

Table 3. Distances and angles involved in hydrogen bonds

	Transformation (on third atom)	Distance (Å)		Angle (°)
N(1)—H...Cl(1)	-x, 1-y, -z	3.260 (6)	Pt(1)—N(1)...Cl(1)	106.1 (2)
N(1)—H...Cl(2)	1-x, -y, -z	3.416 (6)	Pt(1)—N(1)...Cl(2)	104.1 (2)
N(1)—H...Cl(3)	1-x, -y, -z	3.271 (6)	Pt(1)—N(1)...Cl(3)	107.3 (2)
			Cl(1)...N(1)...Cl(2)	116.0 (2)
			Cl(1)...N(1)...Cl(3)	146.3 (2)
			Cl(2)...N(1)...Cl(3)	59.6 (2)
N(2)—H...Cl(1)	-x, 1-y, -z	3.403 (6)	Pt(1)—N(2)...Cl(1)	101.3 (2)
N(2)—H...Cl(2)	x-1, y, z	3.379 (7)	Pt(1)—N(2)...Cl(2)	105.2 (2)
N(2)—H...Cl(3)	x-1, y, z	3.559 (8)	Pt(1)—N(2)...Cl(3)	97.8 (2)
			Cl(1)...N(2)...Cl(2)	153.6 (2)
			Cl(1)...N(2)...Cl(3)	118.6 (2)
			Cl(2)...N(2)...Cl(3)	57.2 (2)

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Structure of Diaquatetrakis(urea)magnesium Bromide

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Abstract. [Mg{CO(NH₂)₂}₄(H₂O)₂]₂Br₂, C₄H₂₀MgN₈O₆²⁺.2Br⁻, monoclinic, *P*2₁/*c*, *a* = 8.455 (1), *b* = 11.206 (1), *c* = 9.127 (1) Å, β = 103.52 (2)°, *Z* = 2, *D*_x = 1.818, *D*_m = 1.804 Mg m⁻³. The Mg²⁺ ions are octahedrally coordinated by the O atoms of the four urea and two water molecules. The urea molecules form a pseudotetragonal arrangement with intra-complex hydrogen bonds.

Introduction. Crystals of the title compound were obtained by slow evaporation of an aqueous solution of

magnesium bromide and urea in the molar ratio 1:4. This is probably the same compound as that described as MgBr₂.4urea.H₂O by Suleimankulov, Noguev, Dushenaliyeva & Naumova (1964) in their study of the magnesium bromide–urea–water system.

A crystal ground to a sphere of diameter 0.38 mm was used to collect intensity data on an Enraf–Nonius CAD-4 diffractometer. Variable ω–2θ scans in the θ range 0–27° and graphite-monochromatized Mo *K*α radiation were used. The cell parameters were obtained from a least-squares fit of the setting angles for 15

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Table 1. Atomic positional coordinates ($\times 10^5$ for Br, $\times 10^4$ for Mg, C, N and O atoms, $\times 10^3$ for H atoms) with e.s.d.'s in parentheses and isotropic thermal parameters

	x	y	z	\bar{U} ($\times 10^3 \text{ \AA}^2$)
Mg	5000	0	0	23
Br	14153 (3)	69307 (2)	6486 (3)	38
O(1)	4229 (2)	989 (1)	-1925 (2)	33
C(1)	2924 (3)	1327 (2)	-2776 (2)	24
N(11)	2916 (3)	1791 (2)	-4131 (2)	38
N(12)	1519 (3)	1228 (2)	-2383 (3)	39
H(111)	202 (4)	207 (3)	-465 (3)	53
H(112)	368 (4)	211 (2)	-423 (3)	38
H(121)	70 (4)	139 (3)	-300 (4)	78
H(122)	152 (3)	90 (2)	-155 (3)	27
O(2)	7167 (2)	-347 (1)	-623 (2)	30
C(2)	7712 (3)	-341 (2)	-1786 (2)	29
N(21)	9197 (3)	-778 (2)	-1747 (3)	42
N(22)	6857 (3)	98 (3)	-3070 (3)	57
H(211)	946 (4)	-89 (2)	-255 (3)	53
H(212)	970 (4)	-121 (3)	-91 (3)	61
H(221)	728 (4)	29 (3)	-338 (4)	71
H(222)	598 (4)	47 (3)	-305 (4)	76
W	6048 (2)	1594 (2)	1009 (2)	33
HW(1)	661 (4)	190 (3)	51 (3)	49
HW(2)	652 (4)	164 (2)	193 (4)	52

reflections. The space group was determined from systematic absences to be $P2_1/c$. Lorentz, polarization and absorption corrections were applied in the usual manner. Of the 1956 intensities measured, 1902 were positive and yielded 1789 unique $|F|$ values giving an internal consistency factor of 1.6% in a sort-merge procedure. The structure was determined by the heavy-atom method and refined by a full-matrix least-squares procedure using weights $w^{-1} = \sigma^2(|F|)$.

All H atoms were identified in difference Fourier maps and refined using isotropic temperature factors. Neutral-atom scattering factors were used (*International Tables for X-ray Crystallography*, 1974).

Discrepancy indices were $R = 2.9\%$ and $R_w = 2.3\%$ for all structure factors. On the final difference Fourier map the highest peak of 0.5 e \AA^{-3} was of no chemical significance. The final atomic coordinates and their standard deviations are given in Table 1.* Most of the calculations were performed with the systems of programs written by Sheldrick (1976) and Roberts & Sheldrick (1972).

Discussion. This structure was examined in order to compare it with those of $[\text{Mg}(\text{urea})_6]\text{Br}_2 \cdot 4\text{urea}$ (MBD) (Lebioda, Stadnicka & Sliwinski, 1979) and

* Lists of structure factors, thermal parameters and distances and angles involving the H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34845 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

$[\text{Mg}(\text{urea})_6]\text{Br}_2 \cdot \text{MgBr}_2$ (3:1) (MBH) (Lebioda & Lewinski, 1979). The coordination of the Mg^{2+} ion is shown in Fig. 1. The complex cation is in a special position $(0, \frac{1}{2}, \frac{1}{2})$ of symmetry $\bar{1}$. The Mg^{2+} ion is approximately in the planes of both urea molecules, which form an angle of 20.4° with each other. The $\text{Mg}-\text{O}=\text{C}$ angles of 139° are close to the expected value of 138° (Lebioda, 1980). The $\text{O}=\text{C}-\text{N}$ angles nearest to the cation are $121.6(2)$ and $121.4(2)^\circ$ while those on the opposite side are $120.2(2)$ and $120.0(2)^\circ$; these differences are accompanied by differences in the lengths of the C-N bonds: $1.323(3)$ and $1.320(3) \text{ \AA}$ at the greater angle, $1.341(3)$ and $1.340(3) \text{ \AA}$ at the smaller. Both these distortions reflect the asymmetrical polarization of the urea molecules.

Table 2 shows the distances and angles in the Mg^{2+} coordination polyhedra.

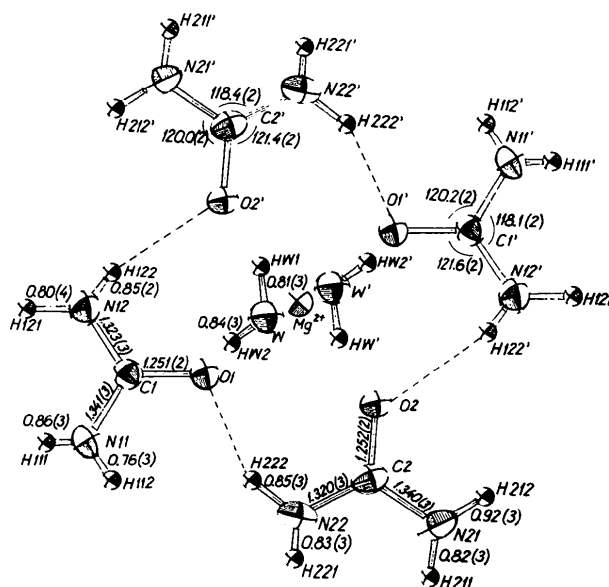


Fig. 1. The $[\text{Mg}(\text{urea})_4(\text{H}_2\text{O})_2]^{2+}$ complex cation with some distances (\AA) and angles ($^\circ$). Standard deviations are in parentheses. The figure was drawn with the ORTEP program (Johnson, 1965) using arbitrary temperature factors for the H atoms.

Table 2. Distances (\AA) and angles ($^\circ$) within the Mg^{2+} coordination polyhedra

Standard deviations are in parentheses.			
Mg-O(1)	2.050 (1)	O(1)-Mg-O(2)	89.5 (1)
Mg-O(2)	2.078 (1)	O(1)-Mg-W	86.2 (1)
Mg-W	2.108 (2)	O(2)-Mg-W	88.3 (1)
Mg-urea(1) plane	0.308	Mg-O(1)-C(1)	138.9 (1)
Mg-urea(2) plane	0.200	Mg-O(2)-C(2)	138.9 (1)
Mg-water plane	1.323	Mg-W-HW(1)	111 (2)
Plane(1)-plane(2)	20.29°	Mg-W-HW(2)	122 (2)

Table 3. Distances (Å) and angles (°) in the hydrogen-bonding system

D-H...A	Acceptor position	D-H	D...A	H...A	D-H...A	C=O...H
N(11)-H(111)...Br	-x, $-\frac{1}{2} + y$, $\frac{1}{2} - z$	0.86 (3)	3.603 (2)	2.84 (3)	150 (2)	
N(11)-H(112)...W	x, $\frac{1}{2} - y$, $\frac{1}{2} + z$	0.76 (3)	3.185 (3)	2.44 (4)	165 (3)	
N(12)-H(121)...Br	-x, $-\frac{1}{2} + y$, $\frac{1}{2} - z$	0.80 (4)	3.493 (2)	2.72 (3)	163 (2)	
N(12)-H(122)...O(2)	1 - x, -y, 2 - z	0.85 (2)	2.883 (3)	2.12 (4)	149 (3)	125 (3)
N(21)-H(211)...Br	1 + x, $\frac{1}{2} - y$, $\frac{1}{2} + z$	0.82 (3)	3.595 (2)	2.84 (3)	155 (2)	
N(21)-H(212)...Br	x, -1 + y, 1 + z	0.92 (3)	3.601 (2)	2.74 (3)	157 (2)	
N(22)-H(221)...Br	1 - x, $-\frac{1}{2} + y$, $\frac{1}{2} - z$	0.83 (3)	3.673 (2)	2.90 (3)	128 (2)	
N(22)-H(222)...O(1)	x, y, z	0.85 (3)	2.848 (3)	2.07 (4)	151 (3)	114 (3)
W-HW(1)...Br	1 - x, 1 - y, -z	0.81 (3)	3.338 (2)	2.54 (3)	170 (2)	
W-HW(2)...Br	1 - x, $-\frac{1}{2} + y$, $\frac{1}{2} - z$	0.84 (3)	3.315 (2)	2.50 (3)	164 (2)	

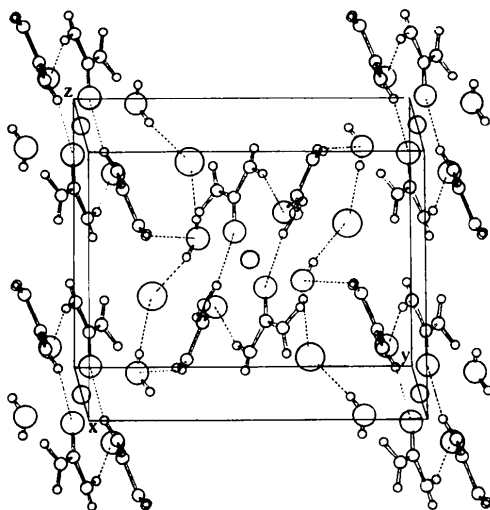


Fig. 2. Hydrogen bonding in the structure.

Hydrogen bonding at the carbonyl groups reflects well the sp^2 hybridization at the O atoms as shown in Fig. 1. The O atoms of the urea molecules are acceptors of intracomplex hydrogen bonds from neighbouring molecules forming a pseudotetragonal arrangement. This situation is different from that found in MBD, where there is only a pair of intracomplex hydrogen bonds, and that in MBH where there are six intracomplex hydrogen bonds of symmetry $\bar{3}$. A similar pseudotetragonal arrangement of urea ligands was found in $\text{CaSO}_4 \cdot 4\text{urea}$ (de Villiers & Boeyens, 1975).

The water molecule is positioned with one of its free electron pairs directed towards the cation; the

H(112)...W distance of 2.44 (4) Å is too long for a hydrogen bond, so it can be placed in type J of the hydrate-classification scheme of Ferraris & Franchini-Angela (1972).

The hydrogen bonding is shown in Fig. 2 and described in Table 3. All available H atoms form or tend to form hydrogen bonds to Br^- ions thus connecting complex cations and anions in a three-dimensional network.

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