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Supporting information for article:

Molecular structures of two copper complexes with the pharmaceuticals norfloxacin and tinidazole, when PXRD assists multi-domain SCXRD

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Tables of fractional coordinates and equivalent isotropic displacement parameters of the non-H atoms (Tables S1 y S2), full bond distances and angle (Tables S3 y S4), atomic anisotropic displacement parameters (Tables S5 y S6), hydrogen atoms positions (Tables S7 y S8), and hydrogen bond distances and angles (Tables S9 y S10). CIF files with further details of the crystal structures reported in the paper has been deposited with the Cambridge Crystallographic Data Centre, under deposition number CCDC 900244 (nor) and 2082848 (tnz).

Table S1 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Cu(nor)_2]SO_4 \cdot 7H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

C(11)	-1186(3)	824(1)	7887(2)	31(1)
C(12)	-212(3)	858(1)	9016(2)	29(1)
C(13)	638(3)	522(1)	9514(2)	26(1)
C(14)	1427(3)	599(1)	10657(2)	26(1)
C(15)	2225(3)	271(1)	11261(2)	28(1)
C(16)	2988(3)	348(1)	12312(2)	29(1)
C(17)	3084(3)	757(1)	12835(2)	27(1)
C(18)	2265(3)	1077(1)	12257(2)	27(1)
C(19)	1420(3)	999(1)	11185(2)	25(1)
C(21)	1295(3)	-745(1)	7028(2)	30(1)
C(22)	315(3)	-789(1)	5910(2)	28(1)
C(23)	-658(3)	-481(1)	5456(2)	27(1)
C(24)	-1452(3)	-565(1)	4328(2)	25(1)
C(25)	-2352(3)	-254(1)	3761(2)	28(1)
C(26)	-3115(3)	-336(1)	2710(2)	29(1)
C(27)	-3131(3)	-737(1)	2164(2)	26(1)
C(28)	-2217(3)	-1039(1)	2707(2)	26(1)
C(29)	-1354(3)	-953(1)	3761(2)	25(1)
C(110)	-180(3)	1240(1)	9584(2)	30(1)

C(111)	559(3)	1752(1)	11114(2)	34(1)
C(112)	-161(4)	1758(1)	12042(3)	48(1)
C(113)	5361(3)	759(1)	13852(2)	36(1)
C(114)	6244(3)	731(1)	15033(3)	42(1)
C(115)	4703(3)	1191(1)	15686(2)	42(1)
C(116)	3832(3)	1213(1)	14490(2)	35(1)
C(210)	400(3)	-1156(1)	5300(2)	30(1)
C(211)	-272(3)	-1673(1)	3794(3)	43(1)
C(212)	-1185(5)	-1991(1)	4114(4)	72(1)
C(213)	-5431(3)	-748(1)	1142(2)	35(1)
C(214)	-6282(3)	-710(1)	-55(3)	41(1)
C(215)	-4697(3)	-1162(1)	-697(2)	39(1)
C(216)	-3870(3)	-1195(1)	511(2)	31(1)
N(11)	601(2)	1321(1)	10609(2)	29(1)
N(12)	3971(2)	817(1)	13891(2)	29(1)
N(13)	6096(2)	1125(1)	15661(2)	36(1)
N(21)	-394(2)	-1245(1)	4287(2)	29(1)
N(22)	-4034(2)	-805(1)	1124(2)	29(1)
N(23)	-6101(2)	-1095(1)	-710(2)	37(1)
O(1)	6929(3)	1797(1)	14610(2)	54(1)
O(2)	5560(3)	2413(1)	14655(3)	76(1)
O(1W)	5280(4)	1925(1)	17676(3)	91(1)
O(3)	6948(3)	2136(1)	16361(2)	75(1)
O(2W)	9107(3)	2736(1)	13321(2)	65(1)
O(4)	7907(3)	2484(1)	15053(3)	60(1)
O(3W)	6432(4)	1906(1)	12156(3)	80(1)
O(4W)	-7155(3)	-1685(1)	375(3)	69(1)
O(5W)	11771(3)	2917(1)	13659(3)	81(1)
O(6W)	13591(3)	2784(1)	15645(3)	84(1)

O(7W)	13296(4)	2777(1)	17932(3)	94(1)
O(11)	-1095(2)	516(1)	7225(2)	36(1)
O(12)	-2054(2)	1101(1)	7652(2)	54(1)
O(13)	771(2)	164(1)	9049(2)	33(1)
O(21)	1072(2)	-476(1)	7746(2)	37(1)
O(22)	2278(2)	-979(1)	7210(2)	43(1)
O(23)	-864(2)	-137(1)	5954(2)	32(1)
F(1)	3698(2)	25(1)	12901(1)	39(1)
F(2)	-3885(2)	-19(1)	2142(1)	40(1)
Cu	-29(1)	16(1)	7497(1)	29(1)
S	6825(1)	2210(1)	15167(1)	40(1)

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Cu(tnz)_2(NO_3)_2]$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

C(1)	3168(4)	6549(3)	3700(2)	25(1)
C(2)	3393(4)	5418(3)	2609(2)	26(1)
C(3)	4058(4)	4765(3)	3247(2)	28(1)
C(4)	1939(4)	7562(3)	2446(2)	29(1)
C(5)	-135(4)	7542(3)	2511(2)	31(1)
C(6)	-1054(5)	6964(3)	887(2)	41(1)
C(7)	-2127(6)	6140(4)	309(2)	64(1)
C(8)	2742(5)	7587(3)	4240(2)	37(1)
N(1)	3916(3)	5482(2)	3930(1)	25(1)
N(2)	2837(3)	6547(2)	2886(1)	24(1)
N(3)	3499(3)	5053(3)	1775(1)	36(1)
N(4)	8211(3)	5157(3)	4276(1)	33(1)
O(1)	3957(4)	3990(3)	1655(1)	59(1)
O(2)	3176(3)	5801(3)	1236(1)	47(1)
O(3)	-547(3)	5277(2)	1992(1)	43(1)
O(4)	-3248(3)	6618(3)	2100(2)	55(1)
O(5)	7140(3)	4248(2)	4373(1)	42(1)
O(6)	9632(4)	5017(3)	3922(2)	74(1)
O(7)	7692(4)	6141(3)	4556(2)	66(1)
S	-1353(1)	6471(1)	1899(1)	30(1)
Cu	5000	5000	5000	24(1)

Table S3 Full bond lengths [Å] and angles [°] for $[Cu(nor)_2]SO_4 \cdot 7H_2O$.

C(11)-O(12)	1.235(3)	C(27)-N(22)	1.397(3)
C(11)-O(11)	1.274(3)	C(28)-C(29)	1.402(3)
C(11)-C(12)	1.501(3)	C(29)-N(21)	1.390(3)
C(12)-C(110)	1.377(4)	C(110)-N(11)	1.338(3)
C(12)-C(13)	1.410(4)	C(111)-N(11)	1.486(3)
C(13)-O(13)	1.278(3)	C(111)-C(112)	1.511(4)
C(13)-C(14)	1.454(3)	C(113)-N(12)	1.478(3)
C(14)-C(19)	1.407(4)	C(113)-C(114)	1.509(4)
C(14)-C(15)	1.407(4)	C(114)-N(13)	1.479(4)
C(15)-C(16)	1.355(4)	C(115)-N(13)	1.479(4)
C(16)-F(1)	1.348(3)	C(115)-C(116)	1.518(4)
C(16)-C(17)	1.422(4)	C(116)-N(12)	1.464(4)
C(17)-C(18)	1.387(4)	C(210)-N(21)	1.337(3)
C(17)-N(12)	1.401(3)	C(211)-N(21)	1.484(3)
C(18)-C(19)	1.407(3)	C(211)-C(212)	1.498(5)
C(19)-N(11)	1.392(3)	C(213)-N(22)	1.478(3)
C(21)-O(22)	1.237(3)	C(213)-C(214)	1.515(4)
C(21)-O(21)	1.277(3)	C(214)-N(23)	1.481(4)
C(21)-C(22)	1.497(3)	C(215)-N(23)	1.481(4)
C(22)-C(210)	1.381(4)	C(215)-C(216)	1.517(4)
C(22)-C(23)	1.409(4)	C(216)-N(22)	1.463(3)
C(23)-O(23)	1.279(3)	O(1)-S	1.474(2)
C(23)-C(24)	1.445(3)	O(2)-S	1.460(3)
C(24)-C(25)	1.407(4)	O(3)-S	1.451(3)
C(24)-C(29)	1.412(4)	O(4)-S	1.454(3)
C(25)-C(26)	1.357(4)	O(11)-Cu	1.900(2)
C(26)-F(2)	1.352(3)	O(13)-Cu	1.929(2)
C(26)-C(27)	1.420(4)	O(21)-Cu	1.898(2)

C(27)-C(28)	1.386(4)	O(23)-Cu	1.931(2)
O(12)-C(11)-O(11)	123.2(3)	O(23)-C(23)-C(22)	125.2(2)
O(12)-C(11)-C(12)	117.1(3)	O(23)-C(23)-C(24)	118.6(2)
O(11)-C(11)-C(12)	119.7(2)	C(22)-C(23)-C(24)	116.1(2)
C(110)-C(12)-C(13)	119.5(2)	C(25)-C(24)-C(29)	118.1(2)
C(110)-C(12)-C(11)	116.7(2)	C(25)-C(24)-C(23)	120.0(2)
C(13)-C(12)-C(11)	123.7(2)	C(29)-C(24)-C(23)	121.8(2)
O(13)-C(13)-C(12)	125.8(2)	C(26)-C(25)-C(24)	120.0(3)
O(13)-C(13)-C(14)	118.2(2)	F(2)-C(26)-C(25)	118.9(2)
C(12)-C(13)-C(14)	116.0(2)	F(2)-C(26)-C(27)	117.9(2)
C(19)-C(14)-C(15)	118.4(2)	C(25)-C(26)-C(27)	123.1(2)
C(19)-C(14)-C(13)	120.3(2)	C(28)-C(27)-N(22)	124.3(2)
C(15)-C(14)-C(13)	123.2(3)	C(28)-C(27)-C(26)	116.6(2)
C(16)-C(15)-C(14)	120.1(3)	N(22)-C(27)-C(26)	119.1(2)
F(1)-C(16)-C(15)	119.3(3)	C(27)-C(28)-C(29)	121.3(2)
F(1)-C(16)-C(17)	117.7(2)	N(21)-C(29)-C(28)	121.6(2)
C(15)-C(16)-C(17)	123.0(3)	N(21)-C(29)-C(24)	117.9(2)
C(18)-C(17)-N(12)	123.8(2)	C(28)-C(29)-C(24)	120.4(2)
C(18)-C(17)-C(16)	116.8(2)	N(11)-C(110)-C(12)	124.6(3)
N(12)-C(17)-C(16)	119.3(2)	N(11)-C(111)-C(112)	113.3(3)
C(17)-C(18)-C(19)	121.0(2)	N(12)-C(113)-C(114)	110.4(2)
N(11)-C(19)-C(14)	120.7(2)	N(13)-C(114)-C(113)	109.3(2)
N(11)-C(19)-C(18)	118.8(2)	N(13)-C(115)-C(116)	110.2(2)
C(14)-C(19)-C(18)	120.4(2)	N(12)-C(116)-C(115)	109.4(3)
O(22)-C(21)-O(21)	123.6(2)	N(21)-C(210)-C(22)	124.3(3)
O(22)-C(21)-C(22)	117.2(2)	N(21)-C(211)-C(212)	111.5(3)
O(21)-C(21)-C(22)	119.2(3)	N(22)-C(213)-C(214)	109.9(2)
C(210)-C(22)-C(23)	119.4(2)	N(23)-C(214)-C(213)	109.7(2)

C(210)-C(22)-C(21)	116.7(3)	N(23)-C(215)-C(216)	110.1(2)
C(23)-C(22)-C(21)	124.0(2)	N(22)-C(216)-C(215)	109.4(2)
C(110)-N(11)-C(19)	119.5(2)	C(13)-O(13)-Cu	125.3(2)
C(110)-N(11)-C(111)	119.1(2)	C(21)-O(21)-Cu	129.0(2)
C(19)-N(11)-C(111)	121.5(2)	C(23)-O(23)-Cu	125.7(2)
C(17)-N(12)-C(116)	116.5(2)	O(21)-Cu-O(11)	178.3(1)
C(17)-N(12)-C(113)	112.6(2)	O(21)-Cu-O(13)	86.50(8)
C(116)-N(12)-C(113)	110.0(2)	O(11)-Cu-O(13)	93.82(8)
C(114)-N(13)-C(115)	110.9(2)	O(21)-Cu-O(23)	93.71(8)
C(210)-N(21)-C(29)	120.2(2)	O(11)-Cu-O(23)	86.01(8)
C(210)-N(21)-C(211)	117.8(2)	O(13)-Cu-O(23)	178.69(9)
C(29)-N(21)-C(211)	121.9(2)	O(3)-S-O(4)	108.3(2)
C(27)-N(22)-C(216)	116.9(2)	O(3)-S-O(2)	110.2(2)
C(27)-N(22)-C(213)	114.5(2)	O(4)-S-O(2)	110.2(2)
C(216)-N(22)-C(213)	110.5(2)	O(3)-S-O(1)	109.1(2)
C(214)-N(23)-C(215)	111.7(2)	O(4)-S-O(1)	108.9(2)
C(11)-O(11)-Cu	130.0(2)	O(2)-S-O(1)	110.2(2)

Table S4 Full bond lengths [Å] and angles [°] for $[Cu(tnz)_2(NO_3)_2]$.

C(1)-N(1)	1.337(4)	C(2)-C(3)-N(1)	107.8(3)
C(1)-N(2)	1.357(3)	N(2)-C(4)-C(5)	113.2(2)
C(1)-C(8)	1.472(4)	C(4)-C(5)-S	117.6(2)
C(2)-C(3)	1.353(4)	C(7)-C(6)-S	110.0(2)
C(2)-N(2)	1.375(4)	C(1)-N(1)-C(3)	107.3(2)
C(2)-N(3)	1.430(3)	C(1)-N(1)-Cu	129.56(19)
C(3)-N(1)	1.373(3)	C(3)-N(1)-Cu	122.6(2)
C(4)-N(2)	1.472(4)	C(1)-N(2)-C(2)	106.1(2)
C(4)-C(5)	1.520(4)	C(1)-N(2)-C(4)	123.9(2)
C(5)-S	1.773(3)	C(2)-N(2)-C(4)	129.9(2)
C(6)-C(7)	1.518(5)	O(2)-N(3)-O(1)	124.4(3)
C(6)-S	1.765(3)	O(2)-N(3)-C(2)	119.8(3)
N(1)-Cu	1.990(2)	O(1)-N(3)-C(2)	115.8(3)
N(3)-O(2)	1.223(3)	O(6)-N(4)-O(7)	124.3(3)
N(3)-O(1)	1.222(4)	O(6)-N(4)-O(5)	119.8(3)
N(4)-O(6)	1.205(3)	O(7)-N(4)-O(5)	116.0(3)
N(4)-O(7)	1.229(4)	N(4)-O(5)-Cu	103.06(19)
N(4)-O(5)	1.273(3)	O(4)-S-O(3)	118.17(16)
O(3)-S	1.436(2)	O(4)-S-C(6)	108.24(16)
O(4)-S	1.436(2)	O(3)-S-C(6)	108.68(16)
O(5)-Cu	2.053(2)	O(4)-S-C(5)	106.03(15)
Cu-N(1)#1	1.990(2)	O(3)-S-C(5)	109.48(14)
Cu-O(5)#1	2.053(2)	C(6)-S-C(5)	105.53(15)
		N(1)#1-Cu-N(1)	180.0
N(1)-C(1)-N(2)	110.2(2)	N(1)#1-Cu-O(5)#1	87.65(9)
N(1)-C(1)-C(8)	125.8(2)	N(1)-Cu-O(5)#1	92.35(9)
N(2)-C(1)-C(8)	124.0(3)	N(1)#1-Cu-O(5)	92.35(9)
C(3)-C(2)-N(2)	108.5(2)	N(1)-Cu-O(5)	87.65(9)

C(3)-C(2)-N(3)	125.1(3)	O(5)#1-Cu-O(5)	180.0
N(2)-C(2)-N(3)	125.8(3)		

Table S5 Anisotropic displacement parameters ($Å^2$ x 10^3) for $[Cu(nor)_2]SO_4 \cdot 7H_2O$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(11)	31(2)	35(2)	21(1)	-2(1)	-4(1)	0(1)
C(12)	28(1)	36(2)	18(1)	-3(1)	-3(1)	0(1)
C(13)	26(1)	30(1)	22(1)	-3(1)	3(1)	-3(1)
C(14)	24(1)	29(1)	21(1)	-3(1)	0(1)	-1(1)
C(15)	29(1)	27(1)	26(1)	-5(1)	1(1)	-2(1)
C(16)	28(1)	30(1)	24(1)	3(1)	0(1)	1(1)
C(17)	23(1)	35(2)	21(1)	-1(1)	1(1)	-3(1)
C(18)	28(1)	30(1)	21(1)	-4(1)	1(1)	-1(1)
C(19)	26(1)	26(1)	20(1)	-3(1)	-1(1)	-1(1)
C(21)	31(2)	34(2)	20(1)	-2(1)	-3(1)	-1(1)
C(22)	25(1)	35(2)	19(1)	-3(1)	-2(1)	-2(1)
C(23)	28(1)	27(1)	22(1)	-2(1)	2(1)	-4(1)
C(24)	25(1)	26(1)	19(1)	-1(1)	-1(1)	-2(1)
C(25)	30(1)	24(1)	26(1)	-3(1)	-1(1)	-1(1)
C(26)	28(1)	28(1)	24(1)	3(1)	-3(1)	2(1)
C(27)	26(1)	31(1)	17(1)	-2(1)	1(1)	-3(1)
C(28)	25(1)	29(1)	22(1)	-4(1)	1(1)	-1(1)
C(29)	24(1)	26(1)	22(1)	-1(1)	2(1)	-2(1)
C(110)	29(1)	34(2)	22(1)	-1(1)	-1(1)	6(1)
C(111)	45(2)	24(1)	28(1)	-3(1)	-1(1)	4(1)
C(112)	52(2)	51(2)	43(2)	-9(2)	13(2)	10(2)
C(113)	26(2)	46(2)	32(2)	-8(1)	-1(1)	3(1)
C(114)	33(2)	42(2)	41(2)	-2(1)	-12(1)	3(1)
C(115)	39(2)	60(2)	23(1)	-10(1)	0(1)	-5(2)
C(116)	28(2)	48(2)	26(1)	-9(1)	-3(1)	2(1)
C(210)	27(1)	35(2)	23(1)	0(1)	-3(1)	3(1)

C(211)	44(2)	38(2)	36(2)	-14(1)	-10(1)	14(1)
C(212)	106(4)	35(2)	63(3)	-8(2)	0(2)	-11(2
C(213)	27(1)	44(2)	28(1)	-8(1)	-3(1)	2(1)
C(214)	34(2)	43(2)	35(2)	-1(1)	-11(1)	3(1)
C(215)	36(2)	57(2)	20(1)	-9(1)	0(1)	-5(2)
C(216)	27(1)	41(2)	23(1)	-7(1)	0(1)	3(1)
N(11)	30(1)	29(1)	23(1)	-4(1)	-2(1)	4(1)
N(12)	26(1)	36(1)	20(1)	-3(1)	-2(1)	-1(1)
N(13)	36(1)	42(1)	22(1)	-1(1)	-6(1)	-4(1)
N(21)	28(1)	29(1)	25(1)	-6(1)	-3(1)	5(1)
N(22)	25(1)	36(1)	22(1)	-3(1)	-2(1)	0(1)
N(23)	33(1)	49(2)	23(1)	-3(1)	-7(1)	-5(1)
O(1)	70(2)	41(1)	55(2)	-4(1)	20(1)	-4(1)
O(2)	48(2)	86(2)	84(2)	-13(2)	-2(2)	20(2)
O(1W)	126(3)	75(2)	82(2)	-10(2)	44(2)	-18(2)
O(3)	79(2)	104(3)	43(2)	-7(2)	19(2)	-6(2)
O(2W)	51(2)	86(2)	56(2)	-5(2)	12(1)	-5(2)
O(4)	58(2)	47(2)	74(2)	3(1)	13(2)	-9(1)
O(3W)	101(3)	72(2)	57(2)	-9(2)	2(2)	-14(2)
O(4W)	89(2)	49(2)	77(2)	-7(1)	35(2)	-14(2)
O(5W)	54(2)	125(3)	56(2)	28(2)	4(1)	-2(2)
O(6W)	56(2)	125(3)	65(2)	11(2)	4(2)	10(2)
O(7W)	84(3)	120(3)	64(2)	13(2)	-9(2)	-11(2)
O(11)	39(1)	40(1)	22(1)	-6(1)	-7(1)	5(1)
O(12)	51(1)	59(2)	35(1)	-16(1)	-20(1)	25(1)
O(13)	39(1)	31(1)	22(1)	-4(1)	-5(1)	3(1)
O(21)	40(1)	40(1)	23(1)	-7(1)	-7(1)	7(1)
O(22)	33(1)	54(1)	31(1)	-10(1)	-10(1)	13(1)
O(23)	36(1)	32(1)	21(1)	-6(1)	-5(1)	3(1)

F(1)	43(1)	31(1)	32(1)	4(1)	-8(1)	4(1)
F(2)	45(1)	32(1)	32(1)	1(1)	-10(1)	8(1)
Cu	32(1)	30(1)	19(1)	-5(1)	-3(1)	-1(1)
S	41(1)	39(1)	39(1)	-2(1)	7(1)	2(1)

Table S6 Anisotropic displacement parameters ($Å^2$ x 10^3) for $[Cu(tnz)_2(NO_3)_2]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(1)	30(2)	22(1)	-1(1)	0(1)	-2(1)
C(2)	23(1)	32(2)	23(1)	-3(1)	-2(1)	-1(1)
C(3)	25(1)	33(2)	26(1)	-2(1)	-2(1)	5(1)
C(4)	31(2)	28(2)	28(1)	8(1)	-3(1)	-5(1)
C(5)	32(2)	27(2)	33(1)	0(1)	-6(1)	0(1)
C(6)	53(2)	35(2)	33(2)	10(1)	-13(1)	-10(2)
C(7)	91(3)	57(3)	43(2)	3(2)	-22(2)	-23(2)
C(8)	53(2)	31(2)	28(1)	-5(1)	-1(1)	4(2)
N(1)	23(1)	31(1)	21(1)	-3(1)	-1(1)	3(1)
N(2)	24(1)	27(1)	21(1)	2(1)	-1(1)	-3(1)
N(3)	33(1)	50(2)	24(1)	-6(1)	-3(1)	2(1)
N(4)	28(1)	47(2)	26(1)	4(1)	-2(1)	-1(1)
O(1)	88(2)	53(2)	35(1)	-17(1)	-2(1)	17(2)
O(2)	52(2)	64(2)	26(1)	1(1)	-3(1)	3(1)
O(3)	57(2)	26(1)	47(1)	7(1)	-14(1)	-4(1)
O(4)	30(1)	69(2)	65(2)	-6(1)	-1(1)	-11(1)
O(5)	44(1)	41(2)	42(1)	8(1)	-8(1)	-5(1)
O(6)	37(2)	116(3)	69(2)	28(2)	21(1)	5(2)
O(7)	79(2)	49(2)	69(2)	-26(1)	-26(2)	14(2)
S	29(1)	28(1)	34(1)	6(1)	-5(1)	-7(1)
Cu	23(1)	29(1)	20(1)	-1(1)	0(1)	3(1)

Table S7 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $[Cu(nor)_2]SO_4 \cdot 7H_2O$.

H(15)	2228	2	10938	34
H(18)	2276	1346	12582	33
H(25)	-2424	7	4108	34
H(28)	-2176	-1303	2366	31
H(110)	-741	1457	9230	36
H(11A)	129	1950	10524	41
H(11B)	1456	1852	11418	41
H(11C)	-156	2044	12334	73
H(11D)	-1056	1666	11744	73
H(11E)	271	1568	12638	73
H(11F)	5634	998	13457	44
H(11G)	5444	499	13442	44
H(11H)	6005	483	15418	51
H(11I)	7155	699	15000	51
H(11J)	4623	1455	16082	51
H(11K)	4417	956	16088	51
H(11L)	2918	1251	14511	42
H(11M)	4088	1456	14098	42
H(210)	1052	-1354	5615	36
H(21A)	630	-1773	4056	51
H(21B)	-473	-1649	2977	51
H(21C)	-1083	-2264	3783	108
H(21D)	-978	-2019	4921	108
H(21E)	-2081	-1895	3843	108
H(21F)	-5524	-492	1564	42
H(21G)	-5718	-991	1514	42

H(21H)	-7202	-684	-42	49
H(21I)	-6036	-456	-409	49
H(21J)	-4385	-925	-1074	46
H(21K)	-4607	-1423	-1102	46
H(21L)	-4147	-1441	877	37
H(21M)	-2948	-1232	517	37
H(13A)	6373	1350	15334	43
H(13B)	6595	1106	16365	43
H(23A)	-6571	-1065	-1421	45
H(23B)	-6403	-1324	-421	45
H(1A)	5110(60)	2167(9)	17960(50)	136
H(1B)	5700(60)	2003(16)	17180(40)	136
H(2A)	8740(40)	2595(14)	13760(30)	97
H(2B)	8520(30)	2773(16)	12710(20)	97
H(3A)	6460(60)	1887(15)	12865(15)	119
H(3B)	6660(60)	2167(7)	12070(40)	119
H(4A)	-6630(40)	-1705(14)	1050(20)	103
H(4B)	-7230(50)	-1949(6)	150(30)	103
H(5A)	12230(40)	2803(17)	14270(30)	121
H(5B)	11010(30)	2794(17)	13560(40)	121
H(6A)	14100(50)	2583(14)	15510(40)	126
H(6B)	13580(60)	2748(18)	16341(18)	126
H(7A)	14020(40)	2690(20)	18360(50)	141

Table S8 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $[Cu(tnz)_2(NO_3)_2]$.

Atom	x	y	z	U(eq)
H(3)	4527	3972	3227	33
H(4A)	2267	7519	1876	35
H(4B)	2395	8336	2660	35
H(5A)	-586	8357	2378	37
H(5B)	-436	7385	3074	37
H(6A)	-1474	7805	829	49
H(6B)	235	6938	753	49
H(7A)	-1628	5325	327	96
H(7B)	-2045	6456	-235	96
H(7C)	-3387	6119	468	96
H(8A)	1507	7512	4426	55
H(8B)	2874	8344	3946	55
H(8C)	3569	7582	4698	55
H(3)	4527	3972	3227	33

Table S9 H-bond distances (Å) and angles (°) in $[Cu(nor)_2]SO_4 \cdot 7H_2O$.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(D-H···A)
C(110)-H(110)···O(4W)#1	0.93	2.47	3.126(4)	127.4
C(111)-H(11B)···O(7W)#2	0.97	2.59	3.481(5)	153.3
C(113)-H(11F)···O(22)#3	0.97	2.52	3.140(4)	122.0
C(113)-H(11G)···F(1)	0.97	2.31	2.935(3)	121.1
C(113)-H(11G)···F(2)#4	0.97	2.49	3.423(3)	162.0
C(114)-H(11H)···F(1)#5	0.97	2.55	3.448(4)	153.1
C(115)-H(11J)···O(1W)	0.97	2.40	3.288(5)	152.0
C(210)-H(210)···O(1)#3	0.93	2.60	3.417(4)	147.4
C(211)-H(21B)···O(5W)#6	0.97	2.51	3.277(4)	135.5
C(213)-H(21F)···F(1)#7	0.97	2.57	3.502(3)	161.1
C(213)-H(21F)···F(2)	0.97	2.24	2.882(3)	122.8
C(214)-H(21I)···F(2)#8	0.97	2.57	3.457(4)	152.1
C(215)-H(21K)···O(3W)#9	0.97	2.52	3.203(4)	127.3
N(13)-H(13A)···O(1)	0.89	1.82	2.714(4)	177.7
N(13)-H(13B)···O(12)#4	0.89	1.82	2.705(3)	171.9
N(23)-H(23A)···O(22)#7	0.89	1.80	2.666(4)	165.4
N(23)-H(23B)···O(4W)	0.89	1.80	2.666(4)	165.4
O(1W)-H(1A)···O(2)#10	0.87(1)	2.40(4)	3.139(5)	143(5)
O(1W)-H(1B)···O(3)	0.87(1)	1.878(18)	2.732(5)	167(6)
O(2W)-H(2A)···O(4)	0.85(1)	2.02(2)	2.828(4)	158(5)
O(2W)-H(2B)···O(3)#11	0.85(1)	2.036(13)	2.882(4)	173(4)
O(3W)-H(3A)···O(1)	0.86(1)	2.085(16)	2.934(4)	168(6)
O(3W)-H(3B)···O(3)#11	0.86(1)	2.39(2)	3.232(5)	165(5)
O(4W)-H(4A)···O(1W)#12	0.87(1)	1.95(2)	2.785(6)	160(4)
O(4W)-H(4B)···O(2)#13	0.87(1)	2.62(4)	3.279(5)	133(4)
O(4W)-H(4B)···O(4)#13	0.87(1)	1.90(2)	2.723(4)	158(5)
O(5W)-H(5A)···O(6W)	0.86(1)	1.91(2)	2.717(4)	156(5)

O(5W)-H(5B)···O(2W)	0.86(1)	1.95(2)	2.772(4)	159(6)
O(6W)-H(6A)···O(2)#14	0.86(1)	2.13(3)	2.880(5)	146(5)
O(6W)-H(6B)···O(7W)	0.86(1)	2.04(1)	2.889(5)	167(5)
O(7W)-H(7A)···O(2) #15	0.86(1)	1.98(2)	2.812(4)	164(7)

Symmetry transformations to generate equivalent atoms: (#1) -x-1, -y, -z+1; (#2) x-1, -y+1/2, z-1/2; (#3) -x+1, -y, -z+2; (#4) x+1, y, z+1; (#5) -x+1, -y, -z+3; (#6) -x+1, y-1/2, -z+3/2; (#7) x-1, y, z-1; (#8) -x-1, -y, -z; (#9) -x, -y, -z+1; (#10) x, -y+1/2, z+1/2; (#11) x, -y+1/2, z-1/2; (#12) -x, -y, -z+2; (#13) -x, y-1/2, -z+3/2; (#14) x+1, y, z; (#15) x+1, -y+1/2, z+1/2.

Table S10 H-bond distances (Å) and angles (°) in $[Cu(tnz)_2(NO_3)_2]$.

D-H···A	**d(D-H)**	**d(H···A)**	**D···A**	**∠(D-H···A)**
C(4)-H(4A) ··O(2)	0.97	2.25	2.914(4)	124.7
C(4)-H(4B) ··O(3)#2	0.97	2.58	3.263(4)	127.9
C(5)-H(5A)···O(3)#2	0.97	2.47	3.126(4)	124.6
C(6)-H(6A) ···O(7)#3	0.97	2.46	3.136(4)	126.8
C(6)-H(6B) ···O(2)	0.97	2.60	3.383(4)	138.3
C(7)-H(7B)···O(7)#3	0.96	2.65	3.210(5)	118.0
C(8)-H(8B) ··O(1)#4	0.96	2.62	3.224(4)	120.9

Symmetry transformations used to generate equivalent atoms: (#1) -x+1, -y+1, -z+1; (#2) -x, y+1/2, -z+1/2; (#3) x-1, -y+3/2, z-1/2; (#4) -x+1, y+1/2, -z+1/2.