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The Crystal Structure of Ammonium Tricyanomethide, $NH_4C(CN)_3$

BY ROBERT DESIDERATO AND RONALD L. SASS

Department of Chemistry, William Marsh Rice University, Houston, Texas, U.S.A.

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The structure of ammonium tricyanomethide, $NH_4C(CN)_3$ has been determined by X-ray single-crystal diffraction techniques. The crystals are monoclinic in the space group $P2_1/c$. The unit-cell constants are: $a = 9{\cdot}055 \pm 0{\cdot}007$, $b = 3{\cdot}87 \pm 0{\cdot}01$, $c = 17{\cdot}325 \pm 0{\cdot}014$ Å, $\beta = 104{\cdot}6 \pm 0{\cdot}2°$. Atomic and thermal vibrational coordinates were refined by isotropic least-squares methods. The $C(CN)_3^-$ ion is slightly nonplanar with $3m$ (C_{3v}) symmetry indicating a concentration of anion charge on the central carbon atom. The three C–C distances were found to be $1{\cdot}40 \pm 0{\cdot}01$ Å and the C–N distances were $1{\cdot}15 \pm 0{\cdot}01$ Å.

Introduction

Several metal salts of the tricyanomethide ion have been known to exist for many years. Only recently, however, has there been an interest in the structural properties of this ion. Miller & Baer (1962) and Long, Carrington & Cravenor (1962) have reported Raman and infrared spectroscopic studies of solid and aqueous solutions of $KC(CN)_3$. Although both of these sets of authors favor the planar $\bar{6}m2$ (D_{3h}) configuration of the $C(CN)_3^-$ ion, neither claimed to have conclusively eliminated the pyramidal $3m$ (C_{3v}) configuration for the ion.

In an attempt to determine the structure of the tricyanomethide ion, we had initially intended to study the crystal structures of both the potassium and the ammonium salts of the ion by single-crystal X-ray diffraction techniques. All of the crystals of the potassium salt which were examined proved to be badly twinned and unsuited for analysis. This paper therefore reports the structure of only the ammonium salt.

Experimental

Crystals of $NH_4C(CN)_3$ were obtained from $KC(CN)_3$ by means of an ion exchange column containing 120 Amberlite resin charged with ammonium ion. Evaporation of the eluent water solution followed by a double recrystallization with hot ethanol produced long-needled, colorless crystals about 0·2–0·3 mm in diameter and 1-2 mm in length. Kjeldahl analyses determined that the exchange was quantitative.

Suitable crystals were chosen and mounted along the needle axis. Oscillation, Weissenberg and precession photographs showed the Laue symmetry to be $2/m$ (C_{2h}). The space group was determined to be $P2_1/c$ (C_{2h}^5), derived from the following systematic absences:

$$h0l \text{ absent if } l = 2n+1$$
$$0k0 \text{ absent if } k = 2n+1 .$$

The cell constants a, c and the angle β were determined from a zero layer Weissenberg photograph which was calibrated with a superimposed NaCl ($a_0 = 5{\cdot}637$ Å) powder pattern. The b axis was determined from a rotation photograph. The following values were obtained ($\lambda = 1{\cdot}5418$ Å):

$$a = 9{\cdot}055 \pm 0{\cdot}007,\ b = 3{\cdot}87 \pm 0{\cdot}01,\ c = 17{\cdot}325 \pm 0{\cdot}014 \text{ Å};$$
$$\beta = 104{\cdot}6 \pm 0{\cdot}2°.$$

Assuming four molecules per unit cell, the calculated density is 1·18 g.cm^{-3}.

Weissenberg photographs of the $k = 0$, 1 and 2 layers were taken with filtered Cu $K\alpha$ radiation. Sets of three films were used and the intensities of the various reflections were estimated visually with a standard intensity strip. Correlation of the intensities of the various sets of films was made by comparison with a photograph which contained 15-min exposures of a 25° portion of each layer. The intensities were then corrected by the appropriate Lorentz, polarization and Tunell factors; absorption was neglected.

Treatment of data

Because of the relatively short b axis (3·867 Å) and the anticipated planar character of the $C(CN)_3^-$ ion, it was expected that a [010] projection would present a reasonably resolved image of the molecule. The Patterson $P(uw)$ projection was calculated and subsequently led to the solution of the trial structure. The sixfold nature of the near origin peaks of the vector diagram clearly showed the rotational orientation of the anion. Assuming a trigonal ion rotationally oriented as mentioned above, the complete set of interionic vectors between two anions related by a center of symmetry was constructed. Only the position of the center of gravity of this vector set is affected by the position of the center of gravity of the ion.

Table 1. *Observed and calculated structure factors for ammonium tricyanomethide*

h0ℓ

h	ℓ	F_{obs}	F_{calc}
0	16	9.608	-9.425
0	10	22.761	22.179
0	8	15.367	13.110
0	6	60.624	-71.623
0	4	48.500	-56.196
1	16	7.473	7.451
1	14	9.148	-8.261
1	10	5.857	-5.385
1	8	7.757	-6.985
1	6	16.062	-11.865
1	4	20.763	23.005
1	2	28.970	33.417
1	-2	16.072	-25.415
1	-4	36.541	36.893
1	-6	12.262	-9.103
1	-8	38.539	-38.218
1	-10	10.401	-11.188
1	-12	13.134	14.348
1	-14	20.665	21.058
1	-16	10.352	-9.832
2	16	9.520	8.509
2	14	9.294	-9.528
2	10	18.569	-16.749
2	8	6.866	-5.390
2	6	22.291	20.600
2	4	16.072	13.827
2	2	32.506	38.068
2	0	40.596	-48.955
2	-2	38.304	36.282
2	-4	42.261	-48.511
2	-6	8.031	-6.155
2	-8	5.299	-2.637
2	-10	16.718	15.937
2	-14	6.866	-6.596
2	-16	10.861	11.651
2	-20	6.552	-8.697
3	14	4.133	3.957
3	12	12.301	-14.241
3	10	16.718	-18.044
3	8	6.738	6.423
3	6	40.684	44.074
3	4	22.291	20.666
3	2	21.272	-17.327
3	0	51.085	-57.265
3	-6	37.756	35.721
3	-8	10.401	-10.449
3	-10	18.755	-19.489
3	-14	13.134	16.144
3	-16	16.522	16.402
3	-18	16.718	-19.073
4	14	6.552	8.063
4	12	15.367	-15.860
4	8	6.552	3.733
4	6	10.362	11.440
4	4	11.381	13.033
4	2	5.485	-6.194
4	-2	51.085	-53.065
4	-6	8.687	6.681
4	-8	23.221	23.907
4	-10	6.738	4.810
4	-14	7.061	-5.943
4	-16	10.401	-8.241
4	-20	6.552	6.172
5	14	8.315	-11.499
5	12	6.738	9.016
5	10	19.128	22.583
5	6	16.718	-17.951
5	4	7.199	-5.488
5	0	14.671	15.174
5	-2	19.137	-19.912
5	-4	7.199	7.526
5	-6	22.291	-21.762
5	-8	18.569	18.393
5	-10	16.072	16.439
5	-12	6.229	6.063
5	-14	9.294	-11.410
5	-16	16.072	-17.241
5	-18	6.415	5.520
6	12	11.381	14.725
6	2	9.294	-8.454
6	0	7.610	-5.472
6	-2	16.072	16.824
6	-4	6.866	-7.844
6	-8	11.381	9.355
6	-10	8.031	10.464
6	-12	7.473	-6.496
6	-14	10.401	-11.650
7	8	7.199	8.805
7	6	10.401	-11.438
7	4	13.094	-15.057
7	0	9.294	6.886
7	-2	9.294	8.984
7	-4	13.937	-14.029
7	-6	17.972	19.148
7	-12	9.294	-8.640
7	-14	5.396	1.805
8	2	11.371	-10.883
8	0	13.937	-14.483
8	-2	6.552	5.695
8	-4	27.864	29.237
8	-6	9.294	7.868
8	-8	21.782	-22.893
8	-10	13.094	-14.843
8	-14	8.031	9.393
9	-6	9.294	-10.508
9	-8	6.493	6.484
9	-16	8.031	8.034
10	-12	6.866	4.663

h1ℓ

h	ℓ	F_{obs}	F_{calc}
10	-14	5.485	3.246
11	0	6.033	5.834
11	-2	7.424	-4.586
11	-4	13.937	-12.982
0	17	8.697	-8.331
0	16	5.250	5.637
0	11	12.184	9.658
0	10	10.930	9.916
0	9	11.292	-10.155
0	7	6.239	7.715
0	6	5.063	-4.526
0	5	24.191	28.828
0	4	19.891	-20.419
0	3	17.247	18.296
0	2	16.699	17.733
1	19	7.071	5.719
1	13	11.929	-11.774
1	12	11.292	12.637
1	11	7.972	8.047
1	10	4.887	-3.488
1	9	24.681	24.988
1	8	11.390	-12.823
1	7	20.127	18.752
1	6	4.887	-6.069
1	5	13.721	-12.282
1	4	5.680	5.491
1	3	51.163	-81.780
1	2	18.638	19.773
1	1	12.977	12.524
1	0	23.672	-30.075
1	-1	21.116	20.163
1	-2	19.627	20.953
1	-3	40.292	47.402
1	-5	36.923	-38.746
1	-9	9.069	9.553
1	-10	5.112	-1.251
1	-11	9.294	7.516
1	-14	10.000	-10.353
1	-15	5.906	-5.853
1	-19	7.855	-4.629
2	11	5.494	-5.070
2	10	6.043	-4.308
2	9	19.989	18.805
2	8	6.239	6.557
2	7	13.574	12.363
2	6	5.494	-6.269
2	4	9.588	-7.717
2	3	49.303	-46.587
2	2	14.887	-14.071
2	1	24.181	-23.238
2	0	20.362	22.097
2	-1	6.885	-5.863
2	-2	29.010	32.824
2	-3	42.888	51.883
2	-4	19.294	-20.310
2	-5	33.858	36.225
2	-6	5.680	-5.723
2	-7	5.152	-4.820
2	-8	7.345	-7.853
2	-9	26.777	-30.151
2	-11	15.073	-13.484
2	-13	18.589	19.271
2	-16	7.345	6.143
2	-18	6.738	-5.944
2	-19	11.292	-9.000
2	-21	8.325	7.772
3	17	6.043	4.215
3	13	8.325	8.678
3	12	9.069	-10.699
3	7	13.574	-13.252
3	5	14.975	-12.891
3	3	14.505	13.161
3	2	8.472	-6.263
3	1	4.652	-5.011
3	0	18.775	15.982
3	-1	16.503	18.008
3	-2	14.554	-14.128
3	-3	16.503	-16.088
3	-4	10.597	10.611
3	-5	18.540	19.938
3	-6	5.112	3.546
3	-7	4.887	-3.295
3	-8	11.057	-11.844
3	-9	11.763	11.073
3	-10	5.299	-6.165
3	-11	8.325	-8.704
3	-13	13.075	-14.091
3	-14	11.292	12.119
3	-15	8.325	-7.689
3	-17	9.206	10.651
3	-19	11.292	11.544
4	13	9.069	9.574
4	11	6.885	7.621
4	10	6.415	6.649
4	9	15.073	-15.266
4	8	7.345	-6.130
4	7	16.229	-16.060
4	3	24.681	24.160
4	2	11.939	11.463
4	-1	8.834	9.111
4	-2	9.755	-9.010
4	-3	13.623	-14.763
4	-4	10.186	7.353
4	-5	11.763	12.856
4	-6	14.554	-15.668
4	-10	5.112	3.141

h2ℓ

h	ℓ	F_{obs}	F_{calc}
4	-11	13.075	-12.901
4	-12	5.494	5.480
4	-13	11.204	-11.405
4	-15	10.509	9.909
4	-16	3.112	-4.264
4	-17	5.680	6.715
4	-18	6.239	5.992
4	-19	7.620	5.304
4	-21	8.188	-5.514
5	12	4.887	4.705
5	15	8.932	12.667
5	10	7.345	-8.248
5	9	16.650	-19.436
5	6	8.550	9.146
5	5	7.620	5.985
5	4	8.051	5.717
5	3	9.294	8.905
5	1	12.526	13.272
5	0	15.386	-13.939
5	-1	5.680	-4.730
5	-2	6.043	7.238
5	-4	5.494	-4.890
5	-5	12.144	-12.890
5	-7	9.069	9.740
5	-8	7.199	5.406
5	-9	4.691	-3.251
5	-13	4.554	-5.377
5	-15	5.299	5.219
5	-16	5.063	5.748
5	-19	4.084	4.577
5	-20	4.554	-4.472
6	13	7.767	-7.845
6	10	4.887	-4.475
6	9	6.846	7.862
6	8	4.554	5.003
6	5	9.627	-10.213
6	1	21.292	21.474
6	-2	7.610	-5.410
6	-4	17.394	-16.758
6	-5	19.167	-19.476
6	-6	11.390	11.600
6	-7	6.415	-5.636
6	-8	6.415	5.645
6	-9	9.392	-9.547
6	-11	10.098	11.631
6	-13	11.204	12.574
6	-18	4.652	-3.725
6	-19	7.767	-6.229
7	11	5.112	-5.792
7	7	4.368	4.847
7	5	8.325	9.565
7	1	11.576	-11.397
7	3	4.505	-6.187
7	-1	4.368	5.236
7	-2	6.730	-6.441
7	-3	12.644	13.083
7	-4	6.738	6.843
7	-7	18.501	-21.062
7	-8	6.415	-6.403
7	-11	11.488	12.914
7	-13	10.597	13.023
7	-16	6.141	-6.196
7	-19	6.415	-6.525
8	9	5.494	5.580
8	-1	6.415	7.168
8	-3	13.388	-14.602
8	-4	6.415	6.507
8	-5	6.885	-3.949
8	-6	6.885	-7.351
8	-9	13.986	14.113
9	5	6.885	4.916
9	4	5.680	-6.190
9	1	6.484	-6.172
9	-1	12.144	-11.560
9	-2	5.494	5.362
9	-5	10.107	10.778
9	-7	5.494	6.922
10	4	5.299	0.606
10	-1	10.186	-9.460
10	-3	6.043	-3.030
10	-6	8.227	6.826
10	-7	14.426	12.521
10	-8	4.133	-4.127
10	-9	7.022	3.709
10	-10	5.112	-2.667
10	-13	11.763	-11.339
0	14	8.668	-8.952
0	12	7.874	7.601
0	10	10.950	11.419
0	9	15.298	-15.873
0	8	8.031	5.905
0	5	21.106	21.133
0	4	18.941	-19.314
0	2	12.752	11.690
0	1	11.811	11.113
1	12	7.483	7.462
1	10	9.598	-10.307
1	9	7.287	9.821
1	7	13.036	12.539
1	6	11.949	-10.640
1	5	15.700	-14.935
1	4	19.128	18.365
1	3	6.601	-5.847
1	1	14.769	15.004
1	-1	6.689	7.092
1	-2	7.130	6.948

h	ℓ	F_{obs}	F_{calc}
1	-3	11.567	-12.124
1	-5	16.591	-19.725
1	-7	11.684	7.735
1	-8	21.752	-18.336
1	-13	6.004	7.189
1	-14	9.833	9.879
1	-19	5.808	-4.678
2	16	6.444	6.212
2	15	5.622	-5.100
2	12	8.521	-9.970
2	10	6.934	-7.325
2	9	6.787	8.082
2	6	12.311	10.366
2	3	17.570	15.290
2	2	6.503	4.997
2	1	13.094	-12.444
2	-1	7.130	-8.931
2	-3	11.655	-11.901
2	-4	15.053	-15.803
2	-5	13.780	12.970
2	-6	7.483	6.369
2	-8	6.787	-4.661
2	-10	5.622	6.449
2	-11	9.696	10.321
2	-12	7.629	-6.863
2	-14	7.287	6.148
2	-17	5.622	-4.598
3	12	8.521	-10.043
3	9	5.622	6.641
3	8	5.622	-6.124
3	6	23.927	23.287
3	3	10.039	-9.185
3	1	11.567	-10.534
3	0	28.882	-31.907
3	-1	8.717	7.354
3	-2	9.500	-10.014
3	-4	15.896	16.644
3	-6	11.508	10.958
3	-7	6.787	-6.837
3	-9	11.763	12.042
3	-10	14.475	-15.744
3	-12	5.171	5.452
3	-13	8.961	-7.791
3	-14	8.227	9.513
3	-16	6.787	5.257
3	-18	5.416	-5.605
4	15	5.416	7.397
4	7	10.724	11.674
4	6	10.724	11.841
4	5	10.577	9.850
4	4	6.934	3.530
4	3	14.456	-14.939
4	1	10.724	-9.696
4	0	8.521	-8.543
4	-1	10.636	-9.373
4	-3	13.241	12.933
4	-5	12.497	11.694
4	-6	7.287	-6.536
4	-7	9.050	9.764
4	-8	12.938	15.316
4	-9	7.130	-6.479
4	-11	12.987	-16.151
4	-12	5.622	4.844
4	-14	10.088	-11.052
5	10	7.718	7.703
5	8	5.416	6.918
5	6	15.053	-15.305
5	5	11.126	-11.474
5	1	8.668	7.824
5	0	15.053	14.328
5	-1	5.808	-5.129
5	-2	6.787	-7.969
5	-4	10.088	-10.434
5	-7	9.833	10.166
5	-8	9.050	9.601
5	-9	6.934	-7.182
5	-10	8.364	8.724
5	-16	5.553	-6.416
6	12	5.171	4.598
6	7	6.395	-7.189
6	6	6.004	-6.654
6	2	5.171	-4.741
6	1	5.171	-6.428
6	-3	5.808	7.161
6	-7	8.070	-8.672
6	-10	10.195	11.320
6	-11	4.926	5.447
6	-16	11.224	-9.670
7	7	4.926	-5.266
7	4	5.808	-7.664
7	1	6.601	6.496
7	-1	6.601	11.307
7	-3	8.227	-8.029
7	-5	8.070	-7.212
7	-9	9.941	10.229
7	-12	5.553	-6.027
7	-13	5.171	-5.571
8	6	10.088	9.971
8	2	7.629	-6.021
8	1	8.364	9.272
8	0	8.961	-11.501
8	-2	8.668	9.249
8	-4	13.036	12.544
8	-8	8.961	-7.869
8	-10	11.126	-13.553
8	-13	9.050	8.599
9	-16	6.249	6.445
9	-1	6.787	-6.377
10	-8	5.808	-3.458

Table 2. *Final atomic parameters*

Atom	x	y	z	β	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(\beta)$
C(1)	0·2976	0·1451	0·3609	1·66	0·0009	0·0030	0·0004	0·15
C(2)	0·2462	0·3264	0·2891	2·33	0·0009	0·0034	0·0005	0·18
C(3)	0·1928	0·0308	0·4021	1·67	0·0009	0·0031	0·0004	0·15
C(4)	0·4490	0·0274	0·3835	2·39	0·0009	0·0033	0·0004	0·17
N(1)	0·1718	0·5405	0·5945	1·71	0·0007	0·0024	0·0003	0·12
N(2)	0·2055	0·4798	0·2305	3·67	0·0009	0·0029	0·0004	0·18
N(3)	0·1079	0·9407	0·4366	2·57	0·0008	0·0026	0·0004	0·15
N(4)	0·5741	0·9300	0·4024	3·49	0·0009	0·0029	0·0004	0·17

This array was then superimposed on the Patterson projection until a reasonable overlay was found. The coordinates of the center of the vector set then corresponded to twice the coordinates of the actual ion. This procedure led directly to the trial positional parameters of the $C(CN)_3^-$ group. The ammonium ion was then located by packing considerations.

An electron density projection based on this trial structure was well resolved with no spurious peaks. The coordinates obtained from this electron distribution function were used in an isotropic least-squares refinement of the $h0l$ data. A total of 112 observed reflections were used. The reliability index decreased from $R=28{\cdot}9\%$ to $R=8{\cdot}9\%$.

Trial y parameters were obtained by tilting the $C(CN)_3^-$ ion with respect to the xz plane as indicated by the projected dimensions of the ion and then adjusting the y parameter of the center of gravity to give a reasonable packing around the ammonium ion.

The ambiguity between the twofold screw axis and center of symmetry in the projection was resolved from a packing consideration.

A total of 429 observed reflections were then used to refine all trial parameters. Calculated structure factors for unobserved reflections were not included in the Table of structure factors (Table 1) although they were computed and showed no significant discrepancies. The program used was one written for the Rice Computer. The thermal vibration parameters were assumed to be isotropic. Form factors were obtained from *International Tables for X-Ray Crystallography* (1962). A table look-up and linear interpolation was employed. Weights of integral values ranging from 1 to 5 were assigned such that the largest reflections were given a weight of 1 and the smallest reflections were given a weight of 5. The complete normal equation matrix was used in the solution. The final over-all R value obtained was 10·4%. The final calculated and observed structure factors are listed in Table 1. A summary of the final atomic parameters and their estimated standard deviations is presented in Table 2.

Discussion of the structure

The dimensions of the $C(CN)_3^-$ ion are presented in Table 3. Within experimental error the ion is threefold.

Table 3. *Interatomic dimensions in* $C(CN)_3^-$ *ion*

Distances		Angles	
C(1)–C(2)	1·40 ± 0·01 Å	C(2)–C(1)–C(3)	119° 40′ ± 1°
C(1)–C(3)	1·40 ± 0·01	C(3)–C(1)–C(4)	119 31 ± 1
C(1)–C(4)	1·40 ± 0·01	C(4)–C(1)–C(2)	119 32 ± 1
C(2)–N(2)	1·15 ± 0·01	C(1)–C(2)–N(2)	180 0 ± 1
C(3)–N(3)	1·14 ± 0·01	C(1)–C(3)–N(3)	180 0 ± 1
C(4)–N(4)	1·16 ± 0·01	C(1)–C(4)–N(4)	180 0 ± 1

The value of 1·40 Å for the C–C bond length is somewhat shorter than what one would expect for a single sp–sp^2 carbon–carbon bond; compare with the value of 1·44 Å found in vinyl cyanide (Wilcox, Goldstein & Simmons, 1954). The value of 1·15 Å for the C–N distance is normal. The C–C–N bond angles are all 180° as expected; however, the C–C–C angles of 119° 31′, 119° 32′ and 119° 40′ suggest a slight non-planarity of the ion. If one passes a plane through carbon atoms C(2), C(3) and C(4), the central carbon atom C(1) is found to be 0·08 Å above this plane and the nitrogen atoms N(2), N(3), N(4) are all 0·05 Å below this plane. Each C–C–N unit thus makes an angle of 3° with respect to the plane perpendicular to the threefold axis. It is believed by the authors that this deviation from planarity is real and that the central carbon atom does, therefore, possess a significant amount of negative charge. It is difficult to see how the crystal symmetry could be causing this distortion from planarity. Fig. 1 shows a diagram

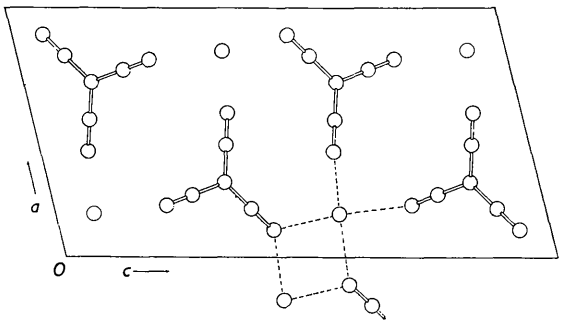

Fig. 1. Projection of the ammonium tricyanomethide structure projected down the [010] axis.

of the packing projected onto the (010) plane. There

are no abnormal interionic attractions. The $C(CN)_3^-$ ions are stacked along the b axis with the ammonium ions to the side. The crystal symmetry around a particular $C(CN)_3^-$ ion is very nearly m (C_s) with the mirror plane passing through C(1)–C(3)–N(3). This feature is not evident in the dimensions of the ion but can readily be seen in the thermal vibration parameters presented in Table 2. The nitrogen atom N(3) approaches four NH_4^+ groups whereas N(2) and N(4) approach only two. The thermal vibration parameters of C(2) and C(4) are comparable as are the thermal parameters of N(2) and N(4). Those of C(3) and N(3) are, however, significantly smaller than their counterparts.

The NH_4^+ environment is rather interesting. Each N(1) atom is surrounded by eight nearest nitrogen neighbors in a distorted tetragonal arrangement rather similar to that found in the ammonium halides. The significant distances and angles are presented in Table 4 and Fig. 2. All distances are normal. The

Table 4. *Interionic dimensions about the* NH_4^+ *ion*

Distances		Distances	
Below N(1)		Above N(1)	
N(3) –N(1)	3·523 Å	N(3)	3·070 Å
N(3′)–N(1)	3·082	N(3′)	3·171
N(2′)–N(1)	3·056	N(2′)	2·954
N(4′)–N(1)	2·925	N(4′)	3·072

Distances		Angles	
Between $C(CN)_3^-$ ions			
N(3) –N(3′)	3·323 Å	N(4′)–N(3′)–N(3′)	87° 29′
N(3′)–N(2′)	3·509	N(3) –N(3′)–N(2)	92 55
N(2′)–N(4′)	3·414	N(3′)–N(2′)–N(4)	86 1
N(4′)–N(3)	3·502	N(2′)–N(4′)–N(3)	91 28

ammonium atom is not in the center of the Coulomb field of the eight neighbor nitrogen atoms, but is displaced from this center by 0·22 Å in a direction away from its only neighboring NH_4^+ ion thus making the distance of this repulsive interaction 3·92 Å rather than 3·49 Å.

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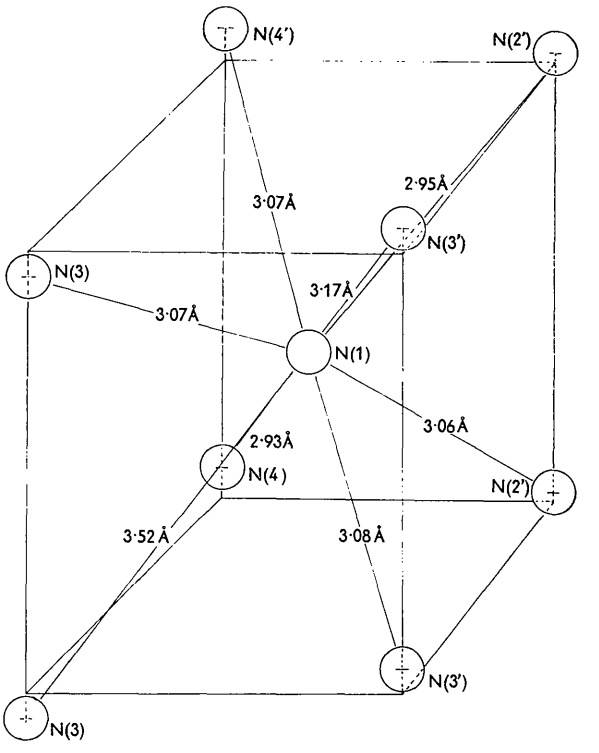

Fig. 2. Environment of the ammonium ion.

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