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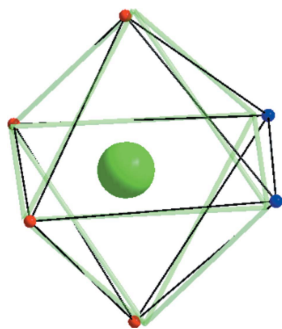
Crystal structure, shape analysis and bioactivity of new Li^{I} , Na^{I} and Mg^{II} complexes with 1,10-phenanthroline and 2-(3,4-dichlorophenyl)acetic acid**Proof instructions**

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Synopsis: Reactions of 1,10-phenanthroline (phen) and 2-(3,4-dichlorophenyl)acetic acid (dcaH) with $M_n(\text{CO}_3)$ ($M = \text{Li}^{\text{I}}$, Na^{I} and Mg^{II} ; $n = 1$ and 2) in MeOH yield the mononuclear lithium complex, the dinuclear sodium complex and the one-dimensional chain magnesium complex. In these complexes, phen binds *via* an N,N' -chelate pocket, while the deprotonated dca^- ligands coordinate either in a monodentate or bidentate fashion.

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Keywords: s-block metals; single-crystal X-ray diffraction; 1,10-phenanthroline; 2-(3,4-dichlorophenyl)acetic acid; bioactivity; crystal structure

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Crystal structure, shape analysis and bioactivity of new Li^I, Na^I and Mg^{II} complexes with 1,10-phenanthroline and 2-(3,4-dichlorophenyl)acetic acid

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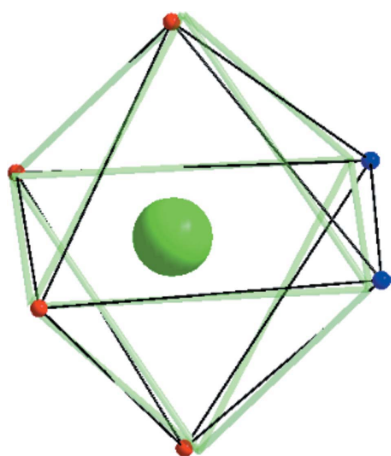
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Reactions of 1,10-phenanthroline (phen) and 2-(3,4-dichlorophenyl)acetic acid (dcaH) with $M_n(\text{CO}_3)$ ($M = \text{Li}^{\text{I}}$, Na^{I} and Mg^{II} ; $n = 1$ and 2) in MeOH yield the mononuclear lithium complex aqua[2-(3,4-dichlorophenyl)acetato- κO](1,10-phenanthroline- $\kappa^2\text{N,N'}$)lithium(I), $[\text{Li}(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_2)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$ or $[\text{Li}(\text{dca})(\text{phen})(\text{H}_2\text{O})]$ (**1**), the dinuclear sodium complex di- μ -aqua-bis[[2-(3,4-dichlorophenyl)acetato- κO](1,10-phenanthroline- $\kappa^2\text{N,N'}$)sodium(I)], $[\text{Na}_2(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$ or $[\text{Na}_2(\text{dca})_2(\text{phen})_2(\text{H}_2\text{O})_2]$ (**2**), and the one-dimensional chain magnesium complex catena-poly[[[diaqua(1,10-phenanthroline- $\kappa^2\text{N,N'}$)magnesium]- μ -2-(3,4-dichlorophenyl)acetato- $\kappa^2\text{O}:\text{O}'$] 2-(3,4-dichlorophenyl)acetate monohydrate], $\{[\text{Mg}(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_2)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2](\text{C}_8\text{H}_5\text{Cl}_2\text{O}_2) \cdot \text{H}_2\text{O}\}_n$ or $\{[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca}) \cdot \text{H}_2\text{O}\}_n$ (**3**). In these complexes, phen binds *via* an N,N' -chelate pocket, while the deprotonated dca^- ligands coordinate either in a monodentate (in **1** and **2**) or bidentate (in **3**) fashion. The remaining coordination sites around the metal ions are occupied by water molecules in all three complexes. Complex **1** crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the asymmetric unit. The Li^+ ion adopts a four-coordinated distorted seesaw geometry comprising an $[\text{N}_2\text{O}_2]$ donor set. Complex **2** crystallizes in the triclinic space group $P\bar{1}$ with half a molecule in the asymmetric unit, in which the Na^+ ion adopts a five-coordinated distorted spherical square-pyramidal geometry, with an $[\text{N}_2\text{O}_3]$ donor set. Complex **3** crystallizes in the orthorhombic space group $P2_12_12_1$, with one Mg^{2+} ion, one phen ligand, two dca^- ligands and three water molecules in the asymmetric unit. Both dcaH ligands are deprotonated, however, one dca^- anion is not coordinated, whereas the second dca^- anion coordinates in a bidentate fashion bridging two Mg^{2+} ions, resulting in a one-dimensional chain structure for **3**. The Mg^{2+} ion adopts a distorted octahedral geometry, with an $[\text{N}_2\text{O}_4]$ donor set. Complexes **1–3** were evaluated against urease and α -glucosidase enzymes for their inhibition potential and were found to be inactive.

1. Introduction

A great deal of work in coordination chemistry has focused on the 'predictable self-assembly' of metal–organic architectures, which involves the design and/or selection of suitable ligands with well-defined coordination sites (Lehn, 2007). In this respect, the 1,10-phenanthroline (phen) ligand has a central position in coordination chemistry due to its predictable and rich coordination chemistry (Li *et al.*, 2018). Phen offers an attractive N,N' -chelate pocket for metal ions in which the two N-donor atoms offer a rigid bidentate coordination environment. In addition to the N-donor sites, the aromaticity involving the σ/π -donor and π^* -acceptor orbitals enhances the



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Table 1

Experimental details.

	1	2	3
Crystal data			
Chemical formula	[Li(C ₈ H ₅ Cl ₂ O ₂)(C ₁₂ H ₈ N ₂)(H ₂ O)]	[Na ₂ (C ₈ H ₅ Cl ₂ O ₂) ₂ (C ₁₂ H ₈ N ₂) ₂ ·(H ₂ O) ₂]	[Mg(C ₈ H ₅ Cl ₂ O ₂)(C ₁₂ H ₈ N ₂)-(H ₂ O) ₂](C ₈ H ₅ Cl ₂ O ₂)·H ₂ O
<i>M_r</i>	409.18	850.46	666.60
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$	Triclinic, <i>P</i> $\bar{1}$	Orthorhombic, <i>P</i> 2 ₁ 2 ₁
Temperature (K)	296	296	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.056 (2), 10.226 (5), 13.451 (5)	6.9518 (10), 10.8369 (16), 13.5077 (17)	8.3889 (4), 11.9459 (6), 29.1630 (15)
α , β , γ (°)	87.21 (2), 86.978 (13), 76.42 (2)	82.823 (6), 83.700 (6), 71.920 (7)	90, 90, 90
<i>V</i> (Å ³)	941.5 (7)	957.1 (2)	2922.5 (3)
<i>Z</i>	2	1	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.37	0.39	0.48
Crystal size (mm)	0.32 × 0.10 × 0.10	0.45 × 0.40 × 0.20	0.45 × 0.21 × 0.10
Data collection			
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2010)	Multi-scan (<i>SADABS</i> ; Bruker, 2010)	Multi-scan (<i>SADABS</i> ; Bruker, 2010)
<i>T_{min}</i> , <i>T_{max}</i>	0.591, 0.745	0.669, 0.745	0.516, 0.745
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	29466, 3827, 3197	29417, 3931, 3119	29717, 5875, 5186
<i>R_{int}</i>	0.033	0.038	0.042
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.625	0.628	0.625
Refinement			
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.044, 0.128, 1.03	0.042, 0.123, 1.03	0.043, 0.095, 1.11
No. of reflections	3827	3931	5875
No. of parameters	259	259	397
No. of restraints	2	2	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.44, -0.44	0.29, -0.44	0.19, -0.30
Absolute structure	–	–	Flack <i>x</i> determined using 1954 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	–	–	-0.02 (2)

Computer programs: *APEX2* (Bruker, 2010), *SAINTE* (Bruker, 2010), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

electronic interaction with the metal centres (Schöne *et al.*, 2018). Phen is often employed with O-donor co-ligands and has produced a range of structural topologies that includes mononuclear (Buttery *et al.*, 2006), polynuclear metal clusters (Ma *et al.*, 2004) and metal-organic frameworks (MOFs) (Platero-Prats *et al.*, 2012). Phen complexes have attracted the continuous interest of coordination chemists, not only due to their predictable chemistry, but also due to their potential applications in the fields of electrochemistry (Happ *et al.*, 2012; Khake *et al.*, 2018) and biology (Viganor *et al.*, 2017). Much of this effort has, however, focused on *d*- and *f*-block elements rather than alkali/alkaline earth metals (*s* block), mainly due to the inherent difficulties arising from these elements, *i.e.* crystallization processes and unpredictable coordination numbers/geometries. These metal salts play a vital role in organic/organometallic transformations, *e.g.* lithium-based reagents are used in over 95% of natural product syntheses (Xavier *et al.*, 2004).

In these current studies, we have investigated the reactions of phen and 2-(3,4-dichlorophenyl)acetic acid (dcaH) with selected *s*-block elements. We chose the combination of these two ligands for two main reasons, based on our interest in their

biological activity. Specifically, phen has predictable coordination chemistry and is a well-known enzyme inhibitor (McCann *et al.*, 2012; Boumans *et al.*, 1997; Sartorius *et al.*, 1988). Conversely, the coordination chemistry of dcaH ligands is less well established with just three complexes containing dcaH reported in the Cambridge Structural Database (CSD, Version of 2018; Groom *et al.*, 2016). Notably, two mononuclear copper complexes (Cui *et al.*, 2011) were found to be urease active, whereas a tetranuclear tin complex (Saeed *et al.*, 2010) showed some antibacterial and antifungal activity. As a continuation of our search for new potential α -glucosidase and urease inhibitors (Avula *et al.*, 2018; Ur Rehman *et al.*, 2018; Alam *et al.*, 2019), we were interested in the bioactivities of alkali/alkaline earth complexes of phen/dcaH.

In this new study, we have investigated the reactions of phen and dcaH with selected *s*-block metals and describe the structures of the mononuclear complex aqua[2-(3,4-dichlorophenyl)acetato- κ O](1,10-phenanthroline- κ^2N,N')lithium(I), [Li(dca)(phen)(H₂O)], **1**, the dinuclear complex di- μ -aqua-bis[[2-(3,4-dichlorophenyl)acetato- κ O](1,10-phenanthroline- κ^2N,N')sodium(I)], [Na₂(dca)₂(phen)₂(H₂O)₂], **2**, and the polymeric chain structure *catena*-poly[[[diaqua(1,10-phen-

anthroline- κ^2N,N' magnesium]- μ -2-(3,4-dichlorophenyl)acetato- $\kappa^2O:O'$] 2-(3,4-dichlorophenyl)acetate monohydrate], $\{[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca})\cdot\text{H}_2\text{O}\}_n$, **3** (Fig. 1). The structures of **1–3** were analysed by single-crystal X-ray diffraction and a detailed description of their crystal structures described along with a *SHAPE* analysis (Version 2.1; Llundell *et al.*, 2013). The bulk compositions were confirmed by elemental analysis, IR spectroscopy and powder X-ray diffraction. *In vitro* urease and α -glucosidase enzyme inhibition studies were performed.

2. Experimental

Commercially available solvents and chemicals were used without further purification. All complexes were prepared under similar reaction conditions and crystals were obtained by slow evaporation from the mother solution.

2.1. Synthesis and crystallization

2.1.1. Preparation of $[\text{Li}(\text{dca})(\text{phen})(\text{H}_2\text{O})]$, **1.** A solution of Li_2CO_3 (0.073 g, 1.0 mmol) and dcaH (0.205 g, 1.0 mmol) in MeOH (15 ml) was refluxed for 1 h, followed by the dropwise addition of a solution of phen (0.198 g, 1.0 mmol) in MeOH (2 ml). The resulting solution was stirred with gentle heating for 1 h. The solution was filtered and the filtrate left undisturbed at room temperature. Colourless crystals suitable for X-ray diffraction analysis formed within a week (yield: 0.308 g, 75%; m.p. 250–253 °C). FT-IR (cm^{-1}): $\nu_{\text{OH}} = 3668\text{--}3050$, $\nu_{\text{C=O}} = 1665$, $\nu_{\text{C=C}} = 1575$ (s), $\nu_{\text{C=N}} = 1514$. Analysis calculated (%) for $\text{C}_{20}\text{H}_{15}\text{Cl}_2\text{LiN}_2\text{O}_3$: C 58.71, H 3.69, N 6.85; found: C 58.36, H 3.55, N 6.83.

2.1.2. Preparation of $[\text{Na}_2(\text{dca})_2(\text{phen})_2(\text{H}_2\text{O})_2]$, **2.** A solution of Na_2CO_3 (0.106 g, 1.0 mmol) and dcaH (0.205 g, 1.0 mmol) in MeOH (15 ml) was refluxed for 1 h, followed by the dropwise addition of a solution of phen (0.198 g, 1.0 mmol) in MeOH (2 ml). The resulting solution was stirred with gentle heating for 1 h. The solution was then filtered and the filtrate left undisturbed at room temperature. Colourless crystals suitable for X-ray diffraction analysis appeared over a period of 10 d (yield: 0.423 g, 50%; m.p. 230 °C). FT-IR (cm^{-1}): $\nu_{\text{OH}} = 3683\text{--}2740$, $\nu_{\text{C=O}} = 1650$ and 1510, $\nu_{\text{C=N}} = 1510$. Analysis calculated (%) for $\text{C}_{40}\text{H}_{30}\text{Cl}_4\text{N}_4\text{Na}_2\text{O}_6$: C 56.49, H 3.56, N 6.59; found: C 56.33, H 3.66, N 6.58.

2.1.3. Preparation of $\{[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca})\cdot\text{H}_2\text{O}\}_n$, **3.** A solution of MgCO_3 (0.843 g, 1.0 mmol) and dcaH (0.410 g, 2.0 mmol) in MeOH (20 ml) was refluxed for 1 h, followed by the dropwise addition of a solution of phen (0.198 g, 1 mmol) in MeOH (2 ml). The resulting solution was stirred with gentle heating for 1 h, and was then filtered and the filtrate left undisturbed at room temperature. Colourless crystals suitable for X-ray diffraction analysis formed over a period of 10 d (yield: 0.412 g, 64%; m.p. 220–224 °C). FT-IR (cm^{-1}): $\nu_{\text{OH}} = 3683\text{--}2740$, $\nu_{\text{C=O}} = 1616$, $\nu_{\text{C=N}} = 1520$. Analysis calculated (%) for $\text{C}_{28}\text{H}_{24}\text{Cl}_4\text{MgN}_2\text{O}_7$: C 50.45, H 3.63, N 4.20; found: C 50.50, H 3.48, N 4.23.

2.2. X-ray crystallography

Crystal data, data collection and structure refinement details for **1–3** are summarized in Table 1. Single crystals were mounted on a MiTeGen loop with grease and examined on a Bruker D8 Venture APEX diffractometer equipped with a

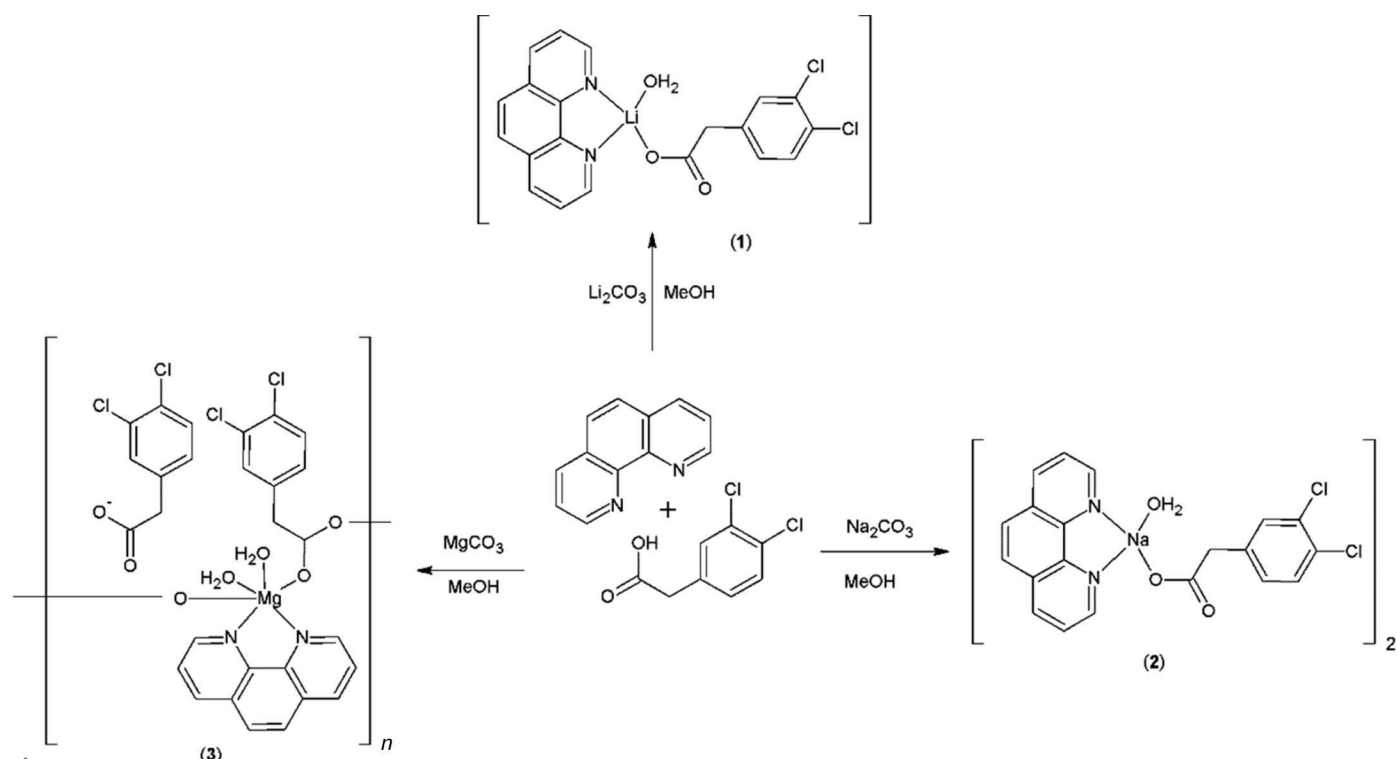


Figure 1

The synthetic routes to $[\text{Li}(\text{dca})(\text{phen})(\text{H}_2\text{O})]$ (**1**), $[\text{Na}_2(\text{dca})_2(\text{phen})_2(\text{H}_2\text{O})_2]$ (**2**) and $\{[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca})\cdot\text{H}_2\text{O}\}_n$ (**3**).

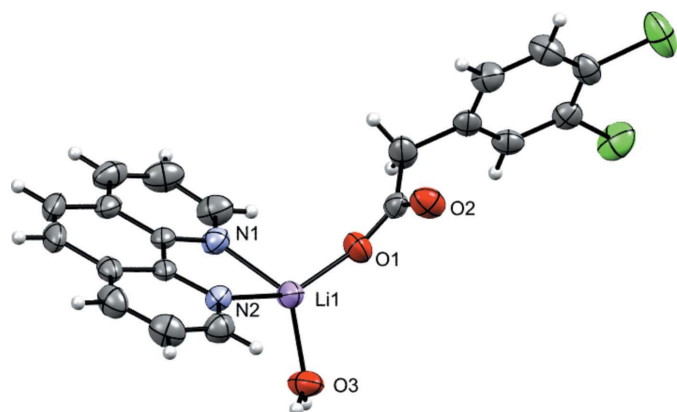


Figure 2
The molecular structure of $[\text{Li}(\text{dca})(\text{phen})(\text{H}_2\text{O})]$ (**1**). Displacement ellipsoids are drawn at the 50% probability level.

Photon 100 CCD area detector at 296 (2) K using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). The phen C atoms in complex **3** have slightly elongated displacement parameters suggesting some slight disorder, but this was insufficient to merit splitting and modelling the atomic positions over two sites. A powder X-ray diffraction (PXRD) scan was performed using a Bruker D8 Discover instrument operated at 40 kV with 2θ ranging from 5 to 40° . [see Note 2]

3. Results and discussion

3.1. Synthesis

Reactions of phen, dcaH and $M_n(\text{CO}_3)$ ($M = \text{Li}^I, \text{Na}^I$ and Mg^{II} ; $n = 1$ and 2) in MeOH afforded the mononuclear Li complex, **1**, the dinuclear Na complex, **2**, and a 1D chain for the Mg complex, **3**. All three complexes were characterized by single-crystal X-ray diffraction, elemental analysis, powder XRD and IR spectroscopy.

3.2. FT-IR

The IR spectra of complexes **1–3** are presented in Fig. S1 of the supporting information, where the broad peaks (2712–

Table 2
Selected geometric parameters (\AA , $^\circ$) for **1**.

Li1–O1	1.918 (4)	N1–C1	1.327 (3)
Li1–O3	1.950 (4)	N1–C12	1.357 (2)
Li1–N1	2.164 (4)	N2–C10	1.324 (3)
Li1–N2	2.132 (4)	N2–C11	1.359 (2)
C13–O1–Li1	140.53 (18)	C10–N2–Li1	128.55 (17)
C1–N1–Li1	129.77 (17)	C11–N2–Li1	113.78 (16)
C12–N1–Li1	112.75 (15)	C1–N1–C12	117.47 (18)

3638 cm^{-1}) are due to the O–H stretching frequency, which is broadened due to hydrogen bonding. The carbonyl peaks fall in the range $1661\text{--}1665 \text{ cm}^{-1}$, in good agreement with literature examples (Deacon, 1980). The peaks in the range $1514\text{--}1520 \text{ cm}^{-1}$ reflect the presence of the heterocyclic phen $\text{C}=\text{N}$ stretching in the complexes (Neykov *et al.*, 2006).

3.3. Description of the crystal structures

3.3.1. $[\text{Li}(\text{dca})(\text{phen})(\text{H}_2\text{O})]$, **1.** The molecular structure of **1** is shown in Fig. 2 and selected interatomic distances and angles are listed in Table 2. The complex crystallizes in the triclinic space group $P\bar{1}$, with one phen ligand, a deprotonated dca[−] anionic ligand, an Li^+ cation and a coordinated water molecule in the asymmetric unit. The Li^+ ion adopts a four-coordinated geometry comprising an $[\text{N}_2\text{O}_2]$ donor set. The bond angles around Li^+ are in the range $78.02(13)\text{--}146.7(2)^\circ$. The phen ligand adopts an N,N' -chelate mode through the N1 and N2 atoms, making a five-membered ring, with Li–N distances of 2.132 (4) and 2.164 (4) \AA . The Li–N bond lengths lie within the normal observed range of 2.06–2.29 \AA for related lithium complexes with phen ligands (Buttery *et al.*, 2006). The Li–O_{water} distance is 1.918 (4) \AA , consistent with hydrated Li^+ complexes reported by others (Buttery *et al.*, 2006). The carboxylate group of the dca[−] anion adopts a monodentate coordination mode [Li–O = 1.950 (4) \AA]. Lithium complexes of phen with carboxylate as co-ligands are rare. A CSD search resulted in only one hit, where the Li^+ coordination geometry is quite similar to that of **1** (Hundal *et al.*, 1991). The uncoordinated dca[−] carboxylate O atom (O2)

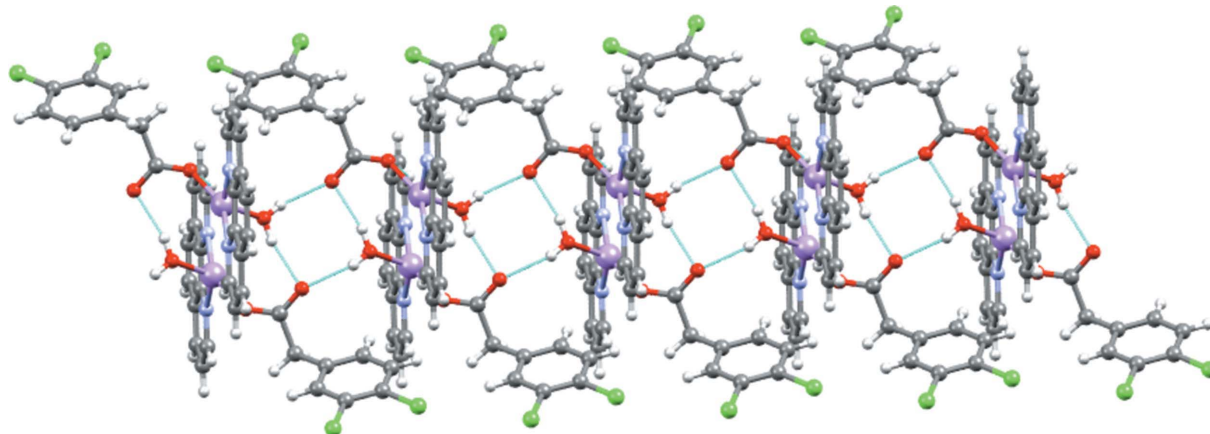


Figure 3
The hydrogen-bonded chain structure in **1**. Hydrogen bonds are shown in blue.

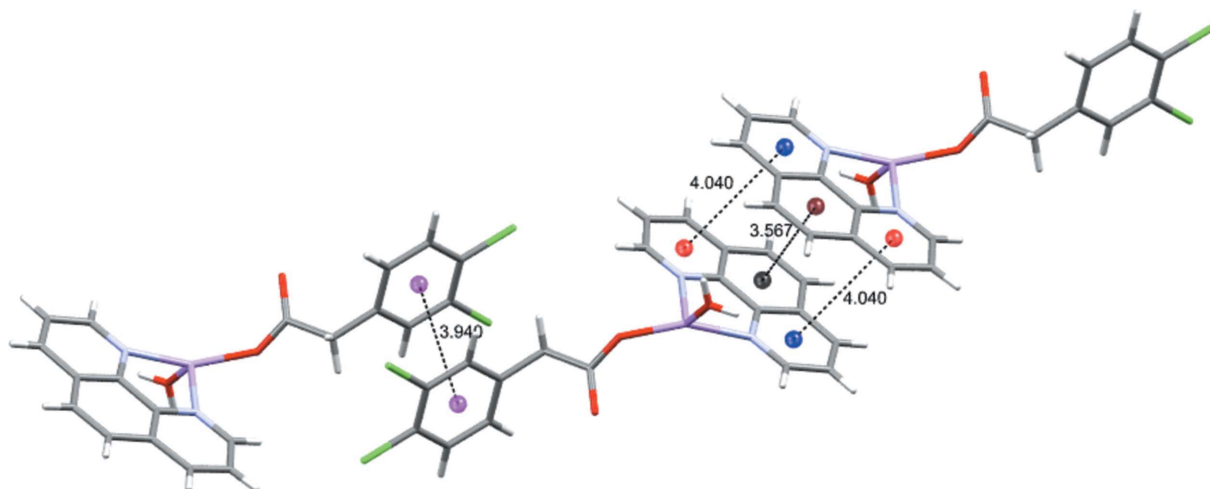


Figure 4
The crystal packing of **1**, highlighting the centroid-centroid ($Cg \cdots Cg$) distances (black dotted lines).

forms hydrogen bonds with two water molecules, each of which is coordinated to neighbouring molecules [$O \cdots O = 2.835$ (4) and 2.841 (2) Å; $O-H \cdots O = 165$ (2) and 168 (2)° [see Note 1]], resulting in a supramolecular hydrogen-bonded chain parallel to the crystallographic a axis, with $Li \cdots O-Li$ and $Li \cdots Li$ separations of 3.108 (4) and 3.734 (7) Å, respectively (Fig. 3 and Fig. S2 in the supporting information). The structure exhibits intermolecular $\pi-\pi$ stacking between phen ligands, with centroid-centroid ($Cg \cdots Cg$) distances of 3.567 and 4.04 Å, while the $Cg \cdots Cg$ distance between dca⁻ rings is 3.940 Å (Fig. 4). The degree of distortion of the $[LiN_2O_2]$ coordination polyhedron with respect to an ideal four-coordinated polyhedron was calculated by the continuous shape measure (CshM) theory utilizing *SHAPE* software (Version 2.1; Llunell *et al.*, 2013), which indicates that the distorted coordination geometry at lithium (Fig. 5) is close to an ideal seesaw (SS-4), with a value for the deviation from standard C_{2v} symmetry of 3.86 (Table S1 in the supporting information). Four-coordinated lithium complexes are not uncommon and distorted geometries have been observed previously (Tacke *et al.*, 2015).

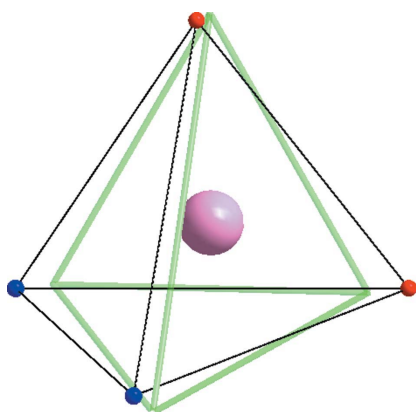


Figure 5
The observed distorted polyhedron (black lines) and the ideal seesaw polyhedron (green lines) in **1**. Colour codes: nitrogen blue, oxygen red and lithium pink. CshM = 3.862 (see Table S1 in the supporting information).

Table 3
Selected geometric parameters (Å, °) for **2**.

Na1—O1	2.3180 (17)	Na1—N2	2.4475 (19)
Na1—O3	2.3834 (17)	Na1—N1	2.4558 (18)
Na1—O3 ⁱ	2.4436 (16)	Na1—Na1 ⁱ	3.5438 (16)
O1—Na1—O3	101.40 (6)	O3 ⁱ —Na1—N1	141.12 (6)
O1—Na1—O3 ⁱ	87.33 (6)	N2—Na1—N1	67.72 (6)
O3—Na1—O3 ⁱ	85.54 (6)	O1—Na1—Na1 ⁱ	95.78 (5)
O1—Na1—N2	157.58 (7)	O3—Na1—Na1 ⁱ	43.43 (4)
O3—Na1—N2	101.02 (6)	O3 ⁱ —Na1—Na1 ⁱ	42.11 (4)
O3 ⁱ —Na1—N2	93.74 (6)	N2—Na1—Na1 ⁱ	99.99 (5)
O1—Na1—N1	97.83 (6)	N1—Na1—Na1 ⁱ	166.14 (6)
O3—Na1—N1	130.20 (6)	Na1—O3—Na1 ⁱ	94.46 (6)

Symmetry code: (i) $-x + 1, -y, -z + 1$.

3.3.2. $[Na_2(dca)_2(phen)_2(H_2O)_2]$, **2.** The molecular structure of **2** is shown in Fig. 6 and selected interatomic distances and angles are listed in Table 3. The complex crystallizes in the triclinic space group $P\bar{1}$ with half a molecule in the asymmetric unit. Two Na^+ cations are charge-balanced by two deproton-

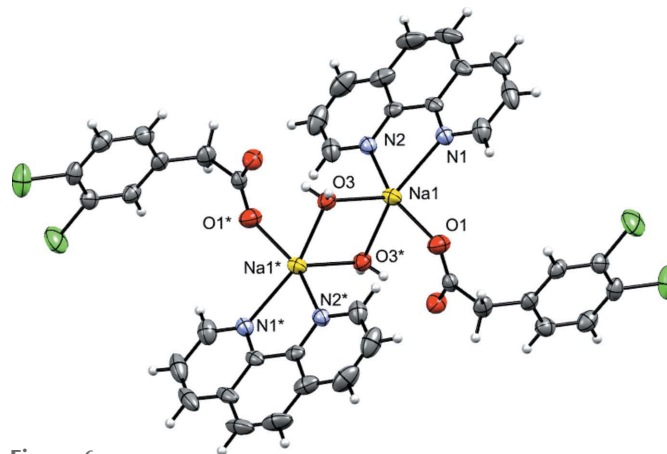


Figure 6
The molecular structure of $[Na_2(dca)_2(phen)_2(H_2O)_2]$ (**2**). Atoms marked with an asterisk (*) are generated by crystallographic inversion centre [symmetry code: (i) $-x + 1, -y, -z + 1$]. Displacement ellipsoids are drawn at the 50% probability level.

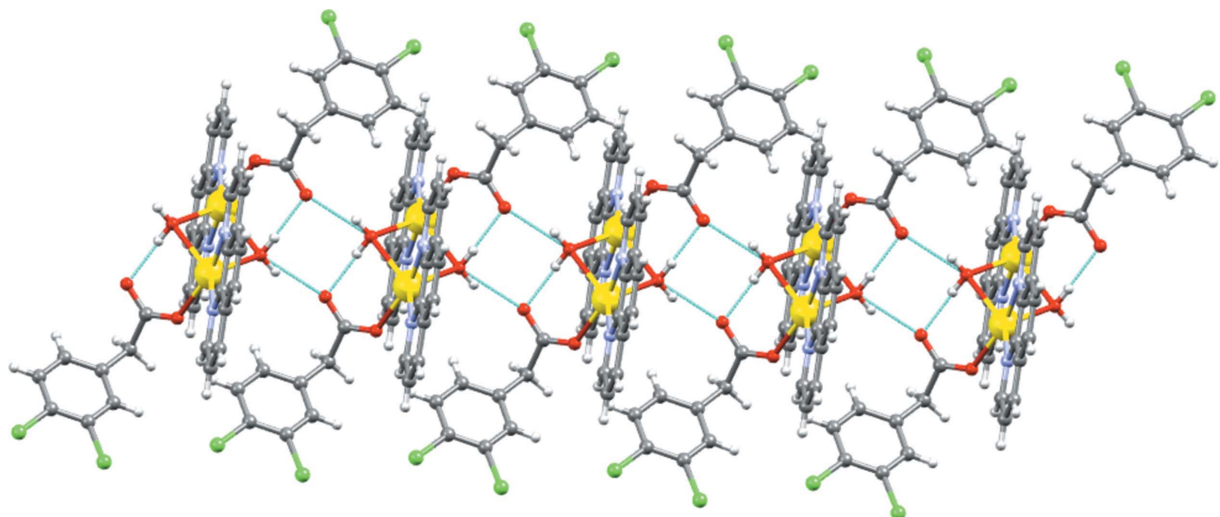


Figure 7
The hydrogen-bonded polymeric arrangement of **2**.

ated dca^- ligands to satisfy the overall charge balance on the complex. Like complex **1**, the dca^- ligands in **2** coordinate only through one of the carboxylate O atoms. Each Na^+ ion is five-coordinated and adopts a distorted spherical square-pyramidal geometry (*vide infra*), with the O3 water atom occupying the axial position. The equatorial sites comprise two chelating phen N (N_{phen}) atoms (N1 and N2), a carboxylate O atom (O1) and the symmetry-related O3ⁱ water molecule [symmetry code: (i) $-x + 1, -y, -z + 1$]. The $Na-N_{phen}$ distances [2.4475 (19) and 2.4558 (18) Å] are consistent with

related pentacoordinated Na complexes (Zhang *et al.*, 2004). The two crystallographically identical Na^+ ions are connected to each other *via* two bridging water ligands [$Na1-O3 = 2.3834 (17)$ Å and $Na1-O3-Na1^i = 94.47 (6)^\circ$], leading to an $Na \cdots Na$ separation of 3.544 (1) Å. The uncoordinated carboxylate O atom forms hydrogen bonds with the water molecule coordinated to the Na^+ ion of a neighbouring complex [$O \cdots O = 2.733 (2)$ and $2.821 (2)$ Å; $O-H \cdots O = 160 (2)$ and $174 (2)^\circ$ [see Note 1]], resulting in a one-dimensional supramolecular chain (Fig. 7). The structure is addi-

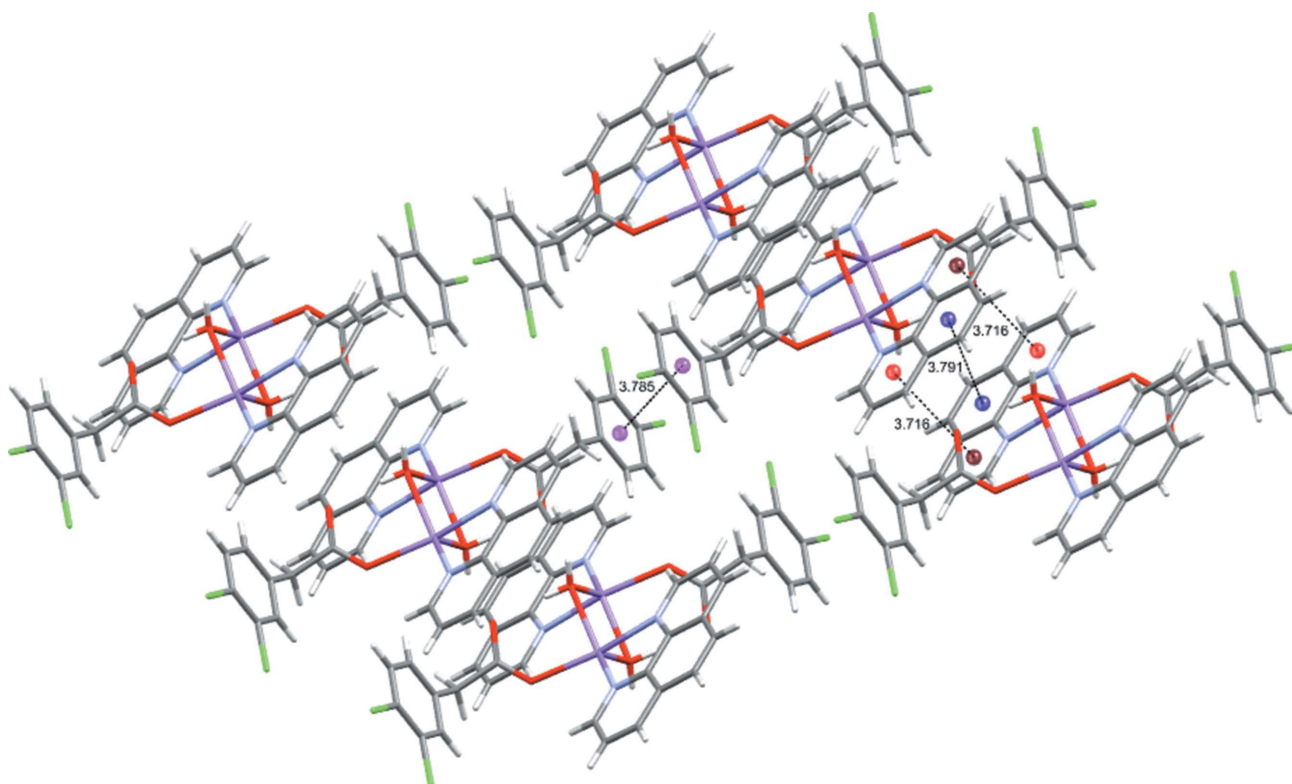
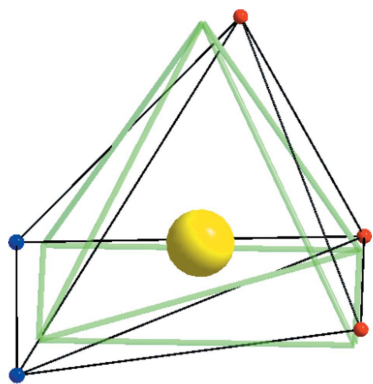


Figure 8
The crystal packing of **2**, highlighting the centroid-centroid ($Cg \cdots Cg$) distances (in Å; black dotted lines) between neighbouring molecules.


Figure 9

The observed polyhedron for **2** (black lines) and the ideal spherical square-pyramidal polyhedron (green lines). Colour codes: nitrogen blue, oxygen red and sodium yellow. CshM = 3.09 (see Table S2 in the supporting information).

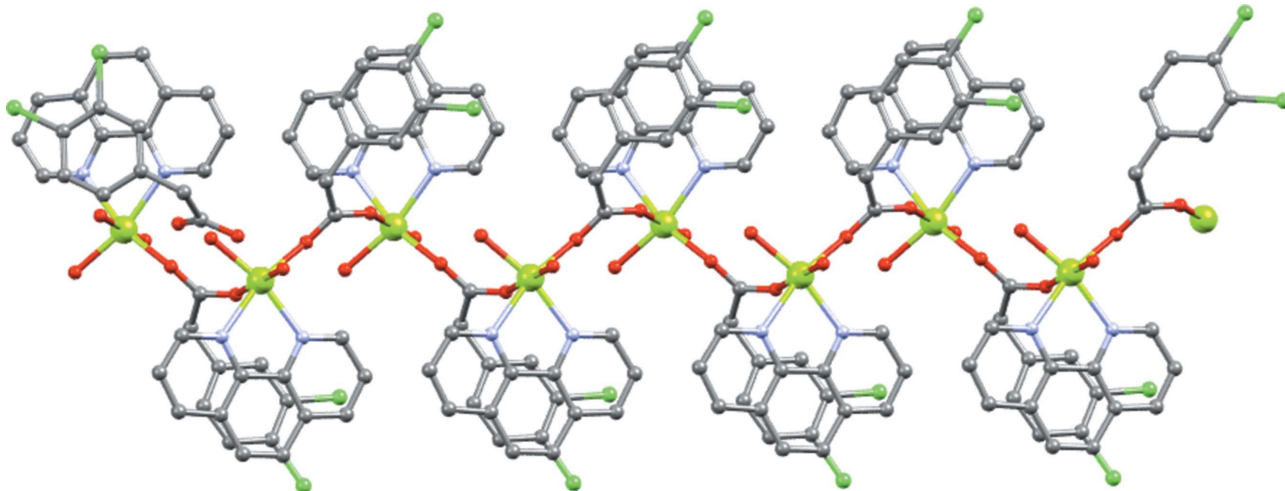
Table 4

Selected geometric parameters (Å, °) for **3**.

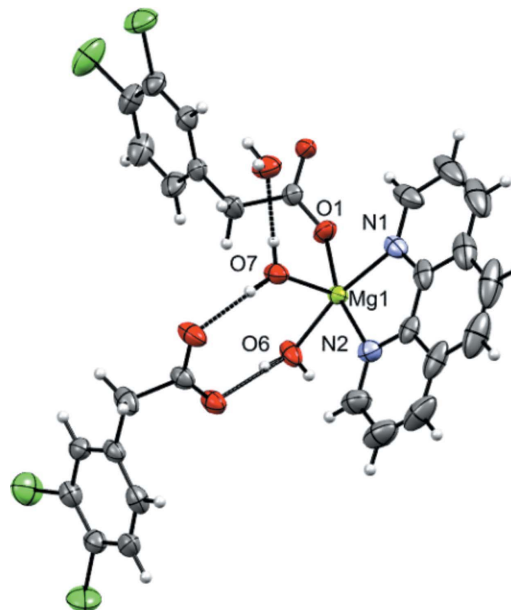
Mg1—O6	2.037 (3)	Mg1—O7	2.054 (3)
Mg1—O1	2.040 (3)	Mg1—N1	2.213 (3)
Mg1—O2 ⁱ	2.044 (3)	Mg1—N2	2.264 (3)
O6—Mg1—O1	102.91 (13)	O2 ⁱ —Mg1—N1	87.92 (11)
O6—Mg1—O2 ⁱ	89.87 (11)	O7—Mg1—N1	91.38 (12)
O1—Mg1—O2 ⁱ	90.07 (12)	O6—Mg1—N2	92.01 (13)
O6—Mg1—O7	89.95 (12)	O1—Mg1—N2	164.72 (13)
O1—Mg1—O7	93.57 (12)	O2 ⁱ —Mg1—N2	86.70 (12)
O2 ⁱ —Mg1—O7	176.30 (13)	O7—Mg1—N2	89.62 (13)
O6—Mg1—N1	166.23 (14)	N1—Mg1—N2	74.29 (12)
O1—Mg1—N1	90.68 (13)		

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

tionally stabilized by intermolecular π - π stacking between dca⁻ rings and between phen rings. The $Cg \cdots Cg$ distances between the peripheral aromatic rings and between the central aromatic rings in phen are 3.716 and 3.791 Å, respectively. The $Cg \cdots Cg$ distance between dca⁻ aromatic rings is


Figure 11

The oxygen-bridged polymer chain in **3**. H atoms, lattice water molecules and dca⁻ ligands have been omitted for clarity.


Figure 10

The asymmetric unit in $[[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca})\cdot\text{H}_2\text{O}]_n$ (**3**). Hydrogen bonds are shown as black dotted lines and displacement ellipsoids are drawn at the 50% probability level.

3.785 Å (Fig. 8). The π - π interactions are shown in Fig. 8 as blue lines between the aromatic rings (*cf.* the interlayer separation in graphite of 3.354 Å; Earnshaw & Greenwood, 1986). The calculation of the degree of distortion of the $[\text{NaN}_2\text{O}_5]$ coordination polyhedron with respect to an idealized five-coordinated polyhedron by CshM theory (*vide supra*) indicated that the arrangement is closest to spherical square pyramidal (SPY-5), with a deviation from ideal C_{4v} symmetry of 3.09 (Fig. 9 and Table S2 in the supporting information).

3.3.3. $[[\text{Mg}(\text{dca})(\text{phen})(\text{H}_2\text{O})_2](\text{dca})\cdot\text{H}_2\text{O}]_n$, **3.** The molecular structure of **3** is shown in Fig. 10 and selected interatomic distances and angles are listed in Table 4. The complex

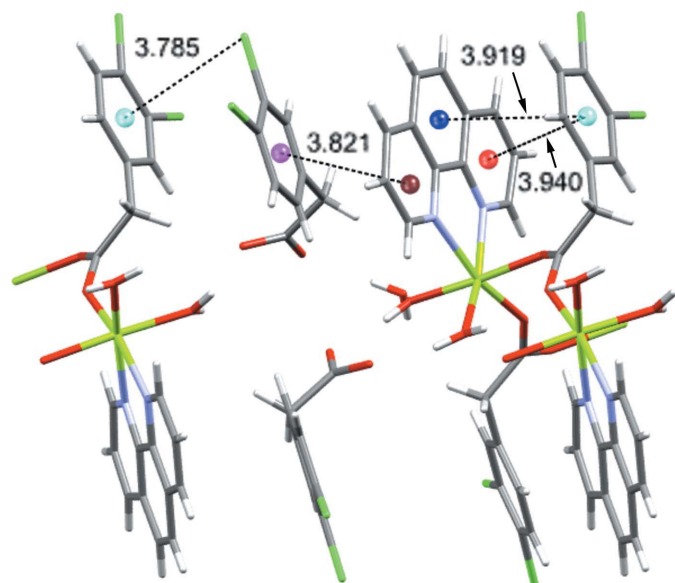


Figure 12
The crystal packing of **3**, highlighting the centroid-centroid ($Cg \cdots Cg$) distances (black dotted lines).

crystallizes in the orthorhombic space group $P2_12_12_1$, with one phen ligand, two dca^- anionic ligands, one Mg^{2+} ion and three water molecules in the asymmetric unit. One of the dca^- anions and a water molecule are uncoordinated. The Mg^{2+} ion adopts a distorted $[N_2O_4]$ octahedral geometry, with one phen ligand acting as an N_2 donor [$Mg-N_{phen} = 2.213$ (3) and 2.264 (3) Å] and one dca^- ligand adopting a 1,3- $O:O'$ -bridging mode [$Mg1-O2 = 2.044$ (3) Å and $Mg1-O1 = 2.040$ (3) Å]. The remaining two coordination sites are occupied by water molecules [$Mg-O6 = 2.037$ (3) Å and $Mg-O7 = 2.054$ (3) Å]. The degree of distortion from ideal octahedral geometry of the Mg^{2+} ion is reflected in the cisoid [range 89.87 (11)– 90.07 (12)°] and transoid angles [range 164.72 (13)– 166.23 (14)°]. The uncoordinated dca^- ligand forms hydrogen

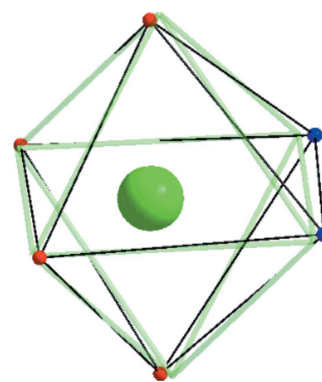


Figure 13
The observed polyhedron for **3** (black lines) and the ideal octahedral polyhedron (green lines). Colour codes: nitrogen blue, oxygen red and magnesium green. CshM = 0.641 (see Table S3 in the supporting information).

bonds with the water coordinated to the Mg^{2+} ion [$O \cdots O = 2.660$ (3) and 2.677 (4) Å; $O-H \cdots O = 169$ (4) and 174 (4)°, respectively [see Note 1]]. The bridging mode of the dca^- ligand results in a one-dimensional chain structure of **3** parallel to the crystallographic a axis (Fig. 11). The uncoordinated dca^- ligands are also connected with each other *via* hydrogen bonding involving the water of crystallization [$O \cdots O = 2.799$ (4) and 2.931 (4) Å; $O-H \cdots O = 167$ (4) and 162 (4)° [see Note 1]] (Fig. S3 in the supporting information). The structure is additionally stabilized by $\pi-\pi$ and $C-Cl \cdots \pi$ interactions (Fig. 12). The calculation of the degree of distortion of the $[MgN_2O_4]$ coordination polyhedron with respect to an idealized six-coordinated polyhedron using the CshM theory indicated that the arrangement is quite close to an ideal octahedron (OC-6), with a small deviation (0.641) from standard O_h symmetry (Fig. 13 and Table S3 in the supporting information).

The experimental powder diffraction patterns of complexes **1–3** (Figs. 14–16) are in good agreement with those calculated

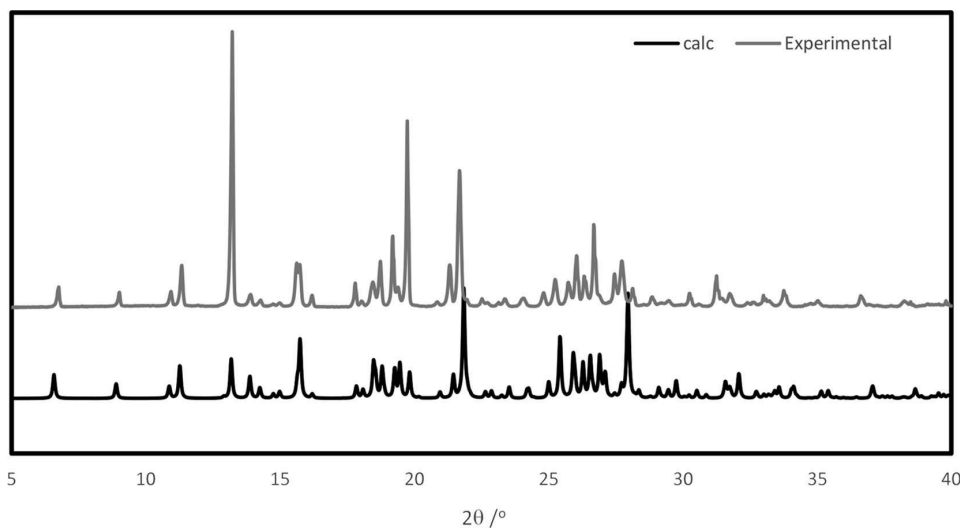


Figure 14
The calculated (bottom) and observed (top) powder X-ray diffraction patterns of **1**.

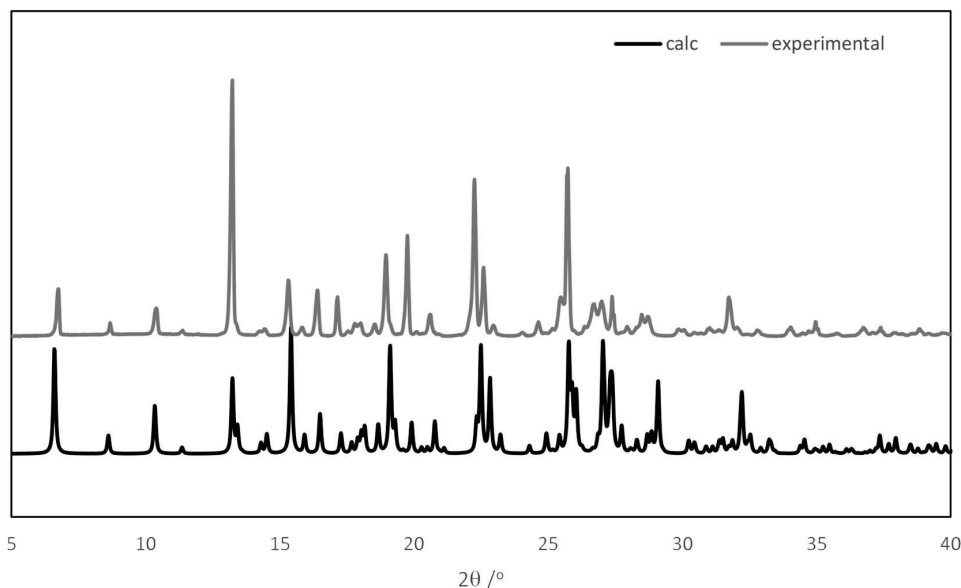


Figure 15
The calculated (bottom) and observed (top) powder X-ray diffraction patterns of **2**.

based on the single-crystal data. Small differences between the intensity profiles may be accounted for by the texture (preferred orientation) of the samples.

3.4. Urease and α -glucosidase enzyme inhibition

Phen is a well-known enzyme inhibitor (McCann *et al.*, 2012; Boumans *et al.*, 1997; Sartorius *et al.*, 1988) and copper–dca[−] complexes (Cui *et al.*, 2011) were found to be urease active, whereas a tin–dca[−] complex (Saeed *et al.*, 2010) showed some antibacterial and antifungal activity (*vide supra*). As an extension of our search for new potential α -glucosidase and urease inhibitors (Avula *et al.*, 2018; Ur Rehman *et al.*, 2018; Arfan *et al.*, 2010), we were interested in comparing the

bioactivities of alkali/alkaline earth complexes of phen/dcaH. Complexes **1–3** were evaluated in *in-vitro* assays against urease and α -glucosidase enzyme for inhibition studies using the literature-reported protocol (Choudhary *et al.*, 2010; Arfan *et al.*, 2010). The complexes were found to be inactive against both urease enzymes, as well as against α -glucosidase.

4. Conclusion

The syntheses and structures of a series of *s*-block complexes containing both 1,10-phenanthroline and 2-(3,4-dichlorophenyl)acetate have been described. In all three complexes, the phen ligand acts as a bidentate ligand, while the acetate

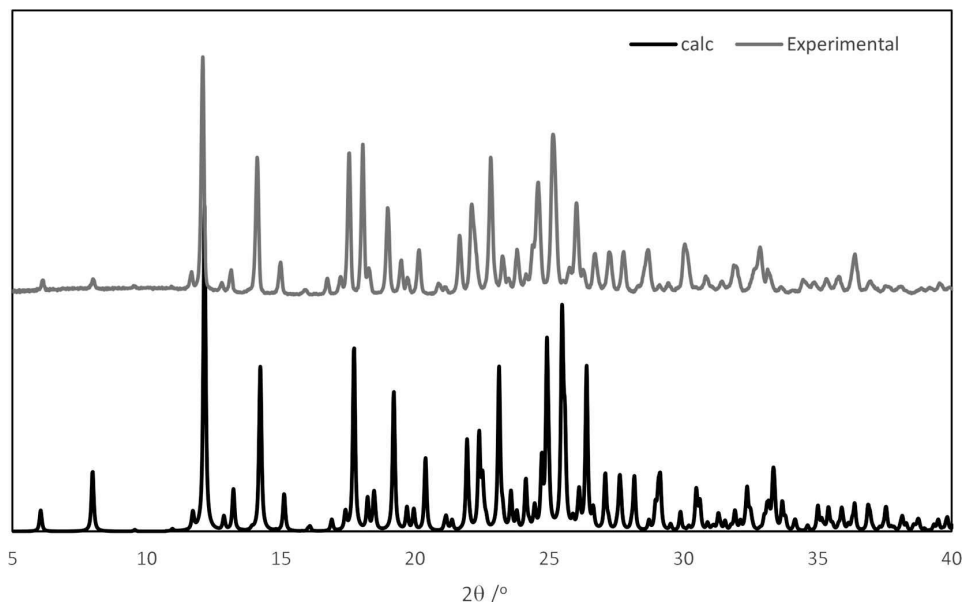


Figure 16
The calculated (bottom) and observed (top) powder X-ray diffraction patterns of **3**.

ligand coordinates in either a monodentate or a 1,3-bridging fashion. Complex **1** is a mononuclear complex in which the Li⁺ ion adopts a four-coordinated distorted seesaw geometry. Complex **2** crystallizes as a dinuclear complex, where both Na⁺ ions adopts a five-coordinated distorted spherical square-pyramidal geometry. Complex **3** is a one-dimensional chain structure where the metal ions adopt distorted octahedral geometries. *In-vitro* studies on complexes **1–3** showed no inhibition against urease and α -glucosidase enzymes. We are currently working on the antibiofilm potential of these compounds against methicillin-resistant *Staphylococcus aureus* and *Klebsiella pneumoniae*, as well as evaluating their mechanism by microscopy.

Acknowledgements

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FROM THE MAIN EDITORS

1. Please give the specifics of the H-bonding with atom names and symmetry operators. It would be best to provide CIF-format hydrogen-bond tables. These can be added to the article and then just referred to from the text. Also, the Li...O—Li interaction should have the specific labels and any symmetry codes given.

2. The treatment of hydrogen atoms should be described here. This should be done, but without using the specifics of SHELX restraints or constraints such as AFIX and DFIX. C-H or O-H distances should be quoted as should the treatment of the H-atom displacement parameters, such a U(H) = 1.2U(eq)(C).

1 supporting information

2 **Crystal structure, shape analysis, and bioactivity of new Li^I, Na^I and Mg^{II}**
3 **complexes with 1,10-phenanthroline and 2-(3,4-dichlorophenyl)acetic acid**4 **Syed Raza Shah, Zarbad Shah, Najeeb Ullah, Javid Hussain, Rashid Al-Harrasi,* Ajmal Khan,**
5 **Jeremy M. Rawson, Ahmed Al-Harrasi and Muhammad U. Anwar***6 **Computing details**7 For all structures, data collection: *APEX2* (Bruker, 2010); cell refinement: *S SAINT* (Bruker, 2010); data reduction: *S SAINT*
8 (Bruker, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure:
9 *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for
10 publication: *SHELXTL* (Sheldrick, 2008).11 **Aqua[2-(3,4-dichlorophenyl)acetato- κ O](1,10-phenanthroline- κ^2 N,N')lithium(I) (AN_Li_b_0m_a)**12 *Crystal data*13 [Li(C₈H₅Cl₂O₂)(C₁₂H₈N₂)(H₂O)] Z = 2
14 $M_r = 409.18$ $F(000) = 420$
15 Triclinic, $P\bar{1}$ $D_x = 1.443 \text{ Mg m}^{-3}$
16 $a = 7.056 (2) \text{ \AA}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
17 $b = 10.226 (5) \text{ \AA}$ Cell parameters from 8992 reflections
18 $c = 13.451 (5) \text{ \AA}$ $\theta = 3.0\text{--}26.4^\circ$
19 $\alpha = 87.21 (2)^\circ$ $\mu = 0.37 \text{ mm}^{-1}$
20 $\beta = 86.978 (13)^\circ$ $T = 296 \text{ K}$
21 $\gamma = 76.42 (2)^\circ$ Prism, colorless
22 $V = 941.5 (7) \text{ \AA}^3$ $0.32 \times 0.10 \times 0.10 \text{ mm}$ 23 *Data collection*24 Bruker APEXII CCD 3827 independent reflections
diffractionmeter 3197 reflections with $I > 2\sigma(I)$
25 φ and ω scans $R_{\text{int}} = 0.033$
26 Absorption correction: multi-scan $\theta_{\text{max}} = 26.4^\circ$, $\theta_{\text{min}} = 3.0^\circ$
(*SADABS*; Bruker, 2010) $h = -8 \rightarrow 8$
27 $T_{\text{min}} = 0.591$, $T_{\text{max}} = 0.745$ $k = -12 \rightarrow 12$
28 29466 measured reflections $l = -16 \rightarrow 16$ 29 *Refinement*30 Refinement on F^2 Hydrogen site location: mixed
31 Least-squares matrix: full H atoms treated by a mixture of independent
32 $R[F^2 > 2\sigma(F^2)] = 0.044$ and constrained refinement
33 $wR(F^2) = 0.128$ $w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.5649P]$
34 $S = 1.03$ where $P = (F_o^2 + 2F_c^2)/3$
35 3827 reflections $(\Delta/\sigma)_{\text{max}} < 0.001$
36 259 parameters $\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
37 2 restraints $\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$

38 *Special details*

39 **Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

40 *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	
42	Cl1	0.42417 (11)	0.83941 (6)	-0.04450 (4)	0.0642 (2)
43	Cl2	-0.00534 (10)	0.80394 (8)	0.00756 (5)	0.0734 (2)
44	O1	0.9135 (2)	0.43625 (15)	0.31886 (11)	0.0480 (4)
45	O2	0.5988 (2)	0.51587 (16)	0.35839 (10)	0.0492 (4)
46	O3	1.2490 (3)	0.47075 (17)	0.45196 (12)	0.0525 (4)
47	H3A	1.277 (4)	0.475 (3)	0.5101 (9)	0.063*
48	H3B	1.336 (3)	0.493 (3)	0.4178 (18)	0.063*
49	N1	1.1877 (2)	0.16122 (16)	0.34819 (12)	0.0385 (4)
50	N2	1.1291 (2)	0.20964 (15)	0.54463 (12)	0.0341 (3)
51	C1	1.2085 (4)	0.1363 (2)	0.25181 (16)	0.0513 (5)
52	H1	1.176828	0.208714	0.206344	0.062*
53	C2	1.2751 (4)	0.0077 (3)	0.21479 (18)	0.0564 (6)
54	H2	1.285669	-0.004676	0.146514	0.068*
55	C3	1.3247 (3)	-0.0996 (2)	0.28053 (18)	0.0507 (6)
56	H3	1.371415	-0.185925	0.257230	0.061*
57	C4	1.3048 (3)	-0.07914 (19)	0.38359 (16)	0.0373 (4)
58	C5	1.3533 (3)	-0.18614 (19)	0.45715 (19)	0.0458 (5)
59	H5	1.401208	-0.273927	0.437027	0.055*
60	C6	1.3308 (3)	-0.1617 (2)	0.55499 (18)	0.0453 (5)
61	H6	1.365118	-0.232790	0.601357	0.054*
62	C7	1.2549 (3)	-0.02819 (19)	0.58897 (15)	0.0351 (4)
63	C8	1.2275 (3)	0.0026 (2)	0.69018 (16)	0.0481 (5)
64	H8	1.259113	-0.065244	0.739262	0.058*
65	C9	1.1543 (3)	0.1327 (3)	0.71580 (16)	0.0518 (5)
66	H9	1.136576	0.154414	0.782526	0.062*
67	C10	1.1061 (3)	0.2335 (2)	0.64093 (16)	0.0442 (5)
68	H10	1.055349	0.321598	0.659800	0.053*
69	C11	1.2042 (2)	0.08038 (17)	0.51855 (13)	0.0285 (4)
70	C12	1.2321 (2)	0.05443 (17)	0.41369 (14)	0.0300 (4)
71	C13	0.7370 (3)	0.46480 (17)	0.29992 (13)	0.0340 (4)
72	C14	0.6895 (3)	0.4312 (2)	0.19580 (15)	0.0472 (5)
73	H14A	0.802539	0.430821	0.151473	0.057*
74	H14B	0.668305	0.340659	0.198980	0.057*
75	C15	0.5147 (3)	0.52449 (19)	0.15057 (13)	0.0360 (4)
76	C16	0.3249 (3)	0.5126 (2)	0.17414 (15)	0.0442 (5)
77	H16	0.304035	0.445914	0.220043	0.053*
78	C17	0.1666 (3)	0.5981 (2)	0.13063 (16)	0.0479 (5)
79	H17	0.040880	0.588283	0.147095	0.058*
80	C18	0.1957 (3)	0.6986 (2)	0.06227 (14)	0.0414 (5)

81	C19	0.3828 (3)	0.71335 (19)	0.03927 (13)	0.0369 (4)
82	C20	0.5416 (3)	0.6266 (2)	0.08266 (14)	0.0382 (4)
83	H20	0.667061	0.636774	0.066162	0.046*
84	Li1	1.0846 (5)	0.3505 (3)	0.4211 (3)	0.0436 (8)

85 *Atomic displacement parameters (Å²)*

86		U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
87	C11	0.0972 (5)	0.0556 (4)	0.0443 (3)	-0.0300 (3)	-0.0044 (3)	0.0129 (3)
88	C12	0.0581 (4)	0.0924 (5)	0.0540 (4)	0.0152 (3)	-0.0162 (3)	0.0057 (3)
89	O1	0.0454 (8)	0.0467 (8)	0.0490 (9)	-0.0027 (6)	-0.0169 (7)	0.0015 (7)
90	O2	0.0505 (9)	0.0629 (10)	0.0339 (7)	-0.0104 (7)	-0.0034 (6)	-0.0113 (7)
91	O3	0.0636 (10)	0.0559 (9)	0.0484 (9)	-0.0328 (8)	-0.0240 (8)	0.0125 (7)
92	N1	0.0474 (9)	0.0325 (8)	0.0382 (9)	-0.0138 (7)	-0.0065 (7)	0.0022 (6)
93	N2	0.0355 (8)	0.0285 (8)	0.0389 (8)	-0.0086 (6)	-0.0027 (6)	-0.0013 (6)
94	C1	0.0676 (15)	0.0554 (13)	0.0367 (11)	-0.0260 (11)	-0.0044 (10)	0.0019 (9)
95	C2	0.0663 (15)	0.0681 (16)	0.0413 (12)	-0.0280 (12)	0.0056 (10)	-0.0142 (11)
96	C3	0.0467 (12)	0.0476 (12)	0.0610 (14)	-0.0155 (10)	0.0082 (10)	-0.0238 (11)
97	C4	0.0298 (9)	0.0307 (9)	0.0535 (12)	-0.0102 (7)	-0.0012 (8)	-0.0081 (8)
98	C5	0.0384 (10)	0.0237 (9)	0.0747 (15)	-0.0046 (8)	-0.0055 (10)	-0.0036 (9)
99	C6	0.0416 (11)	0.0282 (9)	0.0654 (14)	-0.0075 (8)	-0.0118 (10)	0.0131 (9)
100	C7	0.0286 (9)	0.0341 (9)	0.0438 (10)	-0.0106 (7)	-0.0069 (7)	0.0094 (8)
101	C8	0.0490 (12)	0.0528 (13)	0.0426 (11)	-0.0143 (10)	-0.0085 (9)	0.0157 (9)
102	C9	0.0559 (13)	0.0654 (15)	0.0355 (11)	-0.0173 (11)	-0.0002 (9)	-0.0009 (10)
103	C10	0.0454 (11)	0.0424 (11)	0.0446 (11)	-0.0095 (9)	0.0007 (9)	-0.0068 (9)
104	C11	0.0235 (8)	0.0259 (8)	0.0379 (9)	-0.0094 (6)	-0.0038 (7)	0.0023 (7)
105	C12	0.0261 (8)	0.0266 (8)	0.0393 (9)	-0.0097 (6)	-0.0035 (7)	-0.0009 (7)
106	C13	0.0451 (10)	0.0247 (8)	0.0326 (9)	-0.0077 (7)	-0.0101 (8)	0.0017 (7)
107	C14	0.0562 (13)	0.0442 (11)	0.0361 (10)	0.0024 (9)	-0.0129 (9)	-0.0098 (9)
108	C15	0.0448 (10)	0.0375 (10)	0.0259 (8)	-0.0075 (8)	-0.0078 (7)	-0.0074 (7)
109	C16	0.0550 (12)	0.0471 (11)	0.0344 (10)	-0.0203 (10)	-0.0028 (9)	0.0041 (8)
110	C17	0.0419 (11)	0.0651 (14)	0.0390 (11)	-0.0174 (10)	-0.0016 (9)	0.0004 (10)
111	C18	0.0421 (11)	0.0494 (11)	0.0293 (9)	-0.0020 (9)	-0.0079 (8)	-0.0037 (8)
112	C19	0.0512 (11)	0.0382 (10)	0.0225 (8)	-0.0120 (8)	-0.0036 (7)	-0.0020 (7)
113	C20	0.0420 (10)	0.0462 (11)	0.0299 (9)	-0.0156 (8)	-0.0037 (8)	-0.0068 (8)
114	Li1	0.053 (2)	0.0339 (17)	0.0472 (19)	-0.0144 (14)	-0.0205 (15)	0.0085 (14)

115 *Geometric parameters (Å, °)*

116	Li1—O1	1.918 (4)	C6—C7	1.432 (3)
117	Li1—O3	1.950 (4)	C6—H6	0.9300
118	Li1—N1	2.164 (4)	C7—C8	1.405 (3)
119	Li1—N2	2.132 (4)	C7—C11	1.416 (2)
120	N1—C1	1.327 (3)	C8—C9	1.364 (3)
121	N1—C12	1.357 (2)	C8—H8	0.9300
122	N2—C10	1.324 (3)	C9—C10	1.401 (3)
123	N2—C11	1.359 (2)	C9—H9	0.9300
124	C11—C19	1.737 (2)	C10—H10	0.9300

125	C12—C18	1.741 (2)	C11—C12	1.443 (3)
126	O1—C13	1.248 (2)	C13—C14	1.531 (3)
127	O2—C13	1.250 (2)	C14—C15	1.507 (3)
128	O3—H3A	0.822 (10)	C14—H14A	0.9700
129	O3—H3B	0.815 (10)	C14—H14B	0.9700
130	C1—C2	1.395 (3)	C15—C16	1.392 (3)
131	C1—H1	0.9300	C15—C20	1.394 (3)
132	C2—C3	1.367 (4)	C16—C17	1.384 (3)
133	C2—H2	0.9300	C16—H16	0.9300
134	C3—C4	1.407 (3)	C17—C18	1.390 (3)
135	C3—H3	0.9300	C17—H17	0.9300
136	C4—C12	1.413 (3)	C18—C19	1.381 (3)
137	C4—C5	1.431 (3)	C19—C20	1.391 (3)
138	C5—C6	1.346 (3)	C20—H20	0.9300
139	C5—H5	0.9300		
140				
141	C13—O1—Li1	140.53 (18)	N2—C11—C7	123.19 (17)
142	C1—N1—Li1	129.77 (17)	N2—C11—C12	117.59 (15)
143	C12—N1—Li1	112.75 (15)	C7—C11—C12	119.23 (16)
144	C10—N2—Li1	128.55 (17)	N1—C12—C4	122.99 (18)
145	C11—N2—Li1	113.78 (16)	N1—C12—C11	117.75 (16)
146	C1—N1—C12	117.47 (18)	C4—C12—C11	119.26 (16)
147	Li1—O3—H3A	119 (2)	O1—C13—O2	125.84 (18)
148	Li1—O3—H3B	129 (2)	O1—C13—C14	115.85 (18)
149	H3A—O3—H3B	106 (3)	O2—C13—C14	118.30 (18)
150	C10—N2—C11	117.48 (17)	C15—C14—C13	115.93 (16)
151	N1—C1—C2	123.8 (2)	C15—C14—H14A	108.3
152	N1—C1—H1	118.1	C13—C14—H14A	108.3
153	C2—C1—H1	118.1	C15—C14—H14B	108.3
154	C3—C2—C1	118.9 (2)	C13—C14—H14B	108.3
155	C3—C2—H2	120.6	H14A—C14—H14B	107.4
156	C1—C2—H2	120.6	C16—C15—C20	118.15 (18)
157	C2—C3—C4	119.7 (2)	C16—C15—C14	122.23 (19)
158	C2—C3—H3	120.1	C20—C15—C14	119.62 (19)
159	C4—C3—H3	120.1	C17—C16—C15	121.32 (19)
160	C3—C4—C12	117.09 (19)	C17—C16—H16	119.3
161	C3—C4—C5	123.16 (19)	C15—C16—H16	119.3
162	C12—C4—C5	119.75 (18)	C16—C17—C18	119.9 (2)
163	C6—C5—C4	121.04 (18)	C16—C17—H17	120.0
164	C6—C5—H5	119.5	C18—C17—H17	120.0
165	C4—C5—H5	119.5	C19—C18—C17	119.57 (19)
166	C5—C6—C7	121.15 (18)	C19—C18—C12	121.32 (17)
167	C5—C6—H6	119.4	C17—C18—C12	119.12 (17)
168	C7—C6—H6	119.4	C18—C19—C20	120.31 (18)
169	C8—C7—C11	117.05 (18)	C18—C19—C11	120.77 (16)
170	C8—C7—C6	123.39 (18)	C20—C19—C11	118.92 (16)
171	C11—C7—C6	119.55 (18)	C19—C20—C15	120.74 (18)
172	C9—C8—C7	119.44 (19)	C19—C20—H20	119.6

173	C9—C8—H8	120.3	C15—C20—H20	119.6
174	C7—C8—H8	120.3	O1—Li1—O3	108.37 (17)
175	C8—C9—C10	119.6 (2)	O1—Li1—N2	146.7 (2)
176	C8—C9—H9	120.2	O3—Li1—N2	101.65 (16)
177	C10—C9—H9	120.2	O1—Li1—N1	95.98 (16)
178	N2—C10—C9	123.3 (2)	O3—Li1—N1	124.7 (2)
179	N2—C10—H10	118.4	N2—Li1—N1	78.02 (13)
180	C9—C10—H10	118.4		

181 **Di- μ -aqua-bis[2-(3,4-dichlorophenyl)acetato- κ O](1,10-phenanthroline- κ^2 N,N')sodium(I)] (An_Na_b_0m_a)**

182 *Crystal data*

183	[Na ₂ (C ₈ H ₅ Cl ₂ O ₂) ₂ (C ₁₂ H ₈ N ₂) ₂ (H ₂ O) ₂]	$Z = 1$
184	$M_r = 850.46$	$F(000) = 436$
185	Triclinic, $P\bar{1}$	$D_x = 1.476 \text{ Mg m}^{-3}$
186	$a = 6.9518 (10) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
187	$b = 10.8369 (16) \text{ \AA}$	Cell parameters from 9990 reflections
188	$c = 13.5077 (17) \text{ \AA}$	$\theta = 3.1\text{--}26.4^\circ$
189	$\alpha = 82.823 (6)^\circ$	$\mu = 0.39 \text{ mm}^{-1}$
190	$\beta = 83.700 (6)^\circ$	$T = 296 \text{ K}$
191	$\gamma = 71.920 (7)^\circ$	Plate, colorless
192	$V = 957.1 (2) \text{ \AA}^3$	$0.45 \times 0.40 \times 0.20 \text{ mm}$

193 *Data collection*

194	Bruker APEXII CCD diffractometer	3931 independent reflections
195	φ and ω scans	3119 reflections with $I > 2\sigma(I)$
196	Absorption correction: multi-scan (SADABS; Bruker, 2010)	$R_{\text{int}} = 0.038$
197	$T_{\text{min}} = 0.669$, $T_{\text{max}} = 0.745$	$\theta_{\text{max}} = 26.5^\circ$, $\theta_{\text{min}} = 3.1^\circ$
198	29417 measured reflections	$h = -8 \rightarrow 8$
		$k = -13 \rightarrow 13$
		$l = -16 \rightarrow 16$

199 *Refinement*

200	Refinement on F^2	Hydrogen site location: mixed
201	Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
202	$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.6986P]$
203	$wR(F^2) = 0.123$	where $P = (F_o^2 + 2F_c^2)/3$
204	$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.001$
205	3931 reflections	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
206	259 parameters	$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$
207	2 restraints	

208 *Special details*

209 **Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

210 *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	
211					
212	Cl1	0.73690 (12)	0.33088 (8)	1.02936 (5)	0.0677 (2)
213	Cl2	1.19017 (13)	0.32639 (8)	0.96614 (5)	0.0672 (2)

214	Na1	0.44884 (12)	0.14776 (7)	0.55547 (6)	0.0361 (2)
215	O1	0.6010 (2)	0.05309 (16)	0.70211 (11)	0.0449 (4)
216	O2	0.9153 (2)	-0.03743 (15)	0.64207 (11)	0.0413 (4)
217	O3	0.2655 (2)	0.00151 (14)	0.53343 (11)	0.0346 (3)
218	H3A	0.207 (3)	0.018 (2)	0.4819 (12)	0.041*
219	H3B	0.179 (3)	-0.008 (2)	0.5767 (14)	0.041*
220	N1	0.3257 (3)	0.37406 (16)	0.59860 (12)	0.0330 (4)
221	N2	0.3647 (2)	0.30471 (16)	0.40809 (12)	0.0317 (4)
222	C1	0.3072 (4)	0.4094 (3)	0.69022 (18)	0.0484 (6)
223	H1	0.347749	0.344601	0.742320	0.058*
224	C2	0.2299 (4)	0.5391 (3)	0.7131 (2)	0.0601 (8)
225	H2	0.217555	0.559060	0.778982	0.072*
226	C3	0.1737 (4)	0.6346 (3)	0.6383 (2)	0.0558 (7)
227	H3	0.122959	0.721198	0.652161	0.067*
228	C4	0.1920 (3)	0.60284 (19)	0.53966 (19)	0.0410 (5)
229	C5	0.1372 (4)	0.6986 (2)	0.4573 (3)	0.0569 (7)
230	H5	0.087498	0.786278	0.468486	0.068*
231	C6	0.1561 (4)	0.6648 (2)	0.3641 (3)	0.0592 (8)
232	H6	0.118970	0.729497	0.311598	0.071*
233	C7	0.2322 (3)	0.5311 (2)	0.34337 (18)	0.0436 (5)
234	C8	0.2562 (4)	0.4910 (3)	0.2468 (2)	0.0609 (7)
235	H8	0.219631	0.552553	0.192310	0.073*
236	C9	0.3325 (4)	0.3629 (3)	0.23263 (19)	0.0596 (7)
237	H9	0.349448	0.335885	0.168699	0.071*
238	C10	0.3850 (3)	0.2726 (2)	0.31511 (17)	0.0440 (5)
239	H10	0.437204	0.184806	0.304577	0.053*
240	C11	0.2892 (3)	0.43332 (18)	0.42262 (15)	0.0288 (4)
241	C12	0.2692 (3)	0.46939 (18)	0.52317 (15)	0.0292 (4)
242	C13	0.7807 (3)	-0.00943 (18)	0.71201 (14)	0.0295 (4)
243	C14	0.8441 (4)	-0.0577 (2)	0.81847 (15)	0.0398 (5)
244	H14A	0.727192	-0.065924	0.861954	0.048*
245	H14B	0.944496	-0.142986	0.818607	0.048*
246	C15	0.9319 (3)	0.03660 (19)	0.85735 (13)	0.0325 (4)
247	C16	0.8132 (3)	0.1291 (2)	0.91919 (14)	0.0353 (4)
248	H16	0.679484	0.131581	0.938336	0.042*
249	C17	0.8921 (3)	0.2177 (2)	0.95257 (14)	0.0376 (5)
250	C18	1.0895 (3)	0.2160 (2)	0.92540 (15)	0.0391 (5)
251	C19	1.2095 (3)	0.1249 (2)	0.86338 (16)	0.0429 (5)
252	H19	1.342765	0.123290	0.843997	0.051*
253	C20	1.1304 (3)	0.0360 (2)	0.83028 (15)	0.0399 (5)
254	H20	1.212240	-0.025365	0.789021	0.048*

255 *Atomic displacement parameters (\AA^2)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}	
257	Cl1	0.0699 (5)	0.0735 (5)	0.0584 (4)	-0.0125 (4)	0.0097 (3)	-0.0377 (3)
258	Cl2	0.0903 (5)	0.0815 (5)	0.0521 (4)	-0.0536 (4)	-0.0108 (3)	-0.0127 (3)
259	Na1	0.0412 (5)	0.0245 (4)	0.0401 (4)	-0.0048 (3)	-0.0071 (3)	-0.0033 (3)

260	O1	0.0378 (9)	0.0514 (9)	0.0371 (8)	-0.0009 (7)	-0.0036 (6)	-0.0041 (7)
261	O2	0.0356 (8)	0.0535 (9)	0.0332 (8)	-0.0106 (7)	0.0011 (6)	-0.0084 (7)
262	O3	0.0301 (8)	0.0395 (8)	0.0339 (8)	-0.0093 (6)	-0.0027 (6)	-0.0054 (6)
263	N1	0.0339 (9)	0.0318 (9)	0.0351 (9)	-0.0114 (7)	-0.0005 (7)	-0.0076 (7)
264	N2	0.0304 (8)	0.0299 (8)	0.0365 (9)	-0.0103 (7)	-0.0012 (7)	-0.0074 (7)
265	C1	0.0522 (14)	0.0579 (15)	0.0414 (12)	-0.0238 (12)	0.0024 (10)	-0.0151 (11)
266	C2	0.0543 (15)	0.0766 (19)	0.0635 (17)	-0.0329 (14)	0.0169 (13)	-0.0446 (16)
267	C3	0.0355 (12)	0.0472 (14)	0.092 (2)	-0.0170 (11)	0.0159 (12)	-0.0423 (15)
268	C4	0.0203 (9)	0.0266 (10)	0.0772 (16)	-0.0069 (8)	0.0041 (9)	-0.0161 (10)
269	C5	0.0339 (12)	0.0219 (10)	0.109 (2)	-0.0024 (9)	-0.0054 (13)	-0.0005 (12)
270	C6	0.0442 (14)	0.0334 (12)	0.092 (2)	-0.0087 (11)	-0.0157 (14)	0.0242 (13)
271	C7	0.0305 (11)	0.0420 (12)	0.0558 (14)	-0.0132 (9)	-0.0092 (9)	0.0158 (10)
272	C8	0.0566 (16)	0.082 (2)	0.0448 (14)	-0.0292 (15)	-0.0163 (12)	0.0230 (13)
273	C9	0.0576 (16)	0.098 (2)	0.0334 (12)	-0.0392 (16)	-0.0029 (11)	-0.0061 (13)
274	C10	0.0432 (12)	0.0537 (14)	0.0421 (12)	-0.0219 (11)	0.0023 (10)	-0.0163 (10)
275	C11	0.0200 (9)	0.0265 (9)	0.0396 (10)	-0.0082 (7)	-0.0030 (7)	0.0014 (8)
276	C12	0.0181 (8)	0.0236 (9)	0.0464 (11)	-0.0071 (7)	0.0022 (8)	-0.0069 (8)
277	C13	0.0377 (11)	0.0259 (9)	0.0272 (9)	-0.0122 (8)	-0.0037 (8)	-0.0035 (7)
278	C14	0.0557 (13)	0.0357 (11)	0.0293 (10)	-0.0160 (10)	-0.0103 (9)	0.0040 (8)
279	C15	0.0410 (11)	0.0344 (10)	0.0210 (9)	-0.0096 (9)	-0.0087 (8)	0.0029 (7)
280	C16	0.0339 (10)	0.0447 (12)	0.0263 (9)	-0.0100 (9)	-0.0041 (8)	-0.0023 (8)
281	C17	0.0436 (12)	0.0423 (11)	0.0236 (9)	-0.0068 (9)	-0.0029 (8)	-0.0064 (8)
282	C18	0.0484 (13)	0.0468 (12)	0.0277 (10)	-0.0211 (10)	-0.0100 (9)	-0.0011 (9)
283	C19	0.0357 (11)	0.0573 (14)	0.0350 (11)	-0.0143 (10)	-0.0030 (9)	-0.0012 (10)
284	C20	0.0398 (12)	0.0420 (12)	0.0325 (11)	-0.0040 (9)	-0.0016 (9)	-0.0059 (9)

285 *Geometric parameters (Å, °)*

286	Na1—O1	2.3180 (17)	C5—H5	0.9300
287	Na1—O3	2.3834 (17)	C6—C7	1.432 (4)
288	Na1—O3 ⁱ	2.4436 (16)	C6—H6	0.9300
289	Na1—N2	2.4475 (19)	C7—C8	1.403 (4)
290	Na1—N1	2.4558 (18)	C7—C11	1.406 (3)
291	Na1—Na1 ⁱ	3.5438 (16)	C8—C9	1.353 (4)
292	Cl1—C17	1.730 (2)	C8—H8	0.9300
293	Cl2—C18	1.730 (2)	C9—C10	1.389 (4)
294	O1—C13	1.235 (2)	C9—H9	0.9300
295	O2—C13	1.250 (2)	C10—H10	0.9300
296	O3—H3A	0.816 (10)	C11—C12	1.440 (3)
297	O3—H3B	0.813 (10)	C13—C14	1.531 (3)
298	N1—C1	1.322 (3)	C14—C15	1.511 (3)
299	N1—C12	1.354 (3)	C14—H14A	0.9700
300	N2—C10	1.326 (3)	C14—H14B	0.9700
301	N2—C11	1.359 (2)	C15—C20	1.387 (3)
302	C1—C2	1.401 (4)	C15—C16	1.389 (3)
303	C1—H1	0.9300	C16—C17	1.384 (3)
304	C2—C3	1.349 (4)	C16—H16	0.9300
305	C2—H2	0.9300	C17—C18	1.376 (3)

306	C3—C4	1.400 (4)	C18—C19	1.384 (3)
307	C3—H3	0.9300	C19—C20	1.386 (3)
308	C4—C12	1.415 (3)	C19—H19	0.9300
309	C4—C5	1.421 (4)	C20—H20	0.9300
310	C5—C6	1.336 (4)		
311				
312	O1—Na1—O3	101.40 (6)	C8—C7—C11	117.1 (2)
313	O1—Na1—O3 ⁱ	87.33 (6)	C8—C7—C6	123.5 (2)
314	O3—Na1—O3 ⁱ	85.54 (6)	C11—C7—C6	119.3 (2)
315	O1—Na1—N2	157.58 (7)	C9—C8—C7	120.2 (2)
316	O3—Na1—N2	101.02 (6)	C9—C8—H8	119.9
317	O3 ⁱ —Na1—N2	93.74 (6)	C7—C8—H8	119.9
318	O1—Na1—N1	97.83 (6)	C8—C9—C10	118.9 (2)
319	O3—Na1—N1	130.20 (6)	C8—C9—H9	120.5
320	O3 ⁱ —Na1—N1	141.12 (6)	C10—C9—H9	120.5
321	N2—Na1—N1	67.72 (6)	N2—C10—C9	123.5 (2)
322	O1—Na1—Na1 ⁱ	95.78 (5)	N2—C10—H10	118.2
323	O3—Na1—Na1 ⁱ	43.43 (4)	C9—C10—H10	118.2
324	O3 ⁱ —Na1—Na1 ⁱ	42.11 (4)	N2—C11—C7	122.4 (2)
325	N2—Na1—Na1 ⁱ	99.99 (5)	N2—C11—C12	118.20 (17)
326	N1—Na1—Na1 ⁱ	166.14 (6)	C7—C11—C12	119.39 (18)
327	C13—O1—Na1	128.00 (13)	N1—C12—C4	122.3 (2)
328	Na1—O3—Na1 ⁱ	94.46 (6)	N1—C12—C11	118.66 (16)
329	Na1—O3—H3A	114.5 (17)	C4—C12—C11	118.99 (19)
330	Na1 ⁱ —O3—H3A	87.9 (17)	O1—C13—O2	125.36 (18)
331	Na1—O3—H3B	118.6 (18)	O1—C13—C14	117.57 (18)
332	Na1 ⁱ —O3—H3B	134.0 (18)	O2—C13—C14	117.07 (18)
333	H3A—O3—H3B	104 (2)	C15—C14—C13	110.28 (16)
334	C1—N1—C12	117.66 (19)	C15—C14—H14A	109.6
335	C1—N1—Na1	124.80 (16)	C13—C14—H14A	109.6
336	C12—N1—Na1	117.52 (12)	C15—C14—H14B	109.6
337	C10—N2—C11	117.77 (19)	C13—C14—H14B	109.6
338	C10—N2—Na1	124.38 (15)	H14A—C14—H14B	108.1
339	C11—N2—Na1	117.84 (13)	C20—C15—C16	118.07 (19)
340	N1—C1—C2	123.6 (3)	C20—C15—C14	121.28 (19)
341	N1—C1—H1	118.2	C16—C15—C14	120.62 (19)
342	C2—C1—H1	118.2	C17—C16—C15	120.6 (2)
343	C3—C2—C1	119.0 (2)	C17—C16—H16	119.7
344	C3—C2—H2	120.5	C15—C16—H16	119.7
345	C1—C2—H2	120.5	C18—C17—C16	120.83 (19)
346	C2—C3—C4	119.8 (2)	C18—C17—C11	120.65 (17)
347	C2—C3—H3	120.1	C16—C17—C11	118.52 (17)
348	C4—C3—H3	120.1	C17—C18—C19	119.3 (2)
349	C3—C4—C12	117.6 (2)	C17—C18—C12	121.41 (17)
350	C3—C4—C5	122.6 (2)	C19—C18—C12	119.25 (18)
351	C12—C4—C5	119.8 (2)	C18—C19—C20	119.7 (2)
352	C6—C5—C4	121.1 (2)	C18—C19—H19	120.1
353	C6—C5—H5	119.5	C20—C19—H19	120.1

354	C4—C5—H5	119.5	C19—C20—C15	121.4 (2)
355	C5—C6—C7	121.4 (2)	C19—C20—H20	119.3
356	C5—C6—H6	119.3	C15—C20—H20	119.3
357	C7—C6—H6	119.3		

358 Symmetry code: (i) $-x+1, -y, -z+1$.

359 **catena-Poly[[[diaqua(1,10-phenanthroline- κ^2N,N')magnesium]- μ -2-(3,4-dichlorophenyl)acetato- $\kappa^2O:O'$] 2-(3,4-**
 360 **dichlorophenyl)acetate monohydrate] (ANMGB_0m_a)**

361 *Crystal data*

362 [Mg(C₈H₅Cl₂O₂)(C₁₂H₈N₂)(H₂O)₂]
 (C₈H₅Cl₂O₂)·H₂O

363 $M_r = 666.60$

364 Orthorhombic, $P2_12_12_1$

365 $a = 8.3889$ (4) Å

366 $b = 11.9459$ (6) Å

367 $c = 29.1630$ (15) Å

368 $V = 2922.5$ (3) Å³

369 $Z = 4$

$F(000) = 1368$

$D_x = 1.515$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9986 reflections

$\theta = 3.0$ – 26.4°

$\mu = 0.48$ mm⁻¹

$T = 296$ K

Plate, colorless

$0.45 \times 0.21 \times 0.10$ mm

370 *Data collection*

371 Bruker APEXII CCD
 diffractometer

5875 independent reflections

5186 reflections with $I > 2\sigma(I)$

372 φ and ω scans

$R_{\text{int}} = 0.042$

373 Absorption correction: multi-scan
 (SADABS; Bruker, 2010)

$\theta_{\text{max}} = 26.4^\circ$, $\theta_{\text{min}} = 3.0^\circ$

$h = -10 \rightarrow 10$

374 $T_{\text{min}} = 0.516$, $T_{\text{max}} = 0.745$

$k = -14 \rightarrow 12$

375 29717 measured reflections

$l = -36 \rightarrow 35$

376 *Refinement*

377 Refinement on F^2

H atoms treated by a mixture of independent
 and constrained refinement

378 Least-squares matrix: full

$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 1.6964P]$

379 $R[F^2 > 2\sigma(F^2)] = 0.043$

where $P = (F_o^2 + 2F_c^2)/3$

380 $wR(F^2) = 0.095$

$(\Delta/\sigma)_{\text{max}} = 0.001$

381 $S = 1.11$

$\Delta\rho_{\text{max}} = 0.19$ e Å⁻³

382 5875 reflections

$\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

383 397 parameters

Absolute structure: Flack x determined using

384 6 restraints

1954 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)

385 Hydrogen site location: mixed

Absolute structure parameter: -0.02 (2)

386 *Special details*

387 **Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

388 *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

389		x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
390	Mg1	0.74975 (13)	0.61684 (9)	0.47862 (4)	0.0267 (2)
391	N1	0.9037 (4)	0.6149 (3)	0.41702 (11)	0.0365 (7)

392	O1	0.9217 (3)	0.6992 (2)	0.51478 (9)	0.0385 (6)
393	Cl1	1.54405 (14)	0.55375 (12)	0.66319 (5)	0.0633 (3)
394	C1	1.0494 (5)	0.6545 (4)	0.41426 (18)	0.0530 (12)
395	H1	1.099013	0.679111	0.440952	0.064*
396	C2	1.1337 (7)	0.6614 (5)	0.3727 (2)	0.0780 (19)
397	H2	1.236266	0.690840	0.371965	0.094*
398	N2	0.6022 (4)	0.5362 (3)	0.42262 (11)	0.0369 (7)
399	O2	1.1607 (3)	0.7335 (2)	0.54372 (9)	0.0357 (6)
400	Cl2	1.4063 (2)	0.67185 (14)	0.75186 (5)	0.0790 (5)
401	Cl3	0.15576 (17)	0.37562 (13)	0.73575 (4)	0.0663 (4)
402	O3	0.6602 (4)	0.3036 (2)	0.54131 (11)	0.0493 (7)
403	C3	1.0631 (8)	0.6243 (5)	0.3337 (2)	0.082 (2)
404	H3	1.117209	0.629134	0.305907	0.099*
405	Cl4	-0.16156 (14)	0.37371 (13)	0.67738 (5)	0.0699 (4)
406	O4	0.4435 (3)	0.4096 (2)	0.55004 (10)	0.0419 (6)
407	C4	0.9097 (7)	0.5789 (4)	0.33488 (16)	0.0610 (14)
408	C5	0.8254 (11)	0.5346 (5)	0.29550 (17)	0.084 (2)
409	H5	0.875538	0.534589	0.267065	0.101*
410	O5	1.1543 (4)	0.4146 (3)	0.49366 (11)	0.0479 (7)
411	H5A	1.171 (6)	0.351 (2)	0.4841 (16)	0.057*
412	H5B	1.222 (5)	0.418 (4)	0.5141 (12)	0.057*
413	C6	0.6766 (11)	0.4933 (5)	0.29891 (18)	0.080 (2)
414	H6	0.626427	0.465292	0.272900	0.096*
415	O6	0.5677 (3)	0.6048 (2)	0.52461 (10)	0.0398 (6)
416	H6A	0.534 (5)	0.547 (2)	0.5358 (14)	0.048*
417	H6B	0.499 (4)	0.652 (3)	0.5197 (15)	0.048*
418	C7	0.5954 (7)	0.4920 (4)	0.34131 (15)	0.0577 (14)
419	O7	0.8298 (3)	0.4614 (2)	0.49807 (10)	0.0392 (6)
420	H7A	0.9266 (18)	0.452 (4)	0.4979 (15)	0.047*
421	H7B	0.780 (5)	0.416 (3)	0.5129 (13)	0.047*
422	C8	0.4402 (8)	0.4523 (4)	0.3470 (2)	0.0694 (16)
423	H8	0.384505	0.424534	0.321840	0.083*
424	C9	0.3702 (7)	0.4541 (4)	0.3887 (2)	0.0673 (15)
425	H9	0.267073	0.427043	0.392538	0.081*
426	C10	0.4546 (5)	0.4969 (4)	0.42594 (17)	0.0522 (11)
427	H10	0.405179	0.497982	0.454485	0.063*
428	C11	0.6733 (5)	0.5346 (3)	0.38090 (13)	0.0367 (9)
429	C12	0.8325 (6)	0.5775 (3)	0.37770 (13)	0.0402 (9)
430	C13	1.0286 (4)	0.6864 (3)	0.54477 (12)	0.0290 (7)
431	C14	0.9945 (5)	0.6065 (4)	0.58447 (13)	0.0408 (9)
432	H14A	0.883664	0.614531	0.593312	0.049*
433	H14B	1.009482	0.530295	0.573815	0.049*
434	C15	1.0973 (4)	0.6245 (3)	0.62627 (12)	0.0336 (8)
435	C16	1.0394 (5)	0.6754 (4)	0.66536 (14)	0.0457 (10)
436	H16	0.934188	0.699894	0.666065	0.055*
437	C17	1.1349 (6)	0.6905 (4)	0.70345 (14)	0.0538 (12)
438	H17	1.093717	0.725093	0.729441	0.065*
439	C18	1.2902 (5)	0.6546 (4)	0.70310 (14)	0.0465 (11)

440	C19	1.3500 (5)	0.6034 (3)	0.66423 (14)	0.0404 (9)
441	C20	1.2544 (5)	0.5880 (3)	0.62600 (13)	0.0351 (8)
442	H20	1.295637	0.553031	0.600080	0.042*
443	C21	0.5252 (5)	0.3253 (3)	0.55813 (13)	0.0352 (8)
444	C22	0.4613 (5)	0.2369 (3)	0.59174 (16)	0.0479 (11)
445	H22A	0.448975	0.166578	0.575469	0.057*
446	H22B	0.539763	0.225382	0.615715	0.057*
447	C24	0.0211 (5)	0.2985 (4)	0.60812 (14)	0.0434 (10)
448	H24	-0.072029	0.297885	0.590816	0.052*
449	C23	0.0185 (5)	0.3335 (3)	0.65342 (14)	0.0386 (9)
450	C26	0.3042 (4)	0.2669 (3)	0.61370 (14)	0.0351 (9)
451	C27	0.1555 (5)	0.3334 (3)	0.67863 (13)	0.0386 (9)
452	C28	0.2987 (5)	0.3005 (3)	0.65896 (14)	0.0379 (9)
453	H28	0.391555	0.301079	0.676383	0.045*
454	C25	0.1641 (6)	0.2645 (3)	0.58899 (13)	0.0423 (9)
455	H25	0.165698	0.239476	0.558795	0.051*

456 *Atomic displacement parameters (\AA^2)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}	
458	Mg1	0.0224 (5)	0.0244 (6)	0.0333 (6)	-0.0004 (5)	0.0015 (5)	0.0023 (5)
459	N1	0.0324 (16)	0.0279 (16)	0.0491 (19)	0.0050 (14)	0.0122 (14)	0.0064 (14)
460	O1	0.0354 (14)	0.0318 (14)	0.0483 (15)	-0.0068 (11)	-0.0164 (12)	0.0089 (12)
461	Cl1	0.0390 (6)	0.0676 (8)	0.0833 (9)	0.0155 (6)	-0.0107 (6)	0.0032 (6)
462	C1	0.035 (2)	0.040 (2)	0.084 (3)	0.0020 (19)	0.021 (2)	0.006 (2)
463	C2	0.053 (3)	0.062 (3)	0.119 (5)	0.014 (3)	0.049 (4)	0.029 (3)
464	N2	0.0324 (17)	0.0345 (17)	0.0437 (18)	0.0013 (14)	-0.0041 (14)	0.0000 (14)
465	O2	0.0279 (13)	0.0329 (13)	0.0463 (14)	-0.0072 (12)	-0.0067 (12)	0.0130 (11)
466	Cl2	0.0955 (11)	0.0839 (10)	0.0576 (7)	0.0175 (8)	-0.0370 (7)	-0.0105 (7)
467	Cl3	0.0697 (8)	0.0861 (9)	0.0433 (6)	-0.0050 (8)	0.0050 (6)	-0.0119 (6)
468	O3	0.0368 (16)	0.0370 (15)	0.074 (2)	-0.0009 (14)	0.0198 (15)	0.0066 (14)
469	C3	0.090 (4)	0.080 (4)	0.077 (4)	0.031 (4)	0.052 (4)	0.029 (3)
470	Cl4	0.0393 (6)	0.0871 (9)	0.0832 (9)	0.0180 (7)	0.0161 (6)	0.0076 (7)
471	O4	0.0367 (15)	0.0297 (14)	0.0592 (17)	-0.0010 (12)	0.0094 (13)	0.0089 (12)
472	C4	0.085 (4)	0.050 (3)	0.049 (3)	0.030 (3)	0.027 (3)	0.013 (2)
473	C5	0.148 (7)	0.074 (4)	0.031 (2)	0.056 (5)	0.015 (4)	0.004 (2)
474	O5	0.0343 (16)	0.0431 (16)	0.066 (2)	0.0036 (14)	-0.0050 (14)	0.0015 (15)
475	C6	0.136 (6)	0.062 (4)	0.041 (3)	0.041 (4)	-0.017 (4)	-0.008 (2)
476	O6	0.0416 (16)	0.0282 (14)	0.0496 (16)	0.0068 (12)	0.0166 (13)	0.0102 (12)
477	C7	0.093 (4)	0.035 (2)	0.045 (2)	0.027 (3)	-0.022 (2)	-0.0044 (19)
478	O7	0.0267 (13)	0.0284 (14)	0.0624 (17)	0.0009 (12)	0.0034 (13)	0.0110 (12)
479	C8	0.084 (4)	0.041 (3)	0.082 (4)	0.006 (3)	-0.049 (3)	-0.007 (3)
480	C9	0.057 (3)	0.048 (3)	0.097 (4)	-0.004 (2)	-0.033 (3)	-0.001 (3)
481	C10	0.041 (2)	0.050 (3)	0.066 (3)	-0.004 (2)	-0.009 (2)	0.000 (2)
482	C11	0.049 (2)	0.0243 (18)	0.037 (2)	0.0141 (18)	-0.0069 (18)	0.0015 (15)
483	C12	0.058 (3)	0.0239 (18)	0.039 (2)	0.0165 (19)	0.011 (2)	0.0077 (15)
484	C13	0.0307 (19)	0.0209 (17)	0.0355 (18)	0.0004 (15)	-0.0020 (16)	0.0004 (14)
485	C14	0.040 (2)	0.039 (2)	0.044 (2)	-0.0130 (18)	-0.0047 (17)	0.0107 (18)

486	C15	0.0352 (19)	0.0263 (18)	0.0393 (19)	-0.0034 (17)	-0.0025 (15)	0.0086 (16)
487	C16	0.041 (2)	0.050 (2)	0.045 (2)	0.017 (2)	0.0015 (19)	0.0063 (19)
488	C17	0.068 (3)	0.054 (3)	0.039 (2)	0.020 (2)	0.003 (2)	-0.003 (2)
489	C18	0.058 (3)	0.042 (2)	0.040 (2)	0.008 (2)	-0.0133 (19)	0.0016 (18)
490	C19	0.039 (2)	0.033 (2)	0.050 (2)	0.0084 (18)	-0.0059 (19)	0.0059 (17)
491	C20	0.039 (2)	0.0276 (18)	0.039 (2)	0.0016 (17)	0.0013 (17)	0.0012 (15)
492	C21	0.035 (2)	0.028 (2)	0.042 (2)	-0.0031 (17)	0.0055 (17)	0.0000 (16)
493	C22	0.049 (3)	0.032 (2)	0.063 (3)	0.007 (2)	0.019 (2)	0.012 (2)
494	C24	0.040 (2)	0.042 (2)	0.048 (2)	-0.0087 (19)	-0.0048 (19)	0.0126 (19)
495	C23	0.035 (2)	0.034 (2)	0.047 (2)	0.0030 (17)	0.0057 (17)	0.0075 (17)
496	C26	0.034 (2)	0.0256 (18)	0.046 (2)	-0.0005 (16)	0.0087 (17)	0.0077 (16)
497	C27	0.043 (2)	0.036 (2)	0.0369 (19)	-0.0023 (18)	0.0060 (18)	0.0029 (16)
498	C28	0.032 (2)	0.035 (2)	0.046 (2)	0.0009 (16)	-0.0006 (17)	0.0082 (17)
499	C25	0.052 (2)	0.038 (2)	0.036 (2)	-0.008 (2)	0.008 (2)	0.0029 (17)

500 *Geometric parameters (Å, °)*

501	Mg1—O6	2.037 (3)	C7—C11	1.421 (6)
502	Mg1—O1	2.040 (3)	O7—H7A	0.820 (14)
503	Mg1—O2 ⁱ	2.044 (3)	O7—H7B	0.815 (14)
504	Mg1—O7	2.054 (3)	C8—C9	1.352 (8)
505	Mg1—N1	2.213 (3)	C8—H8	0.9300
506	Mg1—N2	2.264 (3)	C9—C10	1.394 (7)
507	N1—C1	1.313 (5)	C9—H9	0.9300
508	N1—C12	1.368 (5)	C10—H10	0.9300
509	O1—C13	1.262 (4)	C11—C12	1.434 (6)
510	C11—C19	1.732 (4)	C13—C14	1.528 (5)
511	C1—C2	1.405 (7)	C14—C15	1.509 (5)
512	C1—H1	0.9300	C14—H14A	0.9700
513	C2—C3	1.358 (9)	C14—H14B	0.9700
514	C2—H2	0.9300	C15—C16	1.380 (6)
515	N2—C10	1.328 (6)	C15—C20	1.389 (5)
516	N2—C11	1.355 (5)	C16—C17	1.382 (6)
517	O2—C13	1.243 (4)	C16—H16	0.9300
518	C12—C18	1.736 (4)	C17—C18	1.371 (7)
519	C13—C27	1.741 (4)	C17—H17	0.9300
520	O3—C21	1.261 (5)	C18—C19	1.383 (6)
521	C3—C4	1.397 (9)	C19—C20	1.386 (5)
522	C3—H3	0.9300	C20—H20	0.9300
523	C14—C23	1.732 (4)	C21—C22	1.537 (5)
524	O4—C21	1.241 (5)	C22—C26	1.509 (6)
525	C4—C12	1.407 (6)	C22—H22A	0.9700
526	C4—C5	1.449 (9)	C22—H22B	0.9700
527	C5—C6	1.345 (10)	C24—C25	1.384 (6)
528	C5—H5	0.9300	C24—C23	1.386 (6)
529	O5—H5A	0.826 (14)	C24—H24	0.9300
530	O5—H5B	0.822 (14)	C23—C27	1.364 (6)
531	C6—C7	1.412 (8)	C26—C25	1.379 (6)

532	C6—H6	0.9300	C26—C28	1.380 (6)
533	O6—H6A	0.817 (14)	C27—C28	1.388 (6)
534	O6—H6B	0.817 (13)	C28—H28	0.9300
535	C7—C8	1.395 (8)	C25—H25	0.9300
536				
537	O6—Mg1—O1	102.91 (13)	N2—C11—C7	122.2 (4)
538	O6—Mg1—O2 ⁱ	89.87 (11)	N2—C11—C12	117.6 (3)
539	O1—Mg1—O2 ⁱ	90.07 (12)	C7—C11—C12	120.2 (4)
540	O6—Mg1—O7	89.95 (12)	N1—C12—C4	122.6 (5)
541	O1—Mg1—O7	93.57 (12)	N1—C12—C11	118.0 (3)
542	O2 ⁱ —Mg1—O7	176.30 (13)	C4—C12—C11	119.4 (4)
543	O6—Mg1—N1	166.23 (14)	O2—C13—O1	124.2 (3)
544	O1—Mg1—N1	90.68 (13)	O2—C13—C14	117.9 (3)
545	O2 ⁱ —Mg1—N1	87.92 (11)	O1—C13—C14	117.9 (3)
546	O7—Mg1—N1	91.38 (12)	C15—C14—C13	114.6 (3)
547	O6—Mg1—N2	92.01 (13)	C15—C14—H14A	108.6
548	O1—Mg1—N2	164.72 (13)	C13—C14—H14A	108.6
549	O2 ⁱ —Mg1—N2	86.70 (12)	C15—C14—H14B	108.6
550	O7—Mg1—N2	89.62 (13)	C13—C14—H14B	108.6
551	N1—Mg1—N2	74.29 (12)	H14A—C14—H14B	107.6
552	C1—N1—C12	118.2 (4)	C16—C15—C20	118.5 (4)
553	C1—N1—Mg1	126.1 (3)	C16—C15—C14	121.9 (4)
554	C12—N1—Mg1	115.4 (3)	C20—C15—C14	119.5 (4)
555	C13—O1—Mg1	143.3 (2)	C15—C16—C17	121.1 (4)
556	N1—C1—C2	122.8 (5)	C15—C16—H16	119.4
557	N1—C1—H1	118.6	C17—C16—H16	119.4
558	C2—C1—H1	118.6	C18—C17—C16	120.3 (4)
559	C3—C2—C1	119.0 (5)	C18—C17—H17	119.9
560	C3—C2—H2	120.5	C16—C17—H17	119.9
561	C1—C2—H2	120.5	C17—C18—C19	119.3 (4)
562	C10—N2—C11	118.1 (4)	C17—C18—C12	119.3 (3)
563	C10—N2—Mg1	127.4 (3)	C19—C18—C12	121.3 (3)
564	C11—N2—Mg1	114.4 (3)	C18—C19—C20	120.5 (4)
565	C13—O2—Mg1 ⁱⁱ	136.9 (2)	C18—C19—C11	120.5 (3)
566	C2—C3—C4	120.5 (5)	C20—C19—C11	119.0 (3)
567	C2—C3—H3	119.8	C19—C20—C15	120.2 (4)
568	C4—C3—H3	119.8	C19—C20—H20	119.9
569	C3—C4—C12	116.8 (5)	C15—C20—H20	119.9
570	C3—C4—C5	124.8 (6)	O4—C21—O3	126.1 (4)
571	C12—C4—C5	118.3 (6)	O4—C21—C22	119.1 (3)
572	C6—C5—C4	121.9 (5)	O3—C21—C22	114.8 (3)
573	C6—C5—H5	119.1	C26—C22—C21	114.3 (3)
574	C4—C5—H5	119.1	C26—C22—H22A	108.7
575	H5A—O5—H5B	100 (5)	C21—C22—H22A	108.7
576	C5—C6—C7	121.1 (6)	C26—C22—H22B	108.7
577	C5—C6—H6	119.4	C21—C22—H22B	108.7
578	C7—C6—H6	119.4	H22A—C22—H22B	107.6
579	Mg1—O6—H6A	126 (3)	C25—C24—C23	119.1 (4)

580	Mg1—O6—H6B	112 (3)	C25—C24—H24	120.4
581	H6A—O6—H6B	114 (5)	C23—C24—H24	120.4
582	C8—C7—C6	123.9 (6)	C27—C23—C24	120.0 (4)
583	C8—C7—C11	117.0 (5)	C27—C23—C14	121.2 (3)
584	C6—C7—C11	119.1 (6)	C24—C23—C14	118.8 (3)
585	Mg1—O7—H7A	117 (3)	C25—C26—C28	118.5 (4)
586	Mg1—O7—H7B	126 (3)	C25—C26—C22	121.2 (4)
587	H7A—O7—H7B	115 (5)	C28—C26—C22	120.3 (4)
588	C9—C8—C7	120.4 (5)	C23—C27—C28	120.4 (3)
589	C9—C8—H8	119.8	C23—C27—C13	121.1 (3)
590	C7—C8—H8	119.8	C28—C27—C13	118.4 (3)
591	C8—C9—C10	119.1 (5)	C26—C28—C27	120.4 (4)
592	C8—C9—H9	120.4	C26—C28—H28	119.8
593	C10—C9—H9	120.4	C27—C28—H28	119.8
594	N2—C10—C9	123.2 (5)	C26—C25—C24	121.5 (4)
595	N2—C10—H10	118.4	C26—C25—H25	119.3
596	C9—C10—H10	118.4	C24—C25—H25	119.3

597 Symmetry codes: (i) $x-1/2, -y+3/2, -z+1$; (ii) $x+1/2, -y+3/2, -z+1$.

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