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Synthesis, X-ray crystal structure and spectroscopic characterization of a hybrid material based on glycine and *α*-Keggin type polyoxotungstate

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Table 1S. Crystal data and structure refinement for GL2.

Identification code	gl2	
Empirical formula	C6 H28 N3 O51 P W12	
Formula weight	3195.48	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.4816(14) Å	α= 90°.
	b = 19.972(2) Å	β= 102.218(2)°.
	c = 17.933(2) Å	γ = 90°.
Volume	4369.2(8) $Å^3$	
Z	4	
Density (calculated)	4.858 Mg/m^3	
Absorption coefficient	31.622 mm^{-1}	
F(000)	5584	
Crystal size	0.19 x 0.14 x 0.13 mm^3	
Theta range for data collection	1.55 to 30.00°.	
Index ranges	-17<=h<=17, -28<=k<=28, -25<=l<=25	
Reflections collected	56448	
Independent reflections	12722 [R(int) = 0.0689]	
Observed reflections [I>2sigma(I)]	9481	
Completeness to theta = 30.00°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.1399 and 0.0232	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	12722 / 0 / 658
Goodness-of-fit on F^2	0.998
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0790
R indices (all data)	R1 = 0.0599, wR2 = 0.0882
Largest diff. peak and hole	2.825 and -2.606 e.Å^{-3}

Table 2S Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for GL2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
W(1)	1902(1)	2875(1)	3586(1)	16(1)
W(2)	1943(1)	4719(1)	3660(1)	16(1)
W(3)	4383(1)	3761(1)	4599(1)	16(1)
W(4)	1187(1)	2952(1)	1640(1)	15(1)
W(5)	1223(1)	4797(1)	1707(1)	15(1)
W(6)	3525(1)	5617(1)	2665(1)	15(1)
W(7)	5956(1)	4649(1)	3606(1)	15(1)
W(8)	5929(1)	2939(1)	3520(1)	15(1)
W(9)	3450(1)	2060(1)	2504(1)	15(1)
W(10)	2880(1)	3901(1)	543(1)	15(1)
W(11)	5176(1)	4715(1)	1502(1)	15(1)
W(12)	5126(1)	3004(1)	1415(1)	15(1)
P(1)	3554(2)	3835(1)	2571(1)	13(1)
O(1)	1186(6)	2552(3)	4213(4)	17(2)
O(2)	1233(6)	5025(4)	4303(4)	23(2)
O(3)	4490(6)	3719(4)	5554(4)	20(2)
O(4)	23(6)	2672(4)	1044(4)	20(2)
O(5)	68(6)	5128(4)	1151(4)	19(2)
O(6)	3752(6)	6451(4)	2697(4)	19(2)
O(7)	7060(6)	5144(4)	3961(4)	21(2)
O(8)	6973(6)	2396(4)	3822(4)	20(2)
O(9)	3632(6)	1214(4)	2464(4)	17(1)
O(10)	2287(6)	3954(3)	-401(4)	16(1)
O(11)	6023(6)	5245(4)	1147(4)	21(2)
O(12)	5915(6)	2494(4)	1002(4)	21(2)

O(13)	1517(6)	3807(4)	3565(4)	18(1)
O(14)	3249(6)	3130(3)	4219(4)	17(2)
O(15)	2603(6)	2097(4)	3271(4)	19(2)
O(16)	883(6)	2806(4)	2616(4)	19(2)
O(17)	952(6)	4895(3)	2711(4)	18(2)
O(18)	2698(6)	5520(3)	3450(4)	16(1)
O(19)	3264(6)	4412(3)	4282(4)	15(1)
O(20)	5470(6)	4420(4)	4515(4)	18(2)
O(21)	5433(6)	3097(3)	4451(4)	16(1)
O(22)	2063(6)	2161(4)	1777(4)	19(2)
O(23)	2025(6)	3255(3)	928(4)	18(2)
O(24)	877(6)	3875(3)	1746(4)	18(1)
O(25)	2064(6)	4555(4)	972(4)	19(2)
O(26)	2154(6)	5567(3)	1932(4)	17(2)
O(27)	4211(6)	5306(4)	1867(4)	20(2)
O(28)	4760(6)	5249(4)	3338(4)	18(2)
O(29)	5924(6)	4625(4)	2532(4)	19(2)
O(30)	6647(6)	3786(3)	3673(4)	17(1)
O(31)	5890(6)	3017(4)	2456(4)	19(2)
O(32)	4676(6)	2361(4)	3211(4)	18(2)
O(33)	4130(6)	2409(4)	1740(4)	18(2)
O(34)	4012(6)	4561(3)	623(4)	19(2)
O(35)	3983(6)	3237(4)	552(4)	18(2)
O(36)	5741(6)	3863(3)	1292(4)	18(1)
O(37)	2834(6)	3212(3)	2561(4)	15(1)
O(38)	2864(6)	4459(3)	2623(4)	18(2)
O(39)	4537(6)	3809(4)	3264(4)	17(1)
O(40)	3982(6)	3866(3)	1834(4)	16(1)
O(1A)	-475(7)	1442(4)	1788(4)	23(2)
O(2A)	117(6)	1438(4)	3079(5)	23(2)
N(1A)	1774(8)	609(5)	3042(5)	25(2)
C(1A)	168(8)	1252(5)	2441(6)	18(2)
C(2A)	1058(8)	783(6)	2306(6)	22(2)
O(1B)	7878(6)	3255(4)	852(4)	23(2)
O(2B)	8279(7)	4152(4)	1616(4)	25(2)
N(1B)	7483(8)	3943(4)	-435(5)	21(2)
C(1B)	7998(8)	3894(5)	991(6)	17(2)

C(2B)	7753(10)	4334(5)	270(6)	21(2)
O(1C)	8749(7)	794(4)	8095(4)	28(2)
O(2C)	8887(6)	1877(4)	8395(4)	19(2)
N(1C)	9339(8)	1674(5)	9907(5)	25(2)
C(1C)	8922(9)	1320(6)	8576(6)	21(2)
C(2C)	9180(10)	1077(6)	9387(6)	26(2)
O(1W)	8163(6)	2444(4)	2056(4)	21(2)
O(2W)	5345(7)	1400(4)	4468(5)	29(2)
O(3W)	1571(7)	3726(4)	5464(5)	32(2)
O(4W)	7563(6)	3397(4)	5554(4)	23(2)
O(5W)	9346(8)	3253(5)	9454(5)	41(2)

Table 3S Bond lengths [Å] and angles [°] for GL2.

W(1)-O(1)	1.702(7)
W(1)-O(14)	1.889(7)
W(1)-O(13)	1.921(7)
W(1)-O(15)	1.926(7)
W(1)-O(16)	1.930(7)
W(1)-O(37)	2.469(7)
W(2)-O(2)	1.708(7)
W(2)-O(19)	1.887(7)
W(2)-O(13)	1.896(7)
W(2)-O(17)	1.913(7)
W(2)-O(18)	1.933(7)
W(2)-O(38)	2.441(7)
W(3)-O(3)	1.692(7)
W(3)-O(19)	1.905(7)
W(3)-O(14)	1.909(7)
W(3)-O(20)	1.920(7)
W(3)-O(21)	1.921(7)
W(3)-O(39)	2.445(7)
W(4)-O(4)	1.706(7)
W(4)-O(16)	1.891(7)
W(4)-O(24)	1.902(7)
W(4)-O(22)	1.906(7)

W(4)-O(23)	1.913(7)
W(4)-O(37)	2.406(7)
W(5)-O(5)	1.703(7)
W(5)-O(24)	1.896(7)
W(5)-O(17)	1.911(7)
W(5)-O(25)	1.914(7)
W(5)-O(26)	1.918(7)
W(5)-O(38)	2.435(7)
W(6)-O(6)	1.688(7)
W(6)-O(28)	1.892(7)
W(6)-O(27)	1.920(7)
W(6)-O(18)	1.923(7)
W(6)-O(26)	1.928(7)
W(6)-O(38)	2.452(7)
W(7)-O(7)	1.706(7)
W(7)-O(28)	1.896(7)
W(7)-O(20)	1.911(7)
W(7)-O(29)	1.919(7)
W(7)-O(30)	1.919(7)
W(7)-O(39)	2.423(7)
W(8)-O(8)	1.695(7)
W(8)-O(31)	1.906(7)
W(8)-O(30)	1.907(7)
W(8)-O(21)	1.925(7)
W(8)-O(32)	1.928(7)
W(8)-O(39)	2.430(7)
W(9)-O(9)	1.708(7)
W(9)-O(32)	1.868(7)
W(9)-O(33)	1.890(7)
W(9)-O(15)	1.905(7)
W(9)-O(22)	1.945(7)
W(9)-O(37)	2.435(7)
W(10)-O(10)	1.701(7)
W(10)-O(23)	1.895(7)
W(10)-O(35)	1.908(7)
W(10)-O(25)	1.915(7)
W(10)-O(34)	1.917(7)

W(10)-O(40)	2.432(7)
W(11)-O(11)	1.711(7)
W(11)-O(29)	1.895(7)
W(11)-O(27)	1.900(7)
W(11)-O(36)	1.909(7)
W(11)-O(34)	1.928(7)
W(11)-O(40)	2.415(7)
W(12)-O(12)	1.693(7)
W(12)-O(33)	1.900(7)
W(12)-O(31)	1.908(7)
W(12)-O(36)	1.910(7)
W(12)-O(35)	1.926(7)
W(12)-O(40)	2.453(7)
P(1)-O(40)	1.528(7)
P(1)-O(38)	1.528(7)
P(1)-O(37)	1.531(7)
P(1)-O(39)	1.552(7)
O(1A)-C(1A)	1.328(12)
O(1A)-H(1OA)	0.8401
O(2A)-C(1A)	1.217(13)
N(1A)-C(2A)	1.471(14)
N(1A)-H(1AA)	0.9100
N(1A)-H(1AB)	0.9100
N(1A)-H(1AC)	0.9100
C(1A)-C(2A)	1.511(15)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
O(1B)-C(1B)	1.302(12)
O(1B)-H(1OB)	0.8402
O(2B)-C(1B)	1.215(12)
N(1B)-C(2B)	1.462(13)
N(1B)-H(1BA)	0.9100
N(1B)-H(1BB)	0.9100
N(1B)-H(1BC)	0.9101
C(1B)-C(2B)	1.540(14)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900

O(1C)-C(1C)	1.346(13)
O(1C)-H(1OC)	0.8401
O(2C)-C(1C)	1.158(13)
N(1C)-C(2C)	1.500(14)
N(1C)-H(1CA)	0.9101
N(1C)-H(1CB)	0.9101
N(1C)-H(1CC)	0.9099
C(1C)-C(2C)	1.502(15)
C(2C)-H(2CA)	0.9900
C(2C)-H(2CB)	0.9900
O(1W)-H(1WA)	0.8499
O(1W)-H(1WB)	0.8500
O(2W)-H(2WA)	0.8499
O(2W)-H(2WB)	0.8501
O(3W)-H(3WA)	0.8500
O(3W)-H(3WB)	0.8501
O(4W)-H(4WA)	0.8500
O(4W)-H(4WB)	0.8500
O(5W)-H(5WA)	0.8502
O(5W)-H(5WB)	0.8500

O(1)-W(1)-O(14)	103.3(3)
O(1)-W(1)-O(13)	102.5(3)
O(14)-W(1)-O(13)	86.4(3)
O(1)-W(1)-O(15)	102.9(3)
O(14)-W(1)-O(15)	89.5(3)
O(13)-W(1)-O(15)	154.6(3)
O(1)-W(1)-O(16)	103.3(3)
O(14)-W(1)-O(16)	153.4(3)
O(13)-W(1)-O(16)	86.4(3)
O(15)-W(1)-O(16)	86.0(3)
O(1)-W(1)-O(37)	172.0(3)
O(14)-W(1)-O(37)	82.8(3)
O(13)-W(1)-O(37)	82.9(3)
O(15)-W(1)-O(37)	71.7(3)
O(16)-W(1)-O(37)	70.9(3)
O(2)-W(2)-O(19)	103.4(3)

O(2)-W(2)-O(13)	103.2(3)
O(19)-W(2)-O(13)	86.2(3)
O(2)-W(2)-O(17)	101.8(3)
O(19)-W(2)-O(17)	154.8(3)
O(13)-W(2)-O(17)	88.8(3)
O(2)-W(2)-O(18)	100.4(3)
O(19)-W(2)-O(18)	89.0(3)
O(13)-W(2)-O(18)	156.4(3)
O(17)-W(2)-O(18)	85.7(3)
O(2)-W(2)-O(38)	170.2(3)
O(19)-W(2)-O(38)	83.5(3)
O(13)-W(2)-O(38)	84.0(3)
O(17)-W(2)-O(38)	71.4(3)
O(18)-W(2)-O(38)	72.5(3)
O(3)-W(3)-O(19)	103.4(3)
O(3)-W(3)-O(14)	102.8(3)
O(19)-W(3)-O(14)	84.4(3)
O(3)-W(3)-O(20)	102.0(3)
O(19)-W(3)-O(20)	89.6(3)
O(14)-W(3)-O(20)	155.2(3)
O(3)-W(3)-O(21)	101.3(3)
O(19)-W(3)-O(21)	155.2(3)
O(14)-W(3)-O(21)	88.3(3)
O(20)-W(3)-O(21)	87.1(3)
O(3)-W(3)-O(39)	171.1(3)
O(19)-W(3)-O(39)	83.4(3)
O(14)-W(3)-O(39)	83.3(3)
O(20)-W(3)-O(39)	72.1(3)
O(21)-W(3)-O(39)	72.2(3)
O(4)-W(4)-O(16)	102.6(3)
O(4)-W(4)-O(24)	102.5(3)
O(16)-W(4)-O(24)	88.4(3)
O(4)-W(4)-O(22)	101.4(3)
O(16)-W(4)-O(22)	88.6(3)
O(24)-W(4)-O(22)	156.0(3)
O(4)-W(4)-O(23)	101.4(3)
O(16)-W(4)-O(23)	155.9(3)

O(24)-W(4)-O(23)	84.9(3)
O(22)-W(4)-O(23)	88.2(3)
O(4)-W(4)-O(37)	172.8(3)
O(16)-W(4)-O(37)	73.0(3)
O(24)-W(4)-O(37)	83.3(3)
O(22)-W(4)-O(37)	73.0(3)
O(23)-W(4)-O(37)	83.2(3)
O(5)-W(5)-O(24)	103.2(3)
O(5)-W(5)-O(17)	102.5(3)
O(24)-W(5)-O(17)	88.7(3)
O(5)-W(5)-O(25)	102.4(3)
O(24)-W(5)-O(25)	86.7(3)
O(17)-W(5)-O(25)	155.1(3)
O(5)-W(5)-O(26)	102.3(3)
O(24)-W(5)-O(26)	154.6(3)
O(17)-W(5)-O(26)	86.6(3)
O(25)-W(5)-O(26)	87.2(3)
O(5)-W(5)-O(38)	171.8(3)
O(24)-W(5)-O(38)	82.6(3)
O(17)-W(5)-O(38)	71.6(3)
O(25)-W(5)-O(38)	83.6(3)
O(26)-W(5)-O(38)	72.2(3)
O(6)-W(6)-O(28)	104.7(3)
O(6)-W(6)-O(27)	104.2(3)
O(28)-W(6)-O(27)	85.3(3)
O(6)-W(6)-O(18)	100.8(3)
O(28)-W(6)-O(18)	89.2(3)
O(27)-W(6)-O(18)	155.0(3)
O(6)-W(6)-O(26)	101.1(3)
O(28)-W(6)-O(26)	154.2(3)
O(27)-W(6)-O(26)	86.9(3)
O(18)-W(6)-O(26)	87.5(3)
O(6)-W(6)-O(38)	170.0(3)
O(28)-W(6)-O(38)	82.9(3)
O(27)-W(6)-O(38)	82.7(3)
O(18)-W(6)-O(38)	72.4(3)
O(26)-W(6)-O(38)	71.7(3)

O(7)-W(7)-O(28)	105.0(3)
O(7)-W(7)-O(20)	101.4(3)
O(28)-W(7)-O(20)	89.6(3)
O(7)-W(7)-O(29)	103.4(3)
O(28)-W(7)-O(29)	85.0(3)
O(20)-W(7)-O(29)	155.1(3)
O(7)-W(7)-O(30)	100.4(3)
O(28)-W(7)-O(30)	154.5(3)
O(20)-W(7)-O(30)	87.3(3)
O(29)-W(7)-O(30)	87.3(3)
O(7)-W(7)-O(39)	170.2(3)
O(28)-W(7)-O(39)	83.1(3)
O(20)-W(7)-O(39)	72.8(3)
O(29)-W(7)-O(39)	82.5(3)
O(30)-W(7)-O(39)	71.9(3)
O(8)-W(8)-O(31)	103.1(3)
O(8)-W(8)-O(30)	102.4(3)
O(31)-W(8)-O(30)	89.0(3)
O(8)-W(8)-O(21)	101.2(3)
O(31)-W(8)-O(21)	155.6(3)
O(30)-W(8)-O(21)	87.6(3)
O(8)-W(8)-O(32)	103.4(3)
O(31)-W(8)-O(32)	85.0(3)
O(30)-W(8)-O(32)	154.2(3)
O(21)-W(8)-O(32)	87.6(3)
O(8)-W(8)-O(39)	171.4(3)
O(31)-W(8)-O(39)	83.5(3)
O(30)-W(8)-O(39)	71.9(3)
O(21)-W(8)-O(39)	72.5(3)
O(32)-W(8)-O(39)	82.5(3)
O(9)-W(9)-O(32)	104.5(3)
O(9)-W(9)-O(33)	104.5(3)
O(32)-W(9)-O(33)	86.8(3)
O(9)-W(9)-O(15)	99.6(3)
O(32)-W(9)-O(15)	89.9(3)
O(33)-W(9)-O(15)	155.7(3)
O(9)-W(9)-O(22)	100.5(3)

O(32)-W(9)-O(22)	155.0(3)
O(33)-W(9)-O(22)	87.1(3)
O(15)-W(9)-O(22)	85.9(3)
O(9)-W(9)-O(37)	169.2(3)
O(32)-W(9)-O(37)	83.5(3)
O(33)-W(9)-O(37)	82.9(3)
O(15)-W(9)-O(37)	72.8(3)
O(22)-W(9)-O(37)	71.7(3)
O(10)-W(10)-O(23)	104.2(3)
O(10)-W(10)-O(35)	102.3(3)
O(23)-W(10)-O(35)	89.2(3)
O(10)-W(10)-O(25)	101.6(3)
O(23)-W(10)-O(25)	85.9(3)
O(35)-W(10)-O(25)	156.0(3)
O(10)-W(10)-O(34)	101.0(3)
O(23)-W(10)-O(34)	154.7(3)
O(35)-W(10)-O(34)	87.6(3)
O(25)-W(10)-O(34)	86.9(3)
O(10)-W(10)-O(40)	171.4(3)
O(23)-W(10)-O(40)	83.2(3)
O(35)-W(10)-O(40)	73.1(3)
O(25)-W(10)-O(40)	83.0(3)
O(34)-W(10)-O(40)	71.9(3)
O(11)-W(11)-O(29)	101.9(3)
O(11)-W(11)-O(27)	103.3(3)
O(29)-W(11)-O(27)	86.6(3)
O(11)-W(11)-O(36)	101.3(3)
O(29)-W(11)-O(36)	88.9(3)
O(27)-W(11)-O(36)	155.4(3)
O(11)-W(11)-O(34)	102.3(3)
O(29)-W(11)-O(34)	155.8(3)
O(27)-W(11)-O(34)	87.6(3)
O(36)-W(11)-O(34)	86.7(3)
O(11)-W(11)-O(40)	171.4(3)
O(29)-W(11)-O(40)	83.9(3)
O(27)-W(11)-O(40)	83.2(3)
O(36)-W(11)-O(40)	72.3(3)

O(34)-W(11)-O(40)	72.1(3)
O(12)-W(12)-O(33)	103.6(3)
O(12)-W(12)-O(31)	102.7(3)
O(33)-W(12)-O(31)	86.1(3)
O(12)-W(12)-O(36)	101.8(3)
O(33)-W(12)-O(36)	154.5(3)
O(31)-W(12)-O(36)	88.4(3)
O(12)-W(12)-O(35)	101.2(3)
O(33)-W(12)-O(35)	88.6(3)
O(31)-W(12)-O(35)	156.1(3)
O(36)-W(12)-O(35)	86.4(3)
O(12)-W(12)-O(40)	170.6(3)
O(33)-W(12)-O(40)	83.3(3)
O(31)-W(12)-O(40)	83.9(3)
O(36)-W(12)-O(40)	71.3(3)
O(35)-W(12)-O(40)	72.3(3)
O(40)-P(1)-O(38)	108.9(4)
O(40)-P(1)-O(37)	109.5(4)
O(38)-P(1)-O(37)	109.0(4)
O(40)-P(1)-O(39)	109.3(4)
O(38)-P(1)-O(39)	109.8(4)
O(37)-P(1)-O(39)	110.2(4)
W(2)-O(13)-W(1)	150.0(4)
W(1)-O(14)-W(3)	152.9(4)
W(9)-O(15)-W(1)	126.8(4)
W(4)-O(16)-W(1)	126.9(4)
W(5)-O(17)-W(2)	127.6(4)
W(6)-O(18)-W(2)	125.9(4)
W(2)-O(19)-W(3)	153.2(4)
W(7)-O(20)-W(3)	126.0(4)
W(3)-O(21)-W(8)	125.9(4)
W(4)-O(22)-W(9)	125.3(4)
W(10)-O(23)-W(4)	152.8(4)
W(5)-O(24)-W(4)	152.3(4)
W(5)-O(25)-W(10)	150.0(4)
W(5)-O(26)-W(6)	126.6(4)
W(11)-O(27)-W(6)	150.8(4)

W(6)-O(28)-W(7)	154.0(4)
W(11)-O(29)-W(7)	151.4(4)
W(8)-O(30)-W(7)	126.6(4)
W(8)-O(31)-W(12)	151.7(4)
W(9)-O(32)-W(8)	152.4(4)
W(9)-O(33)-W(12)	151.2(4)
W(10)-O(34)-W(11)	126.0(4)
W(10)-O(35)-W(12)	125.8(4)
W(11)-O(36)-W(12)	127.1(4)
P(1)-O(37)-W(4)	126.7(4)
P(1)-O(37)-W(9)	125.3(4)
W(4)-O(37)-W(9)	89.9(2)
P(1)-O(37)-W(1)	125.5(4)
W(4)-O(37)-W(1)	89.0(2)
W(9)-O(37)-W(1)	88.6(2)
P(1)-O(38)-W(5)	126.1(4)
P(1)-O(38)-W(2)	125.6(4)
W(5)-O(38)-W(2)	89.4(2)
P(1)-O(38)-W(6)	125.5(4)
W(5)-O(38)-W(6)	89.3(2)
W(2)-O(38)-W(6)	89.1(2)
P(1)-O(39)-W(7)	126.3(4)
P(1)-O(39)-W(8)	126.0(4)
W(7)-O(39)-W(8)	89.6(2)
P(1)-O(39)-W(3)	124.9(4)
W(7)-O(39)-W(3)	89.1(2)
W(8)-O(39)-W(3)	89.3(2)
P(1)-O(40)-W(11)	126.1(4)
P(1)-O(40)-W(10)	126.5(4)
W(11)-O(40)-W(10)	89.9(2)
P(1)-O(40)-W(12)	124.7(4)
W(11)-O(40)-W(12)	89.2(2)
W(10)-O(40)-W(12)	88.7(2)
C(1A)-O(1A)-H(1OA)	109.5
C(2A)-N(1A)-H(1AA)	109.5
C(2A)-N(1A)-H(1AB)	109.5
H(1AA)-N(1A)-H(1AB)	109.5

C(2A)-N(1A)-H(1AC)	109.5
H(1AA)-N(1A)-H(1AC)	109.5
H(1AB)-N(1A)-H(1AC)	109.5
O(2A)-C(1A)-O(1A)	126.9(10)
O(2A)-C(1A)-C(2A)	121.8(9)
O(1A)-C(1A)-C(2A)	111.3(9)
N(1A)-C(2A)-C(1A)	109.2(9)
N(1A)-C(2A)-H(2AA)	109.8
C(1A)-C(2A)-H(2AA)	109.8
N(1A)-C(2A)-H(2AB)	109.8
C(1A)-C(2A)-H(2AB)	109.8
H(2AA)-C(2A)-H(2AB)	108.3
C(1B)-O(1B)-H(1OB)	109.5
C(2B)-N(1B)-H(1BA)	109.5
C(2B)-N(1B)-H(1BB)	109.5
H(1BA)-N(1B)-H(1BB)	109.5
C(2B)-N(1B)-H(1BC)	109.4
H(1BA)-N(1B)-H(1BC)	109.5
H(1BB)-N(1B)-H(1BC)	109.5
O(2B)-C(1B)-O(1B)	126.2(10)
O(2B)-C(1B)-C(2B)	119.9(9)
O(1B)-C(1B)-C(2B)	113.8(9)
N(1B)-C(2B)-C(1B)	113.0(8)
N(1B)-C(2B)-H(2BA)	109.0
C(1B)-C(2B)-H(2BA)	109.0
N(1B)-C(2B)-H(2BB)	109.0
C(1B)-C(2B)-H(2BB)	109.0
H(2BA)-C(2B)-H(2BB)	107.8
C(1C)-O(1C)-H(1OC)	109.5
C(2C)-N(1C)-H(1CA)	109.5
C(2C)-N(1C)-H(1CB)	109.5
H(1CA)-N(1C)-H(1CB)	109.5
C(2C)-N(1C)-H(1CC)	109.4
H(1CA)-N(1C)-H(1CC)	109.5
H(1CB)-N(1C)-H(1CC)	109.5
O(2C)-C(1C)-O(1C)	125.4(10)
O(2C)-C(1C)-C(2C)	124.7(10)

O(1C)-C(1C)-C(2C)	110.0(10)
N(1C)-C(2C)-C(1C)	108.6(9)
N(1C)-C(2C)-H(2CA)	110.0
C(1C)-C(2C)-H(2CA)	110.0
N(1C)-C(2C)-H(2CB)	110.0
C(1C)-C(2C)-H(2CB)	110.0
H(2CA)-C(2C)-H(2CB)	108.4
H(1WA)-O(1W)-H(1WB)	107.2
H(2WA)-O(2W)-H(2WB)	119.2
H(3WA)-O(3W)-H(3WB)	102.8
H(4WA)-O(4W)-H(4WB)	87.0
H(5WA)-O(5W)-H(5WB)	88.3

Symmetry transformations used to generate equivalent atoms:

Table 4S Anisotropic displacement parameters ($Å^2 x\ 10^3$) for GL2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W(1)	16(1)	15(1)	17(1)	1(1)	5(1)	-1(1)
W(2)	17(1)	14(1)	16(1)	-1(1)	5(1)	1(1)
W(3)	17(1)	16(1)	14(1)	0(1)	3(1)	0(1)
W(4)	14(1)	14(1)	16(1)	0(1)	2(1)	-1(1)
W(5)	15(1)	14(1)	16(1)	0(1)	3(1)	1(1)
W(6)	15(1)	13(1)	16(1)	0(1)	3(1)	0(1)
W(7)	15(1)	15(1)	16(1)	-1(1)	2(1)	-1(1)
W(8)	15(1)	14(1)	15(1)	0(1)	2(1)	1(1)
W(9)	15(1)	13(1)	17(1)	0(1)	3(1)	0(1)
W(10)	16(1)	15(1)	14(1)	0(1)	3(1)	0(1)
W(11)	15(1)	14(1)	15(1)	0(1)	4(1)	-1(1)
W(12)	15(1)	14(1)	16(1)	-1(1)	4(1)	0(1)
P(1)	12(1)	13(1)	14(1)	1(1)	4(1)	1(1)
O(1)	22(4)	12(3)	19(4)	1(3)	9(3)	2(3)
O(2)	28(4)	22(4)	22(4)	3(3)	16(3)	5(3)
O(3)	23(4)	21(4)	15(4)	4(3)	3(3)	0(3)
O(4)	22(4)	14(4)	23(4)	2(3)	3(3)	0(3)

O(5)	17(4)	17(4)	23(4)	5(3)	5(3)	1(3)
O(6)	21(4)	11(3)	24(4)	-2(3)	2(3)	0(3)
O(7)	20(4)	14(4)	27(4)	0(3)	1(3)	-2(3)
O(8)	17(4)	20(4)	24(4)	2(3)	2(3)	1(3)
O(9)	15(3)	20(4)	13(3)	0(3)	-2(3)	1(3)
O(10)	19(4)	20(4)	7(3)	-2(3)	0(3)	1(3)
O(11)	23(4)	17(4)	24(4)	1(3)	6(3)	-4(3)
O(12)	24(4)	24(4)	15(4)	-2(3)	7(3)	-3(3)
O(13)	18(3)	19(4)	16(4)	3(3)	4(3)	6(3)
O(14)	12(3)	15(3)	28(4)	1(3)	10(3)	-1(3)
O(15)	16(4)	15(4)	23(4)	1(3)	1(3)	-2(3)
O(16)	15(4)	22(4)	21(4)	-2(3)	6(3)	-1(3)
O(17)	12(3)	14(3)	28(4)	1(3)	3(3)	2(3)
O(18)	19(4)	10(3)	20(4)	0(3)	6(3)	1(3)
O(19)	18(3)	13(3)	13(3)	-2(3)	3(3)	0(3)
O(20)	18(4)	21(4)	15(4)	-5(3)	3(3)	2(3)
O(21)	16(3)	18(4)	14(3)	2(3)	4(3)	-2(3)
O(22)	19(4)	17(4)	21(4)	-5(3)	9(3)	-4(3)
O(23)	17(4)	16(4)	21(4)	-4(3)	6(3)	-3(3)
O(24)	19(4)	14(3)	20(4)	1(3)	5(3)	-2(3)
O(25)	18(4)	14(4)	26(4)	0(3)	7(3)	-1(3)
O(26)	22(4)	17(4)	11(3)	-1(3)	-1(3)	1(3)
O(27)	18(4)	21(4)	21(4)	1(3)	3(3)	2(3)
O(28)	16(4)	23(4)	12(3)	2(3)	1(3)	5(3)
O(29)	18(4)	21(4)	17(4)	2(3)	3(3)	3(3)
O(30)	19(3)	14(3)	16(3)	5(3)	2(3)	0(3)
O(31)	16(4)	25(4)	17(4)	2(3)	3(3)	4(3)
O(32)	25(4)	18(4)	10(3)	1(3)	3(3)	0(3)
O(33)	21(4)	18(4)	17(4)	-2(3)	9(3)	-3(3)
O(34)	20(4)	16(4)	21(4)	0(3)	6(3)	1(3)
O(35)	18(4)	24(4)	12(3)	-1(3)	8(3)	4(3)
O(36)	19(4)	16(4)	19(4)	1(3)	6(3)	3(3)
O(37)	17(3)	15(3)	12(3)	-5(3)	4(3)	-6(3)
O(38)	23(4)	12(3)	21(4)	3(3)	8(3)	5(3)
O(39)	16(3)	18(4)	15(3)	-2(3)	2(3)	-2(3)
O(40)	20(4)	13(3)	15(3)	2(3)	5(3)	2(3)
O(1A)	27(4)	20(4)	23(4)	4(3)	7(3)	9(3)

O(2A)	26(4)	21(4)	25(4)	2(3)	9(3)	-3(3)
N(1A)	25(5)	25(5)	23(5)	2(4)	1(4)	-4(4)
C(1A)	16(5)	12(5)	24(5)	6(4)	-2(4)	0(4)
C(2A)	10(5)	29(6)	26(6)	-2(5)	0(4)	-8(4)
O(1B)	31(4)	17(4)	19(4)	-1(3)	4(3)	6(3)
O(2B)	31(4)	27(4)	17(4)	-4(3)	8(3)	-9(3)
N(1B)	23(5)	16(4)	23(5)	-1(3)	3(4)	-3(4)
C(1B)	13(4)	19(5)	18(5)	2(4)	1(4)	3(4)
C(2B)	31(6)	10(5)	18(5)	5(4)	-1(5)	-5(4)
O(1C)	48(5)	23(4)	18(4)	1(3)	14(4)	0(4)
O(2C)	20(4)	15(4)	22(4)	1(3)	9(3)	-2(3)
N(1C)	26(5)	25(5)	24(5)	-5(4)	5(4)	1(4)
C(1C)	17(5)	31(6)	13(5)	-5(4)	2(4)	1(4)
C(2C)	26(6)	30(6)	19(5)	-2(4)	-1(5)	-1(5)
O(1W)	19(4)	28(4)	16(4)	-5(3)	2(3)	-3(3)
O(2W)	35(5)	23(4)	32(5)	-5(3)	15(4)	5(4)
O(3W)	29(4)	21(4)	39(5)	11(4)	-9(4)	-10(3)
O(4W)	16(4)	26(4)	28(4)	-6(3)	2(3)	-4(3)
O(5W)	46(6)	54(6)	24(5)	0(4)	11(4)	19(5)

Table 5S Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for GL2.

	x	y	z	U(eq)
H(1OA)	-1013	1656	1878	35
H(1AA)	2469	544	2977	37
H(1AB)	1525	227	3225	37
H(1AC)	1769	948	3380	37
H(2AA)	725	372	2047	26
H(2AB)	1494	1002	1973	26
H(1OB)	8018	3042	1265	34
H(1BA)	7261	4224	-837	32
H(1BB)	6934	3650	-407	32
H(1BC)	8086	3713	-498	32

H(2BA)	7133	4635	297	25
H(2BB)	8401	4616	258	25
H(1OC)	8827	915	7661	43
H(1CA)	9941	1611	10286	37
H(1CB)	8738	1728	10113	37
H(1CC)	9434	2047	9635	37
H(2CA)	8571	798	9487	31
H(2CB)	9855	802	9480	31
H(1WA)	8237	2554	2522	32
H(1WB)	7602	2192	1946	32
H(2WA)	4795	1140	4359	43
H(2WB)	5262	1790	4638	43
H(3WA)	2169	3907	5689	48
H(3WB)	1590	3348	5685	48
H(4WA)	7292	3735	5735	35
H(4WB)	7130	3158	5750	35
H(5WA)	9658	3039	9150	61
H(5WB)	9926	3205	9796	61

Table 6S Hydrogen bonds for GL2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1OA)...O(1W)#1	0.84	1.94	2.733(11)	156
N(1A)-H(1AA)...O(9)	0.91	2.30	2.988(13)	132
N(1A)-H(1AA)...O(11)#2	0.91	2.26	2.918(12)	129
N(1A)-H(1AB)...O(2B)#2	0.91	2.17	2.977(13)	147
N(1A)-H(1AB)...O(5)#3	0.91	2.49	3.116(12)	127
N(1A)-H(1AC)...O(2A)	0.91	2.24	2.661(13)	107
N(1A)-H(1AC)...O(15)	0.91	2.54	3.145(13)	124
N(1A)-H(1AC)...O(10)#4	0.91	2.15	2.866(11)	135
O(1B)-H(1OB)...O(1W)	0.84	1.83	2.662(10)	169
N(1B)-H(1BA)...O(26)#5	0.91	2.27	2.981(11)	134
N(1B)-H(1BA)...O(27)#5	0.91	2.50	3.319(12)	151
N(1B)-H(1BB)...O(2W)#6	0.91	1.95	2.725(13)	142
N(1B)-H(1BB)...O(8)#6	0.91	2.51	2.996(11)	114

N(1B)-H(1BC)...O(5W)#7	0.91	1.84	2.746(14)	176
O(1C)-H(1OC)...O(2B)#4	0.84	1.86	2.595(10)	145
N(1C)-H(1CA)...O(4)#8	0.91	2.51	2.850(12)	103
N(1C)-H(1CA)...O(3W)#9	0.91	2.10	2.867(13)	141
N(1C)-H(1CB)...O(4W)#4	0.91	1.82	2.715(12)	165
N(1C)-H(1CC)...O(2C)	0.91	2.21	2.681(11)	111
N(1C)-H(1CC)...O(5W)	0.91	2.43	3.257(14)	151
N(1C)-H(1CC)...O(1)#9	0.91	2.59	3.235(12)	129
O(1W)-H(1WA)...O(2C)#6	0.85	1.97	2.739(10)	151
O(1W)-H(1WB)...O(12)	0.85	2.48	3.035(10)	124
O(1W)-H(1WB)...O(6)#2	0.85	2.43	3.208(11)	152
O(2W)-H(2WA)...O(11)#2	0.85	2.16	2.942(11)	153
O(2W)-H(2WB)...O(35)#4	0.85	2.52	2.931(12)	111
O(3W)-H(3WA)...O(7)#10	0.85	2.16	2.886(11)	144
O(3W)-H(3WB)...O(22)#4	0.85	2.17	2.906(11)	144
O(4W)-H(4WA)...O(18)#10	0.85	2.08	2.867(10)	153
O(4W)-H(4WB)...O(12)#4	0.85	2.12	2.957(11)	168
O(5W)-H(5WA)...O(1)#9	0.85	2.23	2.910(12)	138
O(5W)-H(5WA)...O(2A)#9	0.85	2.36	2.897(13)	122
O(5W)-H(5WB)...O(4)#8	0.85	2.46	3.028(11)	125
O(5W)-H(5WB)...O(1)#9	0.85	2.56	2.910(12)	106

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 -x+1,y-1/2,-z+1/2 #3 -x,y-1/2,-z+1/2

#4 x,-y+1/2,z+1/2 #5 -x+1,-y+1,-z #6 x,-y+1/2,z-1/2

#7 x,y,z-1 #8 x+1,y,z+1 #9 x+1,-y+1/2,z+1/2

#10 -x+1,-y+1,-z+1