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All enquiries and manuscripts should be directed to:

Dr Alison Green
Australian Journal of Chemistry – an International Journal for Chemical Science
CSIRO PUBLISHING
PO Box 1139 (150 Oxford St)
Collingwood, Vic. 3066, Australia

Telephone: +61 3 9662 7630
Fax: +61 3 9662 7611
E-mail: publishing.ajc@csiro.au

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Supplementary Table 1. Atomic fractional coordinates, atomic displacement parameters and occupancies for *cis*-[Cu(Gly)$_2$]·H$_2$O obtained by refinement using a combined synchrotron X-ray and neutron data set

Estimated standard deviations in the least significant figure are given in parentheses

Atom	*x*	*y*	*z*	*B* (Å^2)	Occupancy
Cu	0.1046(4)	0.3427(8)	0.4007(4)	2.7(1)	1.00
O(1)	0.083(1)	0.574(2)	0.289(1)	3.5(2)	1.00
O(2)	0.122(1)	0.624(2)	0.1314(9)	3.5(2)	1.00
O(3)	0.007(1)	0.546(2)	0.489(1)	3.5(2)	1.00
O(4)	0.935(1)	0.577(2)	0.6431(9)	3.5(2)	1.00
O(5)	0.2971(7)	0.543(1)	0.4492(7)	3.5(2)	0.941(9)
N(1)	0.1798(7)	0.103(1)	0.3032(4)	2.0(1)	1.00
N(2)	0.1210(6)	0.091(1)	0.5185(4)	2.0(1)	1.00
C(1)	0.196(1)	0.244(2)	0.2060(7)	1.7(1)	1.00
C(2)	0.133(1)	0.501(2)	0.2084(8)	1.7(1)	1.00
C(3)	0.064(1)	0.215(2)	0.6072(8)	1.7(1)	1.00
C(4)	0.995(1)	0.472(2)	0.5786(8)	1.7(1)	1.00
H(1)	0.1548(9)	0.131(2)	0.1475(7)	5.8(4)	1.00
H(2)	0.2664(9)	0.257(2)	0.158(1)	5.8(4)	1.00
D(3)	0.1328(7)	0.936(1)	0.2987(4)	4.5(1)	1.00
D(4)	0.2670(7)	0.056(1)	0.3218(4)	4.5(1)	1.00
D(5)	0.3492(7)	0.679(1)	0.4214(7)	4.5(1)	0.941(9)
D(6)	0.3174(7)	0.514(1)	0.5156(7)	4.5(1)	0.941(9)
D(7)	0.0731(7)	0.930(1)	0.4963(4)	4.5(3)	1.00
D(8)	0.2138(7)	0.084(1)	0.5257(4)	4.5(3)	1.00
H(9)	0.002(1)	0.093(2)	0.6318(8)	5.8(4)	1.00
H(10)	0.087(1)	0.265(2)	0.6668(8)	5.8(4)	1.00

Supplementary Table 2. Atomic fractional coordinates and atomic displacement parameters for *trans*-[Cu(Gly)$_2$]·H$_2$O using synchrotron X-ray and neutron diffraction data

Estimated standard deviations in the least significant figure are given in parentheses

Atom	*x*	*y*	*z*	*B* (Å^2)
Cu	0	0	0	2.6(1)
O(1)	0.0325(4)	0.756(1)	0.8515(6)	1.7(1)
O(2)	0.1218(4)	0.694(1)	0.6608(6)	1.7(1)
O(3w)	¼	0.947(2)	½	2.8(1)
N(1)	0.0924(2)	0.2168(7)	0.9078(3)	1.35(9)
C(1)	0.0974(3)	0.820(1)	0.7694(6)	0.87(7)
C(2)	0.1453(2)	0.0671(8)	0.8001(4)	0.87(7)
D(1Na)	0.1324(2)	0.2870(7)	0.9642(3)	3.2(1)
D(1Nb)	0.0639(2)	0.3526(7)	0.8655(3)	3.2(1)
H(2Ca)	0.2093(3)	0.0156(8)	0.8321(4)	3.9(2)
H(2Cb)	0.1631(8)	0.188(2)	0.706(2)	3.9(2)
D(3w)	0.2865(5)	–0.1451(13)	–0.5564(8)	2.6(2)

Supplementary Table 3. Atomic fractional coordinates and atomic displacement parameters for *cis*-[Cu(Gly)$_2$]

Estimated standard deviations in the least significant figure are given in parentheses

Atom	*x*	*y*	*z*	*B* (Å^2)
Cu	0.0997(8)	0.374(2)	0.3933(6)	5.6(3)
O(1)	0.108(3)	0.610(7)	0.280(3)	5.3(5)
O(2)	0.117(3)	0.722(5)	0.143(3)	5.3(5)
O(3)	0.034(3)	0.618(9)	0.477(2)	5.3(5)
O(4)	0.912(2)	0.608(6)	0.635(2)	5.3(5)
N(1)	0.197(3)	0.192(5)	0.291(2)	0.2
N(2)	0.107(2)	0.148(6)	0.508(2)	0.2
C(1)	0.210(4)	0.318(9)	0.188(3)	5(1)
C(2)	0.172(4)	0.56(1)	0.170(4)	5(1)
C(3)	0.011(4)	0.231(8)	0.592(3)	5(1)
C(4)	0.980(5)	0.53(1)	0.549(3)	5(1)
H(1)	0.209(4)	0.172(9)	0.136(3)	1.0
H(2)	0.307(4)	0.372(9)	0.206(3)	1.0
D(3)	0.121(3)	0.073(5)	0.272(2)	1.0
D(4)	0.296(3)	0.141(5)	0.300(2)	1.0
D(7)	0.113(2)	0.987(6)	0.466(2)	1.0
D(8)	0.207(2)	0.170(6)	0.510(2)	1.0
H(9)	0.935(4)	0.098(8)	0.606(3)	1.0
H(10)	0.002(4)	0.160(8)	0.660(3)	1.0

Supplementary Table 4. Atomic fractional coordinates and atomic displacement parameters for anhydrous *trans*-[Cu(Gly)$_2$] using synchrotron diffraction data

Estimated standard deviations in the least significant figure are given in parentheses. Note the proton coordinates are for idealized atoms

Atom	*x*	*y*	*z*	*B* (Å^2)
Cu	0.000	0.000	0.000	6.0(3)
O(1)	–0.081(3)	–0.219(2)	–0.179(2)	2.7(4)
O(2)	–0.248(2)	–0.234(2)	–0.393(2)	2.7(4)
N(1)	–0.190(3)	0.253(3)	–0.108(2)	0.4(5)
C(1)	–0.315(5)	0.161(5)	–0.261(3)	5.7(7)
C(2)	–0.277(4)	–0.110(6)	–0.283(3)	5.7(7)
H(1)	–0.279	0.276	–0.346	—
H(2)	–0.471	0.184	–0.271	—
H(3)	–0.118	0.417	0.123	—
H(4)	–0.285	0.288	–0.049	—

Supplementary Table 5. Selected bond angles for *cis*-[Cu(Gly)$_2$]·H$_2$O

Angle	θ (deg)	Angle	θ (deg)
N(1)–Cu–O(1)	85.8(4)	D(7)–N(2)–D(8)	119.8
N(2)–Cu–O(3)	85.3(5)	Cu–O(1)–C(2)	120.4(6)
N(1)–Cu–N(2)	94.3(3)	Cu–O(3)–C(4)	119(1)
O(1)–Cu–O(3)	94.3(6)	N(1)–C(1)–C(2)	111.3(8)
N(1)–Cu–O(2)^A	90.1(4)	H(1)–C(1)–H(2)	83.0
N(2)–Cu–O(2)^A	86.3(4)	N(2)–C(3)–C(4)	111.5(8)
O(1)–Cu–O(2)^A	91.7(4)	H(9)–C(3)–C(10)	94.4
O(3)–Cu–O(2)^A	113.5(5)	O(1)–C(2)–O(2)	122(1)
O(5)–Cu–O(2)^A	92.7(3)	O(1)–C(2)–C(1)	118(1)
N(1)–Cu–O(5)	95.6(3)	O(2)–C(2)–C(1)	120(1)
N(2)–Cu–O(5)	89.5(3)	O(3)–C(4)–O(4)	127(1)
O(1)–Cu–O(5)	92.5(4)	O(3)–C(4)–C(3)	116(1)
O(3)–Cu–O(5)	93.6(5)	O(4)–C(4)–C(3)	117(1)
Cu–N(1)–C(1)	108.3(5)	Cu–O(2)–C(2)	115.7(9)
D(3)–N(1)–D(4)	106.1	D(5)–O(5)–D(6)	110.4
Cu–N(2)–C(3)	107.9(5)		

^{A} Carbonyl oxygen group from an adjacent molecule.

Supplementary Table 6. Intermolecular and H-bonding contacts for *cis*-[Cu(Gly)$_2$]·H$_2$O

Contact	*d* (Å)	Contact	*d* (Å)	Contact	*d* (Å)
Cu···D(3)	2.544(8)	O(2)···D(8)	2.73(1)	O(4)···D(8)	2.752(9)
Cu···D(4)	2.539(8)	O(3)···O(4)	2.23(2)	O(5)···H(9)	2.57(1)
Cu···D(7)	2.529(7)	O(3)···N(2)	2.70(1)	N(1)···C(2)	2.49(1)
Cu···D(8)	2.460(7)	O(3)···C(3)	2.43(2)	N(1)···H(1)	2.12(1)
O(1)···O(2)	2.19(2)	O(3)···H(1)	2.58(2)	N(1)···H(2)	2.32(1)
O(1)···N(1)	2.67(1)	O(3)···D(5)	2.54(2)	N(2)···H(9)	2.00(1)
O(1)···C(1)	2.39(2)	O(3)···D(7)	2.12(1)	C(1)···D(4)	2.00(1)
O(1)···D(3)	1.97(1)	O(4)···O(5)	2.78(1)	C(2)···H(1)	2.11(1)
O(2)···O(5)	2.75(2)	O(4)···N(1)	3.01(1)	C(2)···H(2)	2.04(1)
O(2)···C(1)	2.36(1)	O(4)···H(9)	2.78(2)	C(3)···D(7)	2.11(1)
O(2)···H(1)	2.60(1)	O(4)···H(10)	2.33(2)	C(3)···D(8)	2.07(1)
O(2)···H(2)	2.49(2)	O(4)···D(4)	2.00(1)	C(4)···H(10)	1.89(1)
O(2)···D(6)	1.83(1)	O(4)···D(5)	1.80(1)	C(4)···D(5)	2.40(1)

Supplementary Table 7. Selected bond angles for *trans*-[Cu(Gly)$_2$]·H$_2$O

Angle	θ (deg)	Angle	θ (deg)
O(1)–Cu–O(2)	88.4(2)	O(1)–C(1)–O(2)	124.1(5)
O(1)–Cu–N(1)	84.4(2)	O(1)–C(1)–C(2)	116.9(5)
D(3w)–O(3)–D(3w)	115(1)	O(2)–C(1)–C(2)	119.0(5)
Cu–O(1)–C(1)	116.3(5)	N(1)–C(2)–C(1)	110.5(3)
Cu–N(1)–C(2)	110.2(3)	H(2Ca)–C(2)–H(2Cb)	101.6(7)
D(1Na)–N(1)–D(1Nb)	106.22(3)		

Supplementary Table 8. Intermolecular and H-bonding contacts for *trans*-[Cu(Gly)$_2$]·H$_2$O

Contact	*d* (Å)	Contact	*d* (Å)	Contact	*d* (Å)
Cu···.D(1Na)	2.482(3)	O(2)···D(1b)	2.768(6)	N(1)···H(2b)	2.17(1)
Cu···.D(1Nb)	2.421(4)	O(2)···D(1O)	1.853(6)	N(1)···C(1)	2.469(6)
O(1)···O(2)	2.238(8)	O(2)···H(2a)	2.728(7)	C(1)···D(1Nb)	2.651(6)
O(1)···N(1)	2.632(6)	O(2)···H(2b)	2.70(1)	C(1)···H(2a)	2.065(7)
O(1)···C(2)	2.367(7)	O(3)···O(2)	2.734(7)	C(1)···H(2b)	2.003(5)
O(1)···D(1Na)	2.960(6)	O(3)···D(1Na)	2.271(7)	C(2)···D(1Na)	1.959(5)
O(1)···D(1Nb)	2.170(7)	O(3)···H(2a)	2.126(5)	C(2)···D(1Nb)	2.003(5)
O(1)···H(2a)	2.948(7)	O(3)···H(2b)	2.17(1)		
O(2)···C(1)	2.404(7)	N(1)···H(2a)	2.126(5)		

Supplementary Table 9. Selected bond angles for *cis*-[Cu(Gly)$_2$]

Angle	θ (deg)	Angle	θ (deg°)
N(1)–Cu–O(1)	76(1)	Cu–O(1)–C(2)	127(2)
N(2)–Cu–O(3)	89(1)	Cu–O(3)–C(4)	112(4)
N(1)–Cu–N(2)	103(1)	N(1)–C(1)–C(2)	124(3)
O(1)–Cu–O(3)	92(2)	H(1)–C(1)–H(2)	111(0)
N(1)–Cu–O(2)^A	99(1)	N(2)–C(3)–C(4)	98(2)
N(2)–Cu–O(2)^A	89(1)	H(9)–C(3)–H(10)	61(0)
O(1)–Cu–O(2)^A	96(2)	O(1)–C(2)–O(2)	87(4)
O(3)–Cu–O(2)^A	92(1)	O(1)–C(2)–C(1)	96(3)
Cu–N(1)–C(1)	116(2)	O(2)–C(2)–C(1)	162(5)
D(3)–N(1)–D(4)	126(0)	O(3)–C(4)–O(4)	139(5)
Cu–N(2)–C(3)	111(2)	O(3)–C(4)–C(3)	124(3)
D(7)–N(2)–D(8)	92(0)	O(4)–C(4)–C(3)	95(3)

^{A} Carbonyl oxygen group from an adjacent molecule.

Supplementary Table 10. Selected intermolecular and H-bonding contacts for *cis*-[Cu(Gly)$_2$]

Contact	*d* (Å)	Contact	*d* (Å)	Contact	*d* (Å)
Cu···D(3)	2.27(3)	O(3)···O(4)	2.42(4)	N(1)···D(8)	2.90(4)
Cu···D(4)	2.64(4)	O(3)···N(2)	2.63(4)	N(1)···H(9)	2.98(5)
Cu···D(7)	2.28(3)	O(3)···C(3)	2.56(6)	N(2)···H(9)	2.18(5)
Cu···D(8)	2.17(8)	O(3)···H(1)	2.88(6)	N(2)···H(10)	2.27(5)
O(1)···O(2)	1.90(5)	O(3)···D(7)	2.13(5)	C(1)···D(3)	1.94(5)
O(1)···N(1)	2.40(3)	O(3)···D(8)	2.98(5)	C(1)···D(4)	1.96(6)
O(1)···C(1)	2.22(5)	C(1)···D(3)	1.94(5)	C(2)···H(1)	2.14(7)
O(1)···H(2)	2.57(4)	O(4)···H(2)	2.97(5)	C(2)···H(2)	1.75(5)
O(1)···D(3)	2.41(6)	O(4)···D(4)	1.96(4)	C(2)···H(8)	2.84(6)
O(2)···C(1)	2.41(4)	O(4)···H(9)	2.64(4)	C(3)···D(7)	2.35(5)
O(2)···H(1)	2.56(6)	O(4)···H(10)	2.57(4)	C(3)···D(8)	2.28(5)
O(2)···H(2)	2.80(4)	N(1)···C(2)	2.53(7)	C(4)···D(4)	2.86(4)
O(2)···D(3)	2.53(4)	N(1)···H(1)	2.05(5)	C(4)···H(9)	2.45(6)
O(2)···D(7)	3.01(5)	N(1)···H(2)	1.85(5)	C(4)···H(10)	2.46(6)
O(2)···D(8)	2.57(4)	N(1)···D(7)	2.70(4)		

Supplementary Table 11. Selected bond angles for *trans*-[Cu(Gly)$_2$]

Angle	θ (deg)	Angle	θ (deg)
O(1)–Cu–O(1)	180	Cu–O(1)–C(2)	108(1)
O(1)–Cu–O(2)	88.9(5)	Cu–N(1)–C(1)	114(1)
O(1)–Cu–O(2)	91.1(5)	D(3)–N(1)–D(4)	112
O(1)–Cu–N(1)	87.5(8)	O(1)–C(2)–O(2)	90(2)
N(1)–Cu–O(2)	83.5(7)	N(1)–C(1)–C(2)	110(2)
N(1)–Cu–O(2)	96.5(7)	H(1)–C(2)–H(2)	109
O(2)–Cu–O(2)	179		

Supplementary Table 12. H-bonding contacts for *trans*-[Cu(Gly)$_2$] from synchrotron X-ray diffraction data

Contact	*d* (Å)	Contact	*d* (Å)
O(1)···O(2)	2.01(3)	N(1)···C(2)	2.45(3)
O(1)···N(1)	2.70(2)	O(1)···O(2)	2.01(3)
O(1)···C(1)	2.53(4)	Cu···C(1)	2.90(3)
O(2)···C(1)	2.51(3)	Cu···C(2)	2.86(3)
O(2)···N(1)	3.10(2)		