

two carboxylic O atoms to form bonds to two other Nd cations. Each metal ion is thereby involved in coordination to three dipicolinate anions and takes part in two hexameric rings. Each pair of connected hexamers has one Nd atom in common. The coordination figure of Nd may best be described as a tricapped trigonal prism with O1, OW2, OW1, and OW3, OW4, O4 defining the bases, and with O2, O3, N as the caps, $\Delta = 0.038 \text{ \AA}^2$ [$\Delta = \sum d_i^2/9$, where d_i is the distance between the real position of the i th atom and the relevant vertex in the ideal least-squares-fitted polyhedron (Drew, 1977)]. Two alternative descriptions in terms of a capped square antiprism are: (i) non-capped base O2, OW2, O3, OW4; capped base OW1, O1, OW3, O4; cap N; $\Delta = 0.067 \text{ \AA}^2$; and (ii) non-capped base O2, O4, N, OW1; capped base OW4, OW3, O1, OW2; cap O3; $\Delta = 0.078 \text{ \AA}^2$. An ORTEPII view (Johnson, 1976) of the Nd coordination is given in Fig. 1, and the hexameric fragment of the complex cation is presented in Fig. 2. The structure is held together by an elaborate network of

intermolecular hydrogen bonds, some of them disordered and bifurcated.

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Structure of Tetralithium 1,4,5,8-Naphthalenetetracarboxylate Dodecahydrate

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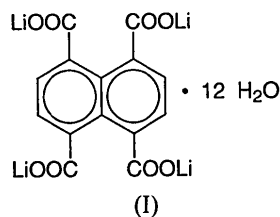
Abstract. $4\text{Li}^+ \cdot \text{C}_{14}\text{H}_4\text{O}_8^{4-} \cdot 12\text{H}_2\text{O}$, $M_r = 544.18$, triclinic, $P\bar{1}$, $a = 9.608$ (2), $b = 10.034$ (2), $c = 7.033$ (1) Å, $\alpha = 94.29$ (1), $\beta = 96.95$ (1), $\gamma = 64.52$ (1)°, $V = 607.4$ (2) Å³, $Z = 1$, $D_x = 1.49 \text{ g cm}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71073 \text{ \AA}$, $\mu = 1.29 \text{ cm}^{-1}$, $T = 295 \text{ K}$, $F(000) = 284$, $R = 0.039$ for 2781 unique reflections having $I > \sigma_I$. The two inequivalent carboxyl groups adopt a non-planar arrangement with respect to the naphthalene core, making dihedral angles of 52.7 (1) and 54.6 (1)° with it. The Li⁺ ions are tetrahedrally coordinated by carboxyl and water O atoms. The Li—O distances are in the range 1.906 (3)–2.041 (3) Å, averaging 1.97 (4) Å; O—Li—O angles are 101.5 (1)–123.9 (1)°, averaging 109 (6)°. Each of the 12 inequivalent water H atoms is involved in hydrogen bonding. Of these bonds, 11 are typical two-centered hydrogen bonds with an average H···O (acceptor) distance of 1.92 (11) Å and

an average O—H···O (acceptor) angle of 172 (5)°. One water H atom is involved in a three-centered hydrogen bond with an average H···O (acceptor) distance of 2.61 (4) Å and an average O—H···O (acceptor) angle of 120 (3)°. Adjacent organic anions are separated by the Li⁺ ions and their coordination polyhedra, with the water molecules occupying positions above and below the naphthalene rings and participating in a three-dimensional hydrogen-bonded network.

Introduction. The structure determination of crystalline Group IA salts of 1,4,5,8-naphthalenetetracarboxylic acid is being undertaken as part of a continuing investigation of hydrogen bonding in organic solids. The effects of cation size on crystal structure and the attendant hydrogen-bond network, as well as on the conformation of the organic anion, are of particular interest. The structure of the tetrasodium salt has previously been reported (Fitzgerald,

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Gallucci & Gerkin, 1991); we report here the structure of crystalline tetralithium 1,4,5,8-naphthalenetetracarboxylate dodecahydrate (I), whose structure has not previously been described.



Experimental. 1,4,5,8-Naphthalenetetracarboxylic acid obtained from Aldrich Chemical Company was suspended in water and reacted with excess analytical reagent grade LiOH to prepare an aqueous solution of tetralithium 1,4,5,8-naphthalenetetracarboxylate. The solution was mixed with Norit-A decolorizing carbon and filtered. The Li salt thus purified was crystallized from water by slow evaporation at room temperature. The experimental sample was a clear colorless plate with approximate principal dimensions $0.19 \times 0.31 \times 0.38$ mm. This was mounted on a glass fiber with epoxy cement and coated with Apiezon L grease; data were collected at room temperature with a Rigaku AFC5S diffractometer utilizing monochromated Mo $K\alpha$ radiation.

Unit-cell parameters were obtained from a least-squares fit of the setting angles for 25 centered reflections with $29 < 2\theta < 30^\circ$. Intensity data were measured for 3746 reflections (exclusive of standards) with $+h, \pm k, \pm l$ indices ($h_{\max} = 13, -14 \leq k \leq 14, -9 \leq l \leq 9$) and 2θ values in the range $4 < 2\theta < 60^\circ$. The ω - 2θ scan technique was employed with scan widths $(1.40 + 0.35 \tan \theta)^\circ$ in ω , and a background/scan time-ratio of 0.5. A variance was assigned to each reflection by means of the formula $\sigma_I^2 = \sigma_{cs}^2(I) + (0.03I)^2$ in which σ_{cs} is based on counting statistics and I is the integrated intensity. Six standard reflections ($110, 21\bar{1}, 10\bar{1}, 632, 12\bar{5}, 3\bar{1}4$) were measured after every 150 reflections. Over the course of the intensity data collection they showed, on average, a relative intensity decay of 5.0%; a linear correction was applied to account for this decay. No correction was made for absorption; the data were corrected for Lorentz and polarization effects. Averaging equivalent reflections gave 3551 independent reflections with $R_{\text{int}} = 0.009$.

The crystal system was found to be triclinic, thus allowing two space groups: $P1$ and $P\bar{1}$. Initial preference was given to the centrosymmetric alternative $P\bar{1}$ and, since refinement proceeded well, it was adopted. The direct methods program *SHELXS86* (Sheldrick, 1985) was used to generate an E map from which the initial positions of the C and O atoms of the anion

were assigned. Fourier difference methods were used to locate the positions of the six O atoms of the water molecules, the two Li atoms, and the H atoms. Full-matrix least-squares refinement (*TEXSAN*; Molecular Structure Corporation, 1989) minimized the function $\sum \sigma_F^{-2} (|F_o| - |F_c|)^2$ in which $\sigma_F = \sigma_I / 2FLp$. Neutral-atom scattering factors and anomalous-dispersion factors were taken from Cromer & Waber (1974) for C, O and Li; the scattering factor for H was taken from Stewart, Davidson & Simpson (1965).

The results of the final refinement cycle were: 2781 observations having $I > \sigma_I$; 229 variables; $R = 0.039$; $wR = 0.044$; $w = \sigma_F^{-2}$; $S = 1.57$; $(\Delta/\sigma)_{\max} < 0.01$. The optimized secondary-extinction coefficient was $9.9(9) \times 10^{-6}$ (Zachariasen, 1967); the maximum correction for extinction was 10% of F_o for the 002 reflection. Maximum and minimum peaks on the final electron-density difference map had values 0.35 and $-0.22 \text{ e } \text{\AA}^{-3}$, respectively. The maximum peak lay at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, the inversion center between C(5) and C(5ⁱ); the minimum peak lay at (0.53, 0.44, 0.34), approximately 1.3 Å from C(6) and C(7). [For the final refinement cycle for 2595 independent observations having $I > 3\sigma_I$: $R = 0.035$; $wR = 0.043$; $S = 1.58$; $(\Delta/\sigma)_{\max} < 0.01$. Similarly, for the final refinement cycle for 3229 independent observations having $I > 0$: $R = 0.049$; $wR = 0.045$; $S = 1.49$; $(\Delta/\sigma)_{\max} < 0.03$. These latter results are for comparison purposes only].

Final atomic coordinates, equivalent isotropic and isotropic displacement parameters and their e.s.d.'s are given in Table 1.* As noted above, a center of inversion lies at the midpoint of the C(5)—C(5ⁱ) ring bond. The hydrocarbon portion of the molecule is shown in Fig. 1 with selected interatomic distances specified in one asymmetric unit and angles in the other. Table 2 lists selected distances and angles in the coordination polyhedra of the two inequivalent Li⁺ ions together with distances and angles for the six inequivalent water molecules.

Discussion. The 1,4,5,8-naphthalenetetracarboxylate anion is shown with bond lengths and angles in Fig. 1. These lengths and angles are very similar, respectively, to those determined for the same anion in tetrasodium 1,4,5,8-naphthalenetetracarboxylate octahydrate (Fitzgerald, Gallucci & Gerkin, 1991), with most differences being less than the combined

* Lists of structure factors, anisotropic displacement parameters, positional parameters and isotropic displacement parameters of ring H atoms and data pertaining to least-squares best-fit planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55025 (30 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0556]

Table 1. Final atomic coordinates and equivalent isotropic and isotropic displacement parameters (Å²) for tetralithium 1,4,5,8-naphthalenetetracarboxylate dodecahydrate

$B_{eq} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$, H atoms were refined isotropically. E.s.d.'s are given in parentheses.

	x	y	z	B_{eq}/B
O(1)	0.6442 (1)	0.8314 (1)	0.6891 (1)	2.13 (5)
O(2)	0.8175 (1)	0.6015 (1)	0.6302 (1)	2.25 (5)
O(3)	0.6116 (1)	0.7377 (1)	0.2493 (1)	2.03 (5)
O(4)	0.8273 (1)	0.5389 (1)	0.1912 (1)	2.25 (5)
O(5)	0.6685 (1)	0.9756 (1)	0.3359 (2)	2.43 (6)
O(6)	0.7048 (1)	1.1297 (1)	0.7500 (2)	2.63 (6)
O(7)	0.8706 (2)	1.0295 (1)	1.1341 (2)	3.70 (8)
O(8)	0.9810 (1)	0.8213 (1)	0.6466 (2)	2.51 (6)
O(9)	0.9143 (1)	0.7149 (1)	1.0156 (2)	2.80 (7)
O(10)	0.8697 (1)	0.2967 (1)	0.6778 (2)	3.08 (7)
C(1)	0.6820 (1)	0.6966 (1)	0.6477 (2)	1.64 (6)
C(2)	0.6960 (1)	0.6012 (1)	0.2520 (2)	1.56 (6)
C(3)	0.4714 (2)	0.6755 (1)	0.7862 (2)	1.78 (6)
C(4)	0.5585 (1)	0.6406 (1)	0.6337 (2)	1.48 (6)
C(5)	0.5464 (1)	0.5378 (1)	0.4870 (2)	1.34 (6)
C(6)	0.6254 (1)	0.5061 (1)	0.3172 (2)	1.46 (6)
C(7)	0.6214 (2)	0.3971 (1)	0.1900 (2)	1.77 (6)
Li(1)	0.9881 (3)	0.6376 (3)	0.7624 (4)	2.2 (1)
Li(2)	0.7520 (3)	0.9408 (3)	0.6084 (4)	2.3 (1)
H(3)	0.571 (3)	1.040 (3)	0.329 (3)	4.9 (5)
H(4)	0.657 (3)	0.892 (3)	0.290 (3)	5.1 (5)
H(5)	0.748 (2)	1.184 (2)	0.719 (3)	4.2 (5)
H(6)	0.600 (3)	1.182 (2)	0.747 (3)	5.4 (6)
H(7)	0.830 (3)	1.052 (3)	1.024 (5)	7.8 (8)
H(8)	0.797 (3)	1.020 (2)	1.190 (4)	5.4 (6)
H(9)	1.031 (3)	0.784 (3)	0.542 (4)	5.2 (5)
H(10)	1.024 (3)	0.869 (3)	0.719 (4)	5.8 (6)
H(11)	0.878 (3)	0.662 (3)	1.076 (3)	5.8 (6)
H(12)	0.845 (4)	0.795 (4)	0.997 (5)	10 (1)
H(13)	0.940 (3)	0.282 (2)	0.777 (3)	5.3 (6)
H(14)	0.834 (3)	0.388 (3)	0.655 (4)	6.9 (7)

e.s.d.'s for the two determinations. The atoms that comprise the naphthalene core in the present case have an average deviation of 0.030 (2) Å from the best least-squares plane describing these atoms, while C(1) and C(2) have positions 0.389 (1) and -0.371 (1) Å, respectively, relative to this plane. The planes describing each of the carboxyl groups form dihedral angles of 52.7 (1) [C(1), O(1), O(2)] and 54.6 (1)° [C(2), O(3), O(4)] with the least-squares plane of the naphthalene core, in very close agreement with corresponding values for the tetrasodium salt (Fitzgerald, Gallucci & Gerkin, 1991). Thus, changing from Na⁺ to Li⁺ cation had very little effect on the geometry of the organic anion despite changes of hydration and crystal packing.

As shown in Fig. 2, both Li⁺ ions are tetrahedrally coordinated: Li(1) by two carboxyl O atoms and two water O atoms, Li(2) by one carbonyl O atom and three water O atoms. The average Li(1)—O distance is 1.97 (6) Å, while the average Li(2)—O distance is 1.98 (2) Å, both comparable to average values reported for other hydrated Li salts of organic acids: lithium formate monohydrate, 1.95 (2) Å (Thomas, Tellgren & Almlöf, 1975); lithium maleate dihydrate, 1.96 (4) Å (Town & Small, 1973); and lithium acetate dihydrate, 1.97 (11) Å (Galigné, Mouvet & Falgueirettes, 1970). In the present study, the Li—O contacts for the carboxyl O

Table 2. Distances (Å) and angles (°) in the coordination polyhedra of the two inequivalent Li⁺ ions and for the six inequivalent water molecules of the title salt

E.s.d.'s are given in parentheses.

Coordination polyhedron I

Li(1)—O(2)	1.943 (3)	O(2)—Li(1)—O(4')	113.0 (1)
Li(1)—O(4')	1.906 (3)	O(2)—Li(1)—O(8)	106.9 (1)
Li(1)—O(8)	2.041 (3)	O(2)—Li(1)—O(9)	102.5 (1)
Li(1)—O(9)	1.976 (3)	O(4')—Li(1)—O(8)	123.9 (1)
Li(1)—O (mean)	1.966 (57)	O(4')—Li(1)—O(9)	106.3 (1)
		O(8)—Li(1)—O(9)	101.6 (1)
		O—Li(1)—O (mean)	109.0 (83)

Coordination polyhedron II

Li(2)—O(1)	1.953 (3)	O(1)—Li(2)—O(5)	101.5 (1)
Li(2)—O(5)	1.981 (3)	O(1)—Li(2)—O(6)	113.3 (1)
Li(2)—O(6)	1.969 (3)	O(1)—Li(2)—O(8)	110.4 (1)
Li(2)—O(8)	1.996 (3)	O(5)—Li(2)—O(6)	110.6 (1)
Li(2)—O (mean)	1.975 (18)	O(5)—Li(2)—O(8)	113.8 (1)
		O(6)—Li(2)—O(8)	107.4 (1)
		O—Li(2)—O (mean)	109.5 (45)

Water molecules

O(5)—H(3)	0.88 (2)	H(3)—O(5)—H(4)	100 (2)
O(5)—H(4)	0.92 (2)		
O(6)—H(5)	0.86 (2)	H(5)—O(6)—H(6)	112 (2)
O(6)—H(6)	0.91 (3)		
O(7)—H(7)	0.82 (3)	H(7)—O(7)—H(8)	103 (3)
O(7)—H(8)	0.90 (3)		
O(8)—H(9)	0.89 (3)	H(9)—O(8)—H(10)	111 (2)
O(8)—H(10)	0.86 (3)		
O(9)—H(11)	0.90 (3)	H(11)—O(9)—H(12)	108 (3)
O(9)—H(12)	0.80 (4)		
O(10)—H(13)	0.88 (3)	H(13)—O(10)—H(14)	105 (2)
O(10)—H(14)	0.85 (3)		

Symmetry code: (none) x, y, z; (i) -x + 2, -y + 1, -z + 1.

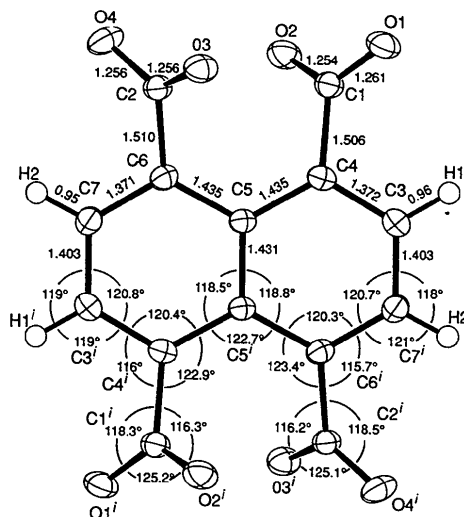


Fig. 1. An ORTEP (Johnson, 1976) view of the 1,4,5,8-naphthalenetetracarboxylate anion, with adopted numbering scheme. Displacement ellipsoids are drawn at 50% probability for all atoms except H, for which they have been set artificially small. An inversion center lies at the midpoint of the C(5)—C(5') bond. Bond lengths (Å) and angles (°) are shown in the diagram; the e.s.d.'s for bond lengths and angles involving C and O atoms are 0.002 Å and 0.2°, respectively, while for lengths and angles involving H atoms they are 0.02 Å and 1°, respectively.

atoms are in the range 1.906–1.953 Å and are significantly shorter than the Li—O contacts for the water O atoms which are 1.969–2.041 Å. This pattern of carboxyl O atoms providing closer contacts than water O atoms is also present in lithium formate monohydrate and lithium acetate dihydrate but not in lithium maleate dihydrate. In addition, the oxygen–cation contacts reported for tetrasodium 1,4,5,8-naphthalenetetracarboxylate octahydrate (Fitzgerald, Gallucci & Gerkin, 1991) show no significant difference between carboxyl and water O atoms. The average O—Li—O angle for Li(1) is 109 (8)° and for Li(2) is 110 (5)°, both close to the 109.5° value expected for regular tetrahedral coordination. One water O atom, O(8), is coordinated to both Li atoms such that the Li(1)—O(8)—Li(2) angle is 99.8 (1)°.

Table 3 lists the hydrogen-bond parameters for each of the water molecules. Each of the H atoms, except H(12), is involved in a typical two-centered hydrogen bond with an average H—O (acceptor) distance of 1.92 (11) Å and an average O—H—O (acceptor) angle of 172 (5)°. Again, these values are comparable to averages of those reported for X-ray studies of similar compounds: lithium formate monohydrate, 2.07 (10) Å and 169 (2)° (Thomas, Tellgren & Almlöf, (1975); lithium maleate dihydrate, 1.94 (15) and 168 (11)° (Town & Small, 1973); and trillithium citrate pentahydrate, 1.98 (9) Å and 166 (7)° (Rossi, Rickles & Glusker, 1983). H(12), however, is approximately equidistant from two O atoms: 2.57 (3) Å from O(7) and 2.65 (4) Å from O(1), the average of which is considerably greater

Table 3. *Hydrogen-bond parameters (Å, °) for the 12 inequivalent water H atoms of the title salt*

H(12), denoted by an asterisk, is involved in a three-center hydrogen bond. E.s.d.'s are given in parentheses

O—H...A	O...A	H...A	O—H...A
O(5)—H(3)···O(1 ^{iv})	2.779 (2)	1.90 (3)	176 (2)
O(5)—H(4)···O(3)	2.682 (1)	1.77 (2)	167 (2)
O(6)—H(5)···O(10 ⁱⁱⁱ)	2.860 (2)	2.00 (2)	172 (2)
O(6)—H(6)···O(3 ⁱⁱ)	2.745 (2)	1.84 (3)	172 (2)
O(7)—H(7)···O(6)	2.972 (2)	2.15 (3)	174 (3)
O(7)—H(8)···O(5 ⁱⁱ)	2.787 (2)	1.90 (3)	170 (2)
O(8)—H(9)···O(10 ⁱ)	2.755 (2)	1.86 (3)	178 (2)
O(8)—H(10)···O(7 ⁱⁱ)	2.759 (2)	1.90 (3)	176 (2)
O(9)—H(11)···O(4 ⁱⁱ)	2.681 (2)	1.79 (3)	174 (2)
*O(9)—H(12)···O(7)	3.064 (2)	2.57 (3)	121 (3)
*O(9)—H(12)···O(1)	3.118 (2)	2.65 (4)	119 (3)
O(10)—H(13)···O(9 ⁱ)	2.778 (2)	1.90 (3)	170 (2)
O(10)—H(14)···O(2)	2.917 (2)	2.10 (3)	162 (3)

Symmetry code: (none) x, y, z ; (i) $-x + 2, -y + 1, -z + 1$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) $x, y + 1, z$; (iv) $-x + 2, -y + 2, -z + 2$; (v) $-x + 2, -y + 1, -z + 2$; (vi) $x, y, z + 1$.

than the average H—O (acceptor) distance for the other H atoms; the O—H—O (acceptor) angles for these two bonds are 121 (3)° for O(7) and 119 (3)° for O(1), considerably smaller than the average value for the other H atoms. Additionally, the O(7)—H(12)—O(1) angle is 116 (3)° indicating that H(12) is close to the plane formed by O(7), O(1) and O(9). These comparisons make it clear that H(12) is involved in a three-centered hydrogen bond, which, according to Jeffrey (1987), is the result of an insufficient number of H-atom donors to satisfy the available O-atom acceptors. The hydrogen-bonding network for tetrasodium 1,4,5,8-naphthalenetetracarboxylate octahydrate (Fitzgerald, Gallucci & Gerkin, 1991), contrary to the situation here, does not involve a three-centered hydrogen bond; the ratio of O-atom acceptors to H-atom donors being 1.25 for the tetrasodium case compared to 1.33 for the present case.

An analysis of the charge distribution for the tetracarboxylate anion was carried out using the equations of Brown & Shannon (1973).^{*} For the C(1), O(1), O(2) carboxylate group a charge of 0.90 was found and for the C(2), O(3), O(4) carboxylate group a charge of 0.87 was determined. The slightly larger charge for the C(1) group is consistent with that group having two Li—O contacts while the C(2) group has only one. The same pattern is found in the tetrasodium study: the carboxylate group having the larger charge also has more cation contacts.

A unit cell for tetralithium 1,4,5,8-naphthalenetetracarboxylate dodecahydrate is illustrated in Fig. 3, which shows that the Li⁺ ions occupy positions between the organic anions and that these ions, together with their coordinated water molecules, separate adjacent organic anions. The space above

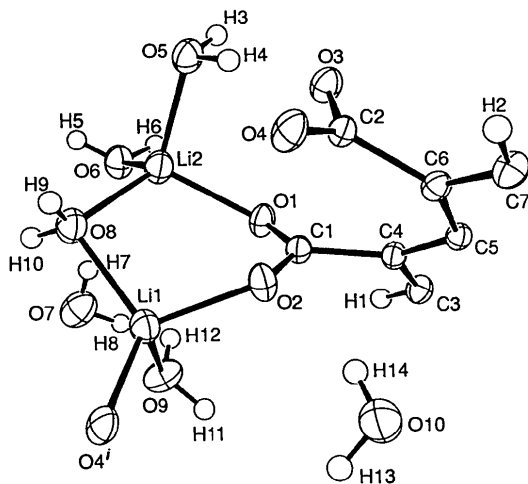


Fig. 2. An ORTEPII (Johnson, 1976) view of the Li⁺ ion coordination in the title compound, with adopted numbering scheme. Displacement ellipsoids are drawn at 50% probability for all atoms except H, for which they have been set artificially small. Only one half of the naphthalenetetracarboxylate anion is shown in this view.

^{*} For Li...O, $s = (r/1.378)^{-4.065}$ and for H...O, $s = (r/0.86)^{-2.17}$, where s = bond strength and r = coordination distance.

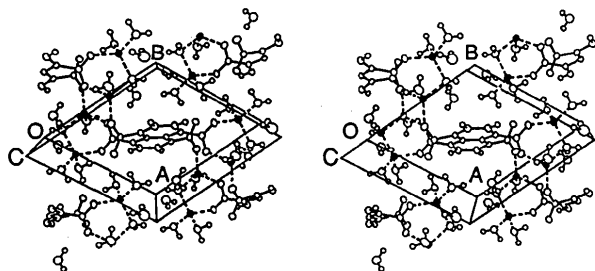


Fig. 3. A unit cell (ORTEPII; Johnson, 1976) of the title compound. Li⁺ ions are filled; Li—O coordination is represented by dashed lines. One formula unit is shown within the central portion of the cell while four additional asymmetric units are shown outside the cell.

and below the naphthalene rings is occupied by water molecules; altogether, the water molecules participate in a three-dimensional network of hydrogen bonds. The two water molecules not involved in coordination of Li⁺ ions supplement the packing around the naphthalene ring.

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The Structure of Copper(II) 5,7,12,14-Tetramethyldibenzo[*b*,*d*][1,4,8,11]-tetraazacyclotetradeca-2,4,7,9,11,14-hexaenediide*

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Abstract. [Cu(C₂₂H₂₂N₄)], *M_r* = 405.99, monoclinic, *P*2₁/*c*, *a* = 14.318 (2), *b* = 16.427 (2), *c* = 16.299 (2) Å, β = 100.01 (1)°, *V* = 3775 (1) Å³, *Z* = 8, *D_x* = 1.429 g cm⁻³, λ(Cu *K*α) = 1.54183 Å, μ = 16.88 cm⁻¹, *F*(000) = 1688, *T* = 296 K, *R* = 0.0355, 4237 unique observations with *I* > 3σ(*I*). There are two crystallographically independent molecules but they are virtually identical. Each has the ligand, tmtaa, in a flattened saddle conformation, whereby the Cu ion can have nearly planar coordination. The

Cu—N distances range from 1.922 (2) to 1.948 (2) Å with a mean value of 1.930 Å.

Introduction. The coordination chemistry of the title macrocyclic ligand has recently been reviewed (Cotton & Czuchajowska, 1990*a*). It is well established that, because of the small size of the 'hole' together with a tendency to minimize internal non-bonded repulsions, this ligand characteristically adopts a saddle shape. This, in turn, causes the metal ion to sit above the plane of the four N atoms. Only two exceptions to this have been reported, namely [Ru(tmtaa)(PMePh₂)₂] (Cotton & Czuchajowska, 1990*b*) and [Pd(tmtaa)] (Tsutsui, Bobsein, Cash &

* IUPAC name: {6,8,15,17-tetramethyl-7*H*,16*H*-5,9,14,18-tetraazadibenzo[*b*,*d*]cyclotetradecanato(2-)-κ⁴*N,N',N'',N'''*}copper(II).

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