Table 3. *Selected structural data for copper(II) complexes of diaminodiamides*

	$[Cu(NO_3)(bcen)(H_2O)]NO_3.H_2O$	$[Cu(H_2O)(N\text{-Mebcen})](ClO_4)_2$ (*A*)	$[Cu(ClO_4)(N\text{-Mebcen})](ClO_4).H_2O$ (*B*)	$[\{Cu(N\text{-}Me_2bcen)\}_2(ClO_4)](ClO_4)_3$	$[Cu(bcen)(H_2O)(ClO_4)](ClO_4).H_2O$	$[Cu(bchtn)](ClO_4)_2$
Cu–N (Å)	1·983 (7)	2·007 (10)	1·979 (10)	1·977 (6)	2·006 (5)	1·998 (10)
	2·002 (6)	2·005 (9)	1·990 (10)	2·010 (6)	2·009 (4)	2·008 (7)
Equatorial Cu–O (Å)	1·957 (5)	1·938 (8)	1·926 (8)	1·945 (5)	1·972 (4)	1·966 (7)
	1·974 (6)	1·961 (8)	1·949 (8)	1·952 (5)	1·987 (4)	1·970 (7)
Axial Cu–O (Å)	2·548 (9)			2·483 (13)	2·500 (4)	2·448 (11)
	2·399 (9)*	2·312 (20)*	2·673 (20)		2·702 (5)*	2·641 (11)
Chelate angle for 5-membered ring (°)	85·6 (3)	88·6 (4)	88·2 (4)	87·3 (3)	–	–
Chelate angle for 6-membered ring (°)	95·3 (2)	93·4 (4)	92·0 (4)	91·8 (2)	93·3 (2)	93·1 (3)
	95·0 (2)	90·6 (4)	92·6 (4)	92·9 (2)	94·1 (2)	93·1 (4)
					93·6 (2)	93·4 (3)
Coordination geometry about Cu^{II}	Tetragonally distorted octahedral	Distorted square-pyramidal	Distorted square-pyramidal	Distorted square-pyramidal	Tetragonally distorted octahedral	Tetragonally distorted octahedral
Conformation of chelate rings	chair	chair	chair	chair	chair	chair
	gauche	*gauche*	*gauche*	*gauche*	chair	chair
	chair	twist	chair	chair	chair	chair
Coordination number	6	5	5	5 (binuclear)	6	6
Configuration for the two chiral N centres	*SS* or *RR*	*SS* or *RR*	*SS* or *RR*	*SS* or *RR*	*RS*	*RS*
Crystal system	Monoclinic	Triclinic	Triclinic	Orthorhombic	Triclinic	Monoclinic
Reference	Lee, Lu, Liu, Chung & Lee (1984)	Present work	Present work	Lu *et al.* (1987)	Hong *et al.* (1987)	Lee, Hong, Liu, Chung & Lee (1984)

* $Cu–OH_2$ bond distance.

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Structure of Poly-diaqua-bis(μ-4,4′-bi-1,2,4-triazole-N^1,$N^{1'}$)-manganese(II) Dinitrate Dihydrate

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Abstract. $[Mn(C_4H_4N_6)_2(H_2O)_2](NO_3)_2.2H_2O$, $M_r = 523{\cdot}24$, orthorhombic, *Pbca*, $a = 13{\cdot}648\ (2)$, $b = 21{\cdot}312\ (3)$, $c = 13{\cdot}979\ (3)$ Å, $V = 4066$ Å^3, $Z = 8$, $D_m = 1{\cdot}69\ (2)$, $D_x = 1{\cdot}71$ Mg m^{-3}, $\lambda(Cu\ K\alpha) = 1{\cdot}54184$ Å, $\mu = 61{\cdot}5$ mm^{-1}, $F(000) = 2083$, $T = 293$ K, $R = 0{\cdot}063$ for 1583 independent reflections. The Mn atoms are octahedrally surrounded by two *trans* oriented water molecules and four ligand N atoms. Each ligand coordinates through its N1 and N1′ atoms constituting a bridge between adjacent Mn atoms. In this way, two-dimensional arrays of Mn atoms are formed. The layers are connected to each other by means of hydrogen bridges through the water molecules. The nitrate anions are not coordinated and are fixed in the lattice by hydrogen bridging with the water ligands and lattice water.

Introduction. In order to be able to study magnetic interactions between first-row transition-metal ions, magnetochemists need ligands which can create a

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pathway for the magnetic exchange between metal ions. During the last decade one of the ligands used for this purpose is 1,2,4-triazole (Engelfriet, Groeneveld & Nap, 1980, and references cited therein). 4-Alkyl-substituted triazoles have been studied extensively (Vos, Haasnoot, Verschoor, Reedijk & Schaminee, 1985, and references cited therein). 4,4′-Bi-1,2,4-triazole (abbreviated as btr), which has been studied earlier (Haasnoot & Groeneveld, 1979) may be regarded as a 4-substituted triazole with 1,2,4-triazole itself as a substituent. Structures have been solved of a thiocyanate compound, $[Co(NCS)_2(btr)_2].H_2O$ (Vreugdenhil, Gorter, Haasnoot & Reedijk, 1985) and of a trifluoromethanesulfonate compound $[Co(btr)_3](CF_3SO_3)_2$ (Vreugdenhil, 1987). In both compounds btr acts as an N1, N1′ bidentate ligand, in spite of it being potentially tetranucleating.

Experimental. Solution of 2 mmol of $Mn(NO_3)_2.4H_2O$ in 10 ml of ethanol added to solution of 4 mmol of btr in 10 ml of water. Volume reduced to 4 ml. Crystals grown upon standing at room temperature. Single crystal: $0.36 \times 0.42 \times 0.32$ mm. D_m determined by flotation in a mixture of chloroform and 1,2-dibromoethane. Enraf–Nonius CAD-4 diffractometer. Cu $K\alpha$ radiation monochromated with graphite. Setting angles of 24 reflections with θ between 14 and 15° used to calculate the lattice parameters. 8259 reflections measured, $2 < \theta < 70°$, $-16 \le h \le 16$, $0 \le k \le 25$, $-17 \le l \le 0$, intensities of standard reflections $20\bar{4}$, $13\bar{4}$, $43\bar{1}$ varied 9% during the data collection, a polynomial correction according to this variation was applied to all reflections. Absorption correction applied using Monte-Carlo methods (de Graaff, 1973), transmission coefficients 0·17 to 0·30. After merging equivalent reflections ($R_{int} = 0.064$), 4312 independent reflections remained, 1583 considered observed [$I > 2\sigma(I)$]. Scattering factors and corrections for anomalous dispersion from *International Tables for X-ray Crystallography* (1974). Structure solved by Patterson and automatic Fourier techniques, using the program *AUTOFOUR* (Kinneging & de Graaff, 1984). All atoms except H atoms refined anisotropically. Positions of H atoms located from difference Fourier maps, except for H(215), which was calculated. H atoms kept at fixed distances from C atoms. 299 parameters refined on F. Final wR value was 0·069 with $w = (\sigma_F)^{-2}$. $S = 3.64$. Ratio of the maximum least-squares shift to e.s.d. 0·33 for atoms with high thermal motion and 0·02 for other atoms. Maximum and minimum heights in the final difference Fourier map 0·49 and 0·57 e Å^{-3}, respectively, with a statistical height of 0·36 e Å^{-3}. One of the nitrate anions displays high thermal motion, most likely due to disorder, which was not further investigated. All computer programs used were written or modified by the crystallography section in our laboratory. Illustrations were prepared with the aid of a modified version of the computer program *ORTEP* (Johnson, 1965).

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *for* $[Mn(btr)_2(H_2O)_2](H_2O)_2(NO_3)_2$ *with e.s.d.'s in parentheses*

	x	y	z	B_{eq}*(Å^2)
Mn	2236 (1)	3725 (1)	4989 (1)	162 (3)
O1	2167 (6)	4739 (3)	5031 (6)	41 (2)
O2	2444 (5)	2716 (3)	4798 (5)	25 (2)
N111	1554 (7)	3722 (5)	3539 (7)	22 (3)
N112	1977 (7)	3307 (5)	2867 (7)	30 (3)
C113	1471 (9)	3355 (6)	2061 (10)	31 (4)
N114	758 (7)	3782 (5)	2214 (7)	21 (3)
C115	822 (9)	4000 (5)	3135 (8)	20 (3)
N121	−1253 (6)	3884 (4)	660 (7)	19 (3)
N122	−633 (7)	4333 (4)	269 (6)	23 (3)
C123	145 (9)	4345 (5)	800 (8)	21 (3)
N124	47 (7)	3928 (4)	1533 (7)	18 (3)
C125	−833 (8)	3635 (5)	1413 (9)	18 (3)
N211	2919 (7)	3604 (4)	−3547 (6)	22 (3)
N212	2491 (6)	3129 (5)	−2983 (7)	24 (3)
C213	3013 (8)	3105 (5)	−2191 (8)	23 (4)
N214	3764 (6)	3541 (4)	−2233 (7)	17 (3)
C215	3677 (9)	3844 (6)	−3100 (9)	24 (4)
N221	5758 (7)	3686 (5)	−677 (7)	23 (3)
N222	5070 (8)	4099 (5)	−274 (7)	35 (3)
C223	4281 (9)	4097 (7)	−790 (9)	41 (5)
N224	4426 (7)	3677 (5)	−1517 (7)	24 (3)
C225	5352 (8)	3430 (5)	−1419 (9)	19 (3)
N1	4240 (10)	2148 (6)	6221 (10)	43 (5)
O11	4266 (7)	2403 (5)	5393 (7)	58 (4)
O12	3654 (8)	1724 (6)	6333 (9)	79 (5)
O13	4794 (8)	2344 (5)	6871 (8)	63 (4)
N2	356 (2)	548 (1)	323 (2)	96 (10)
O22	424 (1)	556 (1)	295 (2)	214 (13)
O23	3277 (13)	5812 (8)	4027 (14)	138 (9)
O21	2858 (9)	5139 (6)	3149 (9)	73 (5)
O3	977 (6)	1898 (4)	4844 (6)	41 (3)
O4	2151 (11)	5507 (5)	6446 (8)	126 (6)

* $B_{eq} = \frac{8}{3}\pi^2$ trace U.

Discussion. Final atomic coordinates are given in Table 1* and geometric data in Table 2; the atom numbering is shown in Fig. 1. The Mn ions in $[Mn(btr)_2(H_2O)_2](NO_3)_2.2H_2O$ are octahedrally surrounded by four ligand N atoms, which lie in a plane, and two water O atoms, which occupy the axial positions of the octahedron. Mn—O distances (2·16; 2·19 Å) are somewhat shorter than the Mn—N distances (2·23–2·28 Å). Each ligand coordinates through its N1 and N1′ atom, thus bridging between two Mn ions. In this way, two-dimensional almost rectangular arrays of Mn ions are formed [Mn–Mn–Mn angles 88·87 (3) and 91·37 (2)°]. The layers, which are planar due to the space-group symmetry, are parallel to the *ac* plane of the unit cell. The volume between the layers is occupied by the nitrate anions and non-coordinating water molecules. One of the anions has a regular geometry, whereas the other shows large variations in the N—O distances [1·02 (3)–1·38 (1) Å] and the

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and additional geometric data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43953 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic bond distances* (Å) *and angles* (°) *in* $[Mn(btr)_2(H_2O)_2](NO_3)_2.2H_2O$

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

Mn–O1	2·164 (7)	Mn–O2	2·187 (7)
Mn–N111	2·231 (9)	Mn–N221^{ii}	2·236 (9)
Mn–N211^{i}	2·263 (9)	Mn–N121^{iii}	2·278 (9)
N111–N112	1·41 (1)	N211–N212	1·41 (1)
N111–C115	1·29 (1)	N211–C215	1·31 (1)
N112–C113	1·33 (1)	N212–C213	1·32 (1)
C113–N114	1·35 (1)	C213–N214	1·38 (1)
N114–C115	1·37 (1)	N214–C215	1·38 (1)
N114–N124	1·39 (1)	N214–N224	1·38 (1)
N121–N122	1·39 (1)	N221–N222	1·41 (1)
N121–C125	1·31 (1)	N221–C225	1·30 (1)
N122–C123	1·30 (1)	N222–C223	1·30 (1)
C123–N124	1·36 (1)	C223–N224	1·37 (1)
N124–C125	1·36 (1)	N224–C225	1·38 (1)
N1–O11	1·28 (1)	N2–O22	1·02 (3)
N1–O12	1·22 (1)	N2–O23	1·38 (3)
N1–O13	1·25 (1)	N2–O21	1·21 (2)
	Mn–Mn^{iii} (intra)	9·746 (3)	
	Mn–Mn^{iv} (inter)	8·171 (3)	
O1–Mn–O2	172·6 (3)	N211^{ii}–Mn–N221^{iii}	88·8 (4)
O1–Mn–111	90·6 (4)	N211^{ii}–Mn–N121^{iv}	90·3 (3)
O1–Mn–N211^{i}	96·2 (4)	N221^{iii}–Mn–N121^{iv}	173·4 (4)
O1–Mn–N221^{ii}	89·3 (3)	Mn–N111–N112	115·8 (7)
O1–Mn–N121^{iii}	84·4 (3)	Mn–N111–C115	135·9 (8)
O2–Mn–N111	86·5 (3)	N122–N121–Mn^{iii}	119·7 (7)
O2–Mn–N211^{ii}	86·8 (3)	C125–N121–Mn^{iii}	131·0 (8)
O2–Mn–N221^{iii}	97·6 (3)	N212–N211–Mn^{i}	114·7 (7)
O2–Mn–N121^{iv}	88·8 (3)	C215–N211–Mn^{i}	135·3 (9)
N111–Mn–N211^{ii}	173·2 (4)	N222–N221–Mn^{iv}	114·0 (7)
N111–Mn–N221^{iii}	90·8 (3)	C225–N221–Mn^{iv}	138·2 (8)
N111–Mn–N121^{iv}	90·9 (3)		

Hydrogen-bridging system

O1···O4	2·57 (1)	O2···N112	3·05 (1)
O1···O21	2·92 (1)	O2···N212^{i}	3·22 (1)
O1···O23	3·08 (2)	O3···O23^{v}	2·77 (2)
O1···N122^{iii}	3·15 (1)	O3···O11^{vi}	2·79 (1)
O1···N222^{ii}	3·19 (1)	O4···O21^{vii}	2·75 (2)
O2···O3	2·65 (1)	O4···O12^{viii}	2·82 (2)
O2···O11	2·71 (1)		

Torsion angles

Least-squares planes ring11–ring12	85·7 (5)°
Least-squares planes ring21–ring22	87·6 (5)°

Symmetry operations (i) $x, y, z+1$; (ii) $-\frac{1}{2}+x, y, \frac{1}{2}-z$; (iii) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (iv) $-x, 1-y, 1-z$; (v) $\frac{1}{2}-x, -\frac{1}{2}+y, z$; (vi) $-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (vii) $\frac{1}{2}-x, 1-y, \frac{1}{2}-z$; (viii) $\frac{1}{2}-x, \frac{1}{2}+y, z$.

O–N–O angles [99 (3)–142 (4)°]. This nitrate also shows high thermal motion. These features can be ascribed to the unresolved disorder.

The structure is held together by hydrogen bonding between the coordinating water molecules, the non-coordinated N atoms of the ligand, the lattice water molecules and the anions (see Table 2 and Fig. 2). Surprisingly, the N atoms are involved in rather weak hydrogen bonding, O···N 3·05 (1), 3·15 (1), 3·19 (1) and 3·22 (1) Å, whereas the O···O distances vary from 2·57 (1) to 3·08 (2) Å. The number of hydrogen bridges between the coordinated water molecules and nitrate O and btr N atoms (see Table 2) suggests possible disorder in the H atoms on these water molecules. This agrees with the observation that these H atoms could not be located from difference Fourier maps.

The structures of four compounds containing btr have been determined so far, *i.e.* btr itself (Domiano, 1977), $[Co(NCS)_2(btr)_2].H_2O$ (Vreugdenhil, Gorter, Haasnoot & Reedijk, 1985), $[Co(btr)_3](CF_3SO_3)_2$ (Vreugdenhil, 1987) and the compound $[Mn(btr)_2(H_2O)_2](NO_3)_2.2H_2O$ discussed in this paper. Owing to disorder, only partial structure determination was possible for $[Co(btr)_3](CF_3SO_3)_2$. The structure described here closely resembles the structure of $[Co(NCS)_2(btr)_2].H_2O$ (Vreugdenhil, Gorter, Haasnoot & Reedijk, 1985). The main differences concern the anions, which coordinate in the thiocyanate compound, and the H-bonding pattern, which is only very weak in $[Co(NCS)_2(btr)_2].H_2O$. The interatomic distances in the btr ligand are almost equal for both compounds. Thus, the differences between the longest (N1–N2) and the shortest (N2–C3 and N1–C5) endocyclic bonds are almost equal for both

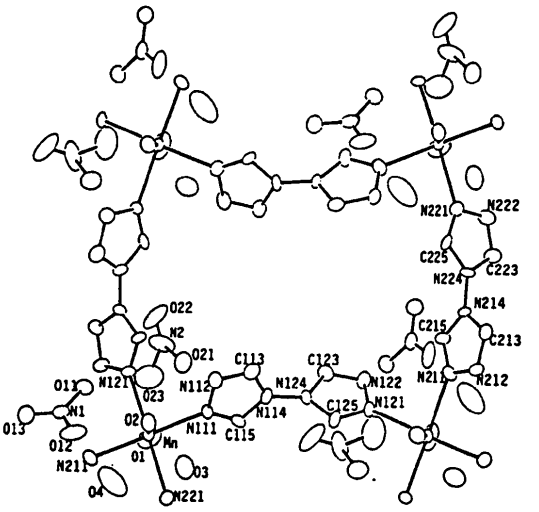

Fig. 1. *ORTEP* drawing of a part of the two-dimensional layer in $[Mn(btr)_2(H_2O)_2](NO_3)_2.2H_2O$, showing the atom labelling as used in Table 1.

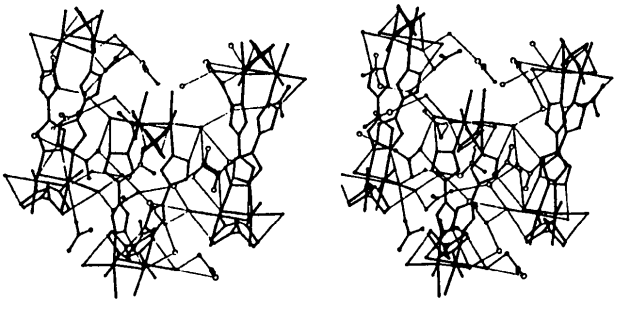

Fig. 2. Stereoscopic *ORTEP* drawing showing the packing and the hydrogen-bond interactions between the layers in $[Mn(btr)_2(H_2O)_2](NO_3)_2.2H_2O$.

compounds. This difference is significantly larger than for coordination compounds with unsubstituted 1,2,4-triazole (Engelfriet, Groeneveld & Nap, 1980, and references cited therein). This indicates a more defined localization of the double-bond character between N1—C5 and N2—C3. The in-plane metal–metal distance is larger in the manganese compound. This effect can be ascribed to the larger ionic radius of Mn. Because of hydrogen bridges between the coordinating water molecules and the non-coordinating N2 of the triazole rings, the *M*—N(1)—N(2) angle is significantly smaller than the *M*—N(1)—C(5) angle. This effect, which has been observed earlier in some pyrazole-containing compounds (Reimann, Mighell & Mauer, 1967; Mighell, Reimann & Santoro, 1969), accounts for an additional lengthening of the metal–metal distance in $[Mn(btr)_2(H_2O)_2].H_2O$. The angle between the least-squares planes through the triazole rings is the same in the free ligand and in the three coordination compounds. The angle of about 90° prohibits any conjugation between the two rings. The absence of conjugation through the N4—N(substituent) or N4—C(substituent) bonds has been observed in other 4-substituted triazoles such as 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole (Key, de Graaff, Haasnoot & Reedijk, 1984) and 3-(2-hydroxyphenyl)-4-phenyl-1,2,4-triazole (van Roosmalen, Vreugdenhil, de Graaff, Haasnoot & Reedijk, 1987).

The anion vibrations in the infrared spectrum [*i.e.* 1760, 1410 (broad), 1050, 830, 730 cm^{-1}] are consistent with the non-coordinating behaviour of the nitrate groups. The ligand vibrations are similar to those of $[Co(NCS)_2(btr)_2].H_2O$, as might be expected because of the similarity between the two compounds. It is not clear why some splittings (at 1012 and 870 cm^{-1}), which were observed in the thiocyanate compound, do not appear.

Although btr is a potentially tetradentate ligand, the synthesis of coordination compounds with btr as a tetranucleating ligand have so far been unsuccessful.

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Tetrakis(2,6-dimethyl-4-pyridinone)zinc(II) Nitrate

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Abstract. $[Zn(C_7H_9NO)_4](NO_3)_2$, $M_r = 682$, orthorhombic, *Pbcn*, $a = 27{\cdot}471$ (20), $b = 9{\cdot}509$ (5), $c = 12{\cdot}666$ (4) Å, $V = 3309$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}37$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}831$ mm^{-1}, $F(000) = 1424$, $T = 291$ K, $R = 0{\cdot}081$ for 1183 observed reflections. The Zn atom lies on a

0108-2701/87/081530-04$01.50