meters. We believe that where there are two solutions possible, it is preferable to choose the more general case, *i.e.* the noncentric interpretation.

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The Crystal Structure of $NaCl\,.\,5\frac{1}{7}NH_3$ and $NaBr\,.\,5\frac{1}{7}NH_3$

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The crystal structures of $NaCl\,.\,5\frac{1}{7}NH_3$ and $NaBr\,.\,5\frac{1}{7}NH_3$ have been determined from single-crystal X-ray data, collected in a low-temperature Weissenberg camera with Cu *K* radiation. Both compounds are trigonal, space group $R\bar{3}$, with 21 formula units in a hexagonal cell for which the measured dimensions are:

$$NaCl\,.\,5\tfrac{1}{7}NH_3\colon a=23{\cdot}67,\ c=9{\cdot}25\ \text{Å}\ (t=-58\ ^\circ\text{C})\ ;$$
$$NaBr\,.\,5\tfrac{1}{7}NH_3\colon a=24{\cdot}34,\ c=9{\cdot}46\ \text{Å}\ (t=-35\ ^\circ\text{C})\ .$$

The ammonia molecules and halide ions together form a roughly cubic close-packed arrangement, the sodium ions occupying certain of the octahedral interstices, so that only ammonia molecules are closest neighbours. The octahedra, which enclose some of the sodium ions, share two corners with adjacent octahedra; in this case the effective coordination of the sodium is only fivefold, the sixth ammonia molecule lying at a greater distance.

Introduction

The present investigation forms part of a series of structure determinations of some ammines formed with salts of the alkali metals and ammonium. The structures of $NH_4\,.\,3NH_3$ (X=Cl, Br, I) and $NH_4I\,.\,4NH_3$ have been reported earlier (Olovsson, 1960 *a*, *b*)

In the systems NaX–NH_3 (X=F, Cl, Br, I) the following compounds have been reported: $NaCl\,.\,2{\cdot}5NH_3$ (Friedrichs, 1921), $NaCl\,.\,5NH_3$ (Joannis, 1891; Biltz & Hansen, 1923; Biltz, 1923; Patscheke, 1933), $NaBr\,.\,5{\cdot}25NH_3$ and $NaBr\,.\,5{\cdot}75NH_3$ (Biltz & Hansen, 1923; Biltz, 1923), $NaI\,.\,4NH_3$ (Picon, 1919; Leonard, Lippincott, Nelson & Sellers, 1955), $NaI\,.\,4{\cdot}5NH_3$ and $NaI\,.\,6NH_3$ (Biltz & Hansen, 1923; Biltz, 1923). A phase with the composition $NaCl\,.\,2{\cdot}5NH_3$ does not exist according to later investigations (Biltz & Hansen, 1923). The phase reported as $NaI\,.\,4NH_3$ has the composition $NaI\,.\,4{\cdot}5NH_3$ according to Biltz & Hansen (1923). The structures of the ammines of sodium iodide are currently being investigated in this laboratory.

In this paper the structures of the compounds formulated above as $NaCl\,.\,5NH_3$ and $NaBr\,.\,5{\cdot}25NH_3$ are reported. The X-ray crystallographic investigation shows that these compounds are isomorphous and have the exact composition $NaCl\,.\,5\frac{1}{7}NH_3$ and $NaBr\,.\,5\frac{1}{7}NH_3$, respectively. This point is further discussed below. For covenience these compounds are called 'pentammines' in the following text, although it should be kept in mind that this designation is not altogether adequate.

Experimental

The solubility curve of sodium chloride in ammonia is shown in Fig. 1. The values were taken from the work by Patscheke (1933) (*cf.* also Patscheke & Tanne, 1935), but the results of Guyer, Bieler & Schmid (1934) and Distanov (1938) are very similar. The curves give the composition of the solution in equilibrium with 'pentammine' (lower curve) and with ammonia-free sodium chloride (upper curve), respectively. Thus the 'pentammine' decomposes at temperatures above −9·5 °C into pure sodium chloride and a solution of sodium chloride in ammonia. As shown in the figure, the maximum solubility of sodium chloride is 15·37 wt.% NaCl (18·90 moles NH_3/mole NaCl) at the transformation temperature −9·5 °C. The corresponding solubility curve for sodium bromide in ammonia is analogous. Sodium bromide is, however, considerably more soluble; the maximum solubility is about 54·5 wt.% NaBr (about 5·05 moles NH_3/mole NaBr) at +13 °C (Distanov, 1938). At this point the saturated solution evidently has a composition very close to that of the solid phase $NaBr.5\frac{1}{7}NH_3$ (5·143 moles NH_3/mol NaBr).

It is obviously not possible to grow single crystals of $NaCl.5\frac{1}{7}NH_3$ in the ordinary way from a liquid of the same composition. The crystals of the 'pentammine' would have to be formed by reaction between solid sodium chloride and ammonia–sodium chloride solution by cooling to a temperature below −9·5 °C. To obtain single crystals this way seems rather difficult. It was therefore decided to grow the crystals from a homogeneous liquid containing as much sodium chloride as possible (maximum 15·37 wt.% NaCl at −9·5 °C, as stated above); the details of the procedure are described in the following section.

Glass capillaries were made by drawing out one end of a thin-walled glass tube (diameter about 2 mm) to a diameter of 0·1 to 0·2 mm and a wall thickness of 0·01 to 0·02 mm. Sodium chloride was weighed into the capillary and carefully dried ammonia was condensed over it. Reweighing, after sealing the capillary with a micro-flame, gave the amount of ammonia present. This amount was adjusted to a percentage by weight of sodium chloride somewhat greater than 15·37 in a series of preparations. The capillary was then kept for some time at about −10 °C to allow as much sodium chloride as possible to dissolve, the small excess of sodium chloride then being transferred to the rear end of the capillary. Single crystals were grown from this saturated solution in the Weissenberg camera by blowing a cooled stream of gas parallel to the capillary axis and following the growth with a polarizing microscope. The details of the low-temperature apparatus were described in an earlier paper (Olovsson, 1960*c*). The bromide was prepared by an analogous method, but it was considerably easier to grow single crystals of the bromide than of the chloride. The crystals of the bromide compound grew preferably with their *c* axes parallel to the capillary axis. If the pentammine of the chloride has an extended range of homogeneity, the crystals formed by the above procedure may not attain the ideal composition of $NaCl.5\frac{1}{7}NH_3$ but may instead have a (small) excess of ammonia. If this is the case the cell dimensions and other properties will be affected to a certain extent. Experience obtained from related systems indicates, however, that solid solutions probably do not exist, or at least only to a very limited extent. In the case of the bromide the problem posed by solid solution formation does not arise in practice since the crystals may be grown from a solution of the ideal composition. During the crystal growth good agreement was observed with the earlier determined melting points.

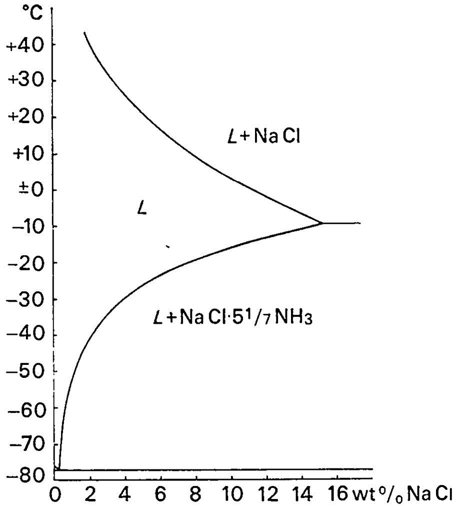

Fig. 1. The solubility curve of sodium chloride in ammonia (values taken from the work by Patscheke, 1933).

Equi-inclination Weissenberg photographs were taken of the chloride at −58 °C and of the bromide at −35 °C with Cu *K* radiation. With [001] as the rotation axis layers $0 \leq l \leq 6$ were collected for the chloride and $0 \leq l \leq 8$ for the bromide. The relative intensities were estimated visually with the use of the multiple-film technique (five films), the intensities being compared with a calibrated scale. The intensity range was 1 to 9000. The data were corrected for the Lorentz and polarization effects. The radii and absorption coefficients of the cylindrical crystals used were:

$$NaCl.5\tfrac{1}{7}NH_3\colon r=0{\cdot}010 \text{ cm}, \mu=37{\cdot}7 \text{ cm}^{-1}$$
$$NaBr.5\tfrac{1}{7}NH_3\colon r=0{\cdot}008 \text{ cm}, \mu=65{\cdot}7 \text{ cm}^{-1}.$$

In addition, rotation photographs were taken of a single crystal of the chloride at −94°, −133° and −190 °C, but no changes in structure were indicated in these photographs.

Unit cell and space group

The data showed the diffraction symmetry to be that of the trigonal Laue group $\bar{3}$. On referring the crystal to hexagonal axes all reflexions missing for which $-h+k+l \neq 3n$ indicating a rhombohedral lattice (with the rhombohedral axes in the 'obverse' orientation relative to the corresponding hexagonal axes; *cf. International Tables for X-ray Crystallography*, 1952, p. 20). These results suggest the space groups $R3$ or $R\bar{3}$. As shown in the next section, the structure is satisfactorily described by $R\bar{3}$ (C_{3i}^2) and the subsequent refinement of the structure using this space group gave good agreement with the intensity data indicating the suitability of this choice. The crystals are here consistently referred to hexagonal axes and the general 18-fold equivalent positions in $R\bar{3}$ are as follows:

$$(0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3})+(x,y,z);\ (\bar{x},\bar{y},\bar{z});\ (\bar{y},x-y,z);$$
$$(y,y-x,\bar{z});\ (y-x,\bar{x},z);\ (x-y,x,\bar{z})\,.$$

The unit-cell parameters as determined from rotation and quartz-calibrated zero-layer Weissenberg photographs are:

$\mathrm{NaCl}\,.\,5\tfrac{1}{7}\mathrm{NH_3}$: $a=23{\cdot}665\pm0{\cdot}010$, $c=9{\cdot}253\pm0{\cdot}020$ Å ($t=-58$ °C)

$\mathrm{NaBr}\,.\,5\tfrac{1}{7}\mathrm{NH_3}$: $a=24{\cdot}343\pm0{\cdot}015$, $c=9{\cdot}462\pm0{\cdot}020$ Å. ($t=-35$ °C)

($a=4{\cdot}913$ Å for α-quartz ($t=20$ °C); λ Cu $K\alpha_1=1{\cdot}54051$ Å, λ Cu $K\alpha_2=1{\cdot}54433$ Å). The uncertainties in the cell dimensions given above are not standard deviations but correspond to estimated maximum errors.

The density of the bromide was estimated from the volume and weight of a completely homogeneous crystal contained in a cylindrical capillary of uniform thickness; the volume was measured microscopically and the weight was given by the preparative technique. The observed density was: $\mathrm{NaBr}\,.\,5\tfrac{1}{7}\mathrm{NH_3}$: $d_{\mathrm{obs}}=1.37$ g.cm^{-3}. In view of the symmetry the number of formula units in the hexagonal unit cell must be a multiple of three; with 21 formula units d_{calc} is 1·36 g.cm^{-3} for the bromide and 1·13 for the chloride. The weighted mean of the densities of the sodium halide and solid ammonia is 1·22 for the bromide and 1·04 for the chloride.

Determination of the atomic coordinates

The positions of the halogen atoms were determined by comparison between the peaks in three-dimensional Patterson syntheses for the chloride and bromide. Subsequent interpretation was based on the space group $R3$. Here the general ninefold positions (in the hexagonal unit cell) are: $(0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3})+(x,y,z)$; $(\bar{y},x-y,z)$; $(y-x,\bar{x},z)$. The only special positions are threefold and of the form $(0,0,z)$. With 21 halogen atoms per unit cell the only practical possibility is to locate two independent atoms in general positions (x_1,y_1,z_1) and (x_2,y_2,z_2) and one atom in a special position $(0,0,z_3)$. The z coordinate of one atom is arbitrary and z_3 was set equal to zero. The only possible atomic coordinates for the other halogen atoms, consistent with the Patterson maps, were found to be approximately $x_1=0{\cdot}09$, $y_1=0{\cdot}45$, $z_1=0$ and $x_2=-0{\cdot}09$, $y_2=-0{\cdot}45$, $z_2=0$. Clearly these atomic positions are equally consistent with the centrosymmetric space group $R\bar{3}$. It is noteworthy that an independent interpretation of the Patterson maps starting with $R\bar{3}$ led to the same coordinates. From three-dimensional F_o syntheses based on these halogen positions, the coordinates of the sodium and nitrogen atoms were then determined. Since satisfactory coordinates for these atoms were obtained assuming the space group $R\bar{3}$ and the subsequent refinements proceeded successfully, the space group $R\bar{3}$ is considered to be the appropriate one. In the structure thus obtained the halogen and sodium atoms are each located in one general 18-fold and one special threefold position and the nitrogen atoms ($21\times5\tfrac{1}{7}$ atoms $=108$ atoms) in six 18-fold positions.

The preliminary atomic coordinates were first improved in a series of three-dimensional electron density calculations and then further refined by the method of least squares. The least-squares treatment also involved refinement of individual isotropic temperature factors and inter-layer scale factors.

The Fourier calculations were made on the computer FACIT EDB with programs (designated STRIX and PROFFS) written by Liminga & Olovsson (1964). The electron-density maxima were located with a program (LOKE) written by Lundberg & Olovsson.

The first series of least-squares calculations (about 20 cycles) was performed on FACIT EDB with a program (SFLS) written by Brändén & Åsbrink (to be published). A block-diagonal approximation is used in this program to minimize the function $\Sigma w(|F_o|-|F_c|)^2$. The weighting scheme used was that due to Cruickshank, Pilling, Bujosa, Lovell & Truter (1961). In this $w=1/(a+|F_o|+c|F_o|^2)$, where the constants a and c were chosen as follows: $a=2\,.\,|F_{o,\,\mathrm{min}}|$ and $c=2/|F_{o,\,\mathrm{max}}|$. Reflexions too weak to be observed were given zero weight. Orthorhombic symmetry is the highest symmetry that this program can handle correctly. Structures of higher symmetry can be refined if they are treated as having lower symmetry, which necessitates the inclusion of more than the independent data. The standard deviations obtained are then incorrect. In the present case the least-squares refinements were performed for the structure described in terms of the corresponding monoclinic symmetry.

Finally five cycles of least-squares calculations were performed with a full matrix program, ORFLS, written by Busing, Martin & Levy (1962). The same weighting scheme as above was used. The shifts in the atomic positions in the final cycles were less than one tenth of the standard deviation for the coordinate in question. The 'discrepancy indices' at this point were:

For the chloride:

$$R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|=0{\cdot}093$$
$$R_2=[\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{\frac{1}{2}}=0{\cdot}125$$

For the bromide:

$$R_1=0{\cdot}067,\ R_2=0{\cdot}089\,.$$

The atomic parameters together with the standard deviations after the final least-squares refinement are listed in Table 1.* The observed and calculated structure factors at this stage are compared in Table 2. The number of reflexions recorded was 756 for the chloride and 1985 for the bromide. Distances and angles together with their standard deviations were calculated using the program ORFFE (Busing, Martin & Levy, 1964). The standard errors of the distances and angles were then computed from the errors of the atomic coordinates obtained in the form of a variance–covariance matrix at the final least-squares cycle using ORFLS. The errors of the cell parameters were also included in these calculations.

The atomic scattering factors used in the above calculations were those given for N°, Na^+, Cl^- and Br^- in *International Tables for X-ray Crystallography* (1962, p. 202 and 206), based on wave functions obtained by the method of the self-consistent field. Hydrogen atoms were not included in the calculations.

Table 1. *Atomic parameters and standard deviations*

	$NaCl\,.\,5\frac{1}{7}NH_3$	$NaBr\,.\,5\frac{1}{7}NH_3$
X(1)	$x=0{\cdot}0947(9)\pm0{\cdot}0001(7)$	$0{\cdot}09470\pm0{\cdot}00003$
	$y=0{\cdot}4461(1)\pm0{\cdot}0002(0)$	$0{\cdot}44645\pm0{\cdot}00003$
	$z=0{\cdot}9948(2)\pm0{\cdot}0005(0)$	$0{\cdot}99502\pm0{\cdot}00007$
	$B=1{\cdot}93\pm0{\cdot}09$	$3{\cdot}54\pm0{\cdot}03$
X(2)	$x=0$	0
	$y=0$	0
	$z=0$	0
	$B=2{\cdot}19\pm0{\cdot}20$	$3{\cdot}44\pm0{\cdot}04$
Na(1)	$x=0{\cdot}4376(5)\pm0{\cdot}0002(6)$	$0{\cdot}4380(5)\pm0{\cdot}0001(4)$
	$y=0{\cdot}1320(1)\pm0{\cdot}0003(2)$	$0{\cdot}1311(5)\pm0{\cdot}0001(8)$
	$z=0{\cdot}1526(7)\pm0{\cdot}0007(4)$	$0{\cdot}1507(0)\pm0{\cdot}0002(9)$
	$B=1{\cdot}58\pm0{\cdot}13$	$3{\cdot}71\pm0{\cdot}06$
Na(2)	$x=0$	0
	$y=0$	0
	$z=0{\cdot}50$	$0{\cdot}50$
	$B=1{\cdot}47\pm0{\cdot}26$	$3{\cdot}93\pm0{\cdot}14$
N(1)	$x=0{\cdot}2551(4)\pm0{\cdot}0006(4)$	$0{\cdot}2557(2)\pm0{\cdot}0003(1)$
	$y=0{\cdot}4742(4)\pm0{\cdot}0006(8)$	$0{\cdot}4711(2)\pm0{\cdot}0003(1)$
	$z=0{\cdot}0429(8)\pm0{\cdot}0015(4)$	$0{\cdot}0297(6)\pm0{\cdot}0007(7)$
	$B=2{\cdot}91\pm0{\cdot}28$	$4{\cdot}26\pm0{\cdot}12$
N(2)	$x=0{\cdot}3363(5)\pm0{\cdot}0006(3)$	$0{\cdot}3379(2)\pm0{\cdot}0003(2)$
	$y=0{\cdot}0513(2)\pm0{\cdot}0006(3)$	$0{\cdot}0524(6)\pm0{\cdot}0003(1)$
	$z=0{\cdot}0292(0)\pm0{\cdot}0015(4)$	$0{\cdot}0216(2)\pm0{\cdot}0007(6)$
	$B=2{\cdot}95\pm0{\cdot}31$	$4{\cdot}48\pm0{\cdot}13$
N(3)	$x=0{\cdot}4817(5)\pm0{\cdot}0006(3)$	$0{\cdot}4807(6)\pm0{\cdot}0002(8)$
	$y=0{\cdot}0715(6)\pm0{\cdot}0006(3)$	$0{\cdot}0721(3)\pm0{\cdot}0002(8)$
	$z=0{\cdot}0157(8)\pm0{\cdot}0015(8)$	$0{\cdot}0103(4)\pm0{\cdot}0008(0)$
	$B=2{\cdot}80\pm0{\cdot}31$	$4{\cdot}10\pm0{\cdot}13$
N(4)	$x=0{\cdot}3025(8)\pm0{\cdot}0006(9)$	$0{\cdot}3000(4)\pm0{\cdot}0003(3)$
	$y=0{\cdot}1915(1)\pm0{\cdot}0006(6)$	$0{\cdot}1894(3)\pm0{\cdot}0003(3)$
	$z=0{\cdot}0051(7)\pm0{\cdot}0016(7)$	$0{\cdot}0081(5)\pm0{\cdot}0007(9)$
	$B=3{\cdot}75\pm0{\cdot}35$	$4{\cdot}64\pm0{\cdot}14$
N(5)	$x=0{\cdot}2366(7)\pm0{\cdot}0007(2)$	$0{\cdot}2373(9)\pm0{\cdot}0003(0)$
	$y=0{\cdot}6099(6)\pm0{\cdot}0007(5)$	$0{\cdot}6118(0)\pm0{\cdot}0003(0)$
	$z=0{\cdot}9829(4)\pm0{\cdot}0018(5)$	$0{\cdot}9922(5)\pm0{\cdot}0007(3)$
	$B=4{\cdot}13\pm0{\cdot}38$	$4{\cdot}19\pm0{\cdot}13$
N(6)	$x=0{\cdot}1432(1)\pm0{\cdot}0006(7)$	$0{\cdot}1433(2)\pm0{\cdot}0003(1)$
	$y=0{\cdot}1696(2)\pm0{\cdot}0006(1)$	$0{\cdot}1681(2)\pm0{\cdot}0003(1)$
	$z=0{\cdot}9941(0)\pm0{\cdot}0016(1)$	$0{\cdot}0003(0)\pm0{\cdot}0007(4)$
	$B=3{\cdot}23\pm0{\cdot}32$	$4{\cdot}33\pm0{\cdot}13$

Description of the structure

The structure can perhaps be most easily described with reference to Fig. 2. Both the ammonia molecules

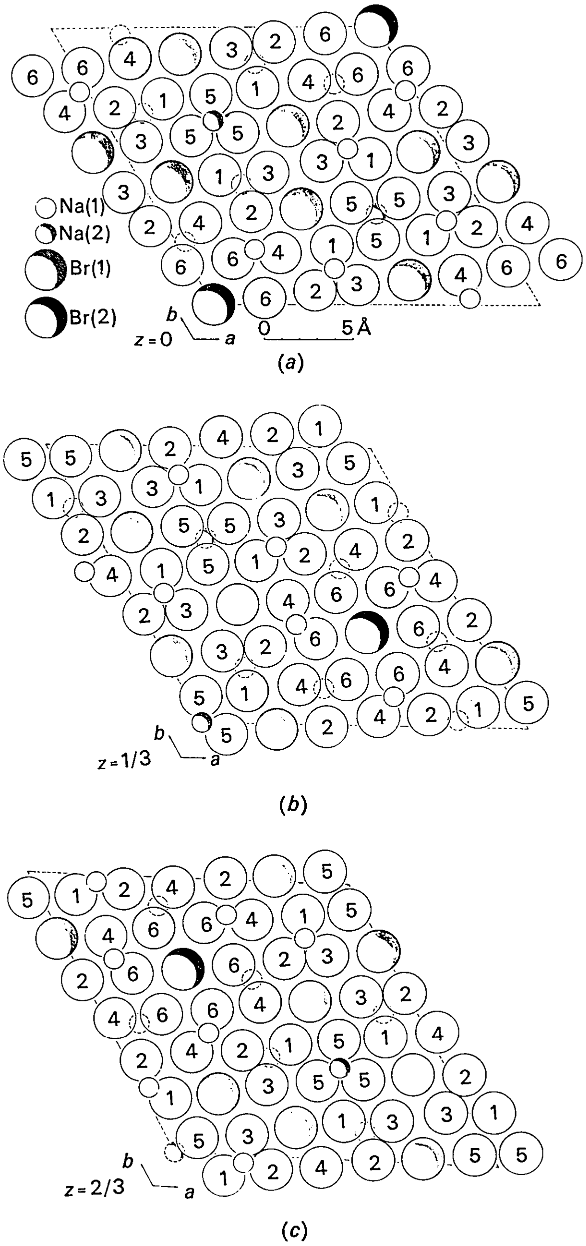

Fig. 2. The crystal structure of $NaBr\,.\,5\frac{1}{7}NH_3$. The ammonia molecules and halide ions are approximately located in three separate layers parallel to (001) with the z coordinates 0, $\frac{1}{3}$ and $\frac{2}{3}$ as shown in (*a*), (*b*) and (*c*). The sodium ions are situated above and below these layers in some of the octahedral interstices. The nitrogen atoms have been numbered as in Table 1.

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* It is noticeable that the temperature factors for the bromide are considerably higher than those for the chloride, more than expected for the difference in temperature. As the slightly stronger absorption in the bromide contributes in the opposite direction the effect is evidently due to other factors (*e.g.* disorder).

Table 2. *Observed and calculated structure factors*

F_o and F_c are $\frac{1}{3}$ of absolute scale. Unobserved reflexions are marked with an asterisk.

NaCl . $5\frac{1}{7}NH_3$

H	K	L	F_o	F_c
3	0	0	20.3	22.5
6	0	0	10.6*	5.7
9	0	0	66.3	60.3
12	0	0	17.1*	3.0
-23	1	0	18.9	15.4
-20	1	0	21.9*	9.1
-17	1	0	13.3	14.6
-14	1	0	60.6	62.7
-11	1	0	23.8	21.8
-8	1	0	13.5	15.6
-5	1	0	82.3	117.9
-2	1	0	5.5*	2.6
4	1	0	40.4	45.9
7	1	0	36.3	35.0
10	1	0	17.8	17.7
13	1	0	26.0	26.7
-22	2	0	16.1	15.3
-19	2	0	44.6	43.8
-16	2	0	19.8*	2.4
-13	2	0	16.8*	4.3
-10	2	0	52.9	46.9
-7	2	0	18.7	19.4
-4	2	0	21.9	22.8
5	2	0	10.9*	6.1
8	2	0	26.8	23.4
11	2	0	45.8	45.6
14	2	0	19.9	15.6
17	2	0	21.9*	3.6
20	2	0	29.6	27.6
23	2	0	22.9	21.0
-24	3	0	30.4	26.9
-21	3	0	21.5*	0.6
-18	3	0	21.2*	10.7
-15	3	0	18.5	14.4
-12	3	0	21.7	19.1
-9	3	0	12.6*	6.7
-6	3	0	29.1	29.7
6	3	0	72.5	70.2
9	3	0	48.6	43.4
12	3	0	18.5*	2.2
15	3	0	36.7	38.3
18	3	0	65.3	56.3
-14	4	0	17.1*	9.4
-11	4	0	29.3	25.7
-8	4	0	51.0	56.7
7	4	0	14.4	13.5
10	4	0	59.8	55.8
13	4	0	20.1	15.2
-13	5	0	146.0	172.9
-10	5	0	36.7	36.4
8	5	0	16.1*	2.7
11	5	0	18.9	16.9
-27	6	0	23.2	18.8
-24	6	0	20.2*	10.9
-21	6	0	21.9*	0.1
-18	6	0	60.6	55.2
-15	6	0	28.4	29.3
-12	6	0	15.0*	6.8
9	6	0	29.1	27.2
-23	7	0	24.2	24.5
-20	7	0	21.5*	8.6
-17	7	0	19.7	16.6
-14	7	0	36.5	33.9
10	7	0	50.5	45.0
13	7	0	21.5*	2.1
16	7	0	24.2	23.2
19	7	0	26.8	25.9
-25	8	0	19.5*	2.2
-22	8	0	21.9*	4.1
-19	8	0	20.9*	1.6
-16	8	0	18.8*	7.7
11	8	0	27.4	31.4
14	8	0	21.9	22.3
-18	9	0	22.2	18.1
12	9	0	21.9	19.7
-26	10	0	42.0	38.7
-23	10	0	16.8	13.8
-20	10	0	21.2*	3.5
13	10	0	21.5*	3.9
16	10	0	19.7	17.2
-22	11	0	26.6	27.6
-27	12	0	17.5	14.6
-24	12	0	20.9*	8.3
15	12	0	21.4	21.8
-23	0	1	18.0	17.6
-20	0	1	24.2	19.6
-17	0	1	12.2	11.7
-14	0	1	10.9*	12.4
-11	0	1	9.1*	1.4
-8	0	1	23.2	21.6
-5	0	1	5.5*	0.5
-2	0	1	3.4*	1.2
1	0	1	2.4*	2.4
4	0	1	4.9*	4.0
7	0	1	6.7*	7.2
10	0	1	14.8	13.7
13	0	1	10.3*	1.1
16	0	1	11.9*	5.4
19	0	1	24.5	25.8
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-16	1	1	16.5	18.6
-13	1	1	22.7	23.1
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-7	1	1	6.5*	1.3
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2	1	1	3.9	1.7
5	1	1	5.9*	2.0
8	1	1	7.7*	1.4
11	1	1	10.1*	0.2
14	1	1	19.5	20.7
17	1	1	26.9	20.9
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3	2	1	5.1*	9.5
6	2	1	6.9*	0.1
9	2	1	40.4	37.5
12	2	1	97.6	103.1
15	2	1	12.0	12.7
18	2	1	12.7*	8.3
21	2	1	13.7	15.1
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-8	3	1	9.7	11.0
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7	3	1	12.0	16.5
10	3	1	9.7*	4.0
13	3	1	11.3*	4.4
16	3	1	20.1	17.7
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5	4	1	7.3*	3.8
8	4	1	15.5	16.7
11	4	1	10.5*	3.6
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-21	5	1	12.7*	13.7
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6	5	1	13.1	14.4
9	5	1	9.9*	4.8
12	5	1	11.5*	10.7
15	5	1	28.9	27.1
18	5	1	11.9*	3.6
21	5	1	16.2	14.2
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-17	6	1	22.9	20.9
-14	6	1	9.8	11.4
-2	6	1	8.2	7.7
7	6	1	14.7	16.1
10	6	1	21.9	23.1
13	6	1	17.2	12.0
16	6	1	18.4	20.3
19	6	1	13.2	14.5
22	6	1	11.8	12.4
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11	7	1	11.8	12.3
14	7	1	15.4	13.0
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10	9	1	12.1*	8.4
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16	9	1	13.9	14.5
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11	10	1	17.7	20.3
14	10	1	11.9*	8.3
17	10	1	42.9	38.3
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-15	17	1	12.0	13.4
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-9	17	1	19.7	20.6
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-11	18	1	11.9*	2.3
-8	18	1	11.7*	6.8
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-4	19	1	28.6	24.8
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-18	29	1	7.1*	9.2
-15	29	1	7.5*	1.5
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-9	29	1	14.6	16.8
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2	0	2	47.5	54.5
5	0	2	24.1	21.0
8	0	2	38.7	33.9
11	0	2	77.8	79.8
14	0	2	10.9*	1.2
17	0	2	19.5	22.4
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3	1	2	22.0	23.2
6	1	2	259.1	267.4
9	1	2	22.0	17.8
12	1	2	16.3	16.9
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7	2	2	7.8*	2.2
10	2	2	22.0	22.2
13	2	2	15.7	16.1
16	2	2	12.3	12.0
19	2	2	12.2	12.7
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5	3	2	16.3	12.5
8	3	2	8.5*	1.0
11	3	2	10.3*	0.6
14	3	2	11.9*	8.4
17	3	2	34.4	30.4
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6	4	2	15.9	13.2
9	4	2	11.9	10.8
12	4	2	47.6	48.8
15	4	2	20.4	16.6
18	4	2	11.9*	4.5
21	4	2	11.9	17.9
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-17	5	2	11.7	12.7
-14	5	2	14.3	15.2
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-2	5	2	78.3	88.5
7	5	2	77.3	78.7
10	5	2	22.1	23.8
13	5	2	11.9*	6.6
16	5	2	34.2	28.7
-16	6	2	28.3	26.5
-13	6	2	15.1	15.3
-4	6	2	37.8	35.0
-1	6	2	32.9	30.5
8	6	2	9.9*	0.7
11	6	2	18.2	18.0
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9	7	2	10.9*	4.4
12	7	2	12.1*	5.3
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-20	8	2	12.3*	8.1
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10	8	2	14.6	15.2
13	8	2	34.9	29.2
16	8	2	24.7	25.4
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11	9	2	75.4	71.9
14	9	2	12.1*	11.9
17	9	2	12.4	16.0
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14	12	2	10.5*	3.1
17	12	2	11.8	13.5
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-11	14	2	20.8	23.1
-8	14	2	35.1	34.8
-5	14	2	14.3	10.9
-2	14	2	117.3	121.9
-10	15	2	40.1	39.5
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-4	15	2	13.1	15.6
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-14	17	2	11.9*	9.2
-10	18	2	23.8	22.7
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7	1	3	14.3*	9.0
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11	2	3	19.8*	7.6
14	2	3	22.5*	14.3
17	2	3	24.0*	11.0
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12	3	3	21.3*	10.9
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13	0	4	22.9*	4.0
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-9	20	4	62.6	58.2
-6	20	4	25.4*	3.7
-3	20	4	25.0	26.1
-8	21	4	25.3	20.2
-22	25	4	30.7	31.1
-19	25	4	18.7*	2.4
-16	25	4	20.4*	6.5
-13	25	4	31.6	31.1
-17	27	4	15.7*	5.5
-4	0	5	11.6	13.7
-1	0	5	5.8	6.4
2	0	5	7.8*	0.7
5	0	5	18.9	14.8
-6	1	5	19.9	23.3
-3	1	5	9.5*	4.6
3	1	5	32.2	31.1
6	1	5	83.0	81.6
-17	2	5	16.9	11.9
-14	2	5	22.6*	10.6
-11	2	5	19.9	18.9
-8	2	5	16.1*	1.0
-5	2	5	12.1	11.5
4	2	5	13.6*	11.9
7	2	5	17.5	16.3
10	2	5	20.6*	20.9
13	2	5	23.0*	7.5
16	2	5	23.0*	6.3
19	2	5	20.6*	5.3
-25	3	5	25.6	31.5
-22	3	5	19.8*	3.9
-19	3	5	23.0*	3.3
-16	3	5	23.7	27.4
-13	3	5	21.0*	4.4
-10	3	5	18.1*	10.8
-7	3	5	14.3	14.6
-1	3	5	16.5	16.9
12	4	5	23.7*	5.0
-11	5	5	18.9*	5.8
-2	5	5	12.1	11.8
7	5	5	19.8*	3.2
10	5	5	22.6*	16.3
13	5	5	23.5*	5.8
16	5	5	21.8*	10.0
-4	6	5	23.7	25.7
-1	6	5	13.6*	1.8
8	6	5	21.8*	14.6
11	6	5	16.9	10.4
-17	8	5	23.7	22.6
-5	8	5	15.6*	4.5
-2	8	5	16.1*	4.8
10	8	5	23.5*	3.7
13	8	5	14.4	9.3
11	9	5	46.3	46.0
14	9	5	20.6*	0.7
-3	10	5	18.4	15.3
12	10	5	21.8*	7.2
15	10	5	12.4	10.7
14	12	5	15.7	16.6
-12	13	5	22.3	25.1
-2	14	5	64.5	62.5
-11	17	5	24.0	23.4
-8	17	5	23.7	21.5
-5	17	5	23.5*	11.3
-2	17	5	23.5*	6.1
-15	19	5	46.3	45.1
-14	20	5	23.0*	4.1
-10	27	5	23.8	30.2
-9	0	6	43.4	40.7
-6	0	6	15.3*	2.3
-3	0	6	10.9	10.6
3	0	6	38.1	34.1
6	0	6	15.5	17.9
9	0	6	38.7	35.4
-14	1	6	43.0	44.7
-11	1	6	20.8*	9.2
-8	1	6	17.7	16.6
-5	1	6	59.0	55.3
-2	1	6	8.1*	0.7
4	1	6	25.3	25.8
7	1	6	17.4*	5.2
10	1	6	20.8*	8.2
13	1	6	16.2	18.9
-13	2	6	22.3	22.5
-10	2	6	19.6*	14.1
-7	2	6	15.7*	1.7
-4	2	6	14.1	12.2
-1	2	6	8.1*	4.3
5	2	6	15.7*	3.4
8	2	6	30.8	33.3
11	2	6	22.3	20.5
-6	3	6	42.6	40.4
0	3	6	13.1	10.6
6	3	6	42.6	41.1
9	3	6	21.2	20.7
12	3	6	23.0*	1.5
15	3	6	22.5*	17.7
18	3	6	33.0	37.7
-20	4	6	14.8	6.8
-17	4	6	23.0*	8.3
-14	4	6	22.5*	1.7
-11	4	6	24.5	24.0
-8	4	6	36.0	33.1
-2	4	6	26.1	23.8
7	4	6	20.0*	14.1
10	4	6	31.7	37.8
13	4	6	18.8	19.9
-13	5	6	79.5	77.1
-10	5	6	29.8	31.5
-4	5	6	67.7	68.2
-1	5	6	34.6	31.8
-18	6	6	35.0	34.0
-15	6	6	22.5*	7.5
-12	6	6	20.4*	0.4
-3	6	6	14.0*	5.7
0	6	6	15.3*	2.3
9	6	6	28.1	29.1
-14	7	6	15.8	18.1
-5	7	6	38.7	34.7
-2	7	6	15.7*	2.0
10	7	6	33.0	36.2
-4	8	6	31.4	26.4
-1	8	6	24.8	23.9
-3	9	6	48.6	46.7
0	9	6	43.4	40.7
-26	10	6	20.2	23.0
-23	10	6	18.3*	13.8
-20	10	6	21.7*	7.0
-8	10	6	49.9	46.9
-5	10	6	13.2	12.1
-4	11	6	20.2	18.9
-1	11	6	25.7	25.9
-3	12	6	36.9	36.3
-8	13	6	76.2	78.8
-5	13	6	21.3*	1.9
-2	13	6	22.3	23.3
-13	14	6	36.3	41.4
-10	14	6	22.5*	12.9
-7	14	6	15.8	12.6
-4	14	6	35.5	38.1
-9	15	6	22.9	17.2
-11	16	6	16.3	16.0
-8	16	6	23.0*	5.7
-10	17	6	18.8	15.6
-12	18	6	37.9	44.1
-9	18	6	23.0*	10.4
-6	18	6	23.0*	2.4
-3	18	6	33.7	32.8
-17	19	6	26.0	28.9
-14	19	6	22.1*	1.8
-11	19	6	22.5*	1.3
-8	19	6	16.0	15.7
-3	21	6	27.0	29.8
-11	22	6	24.5	23.9
-16	23	6	21.6	24.5

Table 2 (*cont.*)

$NaBr . 5\frac{1}{7}NH_3$

H	K	L	F_o	F_c
3	0	0	43.2	45.7
6	0	0	4.0	3.4
9	0	0	114.5	121.6
12	0	0	11.4	10.4
15	0	0	22.5	22.9
18	0	0	11.5	11.1
21	0	0	6.5*	3.0
24	0	0	11.4	9.8
-26	1	0	11.8	11.2
-23	1	0	24.5	23.3
-20	1	0	14.2	12.8
-17	1	0	42.2	40.1
-14	1	0	106.8	113.3
-11	1	0	12.7	13.8
-8	1	0	42.4	46.5
4	1	0	78.8	83.6
7	1	0	43.2	41.5
10	1	0	36.1	36.7
13	1	0	27.9	29.7
16	1	0	6.4	5.5
19	1	0	7.6	7.2
22	1	0	12.8	9.5
25	1	0	4.3*	1.5
-28	2	0	10.0	12.4
-25	2	0	5.3*	1.1
-22	2	0	34.3	34.9
-19	2	0	62.2	59.0
-16	2	0	13.4	12.2
-13	2	0	19.2	20.4
-10	2	0	72.3	70.5
-7	2	0	42.0	44.6
-4	2	0	35.9	37.3
5	2	0	3.3*	0.8
8	2	0	42.6	42.0
11	2	0	40.0	42.0
14	2	0	39.2	38.1
17	2	0	8.1	8.5
20	2	0	25.8	24.7
23	2	0	38.7	34.9
-27	3	0	13.5	12.9
-24	3	0	24.3	22.4
-21	3	0	11.6	9.5
-18	3	0	9.0	8.4
-15	3	0	7.9	7.4
-12	3	0	30.5	30.2
-9	3	0	17.6	19.7
-6	3	0	55.7	56.0
6	3	0	101.9	109.9
9	3	0	96.5	98.2
12	3	0	11.0	8.9
15	3	0	50.0	50.0
18	3	0	81.4	79.2
21	3	0	5.9*	1.8
24	3	0	6.6	4.5
-26	4	0	10.7	8.4
-23	4	0	13.8	11.4
-20	4	0	12.1	11.6
-17	4	0	16.6	15.7
-14	4	0	11.7	11.4
-11	4	0	37.2	36.1
-8	4	0	105.7	117.8
7	4	0	28.4	26.7
10	4	0	86.0	84.9
13	4	0	46.7	44.9
16	4	0	18.9	17.4
19	4	0	6.4*	3.2
22	4	0	9.1	7.6
-28	5	0	8.8	7.9
-25	5	0	5.8*	0.1
-22	5	0	32.5	30.5
-19	5	0	6.3*	3.6
-16	5	0	5.6*	3.6
-13	5	0	217.0	239.0
-10	5	0	58.6	60.1
8	5	0	15.4	15.4
11	5	0	27.8	28.5
14	5	0	6.3*	3.8
17	5	0	8.2	9.8
20	5	0	5.8*	3.0
23	5	0	4.0*	0.3
-27	6	0	35.1	28.8
-24	6	0	7.3	7.1
-21	6	0	11.6	11.9
-18	6	0	101.9	98.4
-15	6	0	28.5	29.7
-12	6	0	7.3	7.7
9	6	0	36.6	35.1
12	6	0	9.8	10.3
15	6	0	23.1	22.5
18	6	0	6.2*	3.5
21	6	0	5.0*	0.1
-29	7	0	3.7*	1.2
-26	7	0	5.7*	6.2
-23	7	0	34.9	32.1
-20	7	0	6.4*	3.7
-17	7	0	20.5	21.2
-14	7	0	34.7	34.5
10	7	0	91.0	91.9
13	7	0	6.4*	8.2
16	7	0	14.8	16.1
19	7	0	43.8	40.0
22	7	0	10.5	11.4
-28	8	0	5.9	5.6
-25	8	0	7.2	5.5
-22	8	0	9.4	8.5
-19	8	0	6.2*	14.3
-16	8	0	8.5	9.9
11	8	0	30.1	29.8
14	8	0	48.4	45.8
17	8	0	6.1*	0.8
20	8	0	7.3	5.3
-30	9	0	4.1	3.7
-27	9	0	7.6	5.3
-24	9	0	13.1	11.6
-21	9	0	30.3	32.1
-18	9	0	36.5	35.4
12	9	0	21.0	21.5
15	9	0	11.4	10.7
18	9	0	6.8	8.6
21	9	0	5.0	2.4
-29	10	0	4.3*	0.4
-26	10	0	55.6	51.1
-23	10	0	20.1	21.7
-20	10	0	6.4*	5.7
13	10	0	15.0	12.7
16	10	0	17.0	14.7
19	10	0	6.7	8.0
-28	11	0	12.8	11.4
-25	11	0	6.2*	2.5
-22	11	0	40.5	42.2
14	11	0	28.1	25.0
17	11	0	5.1*	1.0
-30	12	0	4.3	4.6
-27	12	0	16.4	14.7
-24	12	0	6.4*	0.1
15	12	0	32.5	28.3
18	12	0	9.8	10.3
-29	13	0	5.7	4.2
-26	13	0	6.0*	1.0
16	13	0	5.7	7.1
-31	14	0	7.6	8.3
-28	14	0	11.8	9.9
17	14	0	3.9	1.9
-30	15	0	21.9	22.7
-26	0	1	10.1	8.2
-23	0	1	23.7	21.6
-20	0	1	49.0	45.8
-17	0	1	12.1	8.7
-14	0	1	26.1	26.9
-11	0	1	76.0	76.2
-8	0	1	12.9	13.0
-5	0	1	5.5	6.6
4	0	1	30.3	32.2
7	0	1	14.4	16.0
10	0	1	20.5	23.3
13	0	1	7.2	7.0
16	0	1	13.1	13.4
19	0	1	23.5	23.6
22	0	1	15.5	15.0
-25	1	1	20.4	19.4
-22	1	1	17.9	17.0
-19	1	1	12.5	14.4
-16	1	1	11.5	9.2
-13	1	1	31.8	33.2
-10	1	1	14.1	15.3
-7	1	1	3.1*	1.5
-4	1	1	10.8	12.0
2	1	1	26.7	26.8
5	1	1	2.9	1.2
8	1	1	36.0	39.2
11	1	1	9.3	7.4
14	1	1	7.7	8.4
17	1	1	62.8	61.2
20	1	1	8.7	8.6
23	1	1	5.1*	2.4
26	1	1	23.9	23.5
-27	2	1	8.8	10.0
-24	2	1	8.8	6.8
-21	2	1	7.6	7.7
-18	2	1	17.2	17.2
-15	2	1	5.2*	0.1
-12	2	1	27.2	26.6
-9	2	1	37.9	38.9
-6	2	1	21.7	24.5
3	2	1	84.9	92.2
6	2	1	7.6	7.9
9	2	1	6.0	3.1
12	2	1	159.3	161.4
15	2	1	13.1	11.9
18	2	1	6.2*	3.3
21	2	1	30.1	27.6
-26	3	1	9.9	8.2
-23	3	1	11.9	9.6
-20	3	1	6.1*	0.6
-14	3	1	58.3	61.7
-11	3	1	37.8	40.1
-8	3	1	25.5	26.2
-2	3	1	85.2	90.0
4	3	1	36.1	36.0
7	3	1	65.7	70.7
10	3	1	17.9	16.0
13	3	1	5.4*	1.5
16	3	1	21.8	23.4
19	3	1	10.7	10.5
22	3	1	5.1*	2.9
-28	4	1	15.0	15.0
-25	4	1	5.2*	2.0
-22	4	1	7.6	5.7
-19	4	1	103.8	103.8
-16	4	1	12.2	12.8
-13	4	1	4.6*	2.7
-10	4	1	80.9	87.9
-1	4	1	21.8	22.3
5	4	1	19.8	23.0
8	4	1	4.3*	5.4
11	4	1	12.7	12.7
14	4	1	10.3	9.1
17	4	1	8.8	8.5
20	4	1	16.3	15.1
23	4	1	9.8	8.3
-27	5	1	7.8	7.0
-24	5	1	50.9	42.9
-21	5	1	6.2*	1.7
-18	5	1	5.7*	1.7
-15	5	1	29.5	30.0
-12	5	1	11.9	10.1
-3	5	1	10.7	13.1
6	5	1	32.9	33.7
9	5	1	21.7	19.1
12	5	1	15.5	17.5
15	5	1	29.8	27.3
18	5	1	21.6	23.8
21	5	1	24.9	22.8
24	5	1	6.5	6.7
-29	6	1	9.5	10.0
-26	6	1	14.7	13.3
-23	6	1	6.2	7.7
-20	6	1	6.0*	5.4
-17	6	1	25.9	23.6
-14	6	1	16.8	18.0
-5	6	1	37.7	43.2
-2	6	1	11.5	9.2
7	6	1	32.2	30.4
10	6	1	18.9	19.2
13	6	1	61.5	58.0
16	6	1	30.0	31.5
19	6	1	16.0	12.6
22	6	1	15.3	16.8
-28	7	1	4.2*	1.2
-25	7	1	14.7	12.1
-22	7	1	6.2*	3.0
-19	7	1	16.9	14.7
-16	7	1	18.6	18.9
-4	7	1	9.6	13.7
-1	7	1	310.3	300.2
8	7	1	63.6	59.4
11	7	1	17.8	17.1
14	7	1	18.7	17.9
17	7	1	12.0	12.0
20	7	1	4.7*	2.6
-27	8	1	18.4	16.4
-24	8	1	21.5	22.5
-21	8	1	18.7	15.4
-18	8	1	59.1	55.1
-6	8	1	66.5	72.4
-3	8	1	11.9	12.8
9	8	1	19.2	18.8
12	8	1	10.7	10.6
15	8	1	6.1*	6.3
18	8	1	5.3*	6.6
21	8	1	10.2	8.1
-29	9	1	8.3	9.8
-26	9	1	5.4*	1.8
-23	9	1	47.3	47.7
-20	9	1	27.1	27.9
-8	9	1	22.9	24.3
-5	9	1	16.3	17.7
-2	9	1	9.8	9.2
10	9	1	14.6	12.0
13	9	1	24.8	24.6
16	9	1	13.5	12.9
-28	10	1	18.2	17.8
-25	10	1	5.8*	2.2
-22	10	1	15.4	15.0
-7	10	1	35.3	36.1
-4	10	1	31.3	32.9
-1	10	1	28.7	28.0
11	10	1	19.3	17.8
14	10	1	12.3	11.1
17	10	1	49.0	46.1
-30	11	1	8.3	8.0
-24	11	1	11.5	11.1
-9	11	1	81.5	77.0
-6	11	1	38.6	41.1
-3	11	1	18.8	18.4
12	11	1	30.3	31.2
15	11	1	14.4	12.0
-29	12	1	9.1	7.4
-26	12	1	5.5*	1.4
-11	12	1	26.6	28.2
-8	12	1	15.5	16.2
-5	12	1	73.0	74.1
-2	12	1	41.2	40.3
13	12	1	5.8*	1.9
-31	13	1	8.4	12.0
-28	13	1	29.2	26.0
-10	13	1	23.3	24.9
-7	13	1	18.2	15.8
-4	13	1	34.0	34.1
-1	13	1	15.6	14.1
14	13	1	13.6	12.9
-12	14	1	20.4	20.8
-9	14	1	17.2	18.4
-6	14	1	32.3	32.0
-3	14	1	15.9	11.3
-14	15	1	13.0	13.5
-11	15	1	20.7	20.9
-8	15	1	30.5	32.1
-5	15	1	61.1	61.4
-2	15	1	13.1	15.4
-13	16	1	63.3	64.8
-10	16	1	56.5	54.0
-7	16	1	5.2*	2.1
-4	16	1	26.1	28.1
-1	16	1	54.3	51.7
-15	17	1	33.6	34.3
-12	17	1	13.8	13.4
-6	17	1	15.8	15.0
-3	17	1	19.4	19.5
-17	18	1	17.4	15.3
-14	18	1	5.8*	2.1
-11	18	1	5.6*	2.9
-5	18	1	28.8	27.5
-2	18	1	15.6	14.9
-16	19	1	11.5	7.7
-13	19	1	11.8	11.3
-10	19	1	18.8	19.2
-7	19	1	5.8*	4.0
-4	19	1	49.8	51.5
-1	19	1	12.5	11.0
-18	20	1	30.8	33.3
-15	20	1	16.5	14.6
-12	20	1	16.3	14.9
-9	20	1	103.0	103.2
-6	20	1	13.4	14.6
-3	20	1	6.2	7.8
-20	21	1	6.0*	2.1
-17	21	1	25.1	26.9
-14	21	1	47.2	47.4
-11	21	1	6.1*	3.1
-8	21	1	6.1*	1.8
-5	21	1	25.8	27.6
-2	21	1	12.4	11.9
-19	22	1	11.5	12.2
-16	22	1	9.9	9.9
-13	22	1	10.9	10.8
-10	22	1	6.2*	0.2
-7	22	1	12.5	11.2
-4	22	1	15.3	12.6
-1	22	1	12.0	11.3
-21	23	1	9.4	8.0
-18	23	1	15.0	16.6
-15	23	1	17.6	17.4
-12	23	1	6.1*	8.2
-9	23	1	6.1*	0.0
-6	23	1	13.7	12.0
-3	23	1	18.8	19.4
-23	24	1	12.0	12.3
-20	24	1	8.1	7.4
-17	24	1	27.3	28.1
-14	24	1	7.4	7.2
-11	24	1	6.2	6.0
-8	24	1	45.0	43.6
-5	24	1	23.9	24.4
-2	24	1	8.8	6.9
-22	25	1	46.7	46.3
-19	25	1	9.2	7.6
-16	25	1	9.5	10.6
-13	25	1	45.0	43.7
-10	25	1	22.6	19.4
-7	25	1	11.5	10.6
-4	25	1	12.4	12.5
-1	25	1	8.1	6.1
-21	26	1	8.7	8.6
-18	26	1	23.5	21.1
-15	26	1	5.5*	3.0
-12	26	1	16.1	14.1
-9	26	1	5.4*	0.2
-6	26	1	5.1*	1.1
-3	26	1	8.0	8.3
-20	27	1	8.4	6.8
-17	27	1	8.3	10.4
-14	27	1	13.6	13.3
-11	27	1	5.1*	1.2
-8	27	1	4.8*	0.9
-5	27	1	11.7	8.5
-2	27	1	6.3	5.6
-19	28	1	11.2	11.3
-16	28	1	8.3	9.8
-13	28	1	10.9	15.2
-10	28	1	10.0	8.2
-4	28	1	34.4	32.0
-24	29	1	6.5	6.2
-21	29	1	20.8	21.9
-18	29	1	14.4	14.5
-15	29	1	4.3*	1.2
-12	29	1	16.5	17.5
-9	29	1	20.4	20.6
-6	29	1	7.6	5.7
-17	30	1	11.7	11.3
-14	30	1	7.8	8.6
-11	30	1	6.5	7.1
-8	30	1	3.2	1.3
-16	31	1	6.5	6.4
-13	31	1	6.7	8.8
-22	0	2	21.9	18.2
-19	0	2	6.7*	1.2
-16	0	2	15.9	15.2
-13	0	2	12.7	10.9
-10	0	2	14.2	10.8
-7	0	2	28.5	24.6
-4	0	2	71.3	69.1
5	0	2	34.6	32.9
8	0	2	30.9	28.0
11	0	2	127.4	137.5
14	0	2	16.9	16.5
17	0	2	14.2	15.3
20	0	2	54.6	54.0
23	0	2	19.0	17.8
-24	1	2	5.5*	3.5
-21	1	2	6.6*	3.8
-18	1	2	21.5	20.4
-15	1	2	6.0*	9.1
-12	1	2	25.5	23.3
-9	1	2	53.4	49.7
-6	1	2	38.4	38.2
-3	1	2	148.1	165.5
3	1	2	53.6	55.1
6	1	2	298.4	356.4
9	1	2	24.0	25.0
12	1	2	14.5	16.8
15	1	2	59.2	57.5
18	1	2	6.7*	3.4
-23	2	2	14.4	13.9
-20	2	2	22.0	24.1
-17	2	2	45.8	45.9
-14	2	2	35.3	35.8
-11	2	2	79.0	76.3
-8	2	2	151.1	160.8
-5	2	2	2.8*	3.4
4	2	2	27.0	27.2
7	2	2	5.8	7.1
10	2	2	38.3	39.0
13	2	2	18.0	19.9
16	2	2	17.8	17.0
19	2	2	13.5	15.5
22	2	2	5.7*	2.3
-25	3	2	46.3	40.4
-22	3	2	28.7	27.9
-19	3	2	6.5	5.2
-16	3	2	75.6	74.4
-13	3	2	96.6	95.4
-10	3	2	26.1	26.6
-7	3	2	64.7	63.5
-1	3	2	45.4	43.4
5	3	2	28.1	26.5
8	3	2	4.7	7.3
11	3	2	5.6	4.2
14	3	2	22.7	23.0
17	3	2	26.7	26.7
20	3	2	16.1	16.5
-27	4	2	14.4	13.3
-24	4	2	6.0*	1.1
-21	4	2	31.0	29.1
-18	4	2	33.3	36.8
-15	4	2	18.8	19.8
-12	4	2	23.0	21.5
-3	4	2	51.6	47.5
6	4	2	4.2*	4.1
9	4	2	31.5	30.5
12	4	2	71.0	70.6
15	4	2	46.2	43.4
18	4	2	6.6*	0.9
21	4	2	22.2	21.7
24	4	2	29.2	28.7
-26	5	2	9.4	8.4
-23	5	2	6.4*	2.6
-20	5	2	15.3	15.9
-17	5	2	22.7	23.2
-14	5	2	25.2	23.5
-11	5	2	32.1	32.6
-2	5	2	160.9	158.6
7	5	2	136.0	143.1
10	5	2	54.2	57.0
13	5	2	6.4*	3.4
16	5	2	42.1	41.9
19	5	2	22.0	19.6
-25	6	2	5.9*	3.7
-22	6	2	16.7	16.7
-19	6	2	6.5*	1.4
-16	6	2	59.8	61.0
-13	6	2	19.1	18.6
-4	6	2	54.2	52.6
-1	6	2	28.6	26.1
8	6	2	13.2	14.7
11	6	2	28.9	29.9
14	6	2	6.6*	4.1
17	6	2	13.3	13.1
20	6	2	5.5*	2.6
-27	7	2	12.6	10.9
-24	7	2	22.6	18.7
-21	7	2	56.1	56.9
-18	7	2	6.2*	5.4
-15	7	2	25.6	29.1
-6	7	2	14.0	14.8
-3	7	2	107.0	106.3
9	7	2	10.6	12.8
12	7	2	6.4*	0.1
15	7	2	23.3	20.9
18	7	2	6.0*	3.0
-29	8	2	18.6	18.8
-26	8	2	35.7	31.0
-23	8	2	6.6*	4.6
-20	8	2	20.2	18.6
-17	8	2	52.9	50.6
-5	8	2	24.4	24.3
-2	8	2	16.5	16.6
10	8	2	23.3	23.2
13	8	2	23.8	26.0
16	8	2	38.9	44.5
19	8	2	5.1*	4.1
-28	9	2	4.7*	3.7
-25	9	2	10.3	9.5
-22	9	2	11.9	12.1
-19	9	2	13.1	11.7
-7	9	2	12.4	12.6
-4	9	2	58.1	57.5
-1	9	2	66.4	65.7
11	9	2	100.6	102.4
14	9	2	6.6*	7.8
17	9	2	10.3	14.1
20	9	2	18.5	17.3
-27	10	2	5.5*	2.9
-24	10	2	6.4*	6.5
-21	10	2	9.7	9.7
-9	10	2	52.1	49.7
-6	10	2	125.3	131.2
-3	10	2	93.3	90.2
12	10	2	11.9	13.9
15	10	2	16.4	14.5
-29	11	2	14.1	13.6
-26	11	2	8.5	6.5
-23	11	2	6.6*	2.9
-8	11	2	72.6	73.0
-5	11	2	22.6	23.4
-2	11	2	78.8	78.3
13	11	2	6.5*	6.7
16	11	2	5.5*	3.9
-28	12	2	4.9*	5.6
-25	12	2	54.7	47.4
-10	12	2	25.1	26.0
-7	12	2	36.0	34.7
-4	12	2	4.9	3.8
-1	12	2	14.6	12.0
14	12	2	6.1	4.6
17	12	2	19.3	18.8
-30	13	2	14.3	14.7
-27	13	2	5.6*	1.2
-12	13	2	17.6	19.7
-9	13	2	10.4	7.4
-6	13	2	22.9	20.2
-3	13	2	40.0	38.1
15	13	2	16.7	15.1
-29	14	2	4.4*	3.3
-11	14	2	55.3	58.4
-8	14	2	40.1	41.3
-5	14	2	31.2	30.1
-2	14	2	170.9	174.7
16	14	2	7.9	7.8
-13	15	2	14.6	13.3
-10	15	2	63.1	63.9
-7	15	2	92.3	93.9
-4	15	2	16.4	17.4
-1	15	2	35.0	36.9
-15	16	2	49.2	46.5
-12	16	2	41.4	42.6
-9	16	2	21.0	21.1
-6	16	2	21.0	20.4
-3	16	2	6.2	7.6
-11	17	2	9.9	10.2
-8	17	2	24.8	23.7
-5	17	2	12.5	13.7
-2	17	2	6.4*	1.5
-16	18	2	15.0	14.4
-13	18	2	12.2	10.2
-10	18	2	51.9	51.9
-7	18	2	6.2*	3.5
-4	18	2	9.4	9.2
-1	18	2	72.6	71.4
-18	19	2	6.7*	4.4
-15	19	2	97.7	103.3
-12	19	2	6.4*	5.4
-9	19	2	20.9	20.2
-6	19	2	85.4	83.7
-3	19	2	18.0	17.0
-17	20	2	6.7*	6.0
-14	20	2	19.2	19.0
-11	20	2	56.5	56.7
-8	20	2	14.3	12.5
-5	20	2	6.6*	2.7
-2	20	2	6.9	9.2
-19	21	2	6.6*	4.4
-16	21	2	23.3	23.3
-13	21	2	15.4	13.2
-10	21	2	6.6*	2.0
-7	21	2	13.7	11.7
-4	21	2	6.7*	1.7
-1	21	2	6.7	7.4
-21	22	2	6.3*	3.2
-18	22	2	6.6*	4.0
-15	22	2	6.6*	4.8
-12	22	2	16.9	15.8
-9	22	2	15.4	17.0
-6	22	2	23.2	23.6
-3	22	2	16.4	15.2
-17	23	2	15.0	13.4
-14	23	2	42.1	43.5
-11	23	2	23.6	22.6
-8	23	2	6.7	5.7
-5	23	2	41.8	38.4
-2	23	2	25.7	25.5
-22	24	2	5.7*	1.8
-19	24	2	47.9	47.3
-16	24	2	20.8	19.2
-13	24	2	6.5*	6.2
-10	24	2	32.7	33.6
-7	24	2	10.5	9.7
-4	24	2	6.0*	4.3
-1	24	2	8.4	9.1
-24	25	2	23.2	25.3
-21	25	2	5.6*	0.2
-18	25	2	6.0*	7.7
-15	25	2	22.1	20.6
-12	25	2	6.2*	1.6
-9	25	2	6.2*	3.0
-6	25	2	5.9*	5.9
-3	25	2	9.6	9.1
-20	26	2	5.5*	0.0
-17	26	2	5.8*	2.2
-14	26	2	5.9*	4.0
-11	26	2	11.0	9.0
-8	26	2	5.7*	1.0
-5	26	2	22.4	21.1
-22	27	2	4.6*	4.8
-19	27	2	17.2	15.1
-16	27	2	13.7	11.2
-13	27	2	9.9	8.0
-10	27	2	50.5	41.5
-7	27	2	5.0*	0.3
-4	27	2	15.5	13.9
-1	27	2	21.3	22.5
-24	28	2	9.5	12.0
-21	28	2	4.3*	3.8
-18	28	2	21.1	18.3
-15	28	2	29.3	24.6
-12	28	2	7.6	6.2
-9	28	2	16.7	15.0
-6	28	2	17.4	17.1
-23	29	2	10.5	14.1
-20	29	2	7.8	10.4
-14	29	2	11.2	8.3
-24	0	3	8.7	8.6
-21	0	3	6.3*	5.8
-18	0	3	9.7	10.0
-15	0	3	20.1	21.5
-12	0	3	29.1	30.5
-9	0	3	64.4	61.6
-6	0	3	10.7	10.7
-3	0	3	17.1	15.5
3	0	3	51.1	44.2
6	0	3	16.1	13.2
9	0	3	66.4	60.0
12	0	3	19.1	19.5
15	0	3	15.0	14.4
18	0	3	12.7	16.6
21	0	3	6.3*	0.6
24	0	3	4.9*	4.5
-26	1	3	12.1	12.5
-23	1	3	20.2	19.0
-20	1	3	19.0	17.8
-17	1	3	44.7	43.8
-14	1	3	58.9	58.1
-11	1	3	5.0*	5.1
-8	1	3	37.5	38.6
-5	1	3	69.9	69.7
4	1	3	46.5	43.0
7	1	3	18.6	16.2
10	1	3	14.7	13.6
13	1	3	11.1	11.2
16	1	3	15.4	18.8
19	1	3	9.6	11.1
22	1	3	11.3	10.1
25	1	3	12.1	9.2
-25	2	3	4.8*	4.7
-22	2	3	37.9	36.8
-19	2	3	24.9	25.9
-16	2	3	20.2	21.8
-13	2	3	26.8	26.1
-10	2	3	4.4*	5.0
-7	2	3	31.2	29.7
-4	2	3	7.4	7.5
5	2	3	11.8	10.9
8	2	3	22.0	19.4
11	2	3	5.4*	0.5
14	2	3	32.2	34.1
17	2	3	11.8	12.9
20	2	3	6.3*	0.4
23	2	3	35.0	31.2
-27	3	3	11.3	12.5
-24	3	3	5.6*	5.9
-21	3	3	11.7	14.5
-18	3	3	9.5	8.9
-15	3	3	18.0	16.7
-12	3	3	14.8	15.8
-9	3	3	14.7	15.8
-6	3	3	32.1	30.1
6	3	3	28.9	23.9
9	3	3	70.9	65.6
12	3	3	14.0	14.2
15	3	3	6.7	5.9
18	3	3	63.1	67.7
21	3	3	5.6*	1.9
24	3	3	3.5*	2.4
-26	4	3	8.3	8.8
-23	4	3	11.4	11.1
-20	4	3	13.6	13.8
-17	4	3	18.7	20.0
-14	4	3	5.5*	7.1
-11	4	3	7.4	6.4
-8	4	3	77.0	73.1
-2	4	3	23.7	22.1
7	4	3	16.8	14.5
10	4	3	31.7	33.0
13	4	3	40.0	42.0
16	4	3	8.3	10.3
19	4	3	6.2*	3.5
22	4	3	8.3	7.7
-28	5	3	5.8	7.0
-25	5	3	5.5*	2.6
-22	5	3	32.1	30.8
-19	5	3	6.7	8.5
-16	5	3	13.6	15.9
-13	5	3	155.3	160.7
-10	5	3	25.0	25.8
-4	5	3	83.9	79.9
-1	5	3	41.2	40.8

Table 2 (*cont.*)

NaBr . $5\frac{1}{7}NH_3$

H	K	L	F_o	F_c
8	5	3	12.4	12.4
11	5	3	13.7	16.4
14	5	3	6.7	5.6
17	5	3	10.6	11.5
20	5	3	5.5*	0.7
23	5	3	3.2*	2.2
-27	6	3	29.0	25.3
-24	6	3	6.1*	0.8
-21	6	3	18.6	20.6
-18	6	3	56.7	56.5
-15	6	3	8.2	6.4
-12	6	3	6.1	3.7
-3	6	3	29.4	29.9
9	6	3	17.4	17.2
12	6	3	24.5	26.5
15	6	3	19.2	20.4
18	6	3	6.1*	4.4
21	6	3	15.0	12.5
-23	7	3	10.6	9.2
-20	7	3	20.7	20.3
-17	7	3	8.9	7.7
-14	7	3	5.4*	4.3
-5	7	3	36.1	34.1
-2	7	3	3.6*	3.4
10	7	3	60.5	67.0
13	7	3	9.6	10.0
16	7	3	6.5*	7.6
19	7	3	33.2	31.0
-28	8	3	4.2*	2.6
-25	8	3	10.4	11.6
-22	8	3	6.6*	4.5
-19	8	3	24.5	24.4
-16	8	3	16.0	17.1
-7	8	3	38.2	34.1
-4	8	3	69.3	70.0
-1	8	3	10.8	8.4
11	8	3	6.5*	3.0
14	8	3	31.0	34.6
17	8	3	6.0*	2.5
20	8	3	5.2	5.4
-27	9	3	5.0*	2.6
-24	9	3	15.8	12.3
-21	9	3	29.3	32.7
-18	9	3	25.1	27.9
-6	9	3	9.4	9.9
-3	9	3	36.0	32.5
12	9	3	11.8	11.8
18	9	3	8.9	7.3
-29	10	3	3.6*	0.7
-26	10	3	50.5	47.0
-23	10	3	11.5	13.3
-20	10	3	6.6*	5.3
-8	10	3	24.7	18.8
-5	10	3	4.3*	1.9
-2	10	3	22.5	21.8
13	10	3	15.0	15.6
16	10	3	9.9	9.3
19	10	3	9.7	11.2
-28	11	3	4.5*	3.1
-25	11	3	6.1*	3.9
-22	11	3	21.8	23.9
-10	11	3	15.9	15.5
-7	11	3	12.1	11.6
-4	11	3	35.0	32.4
-1	11	3	30.2	32.3
14	11	3	27.7	24.9
17	11	3	11.4	9.6
-27	12	3	5.2*	5.3
-24	12	3	11.8	12.3
-9	12	3	14.5	13.4
-6	12	3	4.9*	0.4
-3	12	3	72.8	72.1
15	12	3	19.0	19.0
18	12	3	8.1	11.1
-26	13	3	5.7*	3.1
-11	13	3	14.7	14.5
-8	13	3	155.8	159.7
-5	13	3	31.8	34.3
-2	13	3	7.8	5.0
16	13	3	5.0	5.6
-28	14	3	11.0	9.5
-13	14	3	58.0	56.8
-10	14	3	5.5*	1.6
-7	14	3	5.4*	1.5
-4	14	3	29.1	28.2
-1	14	3	15.8	14.3
-30	15	3	19.4	23.6
-12	15	3	15.9	12.8
-9	15	3	10.1	8.3
-6	15	3	11.6	11.3
-3	15	3	8.6	10.2
-14	16	3	30.5	31.5
-11	16	3	15.6	17.9
-8	16	3	8.6	8.2
-5	16	3	18.9	19.6
-2	16	3	24.7	25.3
-16	17	3	36.5	41.0
-13	17	3	21.8	22.4
-10	17	3	9.0	11.1
-7	17	3	59.2	57.8
-4	17	3	44.8	45.6
-1	17	3	6.7	7.7
-15	18	3	14.1	13.9
-12	18	3	61.4	60.1
-9	18	3	32.5	33.4
-6	18	3	13.8	15.4
-3	18	3	17.0	14.1
-17	19	3	21.9	23.3
-14	19	3	6.6*	3.5
-11	19	3	21.1	19.3
-8	19	3	6.7	6.9
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-19	20	3	9.6	9.4
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-13	20	3	23.5	25.9
-7	20	3	9.6	9.9
-4	20	3	15.3	14.1
-1	20	3	6.6*	4.2
-18	21	3	17.8	18.2
-15	21	3	11.8	13.5
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-3	21	3	66.6	70.2
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-2	22	3	6.3*	2.1
-22	23	3	21.5	20.3
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-17	25	3	16.5	14.7
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-11	25	3	28.8	25.9
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-5	25	3	5.5*	4.0
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-25	26	3	11.3	11.4
-22	26	3	8.3	10.0
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-13	26	3	5.7*	7.5
-10	26	3	9.9	8.8
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-4	26	3	8.3	9.9
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-18	27	3	5.0*	1.1
-15	27	3	6.5	7.1
-12	27	3	21.0	19.0
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-6	27	3	9.8	9.8
-3	27	3	3.5*	0.1
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-14	28	3	4.8*	4.6
-11	28	3	8.1	8.2
-8	28	3	11.0	8.8
-5	28	3	3.2*	1.7
-16	29	3	4.0*	3.7
-13	29	3	9.4	8.8
-10	29	3	6.5	8.2
-15	30	3	19.0	20.6
-12	30	3	8.1	11.2
-23	0	4	13.1	10.6
-20	0	4	49.8	45.2
-17	0	4	11.4	12.0
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13	0	4	10.1	11.7
16	0	4	28.6	28.3
19	0	4	5.5*	5.6
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-13	1	4	5.0	4.3
-10	1	4	4.1*	6.0
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5	1	4	15.2	13.7
8	1	4	60.1	58.0
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14	1	4	26.7	26.1
17	1	4	60.9	63.7
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23	1	4	5.0	7.2
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6	2	4	23.9	21.3
9	2	4	47.4	46.4
12	2	4	139.0	139.7
15	2	4	11.3	13.0
18	2	4	7.9	10.0
21	2	4	22.9	21.5
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-23	3	4	4.8*	7.5
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-17	3	4	26.2	27.2
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-2	3	4	138.7	129.1
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7	3	4	84.5	80.9
10	3	4	8.3	10.1
13	3	4	5.3*	3.8
16	3	4	15.6	16.3
19	3	4	6.0	6.8
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-22	4	4	5.2*	5.4
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5	4	4	18.8	20.9
8	4	4	4.4	5.1
11	4	4	14.2	16.4
14	4	4	5.5*	0.2
17	4	4	5.6	4.7
20	4	4	7.1	8.6
23	4	4	7.7	10.7
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-15	5	4	52.2	50.2
-12	5	4	31.8	31.9
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6	5	4	36.9	39.4
9	5	4	42.8	42.9
12	5	4	5.5	4.7
15	5	4	10.6	10.0
18	5	4	34.6	30.6
21	5	4	15.0	16.3
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-23	6	4	5.1*	3.9
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-17	6	4	5.3*	3.2
-14	6	4	11.8	13.1
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7	6	4	8.7	9.8
10	6	4	9.2	10.9
13	6	4	61.2	67.5
16	6	4	21.4	24.2
19	6	4	4.5*	1.0
19	6	4	5.6	1.0
22	6	4	9.4	15.7
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11	7	4	11.8	12.3
14	7	4	5.7	5.7
17	7	4	11.7	10.3
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-24	8	4	20.4	19.0
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-18	8	4	33.4	33.4
-6	8	4	132.8	125.4
-3	8	4	7.7	10.2
9	8	4	12.1	11.3
12	8	4	12.5	13.9
15	8	4	5.2*	4.7
18	8	4	4.3*	1.0
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-8	9	4	17.7	17.9
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10	9	4	16.9	17.9
13	9	4	10.5	12.6
16	9	4	10.3	9.3
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-22	10	4	8.4	8.4
-7	10	4	43.1	44.7
-4	10	4	39.9	37.0
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11	10	4	5.7	6.0
14	10	4	21.4	23.5
17	10	4	38.0	35.9
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12	11	4	23.8	25.7
15	11	4	4.5*	2.9
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13	12	4	4.6*	0.3
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13	15	4	19.4	21.5
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-19	22	4	17.2	19.9
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-7	0	5	11.2	12.2
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5	0	5	2.9*	0.9
8	0	5	3.8*	6.8
11	0	5	65.3	62.4
14	0	5	15.1	15.2
17	0	5	9.7	7.3
20	0	5	34.2	32.0
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12	1	5	5.1	3.8
15	1	5	33.4	34.3
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-20	2	5	22.6	24.9
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7	2	5	5.6	5.6
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13	2	5	9.3	10.9
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14	3	5	17.5	19.1
17	3	5	6.1	4.5
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6	4	5	13.7	15.5
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12	4	5	19.7	21.6
15	4	5	31.9	32.9
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16	5	5	20.9	22.6
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10	8	5	9.9	11.6
13	8	5	5.3*	0.1
16	8	5	36.0	34.5
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-22	9	5	5.2*	7.6
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-7	9	5	7.9	8.3
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14	9	5	5.0*	2.8
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12	10	5	5.2*	1.9
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-3	19	5	18.3	19.4
-17	20	5	5.3*	3.6
-14	20	5	6.7	8.1
-11	20	5	18.2	21.2
-8	20	5	5.4*	3.5
-5	20	5	14.6	14.3
-2	20	5	5.2*	4.6
-19	21	5	5.0*	2.1
-16	21	5	5.2*	1.6
-13	21	5	5.5	4.6
-10	21	5	6.7	9.1
-7	21	5	15.8	17.9
H	K	L	F_c	F_c
-4	21	5	5.2*	1.5
-1	21	5	7.4	8.7
-21	22	5	15.8	15.6
-18	22	5	6.1	5.2
-15	22	5	5.1*	2.1
-12	22	5	15.1	15.3
-9	22	5	11.3	11.8
-6	22	5	25.4	22.5
-3	22	5	8.5	8.5
-17	23	5	5.9	7.8
-14	23	5	32.5	29.0
-11	23	5	22.8	22.4
-8	23	5	4.9*	0.2
-5	23	5	21.7	19.5
-2	23	5	25.9	23.5
-22	24	5	3.7*	4.9
-19	24	5	32.1	31.6
-16	24	5	19.1	19.2
-13	24	5	4.7*	1.9
-10	24	5	13.8	13.8
-7	24	5	6.9	8.0
-4	24	5	7.2	7.7
-1	24	5	3.3*	1.7
-24	25	5	12.6	13.8
-21	25	5	3.5*	2.4
-18	25	5	5.1	5.6
-15	25	5	4.3*	0.8
-12	25	5	4.3*	0.2
-9	25	5	4.2*	4.5
-6	25	5	13.0	12.9
-3	25	5	7.1	9.0
-20	26	5	9.9	11.3
-17	26	5	3.8*	2.4
-14	26	5	4.0*	0.7
-11	26	5	10.4	11.0
-8	26	5	3.7*	0.2
-5	26	5	17.3	18.6
-19	27	5	8.5	10.4
-16	27	5	8.7	8.0
-13	27	5	3.5*	4.5
-10	27	5	34.5	32.7
-7	27	5	2.7*	3.8
-18	28	5	11.8	13.0
-15	28	5	18.0	20.4
-12	28	5	2.6*	0.7
-21	0	6	3.9*	1.5
-18	0	6	10.8	7.8
-15	0	6	18.7	21.6
-12	0	6	4.7*	1.4
-9	0	6	69.5	69.9
-6	0	6	8.3	7.1
-3	0	6	6.4	4.5
3	0	6	47.2	41.9
6	0	6	15.6	13.7
9	0	6	65.5	64.4
12	0	6	21.9	18.9
15	0	6	6.3	7.8
18	0	6	5.7	7.1
21	0	6	3.9*	2.1
-23	1	6	14.7	14.9
-20	1	6	13.2	13.5
-17	1	6	19.5	18.2
-14	1	6	61.3	64.0
-11	1	6	4.5*	6.6
-8	1	6	37.1	33.4
-5	1	6	102.1	96.1
4	1	6	43.3	37.0
7	1	6	3.7*	0.2
10	1	6	10.8	10.9
13	1	6	19.8	21.9
16	1	6	5.0*	6.2
19	1	6	4.5*	4.8
22	1	6	9.2	9.8
-22	2	6	22.6	22.5
-19	2	6	38.2	36.0
-16	2	6	5.1*	2.2
-13	2	6	27.6	27.9
-10	2	6	28.9	26.6
-7	2	6	8.5	7.1
-4	2	6	9.5	6.5
5	2	6	3.3*	0.1
8	2	6	46.6	43.9
11	2	6	19.2	17.5
14	2	6	21.9	23.7
17	2	6	9.0	11.1
20	2	6	13.4	11.5
-24	3	6	11.1	13.1
-21	3	6	4.5*	2.5
-18	3	6	10.3	8.0
-15	3	6	5.0*	2.2
-12	3	6	4.5*	3.2
-9	3	6	10.8	13.1
-6	3	6	56.4	53.0
6	3	6	59.1	54.5
9	3	6	49.8	49.0
12	3	6	5.1	6.9
15	3	6	23.2	23.8
18	3	6	49.6	47.3
21	3	6	5.4	5.1
-23	4	6	9.0	9.1
-20	4	6	11.2	10.7
-17	4	6	15.2	15.0
-14	4	6	5.0	5.4
-11	4	6	35.6	32.6
-8	4	6	67.5	65.3
-2	4	6	37.5	34.2
7	4	6	4.4	4.2
10	4	6	47.6	49.7
13	4	6	30.1	33.5
16	4	6	4.7*	2.0
19	4	6	3.7*	0.8
-25	5	6	2.8*	1.7
-22	5	6	25.0	21.8
-19	5	6	5.0*	3.5
-16	5	6	9.7	9.0
-13	5	6	108.1	112.6
-10	5	6	39.7	39.3
-4	5	6	110.6	104.3
-1	5	6	55.8	51.7
8	5	6	11.1	8.9
11	5	6	8.9	9.3
14	5	6	5.8	5.6
17	5	6	4.3*	6.0
20	5	6	2.8*	0.4
-24	6	6	3.6*	2.9
-21	6	6	7.3	6.9

Table 2 (*cont.*)

$NaBr.5\frac{1}{7}NH_3$

H	K	L	F_o	F_c
-18	6	6	52.4	53.5
-15	6	6	13.8	14.8
-12	6	6	4.5	5.4
-3	6	6	10.4	9.5
9	6	6	29.1	32.4
12	6	6	12.8	14.3
15	6	6	19.9	18.6
18	6	6	3.6*	1.6
-23	7	6	15.2	15.4
-20	7	6	4.9*	0.2
-17	7	6	5.1*	0.6
-14	7	6	16.3	12.8
-5	7	6	46.5	46.0
-2	7	6	3.5	1.9
10	7	6	52.5	55.2
13	7	6	4.9*	3.7
16	7	6	4.2*	7.1
19	7	6	22.1	24.2
-25	8	6	3.3*	0.3
-22	8	6	4.5*	2.3
-19	8	6	15.7	15.6
-16	8	6	12.6	13.1
-7	8	6	30.0	24.9
-4	8	6	62.7	60.4
-1	8	6	32.9	30.1
11	8	6	17.4	18.0
14	8	6	29.5	28.4
17	8	6	3.3*	4.0
-24	9	6	12.6	12.0
-21	9	6	20.0	18.9
-18	9	6	23.3	23.4
-6	9	6	7.9	7.1
-3	9	6	59.1	62.9
12	9	6	6.0	3.5
15	9	6	5.0	4.4
-26	10	6	31.3	29.1
-23	10	6	14.8	15.5
-20	10	6	5.8	6.6
-8	10	6	56.1	51.8
-5	10	6	28.2	25.0
-2	10	6	7.4	8.6
13	10	6	10.9	12.6
16	10	6	7.6	7.8
-25	11	6	3.6*	0.7
-22	11	6	24.6	23.7
-10	11	6	4.5*	1.5
-7	11	6	4.3*	1.4
-4	11	6	26.5	27.3
-1	11	6	31.6	32.9
14	11	6	11.1	12.3
-27	12	6	5.7	7.2
-24	12	6	4.0*	4.3
-9	12	6	22.9	24.0
-6	12	6	9.7	10.8
-3	12	6	61.8	62.8
15	12	6	14.8	18.6
-26	13	6	3.1*	2.8
-11	13	6	4.7*	2.5
-8	13	6	116.3	114.0
-5	13	6	8.3	10.0
-2	13	6	21.2	19.7
-13	14	6	56.4	63.0
-10	14	6	4.8*	5.1
-7	14	6	19.0	19.1
-4	14	6	44.9	45.3
-1	14	6	4.9*	2.6
-12	15	6	8.9	8.8
-9	15	6	14.7	11.9
-6	15	6	4.9*	1.0
-3	15	6	5.0*	1.3
-14	16	6	17.3	17.2
-11	16	6	16.4	17.7
-8	16	6	5.0*	1.5
-5	16	6	24.1	26.5
-2	16	6	24.7	24.5
-16	17	6	30.4	30.8
-13	17	6	6.3	8.2
-10	17	6	19.0	19.4
-7	17	6	47.8	51.3
-4	17	6	19.2	21.9
-1	17	6	5.0*	0.4
-15	18	6	5.0*	0.3
-12	18	6	53.5	58.9
-9	18	6	17.7	21.3
-6	18	6	5.1*	2.4
-3	18	6	36.0	32.9
-17	19	6	29.5	32.9
-14	19	6	4.9*	2.2
-11	19	6	5.0*	4.6
-8	19	6	13.3	12.1
-5	19	6	4.9*	0.4
-2	19	6	4.8*	2.4
-19	20	6	4.5*	0.4
-16	20	6	4.7*	0.6
-13	20	6	8.1	9.7
-10	20	6	4.9*	1.3
-7	20	6	8.1	8.3
-4	20	6	15.5	16.3
-1	20	6	4.5*	4.3
-18	21	6	10.5	12.3
-15	21	6	9.3	10.0
-12	21	6	22.0	19.3
-9	21	6	20.0	17.1
-6	21	6	10.2	11.1
-3	21	6	45.9	42.8
-20	22	6	22.6	21.3
-17	22	6	16.4	16.9
-14	22	6	5.7	6.8
-11	22	6	30.6	27.4
-8	22	6	30.1	27.9
-5	22	6	4.3*	4.4
-2	22	6	14.7	14.1
-22	23	6	13.1	14.9
-19	23	6	3.8*	5.2
-16	23	6	25.8	23.3
-13	23	6	11.4	10.9
-10	23	6	5.4	4.6
-7	23	6	7.4	8.3
-4	23	6	3.7*	2.3
-1	23	6	3.1*	0.2
-21	24	6	10.0	11.0
-18	24	6	3.6*	3.4
-15	24	6	3.9*	0.6
-12	24	6	4.0*	5.1
-9	24	6	8.7	9.6
-6	24	6	6.4	7.9
-3	24	6	3.0*	2.7
-20	25	6	2.8*	2.6
-17	25	6	6.0	6.5
-14	25	6	3.6*	2.1
-11	25	6	19.0	19.0
-8	25	6	3.3*	1.4
-5	25	6	2.8*	1.9
-19	26	6	2.4*	3.0
-16	26	6	30.1	31.0
-13	26	6	3.1*	0.7
-10	26	6	8.0	8.2
-7	26	6	22.0	24.5
-15	27	6	7.6	9.3
-12	27	6	11.8	16.5
-20	0	7	24.3	25.3
-17	0	7	4.4*	2.3
-14	0	7	17.2	16.1
-11	0	7	41.1	39.8
-8	0	7	3.8*	2.5
-5	0	7	3.0*	4.1
-2	0	7	21.2	23.1
4	0	7	14.4	15.0
7	0	7	3.6*	3.2
10	0	7	20.1	18.1
13	0	7	4.6*	7.4
16	0	7	7.6	8.0
19	0	7	12.8	14.7
-22	1	7	2.7*	5.3
-19	1	7	8.7	10.9
-16	1	7	4.7	4.3
-13	1	7	11.6	11.6
-10	1	7	4.3	4.7
-7	1	7	3.5*	2.3
-4	1	7	2.6*	1.7
2	1	7	17.1	20.9
5	1	7	3.2*	4.2
8	1	7	33.1	28.7
11	1	7	4.5*	6.1
14	1	7	4.7*	3.2
17	1	7	35.8	34.0
20	1	7	3.2*	2.7
-21	2	7	3.4*	4.3
-18	2	7	4.4*	4.8
-15	2	7	9.5	8.8
-12	2	7	19.8	19.7
-9	2	7	22.5	21.8
-6	2	7	3.1*	2.0
3	2	7	51.6	44.2
6	2	7	3.7*	5.9
9	2	7	4.3*	1.6
12	2	7	63.9	66.8
15	2	7	7.5	6.5
18	2	7	4.8	3.0
-23	3	7	2.6*	6.2
-20	3	7	3.9*	4.3
-17	3	7	9.9	9.1
-14	3	7	32.1	31.2
-11	3	7	21.3	20.7
-8	3	7	12.3	13.1
-2	3	7	43.6	46.2
4	3	7	29.1	28.2
7	3	7	38.4	35.9
10	3	7	4.5*	7.1
13	3	7	4.7*	2.4
16	3	7	11.9	9.9
19	3	7	3.2*	3.0
-22	4	7	3.4*	1.6
-19	4	7	50.4	48.6
-16	4	7	13.9	14.3
-13	4	7	6.5	4.4
-10	4	7	54.4	49.9
-1	4	7	24.2	24.2
5	4	7	14.7	16.8
8	4	7	4.5	5.8
14	4	7	4.5*	1.0
17	4	7	3.7*	5.0
-21	5	7	3.8*	1.8
-18	5	7	5.3	3.6
-15	5	7	17.5	17.2
-12	5	7	4.3*	1.0
-3	5	7	14.6	14.4
6	5	7	25.0	26.8
9	5	7	19.8	20.9
15	5	7	13.8	16.4
-23	6	7	3.2*	1.4
-20	6	7	4.2*	0.4
-17	6	7	4.7	3.4
-14	6	7	6.9	7.6
-5	6	7	25.3	20.5
-2	6	7	3.1*	2.5
7	6	7	16.3	16.5
10	6	7	9.5	9.0
13	6	7	30.1	30.6
16	6	7	13.6	14.1
-22	7	7	3.7*	4.0
-19	7	7	4.4*	1.3
-16	7	7	16.9	17.1
-4	7	7	3.4*	6.0
-1	7	7	104.7	98.6
8	7	7	31.0	32.4
11	7	7	4.5*	6.5
14	7	7	4.0*	5.8
-21	8	7	10.2	10.6
-18	8	7	27.2	27.3
-6	8	7	43.1	42.4
-3	8	7	3.6*	4.4
9	8	7	4.7*	3.5
12	8	7	4.3*	6.7
15	8	7	3.4*	5.9
-20	9	7	19.6	19.5
-8	9	7	13.5	14.6
-5	9	7	3.7*	3.7
-2	9	7	3.8*	5.9
10	9	7	4.5*	3.1
13	9	7	15.9	15.8
16	9	7	2.2*	8.6
-22	10	7	3.8*	6.0
-4	10	7	18.3	18.0
-1	10	7	8.0	8.1
11	10	7	4.1*	8.6
14	10	7	3.0*	6.0
-9	11	7	36.6	37.2
-6	11	7	22.3	22.9
-3	11	7	8.1	8.9
12	11	7	13.6	15.5
-11	12	7	20.4	20.7
-8	12	7	10.4	9.1
-5	12	7	46.2	44.3
-2	12	7	22.5	22.5
13	12	7	2.6*	0.3
-10	13	7	17.8	18.5
-7	13	7	4.5*	2.6
-4	13	7	13.4	13.7
-1	13	7	8.2	6.4
-12	14	7	4.6*	3.9
-9	14	7	4.6*	5.8
-6	14	7	20.4	21.8
-3	14	7	4.6*	2.4
-14	15	7	4.7*	0.5
-11	15	7	15.8	16.7
-8	15	7	10.6	12.3
-5	15	7	28.5	29.8
-2	15	7	4.8	6.6
-13	16	7	28.5	29.7
-10	16	7	27.3	28.3
-7	16	7	4.7*	4.3
-4	16	7	22.8	22.3
-1	16	7	30.7	30.2
-15	17	7	22.1	22.2
-12	17	7	4.6*	0.9
-9	17	7	13.8	16.3
-6	17	7	4.6*	5.9
-3	17	7	8.7	9.1
-17	18	7	4.2*	5.7
-14	18	7	4.5*	0.9
-11	18	7	4.5*	4.9
-8	18	7	4.6*	3.2
-5	18	7	15.6	15.8
-2	18	7	16.3	17.5
-16	19	7	4.2*	5.8
-13	19	7	4.4*	4.0
-10	19	7	10.3	10.7
-7	19	7	5.2	3.3
-4	19	7	30.8	28.0
-1	19	7	4.0*	7.2
-15	20	7	4.1*	7.0
-12	20	7	4.3*	4.3
-9	20	7	52.4	47.3
-6	20	7	11.2	10.6
-3	20	7	3.9*	5.2
-20	21	7	3.2*	2.0
-17	21	7	14.2	16.3
-14	21	7	25.1	26.4
-11	21	7	4.1*	1.7
-8	21	7	4.0*	4.1
-5	21	7	13.7	15.4
-2	21	7	3.4*	3.2
-19	22	7	3.2*	6.8
-16	22	7	3.6*	2.4
-13	22	7	3.8*	2.3
-10	22	7	3.8*	1.2
-7	22	7	3.7*	2.5
-4	22	7	3.4*	3.4
-12	23	7	3.6*	4.9
-9	23	7	3.4*	1.7
-14	24	7	3.0*	4.3
-11	24	7	3.0*	4.8
-16	25	7	2.2*	4.5
-10	25	7	15.0	12.4
-7	25	7	1.6*	2.7
-19	0	8	4.1*	1.1
-16	0	8	5.4*	2.9
-13	0	8	5.9*	1.6
-10	0	8	5.7*	0.2
-7	0	8	7.2	6.7
-4	0	8	35.0	38.9
2	0	8	36.4	39.7
5	0	8	17.9	18.8
8	0	8	5.2*	2.7
14	0	8	9.6	8.5
17	0	8	5.0*	3.5
-21	1	8	2.3*	0.3
-18	1	8	11.7	12.3
-15	1	8	5.7*	4.7
-12	1	8	12.8	10.3
-9	1	8	29.5	32.0
-6	1	8	13.0	12.5
-3	1	8	57.9	57.0
3	1	8	13.9	14.4
6	1	8	91.8	96.6
9	1	8	18.2	18.8
12	1	8	8.6	10.4
15	1	8	24.2	24.2
18	1	8	4.4*	6.3
-17	2	8	22.6	19.7
-14	2	8	21.6	19.5
-11	2	8	29.7	27.8
-8	2	8	60.1	57.5
-5	2	8	3.9*	2.2
4	2	8	8.9	5.7
7	2	8	5.3*	5.7
10	2	8	14.6	15.6
13	2	8	5.8*	2.0
16	2	8	5.0*	4.9
-19	3	8	4.8*	2.1
-16	3	8	31.9	32.7
-13	3	8	38.0	38.3
-10	3	8	5.4*	3.1
-7	3	8	34.1	32.8
-1	3	8	3.1*	2.4
5	3	8	11.4	13.4
8	3	8	5.7*	6.6
11	3	8	5.9*	3.5
14	3	8	19.1	17.3
17	3	8	7.7	8.3
-21	4	8	11.1	12.9
-18	4	8	12.6	13.6
-15	4	8	5.8*	2.8
-12	4	8	8.3	6.5
-3	4	8	17.2	20.2
6	4	8	5.4*	3.9
9	4	8	20.0	22.4
12	4	8	28.1	26.8
15	4	8	18.3	17.6
18	4	8	2.8*	1.2
-20	5	8	4.6*	0.4
-17	5	8	13.3	14.4
-14	5	8	11.3	12.5
-11	5	8	22.0	22.1
-2	5	8	52.7	58.1
7	5	8	51.5	52.2
10	5	8	28.3	26.2
16	5	8	18.0	19.2
-22	6	8	10.1	9.9
-19	6	8	5.2*	0.7
-16	6	8	32.7	29.4
-13	6	8	8.5	10.3
-4	6	8	21.9	21.6
-1	6	8	9.7	10.6
8	6	8	5.9*	1.6
11	6	8	16.0	13.6
14	6	8	4.8*	3.5
-21	7	8	26.2	24.4
-18	7	8	5.4*	0.0
-15	7	8	17.1	14.1
-6	7	8	13.1	11.2
-3	7	8	35.4	35.1
9	7	8	5.8*	4.0
12	7	8	5.2*	2.7
-23	8	8	3.0*	0.8
-20	8	8	13.9	12.8
-17	8	8	17.9	16.5
-5	8	8	5.0	6.9
-2	8	8	5.0*	2.0
10	8	8	13.9	14.6
13	8	8	8.0	7.5
-22	9	8	4.0*	2.6
-19	9	8	5.3*	1.1
-7	9	8	5.3*	2.0
-4	9	8	33.5	35.9
-1	9	8	25.2	26.1
11	9	8	44.4	39.5
-21	10	8	4.5*	3.0
-9	10	8	23.0	24.5
-6	10	8	46.8	47.5
-3	10	8	36.3	34.1
12	10	8	4.1*	5.0
-23	11	8	3.4*	4.0
-11	11	8	50.2	53.2
-8	11	8	29.9	31.1
-5	11	8	5.5*	3.2
-2	11	8	34.9	32.6
-10	12	8	5.8*	3.7
-4	12	8	5.7*	1.8
-1	12	8	5.8*	5.5
-12	13	8	16.7	17.7
-9	13	8	5.8*	1.7
-6	13	8	16.9	15.6
-3	13	8	20.1	20.8
-11	14	8	29.6	26.3
-8	14	8	20.1	19.9
-5	14	8	10.6	9.5
-2	14	8	60.1	58.9
-13	15	8	5.8*	6.8
-10	15	8	29.0	27.6
-7	15	8	38.0	38.3
-4	15	8	5.8*	2.4
-1	15	8	14.5	13.2
-15	16	8	24.2	23.0
-12	16	8	14.5	14.5
-9	16	8	5.8*	3.8
-6	16	8	6.9	7.2
-3	16	8	5.7*	1.9
-14	17	8	5.4*	2.1
-11	17	8	5.7*	8.3
-8	17	8	15.9	15.5
-5	17	8	12.3	14.5
-2	17	8	5.4*	4.9
-16	18	8	5.0*	8.4
-13	18	8	5.4*	6.4
-10	18	8	29.6	26.5
-7	18	8	5.4*	0.1
-4	18	8	5.3*	5.9
-1	18	8	31.9	28.9
-18	19	8	4.4*	0.5
-15	19	8	42.9	40.9
-12	19	8	5.2*	2.0
-9	19	8	5.3*	6.1
-6	19	8	36.8	34.5
-3	19	8	4.8*	9.3
-17	20	8	4.3*	2.7
-14	20	8	4.8*	8.0
-11	20	8	21.7	22.2
-8	20	8	4.9*	0.3
-5	20	8	4.6*	0.1
-19	21	8	3.1*	2.9
-16	21	8	4.1*	6.5
-13	21	8	4.5*	1.5
-10	21	8	4.5*	1.9
-7	21	8	7.8	9.1
-4	21	8	3.9*	3.4
-1	21	8	2.3*	3.7
-18	22	8	2.8*	6.4
-15	22	8	3.7*	0.5
-6	22	8	7.8	8.5
-11	23	8	3.4*	8.2
-8	23	8	3.0*	2.1

and the halide ions are approximately situated in three separate layers *A*, *B* and *C* parallel to (001) having the z coordinates 0, $\frac{1}{3}$ and $\frac{2}{3}$, respectively. The relative arrangement of the ammonia molecules and halide ions in these layers is illustrated in Fig. 2(*a*), (*b*) and (*c*); it is noteworthy that the layers are almost close-packed. These layers are superimposed in such a way that an approximately cubic close-packed structure of the ammonia molecules and halide ions is formed. In this close-packed arrangement the sodium ions are located in 21 of the available 129 octahedral holes per unit cell, those holes being utilized which provide only ammonia molecules as closest neighbours. Each sodium ion is accordingly surrounded by six ammonia molecules in roughly octahedral coordination. The details of the coordination are described in the next two sections.

1(*a*) *Coordination of sodium ions in special positions*

The octahedron enclosing a sodium ion in a special (threefold) position [Na(2)] does not share corners with other octahedra and the coordination of the ammonia molecules is quite regular. Distances and angles for the bromide are shown in Fig. 3 and are listed for both compounds in Table 3. Notice that the ammonia molecules surrounding this kind of sodium ion are

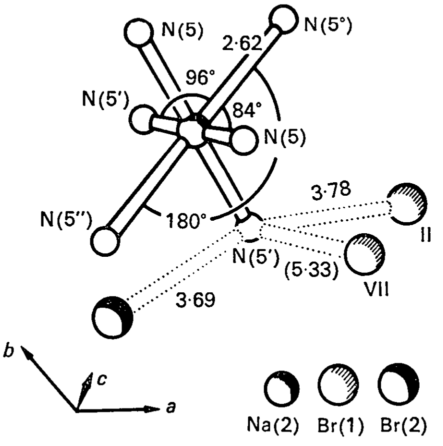

Fig. 3. Bond distances to the neighbours of sodium in special position [Na(2)]. *cf.* also Table 3.

all crystallographically equivalent and are related to each other by the $\bar{3}$ axis which passes through the sodium ion.

Table 3. *Distances and angles with their standard deviations to the neighbours of the sodium ions* (*cf.* Figs. 3 and 5).

Distance	NaCl . $5\frac{1}{7}NH_3$	NaBr . $5\frac{1}{7}NH_3$
Na(1)–N(1)	2·548 ± 0·015 Å	2·474 ± 0·008 Å
Na(1)–N(2)	2·474 ± 0·014	2·536 ± 0·008
Na(1)–N(3)	2·497 ± 0·015	2·530 ± 0·007
Na(1)–N(4)	2·475 ± 0·017	2·527 ± 0·007
Na(1)–N(6)	2·478 ± 0·016	2·501 ± 0·007
Na(1)–N(2′)	3·392 ± 0·015	3·463 ± 0·008
Na(1)–other atoms	> 3·99 Å	> 4·18 Å
Na(2)–N(5)	2·618 ± 0·016	2·616 ± 0·007
[Six equal distances Na(2)–N(5)]		
Na(2)–other atoms	> 4·13 Å	> 4·35 Å
Angle		
N(1)–Na(1)–N(2)	95·88 ± 0·49°	94·89 ± 0·24°
N(1)–Na(1)–N(3)	91·87 ± 0·49	93·02 ± 0·24
N(1)–Na(1)–N(4)	111·15 ± 0·51	107·93 ± 0·25
N(1)–Na(1)–N(6)	110·76 ± 0·47	109·22 ± 0·26
N(1)–Na(1)–N(2′)	169·64 ± 0·44	170·17 ± 0·23
N(2)–Na(1)–N(3)	81·07 ± 0·49	80·27 ± 0·22
N(2)–Na(1)–N(4)	85·40 ± 0·52	86·96 ± 0·24
N(2)–Na(1)–N(6)	152·41 ± 0·54	155·19 ± 0·27
N(3)–Na(1)–N(4)	154·39 ± 0·56	156·35 ± 0·27
N(3)–Na(1)–N(6)	90·74 ± 0·51	92·39 ± 0·24
N(4)–Na(1)–N(6)	91·31 ± 0·56	90·96 ± 0·25
N(5°)–Na(2)–N(5)	82·39 ± 0·54	84·43 ± 0·22
N(5°)–Na(2)–N(5′)	97·61 ± 0·54	95·57 ± 0·22
N(5°)–Na(2)–N(5″)	180·00 ± 0	180·00 ± 0

(the other angles involved are equal to these three by symmetry)

1(*b*) *Coordination of sodium ions in general positions*

The octahedron enclosing a sodium ion in a general (18-fold) position [Na(1)] shares two corners with adjacent octahedra as shown in Fig. 4. The nitrogen atom [N(2)] on one of these shared corners is located very close to the line which connects the two sodium ions of the coupled octahedra. Considering that an ammonia molecule can form a bond to sodium only by utilizing its lone pair it is evidently impossible for ammonia on one of the shared corners to form a strong chemical bond to more than one of the sodium ions. The observed bond distances confirm this. Bond distances for the bromide are shown in Fig. 5 and values for both compounds are listed in Table 3. It is significant that one of the six nitrogen atoms coordinating sodium is much more remote (3·46 Å in the bromide; 3·39 Å in the chloride) than the other five (average distance in the bromide 2·52 and in the chloride 2·48 Å). Evidently, the lone pair of the sixth ammonia molecule is not directed towards this sodium ion which must therefore be described as *5-coordinated.* With one nitrogen atom of the octahedron situated more remotely, the bond angles subtended at the sodium ion by the other five nitrogen atoms are quite naturally somewhat altered from the normal octahedral values as illustrated in Fig. 5 and Table 3. There is also a significant difference in the Na–NH_3 distances for the two different kinds of sodium atom. This distance is 2·62 Å for the 6-coordinated sodium ions (in special positions) but 2·50 Å (2·52 in the bromide, 2·48 in the chloride) for the effectively 5-coordinated sodium ions (in general positions). These relative differences are approximately of the same order of magnitude as those commonly observed when the coordination number is changed from 6 to 5.

In contrast to sodium in special positions the ammonia molecules surrounding sodium in general positions are not all crystallographically equivalent.

2. *Coordination of ammonia*

As described above, each ammonia molecule is coordinated to sodium by means of its lone pair.

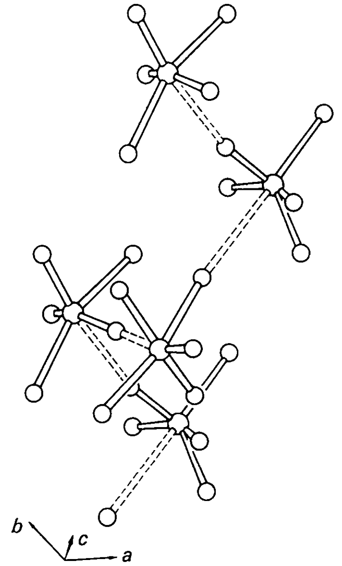

Fig. 4. The environment of sodium in general positions [Na(1)]. The picture illustrates mutual corner sharing by octahedra.

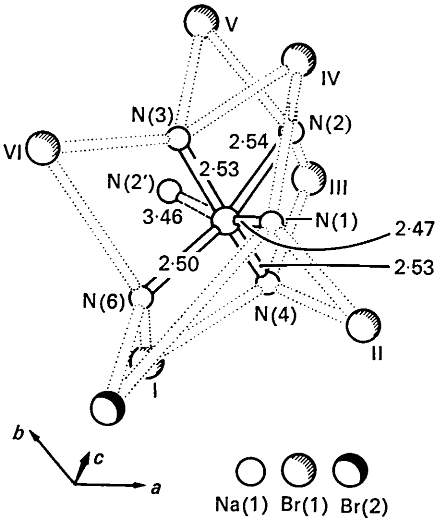

Fig. 5. Bond distances to the neighbours of sodium in general position [Na(1)]. *cf.* also Tables 3 and 4.

Furthermore, the ammonia molecules and halide ions taken together form an approximately cubic close-packed arrangement. Each ammonia is accordingly surrounded by twelve neighbours which are either ammonia or halogen. A close examination reveals that two or three of these neighbours are halide ions. Since the free electron pair is utilized in bonding to sodium, hydrogen bonding between the ammonia molecules themselves seems impossible. The other kinds of neighbour to be considered are the halide ions. As stated above, each ammonia molecule is surrounded by two or three halide ions in the first coordination shell. Some of the ammonia molecules, together with the three halogen neighbours, form a fairly symmetrical pyramid. In those cases where only two halogen ions belong to the first coordination shell a third halogen ion is situated more remotely. The distribution of the halogen neighbours is illustrated in Figs. 3 and 5; the distances are listed for both compounds in Table 4. The average distances are: N–Cl = 3·63 Å, N–Br = 3·75 Å (the distances N(2)–Cl(1)(VI) = 3·91 Å and N(2)–Br(1)(VI) = 3·92 Å are not included in these average values since they deviate rather significantly from the rest; the distances to other halogen neighbours are larger than 5·0 Å). These values are quite close to the average distances between ammonia and halogen observed in NH_4Cl . $3NH_3$ and NH_4Br . $3NH_3$, namely N–Cl = 3·59 Å, N–Br = 3·72 Å (Olovsson, 1960*a*). In those cases where three negatively charged halide ions are relatively favorably arranged around an ammonia group it may be supposed that the hydrogen atoms are preferably oriented towards the halide ions.

Table 4. *Distances to the halogen neighbours of the ammonia molecules* (*cf.* Figs. 3 and 5)

Distance	NaCl . $5\frac{1}{7}NH_3$	NaBr . $5\frac{1}{7}NH_3$
N(1)–X(2)	> 5·0 Å	> 5·0 Å
N(1)–X(1)(II)	3·501	3·635
N(1)–X(1)(IV)	3·538	3·671
N(2)–X(1)(III)	3·655	3·830
N(2)–X(1)(VI)	3·905	3·918
N(2)–X(1)(V)	3·662	3·770
N(3)–X(1)(IV)	3·814	3·848
N(3)–X(1)(V)	3·593	3·691
N(3)–X(1)(VI)	3·708	3·832
N(4)–X(1)(I)	3·650	3·749
N(4)–X(1)(II)	> 5·0	> 5·0
N(4)–X(1)(III)	3·605	3·773
N(5)–X(2)	3·540	3·689
N(5)–X(1)(VII)	> 5·0	> 5·0
N(5)–X(1)(II)	3·647	3·780
N(6)–X(2)	3·741	3·827
N(6)–X(1)(I)	3·566	3·704
N(6)–X(1)(VI)	> 5·0	> 5·0

3. *Coordination of halogen*

The relative arrangement of the ammonia molecules and halide ions in the roughly close-packed structure is such that all twelve neighbours to a certain halogen are ammonia molecules. Distances may be derived from Table 4.

Summary

The ammonia molecules and halide ions together form a roughly cubic close-packed arrangement with the sodium ions located in certain of the octahedral holes, so that only ammonia molecules are closest neighbours. The octahedra enclosing sodium ions in special threefold positions do not share corners with other octahedra but those octahedra which enclose the remaining sodium ions (in general 18-fold positions) share two corners with other octahedra. The ammonia groups on these corners cannot be considered to be bonded to more than one of the sodium ions which effectively reduces the coordination of this kind of sodium ion to *fivefold*, the sixth ammonia molecule being situated more remotely. The possible rotation of the ammonia molecules about their threefold axes may be relatively restricted by interaction with the halide neighbours.

The exact composition of the present compounds, NaX . $5\frac{1}{7}NH_3$ is easily understood in the light of the structural features: Thus in the hexagonal unit cell there are three sodium ions with sixfold coordination and 18 sodium with fivefold coordination. This corresponds to an average composition of $5\frac{1}{7}$ ammonia molecules per sodium ion $[(3\times 6+18\times 5)/21=5\frac{1}{7}]$.

Discussion

In earlier investigations the compositions of the present compounds were reported to be NaCl . $5NH_3$ and NaBr . $5·25NH_3$, respectively. The structure determinations decribed here, however, clearly demonstrate that both compounds should be formulated as NaX . $5\frac{1}{7}NH_3$ or approximately NaX . $5·143NH_3$. In the absence of a better designation the compounds could be called pentammines although this does not give a completely correct indication of the true composition.

As stated at the beginning of this paper, it was rather more difficult to grow single crystals of the chloride than of the bromide. Sodium iodide evidently does not form a corresponding phase. These differences in behavior may possibly be related to the relative sizes of ammonia and halogen in the different cases.

A comparison with other ammines shows that configurations similar to the close-packed arrangement of ammonia and halogen found in the present compounds occur in many instances. For example, compounds such as MX_2 . $6NH_3$ with the K_2PtCl_6 type of structure may be described as cubic close-packed arrangements of X and NH_3 with M situated in some of the octahedral interstices. In the following paper the structures of some of the earlier studied metal ammine salts will be reviewed to see if packing considerations of this kind find a more general application.

The preliminary work on these compounds was done in collaboration with Miss Marianne Westerman and Mr Peter Lindner. The author is much indebted to them and to Mrs Odette Olsson for very valuable assistance.

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Packing Principles in the Structures of Metal Ammine Salts

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From simple considerations of the different ways in which ammonia may be introduced into the structures of metal ammine salts it is evident that while the ammonia molecules tend to be coordinated to the metal ions they otherwise behave as rather inactive groups towards their remaining environment. Accordingly a factor of major importance for the formation of these structures is the form of the most favourable packing of the large groups, namely the ammonia molecules and negative ions. This will be particularly true for the halides since the interaction between ammonia and halide ions appears to be quite small in general. Some metal ammine salt structures studied earlier, mainly halides, are briefly reviewed with the object of investigating to what extent such simple packing is realized in practice. It is shown that in the majority of such compounds the arrangement of the ammonia molecules and negative ions may be described approximately as cubic or hexagonal close-packed or as body-centred cubic, with the metal ions in tetrahedral or octahedral interstices.

Introduction

In the preceding paper the structure common to NaCl . $5\frac{1}{7}NH_3$ and NaBr . $5\frac{1}{7}NH_3$ is presented (Olovsson, 1965). It is found that this structure can be described as a nearly cubic close-packed arrangement of ammonia molecules and halide ions with sodium ions occupying some of the octahedral interstices. Subsequent interest has become focused on the structures of metal ammine halides in general since it appears very probable that simple building principles such as the close-packing of ammonia molecules and halide ions would be an important factor in the structures of many other ammines. A survey of some of the earlier published structures with this concept in mind therefore seems valuable.

General considerations

Let us first consider the different ways of inserting an ammonia molecule into the structure of a metal ammine salt. It is found by experience that ammonia is