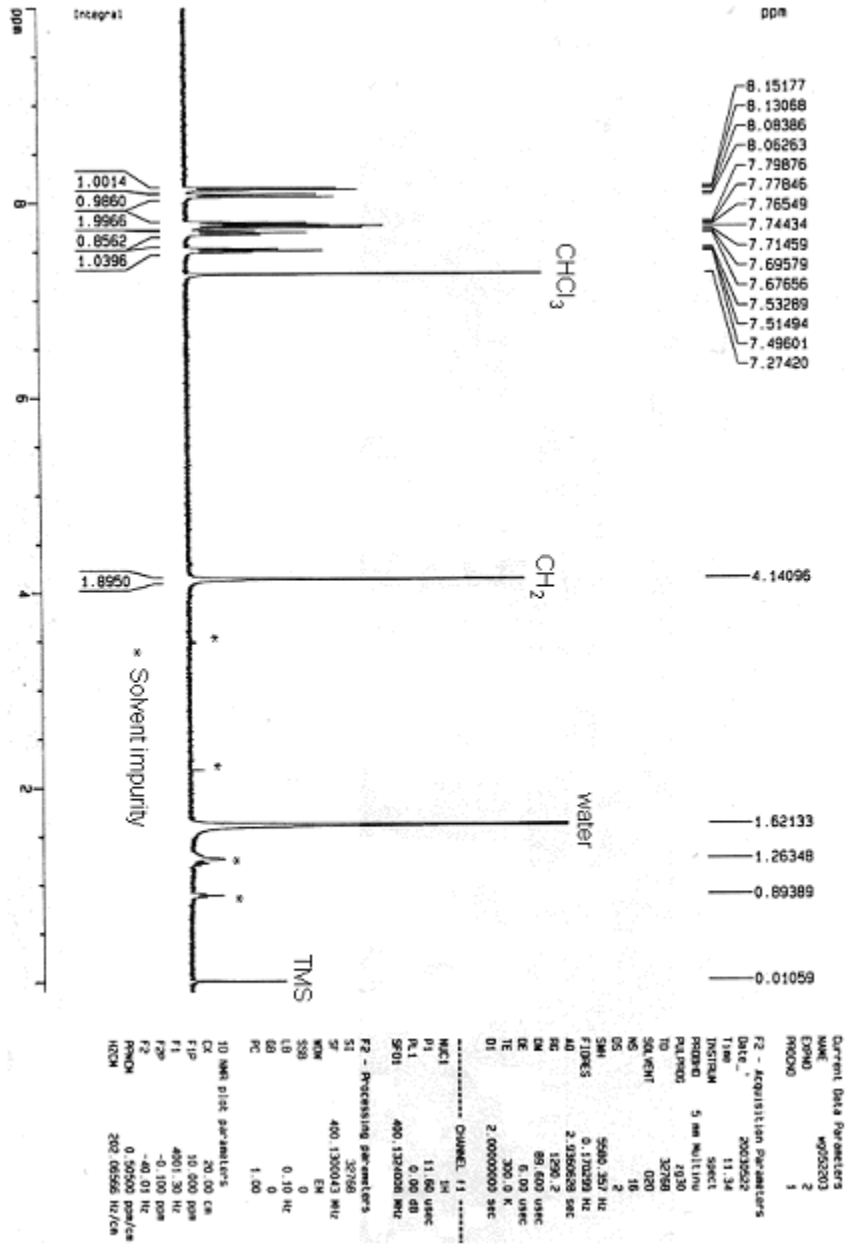
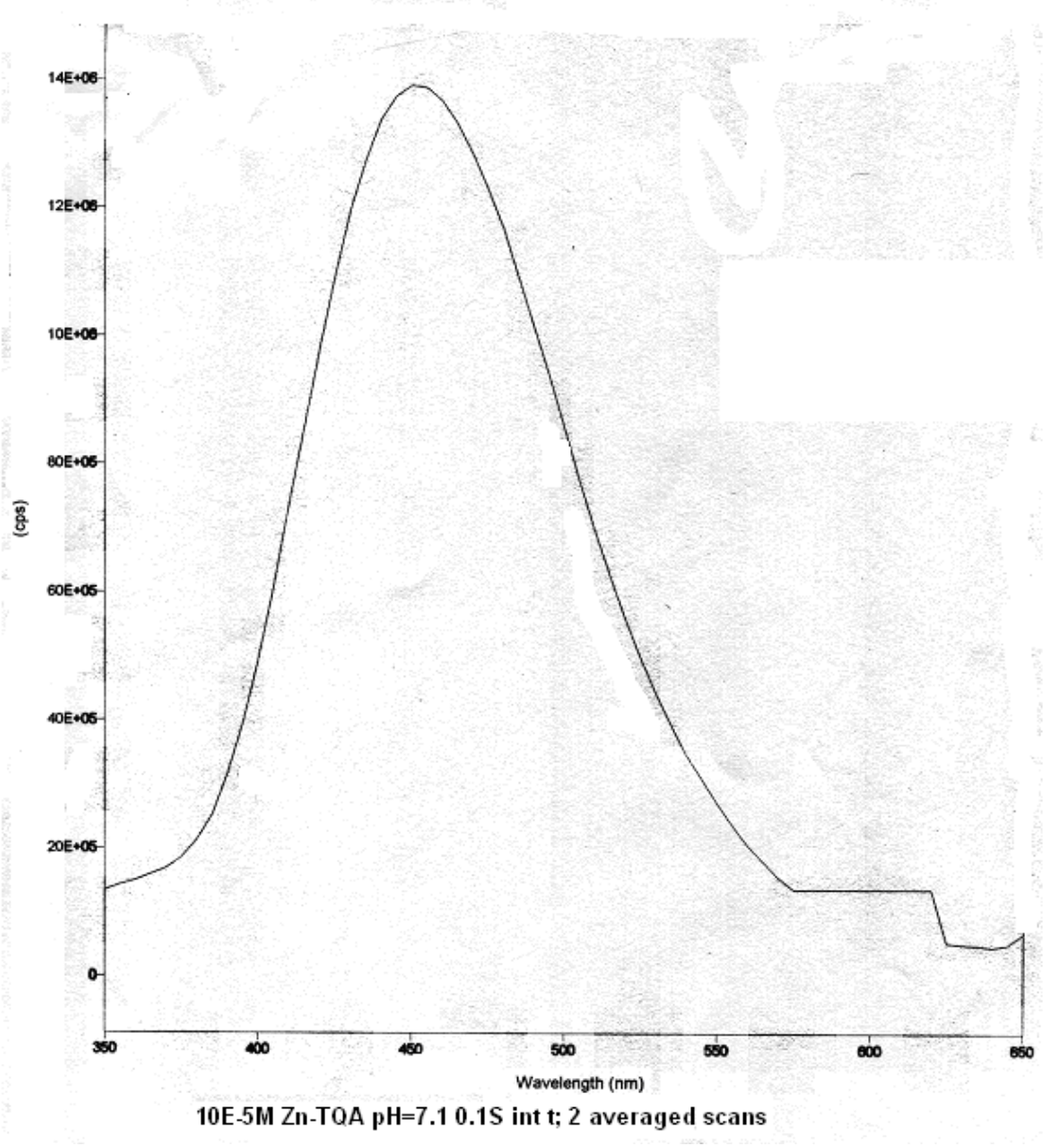
APPENDICES

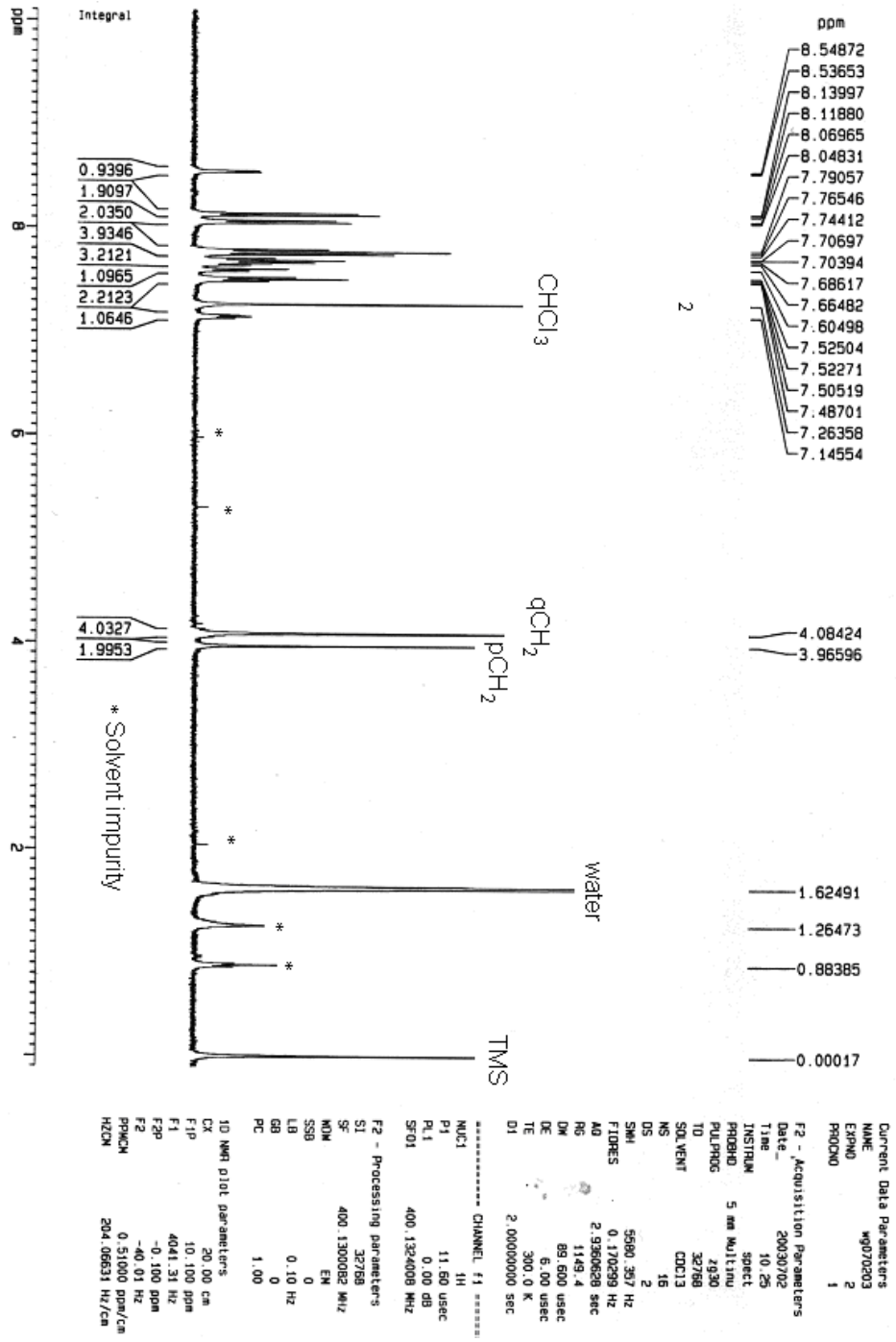
Appendix-1. $^{1}H$ NMR spectrum of TQA



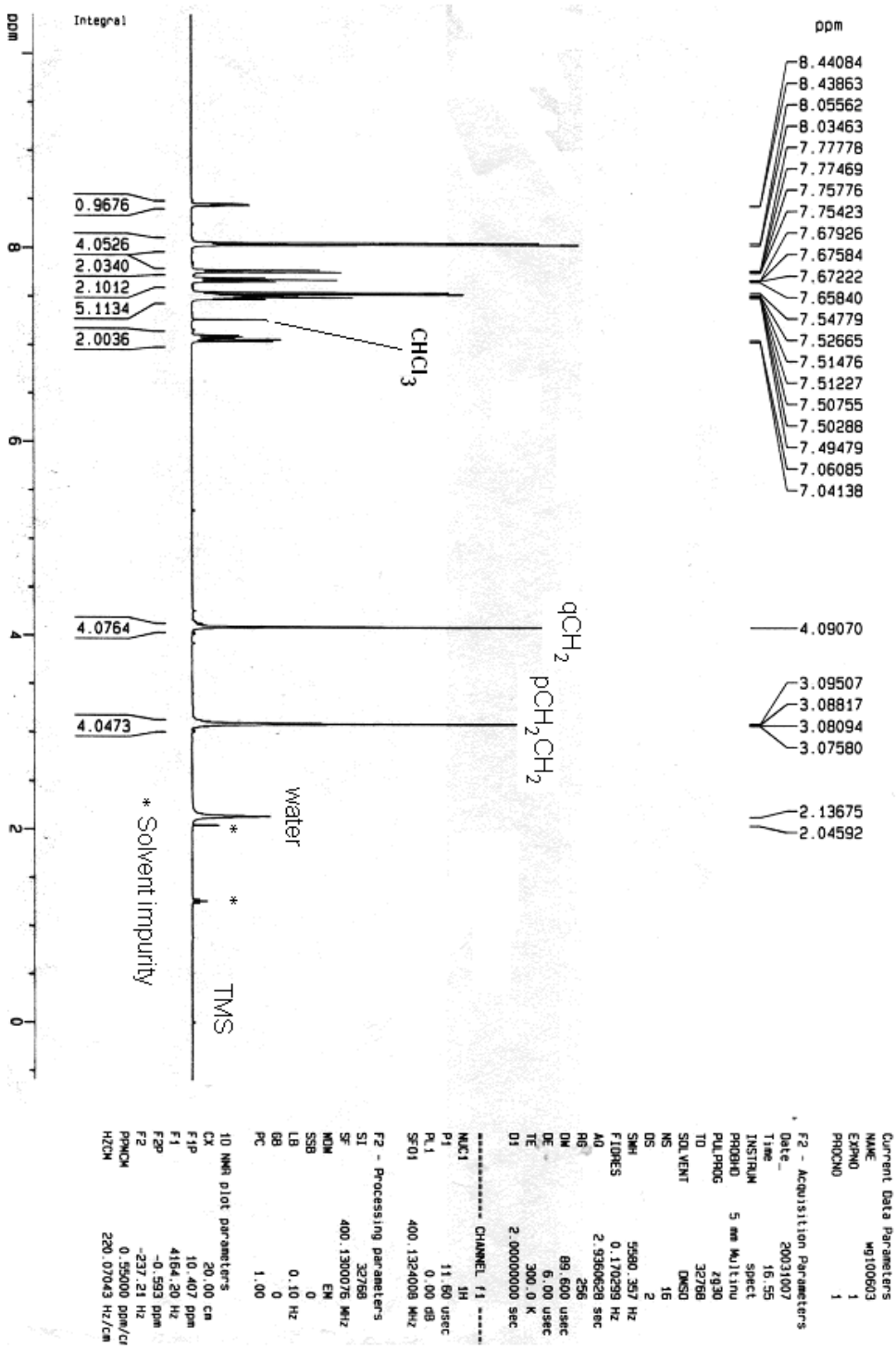
Appendix-2. The Fluorescence spectrum of $Zn^{2+}$-TQA



Appendix-3. $^{1}H$ NMR spectrum of DQPMA

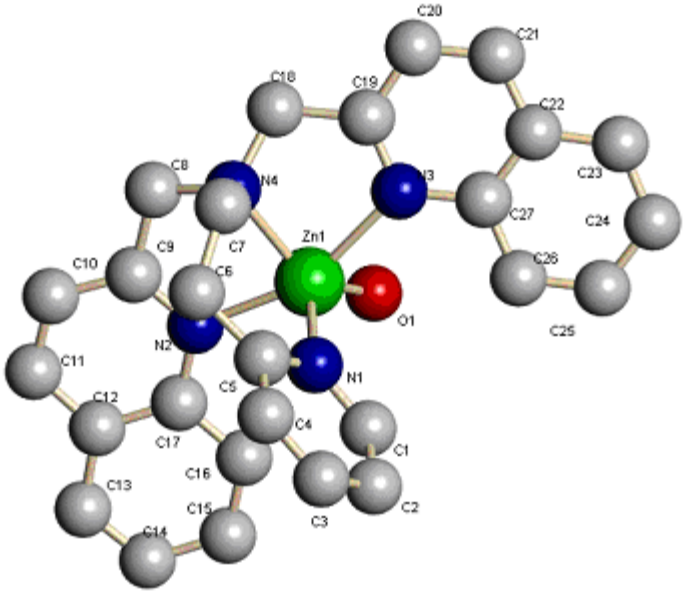


Appendix-4. $^{1}H$ NMR spectrum of DQPEA

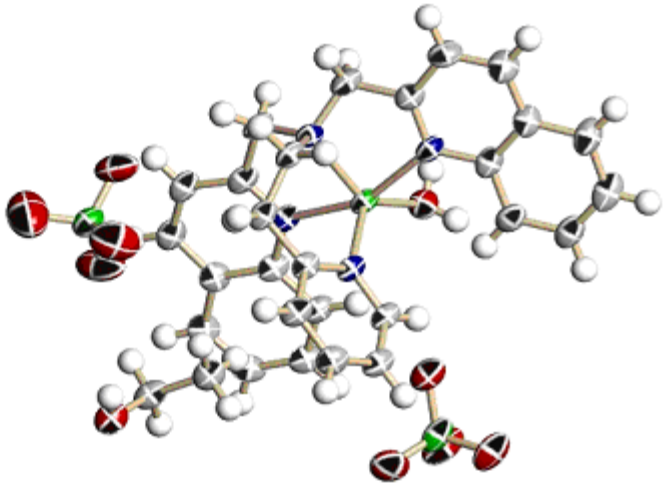


Appendix-5. The crystal structure of $Zn^{2+}$-DQPEA. a) HyperChem (Std. 5.1) drawing of $Zn^{2+}$-DQPEA; b) ORTEP diagram of $Zn^{2+}$-DQPEA

a




b



Appendix-6. Crystal data and structure refinement for $Zn^{2+}$-DQPEA

| | | |
|---|---|---|
| Identification code | rh52 | |
| Empirical formula | C14.50 H16 Cl N2 O5 Zn0.50 | |
| Formula weight | 366.43 | |
| Temperature | 110(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 9.2906(10) Å | α= 82.748(7)°. |
| | b = 10.3943(10) Å | β= 88.519(7)°. |
| | c = 17.3880(18) Å | γ = 66.957(6)°. |
| Volume | 1532.3(3) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.588 $Mg/m^3$ | |
| Absorption coefficient | 1.041 $mm^{-1}$ | |
| F(000) | 756 | |
| Crystal size | 0.20 x 0.10 x 0.10 $mm^3$ | |
| Theta range for data collection | 2.15 to 25.00°. | |
| Index ranges | -9<=h<=11, -12<=k<=12, -20<=l<=20 | |
| Reflections collected | 10644 | |
| Independent reflections | 5042 [R(int) = 0.0479] | |
| Completeness to theta = 25.00° | 93.4 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9031 and 0.8189 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5042 / 0 / 415 | |
| Goodness-of-fit on $F^2$ | 1.053 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0730, wR2 = 0.1850 | |
| R indices (all data) | R1 = 0.0894, wR2 = 0.1988 | |
| Largest diff. peak and hole | 1.285 and -0.805 $e.Å^{-3}$ | |

Appendix-7. Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for $Zn^{2+}$-DQPEA.

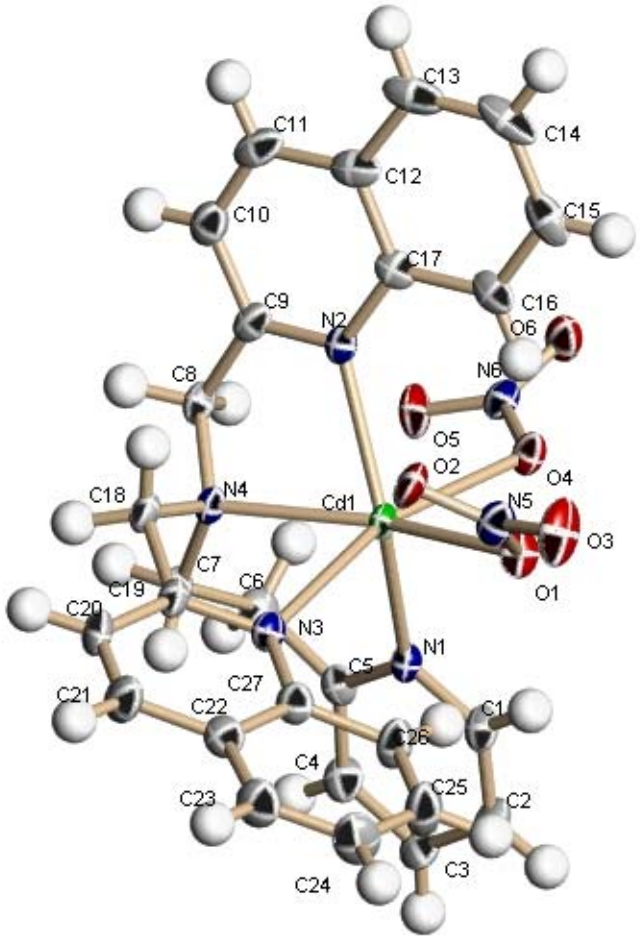
| | x | y | z | U(eq) | | x | y | z | U(eq) |
|---|---|---|---|---|---|---|---|---|---|
| Zn(1) | 478(1) | 1975(1) | 2429(1) | 27(1) | C(8) | 2413(7) | 369(6) | 1226(3) | 33(1) |
| Cl(1) | 7176(2) | 1037(2) | 1019(1) | 39(1) | C(9) | 2126(6) | 1910(6) | 979(3) | 33(1) |
| Cl(2) | 3540(2) | 3520(2) | 6312(1) | 42(1) | C(10) | 2884(7) | 2272(6) | 321(3) | 36(1) |
| O(1) | -1840(4) | 3002(4) | 2263(2) | 38(1) | C(11) | 2616(7) | 3647(7) | 98(3) | 37(1) |
| O(2) | 6376(7) | 140(6) | 915(3) | 68(2) | C(12) | 1623(6) | 4696(6) | 526(3) | 33(1) |
| O(3) | 7637(8) | 725(7) | 1831(3) | 84(2) | C(13) | 1317(7) | 6167(6) | 333(3) | 39(1) |
| O(4) | 6202(6) | 2494(5) | 868(4) | 80(2) | C(14) | 317(7) | 7131(6) | 763(3) | 37(1) |
| O(5) | 8508(8) | 683(7) | 590(5) | 100(2) | C(15) | -417(7) | 6720(6) | 1398(3) | 37(1) |
| O(6) | 3836(5) | 2159(5) | 6084(3) | 49(1) | C(16) | -124(7) | 5299(6) | 1616(3) | 33(1) |
| O(7) | 2995(6) | 3545(6) | 7089(2) | 58(1) | C(17) | 886(6) | 4273(6) | 1178(3) | 31(1) |
| O(8) | 2347(6) | 4575(5) | 5804(3) | 59(1) | C(18) | 1483(7) | -1010(6) | 2210(3) | 37(1) |
| O(9) | 4907(7) | 3756(6) | 6286(3) | 63(1) | C(19) | 578(6) | -887(6) | 2954(3) | 32(1) |
| N(1) | 1791(5) | 2554(4) | 3136(2) | 26(1) | C(20) | 337(7) | -2061(6) | 3326(3) | 39(1) |
| N(2) | 1167(5) | 2869(5) | 1392(2) | 29(1) | C(21) | -578(7) | -1895(6) | 3962(3) | 41(1) |
| N(3) | -7(5) | 382(4) | 3196(2) | 29(1) | C(22) | -1254(6) | -562(6) | 4227(3) | 34(1) |
| N(4) | 2110(5) | 108(4) | 2060(2) | 27(1) | C(23) | -2236(7) | -322(7) | 4883(3) | 45(2) |
| C(1) | 1103(6) | 3608(5) | 3579(3) | 30(1) | C(24) | -2825(7) | 1013(7) | 5126(3) | 46(2) |
| C(2) | 1936(7) | 4039(6) | 4063(3) | 34(1) | C(25) | -2499(7) | 2109(7) | 4738(3) | 39(1) |
| C(3) | 3548(7) | 3374(6) | 4085(3) | 38(1) | C(26) | -1567(7) | 1906(6) | 4101(3) | 36(1) |
| C(4) | 4260(7) | 2320(6) | 3630(3) | 36(1) | C(27) | -945(6) | 561(6) | 3839(3) | 33(1) |
| C(5) | 3357(6) | 1921(6) | 3144(3) | 28(1) | O(10) | 6222(5) | 5528(5) | 1627(2) | 44(1) |
| C(6) | 4171(6) | 828(6) | 2604(3) | 33(1) | C(28) | 4005(7) | 4997(7) | 2079(3) | 41(1) |
| C(7) | 3537(6) | -308(5) | 2548(3) | 30(1) | C(29) | 4683(7) | 5673(6) | 1433(3) | 39(1) |

U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

Appendix-8. Bond lengths [Å] and angles [°] for $Zn^{2+}$-DQPEA.

| | | | | | |
|---|---|---|---|---|---|
| Zn(1)-O(1) | 2.003(4) | C(22)-C(23) | 1.428(8) | C(18)-N(4)-Zn(1) | 108.8(3) |
| Zn(1)-N(1) | 2.050(4) | C(23)-C(24) | 1.394(10) | N(1)-C(1)-C(2) | 123.2(5) |
| Zn(1)-N(4) | 2.107(4) | C(24)-C(25) | 1.383(10) | C(3)-C(2)-C(1) | 118.0(5) |
| Zn(1)-N(2) | 2.123(5) | C(25)-C(26) | 1.375(8) | C(4)-C(3)-C(2) | 119.4(5) |
| Zn(1)-N(3) | 2.172(5) | C(26)-C(27) | 1.418(8) | C(3)-C(4)-C(5) | 120.4(5) |
| Cl(1)-O(5) | 1.375(7) | O(10)-C(29) | 1.423(8) | N(1)-C(5)-C(4) | 119.9(5) |
| Cl(1)-O(4) | 1.422(5) | C(28)-C(29) | 1.504(9) | N(1)-C(5)-C(6) | 120.5(5) |
| Cl(1)-O(2) | 1.430(6) | O(1)-Zn(1)-N(1) | 123.55(16) | C(4)-C(5)-C(6) | 119.6(5) |
| Cl(1)-O(3) | 1.446(6) | O(1)-Zn(1)-N(4) | 132.93(17) | C(5)-C(6)-C(7) | 117.4(5) |
| Cl(2)-O(9) | 1.383(6) | N(1)-Zn(1)-N(4) | 103.36(16) | N(4)-C(7)-C(6) | 116.5(4) |
| Cl(2)-O(7) | 1.430(5) | O(1)-Zn(1)-N(2) | 97.61(16) | N(4)-C(8)-C(9) | 111.6(4) |
| Cl(2)-O(8) | 1.438(4) | N(1)-Zn(1)-N(2) | 94.09(17) | N(2)-C(9)-C(10) | 122.2(6) |
| Cl(2)-O(6) | 1.438(5) | N(4)-Zn(1)-N(2) | 81.34(16) | N(2)-C(9)-C(8) | 118.4(5) |
| N(1)-C(5) | 1.342(7) | O(1)-Zn(1)-N(3) | 87.45(17) | C(10)-C(9)-C(8) | 119.4(5) |
| N(1)-C(1) | 1.357(6) | N(1)-Zn(1)-N(3) | 102.07(16) | C(11)-C(10)-C(9) | 119.2(5) |
| N(2)-C(9) | 1.326(7) | N(4)-Zn(1)-N(3) | 78.65(16) | C(10)-C(11)-C(12) | 120.4(6) |
| N(2)-C(17) | 1.380(7) | N(2)-Zn(1)-N(3) | 156.68(17) | C(11)-C(12)-C(17) | 118.0(5) |
| N(3)-C(19) | 1.334(7) | O(5)-Cl(1)-O(4) | 112.2(4) | C(11)-C(12)-C(13) | 123.2(6) |
| N(3)-C(27) | 1.385(7) | O(5)-Cl(1)-O(2) | 110.3(4) | C(17)-C(12)-C(13) | 118.8(5) |
| N(4)-C(7) | 1.478(7) | O(4)-Cl(1)-O(2) | 113.1(3) | C(14)-C(13)-C(12) | 120.1(6) |
| N(4)-C(8) | 1.481(7) | O(5)-Cl(1)-O(3) | 108.2(5) | C(13)-C(14)-C(15) | 121.1(6) |
| N(4)-C(18) | 1.484(8) | O(4)-Cl(1)-O(3) | 108.0(4) | C(14)-C(15)-C(16) | 120.6(5) |
| C(1)-C(2) | 1.382(8) | O(2)-Cl(1)-O(3) | 104.6(4) | C(15)-C(16)-C(17) | 119.9(6) |
| C(2)-C(3) | 1.381(8) | O(9)-Cl(2)-O(7) | 109.1(3) | N(2)-C(17)-C(16) | 119.8(5) |
| C(3)-C(4) | 1.374(8) | O(9)-Cl(2)-O(8) | 111.3(4) | N(2)-C(17)-C(12) | 120.8(5) |
| C(4)-C(5) | 1.410(8) | O(7)-Cl(2)-O(8) | 109.2(3) | C(16)-C(17)-C(12) | 119.4(5) |
| C(5)-C(6) | 1.517(7) | O(9)-Cl(2)-O(6) | 109.8(3) | N(4)-C(18)-C(19) | 111.4(4) |
| C(6)-C(7) | 1.525(8) | O(7)-Cl(2)-O(6) | 108.6(3) | N(3)-C(19)-C(20) | 123.7(5) |
| C(8)-C(9) | 1.523(8) | O(8)-Cl(2)-O(6) | 108.7(3) | N(3)-C(19)-C(18) | 116.6(5) |
| C(9)-C(10) | 1.416(9) | C(5)-N(1)-C(1) | 119.1(5) | C(20)-C(19)-C(18) | 119.6(5) |
| C(10)-C(11) | 1.357(9) | C(5)-N(1)-Zn(1) | 119.9(3) | C(21)-C(20)-C(19) | 118.4(5) |
| C(11)-C(12) | 1.406(8) | C(1)-N(1)-Zn(1) | 121.0(3) | C(20)-C(21)-C(22) | 119.7(6) |
| C(12)-C(17) | 1.420(8) | C(9)-N(2)-C(17) | 119.4(5) | C(27)-C(22)-C(21) | 119.1(5) |
| C(12)-C(13) | 1.438(9) | C(9)-N(2)-Zn(1) | 113.0(4) | C(27)-C(22)-C(23) | 118.7(5) |
| C(13)-C(14) | 1.361(9) | C(17)-N(2)-Zn(1) | 126.9(3) | C(21)-C(22)-C(23) | 122.1(6) |
| C(14)-C(15) | 1.391(9) | C(19)-N(3)-C(27) | 118.2(5) | C(24)-C(23)-C(22) | 119.0(6) |
| C(15)-C(16) | 1.396(9) | C(19)-N(3)-Zn(1) | 113.3(4) | C(25)-C(24)-C(23) | 121.4(6) |
| C(16)-C(17) | 1.408(7) | C(27)-N(3)-Zn(1) | 128.2(4) | C(26)-C(25)-C(24) | 120.5(6) |
| C(18)-C(19) | 1.515(8) | C(7)-N(4)-C(8) | 112.0(4) | C(25)-C(26)-C(27) | 119.5(6) |
| C(19)-C(20) | 1.403(9) | C(7)-N(4)-C(18) | 108.5(4) | N(3)-C(27)-C(22) | 120.8(5) |
| C(20)-C(21) | 1.364(9) | C(8)-N(4)-C(18) | 111.4(4) | N(3)-C(27)-C(26) | 118.4(6) |
| C(21)-C(22) | 1.411(8) | C(7)-N(4)-Zn(1) | 106.4(3) | C(22)-C(27)-C(26) | 120.8(5) |
| C(22)-C(27) | 1.398(9) | C(8)-N(4)-Zn(1) | 109.6(3) | O(10)-C(29)-C(28) | 111.6(5) |

Appendix-9. The crystal structure of $Cd^{2+}$-DQPEA



Appendix-10. Crystal data and structure refinement for $Cd^{2+}$-DQPEA.

| | | |
|---|---|---|
| Identification code | rh51 | |
| Empirical formula | C27 H24 Cd N6 O6 | |
| Formula weight | 640.92 | |
| Temperature | 110(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | C2/c | |
| Unit cell dimensions | a = 22.160(3) Å | α= 90°. |
| | b = 15.9444(18) Å | β= 119.780(3)°. |
| | c = 16.6962(18) Å | γ = 90°. |
| Volume | 5120.2(10) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.663 $Mg/m^3$ | |
| Absorption coefficient | 0.909 $mm^{-1}$ | |
| F(000) | 2592 | |
| Crystal size | 0.30 x 0.10 x 0.10 $mm^3$ | |
| Theta range for data collection | 1.66 to 25.00°. | |
| Index ranges | -26<=h<=17, -18<=k<=14, -19<=l<=11 | |
| Reflections collected | 12050 | |
| Independent reflections | 4075 [R(int) = 0.0379] | |
| Completeness to theta = 25.00° | 90.2 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9146 and 0.7721 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4075 / 0 / 361 | |
| Goodness-of-fit on $F^2$ | 1.102 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0425, wR2 = 0.0934 | |
| R indices (all data) | R1 = 0.0521, wR2 = 0.0976 | |
| Largest diff. peak and hole | 0.633 and -1.185 e.$Å^{-3}$ | |

Appendix-11. Atomic coordinates (x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for $Cd^{2+}$-DQPEA.

| | x | y | z | U(eq) | | x | y | z | U(eq) |
|---|---|---|---|---|---|---|---|---|---|
| Cd(1) | 2455(1) | 9176(1) | 2816(1) | 15(1) | C(8) | 1693(2) | 10861(3) | 2704(3) | 20(1) |
| O(1) | 2840(2) | 8054(2) | 2315(2) | 23(1) | C(9) | 1400(2) | 10625(3) | 1711(3) | 19(1) |
| O(2) | 2998(2) | 9080(2) | 1586(3) | 31(1) | C(10) | 931(3) | 11174(3) | 1016(4) | 25(1) |
| O(3) | 3250(2) | 7815(2) | 1402(3) | 39(1) | C(11) | 630(3) | 10953(3) | 112(4) | 28(1) |
| O(4) | 1563(2) | 8144(2) | 2342(2) | 21(1) | C(12) | 775(3) | 10151(3) | -122(3) | 26(1) |
| O(5) | 1069(2) | 9113(2) | 2734(2) | 29(1) | C(13) | 482(3) | 9852(4) | -1039(3) | 34(2) |
| O(6) | 457(2) | 8086(2) | 1857(2) | 28(1) | C(14) | 639(3) | 9072(4) | -1217(3) | 35(2) |
| N(1) | 2821(2) | 8672(2) | 4296(3) | 17(1) | C(15) | 1086(3) | 8543(4) | -480(4) | 30(1) |
| N(2) | 1557(2) | 9882(2) | 1514(3) | 16(1) | C(16) | 1384(2) | 8807(3) | 411(3) | 21(1) |
| N(3) | 3635(2) | 9877(2) | 3446(3) | 18(1) | C(17) | 1241(2) | 9617(3) | 614(3) | 19(1) |
| N(4) | 2418(2) | 10567(2) | 3278(3) | 18(1) | C(18) | 2881(3) | 11091(3) | 3096(3) | 20(1) |
| N(5) | 3037(2) | 8320(3) | 1757(3) | 24(1) | C(19) | 3579(3) | 10701(3) | 3393(3) | 18(1) |
| N(6) | 1018(2) | 8458(2) | 2304(3) | 20(1) | C(20) | 4122(3) | 11245(3) | 3537(3) | 24(1) |
| C(1) | 3162(3) | 7942(3) | 4554(3) | 21(1) | C(21) | 4730(3) | 10914(3) | 3680(4) | 30(1) |
| C(2) | 3488(3) | 7653(3) | 5459(4) | 28(1) | C(22) | 4819(3) | 10041(3) | 3729(3) | 24(1) |
| C(3) | 3465(3) | 8153(3) | 6117(3) | 28(1) | C(23) | 5425(3) | 9644(3) | 3843(4) | 31(1) |
| C(4) | 3103(3) | 8900(3) | 5852(3) | 25(1) | C(24) | 5495(3) | 8793(4) | 3898(4) | 35(1) |
| C(5) | 2772(2) | 9142(3) | 4926(3) | 19(1) | C(25) | 4955(3) | 8306(3) | 3852(4) | 37(2) |
| C(6) | 2346(2) | 9935(3) | 4617(3) | 19(1) | C(26) | 4353(3) | 8654(3) | 3724(4) | 28(1) |
| C(7) | 2639(3) | 10630(3) | 4276(3) | 19(1) | C(27) | 4262(3) | 9532(3) | 3637(3) | 22(1) |

U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor

Appendix-12. Bond lengths [Å] and angles [°] for $Cd^{2+}$-DQPEA

| | | | | | |
|---|---|---|---|---|---|
| Cd(1)-O(1) | 2.308(3) | C(22)-C(27) | 1.420(7) | O(5)-N(6)-O(4) | 119.3(4) |
| Cd(1)-N(1) | 2.328(4) | C(23)-C(24) | 1.364(8) | N(1)-C(1)-C(2) | 122.9(5) |
| Cd(1)-N(4) | 2.364(4) | C(24)-C(25) | 1.396(8) | C(3)-C(2)-C(1) | 118.0(5) |
| Cd(1)-N(2) | 2.378(4) | C(25)-C(26) | 1.361(7) | C(2)-C(3)-C(4) | 119.3(5) |
| Cd(1)-O(4) | 2.384(3) | C(26)-C(27) | 1.411(7) | C(3)-C(4)-C(5) | 119.7(5) |
| Cd(1)-N(3) | 2.541(4) | O(1)-Cd(1)-N(1) | 96.91(13) | N(1)-C(5)-C(4) | 120.8(5) |
| O(1)-N(5) | 1.283(5) | O(1)-Cd(1)-N(4) | 157.60(13) | N(1)-C(5)-C(6) | 118.8(4) |
| O(2)-N(5) | 1.239(5) | N(1)-Cd(1)-N(4) | 91.56(13) | C(4)-C(5)-C(6) | 120.5(4) |
| O(3)-N(5) | 1.225(5) | O(1)-Cd(1)-N(2) | 109.17(13) | C(5)-C(6)-C(7) | 115.3(4) |
| O(4)-N(6) | 1.280(5) | N(1)-Cd(1)-N(2) | 145.61(14) | N(4)-C(7)-C(6) | 113.7(4) |
| O(5)-N(6) | 1.240(5) | N(4)-Cd(1)-N(2) | 72.80(13) | N(4)-C(8)-C(9) | 111.9(4) |
| O(6)-N(6) | 1.239(5) | O(1)-Cd(1)-O(4) | 74.90(12) | N(2)-C(9)-C(10) | 122.0(5) |
| N(1)-C(1) | 1.337(6) | N(1)-Cd(1)-O(4) | 84.74(12) | N(2)-C(9)-C(8) | 118.4(4) |
| N(1)-C(5) | 1.341(6) | N(4)-Cd(1)-O(4) | 126.70(13) | C(10)-C(9)-C(8) | 119.4(4) |
| N(2)-C(9) | 1.321(6) | N(2)-Cd(1)-O(4) | 81.01(12) | C(11)-C(10)-C(9) | 120.4(5) |
| N(2)-C(17) | 1.372(6) | O(1)-Cd(1)-N(3) | 90.15(12) | C(10)-C(11)-C(12) | 119.1(5) |
| N(3)-C(19) | 1.319(6) | N(1)-Cd(1)-N(3) | 88.16(13) | C(13)-C(12)-C(11) | 123.8(5) |
| N(3)-C(27) | 1.376(6) | N(4)-Cd(1)-N(3) | 69.37(13) | C(13)-C(12)-C(17) | 118.4(5) |
| N(4)-C(18) | 1.467(6) | N(2)-Cd(1)-N(3) | 113.09(13) | C(11)-C(12)-C(17) | 117.8(5) |
| N(4)-C(8) | 1.478(6) | O(4)-Cd(1)-N(3) | 162.50(12) | C(14)-C(13)-C(12) | 120.9(5) |
| N(4)-C(7) | 1.489(6) | N(5)-O(1)-Cd(1) | 109.1(3) | C(13)-C(14)-C(15) | 119.9(5) |
| C(1)-C(2) | 1.391(7) | N(6)-O(4)-Cd(1) | 110.7(3) | C(16)-C(15)-C(14) | 121.2(5) |
| C(2)-C(3) | 1.378(7) | C(1)-N(1)-C(5) | 119.2(4) | C(15)-C(16)-C(17) | 120.0(5) |
| C(3)-C(4) | 1.380(7) | C(1)-N(1)-Cd(1) | 119.0(3) | N(2)-C(17)-C(16) | 119.4(4) |
| C(4)-C(5) | 1.397(7) | C(5)-N(1)-Cd(1) | 121.3(3) | N(2)-C(17)-C(12) | 121.1(5) |
| C(5)-C(6) | 1.506(7) | C(9)-N(2)-C(17) | 119.6(4) | C(16)-C(17)-C(12) | 119.5(4) |
| C(6)-C(7) | 1.530(7) | C(9)-N(2)-Cd(1) | 113.7(3) | N(4)-C(18)-C(19) | 114.0(4) |
| C(8)-C(9) | 1.498(6) | C(17)-N(2)-Cd(1) | 126.5(3) | N(3)-C(19)-C(20) | 124.1(5) |
| C(9)-C(10) | 1.412(7) | C(19)-N(3)-C(27) | 117.6(4) | N(3)-C(19)-C(18) | 118.7(4) |
| C(10)-C(11) | 1.359(7) | C(19)-N(3)-Cd(1) | 111.6(3) | C(20)-C(19)-C(18) | 117.1(4) |
| C(11)-C(12) | 1.419(8) | C(27)-N(3)-Cd(1) | 129.2(3) | C(21)-C(20)-C(19) | 118.9(5) |
| C(12)-C(13) | 1.417(7) | C(18)-N(4)-C(8) | 109.4(4) | C(20)-C(21)-C(22) | 119.7(5) |
| C(12)-C(17) | 1.429(7) | C(18)-N(4)-C(7) | 108.5(4) | C(21)-C(22)-C(23) | 123.4(5) |
| C(13)-C(14) | 1.364(8) | C(8)-N(4)-C(7) | 110.6(4) | C(21)-C(22)-C(27) | 118.1(5) |
| C(14)-C(15) | 1.413(8) | C(18)-N(4)-Cd(1) | 109.0(3) | C(23)-C(22)-C(27) | 118.5(5) |
| C(15)-C(16) | 1.361(7) | C(8)-N(4)-Cd(1) | 106.8(3) | C(24)-C(23)-C(22) | 121.7(5) |
| C(16)-C(17) | 1.411(7) | C(7)-N(4)-Cd(1) | 112.5(3) | C(23)-C(24)-C(25) | 118.9(5) |
| C(18)-C(19) | 1.505(7) | O(3)-N(5)-O(2) | 122.0(5) | C(26)-C(25)-C(24) | 122.0(5) |
| C(19)-C(20) | 1.404(7) | O(3)-N(5)-O(1) | 119.2(4) | C(25)-C(26)-C(27) | 120.0(5) |
| C(20)-C(21) | 1.353(7) | O(2)-N(5)-O(1) | 118.8(4) | N(3)-C(27)-C(26) | 119.7(5) |
| C(21)-C(22) | 1.402(7) | O(6)-N(6)-O(5) | 121.8(4) | N(3)-C(27)-C(22) | 121.4(5) |
| C(22)-C(23) | 1.410(7) | O(6)-N(6)-O(4) | 118.9(4) | C(26)-C(27)-C(22) | 118.9(5) |