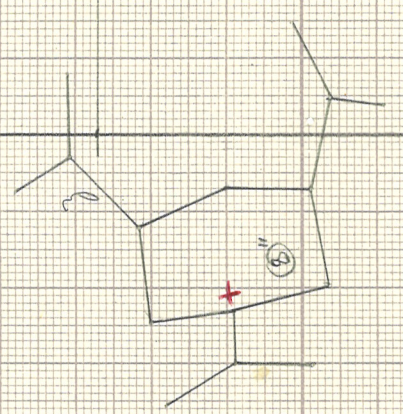


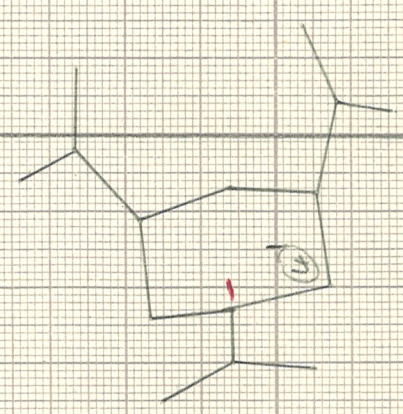


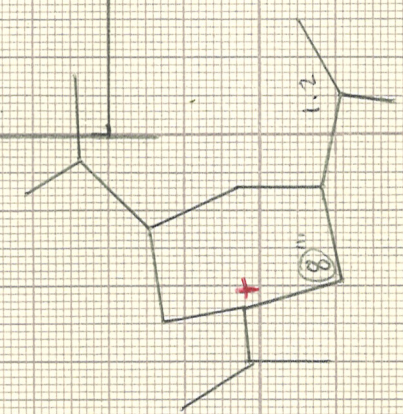


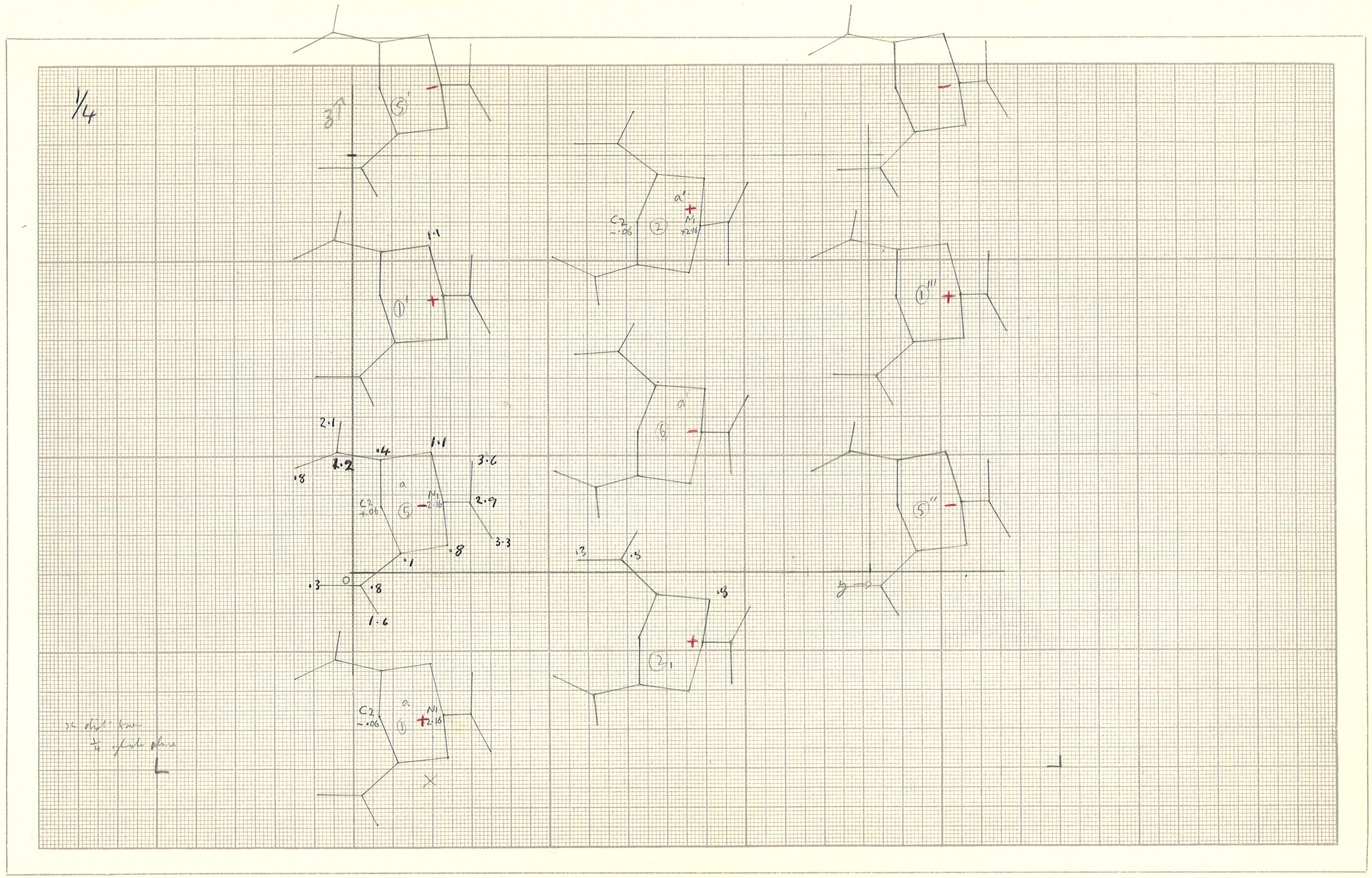




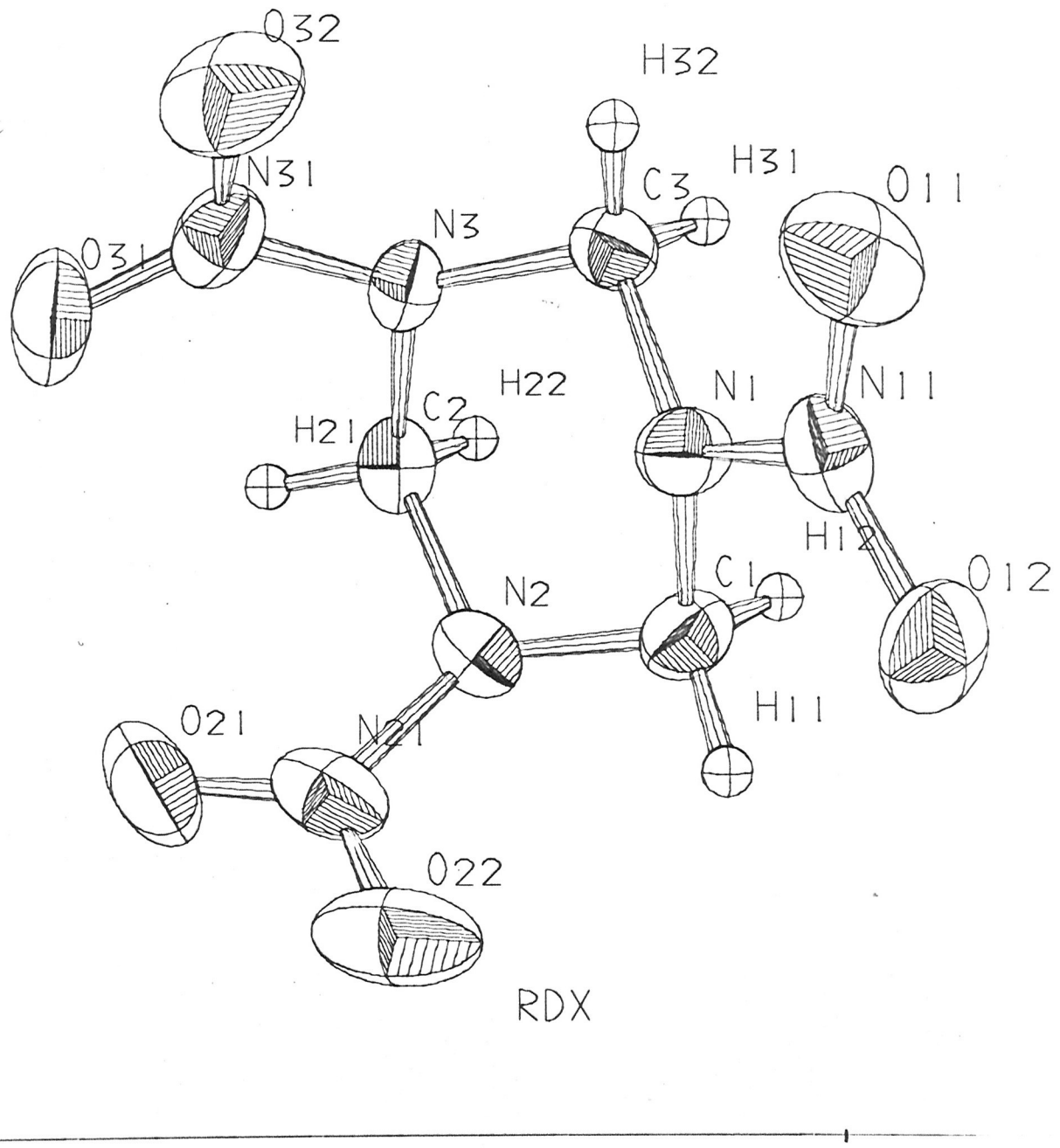








1/4
C2
−.06
N1
+2.16
a
a'
2.1
2.2
.4
1.1
3.6
2.9
3.3
.8
.1
.3
1.6


O32
H32
N31
C3
H31
O11
O31
N3
H22
N1
N11
H21
C2
H12
O12
C1
N2
H11
O21
N21
O22
RDX

(3) $(1-x)$ $\frac{1}{2}-y$, $\frac{1}{2}+z$

	y'	z'
C_1	4·2	·7
2	5·9	1·7
3	4·6	3·1
N_1	4·3	1·8
2	5·4	15
3	5·9	2·9
11	3·6	1·8
21	6·4	−·3
31	7·0	3·1
O 11	3·6	2·8
12	3·1	·7
21	7·5	−·3
22	6·0	−1·1
31	8·1	2·7
32	6·9	3·9

(3)'

	y'	$z'+1$
C_2	5·9	12·4
N_1	4·3	12·5

(4) $(1-x)$, $1-y$, $1-z$

y'	z'
10·8	4·7
12·5	3·6
11·2	2·3
10·9	3·6
12·0	4·9
12·5	2·5
10·2	3·6
13·0	5·7
13·6	2·2
10·2	2·6
9·7	4·6
14·1	5·6
12·6	6·4
14·7	2·7
13·5	1·5

(4)'

	$y'-1$	z'
C_2	−·7	3·6
N_1	−2·3	3·6

(7) $(\frac{1}{2}+x)$ $\frac{1}{2}-y$, z

	y'	z'
C_1	4·2	−4·7
2	5·9	−3·6
3	4·6	−2·3
N_1	4·3	−3·6
2	5·4	−4·9
3	5·9	−2·5
11	3·6	−3·6
21	6·4	−5·7
31	7·0	−2·2
O 11	3·6	−2·6
12	3·1	−4·6
21	7·5	−5·6
22	6·0	−6·4
31	8·1	−2·7
32	6·9	−1·5

(8) $(\frac{1}{2}+x)$, $1-z$, $\frac{1}{2}-z$

y'	z'
10·8	10·1
12·5	9·0
11·2	7·7
10·9	8·9
12·0	10·2
12·5	7·9
10·2	9·0
13·0	11·0
13·6	7·6
10·2	7·9
9·7	10·0
14·1	11·0
12·6	11·8
14·7	8·1
13·5	6·9

(8)'''

$y'-1$	$z'-1$
−·7	−1·7
−2·3	−1·8

(7)'

	y'	$z'+1$
C_2	5·9	7·1
N_1	4·3	7·1

(8)'

y'	$z'-1$
12·5	−1·7
10·9	−1·8

(8)''

$y'-1$	z'
−·7	9·0
−2·3	8·9

(4)'

$y'-1$	z'
−·7	3·6
−2·3	3·6

(1) (2)

x, y, z ; $x, \frac{1}{2}+y, \frac{1}{2}-z$;

(3) $1-x, \frac{1}{2}-y, z+\frac{1}{2}$; (4) $1-x, 1-y, 1-z$

② (x) ½+y , ½−z

	y′	z′
C1	9.0	10.1
2	7.3	9.0
3	8.6	7.7
N1	8.9	8.9
2	7.8	10.2
3	7.3	8.9
11	9.6	9.0
21	6.8	11.0
31	6.2	7.6
O 11	9.6	7.9
12	10.1	10.0
21	5.7	11.0
22	7.2	11.8
31	5.1	8.1
32	6.3	6.9

⑤ (½−x) , y , ½+z

	y′	z′
	2.4	0.7
	0.7	1.7
	2.0	3.1
	2.3	1.8
	1.2	0.5
	0.7	2.9
	3.0	1.8
	0.2	−0.3
	−0.4	3.1
	3.0	2.8
	3.5	0.7
	−0.9	−0.3
	0.6	−1.1
	−1.5	2.7
	−0.3	3.9

⑥ (½−x) ½+y 1−z

	y′	z′
C1	9.0	4.71
2	7.3	3.6
3	8.6	2.3
N1	8.9	3.6
2	7.8	4.9
3	7.3	2.5
11	9.6	3.6
21	6.8	5.7
31	6.2	2.2
O 11	9.6	2.6
12	10.1	4.6
21	5.7	5.6
22	7.2	6.4
31	5.1	2.7
32	6.3	1.5

① (x) y z+1

	y′	z′
C2	0.7	7.1
N1	2.3	7.1

⑤′

	y′	z′+1
C2	.7	12.4
N1	2.3	12.5

⑤″

	y′+1	z′
C2	13.9	1.7
N1	15.5	1.8

①‴

	y+1	z+1
C2	13.9	7.1
N1	15.5	7.1

②

	y′	z′−1
C2	9.3	−1.7
N1	8.9	−1.8

(5) (6)

$1/2 - x, y, 1/2 + z$; $\frac{1}{2} - x, 1/2 + y, 1 - z$;

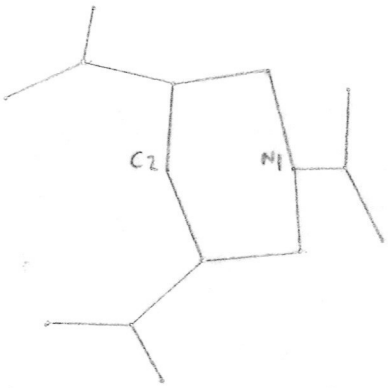
(7) (8)

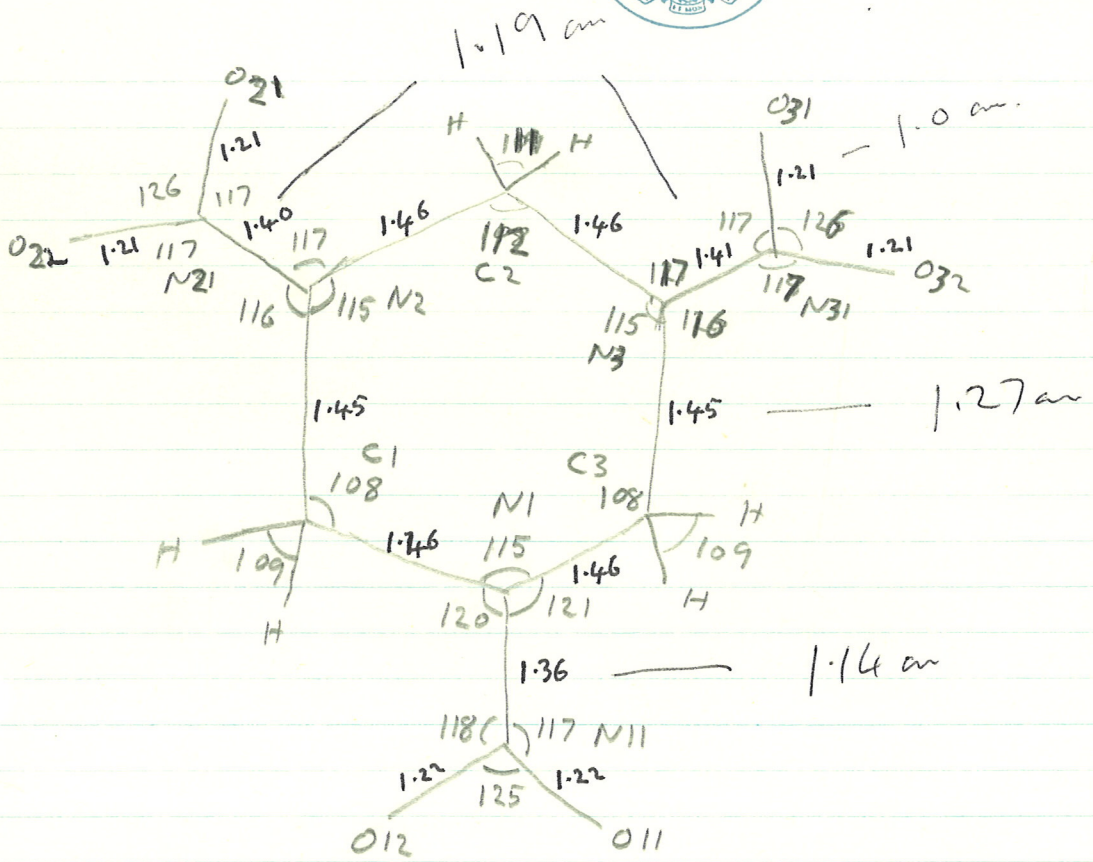
$1/2 + x, 1/2 - y, z$; $1/2 + x, 1 - y, 1/2 - z$;

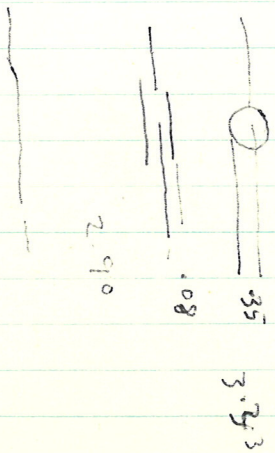
a = 11.602 ¼ 5.800 ¼ 2.900 ¾ 8.700
b = 13.194 6.597 3.298
c = 10.714 5.357 2.678

	x	y	z	½ − x	½ + x	1 − x	½ − y	½ + y	1 − y	½ − z	½ + z	1 − z = + z
C 1	4.15	2.43	−4.71	1.65	9.95	7.45	4.17	9.03	10.76	10.07	0.65	15.42
C 2	2.84	0.66	−3.64	2.96	8.64	8.76	5.94	7.26	12.53	9.00	1.72	14.35
C 3	4.42	1.97	−2.31	1.38	10.22	7.18	4.63	8.57	11.22	7.67	3.05	13.02
N 1	5.06	2.32	−3.57	0.74	10.86	6.54	4.28	8.92	10.87	8.93	1.79	14.28
N 2	3.47	1.16	−4.86	2.33	9.27	8.13	5.44	7.76	12.03	10.22	0.50	15.57
N 3	3.73	0.71	−2.49	2.07	9.53	7.87	5.89	7.31	12.48	7.85	2.87	13.20
N 11	6.24	2.98	−3.59	−0.44	12.04	5.36	3.62	9.58	10.21	8.95	1.77	14.30
N 21	4.09	0.21	−5.68	1.71	9.84	7.51	6.39	6.81	12.98	11.04	−0.32	16.39
N 31	4.50	−0.44	−2.23	1.30	10.30	7.10	7.04	6.16	13.63	7.59	3.13	12.94
O 11	6.89	3.01	−2.55	−1.09	12.69	4.71	3.59	9.61	10.18	7.91	2.81	13.26
O 12	6.54	3.49	−4.64	−0.79	12.39	5.01	3.11	10.09	9.70	10.00	0.72	15.35
O 21	3.66	−0.91	−5.64	2.14	9.46	7.94	7.51	5.69	14.10	11.00	−0.28	16.35
O 22	4.96	0.61	−6.43	0.84	10.76	6.64	5.99	7.21	12.58	11.79	−1.07	17.14
O 31	4.10	−1.49	−2.70	1.70	9.90	7.50	8.09	5.11	14.68	8.06	2.66	13.41
O 32	5.45	−0.32	−1.49	0.35	11.25	6.15	6.92	6.28	13.51	6.85	3.87	12.20
H 21	2.54			3.26	8.34	9.06						
H 22	2.16			3.64	7.96	9.44						

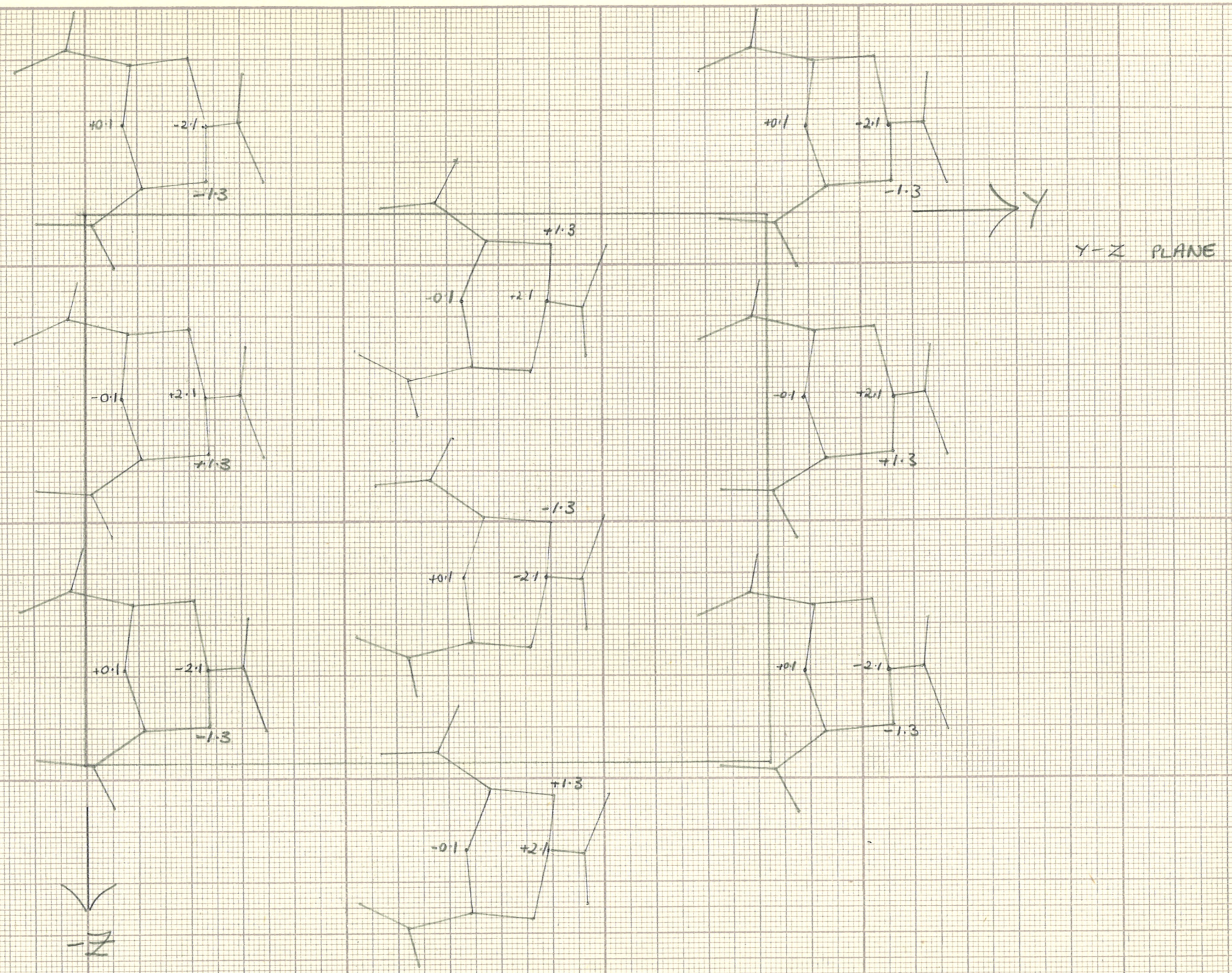
a

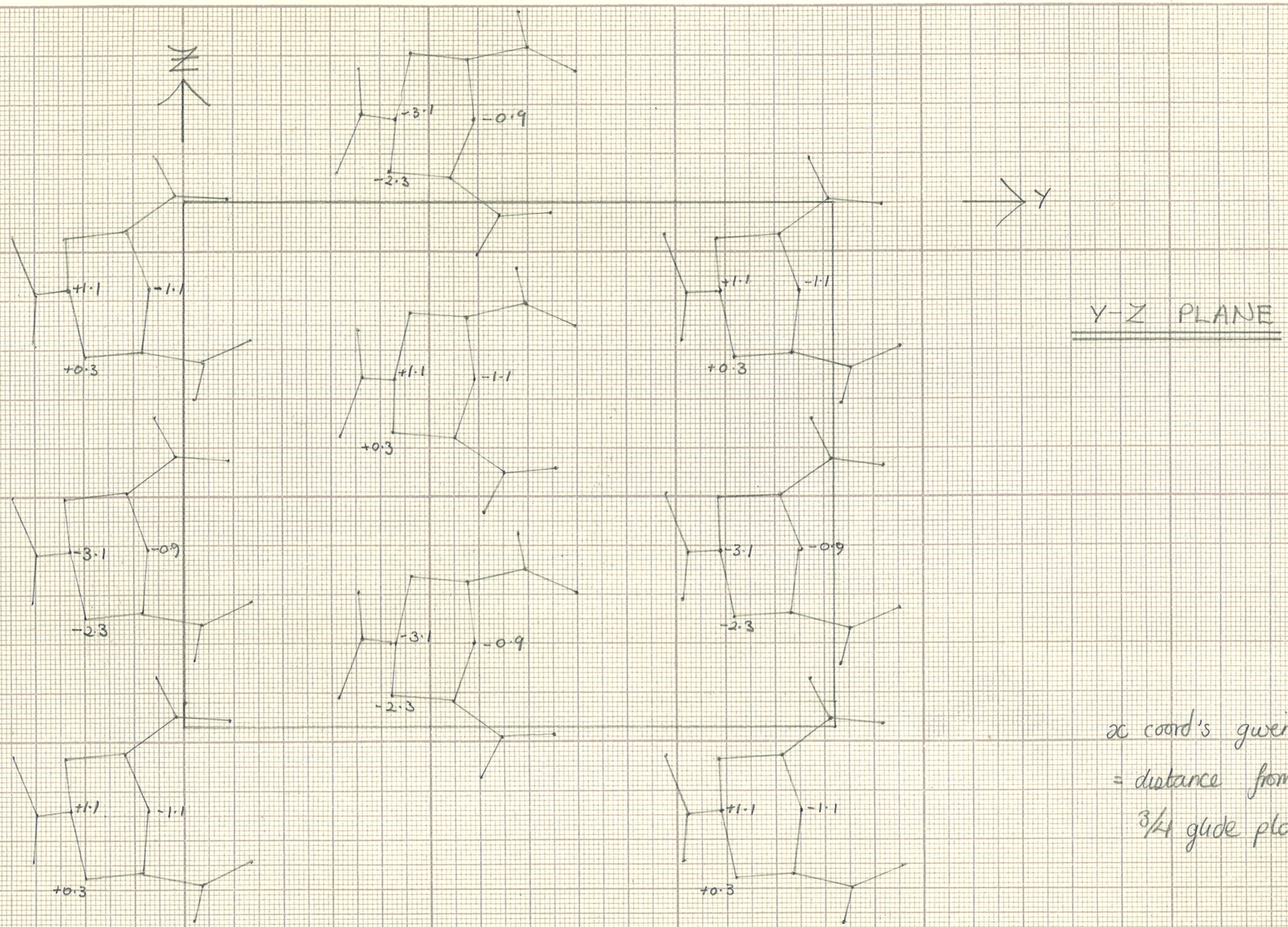



1.19 Å
O21
1.21
126
117
O22
1.21
117
N21
1.40
117
116
115 N2
1.46
H
111
H
1.46
112
C2
1.46
117
115
N3
116
O31
1.21
117
N31
1.41
117
126
1.21
O32
1.0 Å
1.45
1.45
1.27 Å
C1
108
C3
108
N1
115
H
H
109
1.46
109
H
1.46
120
121
H
1.36
1.14 Å
118
117 N11
1.22
125
1.22
O12
O11


2.0
.88
.35
3.23

x co-ords
= distance from
¼ glide plane

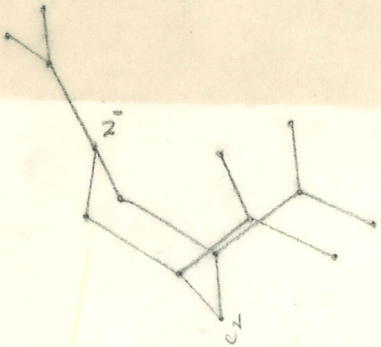


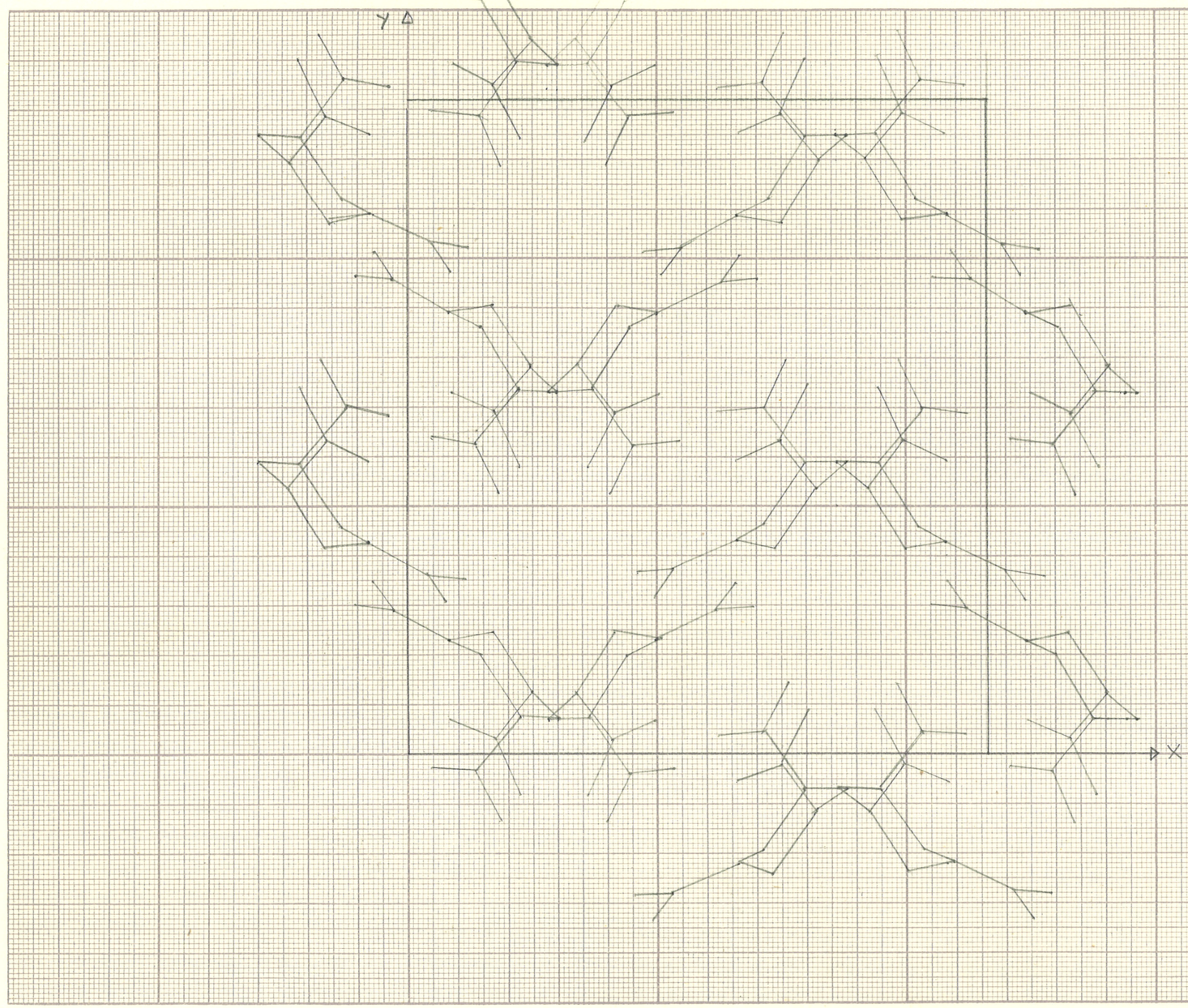


Y-Z PLANE

x coord's given
= distance from
3/4 glide plane

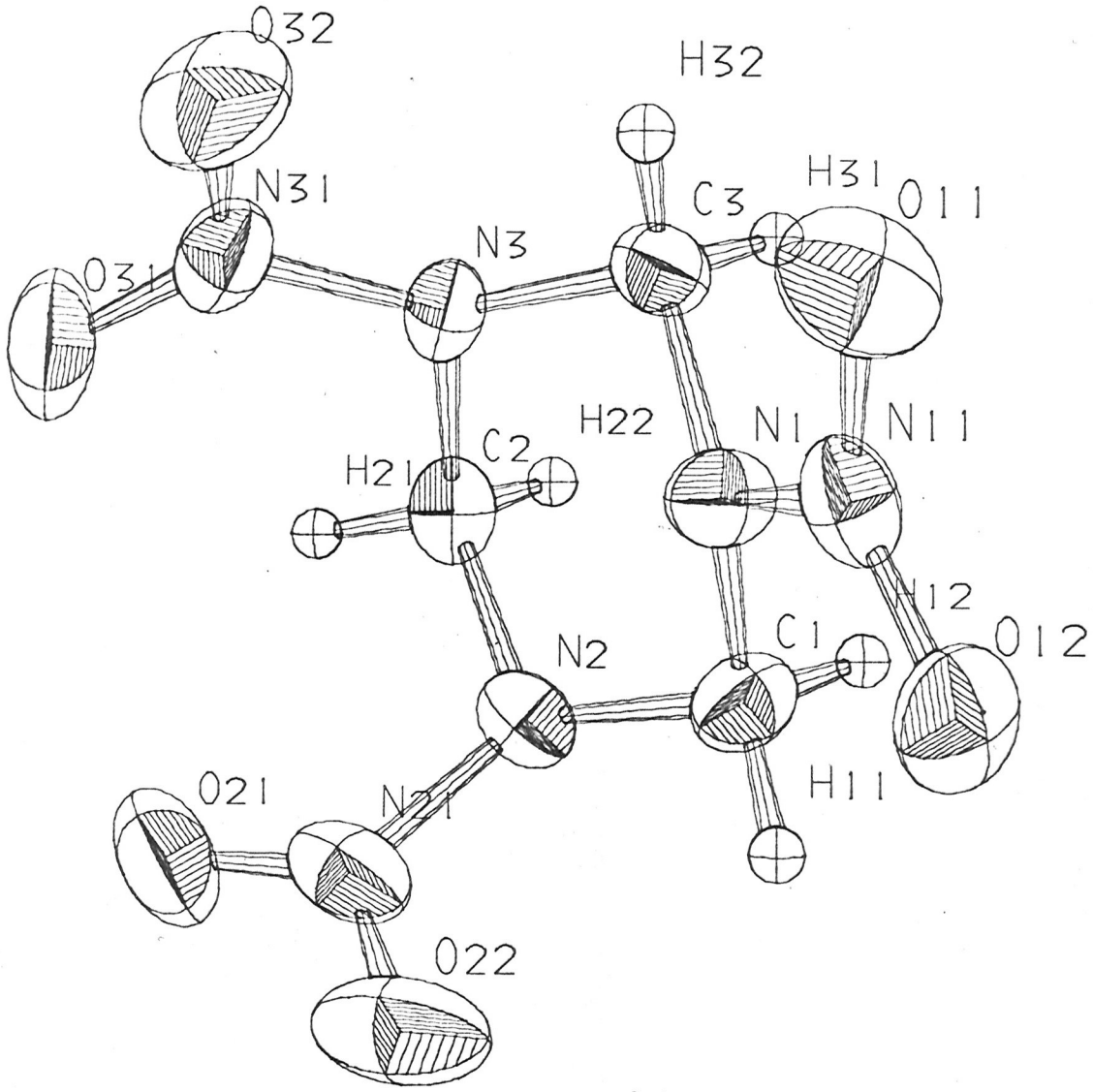
RDX - X-Y PLANE



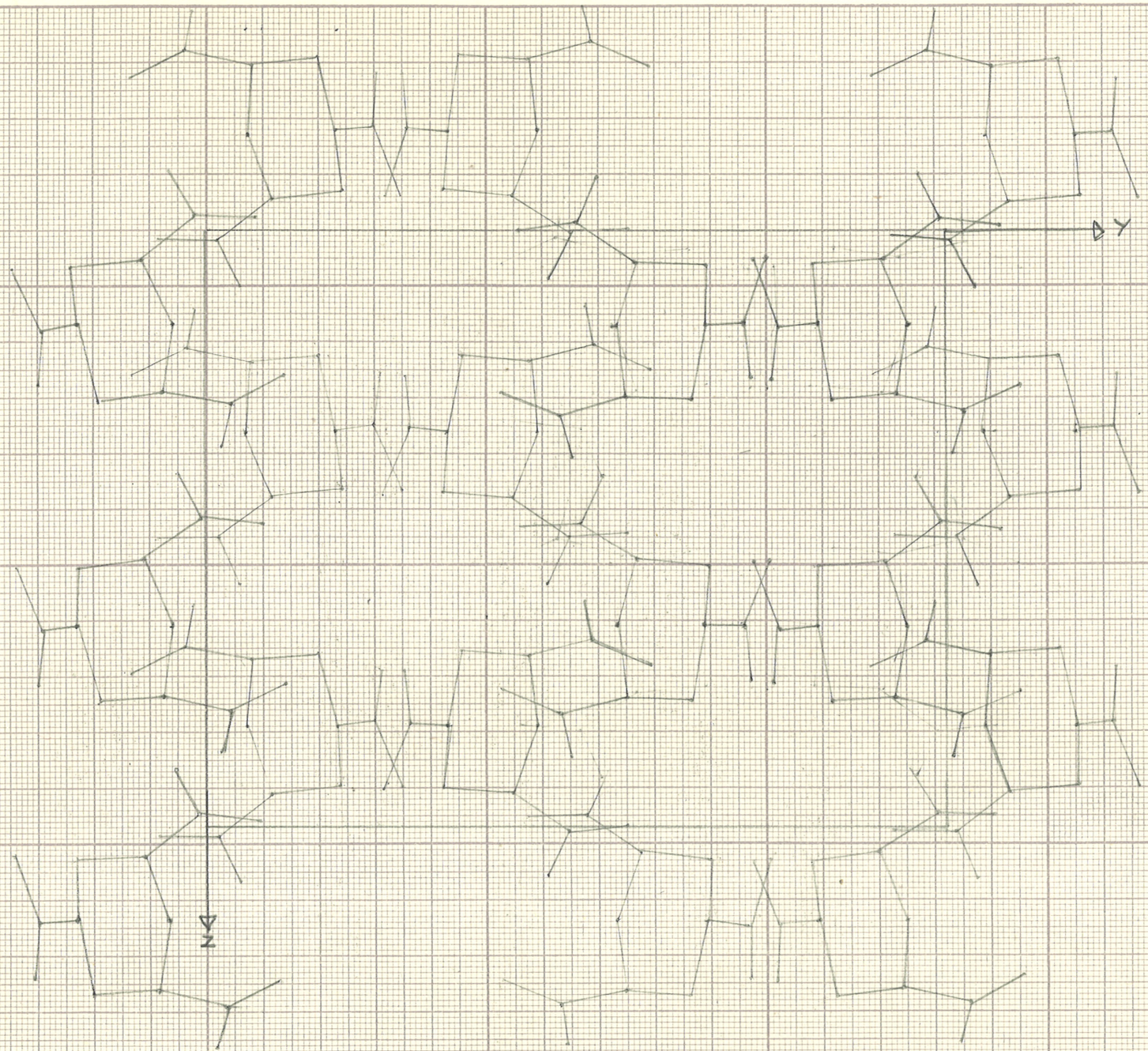


RDX

X-Y PLANE

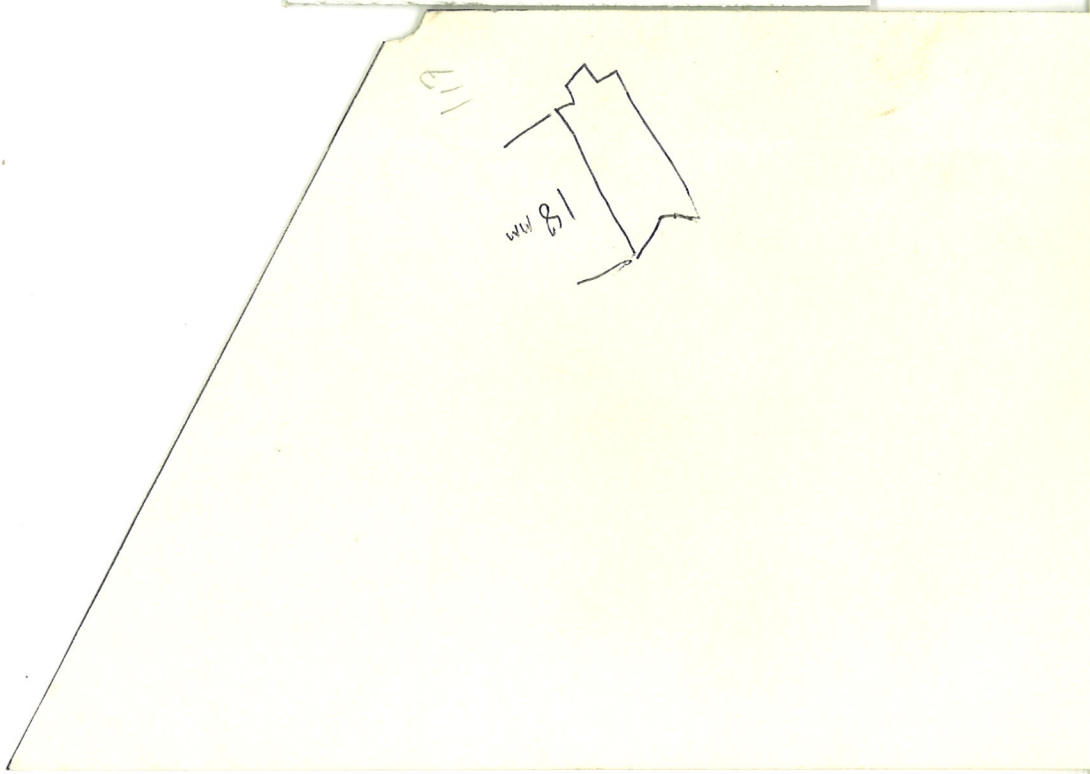

O32
H32
N31
C3
H31
O11
O31
N3
H22
N1
N11
H21
C2
H12
O12
C1
N2
H11
O21
N4
O22

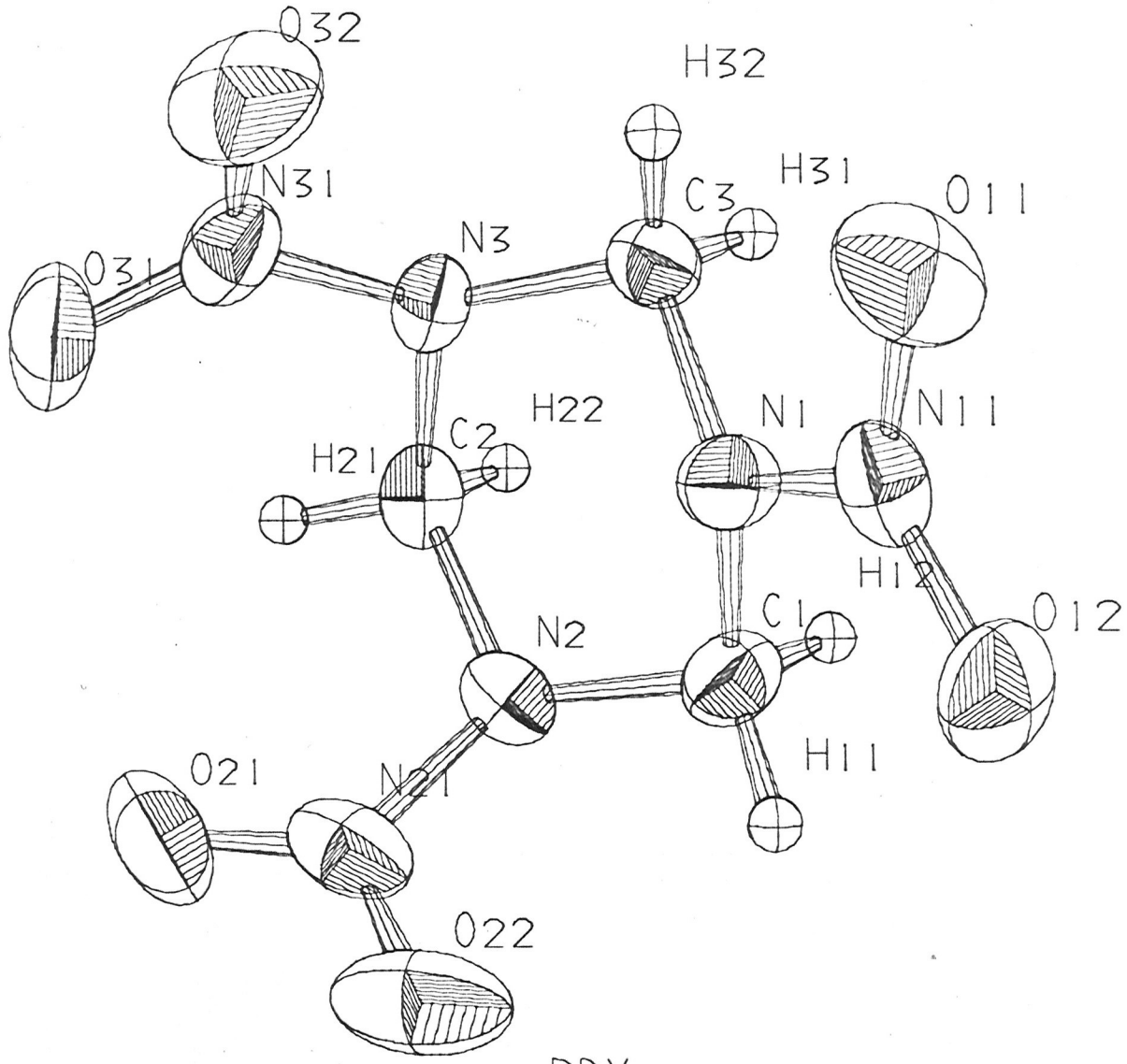
RDX



RDX

Y-Z PLANE


WW 81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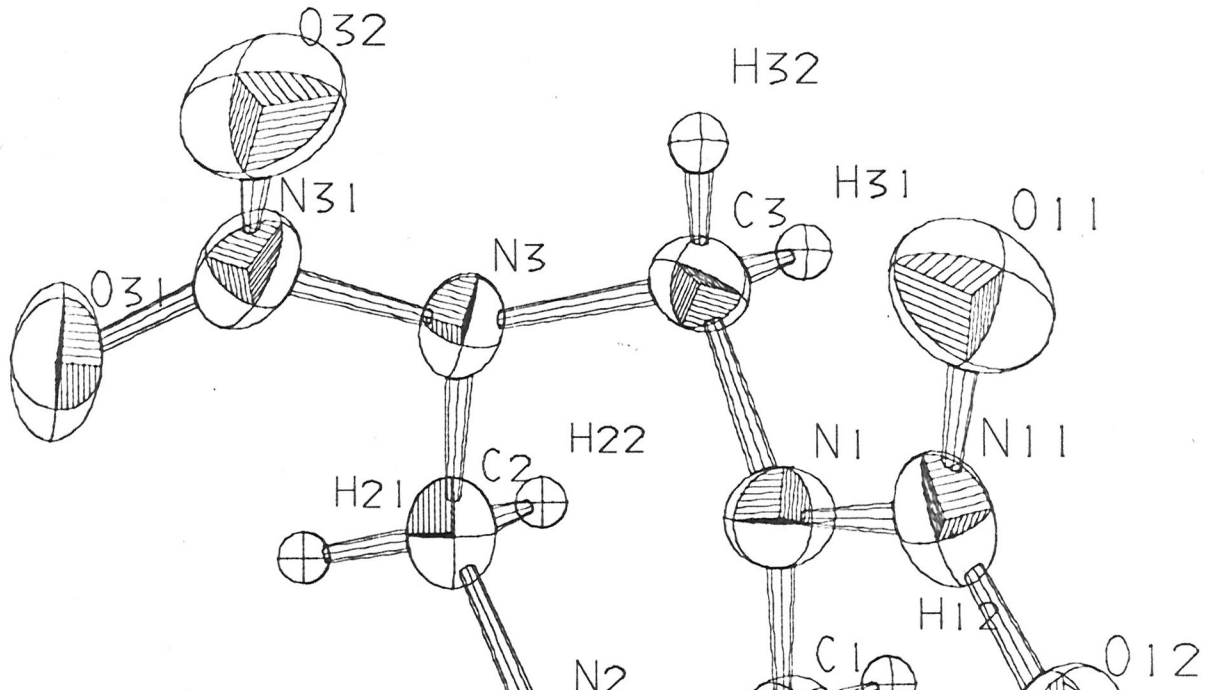
H32
N31
C3
H31
O11
O31
N3
H22
N1
N11
H21
C2
H12
O12
C1
N2
H11
O21
N21
O22

RDX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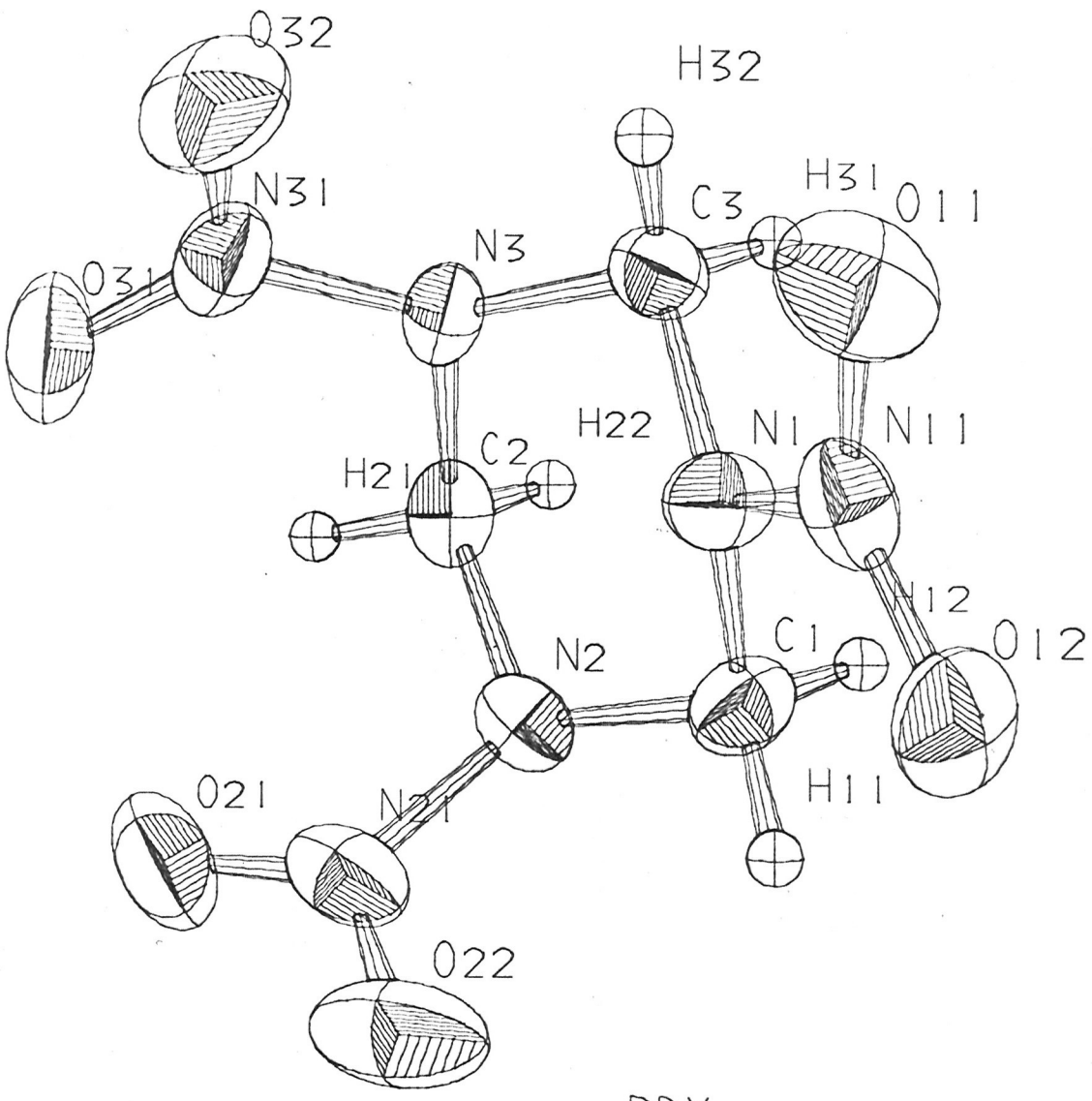
H32
N31
C3
H31
O11
O31
N3
H22
N1
N11
H21
C2
H12
O12
N2
C1
H11
O21
N21
O22

RDX


O32
H32
N31
C3
H31
O11
O31
N3
H22
N1
N11
H21
C2
H12
O12
C1
N2
H11
O21
N4
O22

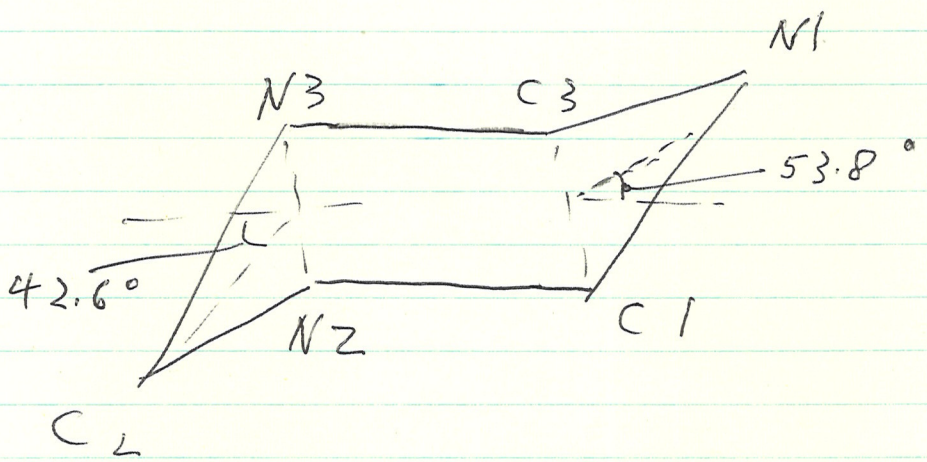
RDX

a 11.600

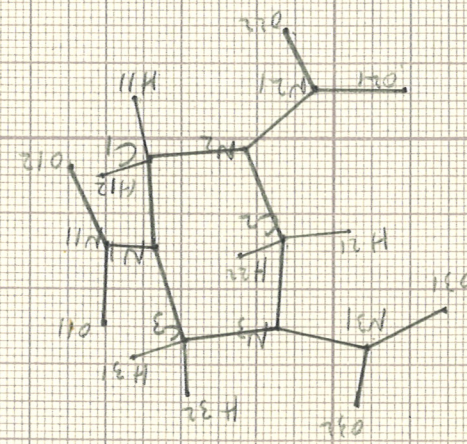
b 13.194

c 10.714

β



-3



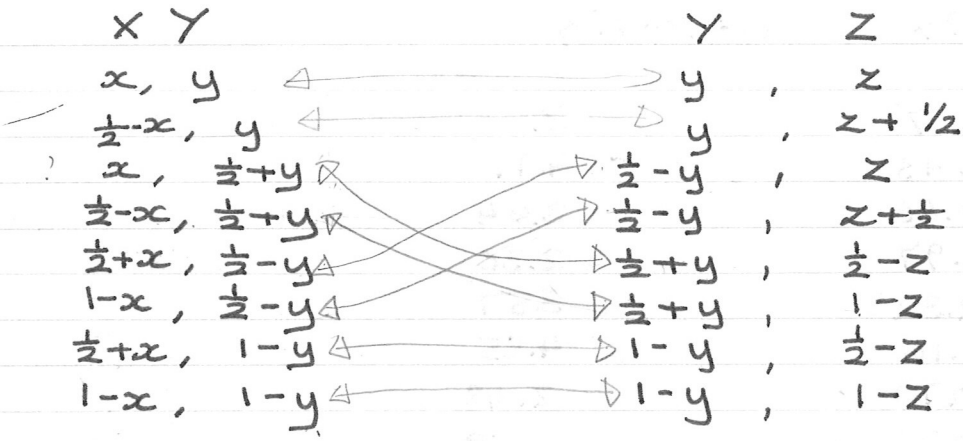
9

RDX

$a = 11.600$ $b = 13.194$ $c = 10.714$

	X	Y	Z
C_1	4.15	2.43	- 4.71
C_2	2.83	0.66	3.64
C_3	4.42	1.97	2.36
N_1	5.05	2.32	3.57
N_2	3.46	1.16	4.85
N_3	3.73	0.70	2.48
N_{11}	6.23	2.98	3.59
N_{21}	4.09	0.21	5.68
N_{31}	4.50	- 0.44	2.23
O_{11}	6.88	3.00	2.55
O_{12}	6.59	3.48	4.64
O_{21}	3.65	- 0.91	5.64
O_{22}	4.96	0.60	6.42
O_{31}	4.10	- 1.48	2.69
O_{32}	5.44	- 0.31	1.49
H_{11}	4.62	2.62	5.51
H_{12}	3.49	3.10	4.51
H_{21}	2.54	- 0.20	3.78
H_{22}	2.16	1.21	3.46
H_{31}	3.74	2.61	2.09
H_{32}	5.01	1.91	1.62

229 cvc + Tim Snook



for X : 1 = 11·6, ½ = 5·8

Y : 1 = 13·2, ½ = 6·6

Z : 1 = -10·7, ½ = -5·3

C_2 :-

	X	Y
①	2·8 x	0·7 y
②	3·0 ½-x	0·7 y
⑤	2·8 x	7·3 y+½
⑥	3·0 ½-x	7·3 y+½
③	8·6 x+½	5·9 ½-y
④	8·8 1-x	5·9 ½-y
⑦	8·6 x+½	12·5 1-y
⑧	8·8 1-x	12·5 1-y

N_1 :-

	X	Y
①	5·0	2·3
②	0·8	2·3
⑤	5·0	8·9
⑥	0·8	8·9
③	10·8	4·3
④	6·6	4·3
⑦	10·8	10·9
⑧	6·6	10·9

C_2 :-

	Y	Z
①	0·7 y	-3·6 z
②	0·7 y	-8·9 ½+z
③	5·9 ½-y	-3·6 z
④	5·9 ½-y	-8·9 ½+z
⑤	7·3 y+½	-1·7 ½-z
⑥	7·3 y+½	-7·1 1-z
⑦	12·5 1-y	-1·7 ½-z
⑧	12·5 1-y	-7·1 1-z

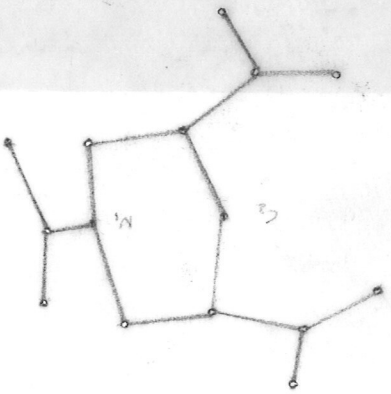
N_1 :-

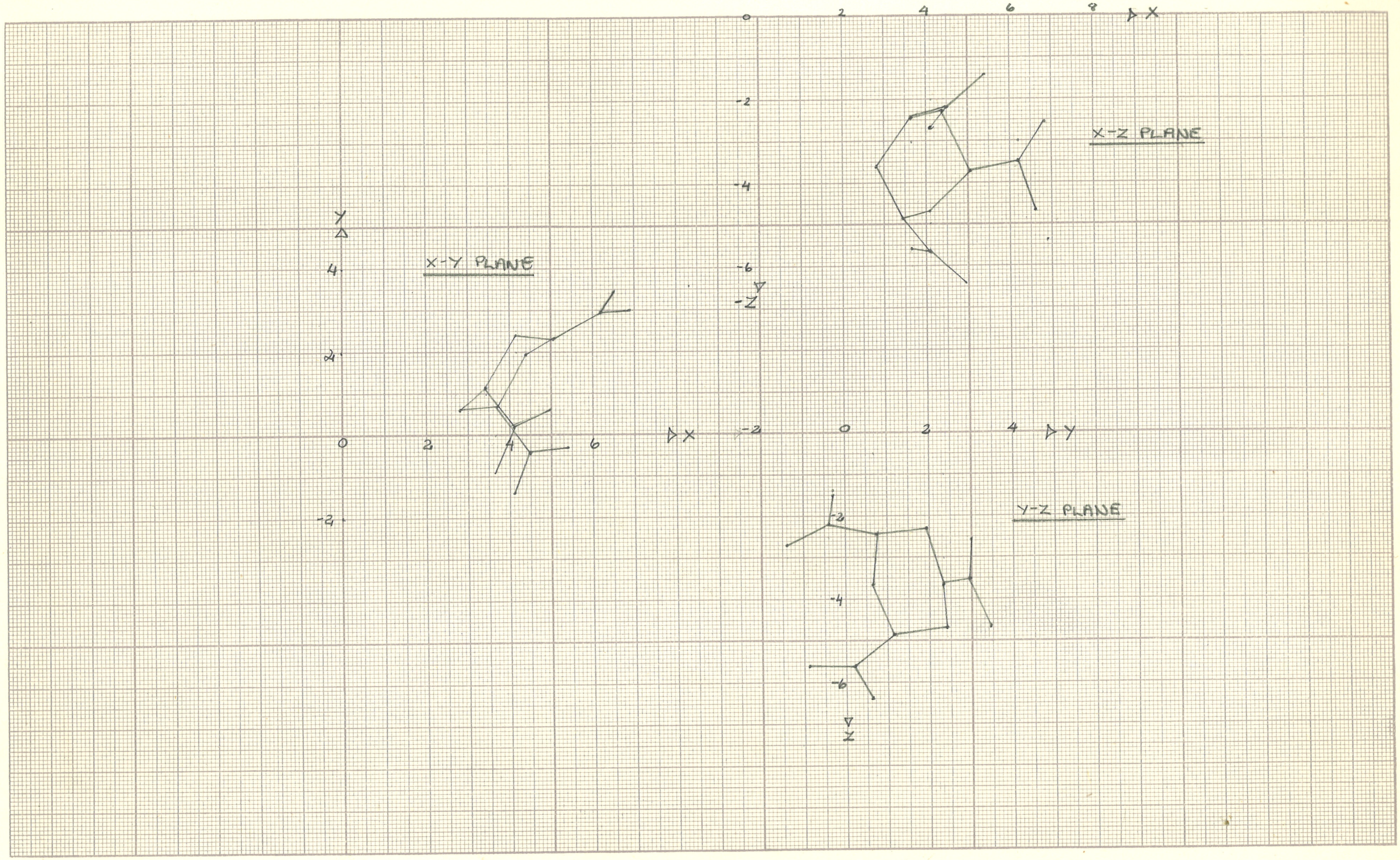
	Y	Z
①	2·3	-3·6
②	2·3	-8·9
③	4·3	-3·6
④	4·3	-8·9
⑤	8·9	-1·7
⑥	8·9	-7·1
⑦	10·9	-1·7
⑧	10·9	-7·1

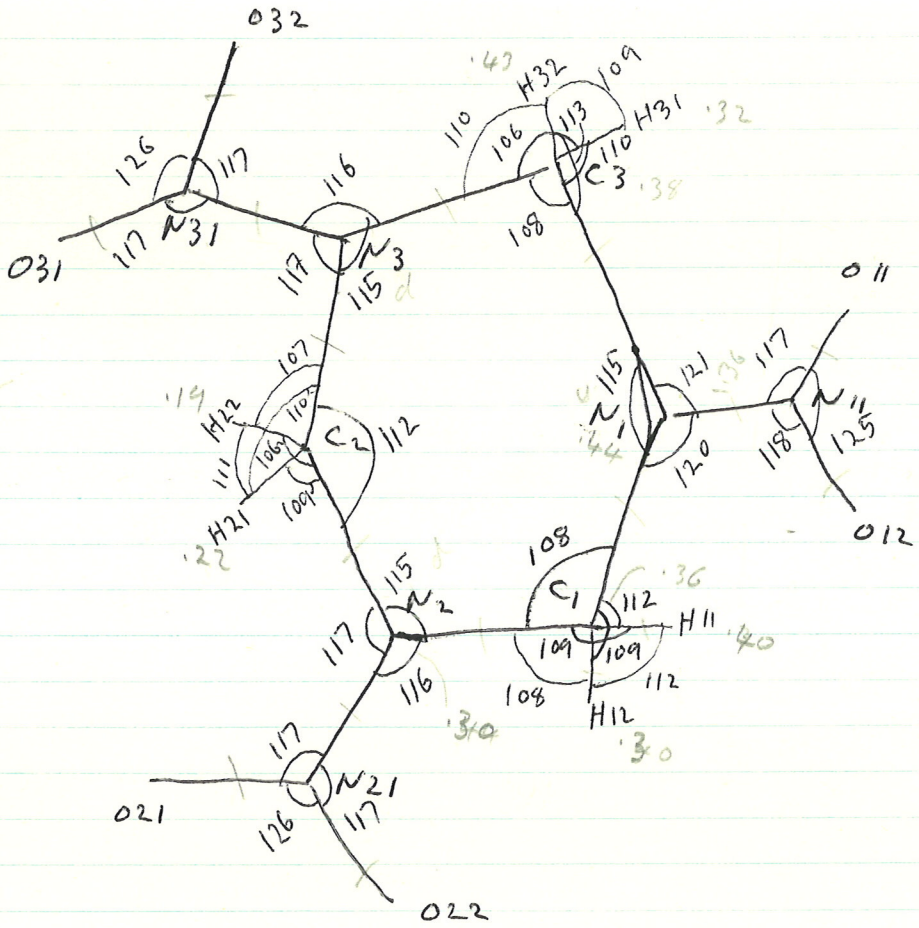
C_1 : -X

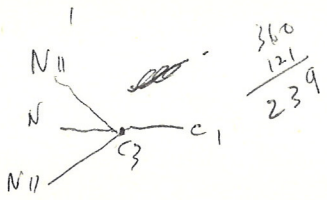
⑤	① 4·2
⑥	② 1·6
⑦	③ 10·0
⑧	④ 7·4

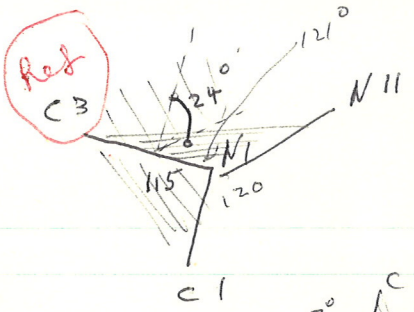
RDX Y-Z PLANE




X-Y PLANE
X-Z PLANE
Y-Z PLANE
Y
X
Z


O32
O31
N31
N3
C3
H32
H31
O11
N11
O12
C2
H22
H21
N1
N2
C1
H11
H12
O21
N21
O22

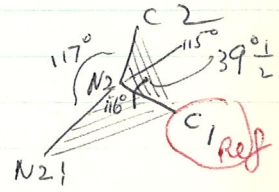


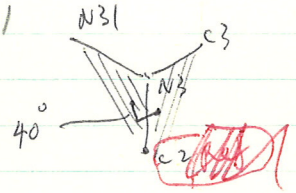


C3, N1, N11 + C3, N1, C1

C1, N2, C2 - C1, N2, N21

C2, N3, C3 - C2, N3, N31





C1	3
C2	3
C3	3
N1	2
N2	2
N3	2
N11	1
N21	1
N31	1

(10) a C3 to C1 115°
C3 to N11 24° about C_3–N1 and then +121° to C_3N1 239

(11) b C_3 to C1 115°
C_3 to N11 336° about C_3–N1 & then +121° to C_3N1 239

(12) a C1 to C2 115°
C1 to N21 39½° about C1 – N2 & then 116½° to C1N2 244

(13) b C1 to C2 115°
C1 to N21 320½° about C–N2 & then 116½° to C1N2 244

20 16 molecules required to furnish 1 cell.

1.00 (111)

a 11.600 ¼a = 2.900
b 13.194
c 10.714

	x	y	z
C_1	·35796 (÷·35)	·18434	−·43971
	4.152	2.432	−4.711
	1.252		
C_2	·24448	·05012	−·33977
	2.836	·661	−3.640
	−0.064		
C_3	·38112	·14942	−·21554
	4.421	1.971	−2.340
N_1	·43594	·17588	−·33336
	5.057	2.324	−3.572
N_2	·29870	·08799	−·45338
	3.465	1.161	−4.858
N_3	·32192	·05380	−·23236
	3.734	·710	−2.490
N_{11}	·53790	·22617	−·33498
	6.240	2.984	−3.589
N_{21}	·35301	·01593	−·52975
	4.095	·210	−5.676
N_{31}	·38801	−·03346	−·20790
	4.501	−·441	−2.227
O_{11}	·59359	·22792	−·23806
	6.886	3.007	−2.551
O_{12}	·56832	·26416	−·43346
	6.593	3.485	−4.644
O_{21}	·31506	−·06930	−·52643
	3.655	−·914	−5.640
O_{22}	·42792	·04601	−·59968
	4.964	·607	−6.425
O_{31}	·35373	−·11255	−·25159
	4.103	−1.485	−2.696

O 32	·46974	−·02393	−·13872
	5·449	−·316	−1·486
	2·771		
H 11	·39803 (±·25)	·19848	−·51462
	4·617	2·619	−5·514
	1·939 1·69		
H 12	·30085	·23543	−·42128
	3·490	3·106	−4·514
	·812 ·56		
H 21	·21884	−·01539	−·35290
	2·539	−·203	−3·781
	−·139 n.s.g.p.		
H 22	·18594	·09206	−·32304
	2·157	1,215	−3·461
	−·521 −·27		
H 31	·32312	·19782	−·19523
	3·748	2·610	−2·092
	1·070 ·82		
H 32	·43240	·14506	−·15155
	5·016	1·914	−1·624
	2·337 2·09		

For 1 Molecule.

					For 20 molecules
(5)	Rods.	1·27 cm	6 off		120
(3)		1·14	1		20
(4)		1·19	2		40
(2)		1·00	6		120
(1)		0·80	6		120
(6)	Balls.	4·9 mm	White 1 hole	6 off.	120
(7)	Balls	6·9 mm	Red 1 hole	6 off.	120
(8)		Block	Tetrahedral 4 holes 109½°	3 off.	60
(9)	Blue.	Initial hole with 1·19 cm rod.		3 off.	60

To I.H.	around IH
~~127~~°	0
117°	180

* (10) a Blue. Initial hole with 1·27 cm rod. 1 off. 20

Ni

To IH	around IH
121	~~0~~ 24
115	~~+x~~ 0

(11) b

To IH	around IH
121	~~0~~ 336
115	~~−x~~ 0

* (12) a 2 off 40

116 ½	0 39½
115	~~+5~~ 0

(13) b 2 off 40

116 ½	0 320½
115	~~−5~~ 0

* (14) a

117	0
115	+3

(15) b

117	0
115	−3

1 each of a or b.

BEEVERS MINIATURE MODELS

August 1970

DRILLED BALLS AND CUT RODS

BALLS are of methylmethacrylate polymer, of diameter about 6.9 mm, (4.9 mm for HYDROGEN). They are drilled to 1 mm from the centre, so that each interatomic distance is 2 mm greater than the rod length.

RODS are 1 mm diameter steel (stainless). The recommended scale is 1 cm = 1 Å, i.e. a magnification of exactly 10^8. Useful models can, however, be made on other scales using these materials. The rods are cut from No.19 gauge wire.

ASSEMBLY can be done using pliers, holding the rod with only 2 mm protruding and pressing into the hole with a twisting movement. Any burr on the rods must first be removed preferably on a cup grinder. Rods should be finally pushed firmly home with large pliers or by the use of a hammer and anvil for the balls.

PRICES

	1	10	100	1000
Balls 6.9mm	6d (£0.025)	5/- (£0.25)	£2/10/- (£2.50)	£25.00
Balls 4.9mm	4d (£0.015)	3/- (£0.15)	£1/10/- (£1.50)	£15.00
Rods	2d (£0.01)	1/- (£0.05)	10/- (£0.50)	£5.00

BALLS 6.9mm

OPAQUE (Non-metals)		No.	Drilling
Black	(Carbon)		
Red	(Oxygen)		
Blue	(Nitrogen)		
Orange	(B, Se, Te)		
Yellow	(Sulphur)		
Green	(F, Cl)		
White	(Rare Gases)		
Dark Blue	(I, At)		
Turquoise	(Br)		
Lilac	(P)		
Pink	(As)		
Brown	(Si)		

TRANSPARENT (Metals)

Clear (Zn, Cd, Hg)		
Ruby (Li, Na, K, Rb, Cs, Fr, Mg, Ca, Sr, Ba, Ra)		
Emerald (Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag)		
Topaz (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu)		
Pink (Be)		
Orange (Ge, Sn, Sb, Pb, Bi, Po)		
Sapphire (La, Hf, Ta, W, Re, Os, Ir, Pt, Au)		
Amethyst (Al, Ga, In, Tl)		
TOTAL No. of 6.9mm		

BALLS 4.9mm

White Hydrogen (opaque)		
TOTAL No. of 4.9mm		

DRILLINGS

OCT; Six holes, 90° angles
TET: Four holes, 109½° angles (sp^3 hybrid)
TRIG: Three holes in plane, 120° angles
THREE AT 109½°: non-planar
TWO AT . . .
ONE:
GENERAL: For each type of drilling specify:
Initial hole with rod . . . .cm.

TO I.H.	AROUND I.H*

in degrees

Are drillings to be centrosymmetrical? YES/NO. (If Yes only the non-symmetric drillings need be specified).

* Measure clockwise looking at the ball. (to get correct enantiomorph).

RODS

cm	Å	for:	No.
0.80	1.00	O-H, N-H	
0.90	1.10	C-H	
1.00	1.20	C-C triple	
1.14	1.34	C-C double	
1.19	1.39	C-C aromatic	
1.23	1.43	C-O, S-O	
1.27	1.47	C-N	
1.34	1.54	C-C single	
1.55	1.75	C-Cl, N-Cl	
1.80	2.00	P-Cl	
2.61	2.81	Na-Cl	
3.15	3.35	C, C (no bond)	

(Insert any special lengths required)

COST:

6.9mm balls	
4.9mm balls	
Rods	
TOTAL	
Packing and postage	
GRAND TOTAL	

BEEVERS MINIATURE MODELS

ASSEMBLED MODELS

August 1970

The list has been extended to include some models of special interest. For example the Apatite model shows well the place of Fluorine in the lattice of bone-mineral. The Corundum model shows the curious distortion of the structure which was an early suggestion of unexpected metal-to-metal bonds. The Cuprite model shows the interpenetration of two independent copper-oxygen lattices. In Pb_3O_4 we have evidence for the co-existence of two oxidation states in the one crystal. The Molybdenum Sulphide structure shows why this compound acts like a lubricant. The Quartz model shows the existence of screw axes all of the same sign, giving optical activity, while in the Zircon model there are screw axes of both senses, resulting in no optical activity. The Regular Solids are those known to the ancient Greek philosophers, and the Snowflake model shows the six arms of the typical snowflake.

There are many other features of interest brought out by this series of models and they are described in the Legends which accompany each model.

The range of colours used now includes transparent balls, and this adds further to the beauty of these models, which are outstanding in their compactness, accuracy, permanence and cheapness.

The lower portion of this sheet can be used to Order:
NOTE: Special boxes or stands, and postages EXTRA at cost.

To: BEEVERS MINIATURE MODELS,
SIMON SQUARE CENTRE,
PLEASANCE, EDINBURGH 8,
EH8 9HW, SCOTLAND.

From:

Date: Order No:

Name	Code	£ s d	£	No. Required
ALPHA HELIX	75 52 116	3 13 0	3.65	
APATITE	150 0 285	10 0 0	10.00	
BODY-CENTRED CUBIC	19 0 36	1 0 0	1.00	
CAESIUM CHLORIDE	35 0 64	1 14 0	1.70	
CADMIUM IODIDE	38 0 72	1 15 0	1.75	
CALCITE	74 0 93	2 8 0	2.40	
CORUNDUM (RUBY)	106 0 202	5 4 0	5.20	
CUPRITE	87 0 104	2 15 0	2.75	
DIAMOND (Showing Cell)	78 0 128	2 18 0	2.90	
" (12 edge tetrahedr)	652 0 1144	25 4 0	25.20	
FACE-CENTRED CUBIC	17 0 36	1 0 0	1.00	
FAUJASITE (Zeolite)	672 0 864	22 0 0	22.00	
FLUORITE	46 0 80	2 0 0	2.00	
GRAPHITE	67 0 105	2 16 0	2.80	
HEXAGONAL CLOSE-PACKED	18 0 45	1 0 0	1.00	
ICE	26 50 50	1 15 0	1.75	
LATTICE, SEVEN PRIMITIVE	56 0 86	2 16 0	2.80	
LEAD OXIDE Pb_3O_4	51 0 80	2 6 0	2.30	
LINDE MOLECULAR SIEVE	120 0 144	3 16 0	3.80	
LITHIUM HYDROXIDE	50 0 88	2 7 0	2.35	
MOLYBDENUM SULPHIDE	45 0 90	2 5 0	2.25	
PERIODIC TABLE IN COLOUR	94 1 95	3 10 0	3.50	
PEROVSKITE	89 0 204	4 2 0	4.10	
PLATINUM SULPHIDE	51 0 72	3 12 0	3.60	
QUARTZ (Two Helices)	62 0 64	2 6 0	2.30	
REGULAR SOLIDS (Five)	50 0 90	2 0 0	2.00	
ROCK SALT (3 balls/edge)	27 0 54	1 4 0	1.20	
" (4 balls/edge)	64 0 144	2 18 0	2.90	
" (8 balls/edge)	512 0 1344	25 8 0	25.40	
" (12 balls/edge)	1728 0 4752	88 4 0	88.20	
RHENIUM OXIDE	135 0 162	4 6 0	4.30	
RUTILE	52 0 78	2 6 0	2.30	
SCANDIUM HYDROXIDE	135 0 162	4 6 0	4.30	
SET(Diamond, Blende, Rocksalt glucose, benzene, naphthaln, hexameth-tetramine)	162 38 303	6 0 0	6.00	
SILICATES (Partial)	177 0 224	5 15 0	5.75	
SNOWFLAKE (Six Arms)	312 0 540	12 0 0	12.00	
SODIUM NITRITE	40 0 50	1 12 0	1.60	
WURTZITE	39 0 58	1 9 0	1.45	
ZINC BLENDE	30 0 44	1 2 0	1.10	
ZIRCON	103 0 168	4 14 0	4.70	