Table 1. Crystal data and structure refinement for pgamat24.

Identification code pgamat24

Empirical formula C45 H69 Cl3 Mg2 O6 Zn

Formula weight 926.34

Temperature 123(2) K

Wavelength 0.71073 Å

Crystal system MONOCLINIC

Space group P21/c

Unit cell dimensions a = 14.6632(14) Å = 90°.

b = 21.3537(19) Å = 107.164(10)°.

c = 15.8903(16) Å  = 90°.

Volume 4753.9(8) Å3

Z 4

Density (calculated) 1.294 Mg/m3

Absorption coefficient 0.756 mm-1

F(000) 1968

Crystal size 0.25 x 0.12 x 0.04 mm3

Theta range for data collection 2.40 to 23.50°.

Index ranges -16<=h<=16, -23<=k<=23, -17<=l<=17

Reflections collected 26225

Independent reflections 6899 [R(int) = 0.1164]

Completeness to theta = 23.50° 98.2 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 1.00000 and 0.59124

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 6899 / 0 / 509

Goodness-of-fit on F2 0.706

Final R indices [I>2sigma(I)] R1 = 0.0498, wR2 = 0.0682

R indices (all data) R1 = 0.1480, wR2 = 0.0785

Largest diff. peak and hole 0.595 and -0.393 e.Å-3

Table 2. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103)

for pgamat24. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn(1) 2414(1) 1773(1) 9868(1) 27(1)

Mg(1) 6460(1) 1875(1) 10165(1) 22(1)

Mg(2) 8309(1) 1844(1) 9572(1) 24(1)

Cl(1) 6708(1) 2317(1) 8791(1) 26(1)

Cl(2) 7367(1) 955(1) 9891(1) 27(1)

Cl(3) 8080(1) 2337(1) 10923(1) 26(1)

O(1) 6292(2) 1435(2) 11259(2) 25(1)

O(2) 5120(2) 1564(2) 9388(2) 28(1)

O(3) 5851(2) 2669(2) 10515(2) 29(1)

O(4) 8465(2) 1385(2) 8482(2) 28(1)

O(5) 9625(2) 1507(2) 10349(2) 29(1)

O(6) 8949(2) 2622(2) 9215(2) 31(1)

C(1) 1762(4) 1330(3) 8738(4) 29(2)

C(2) 1290(3) 1663(3) 7977(4) 29(2)

C(3) 822(4) 1385(3) 7181(4) 34(2)

C(4) 791(4) 747(3) 7072(4) 33(2)

C(5) 1258(4) 389(3) 7801(4) 33(2)

C(6) 1729(3) 676(3) 8599(4) 32(2)

C(7) 286(4) 437(3) 6211(4) 53(2)

C(8) 3045(3) 1309(3) 10985(4) 25(2)

C(9) 3056(3) 651(3) 11058(4) 31(2)

C(10) 3500(4) 338(3) 11820(4) 32(2)

C(11) 3962(4) 642(3) 12602(4) 32(2)

C(12) 3963(4) 1289(3) 12548(4) 37(2)

C(13) 3519(4) 1607(3) 11780(4) 32(2)

C(14) 4439(4) 299(3) 13427(4) 55(2)

C(15) 2412(4) 2727(2) 9890(5) 28(1)

C(16) 2330(3) 3070(3) 10619(4) 29(2)

C(17) 2346(3) 3722(3) 10654(4) 30(2)

C(18) 2432(4) 4072(2) 9957(5) 29(1)

C(19) 2518(3) 3749(3) 9223(4) 30(2)

C(20) 2498(3) 3100(3) 9194(4) 29(2)

C(21) 2496(5) 4779(2) 10010(5) 48(2)

C(22) 5720(4) 866(3) 11209(4) 34(2)

C(23) 6160(4) 515(3) 12051(4) 41(2)

C(24) 6599(4) 1035(3) 12685(4) 50(2)

C(25) 6984(4) 1460(3) 12113(4) 37(2)

C(27) 4305(15) 1095(10) 8084(13) 83(8)

C(26) 4845(10) 983(7) 8988(9) 42(4)

C(31) 5031(11) 3373(7) 11229(10) 28(5)

C(32) 5081(8) 3645(5) 10340(7) 10(3)

C(35) 8080(11) 988(8) 7072(10) 35(5)

C(38) 9676(8) 1041(7) 11090(9) 26(4)

C(40) 10919(11) 1714(9) 11556(10) 24(5)

C(43) 9185(10) 3714(6) 8987(9) 30(4)

C(44) 10025(9) 3307(6) 8871(12) 31(4)

C(261) 5117(7) 1067(5) 8671(8) 10(3)

C(271) 4015(8) 1121(6) 8115(8) 3(3)

C(311) 4896(12) 3380(8) 10935(13) 43(6)

C(321) 5522(12) 3748(7) 10588(11) 46(5)

C(381) 9784(10) 935(8) 10821(10) 41(5)

C(401) 10773(14) 1759(11) 11726(12) 47(6)

C(431) 9649(13) 3597(8) 9180(10) 50(5)

C(441) 9778(10) 3247(7) 8462(11) 38(4)

C(351) 8348(10) 1100(7) 7007(8) 14(3)

C(28) 3942(4) 1804(3) 8057(4) 46(2)

C(29) 4365(3) 2009(3) 8995(4) 33(2)

C(30) 5217(4) 2693(3) 11082(4) 38(2)

C(33) 5983(4) 3294(3) 10217(4) 40(2)

C(34) 7802(4) 1445(3) 7606(4) 37(2)

C(36) 8613(4) 501(3) 7625(4) 39(2)

C(37) 8998(4) 806(3) 8514(4) 40(2)

C(39) 10644(4) 1055(3) 11633(4) 50(2)

C(41) 10435(3) 1903(3) 10685(4) 42(2)

C(42) 8805(3) 3258(3) 9475(4) 37(2)

C(45) 9580(4) 2642(3) 8664(4) 43(2)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_Table 3. Bond lengths [Å] and angles [°] for pgamat24.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn(1)-C(1) 2.004(6)

Zn(1)-C(8) 2.005(6)

Zn(1)-C(15) 2.039(5)

Mg(1)-O(1) 2.054(4)

Mg(1)-O(3) 2.067(4)

Mg(1)-O(2) 2.096(3)

Mg(1)-Cl(2) 2.483(2)

Mg(1)-Cl(1) 2.503(2)

Mg(1)-Cl(3) 2.5253(19)

Mg(1)-Mg(2) 3.1236(18)

Mg(2)-O(4) 2.059(4)

Mg(2)-O(6) 2.067(4)

Mg(2)-O(5) 2.088(3)

Mg(2)-Cl(2) 2.487(2)

Mg(2)-Cl(3) 2.502(2)

Mg(2)-Cl(1) 2.5206(19)

O(1)-C(25) 1.436(5)

O(1)-C(22) 1.463(6)

O(2)-C(26) 1.399(13)

O(2)-C(29) 1.453(6)

O(2)-C(261) 1.557(12)

O(3)-C(33) 1.447(7)

O(3)-C(30) 1.475(6)

O(4)-C(34) 1.449(5)

O(4)-C(37) 1.457(7)

O(5)-C(381) 1.415(15)

O(5)-C(41) 1.429(6)

O(5)-C(38) 1.526(14)

O(6)-C(45) 1.449(6)

O(6)-C(42) 1.455(7)

C(1)-C(2) 1.399(7)

C(1)-C(6) 1.412(8)

C(2)-C(3) 1.382(7)

C(2)-H(2) 0.9500

C(3)-C(4) 1.373(8)

C(3)-H(3) 0.9500

C(4)-C(5) 1.388(8)

C(4)-C(7) 1.503(7)

C(5)-C(6) 1.393(8)

C(5)-H(5) 0.9500

C(6)-H(6) 0.9500

C(7)-H(7A) 0.9800

C(7)-H(7B) 0.9800

C(7)-H(7C) 0.9800

C(8)-C(13) 1.401(7)

C(8)-C(9) 1.410(8)

C(9)-C(10) 1.369(8)

C(9)-H(9) 0.9500

C(10)-C(11) 1.389(8)

C(10)-H(10) 0.9500

C(11)-C(12) 1.384(9)

C(11)-C(14) 1.484(8)

C(12)-C(13) 1.381(7)

C(12)-H(12) 0.9500

C(13)-H(13) 0.9500

C(14)-H(14A) 0.9800

C(14)-H(14B) 0.9800

C(14)-H(14C) 0.9800

C(15)-C(20) 1.399(8)

C(15)-C(16) 1.405(8)

C(16)-C(17) 1.394(8)

C(16)-H(16) 0.9500

C(17)-C(18) 1.372(8)

C(17)-H(17) 0.9500

C(18)-C(19) 1.393(8)

C(18)-C(21) 1.514(6)

C(19)-C(20) 1.386(8)

C(19)-H(19) 0.9500

C(20)-H(20) 0.9500

C(21)-H(21A) 0.9800

C(21)-H(21B) 0.9800

C(21)-H(21C) 0.9800

C(22)-C(23) 1.503(7)

C(22)-H(22A) 0.9900

C(22)-H(22B) 0.9900

C(23)-C(24) 1.511(8)

C(23)-H(23A) 0.9900

C(23)-H(23B) 0.9900

C(24)-C(25) 1.507(8)

C(24)-H(24A) 0.9900

C(24)-H(24B) 0.9900

C(25)-H(25A) 0.9900

C(25)-H(25B) 0.9900

C(27)-C(26) 1.44(2)

C(27)-C(28) 1.60(2)

C(27)-H(27Y) 0.9900

C(27)-H(27Z) 0.9900

C(26)-H(26Y) 0.9900

C(26)-H(26Z) 0.9900

C(31)-C(30) 1.509(16)

C(31)-C(32) 1.549(19)

C(31)-H(31Y) 0.9900

C(31)-H(31Z) 0.9900

C(32)-C(33) 1.583(11)

C(32)-H(32Y) 0.9900

C(32)-H(32Z) 0.9900

C(35)-C(34) 1.429(16)

C(35)-C(36) 1.436(16)

C(35)-H(35A) 0.9900

C(35)-H(35B) 0.9900

C(38)-C(39) 1.427(11)

C(38)-H(38Y) 0.9900

C(38)-H(38Z) 0.9900

C(40)-C(41) 1.415(16)

C(40)-C(39) 1.479(18)

C(40)-H(40Y) 0.9900

C(40)-H(40Z) 0.9900

C(43)-C(42) 1.454(12)

C(43)-C(44) 1.562(18)

C(43)-H(43Y) 0.9900

C(43)-H(43Z) 0.9900

C(44)-C(45) 1.558(15)

C(44)-H(44Y) 0.9900

C(44)-H(44Z) 0.9900

C(261)-C(271) 1.600(15)

C(261)-H(26A) 0.9900

C(261)-H(26B) 0.9900

C(271)-C(28) 1.463(13)

C(271)-H(27A) 0.9900

C(271)-H(27B) 0.9900

C(311)-C(321) 1.44(2)

C(311)-C(30) 1.538(18)

C(311)-H(31C) 0.9900

C(311)-H(31D) 0.9900

C(321)-C(33) 1.409(14)

C(321)-H(32C) 0.9900

C(321)-H(32D) 0.9900

C(381)-C(39) 1.536(14)

C(381)-H(38C) 0.9900

C(381)-H(38D) 0.9900

C(401)-C(39) 1.52(2)

C(401)-C(41) 1.611(19)

C(401)-H(40C) 0.9900

C(401)-H(40D) 0.9900

C(431)-C(441) 1.42(2)

C(431)-C(42) 1.618(16)

C(431)-H(43C) 0.9900

C(431)-H(43D) 0.9900

C(441)-C(45) 1.382(14)

C(441)-H(44C) 0.9900

C(441)-H(44D) 0.9900

C(351)-C(36) 1.589(15)

C(351)-C(34) 1.594(15)

C(351)-H(35C) 0.9900

C(351)-H(35D) 0.9900

C(28)-C(29) 1.500(7)

C(28)-H(28A) 0.9900

C(28)-H(28B) 0.9900

C(29)-H(29A) 0.9900

C(29)-H(29B) 0.9900

C(30)-H(30A) 0.9900

C(30)-H(30B) 0.9900

C(33)-H(33A) 0.9900

C(33)-H(33B) 0.9900

C(34)-H(34A) 0.9900

C(34)-H(34B) 0.9900

C(36)-C(37) 1.505(8)

C(36)-H(36A) 0.9900

C(36)-H(36B) 0.9900

C(37)-H(37A) 0.9900

C(37)-H(37B) 0.9900

C(39)-H(39A) 0.9900

C(39)-H(39B) 0.9900

C(41)-H(41A) 0.9900

C(41)-H(41B) 0.9900

C(42)-H(42A) 0.9900

C(42)-H(42B) 0.9900

C(45)-H(45A) 0.9900

C(45)-H(45B) 0.9900

C(1)-Zn(1)-C(8) 122.2(2)

C(1)-Zn(1)-C(15) 119.0(3)

C(8)-Zn(1)-C(15) 118.8(3)

O(1)-Mg(1)-O(3) 88.81(17)

O(1)-Mg(1)-O(2) 91.59(15)

O(3)-Mg(1)-O(2) 90.81(15)

O(1)-Mg(1)-Cl(2) 89.47(13)

O(3)-Mg(1)-Cl(2) 173.09(11)

O(2)-Mg(1)-Cl(2) 95.93(13)

O(1)-Mg(1)-Cl(1) 174.80(15)

O(3)-Mg(1)-Cl(1) 96.33(14)

O(2)-Mg(1)-Cl(1) 87.57(12)

Cl(2)-Mg(1)-Cl(1) 85.52(8)

O(1)-Mg(1)-Cl(3) 96.11(11)

O(3)-Mg(1)-Cl(3) 88.35(11)

O(2)-Mg(1)-Cl(3) 172.24(14)

Cl(2)-Mg(1)-Cl(3) 85.17(6)

Cl(1)-Mg(1)-Cl(3) 84.85(7)

O(1)-Mg(1)-Mg(2) 125.28(12)

O(3)-Mg(1)-Mg(2) 125.50(14)

O(2)-Mg(1)-Mg(2) 124.16(13)

Cl(2)-Mg(1)-Mg(2) 51.11(6)

Cl(1)-Mg(1)-Mg(2) 51.81(5)

Cl(3)-Mg(1)-Mg(2) 51.26(6)

O(4)-Mg(2)-O(6) 88.82(18)

O(4)-Mg(2)-O(5) 91.22(16)

O(6)-Mg(2)-O(5) 91.42(14)

O(4)-Mg(2)-Cl(2) 90.82(14)

O(6)-Mg(2)-Cl(2) 173.55(12)

O(5)-Mg(2)-Cl(2) 95.03(13)

O(4)-Mg(2)-Cl(3) 176.33(15)

O(6)-Mg(2)-Cl(3) 94.84(14)

O(5)-Mg(2)-Cl(3) 88.42(12)

Cl(2)-Mg(2)-Cl(3) 85.58(8)

O(4)-Mg(2)-Cl(1) 95.44(11)

O(6)-Mg(2)-Cl(1) 88.56(11)

O(5)-Mg(2)-Cl(1) 173.35(14)

Cl(2)-Mg(2)-Cl(1) 85.06(6)

Cl(3)-Mg(2)-Cl(1) 84.96(7)

O(4)-Mg(2)-Mg(1) 125.82(12)

O(6)-Mg(2)-Mg(1) 124.79(14)

O(5)-Mg(2)-Mg(1) 124.16(13)

Cl(2)-Mg(2)-Mg(1) 51.00(6)

Cl(3)-Mg(2)-Mg(1) 51.92(5)

Cl(1)-Mg(2)-Mg(1) 51.30(6)

Mg(1)-Cl(1)-Mg(2) 76.89(6)

Mg(1)-Cl(2)-Mg(2) 77.89(5)

Mg(2)-Cl(3)-Mg(1) 76.82(6)

C(25)-O(1)-C(22) 108.5(4)

C(25)-O(1)-Mg(1) 123.6(3)

C(22)-O(1)-Mg(1) 122.9(3)

C(26)-O(2)-C(29) 107.7(5)

C(26)-O(2)-C(261) 28.8(7)

C(29)-O(2)-C(261) 107.1(5)

C(26)-O(2)-Mg(1) 130.1(6)

C(29)-O(2)-Mg(1) 120.6(3)

C(261)-O(2)-Mg(1) 116.6(4)

C(33)-O(3)-C(30) 109.8(4)

C(33)-O(3)-Mg(1) 123.9(3)

C(30)-O(3)-Mg(1) 126.3(4)

C(34)-O(4)-C(37) 108.0(4)

C(34)-O(4)-Mg(2) 123.8(3)

C(37)-O(4)-Mg(2) 124.5(3)

C(381)-O(5)-C(41) 108.9(6)

C(381)-O(5)-C(38) 21.0(9)

C(41)-O(5)-C(38) 104.6(5)

C(381)-O(5)-Mg(2) 126.2(6)

C(41)-O(5)-Mg(2) 122.5(3)

C(38)-O(5)-Mg(2) 120.5(5)

C(45)-O(6)-C(42) 108.4(4)

C(45)-O(6)-Mg(2) 127.8(4)

C(42)-O(6)-Mg(2) 123.8(3)

C(2)-C(1)-C(6) 112.5(5)

C(2)-C(1)-Zn(1) 121.2(5)

C(6)-C(1)-Zn(1) 126.3(5)

C(3)-C(2)-C(1) 123.9(6)

C(3)-C(2)-H(2) 118.1

C(1)-C(2)-H(2) 118.1

C(4)-C(3)-C(2) 122.1(6)

C(4)-C(3)-H(3) 118.9

C(2)-C(3)-H(3) 118.9

C(3)-C(4)-C(5) 116.8(6)

C(3)-C(4)-C(7) 122.7(6)

C(5)-C(4)-C(7) 120.4(6)

C(4)-C(5)-C(6) 120.5(7)

C(4)-C(5)-H(5) 119.8

C(6)-C(5)-H(5) 119.8

C(5)-C(6)-C(1) 124.2(5)

C(5)-C(6)-H(6) 117.9

C(1)-C(6)-H(6) 117.9

C(4)-C(7)-H(7A) 109.5

C(4)-C(7)-H(7B) 109.5

H(7A)-C(7)-H(7B) 109.5

C(4)-C(7)-H(7C) 109.5

H(7A)-C(7)-H(7C) 109.5

H(7B)-C(7)-H(7C) 109.5

C(13)-C(8)-C(9) 112.8(5)

C(13)-C(8)-Zn(1) 123.4(5)

C(9)-C(8)-Zn(1) 123.8(5)

C(10)-C(9)-C(8) 123.4(5)

C(10)-C(9)-H(9) 118.3

C(8)-C(9)-H(9) 118.3

C(9)-C(10)-C(11) 122.8(6)

C(9)-C(10)-H(10) 118.6

C(11)-C(10)-H(10) 118.6

C(12)-C(11)-C(10) 114.9(5)

C(12)-C(11)-C(14) 122.6(6)

C(10)-C(11)-C(14) 122.5(7)

C(13)-C(12)-C(11) 122.4(6)

C(13)-C(12)-H(12) 118.8

C(11)-C(12)-H(12) 118.8

C(12)-C(13)-C(8) 123.6(6)

C(12)-C(13)-H(13) 118.2

C(8)-C(13)-H(13) 118.2

C(11)-C(14)-H(14A) 109.5

C(11)-C(14)-H(14B) 109.5

H(14A)-C(14)-H(14B) 109.5

C(11)-C(14)-H(14C) 109.5

H(14A)-C(14)-H(14C) 109.5

H(14B)-C(14)-H(14C) 109.5

C(20)-C(15)-C(16) 113.9(4)

C(20)-C(15)-Zn(1) 123.7(5)

C(16)-C(15)-Zn(1) 122.4(5)

C(17)-C(16)-C(15) 123.3(6)

C(17)-C(16)-H(16) 118.4

C(15)-C(16)-H(16) 118.4

C(18)-C(17)-C(16) 121.1(6)

C(18)-C(17)-H(17) 119.5

C(16)-C(17)-H(17) 119.5

C(17)-C(18)-C(19) 117.3(4)

C(17)-C(18)-C(21) 121.1(7)

C(19)-C(18)-C(21) 121.4(7)

C(20)-C(19)-C(18) 121.1(6)

C(20)-C(19)-H(19) 119.5

C(18)-C(19)-H(19) 119.5

C(19)-C(20)-C(15) 123.3(6)

C(19)-C(20)-H(20) 118.4

C(15)-C(20)-H(20) 118.4

C(18)-C(21)-H(21A) 109.5

C(18)-C(21)-H(21B) 109.5

H(21A)-C(21)-H(21B) 109.5

C(18)-C(21)-H(21C) 109.5

H(21A)-C(21)-H(21C) 109.5

H(21B)-C(21)-H(21C) 109.5

O(1)-C(22)-C(23) 106.1(4)

O(1)-C(22)-H(22A) 110.5

C(23)-C(22)-H(22A) 110.5

O(1)-C(22)-H(22B) 110.5

C(23)-C(22)-H(22B) 110.5

H(22A)-C(22)-H(22B) 108.7

C(22)-C(23)-C(24) 102.3(5)

C(22)-C(23)-H(23A) 111.3

C(24)-C(23)-H(23A) 111.3

C(22)-C(23)-H(23B) 111.3

C(24)-C(23)-H(23B) 111.3

H(23A)-C(23)-H(23B) 109.2

C(25)-C(24)-C(23) 101.7(5)

C(25)-C(24)-H(24A) 111.4

C(23)-C(24)-H(24A) 111.4

C(25)-C(24)-H(24B) 111.4

C(23)-C(24)-H(24B) 111.4

H(24A)-C(24)-H(24B) 109.3

O(1)-C(25)-C(24) 105.1(4)

O(1)-C(25)-H(25A) 110.7

C(24)-C(25)-H(25A) 110.7

O(1)-C(25)-H(25B) 110.7

C(24)-C(25)-H(25B) 110.7

H(25A)-C(25)-H(25B) 108.8

C(26)-C(27)-C(28) 105.3(14)

C(26)-C(27)-H(27Y) 110.7

C(28)-C(27)-H(27Y) 110.7

C(26)-C(27)-H(27Z) 110.7

C(28)-C(27)-H(27Z) 110.7

H(27Y)-C(27)-H(27Z) 108.8

O(2)-C(26)-C(27) 107.8(13)

O(2)-C(26)-H(26Y) 110.1

C(27)-C(26)-H(26Y) 110.1

O(2)-C(26)-H(26Z) 110.1

C(27)-C(26)-H(26Z) 110.1

H(26Y)-C(26)-H(26Z) 108.5

C(30)-C(31)-C(32) 99.2(10)

C(30)-C(31)-H(31Y) 111.9

C(32)-C(31)-H(31Y) 111.9

C(30)-C(31)-H(31Z) 111.9

C(32)-C(31)-H(31Z) 111.9

H(31Y)-C(31)-H(31Z) 109.6

C(31)-C(32)-C(33) 101.6(8)

C(31)-C(32)-H(32Y) 111.4

C(33)-C(32)-H(32Y) 111.4

C(31)-C(32)-H(32Z) 111.4

C(33)-C(32)-H(32Z) 111.4

H(32Y)-C(32)-H(32Z) 109.3

C(34)-C(35)-C(36) 109.2(11)

C(34)-C(35)-H(35A) 109.8

C(36)-C(35)-H(35A) 109.8

C(34)-C(35)-H(35B) 109.8

C(36)-C(35)-H(35B) 109.8

H(35A)-C(35)-H(35B) 108.3

C(39)-C(38)-O(5) 105.5(8)

C(39)-C(38)-H(38Y) 110.6

O(5)-C(38)-H(38Y) 110.6

C(39)-C(38)-H(38Z) 110.6

O(5)-C(38)-H(38Z) 110.6

H(38Y)-C(38)-H(38Z) 108.8

C(41)-C(40)-C(39) 106.4(10)

C(41)-C(40)-H(40Y) 110.5

C(39)-C(40)-H(40Y) 110.5

C(41)-C(40)-H(40Z) 110.5

C(39)-C(40)-H(40Z) 110.5

H(40Y)-C(40)-H(40Z) 108.6

C(42)-C(43)-C(44) 97.6(9)

C(42)-C(43)-H(43Y) 112.3

C(44)-C(43)-H(43Y) 112.3

C(42)-C(43)-H(43Z) 112.3

C(44)-C(43)-H(43Z) 112.3

H(43Y)-C(43)-H(43Z) 109.9

C(45)-C(44)-C(43) 103.6(8)

C(45)-C(44)-H(44Y) 111.0

C(43)-C(44)-H(44Y) 111.0

C(45)-C(44)-H(44Z) 111.0

C(43)-C(44)-H(44Z) 111.0

H(44Y)-C(44)-H(44Z) 109.0

O(2)-C(261)-C(271) 98.0(8)

O(2)-C(261)-H(26A) 112.2

C(271)-C(261)-H(26A) 112.2

O(2)-C(261)-H(26B) 112.2

C(271)-C(261)-H(26B) 112.2

H(26A)-C(261)-H(26B) 109.8

C(28)-C(271)-C(261) 98.7(8)

C(28)-C(271)-H(27A) 112.0

C(261)-C(271)-H(27A) 112.0

C(28)-C(271)-H(27B) 112.0

C(261)-C(271)-H(27B) 112.0

H(27A)-C(271)-H(27B) 109.7

C(321)-C(311)-C(30) 112.3(12)

C(321)-C(311)-H(31C) 109.1

C(30)-C(311)-H(31C) 109.1

C(321)-C(311)-H(31D) 109.1

C(30)-C(311)-H(31D) 109.1

H(31C)-C(311)-H(31D) 107.9

C(33)-C(321)-C(311) 102.9(12)

C(33)-C(321)-H(32C) 111.2

C(311)-C(321)-H(32C) 111.2

C(33)-C(321)-H(32D) 111.2

C(311)-C(321)-H(32D) 111.2

H(32C)-C(321)-H(32D) 109.1

O(5)-C(381)-C(39) 105.5(9)

O(5)-C(381)-H(38C) 110.6

C(39)-C(381)-H(38C) 110.6

O(5)-C(381)-H(38D) 110.6

C(39)-C(381)-H(38D) 110.6

H(38C)-C(381)-H(38D) 108.8

C(39)-C(401)-C(41) 95.6(11)

C(39)-C(401)-H(40C) 112.6

C(41)-C(401)-H(40C) 112.6

C(39)-C(401)-H(40D) 112.6

C(41)-C(401)-H(40D) 112.6

H(40C)-C(401)-H(40D) 110.1

C(441)-C(431)-C(42) 107.0(10)

C(441)-C(431)-H(43C) 110.3

C(42)-C(431)-H(43C) 110.3

C(441)-C(431)-H(43D) 110.3

C(42)-C(431)-H(43D) 110.3

H(43C)-C(431)-H(43D) 108.6

C(45)-C(441)-C(431) 102.5(11)

C(45)-C(441)-H(44C) 111.3

C(431)-C(441)-H(44C) 111.3

C(45)-C(441)-H(44D) 111.3

C(431)-C(441)-H(44D) 111.3

H(44C)-C(441)-H(44D) 109.2

C(36)-C(351)-C(34) 94.4(8)

C(36)-C(351)-H(35C) 112.8

C(34)-C(351)-H(35C) 112.8

C(36)-C(351)-H(35D) 112.8

C(34)-C(351)-H(35D) 112.8

H(35C)-C(351)-H(35D) 110.3

C(271)-C(28)-C(29) 103.1(6)

C(271)-C(28)-C(27) 15.9(10)

C(29)-C(28)-C(27) 102.3(8)

C(271)-C(28)-H(28A) 124.2

C(29)-C(28)-H(28A) 111.3

C(27)-C(28)-H(28A) 111.3

C(271)-C(28)-H(28B) 96.7

C(29)-C(28)-H(28B) 111.3

C(27)-C(28)-H(28B) 111.3

H(28A)-C(28)-H(28B) 109.2

O(2)-C(29)-C(28) 106.0(5)

O(2)-C(29)-H(29A) 110.5

C(28)-C(29)-H(29A) 110.5

O(2)-C(29)-H(29B) 110.5

C(28)-C(29)-H(29B) 110.5

H(29A)-C(29)-H(29B) 108.7

O(3)-C(30)-C(31) 107.6(7)

O(3)-C(30)-C(311) 99.2(8)

C(31)-C(30)-C(311) 17.0(9)

O(3)-C(30)-H(30A) 110.2

C(31)-C(30)-H(30A) 110.2

C(311)-C(30)-H(30A) 127.1

O(3)-C(30)-H(30B) 110.2

C(31)-C(30)-H(30B) 110.2

C(311)-C(30)-H(30B) 100.6

H(30A)-C(30)-H(30B) 108.5

C(321)-C(33)-O(3) 111.8(8)

C(321)-C(33)-C(32) 25.7(6)

O(3)-C(33)-C(32) 101.4(6)

C(321)-C(33)-H(33A) 123.9

O(3)-C(33)-H(33A) 111.5

C(32)-C(33)-H(33A) 111.5

C(321)-C(33)-H(33B) 85.8

O(3)-C(33)-H(33B) 111.5

C(32)-C(33)-H(33B) 111.5

H(33A)-C(33)-H(33B) 109.3

C(35)-C(34)-O(4) 106.4(7)

C(35)-C(34)-C(351) 17.8(9)

O(4)-C(34)-C(351) 102.7(5)

C(35)-C(34)-H(34A) 110.4

O(4)-C(34)-H(34A) 110.4

C(351)-C(34)-H(34A) 127.0

C(35)-C(34)-H(34B) 110.4

O(4)-C(34)-H(34B) 110.4

C(351)-C(34)-H(34B) 96.4

H(34A)-C(34)-H(34B) 108.6

C(35)-C(36)-C(37) 104.3(8)

C(35)-C(36)-C(351) 17.9(8)

C(37)-C(36)-C(351) 100.7(7)

C(35)-C(36)-H(36A) 110.9

C(37)-C(36)-H(36A) 110.9

C(351)-C(36)-H(36A) 96.6

C(35)-C(36)-H(36B) 110.9

C(37)-C(36)-H(36B) 110.9

C(351)-C(36)-H(36B) 127.5

H(36A)-C(36)-H(36B) 108.9

O(4)-C(37)-C(36) 106.6(4)

O(4)-C(37)-H(37A) 110.4

C(36)-C(37)-H(37A) 110.4

O(4)-C(37)-H(37B) 110.4

C(36)-C(37)-H(37B) 110.4

H(37A)-C(37)-H(37B) 108.6

C(38)-C(39)-C(40) 102.5(9)

C(38)-C(39)-C(401) 98.8(10)

C(40)-C(39)-C(401) 15.4(11)

C(38)-C(39)-C(381) 20.9(9)

C(40)-C(39)-C(381) 105.4(9)

C(401)-C(39)-C(381) 107.2(10)

C(38)-C(39)-H(39A) 111.3

C(40)-C(39)-H(39A) 111.3

C(401)-C(39)-H(39A) 125.9

C(381)-C(39)-H(39A) 91.4

C(38)-C(39)-H(39B) 111.3

C(40)-C(39)-H(39B) 111.3

C(401)-C(39)-H(39B) 99.5

C(381)-C(39)-H(39B) 126.5

H(39A)-C(39)-H(39B) 109.2

C(40)-C(41)-O(5) 108.6(8)

C(40)-C(41)-C(401) 13.4(12)

O(5)-C(41)-C(401) 103.9(9)

C(40)-C(41)-H(41A) 110.0

O(5)-C(41)-H(41A) 110.0

C(401)-C(41)-H(41A) 123.1

C(40)-C(41)-H(41B) 110.0

O(5)-C(41)-H(41B) 110.0

C(401)-C(41)-H(41B) 100.9

H(41A)-C(41)-H(41B) 108.4

C(43)-C(42)-O(6) 111.3(7)

C(43)-C(42)-C(431) 25.8(6)

O(6)-C(42)-C(431) 98.5(8)

C(43)-C(42)-H(42A) 109.4

O(6)-C(42)-H(42A) 109.4

C(431)-C(42)-H(42A) 135.0

C(43)-C(42)-H(42B) 109.4

O(6)-C(42)-H(42B) 109.4

C(431)-C(42)-H(42B) 94.4

H(42A)-C(42)-H(42B) 108.0

C(441)-C(45)-O(6) 112.6(8)

C(441)-C(45)-C(44) 24.9(7)

O(6)-C(45)-C(44) 101.7(7)

C(441)-C(45)-H(45A) 86.5

O(6)-C(45)-H(45A) 111.4

C(44)-C(45)-H(45A) 111.4

C(441)-C(45)-H(45B) 122.7

O(6)-C(45)-H(45B) 111.4

C(44)-C(45)-H(45B) 111.4

H(45A)-C(45)-H(45B) 109.3

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for pgamat24. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

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Zn(1) 26(1) 24(1) 31(1) -1(1) 9(1) 0(1)

Mg(1) 21(1) 20(1) 26(1) -4(1) 8(1) -2(1)

Mg(2) 21(1) 24(1) 26(1) 4(1) 8(1) -1(1)

Cl(1) 25(1) 27(1) 27(1) 3(1) 8(1) 3(1)

Cl(2) 28(1) 20(1) 34(1) -2(1) 12(1) -3(1)

Cl(3) 25(1) 27(1) 25(1) -3(1) 8(1) -3(1)

O(1) 28(2) 20(3) 26(2) 2(2) 7(2) -7(2)

O(2) 26(2) 25(3) 30(2) -4(2) 4(2) -6(2)

O(3) 28(2) 23(3) 39(2) -6(2) 16(2) -3(2)

O(4) 29(2) 28(3) 28(3) 2(2) 8(2) 10(2)

O(5) 26(2) 26(3) 31(2) 6(2) 4(2) -3(2)

O(6) 33(2) 29(3) 38(3) -1(2) 19(2) -3(2)

C(1) 27(3) 20(5) 44(5) -4(4) 18(3) 1(3)

C(2) 34(3) 18(4) 40(4) -4(4) 20(3) -5(3)

C(3) 52(4) 19(4) 34(4) -1(3) 17(3) 2(3)

C(4) 34(3) 36(5) 31(4) -2(4) 12(3) -2(3)

C(5) 37(4) 20(4) 39(4) -7(4) 10(3) -2(3)

C(6) 24(3) 38(5) 30(4) 10(4) 3(3) 3(3)

C(7) 74(4) 37(5) 39(4) -8(4) 5(4) 6(4)

C(8) 23(3) 19(5) 37(4) 5(3) 14(3) -3(3)

C(9) 25(3) 30(5) 36(4) -5(4) 9(3) -6(3)

C(10) 41(4) 20(4) 40(4) 2(4) 17(3) -2(3)

C(11) 47(4) 28(5) 26(4) 12(4) 19(3) 4(3)

C(12) 37(4) 42(5) 28(4) 3(4) 3(3) 4(3)

C(13) 39(3) 19(5) 40(4) 4(4) 14(3) -3(3)

C(14) 82(5) 57(5) 30(4) 11(4) 23(4) 17(4)

C(15) 16(2) 34(3) 34(4) -5(5) 8(2) -4(4)

C(16) 16(3) 43(6) 28(4) 5(4) 6(3) -1(3)

C(17) 27(3) 25(5) 32(4) -4(4) 0(3) 10(3)

C(18) 18(3) 16(3) 51(4) 12(4) 5(3) 2(3)

C(19) 29(3) 29(5) 32(4) 9(3) 13(3) -3(3)

C(20) 24(3) 26(5) 37(4) -3(3) 8(3) -4(3)

C(21) 53(3) 28(3) 61(4) 3(5) 15(3) 0(5)

C(22) 39(3) 23(4) 40(4) -5(3) 15(3) -13(3)

C(23) 40(4) 25(5) 62(5) 8(4) 23(4) -5(3)

C(24) 45(4) 57(5) 42(4) 17(4) 5(3) -8(4)

C(25) 43(4) 39(5) 28(4) 1(3) 9(3) -16(3)

C(28) 49(4) 48(4) 33(4) 10(4) -4(3) 1(4)

C(29) 20(3) 34(4) 43(4) 8(3) 4(3) 5(3)

C(30) 39(3) 48(5) 31(4) 6(4) 15(3) 6(3)

C(33) 50(4) 25(5) 42(4) -3(4) 12(3) -7(3)

C(34) 43(4) 36(5) 27(4) 1(3) 3(3) 13(3)

C(36) 37(3) 39(5) 45(4) -10(4) 17(3) -3(3)

C(37) 34(3) 50(6) 40(4) 11(4) 17(3) 20(3)

C(39) 81(5) 40(5) 20(4) 12(3) -1(4) 16(4)

C(41) 27(3) 54(5) 42(4) 15(4) 5(3) -8(3)

C(42) 31(3) 28(5) 58(4) 2(4) 25(3) -13(3)

C(45) 43(4) 58(6) 37(4) 9(4) 25(3) -13(4)

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\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Symmetry transformations used to generate equivalent atoms: