**Electronic Supplementary Information: Adjei, Lough & Gossage**

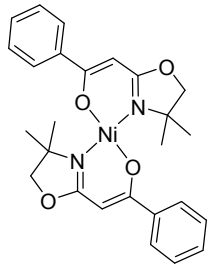
Calculated Diamagnetic Corrections[1]

$X_D(\text{ligand}) = 9X_D(C_{ring}) + X_D(N_{ring}) + 2X_D(O) + 14X_D(H) + 4X_D(C) + \lambda_i(C{=}C) + \lambda_i(\text{benzene}) + \lambda_i(C{=}N)$

$= [9(-6.24) + (-4.61) + 2(-4.6) + 14(-2.93) + 4(-6.0) + (+5.5) + (-1.4) + (+8.15)] \times 10^{-6}$ emu·mol$^{-1}$

$= -122.73 \times 10^{-6}$ emu·mol$^{-1}$

2 ligands = $-257.46 \times 10^{-6}$ emu·mol$^{-1}$




$+ \lambda_i(Ni^{2+})$

$= [-257.46 + (-12)] \times 10^{-6}$ emu·mol$^{-1}$

$= -2.6946 \times 10^{-4}$ emu·mol$^{-1}$

Calculated molar susceptibility (measured)

$X_M = X_g(MW)$

$X_M = 0.000010$ emu·g (491.213 g/mol)

$X_M = +4.9 \times 10^{-3}$ emu·mol$^{-1}$

Overall

$X_p = X_M + X_D = -2.6946 \times 10^{-4} + 4.9 \times 10^{-3}$ emu·mol$^{-1}$ $= +4.6 \times 10^{-3}$ emu·mol$^{-1}$

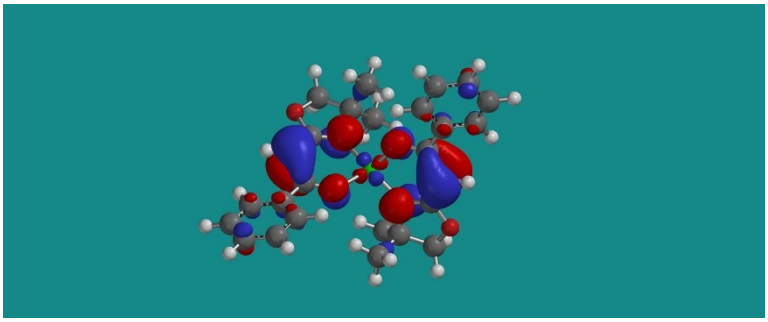
Unpaired Electrons:

$\mu_{eff} = 2.828\sqrt{298.15} * X_p = \mu_{eff} = 2.828\sqrt{1.37} = \mu_{eff} = 3.31$ B. M.

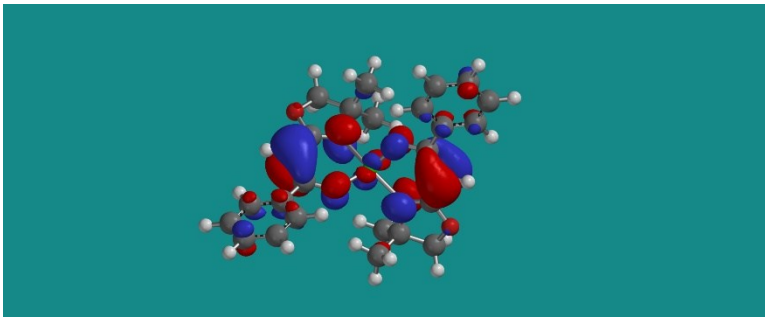
**DFT Treatment Calculations (B3LYP 6-311+G**/LANL2DZ) of Complex 3a.**[2]

HOMO-*a*, and HOMO-*b* and Spin Density: Schematically Representated

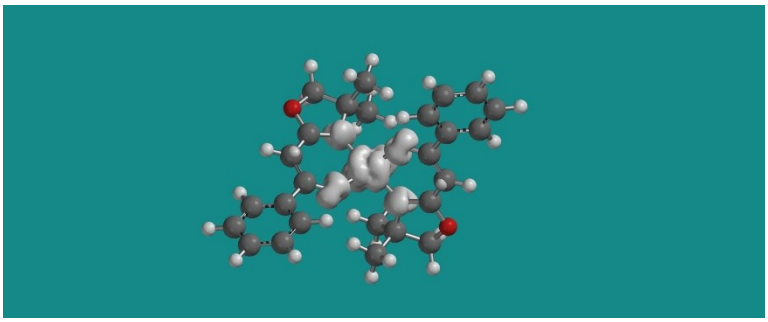
HOMO-*a*



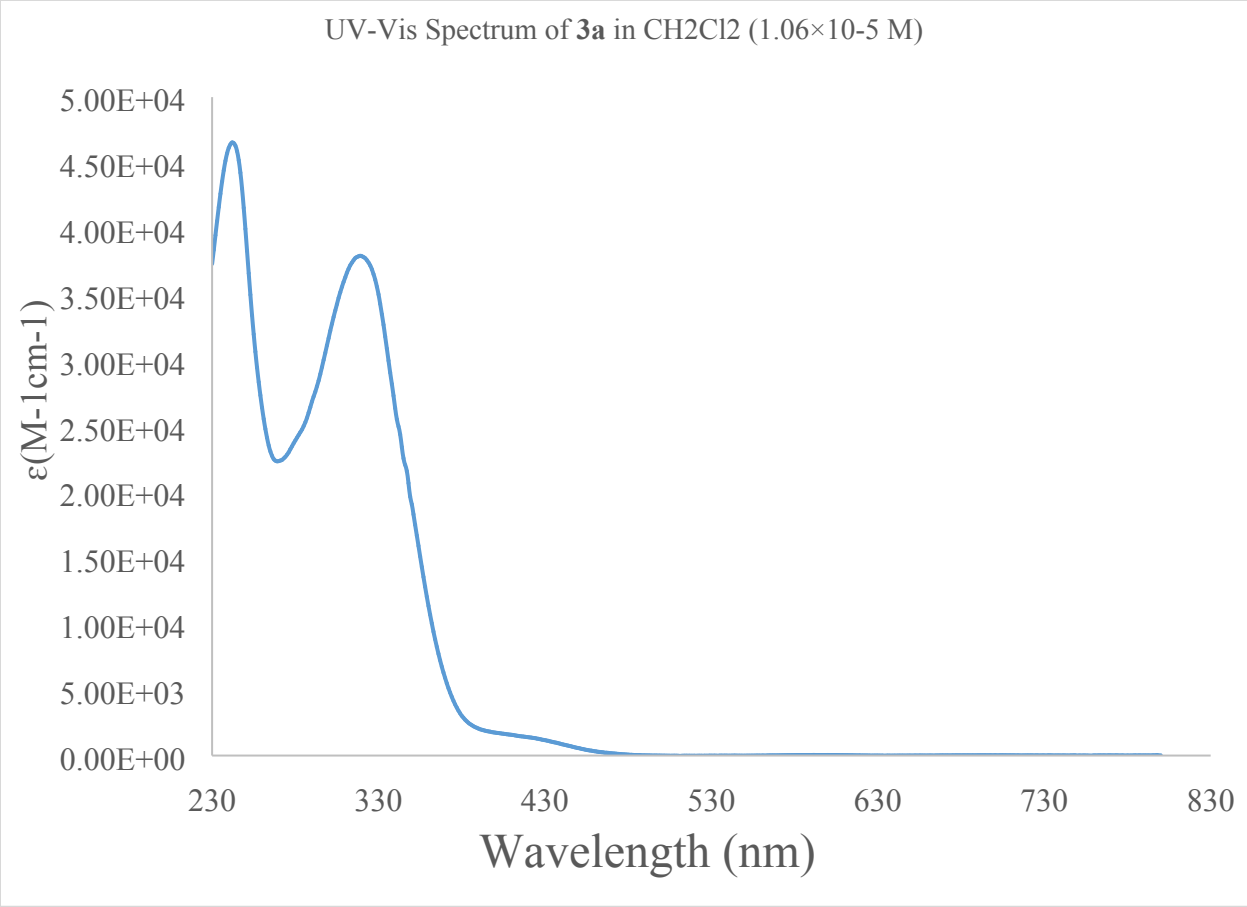
HOMO-*b*



Spin Density



**Typical UV-Vis. Spectrum (Complex 3a).**[3]



## X-ray data: complexes 3a-c and 3e-g.[4-13]

*n.b.*, CCDC numbers 1884791-1884796 have been assigned to the crystallographic data files for complexes **3a-c** and **3e-g**, respectively.

### Complex 3a

Table 1. Crystal data and structure refinement for d1837_a.

| | | |
|---|---|---|
| Identification code | d1837_a | |
| Empirical formula | C26 H28 N2 Ni O4 | |
| Formula weight | 491.21 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1/c$ | |
| Unit cell dimensions | a = 12.0764(17) Å | α= 90°. |
| | b = 9.6715(15) Å | β= 92.155(5)°. |
| | c = 20.657(4) Å | γ = 90°. |
| Volume | 2411.0(7) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.353 $Mg/m^3$ | |
| Absorption coefficient | 0.839 $mm^{-1}$ | |
| F(000) | 1032 | |
| Crystal size | 0.150 x 0.150 x 0.040 $mm^3$ | |
| Theta range for data collection | 1.687 to 24.999°. | |
| Index ranges | -14<=h<=13, -11<=k<=11, -24<=l<=24 | |
| Reflections collected | 35050 | |
| Independent reflections | 4251 [R(int) = 0.1140] | |
| Completeness to theta = 24.999° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.6875 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4251 / 0 / 302 | |
| Goodness-of-fit on $F^2$ | 1.001 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0438, wR2 = 0.0720 | |
| R indices (all data) | R1 = 0.0928, wR2 = 0.0868 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.392 and -0.419 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d1837_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 2636(1) | 7737(1) | 6155(1) | 22(1) |
| O(1) | 3870(2) | 6590(2) | 6414(1) | 23(1) |
| O(2) | 5178(2) | 10462(2) | 5906(1) | 36(1) |
| O(3) | 1323(2) | 8216(2) | 6592(1) | 24(1) |
| O(4) | 297(2) | 6584(2) | 4775(1) | 33(1) |
| N(1) | 3580(2) | 9312(3) | 5998(1) | 21(1) |
| N(2) | 1796(2) | 6970(3) | 5422(1) | 21(1) |
| C(1) | 4655(3) | 9268(3) | 6054(2) | 24(1) |
| C(2) | 5327(3) | 8145(3) | 6250(2) | 26(1) |
| C(3) | 4918(2) | 6897(3) | 6439(2) | 21(1) |
| C(4) | 4336(3) | 11408(4) | 5659(2) | 35(1) |
| C(5) | 3227(3) | 10733(3) | 5821(2) | 26(1) |
| C(6) | 5662(2) | 5782(3) | 6696(2) | 22(1) |
| C(7) | 5221(3) | 4517(3) | 6865(2) | 26(1) |
| C(8) | 5885(3) | 3467(4) | 7115(2) | 33(1) |
| C(9) | 7006(3) | 3671(4) | 7200(2) | 34(1) |
| C(10) | 7464(3) | 4916(4) | 7040(2) | 36(1) |
| C(11) | 6807(3) | 5974(4) | 6791(2) | 30(1) |
| C(12) | 2436(3) | 10696(4) | 5238(2) | 49(1) |
| C(13) | 2736(3) | 11420(4) | 6401(2) | 50(1) |
| C(14) | 307(2) | 8194(3) | 6365(2) | 24(1) |
| C(15) | -20(3) | 7687(4) | 5768(2) | 29(1) |
| C(16) | 726(3) | 7097(3) | 5340(2) | 24(1) |
| C(17) | 1224(3) | 6180(4) | 4395(2) | 33(1) |
| C(18) | 2226(3) | 6160(3) | 4878(2) | 26(1) |
| C(19) | -518(2) | 8771(3) | 6811(2) | 28(1) |
| C(20) | -335(3) | 8631(4) | 7473(2) | 37(1) |
| C(21) | -1073(3) | 9174(4) | 7906(2) | 49(1) |
| C(22) | -2007(3) | 9858(4) | 7671(3) | 52(1) |
| C(23) | -2201(3) | 10006(4) | 7018(3) | 51(1) |
| C(24) | -1457(3) | 9469(4) | 6587(2) | 38(1) |

| | | | | |
|---|---|---|---|---|
| C(25) | 3243(3) | 6848(4) | 4611(2) | 38(1) |
| C(26) | 2494(3) | 4707(3) | 5111(2) | 36(1) |

Table 3. Bond lengths [Å] and angles [°] for d1837_a.

| | |
|---|---|
| Ni(1)-O(3) | 1.912(2) |
| Ni(1)-O(1) | 1.917(2) |
| Ni(1)-N(2) | 1.937(3) |
| Ni(1)-N(1) | 1.937(3) |
| O(1)-C(3) | 1.299(3) |
| O(2)-C(1) | 1.356(4) |
| O(2)-C(4) | 1.447(4) |
| O(3)-C(14) | 1.297(4) |
| O(4)-C(16) | 1.353(4) |
| O(4)-C(17) | 1.444(4) |
| N(1)-C(1) | 1.300(4) |
| N(1)-C(5) | 1.481(4) |
| N(2)-C(16) | 1.302(4) |
| N(2)-C(18) | 1.481(4) |
| C(1)-C(2) | 1.406(4) |
| C(2)-C(3) | 1.367(4) |
| C(2)-H(2A) | 0.9500 |
| C(3)-C(6) | 1.489(4) |
| C(4)-C(5) | 1.538(4) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(12) | 1.508(5) |
| C(5)-C(13) | 1.510(5) |
| C(6)-C(7) | 1.384(4) |
| C(6)-C(11) | 1.401(4) |
| C(7)-C(8) | 1.382(4) |
| C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.373(5) |
| C(8)-H(8A) | 0.9500 |
| C(9)-C(10) | 1.371(5) |
| C(9)-H(9A) | 0.9500 |
| C(10)-C(11) | 1.383(5) |
| C(10)-H(10A) | 0.9500 |
| C(11)-H(11A) | 0.9500 |

| | |
|---|---|
| C(12)-H(12A) | 0.9800 |
| C(12)-H(12B) | 0.9800 |
| C(12)-H(12C) | 0.9800 |
| C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 |
| C(13)-H(13C) | 0.9800 |
| C(14)-C(15) | 1.371(5) |
| C(14)-C(19) | 1.491(5) |
| C(15)-C(16) | 1.407(4) |
| C(15)-H(15A) | 0.9500 |
| C(17)-C(18) | 1.539(5) |
| C(17)-H(17A) | 0.9900 |
| C(17)-H(17B) | 0.9900 |
| C(18)-C(26) | 1.517(5) |
| C(18)-C(25) | 1.518(4) |
| C(19)-C(20) | 1.384(5) |
| C(19)-C(24) | 1.384(5) |
| C(20)-C(21) | 1.389(5) |
| C(20)-H(20A) | 0.9500 |
| C(21)-C(22) | 1.379(6) |
| C(21)-H(21A) | 0.9500 |
| C(22)-C(23) | 1.368(6) |
| C(22)-H(22A) | 0.9500 |
| C(23)-C(24) | 1.389(5) |
| C(23)-H(23A) | 0.9500 |
| C(24)-H(24A) | 0.9500 |
| C(25)-H(25A) | 0.9800 |
| C(25)-H(25B) | 0.9800 |
| C(25)-H(25C) | 0.9800 |
| C(26)-H(26A) | 0.9800 |
| C(26)-H(26B) | 0.9800 |
| C(26)-H(26C) | 0.9800 |

| | |
|---|---|
| O(3)-Ni(1)-O(1) | 131.15(9) |
| O(3)-Ni(1)-N(2) | 92.44(10) |
| O(1)-Ni(1)-N(2) | 112.04(10) |

| | |
|---|---|
| O(3)-Ni(1)-N(1) | 113.07(10) |
| O(1)-Ni(1)-N(1) | 92.62(10) |
| N(2)-Ni(1)-N(1) | 117.71(11) |
| C(3)-O(1)-Ni(1) | 128.7(2) |
| C(1)-O(2)-C(4) | 106.9(2) |
| C(14)-O(3)-Ni(1) | 127.9(2) |
| C(16)-O(4)-C(17) | 106.8(2) |
| C(1)-N(1)-C(5) | 109.3(3) |
| C(1)-N(1)-Ni(1) | 123.5(2) |
| C(5)-N(1)-Ni(1) | 127.2(2) |
| C(16)-N(2)-C(18) | 109.0(3) |
| C(16)-N(2)-Ni(1) | 123.6(2) |
| C(18)-N(2)-Ni(1) | 127.37(19) |
| N(1)-C(1)-O(2) | 115.1(3) |
| N(1)-C(1)-C(2) | 127.9(3) |
| O(2)-C(1)-C(2) | 117.0(3) |
| C(3)-C(2)-C(1) | 123.6(3) |
| C(3)-C(2)-H(2A) | 118.2 |
| C(1)-C(2)-H(2A) | 118.2 |
| O(1)-C(3)-C(2) | 123.5(3) |
| O(1)-C(3)-C(6) | 115.0(3) |
| C(2)-C(3)-C(6) | 121.4(3) |
| O(2)-C(4)-C(5) | 105.1(3) |
| O(2)-C(4)-H(4A) | 110.7 |
| C(5)-C(4)-H(4A) | 110.7 |
| O(2)-C(4)-H(4B) | 110.7 |
| C(5)-C(4)-H(4B) | 110.7 |
| H(4A)-C(4)-H(4B) | 108.8 |
| N(1)-C(5)-C(12) | 110.1(3) |
| N(1)-C(5)-C(13) | 109.3(3) |
| C(12)-C(5)-C(13) | 112.8(3) |
| N(1)-C(5)-C(4) | 101.7(2) |
| C(12)-C(5)-C(4) | 111.5(3) |
| C(13)-C(5)-C(4) | 110.9(3) |
| C(7)-C(6)-C(11) | 118.0(3) |
| C(7)-C(6)-C(3) | 119.8(3) |

| | |
|---|---|
| C(11)-C(6)-C(3) | 122.2(3) |
| C(8)-C(7)-C(6) | 121.3(3) |
| C(8)-C(7)-H(7A) | 119.3 |
| C(6)-C(7)-H(7A) | 119.3 |
| C(9)-C(8)-C(7) | 119.9(3) |
| C(9)-C(8)-H(8A) | 120.1 |
| C(7)-C(8)-H(8A) | 120.1 |
| C(10)-C(9)-C(8) | 120.0(3) |
| C(10)-C(9)-H(9A) | 120.0 |
| C(8)-C(9)-H(9A) | 120.0 |
| C(9)-C(10)-C(11) | 120.6(3) |
| C(9)-C(10)-H(10A) | 119.7 |
| C(11)-C(10)-H(10A) | 119.7 |
| C(10)-C(11)-C(6) | 120.2(3) |
| C(10)-C(11)-H(11A) | 119.9 |
| C(6)-C(11)-H(11A) | 119.9 |
| C(5)-C(12)-H(12A) | 109.5 |
| C(5)-C(12)-H(12B) | 109.5 |
| H(12A)-C(12)-H(12B) | 109.5 |
| C(5)-C(12)-H(12C) | 109.5 |
| H(12A)-C(12)-H(12C) | 109.5 |
| H(12B)-C(12)-H(12C) | 109.5 |
| C(5)-C(13)-H(13A) | 109.5 |
| C(5)-C(13)-H(13B) | 109.5 |
| H(13A)-C(13)-H(13B) | 109.5 |
| C(5)-C(13)-H(13C) | 109.5 |
| H(13A)-C(13)-H(13C) | 109.5 |
| H(13B)-C(13)-H(13C) | 109.5 |
| O(3)-C(14)-C(15) | 124.6(3) |
| O(3)-C(14)-C(19) | 114.5(3) |
| C(15)-C(14)-C(19) | 120.9(3) |
| C(14)-C(15)-C(16) | 122.7(3) |
| C(14)-C(15)-H(15A) | 118.6 |
| C(16)-C(15)-H(15A) | 118.6 |
| N(2)-C(16)-O(4) | 115.1(3) |
| N(2)-C(16)-C(15) | 127.7(3) |

| | |
|---|---|
| O(4)-C(16)-C(15) | 117.2(3) |
| O(4)-C(17)-C(18) | 105.0(3) |
| O(4)-C(17)-H(17A) | 110.8 |
| C(18)-C(17)-H(17A) | 110.8 |
| O(4)-C(17)-H(17B) | 110.8 |
| C(18)-C(17)-H(17B) | 110.8 |
| H(17A)-C(17)-H(17B) | 108.8 |
| N(2)-C(18)-C(26) | 109.0(3) |
| N(2)-C(18)-C(25) | 110.8(3) |
| C(26)-C(18)-C(25) | 110.8(3) |
| N(2)-C(18)-C(17) | 101.3(2) |
| C(26)-C(18)-C(17) | 111.8(3) |
| C(25)-C(18)-C(17) | 112.7(3) |
| C(20)-C(19)-C(24) | 118.5(3) |
| C(20)-C(19)-C(14) | 119.2(3) |
| C(24)-C(19)-C(14) | 122.3(3) |
| C(19)-C(20)-C(21) | 121.1(4) |
| C(19)-C(20)-H(20A) | 119.5 |
| C(21)-C(20)-H(20A) | 119.5 |
| C(22)-C(21)-C(20) | 119.4(4) |
| C(22)-C(21)-H(21A) | 120.3 |
| C(20)-C(21)-H(21A) | 120.3 |
| C(23)-C(22)-C(21) | 120.3(4) |
| C(23)-C(22)-H(22A) | 119.8 |
| C(21)-C(22)-H(22A) | 119.8 |
| C(22)-C(23)-C(24) | 120.1(4) |
| C(22)-C(23)-H(23A) | 119.9 |
| C(24)-C(23)-H(23A) | 119.9 |
| C(19)-C(24)-C(23) | 120.7(4) |
| C(19)-C(24)-H(24A) | 119.7 |
| C(23)-C(24)-H(24A) | 119.7 |
| C(18)-C(25)-H(25A) | 109.5 |
| C(18)-C(25)-H(25B) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 |
| C(18)-C(25)-H(25C) | 109.5 |
| H(25A)-C(25)-H(25C) | 109.5 |

| | |
|---|---|
| H(25B)-C(25)-H(25C) | 109.5 |
| C(18)-C(26)-H(26A) | 109.5 |
| C(18)-C(26)-H(26B) | 109.5 |
| H(26A)-C(26)-H(26B) | 109.5 |
| C(18)-C(26)-H(26C) | 109.5 |
| H(26A)-C(26)-H(26C) | 109.5 |
| H(26B)-C(26)-H(26C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d1837_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 14(1) | 24(1) | 28(1) | 1(1) | 0(1) | -2(1) |
| O(1) | 16(1) | 25(1) | 28(2) | 4(1) | 0(1) | 0(1) |
| O(2) | 27(1) | 26(1) | 54(2) | 14(1) | -3(1) | -7(1) |
| O(3) | 14(1) | 34(1) | 24(2) | 0(1) | -2(1) | 0(1) |
| O(4) | 25(1) | 43(2) | 32(2) | -14(1) | -5(1) | -2(1) |
| N(1) | 24(2) | 19(2) | 20(2) | 1(1) | -2(1) | -1(1) |
| N(2) | 18(1) | 22(2) | 25(2) | -2(1) | 2(1) | -4(1) |
| C(1) | 23(2) | 24(2) | 26(2) | 2(2) | 0(2) | -7(2) |
| C(2) | 14(2) | 29(2) | 36(2) | 5(2) | 0(2) | -1(2) |
| C(3) | 18(2) | 30(2) | 15(2) | -1(2) | 2(1) | 1(2) |
| C(4) | 39(2) | 26(2) | 39(3) | 8(2) | 1(2) | -6(2) |
| C(5) | 28(2) | 17(2) | 32(2) | 1(2) | -3(2) | -1(2) |
| C(6) | 19(2) | 28(2) | 20(2) | -3(2) | 0(2) | 5(2) |
| C(7) | 24(2) | 32(2) | 23(2) | 4(2) | 8(2) | 3(2) |
| C(8) | 40(2) | 35(2) | 25(2) | 7(2) | 6(2) | 6(2) |
| C(9) | 41(2) | 35(2) | 26(2) | 1(2) | -6(2) | 18(2) |
| C(10) | 23(2) | 41(2) | 42(3) | -12(2) | -9(2) | 11(2) |
| C(11) | 26(2) | 30(2) | 34(3) | -3(2) | -5(2) | 3(2) |
| C(12) | 52(3) | 32(2) | 60(3) | 13(2) | -26(2) | -4(2) |
| C(13) | 67(3) | 27(2) | 58(3) | -1(2) | 27(3) | 7(2) |
| C(14) | 18(2) | 21(2) | 33(2) | 2(2) | 0(2) | 1(1) |
| C(15) | 20(2) | 33(2) | 35(2) | -7(2) | -6(2) | 1(2) |
| C(16) | 25(2) | 21(2) | 27(2) | -2(2) | -4(2) | -2(2) |
| C(17) | 34(2) | 37(2) | 30(2) | -10(2) | 2(2) | -2(2) |
| C(18) | 26(2) | 26(2) | 27(2) | -7(2) | 3(2) | -3(2) |
| C(19) | 16(2) | 31(2) | 36(3) | -10(2) | -1(2) | -4(2) |
| C(20) | 20(2) | 48(3) | 45(3) | -8(2) | 6(2) | -6(2) |
| C(21) | 35(2) | 64(3) | 48(3) | -16(2) | 16(2) | -13(2) |
| C(22) | 30(2) | 49(3) | 80(4) | -37(3) | 26(3) | -16(2) |
| C(23) | 24(2) | 44(3) | 84(4) | -35(3) | 2(2) | 2(2) |
| C(24) | 29(2) | 36(2) | 50(3) | -19(2) | -7(2) | 3(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(25) | 39(2) | 42(2) | 34(3) | -6(2) | 14(2) | -13(2) |
| C(26) | 37(2) | 23(2) | 46(3) | -6(2) | 3(2) | 1(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d1837_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 6108 | 8260 | 6251 | 32 |
| H(4A) | 4388 | 11528 | 5185 | 42 |
| H(4B) | 4416 | 12323 | 5870 | 42 |
| H(7A) | 4446 | 4368 | 6808 | 32 |
| H(8A) | 5566 | 2606 | 7227 | 40 |
| H(9A) | 7465 | 2949 | 7370 | 41 |
| H(10A) | 8240 | 5054 | 7102 | 43 |
| H(11A) | 7132 | 6834 | 6683 | 36 |
| H(12A) | 1761 | 10199 | 5349 | 73 |
| H(12B) | 2788 | 10222 | 4881 | 73 |
| H(12C) | 2245 | 11643 | 5108 | 73 |
| H(13A) | 2053 | 10942 | 6510 | 75 |
| H(13B) | 2570 | 12389 | 6298 | 75 |
| H(13C) | 3268 | 11375 | 6770 | 75 |
| H(15A) | -782 | 7736 | 5638 | 35 |
| H(17A) | 1340 | 6854 | 4043 | 40 |
| H(17B) | 1099 | 5254 | 4202 | 40 |
| H(20A) | 305 | 8155 | 7634 | 45 |
| H(21A) | -937 | 9076 | 8359 | 59 |
| H(22A) | -2517 | 10228 | 7964 | 63 |
| H(23A) | -2846 | 10477 | 6858 | 61 |
| H(24A) | -1594 | 9581 | 6134 | 46 |
| H(25A) | 3831 | 6888 | 4951 | 57 |
| H(25B) | 3053 | 7788 | 4469 | 57 |
| H(25C) | 3499 | 6313 | 4243 | 57 |
| H(26A) | 3059 | 4747 | 5464 | 54 |
| H(26B) | 2774 | 4162 | 4753 | 54 |
| H(26C) | 1822 | 4272 | 5269 | 54 |

Table 6. Torsion angles [°] for d1837_a.

| | |
|---|---|
| C(5)-N(1)-C(1)-O(2) | -3.5(4) |
| Ni(1)-N(1)-C(1)-O(2) | 178.2(2) |
| C(5)-N(1)-C(1)-C(2) | 176.1(3) |
| Ni(1)-N(1)-C(1)-C(2) | -2.3(5) |
| C(4)-O(2)-C(1)-N(1) | -6.0(4) |
| C(4)-O(2)-C(1)-C(2) | 174.4(3) |
| N(1)-C(1)-C(2)-C(3) | -2.3(6) |
| O(2)-C(1)-C(2)-C(3) | 177.2(3) |
| Ni(1)-O(1)-C(3)-C(2) | -2.6(5) |
| Ni(1)-O(1)-C(3)-C(6) | 176.9(2) |
| C(1)-C(2)-C(3)-O(1) | 4.9(6) |
| C(1)-C(2)-C(3)-C(6) | -174.6(3) |
| C(1)-O(2)-C(4)-C(5) | 12.3(4) |
| C(1)-N(1)-C(5)-C(12) | 128.9(3) |
| Ni(1)-N(1)-C(5)-C(12) | -52.9(4) |
| C(1)-N(1)-C(5)-C(13) | -106.7(3) |
| Ni(1)-N(1)-C(5)-C(13) | 71.6(4) |
| C(1)-N(1)-C(5)-C(4) | 10.6(4) |
| Ni(1)-N(1)-C(5)-C(4) | -171.1(2) |
| O(2)-C(4)-C(5)-N(1) | -13.6(4) |
| O(2)-C(4)-C(5)-C(12) | -130.8(3) |
| O(2)-C(4)-C(5)-C(13) | 102.5(3) |
| O(1)-C(3)-C(6)-C(7) | 2.3(5) |
| C(2)-C(3)-C(6)-C(7) | -178.1(3) |
| O(1)-C(3)-C(6)-C(11) | -176.2(3) |
| C(2)-C(3)-C(6)-C(11) | 3.4(5) |
| C(11)-C(6)-C(7)-C(8) | -0.5(5) |
| C(3)-C(6)-C(7)-C(8) | -179.0(3) |
| C(6)-C(7)-C(8)-C(9) | 0.1(5) |
| C(7)-C(8)-C(9)-C(10) | 0.3(6) |
| C(8)-C(9)-C(10)-C(11) | -0.2(6) |
| C(9)-C(10)-C(11)-C(6) | -0.2(6) |
| C(7)-C(6)-C(11)-C(10) | 0.5(5) |
| C(3)-C(6)-C(11)-C(10) | 179.0(3) |

| | |
|---|---|
| Ni(1)-O(3)-C(14)-C(15) | 6.3(5) |
| Ni(1)-O(3)-C(14)-C(19) | -173.9(2) |
| O(3)-C(14)-C(15)-C(16) | 1.6(5) |
| C(19)-C(14)-C(15)-C(16) | -178.1(3) |
| C(18)-N(2)-C(16)-O(4) | -5.1(4) |
| Ni(1)-N(2)-C(16)-O(4) | 175.1(2) |
| C(18)-N(2)-C(16)-C(15) | 174.2(3) |
| Ni(1)-N(2)-C(16)-C(15) | -5.5(5) |
| C(17)-O(4)-C(16)-N(2) | -6.6(4) |
| C(17)-O(4)-C(16)-C(15) | 174.0(3) |
| C(14)-C(15)-C(16)-N(2) | -1.9(6) |
| C(14)-C(15)-C(16)-O(4) | 177.5(3) |
| C(16)-O(4)-C(17)-C(18) | 14.7(3) |
| C(16)-N(2)-C(18)-C(26) | -104.4(3) |
| Ni(1)-N(2)-C(18)-C(26) | 75.3(3) |
| C(16)-N(2)-C(18)-C(25) | 133.4(3) |
| Ni(1)-N(2)-C(18)-C(25) | -46.9(4) |
| C(16)-N(2)-C(18)-C(17) | 13.6(3) |
| Ni(1)-N(2)-C(18)-C(17) | -166.7(2) |
| O(4)-C(17)-C(18)-N(2) | -16.7(3) |
| O(4)-C(17)-C(18)-C(26) | 99.1(3) |
| O(4)-C(17)-C(18)-C(25) | -135.2(3) |
| O(3)-C(14)-C(19)-C(20) | -32.1(4) |
| C(15)-C(14)-C(19)-C(20) | 147.7(3) |
| O(3)-C(14)-C(19)-C(24) | 146.7(3) |
| C(15)-C(14)-C(19)-C(24) | -33.5(5) |
| C(24)-C(19)-C(20)-C(21) | 0.0(5) |
| C(14)-C(19)-C(20)-C(21) | 178.9(3) |
| C(19)-C(20)-C(21)-C(22) | 0.4(6) |
| C(20)-C(21)-C(22)-C(23) | -0.3(6) |
| C(21)-C(22)-C(23)-C(24) | -0.1(6) |
| C(20)-C(19)-C(24)-C(23) | -0.4(5) |
| C(14)-C(19)-C(24)-C(23) | -179.3(3) |
| C(22)-C(23)-C(24)-C(19) | 0.5(6) |

Symmetry transformations used to generate equivalent atoms:

## Complex 3b

Table 1. Crystal data and structure refinement for d1839_a.

| | | |
|---|---|---|
| Identification code | d1839_a | |
| Empirical formula | C22 H24 N2 Ni O6 | |
| Formula weight | 471.14 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1/c$ | |
| Unit cell dimensions | a = 10.2574(8) Å | α= 90°. |
| | b = 8.8952(7) Å | β= 95.190(3)°. |
| | c = 23.418(2) Å | γ = 90°. |
| Volume | 2127.9(3) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.471 $Mg/m^3$ | |
| Absorption coefficient | 0.953 $mm^{-1}$ | |
| F(000) | 984 | |
| Crystal size | 0.180 x 0.160 x 0.050 $mm^3$ | |
| Theta range for data collection | 1.746 to 27.559°. | |
| Index ranges | -13<=h<=13, -11<=k<=11, -30<=l<=30 | |
| Reflections collected | 33572 | |
| Independent reflections | 4920 [R(int) = 0.0562] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.6985 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4920 / 0 / 284 | |
| Goodness-of-fit on $F^2$ | 1.001 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0324, wR2 = 0.0643 | |
| R indices (all data) | R1 = 0.0548, wR2 = 0.0714 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.333 and -0.320 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d1839_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 2924(1) | 3758(1) | 2937(1) | 16(1) |
| O(1) | 2763(1) | 3494(1) | 2115(1) | 18(1) |
| O(2) | 6505(1) | 1845(2) | 2759(1) | 24(1) |
| O(3) | 4206(1) | 2534(2) | 840(1) | 25(1) |
| O(4) | 2665(1) | 5258(1) | 3510(1) | 19(1) |
| O(5) | -10(1) | 1710(2) | 3740(1) | 23(1) |
| O(6) | 1051(2) | 6630(2) | 4695(1) | 29(1) |
| N(1) | 4710(2) | 2968(2) | 3041(1) | 16(1) |
| N(2) | 1533(2) | 2475(2) | 3182(1) | 17(1) |
| C(1) | 3657(2) | 2941(2) | 1815(1) | 17(1) |
| C(2) | 4874(2) | 2453(2) | 2023(1) | 19(1) |
| C(3) | 5314(2) | 2465(2) | 2613(1) | 18(1) |
| C(4) | 6802(2) | 2079(2) | 3366(1) | 25(1) |
| C(5) | 5504(2) | 2600(2) | 3588(1) | 19(1) |
| C(6) | 3246(2) | 2796(2) | 1202(1) | 19(1) |
| C(7) | 2061(2) | 2746(3) | 900(1) | 31(1) |
| C(8) | 2286(3) | 2423(3) | 321(1) | 36(1) |
| C(9) | 3576(2) | 2308(2) | 309(1) | 32(1) |
| C(10) | 5696(2) | 3974(2) | 3971(1) | 27(1) |
| C(11) | 4841(2) | 1334(2) | 3890(1) | 25(1) |
| C(12) | 1822(2) | 5222(2) | 3891(1) | 17(1) |
| C(13) | 945(2) | 4093(2) | 3962(1) | 19(1) |
| C(14) | 869(2) | 2784(2) | 3616(1) | 17(1) |
| C(15) | 247(2) | 408(2) | 3390(1) | 24(1) |
| C(16) | 1036(2) | 1034(2) | 2918(1) | 20(1) |
| C(17) | 1890(2) | 6543(2) | 4270(1) | 18(1) |
| C(18) | 2666(2) | 7768(2) | 4291(1) | 24(1) |
| C(19) | 2306(2) | 8682(2) | 4749(1) | 28(1) |
| C(20) | 1339(2) | 7954(3) | 4978(1) | 32(1) |
| C(21) | 159(2) | 1373(2) | 2374(1) | 29(1) |
| C(22) | 2166(2) | 18(2) | 2787(1) | 29(1) |

Table 3. Bond lengths [Å] and angles [°] for d1839_a.

| | |
|---|---|
| Ni(1)-O(4) | 1.9272(13) |
| Ni(1)-O(1) | 1.9325(13) |
| Ni(1)-N(2) | 1.9531(16) |
| Ni(1)-N(1) | 1.9560(16) |
| O(1)-C(1) | 1.301(2) |
| O(2)-C(3) | 1.356(2) |
| O(2)-C(4) | 1.443(2) |
| O(3)-C(9) | 1.364(3) |
| O(3)-C(6) | 1.376(2) |
| O(4)-C(12) | 1.298(2) |
| O(5)-C(14) | 1.362(2) |
| O(5)-C(15) | 1.457(2) |
| O(6)-C(20) | 1.370(2) |
| O(6)-C(17) | 1.375(2) |
| N(1)-C(3) | 1.304(2) |
| N(1)-C(5) | 1.492(2) |
| N(2)-C(14) | 1.303(2) |
| N(2)-C(16) | 1.493(2) |
| C(1)-C(2) | 1.368(3) |
| C(1)-C(6) | 1.466(3) |
| C(2)-C(3) | 1.414(3) |
| C(2)-H(2A) | 0.9500 |
| C(4)-C(5) | 1.544(3) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(10) | 1.518(3) |
| C(5)-C(11) | 1.522(3) |
| C(6)-C(7) | 1.350(3) |
| C(7)-C(8) | 1.426(3) |
| C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.329(3) |
| C(8)-H(8A) | 0.9500 |
| C(9)-H(9A) | 0.9500 |
| C(10)-H(10A) | 0.9800 |

| | |
|---|---|
| C(10)-H(10B) | 0.9800 |
| C(10)-H(10C) | 0.9800 |
| C(11)-H(11A) | 0.9800 |
| C(11)-H(11B) | 0.9800 |
| C(11)-H(11C) | 0.9800 |
| C(12)-C(13) | 1.369(3) |
| C(12)-C(17) | 1.470(3) |
| C(13)-C(14) | 1.417(3) |
| C(13)-H(13A) | 0.9500 |
| C(15)-C(16) | 1.534(3) |
| C(15)-H(15A) | 0.9900 |
| C(15)-H(15B) | 0.9900 |
| C(16)-C(21) | 1.521(3) |
| C(16)-C(22) | 1.522(3) |
| C(17)-C(18) | 1.348(3) |
| C(18)-C(19) | 1.422(3) |
| C(18)-H(18A) | 0.9500 |
| C(19)-C(20) | 1.336(3) |
| C(19)-H(19A) | 0.9500 |
| C(20)-H(20A) | 0.9500 |
| C(21)-H(21A) | 0.9800 |
| C(21)-H(21B) | 0.9800 |
| C(21)-H(21C) | 0.9800 |
| C(22)-H(22A) | 0.9800 |
| C(22)-H(22B) | 0.9800 |
| C(22)-H(22C) | 0.9800 |

| | |
|---|---|
| O(4)-Ni(1)-O(1) | 140.61(6) |
| O(4)-Ni(1)-N(2) | 92.89(6) |
| O(1)-Ni(1)-N(2) | 102.81(6) |
| O(4)-Ni(1)-N(1) | 110.44(6) |
| O(1)-Ni(1)-N(1) | 94.29(6) |
| N(2)-Ni(1)-N(1) | 117.02(7) |
| C(1)-O(1)-Ni(1) | 125.60(12) |
| C(3)-O(2)-C(4) | 107.11(14) |
| C(9)-O(3)-C(6) | 106.20(17) |

| | |
|---|---|
| C(12)-O(4)-Ni(1) | 127.12(12) |
| C(14)-O(5)-C(15) | 106.29(14) |
| C(20)-O(6)-C(17) | 106.05(16) |
| C(3)-N(1)-C(5) | 108.94(16) |
| C(3)-N(1)-Ni(1) | 122.19(13) |
| C(5)-N(1)-Ni(1) | 128.15(12) |
| C(14)-N(2)-C(16) | 108.72(15) |
| C(14)-N(2)-Ni(1) | 123.58(13) |
| C(16)-N(2)-Ni(1) | 127.70(12) |
| O(1)-C(1)-C(2) | 126.38(18) |
| O(1)-C(1)-C(6) | 114.01(17) |
| C(2)-C(1)-C(6) | 119.56(17) |
| C(1)-C(2)-C(3) | 123.08(17) |
| C(1)-C(2)-H(2A) | 118.5 |
| C(3)-C(2)-H(2A) | 118.5 |
| N(1)-C(3)-O(2) | 115.25(17) |
| N(1)-C(3)-C(2) | 128.40(18) |
| O(2)-C(3)-C(2) | 116.33(16) |
| O(2)-C(4)-C(5) | 105.32(16) |
| O(2)-C(4)-H(4A) | 110.7 |
| C(5)-C(4)-H(4A) | 110.7 |
| O(2)-C(4)-H(4B) | 110.7 |
| C(5)-C(4)-H(4B) | 110.7 |
| H(4A)-C(4)-H(4B) | 108.8 |
| N(1)-C(5)-C(10) | 111.23(16) |
| N(1)-C(5)-C(11) | 109.23(16) |
| C(10)-C(5)-C(11) | 111.18(17) |
| N(1)-C(5)-C(4) | 101.34(15) |
| C(10)-C(5)-C(4) | 111.76(17) |
| C(11)-C(5)-C(4) | 111.70(16) |
| C(7)-C(6)-O(3) | 109.44(18) |
| C(7)-C(6)-C(1) | 133.00(19) |
| O(3)-C(6)-C(1) | 117.33(17) |
| C(6)-C(7)-C(8) | 106.8(2) |
| C(6)-C(7)-H(7A) | 126.6 |
| C(8)-C(7)-H(7A) | 126.6 |

| | |
|---|---|
| C(9)-C(8)-C(7) | 106.4(2) |
| C(9)-C(8)-H(8A) | 126.8 |
| C(7)-C(8)-H(8A) | 126.8 |
| C(8)-C(9)-O(3) | 111.13(19) |
| C(8)-C(9)-H(9A) | 124.4 |
| O(3)-C(9)-H(9A) | 124.4 |
| C(5)-C(10)-H(10A) | 109.5 |
| C(5)-C(10)-H(10B) | 109.5 |
| H(10A)-C(10)-H(10B) | 109.5 |
| C(5)-C(10)-H(10C) | 109.5 |
| H(10A)-C(10)-H(10C) | 109.5 |
| H(10B)-C(10)-H(10C) | 109.5 |
| C(5)-C(11)-H(11A) | 109.5 |
| C(5)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 |
| C(5)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| O(4)-C(12)-C(13) | 126.02(17) |
| O(4)-C(12)-C(17) | 113.40(16) |
| C(13)-C(12)-C(17) | 120.57(17) |
| C(12)-C(13)-C(14) | 122.44(17) |
| C(12)-C(13)-H(13A) | 118.8 |
| C(14)-C(13)-H(13A) | 118.8 |
| N(2)-C(14)-O(5) | 114.96(16) |
| N(2)-C(14)-C(13) | 127.84(18) |
| O(5)-C(14)-C(13) | 117.19(16) |
| O(5)-C(15)-C(16) | 104.55(15) |
| O(5)-C(15)-H(15A) | 110.8 |
| C(16)-C(15)-H(15A) | 110.8 |
| O(5)-C(15)-H(15B) | 110.8 |
| C(16)-C(15)-H(15B) | 110.8 |
| H(15A)-C(15)-H(15B) | 108.9 |
| N(2)-C(16)-C(21) | 109.27(16) |
| N(2)-C(16)-C(22) | 110.80(16) |
| C(21)-C(16)-C(22) | 110.72(17) |

| | |
|---|---|
| N(2)-C(16)-C(15) | 101.25(15) |
| C(21)-C(16)-C(15) | 111.43(17) |
| C(22)-C(16)-C(15) | 112.96(17) |
| C(18)-C(17)-O(6) | 109.56(16) |
| C(18)-C(17)-C(12) | 131.54(17) |
| O(6)-C(17)-C(12) | 118.90(16) |
| C(17)-C(18)-C(19) | 107.26(18) |
| C(17)-C(18)-H(18A) | 126.4 |
| C(19)-C(18)-H(18A) | 126.4 |
| C(20)-C(19)-C(18) | 106.13(19) |
| C(20)-C(19)-H(19A) | 126.9 |
| C(18)-C(19)-H(19A) | 126.9 |
| C(19)-C(20)-O(6) | 111.01(18) |
| C(19)-C(20)-H(20A) | 124.5 |
| O(6)-C(20)-H(20A) | 124.5 |
| C(16)-C(21)-H(21A) | 109.5 |
| C(16)-C(21)-H(21B) | 109.5 |
| H(21A)-C(21)-H(21B) | 109.5 |
| C(16)-C(21)-H(21C) | 109.5 |
| H(21A)-C(21)-H(21C) | 109.5 |
| H(21B)-C(21)-H(21C) | 109.5 |
| C(16)-C(22)-H(22A) | 109.5 |
| C(16)-C(22)-H(22B) | 109.5 |
| H(22A)-C(22)-H(22B) | 109.5 |
| C(16)-C(22)-H(22C) | 109.5 |
| H(22A)-C(22)-H(22C) | 109.5 |
| H(22B)-C(22)-H(22C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d1839_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 15(1) | 19(1) | 16(1) | -4(1) | 4(1) | 1(1) |
| O(1) | 18(1) | 21(1) | 17(1) | -3(1) | 4(1) | 2(1) |
| O(2) | 18(1) | 30(1) | 24(1) | 4(1) | 5(1) | 8(1) |
| O(3) | 32(1) | 28(1) | 17(1) | 2(1) | 10(1) | 3(1) |
| O(4) | 19(1) | 20(1) | 18(1) | -4(1) | 6(1) | 0(1) |
| O(5) | 23(1) | 22(1) | 25(1) | -2(1) | 9(1) | -6(1) |
| O(6) | 32(1) | 31(1) | 27(1) | -13(1) | 16(1) | -7(1) |
| N(1) | 17(1) | 16(1) | 16(1) | 0(1) | 2(1) | 0(1) |
| N(2) | 17(1) | 15(1) | 19(1) | -3(1) | 2(1) | 0(1) |
| C(1) | 21(1) | 13(1) | 17(1) | -1(1) | 6(1) | -4(1) |
| C(2) | 20(1) | 19(1) | 18(1) | 0(1) | 7(1) | 1(1) |
| C(3) | 15(1) | 14(1) | 25(1) | 2(1) | 5(1) | 0(1) |
| C(4) | 21(1) | 31(1) | 23(1) | 3(1) | -1(1) | 2(1) |
| C(5) | 19(1) | 20(1) | 18(1) | 1(1) | -1(1) | 1(1) |
| C(6) | 24(1) | 15(1) | 20(1) | -1(1) | 7(1) | 0(1) |
| C(7) | 29(1) | 40(1) | 23(1) | -6(1) | 2(1) | 3(1) |
| C(8) | 44(2) | 42(1) | 20(1) | -6(1) | -3(1) | 4(1) |
| C(9) | 53(2) | 30(1) | 14(1) | -1(1) | 8(1) | 5(1) |
| C(10) | 29(1) | 22(1) | 27(1) | -3(1) | -6(1) | 0(1) |
| C(11) | 27(1) | 24(1) | 23(1) | 4(1) | 0(1) | -1(1) |
| C(12) | 17(1) | 20(1) | 12(1) | 0(1) | 0(1) | 5(1) |
| C(13) | 18(1) | 24(1) | 15(1) | -1(1) | 4(1) | 1(1) |
| C(14) | 13(1) | 20(1) | 18(1) | 2(1) | 1(1) | 1(1) |
| C(15) | 22(1) | 19(1) | 29(1) | -3(1) | 4(1) | -2(1) |
| C(16) | 17(1) | 17(1) | 24(1) | -5(1) | 2(1) | -3(1) |
| C(17) | 18(1) | 22(1) | 14(1) | -3(1) | 4(1) | 3(1) |
| C(18) | 23(1) | 24(1) | 25(1) | -4(1) | 7(1) | 0(1) |
| C(19) | 31(1) | 25(1) | 28(1) | -10(1) | 1(1) | -1(1) |
| C(20) | 39(1) | 35(1) | 25(1) | -17(1) | 11(1) | -4(1) |
| C(21) | 29(1) | 29(1) | 28(1) | -5(1) | -4(1) | -5(1) |
| C(22) | 24(1) | 19(1) | 46(1) | -10(1) | 10(1) | -2(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d1839_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 5449 | 2088 | 1759 | 23 |
| H(4A) | 7487 | 2857 | 3438 | 30 |
| H(4B) | 7111 | 1135 | 3557 | 30 |
| H(7A) | 1236 | 2896 | 1046 | 37 |
| H(8A) | 1642 | 2312 | 6 | 43 |
| H(9A) | 4002 | 2096 | -25 | 38 |
| H(10A) | 4843 | 4329 | 4073 | 40 |
| H(10B) | 6122 | 4770 | 3766 | 40 |
| H(10C) | 6247 | 3709 | 4320 | 40 |
| H(11A) | 3969 | 1661 | 3978 | 37 |
| H(11B) | 5368 | 1076 | 4247 | 37 |
| H(11C) | 4759 | 450 | 3639 | 37 |
| H(13A) | 365 | 4191 | 4254 | 23 |
| H(15A) | -582 | -50 | 3224 | 28 |
| H(15B) | 758 | -360 | 3621 | 28 |
| H(18A) | 3329 | 7981 | 4045 | 28 |
| H(19A) | 2679 | 9620 | 4869 | 33 |
| H(20A) | 908 | 8308 | 5294 | 39 |
| H(21A) | 650 | 1957 | 2110 | 44 |
| H(21B) | -603 | 1953 | 2471 | 44 |
| H(21C) | -136 | 428 | 2190 | 44 |
| H(22A) | 2675 | 507 | 2505 | 44 |
| H(22B) | 1820 | -940 | 2632 | 44 |
| H(22C) | 2731 | -167 | 3140 | 44 |

Table 6. Torsion angles [°] for d1839_a.

| | |
|---|---|
| Ni(1)-O(1)-C(1)-C(2) | -0.3(3) |
| Ni(1)-O(1)-C(1)-C(6) | 176.94(12) |
| O(1)-C(1)-C(2)-C(3) | 1.2(3) |
| C(6)-C(1)-C(2)-C(3) | -175.93(17) |
| C(5)-N(1)-C(3)-O(2) | -4.0(2) |
| Ni(1)-N(1)-C(3)-O(2) | -174.96(12) |
| C(5)-N(1)-C(3)-C(2) | 174.29(18) |
| Ni(1)-N(1)-C(3)-C(2) | 3.3(3) |
| C(4)-O(2)-C(3)-N(1) | -5.8(2) |
| C(4)-O(2)-C(3)-C(2) | 175.71(17) |
| C(1)-C(2)-C(3)-N(1) | -2.9(3) |
| C(1)-C(2)-C(3)-O(2) | 175.31(17) |
| C(3)-O(2)-C(4)-C(5) | 12.5(2) |
| C(3)-N(1)-C(5)-C(10) | 130.00(18) |
| Ni(1)-N(1)-C(5)-C(10) | -59.7(2) |
| C(3)-N(1)-C(5)-C(11) | -106.90(18) |
| Ni(1)-N(1)-C(5)-C(11) | 63.4(2) |
| C(3)-N(1)-C(5)-C(4) | 11.1(2) |
| Ni(1)-N(1)-C(5)-C(4) | -178.61(13) |
| O(2)-C(4)-C(5)-N(1) | -13.95(19) |
| O(2)-C(4)-C(5)-C(10) | -132.48(17) |
| O(2)-C(4)-C(5)-C(11) | 102.24(18) |
| C(9)-O(3)-C(6)-C(7) | -0.6(2) |
| C(9)-O(3)-C(6)-C(1) | 174.61(17) |
| O(1)-C(1)-C(6)-C(7) | -20.0(3) |
| C(2)-C(1)-C(6)-C(7) | 157.5(2) |
| O(1)-C(1)-C(6)-O(3) | 166.25(15) |
| C(2)-C(1)-C(6)-O(3) | -16.3(3) |
| O(3)-C(6)-C(7)-C(8) | 0.6(2) |
| C(1)-C(6)-C(7)-C(8) | -173.6(2) |
| C(6)-C(7)-C(8)-C(9) | -0.3(3) |
| C(7)-C(8)-C(9)-O(3) | 0.0(3) |
| C(6)-O(3)-C(9)-C(8) | 0.4(2) |
| Ni(1)-O(4)-C(12)-C(13) | 0.2(3) |

| | |
|---|---|
| Ni(1)-O(4)-C(12)-C(17) | 179.26(12) |
| O(4)-C(12)-C(13)-C(14) | 0.6(3) |
| C(17)-C(12)-C(13)-C(14) | -178.38(18) |
| C(16)-N(2)-C(14)-O(5) | 4.3(2) |
| Ni(1)-N(2)-C(14)-O(5) | -176.36(12) |
| C(16)-N(2)-C(14)-C(13) | -174.89(19) |
| Ni(1)-N(2)-C(14)-C(13) | 4.5(3) |
| C(15)-O(5)-C(14)-N(2) | 9.5(2) |
| C(15)-O(5)-C(14)-C(13) | -171.24(17) |
| C(12)-C(13)-C(14)-N(2) | -3.3(3) |
| C(12)-C(13)-C(14)-O(5) | 177.57(18) |
| C(14)-O(5)-C(15)-C(16) | -18.4(2) |
| C(14)-N(2)-C(16)-C(21) | 102.49(19) |
| Ni(1)-N(2)-C(16)-C(21) | -76.82(19) |
| C(14)-N(2)-C(16)-C(22) | -135.24(18) |
| Ni(1)-N(2)-C(16)-C(22) | 45.5(2) |
| C(14)-N(2)-C(16)-C(15) | -15.2(2) |
| Ni(1)-N(2)-C(16)-C(15) | 165.53(13) |
| O(5)-C(15)-C(16)-N(2) | 19.88(19) |
| O(5)-C(15)-C(16)-C(21) | -96.20(19) |
| O(5)-C(15)-C(16)-C(22) | 138.41(17) |
| C(20)-O(6)-C(17)-C(18) | 0.0(2) |
| C(20)-O(6)-C(17)-C(12) | 179.61(18) |
| O(4)-C(12)-C(17)-C(18) | -0.1(3) |
| C(13)-C(12)-C(17)-C(18) | 179.1(2) |
| O(4)-C(12)-C(17)-O(6) | -179.57(16) |
| C(13)-C(12)-C(17)-O(6) | -0.4(3) |
| O(6)-C(17)-C(18)-C(19) | 0.0(2) |
| C(12)-C(17)-C(18)-C(19) | -179.6(2) |
| C(17)-C(18)-C(19)-C(20) | 0.1(3) |
| C(18)-C(19)-C(20)-O(6) | -0.1(3) |
| C(17)-O(6)-C(20)-C(19) | 0.0(3) |

Symmetry transformations used to generate equivalent atoms:

## Complex 3c.

Table 1. Crystal data and structure refinement for d1833_a.

| | | |
|---|---|---|
| Identification code | d1833_a | |
| Empirical formula | C26 H26 N4 Ni O8 | |
| Formula weight | 581.22 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 9.5476(10) Å | α= 74.720(3)°. |
| | b = 10.5561(12) Å | β= 70.961(3)°. |
| | c = 14.4705(16) Å | γ = 70.689(3)°. |
| Volume | 1281.1(2) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.507 $Mg/m^3$ | |
| Absorption coefficient | 0.815 $mm^{-1}$ | |
| F(000) | 604 | |
| Crystal size | 0.200 x 0.180 x 0.110 $mm^3$ | |
| Theta range for data collection | 1.512 to 27.698°. | |
| Index ranges | -12<=h<=12, -13<=k<=13, -18<=l<=18 | |
| Reflections collected | 31731 | |
| Independent reflections | 5961 [R(int) = 0.0333] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.7169 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5961 / 0 / 356 | |
| Goodness-of-fit on $F^2$ | 1.024 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0301, wR2 = 0.0681 | |
| R indices (all data) | R1 = 0.0419, wR2 = 0.0733 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.439 and -0.317 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d1833_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 2582(1) | 2283(1) | 6906(1) | 17(1) |
| O(1) | 2972(1) | 1499(1) | 8198(1) | 20(1) |
| O(2) | 779(2) | -1001(1) | 7647(1) | 28(1) |
| O(3) | 4058(2) | 675(1) | 12768(1) | 34(1) |
| O(4) | 3717(2) | -1340(1) | 13155(1) | 28(1) |
| O(5) | 3612(1) | 2843(1) | 5533(1) | 20(1) |
| O(6) | 321(2) | 6369(1) | 6534(1) | 35(1) |
| O(7) | 6376(2) | 3687(2) | 432(1) | 46(1) |
| O(8) | 6587(2) | 5661(1) | 397(1) | 35(1) |
| N(1) | 1718(2) | 821(1) | 6951(1) | 18(1) |
| N(2) | 3749(2) | -252(1) | 12583(1) | 21(1) |
| N(3) | 1273(2) | 4132(1) | 7046(1) | 19(1) |
| N(4) | 6242(2) | 4606(2) | 847(1) | 24(1) |
| C(1) | 2448(2) | 540(2) | 8846(1) | 17(1) |
| C(2) | 1670(2) | -225(2) | 8682(1) | 21(1) |
| C(3) | 1413(2) | -81(2) | 7740(1) | 19(1) |
| C(4) | 538(3) | -614(2) | 6665(1) | 33(1) |
| C(5) | 1343(2) | 514(2) | 6127(1) | 21(1) |
| C(6) | 2743(2) | 310(2) | 9843(1) | 17(1) |
| C(7) | 2669(2) | -896(2) | 10534(1) | 19(1) |
| C(8) | 2995(2) | -1077(2) | 11433(1) | 19(1) |
| C(9) | 3389(2) | -48(2) | 11636(1) | 17(1) |
| C(10) | 3465(2) | 1156(2) | 10972(1) | 19(1) |
| C(11) | 3140(2) | 1320(2) | 10076(1) | 18(1) |
| C(12) | 299(3) | 1778(2) | 5666(2) | 43(1) |
| C(13) | 2826(2) | -7(2) | 5367(2) | 37(1) |
| C(14) | 3383(2) | 4062(2) | 5019(1) | 18(1) |
| C(15) | 2368(2) | 5210(2) | 5363(1) | 24(1) |
| C(16) | 1363(2) | 5172(2) | 6332(1) | 22(1) |
| C(17) | -487(3) | 6120(2) | 7571(2) | 42(1) |
| C(18) | -104(2) | 4574(2) | 7870(1) | 22(1) |

| | | | | |
|---|---|---|---|---|
| C(19) | 4244(2) | 4191(2) | 3943(1) | 17(1) |
| C(20) | 4702(2) | 5369(2) | 3416(1) | 19(1) |
| C(21) | 5390(2) | 5505(2) | 2405(1) | 19(1) |
| C(22) | 5610(2) | 4447(2) | 1930(1) | 18(1) |
| C(23) | 5216(2) | 3253(2) | 2431(1) | 23(1) |
| C(24) | 4537(2) | 3132(2) | 3441(1) | 22(1) |
| C(25) | 246(2) | 4096(3) | 8880(2) | 41(1) |
| C(26) | -1366(2) | 4006(2) | 7862(2) | 34(1) |

Table 3. Bond lengths [Å] and angles [°] for d1833_a.

| | |
|---|---|
| Ni(1)-O(1) | 1.9362(11) |
| Ni(1)-O(5) | 1.9377(11) |
| Ni(1)-N(1) | 1.9547(14) |
| Ni(1)-N(3) | 1.9597(14) |
| O(1)-C(1) | 1.2976(19) |
| O(2)-C(3) | 1.356(2) |
| O(2)-C(4) | 1.445(2) |
| O(3)-N(2) | 1.2238(18) |
| O(4)-N(2) | 1.2291(18) |
| O(5)-C(14) | 1.2927(19) |
| O(6)-C(16) | 1.358(2) |
| O(6)-C(17) | 1.445(2) |
| O(7)-N(4) | 1.2222(19) |
| O(8)-N(4) | 1.2226(19) |
| N(1)-C(3) | 1.300(2) |
| N(1)-C(5) | 1.488(2) |
| N(2)-C(9) | 1.465(2) |
| N(3)-C(16) | 1.299(2) |
| N(3)-C(18) | 1.494(2) |
| N(4)-C(22) | 1.469(2) |
| C(1)-C(2) | 1.369(2) |
| C(1)-C(6) | 1.501(2) |
| C(2)-C(3) | 1.423(2) |
| C(2)-H(2A) | 0.9500 |
| C(4)-C(5) | 1.530(3) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(12) | 1.518(3) |
| C(5)-C(13) | 1.518(3) |
| C(6)-C(11) | 1.391(2) |
| C(6)-C(7) | 1.403(2) |
| C(7)-C(8) | 1.386(2) |
| C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.385(2) |

| | |
|---|---|
| C(8)-H(8A) | 0.9500 |
| C(9)-C(10) | 1.384(2) |
| C(10)-C(11) | 1.384(2) |
| C(10)-H(10A) | 0.9500 |
| C(11)-H(11A) | 0.9500 |
| C(12)-H(12A) | 0.9800 |
| C(12)-H(12B) | 0.9800 |
| C(12)-H(12C) | 0.9800 |
| C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 |
| C(13)-H(13C) | 0.9800 |
| C(14)-C(15) | 1.372(2) |
| C(14)-C(19) | 1.499(2) |
| C(15)-C(16) | 1.416(2) |
| C(15)-H(15A) | 0.9500 |
| C(17)-C(18) | 1.523(3) |
| C(17)-H(17A) | 0.9900 |
| C(17)-H(17B) | 0.9900 |
| C(18)-C(26) | 1.517(3) |
| C(18)-C(25) | 1.523(3) |
| C(19)-C(24) | 1.394(2) |
| C(19)-C(20) | 1.401(2) |
| C(20)-C(21) | 1.385(2) |
| C(20)-H(20A) | 0.9500 |
| C(21)-C(22) | 1.386(2) |
| C(21)-H(21A) | 0.9500 |
| C(22)-C(23) | 1.382(2) |
| C(23)-C(24) | 1.382(2) |
| C(23)-H(23A) | 0.9500 |
| C(24)-H(24A) | 0.9500 |
| C(25)-H(25A) | 0.9800 |
| C(25)-H(25B) | 0.9800 |
| C(25)-H(25C) | 0.9800 |
| C(26)-H(26A) | 0.9800 |
| C(26)-H(26B) | 0.9800 |
| C(26)-H(26C) | 0.9800 |

| | |
|---|---|
| O(1)-Ni(1)-O(5) | 141.83(5) |
| O(1)-Ni(1)-N(1) | 92.16(5) |
| O(5)-Ni(1)-N(1) | 107.53(5) |
| O(1)-Ni(1)-N(3) | 104.36(5) |
| O(5)-Ni(1)-N(3) | 93.04(5) |
| N(1)-Ni(1)-N(3) | 121.31(6) |
| C(1)-O(1)-Ni(1) | 127.32(11) |
| C(3)-O(2)-C(4) | 106.79(13) |
| C(14)-O(5)-Ni(1) | 127.15(11) |
| C(16)-O(6)-C(17) | 106.50(14) |
| C(3)-N(1)-C(5) | 108.79(14) |
| C(3)-N(1)-Ni(1) | 123.38(11) |
| C(5)-N(1)-Ni(1) | 127.81(11) |
| O(3)-N(2)-O(4) | 123.26(14) |
| O(3)-N(2)-C(9) | 118.25(14) |
| O(4)-N(2)-C(9) | 118.49(13) |
| C(16)-N(3)-C(18) | 108.08(14) |
| C(16)-N(3)-Ni(1) | 122.88(12) |
| C(18)-N(3)-Ni(1) | 128.40(11) |
| O(7)-N(4)-O(8) | 122.68(15) |
| O(7)-N(4)-C(22) | 118.60(14) |
| O(8)-N(4)-C(22) | 118.70(14) |
| O(1)-C(1)-C(2) | 125.21(15) |
| O(1)-C(1)-C(6) | 114.59(14) |
| C(2)-C(1)-C(6) | 120.19(14) |
| C(1)-C(2)-C(3) | 122.30(15) |
| C(1)-C(2)-H(2A) | 118.9 |
| C(3)-C(2)-H(2A) | 118.9 |
| N(1)-C(3)-O(2) | 115.57(14) |
| N(1)-C(3)-C(2) | 128.10(15) |
| O(2)-C(3)-C(2) | 116.33(14) |
| O(2)-C(4)-C(5) | 105.81(14) |
| O(2)-C(4)-H(4A) | 110.6 |
| C(5)-C(4)-H(4A) | 110.6 |
| O(2)-C(4)-H(4B) | 110.6 |

| | |
|---|---|
| C(5)-C(4)-H(4B) | 110.6 |
| H(4A)-C(4)-H(4B) | 108.7 |
| N(1)-C(5)-C(12) | 110.00(14) |
| N(1)-C(5)-C(13) | 109.12(15) |
| C(12)-C(5)-C(13) | 111.52(17) |
| N(1)-C(5)-C(4) | 101.97(13) |
| C(12)-C(5)-C(4) | 112.58(17) |
| C(13)-C(5)-C(4) | 111.21(16) |
| C(11)-C(6)-C(7) | 119.04(15) |
| C(11)-C(6)-C(1) | 118.49(14) |
| C(7)-C(6)-C(1) | 122.45(14) |
| C(8)-C(7)-C(6) | 120.28(15) |
| C(8)-C(7)-H(7A) | 119.9 |
| C(6)-C(7)-H(7A) | 119.9 |
| C(9)-C(8)-C(7) | 118.88(15) |
| C(9)-C(8)-H(8A) | 120.6 |
| C(7)-C(8)-H(8A) | 120.6 |
| C(10)-C(9)-C(8) | 122.22(15) |
| C(10)-C(9)-N(2) | 119.18(14) |
| C(8)-C(9)-N(2) | 118.60(14) |
| C(11)-C(10)-C(9) | 118.21(15) |
| C(11)-C(10)-H(10A) | 120.9 |
| C(9)-C(10)-H(10A) | 120.9 |
| C(10)-C(11)-C(6) | 121.36(15) |
| C(10)-C(11)-H(11A) | 119.3 |
| C(6)-C(11)-H(11A) | 119.3 |
| C(5)-C(12)-H(12A) | 109.5 |
| C(5)-C(12)-H(12B) | 109.5 |
| H(12A)-C(12)-H(12B) | 109.5 |
| C(5)-C(12)-H(12C) | 109.5 |
| H(12A)-C(12)-H(12C) | 109.5 |
| H(12B)-C(12)-H(12C) | 109.5 |
| C(5)-C(13)-H(13A) | 109.5 |
| C(5)-C(13)-H(13B) | 109.5 |
| H(13A)-C(13)-H(13B) | 109.5 |
| C(5)-C(13)-H(13C) | 109.5 |

| | |
|---|---|
| H(13A)-C(13)-H(13C) | 109.5 |
| H(13B)-C(13)-H(13C) | 109.5 |
| O(5)-C(14)-C(15) | 125.59(15) |
| O(5)-C(14)-C(19) | 116.06(14) |
| C(15)-C(14)-C(19) | 118.24(14) |
| C(14)-C(15)-C(16) | 122.68(15) |
| C(14)-C(15)-H(15A) | 118.7 |
| C(16)-C(15)-H(15A) | 118.7 |
| N(3)-C(16)-O(6) | 115.45(15) |
| N(3)-C(16)-C(15) | 128.54(16) |
| O(6)-C(16)-C(15) | 115.98(15) |
| O(6)-C(17)-C(18) | 105.16(15) |
| O(6)-C(17)-H(17A) | 110.7 |
| C(18)-C(17)-H(17A) | 110.7 |
| O(6)-C(17)-H(17B) | 110.7 |
| C(18)-C(17)-H(17B) | 110.7 |
| H(17A)-C(17)-H(17B) | 108.8 |
| N(3)-C(18)-C(26) | 108.24(14) |
| N(3)-C(18)-C(25) | 112.31(15) |
| C(26)-C(18)-C(25) | 109.91(17) |
| N(3)-C(18)-C(17) | 101.77(14) |
| C(26)-C(18)-C(17) | 112.23(17) |
| C(25)-C(18)-C(17) | 112.12(17) |
| C(24)-C(19)-C(20) | 119.02(15) |
| C(24)-C(19)-C(14) | 119.01(14) |
| C(20)-C(19)-C(14) | 121.90(14) |
| C(21)-C(20)-C(19) | 120.77(15) |
| C(21)-C(20)-H(20A) | 119.6 |
| C(19)-C(20)-H(20A) | 119.6 |
| C(20)-C(21)-C(22) | 118.23(15) |
| C(20)-C(21)-H(21A) | 120.9 |
| C(22)-C(21)-H(21A) | 120.9 |
| C(23)-C(22)-C(21) | 122.55(15) |
| C(23)-C(22)-N(4) | 118.23(14) |
| C(21)-C(22)-N(4) | 119.20(14) |
| C(22)-C(23)-C(24) | 118.40(15) |

| | |
|---|---|
| C(22)-C(23)-H(23A) | 120.8 |
| C(24)-C(23)-H(23A) | 120.8 |
| C(23)-C(24)-C(19) | 120.96(15) |
| C(23)-C(24)-H(24A) | 119.5 |
| C(19)-C(24)-H(24A) | 119.5 |
| C(18)-C(25)-H(25A) | 109.5 |
| C(18)-C(25)-H(25B) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 |
| C(18)-C(25)-H(25C) | 109.5 |
| H(25A)-C(25)-H(25C) | 109.5 |
| H(25B)-C(25)-H(25C) | 109.5 |
| C(18)-C(26)-H(26A) | 109.5 |
| C(18)-C(26)-H(26B) | 109.5 |
| H(26A)-C(26)-H(26B) | 109.5 |
| C(18)-C(26)-H(26C) | 109.5 |
| H(26A)-C(26)-H(26C) | 109.5 |
| H(26B)-C(26)-H(26C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d1833_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 23(1) | 16(1) | 13(1) | 0(1) | -4(1) | -7(1) |
| O(1) | 26(1) | 22(1) | 13(1) | 2(1) | -6(1) | -11(1) |
| O(2) | 42(1) | 30(1) | 21(1) | -1(1) | -12(1) | -22(1) |
| O(3) | 59(1) | 31(1) | 24(1) | -3(1) | -16(1) | -25(1) |
| O(4) | 45(1) | 25(1) | 19(1) | 4(1) | -13(1) | -16(1) |
| O(5) | 26(1) | 16(1) | 14(1) | 1(1) | -4(1) | -5(1) |
| O(6) | 42(1) | 18(1) | 29(1) | -5(1) | 5(1) | -1(1) |
| O(7) | 82(1) | 32(1) | 22(1) | -13(1) | 6(1) | -27(1) |
| O(8) | 56(1) | 29(1) | 20(1) | -1(1) | 2(1) | -25(1) |
| N(1) | 21(1) | 19(1) | 15(1) | -2(1) | -6(1) | -5(1) |
| N(2) | 25(1) | 22(1) | 15(1) | -3(1) | -4(1) | -9(1) |
| N(3) | 20(1) | 20(1) | 16(1) | -4(1) | -1(1) | -7(1) |
| N(4) | 29(1) | 22(1) | 18(1) | -5(1) | -1(1) | -10(1) |
| C(1) | 19(1) | 17(1) | 13(1) | -1(1) | -2(1) | -5(1) |
| C(2) | 27(1) | 22(1) | 15(1) | 1(1) | -5(1) | -12(1) |
| C(3) | 21(1) | 20(1) | 18(1) | -4(1) | -4(1) | -8(1) |
| C(4) | 44(1) | 45(1) | 20(1) | -4(1) | -11(1) | -26(1) |
| C(5) | 27(1) | 23(1) | 17(1) | -6(1) | -7(1) | -8(1) |
| C(6) | 17(1) | 18(1) | 14(1) | -2(1) | -2(1) | -6(1) |
| C(7) | 24(1) | 18(1) | 18(1) | -2(1) | -5(1) | -10(1) |
| C(8) | 24(1) | 18(1) | 16(1) | 0(1) | -4(1) | -9(1) |
| C(9) | 18(1) | 19(1) | 14(1) | -3(1) | -3(1) | -6(1) |
| C(10) | 22(1) | 17(1) | 19(1) | -4(1) | -4(1) | -8(1) |
| C(11) | 22(1) | 16(1) | 16(1) | 1(1) | -4(1) | -7(1) |
| C(12) | 59(2) | 34(1) | 47(1) | -9(1) | -39(1) | 0(1) |
| C(13) | 41(1) | 43(1) | 28(1) | -17(1) | 4(1) | -17(1) |
| C(14) | 21(1) | 19(1) | 15(1) | 1(1) | -7(1) | -8(1) |
| C(15) | 30(1) | 17(1) | 18(1) | 0(1) | -3(1) | -5(1) |
| C(16) | 25(1) | 16(1) | 23(1) | -5(1) | -5(1) | -4(1) |
| C(17) | 47(1) | 27(1) | 35(1) | -10(1) | 14(1) | -9(1) |
| C(18) | 21(1) | 24(1) | 19(1) | -8(1) | -1(1) | -4(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(19) | 20(1) | 17(1) | 16(1) | 1(1) | -7(1) | -5(1) |
| C(20) | 24(1) | 18(1) | 19(1) | -4(1) | -6(1) | -8(1) |
| C(21) | 22(1) | 17(1) | 20(1) | -1(1) | -5(1) | -9(1) |
| C(22) | 20(1) | 20(1) | 13(1) | -2(1) | -2(1) | -7(1) |
| C(23) | 32(1) | 18(1) | 20(1) | -6(1) | -3(1) | -9(1) |
| C(24) | 30(1) | 16(1) | 18(1) | 0(1) | -4(1) | -10(1) |
| C(25) | 31(1) | 63(2) | 23(1) | -20(1) | -5(1) | 2(1) |
| C(26) | 24(1) | 42(1) | 37(1) | -14(1) | 0(1) | -12(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d1833_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 1287 | -875 | 9216 | 25 |
| H(4A) | -575 | -274 | 6703 | 39 |
| H(4B) | 987 | -1402 | 6313 | 39 |
| H(7A) | 2394 | -1592 | 10385 | 23 |
| H(8A) | 2949 | -1893 | 11903 | 23 |
| H(10A) | 3733 | 1851 | 11127 | 22 |
| H(11A) | 3190 | 2139 | 9611 | 22 |
| H(12A) | 835 | 2496 | 5382 | 64 |
| H(12B) | -638 | 2095 | 6176 | 64 |
| H(12C) | 27 | 1558 | 5140 | 64 |
| H(13A) | 3399 | 686 | 5112 | 55 |
| H(13B) | 2585 | -198 | 4817 | 55 |
| H(13C) | 3451 | -845 | 5680 | 55 |
| H(15A) | 2339 | 6067 | 4933 | 28 |
| H(17A) | -1610 | 6516 | 7666 | 50 |
| H(17B) | -134 | 6522 | 7971 | 50 |
| H(20A) | 4539 | 6082 | 3757 | 23 |
| H(21A) | 5702 | 6303 | 2047 | 23 |
| H(23A) | 5408 | 2532 | 2090 | 28 |
| H(24A) | 4266 | 2315 | 3798 | 26 |
| H(25A) | 1157 | 4355 | 8852 | 61 |
| H(25B) | 442 | 3102 | 9057 | 61 |
| H(25C) | -635 | 4522 | 9382 | 61 |
| H(26A) | -1635 | 4369 | 7227 | 52 |
| H(26B) | -2274 | 4273 | 8406 | 52 |
| H(26C) | -1002 | 3010 | 7948 | 52 |

Table 6. Torsion angles [°] for d1833_a.

| | |
|---|---|
| Ni(1)-O(1)-C(1)-C(2) | 8.9(2) |
| Ni(1)-O(1)-C(1)-C(6) | -170.48(10) |
| O(1)-C(1)-C(2)-C(3) | 3.1(3) |
| C(6)-C(1)-C(2)-C(3) | -177.54(15) |
| C(5)-N(1)-C(3)-O(2) | -3.2(2) |
| Ni(1)-N(1)-C(3)-O(2) | 178.30(11) |
| C(5)-N(1)-C(3)-C(2) | 176.37(17) |
| Ni(1)-N(1)-C(3)-C(2) | -2.1(3) |
| C(4)-O(2)-C(3)-N(1) | -3.8(2) |
| C(4)-O(2)-C(3)-C(2) | 176.55(16) |
| C(1)-C(2)-C(3)-N(1) | -6.7(3) |
| C(1)-C(2)-C(3)-O(2) | 172.91(16) |
| C(3)-O(2)-C(4)-C(5) | 8.8(2) |
| C(3)-N(1)-C(5)-C(12) | 127.93(17) |
| Ni(1)-N(1)-C(5)-C(12) | -53.7(2) |
| C(3)-N(1)-C(5)-C(13) | -109.43(17) |
| Ni(1)-N(1)-C(5)-C(13) | 68.95(18) |
| C(3)-N(1)-C(5)-C(4) | 8.27(19) |
| Ni(1)-N(1)-C(5)-C(4) | -173.35(12) |
| O(2)-C(4)-C(5)-N(1) | -10.16(19) |
| O(2)-C(4)-C(5)-C(12) | -127.99(17) |
| O(2)-C(4)-C(5)-C(13) | 106.03(18) |
| O(1)-C(1)-C(6)-C(11) | 17.0(2) |
| C(2)-C(1)-C(6)-C(11) | -162.43(16) |
| O(1)-C(1)-C(6)-C(7) | -161.44(15) |
| C(2)-C(1)-C(6)-C(7) | 19.1(2) |
| C(11)-C(6)-C(7)-C(8) | -0.3(2) |
| C(1)-C(6)-C(7)-C(8) | 178.11(15) |
| C(6)-C(7)-C(8)-C(9) | 0.2(3) |
| C(7)-C(8)-C(9)-C(10) | 0.1(3) |
| C(7)-C(8)-C(9)-N(2) | -179.32(15) |
| O(3)-N(2)-C(9)-C(10) | 2.4(2) |
| O(4)-N(2)-C(9)-C(10) | -178.08(15) |
| O(3)-N(2)-C(9)-C(8) | -178.20(16) |

| | |
|---|---|
| O(4)-N(2)-C(9)-C(8) | 1.4(2) |
| C(8)-C(9)-C(10)-C(11) | -0.3(3) |
| N(2)-C(9)-C(10)-C(11) | 179.14(15) |
| C(9)-C(10)-C(11)-C(6) | 0.2(2) |
| C(7)-C(6)-C(11)-C(10) | 0.1(2) |
| C(1)-C(6)-C(11)-C(10) | -178.35(15) |
| Ni(1)-O(5)-C(14)-C(15) | 1.3(2) |
| Ni(1)-O(5)-C(14)-C(19) | -174.89(10) |
| O(5)-C(14)-C(15)-C(16) | -4.0(3) |
| C(19)-C(14)-C(15)-C(16) | 172.02(16) |
| C(18)-N(3)-C(16)-O(6) | 5.3(2) |
| Ni(1)-N(3)-C(16)-O(6) | 176.86(12) |
| C(18)-N(3)-C(16)-C(15) | -172.44(18) |
| Ni(1)-N(3)-C(16)-C(15) | -0.9(3) |
| C(17)-O(6)-C(16)-N(3) | 6.4(2) |
| C(17)-O(6)-C(16)-C(15) | -175.53(18) |
| C(14)-C(15)-C(16)-N(3) | 3.9(3) |
| C(14)-C(15)-C(16)-O(6) | -173.83(17) |
| C(16)-O(6)-C(17)-C(18) | -14.9(2) |
| C(16)-N(3)-C(18)-C(26) | 104.54(17) |
| Ni(1)-N(3)-C(18)-C(26) | -66.40(19) |
| C(16)-N(3)-C(18)-C(25) | -133.94(17) |
| Ni(1)-N(3)-C(18)-C(25) | 55.1(2) |
| C(16)-N(3)-C(18)-C(17) | -13.86(19) |
| Ni(1)-N(3)-C(18)-C(17) | 175.21(14) |
| O(6)-C(17)-C(18)-N(3) | 17.1(2) |
| O(6)-C(17)-C(18)-C(26) | -98.44(19) |
| O(6)-C(17)-C(18)-C(25) | 137.28(18) |
| O(5)-C(14)-C(19)-C(24) | 33.1(2) |
| C(15)-C(14)-C(19)-C(24) | -143.32(17) |
| O(5)-C(14)-C(19)-C(20) | -149.76(16) |
| C(15)-C(14)-C(19)-C(20) | 33.8(2) |
| C(24)-C(19)-C(20)-C(21) | 2.2(3) |
| C(14)-C(19)-C(20)-C(21) | -174.96(15) |
| C(19)-C(20)-C(21)-C(22) | 0.1(3) |
| C(20)-C(21)-C(22)-C(23) | -2.2(3) |

| | |
|---|---|
| C(20)-C(21)-C(22)-N(4) | 175.96(15) |
| O(7)-N(4)-C(22)-C(23) | 1.0(3) |
| O(8)-N(4)-C(22)-C(23) | 179.68(17) |
| O(7)-N(4)-C(22)-C(21) | -177.23(17) |
| O(8)-N(4)-C(22)-C(21) | 1.5(2) |
| C(21)-C(22)-C(23)-C(24) | 1.9(3) |
| N(4)-C(22)-C(23)-C(24) | -176.23(16) |
| C(22)-C(23)-C(24)-C(19) | 0.4(3) |
| C(20)-C(19)-C(24)-C(23) | -2.4(3) |
| C(14)-C(19)-C(24)-C(23) | 174.77(16) |

Symmetry transformations used to generate equivalent atoms:

## Complex 3e

Table 1. Crystal data and structure refinement for d1835_a.

| | | |
|---|---|---|
| Identification code | d1835_a | |
| Empirical formula | C22 H24 N2 Ni O4 S2 | |
| Formula weight | 503.26 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1/n$ | |
| Unit cell dimensions | a = 9.8995(5) Å | α= 90°. |
| | b = 14.7668(8) Å | β= 104.652(2)°. |
| | c = 16.2988(9) Å | γ = 90°. |
| Volume | 2305.1(2) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.450 $Mg/m^3$ | |
| Absorption coefficient | 1.054 $mm^{-1}$ | |
| F(000) | 1048 | |
| Crystal size | 0.280 x 0.240 x 0.220 $mm^3$ | |
| Theta range for data collection | 1.889 to 27.519°. | |
| Index ranges | -12<=h<=12, -19<=k<=19, -21<=l<=21 | |
| Reflections collected | 31003 | |
| Independent reflections | 5293 [R(int) = 0.0282] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.7172 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5293 / 180 / 321 | |
| Goodness-of-fit on $F^2$ | 1.052 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0264, wR2 = 0.0607 | |
| R indices (all data) | R1 = 0.0392, wR2 = 0.0667 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.311 and -0.308 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d1835_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 6432(1) | 4916(1) | 7559(1) | 19(1) |
| O(1) | 6472(1) | 5244(1) | 6425(1) | 21(1) |
| O(2) | 4721(1) | 7456(1) | 7460(1) | 27(1) |
| O(3) | 5621(1) | 3983(1) | 8108(1) | 22(1) |
| O(4) | 9947(1) | 4062(1) | 9314(1) | 26(1) |
| N(1) | 5586(1) | 6054(1) | 7764(1) | 19(1) |
| N(2) | 8318(1) | 4671(1) | 8237(1) | 19(1) |
| C(1) | 5284(2) | 6701(1) | 7203(1) | 20(1) |
| C(2) | 5440(2) | 6702(1) | 6364(1) | 21(1) |
| C(3) | 5993(2) | 5980(1) | 6027(1) | 18(1) |
| C(4) | 4877(2) | 7350(1) | 8365(1) | 32(1) |
| C(5) | 5128(2) | 6333(1) | 8528(1) | 24(1) |
| S(1) | 7041(2) | 5237(1) | 4774(1) | 24(1) |
| C(6) | 6100(2) | 6019(1) | 5142(1) | 20(1) |
| C(7) | 5535(9) | 6642(5) | 4532(4) | 17(1) |
| C(8) | 5901(4) | 6496(2) | 3752(2) | 26(1) |
| C(9) | 6721(4) | 5744(2) | 3794(2) | 26(1) |
| S(1A) | 5417(10) | 6740(6) | 4389(4) | 26(1) |
| C(6A) | 6100(2) | 6019(1) | 5142(1) | 20(1) |
| C(7A) | 6870(20) | 5360(10) | 4854(8) | 23(2) |
| C(8A) | 6969(14) | 5524(8) | 4007(6) | 23(2) |
| C(9A) | 6202(14) | 6253(8) | 3670(6) | 25(2) |
| C(10) | 6255(2) | 6133(1) | 9332(1) | 35(1) |
| C(11) | 3769(2) | 5844(2) | 8529(1) | 39(1) |
| C(12) | 6252(2) | 3487(1) | 8748(1) | 18(1) |
| C(13) | 7638(2) | 3556(1) | 9169(1) | 21(1) |
| C(14) | 8584(2) | 4119(1) | 8879(1) | 20(1) |
| C(15) | 10725(2) | 4652(1) | 8895(1) | 32(1) |
| S(2) | 3613(1) | 2759(1) | 8459(1) | 24(1) |
| C(16) | 5355(2) | 2800(1) | 9000(1) | 18(1) |
| C(17) | 5671(2) | 2134(1) | 9606(1) | 22(1) |

| | | | | |
|---|---|---|---|---|
| C(18) | 4498(2) | 1593(1) | 9631(1) | 26(1) |
| C(19) | 3320(2) | 1855(1) | 9051(1) | 27(1) |
| C(20) | 9639(2) | 5100(1) | 8161(1) | 22(1) |
| C(21) | 9900(2) | 4880(2) | 7303(1) | 36(1) |
| C(22) | 9561(2) | 6117(1) | 8284(2) | 42(1) |

Table 3. Bond lengths [Å] and angles [°] for d1835_a.

| | |
|---|---|
| Ni(1)-O(1) | 1.9214(11) |
| Ni(1)-O(3) | 1.9253(11) |
| Ni(1)-N(1) | 1.9437(14) |
| Ni(1)-N(2) | 1.9479(14) |
| O(1)-C(3) | 1.2926(19) |
| O(2)-C(1) | 1.3596(19) |
| O(2)-C(4) | 1.453(2) |
| O(3)-C(12) | 1.2978(18) |
| O(4)-C(14) | 1.358(2) |
| O(4)-C(15) | 1.444(2) |
| N(1)-C(1) | 1.303(2) |
| N(1)-C(5) | 1.487(2) |
| N(2)-C(14) | 1.300(2) |
| N(2)-C(20) | 1.487(2) |
| C(1)-C(2) | 1.415(2) |
| C(2)-C(3) | 1.374(2) |
| C(2)-H(2A) | 0.9500 |
| C(3)-C(6A) | 1.474(2) |
| C(3)-C(6) | 1.474(2) |
| C(4)-C(5) | 1.534(3) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(10) | 1.519(2) |
| C(5)-C(11) | 1.528(3) |
| S(1)-C(6) | 1.6863(18) |
| S(1)-C(9) | 1.720(3) |
| C(6)-C(7) | 1.365(5) |
| C(7)-C(8) | 1.424(6) |
| C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.367(4) |
| C(8)-H(8A) | 0.9500 |
| C(9)-H(9) | 0.9500 |
| S(1A)-C(6A) | 1.637(5) |
| S(1A)-C(9A) | 1.719(7) |

| | |
|---|---|
| C(6A)-C(7A) | 1.386(8) |
| C(7A)-C(8A) | 1.430(8) |
| C(7A)-H(7AA) | 0.9500 |
| C(8A)-C(9A) | 1.352(8) |
| C(8A)-H(8AA) | 0.9500 |
| C(9A)-H(9A) | 0.9500 |
| C(10)-H(10A) | 0.9800 |
| C(10)-H(10B) | 0.9800 |
| C(10)-H(10C) | 0.9800 |
| C(11)-H(11A) | 0.9800 |
| C(11)-H(11B) | 0.9800 |
| C(11)-H(11C) | 0.9800 |
| C(12)-C(13) | 1.374(2) |
| C(12)-C(16) | 1.474(2) |
| C(13)-C(14) | 1.419(2) |
| C(13)-H(13A) | 0.9500 |
| C(15)-C(20) | 1.541(3) |
| C(15)-H(15A) | 0.9900 |
| C(15)-H(15B) | 0.9900 |
| S(2)-C(19) | 1.7145(17) |
| S(2)-C(16) | 1.7282(16) |
| C(16)-C(17) | 1.373(2) |
| C(17)-C(18) | 1.418(2) |
| C(17)-H(17A) | 0.9500 |
| C(18)-C(19) | 1.359(2) |
| C(18)-H(18A) | 0.9500 |
| C(19)-H(19) | 0.9500 |
| C(20)-C(22) | 1.520(2) |
| C(20)-C(21) | 1.520(2) |
| C(21)-H(21A) | 0.9800 |
| C(21)-H(21B) | 0.9800 |
| C(21)-H(21C) | 0.9800 |
| C(22)-H(22A) | 0.9800 |
| C(22)-H(22B) | 0.9800 |
| C(22)-H(22C) | 0.9800 |

| | |
|---|---|
| O(1)-Ni(1)-O(3) | 137.71(5) |
| O(1)-Ni(1)-N(1) | 93.58(5) |
| O(3)-Ni(1)-N(1) | 106.88(5) |
| O(1)-Ni(1)-N(2) | 110.04(5) |
| O(3)-Ni(1)-N(2) | 93.18(5) |
| N(1)-Ni(1)-N(2) | 117.17(6) |
| C(3)-O(1)-Ni(1) | 126.87(10) |
| C(1)-O(2)-C(4) | 106.11(12) |
| C(12)-O(3)-Ni(1) | 127.21(11) |
| C(14)-O(4)-C(15) | 107.16(13) |
| C(1)-N(1)-C(5) | 108.73(13) |
| C(1)-N(1)-Ni(1) | 123.01(11) |
| C(5)-N(1)-Ni(1) | 128.23(11) |
| C(14)-N(2)-C(20) | 109.34(14) |
| C(14)-N(2)-Ni(1) | 122.92(11) |
| C(20)-N(2)-Ni(1) | 127.62(11) |
| N(1)-C(1)-O(2) | 115.07(14) |
| N(1)-C(1)-C(2) | 128.15(15) |
| O(2)-C(1)-C(2) | 116.76(14) |
| C(3)-C(2)-C(1) | 122.47(15) |
| C(3)-C(2)-H(2A) | 118.8 |
| C(1)-C(2)-H(2A) | 118.8 |
| O(1)-C(3)-C(2) | 125.78(14) |
| O(1)-C(3)-C(6A) | 114.58(14) |
| C(2)-C(3)-C(6A) | 119.63(14) |
| O(1)-C(3)-C(6) | 114.58(14) |
| C(2)-C(3)-C(6) | 119.63(14) |
| O(2)-C(4)-C(5) | 104.67(13) |
| O(2)-C(4)-H(4A) | 110.8 |
| C(5)-C(4)-H(4A) | 110.8 |
| O(2)-C(4)-H(4B) | 110.8 |
| C(5)-C(4)-H(4B) | 110.8 |
| H(4A)-C(4)-H(4B) | 108.9 |
| N(1)-C(5)-C(10) | 110.83(14) |
| N(1)-C(5)-C(11) | 108.96(14) |
| C(10)-C(5)-C(11) | 111.25(16) |

| | |
|---|---|
| N(1)-C(5)-C(4) | 101.28(13) |
| C(10)-C(5)-C(4) | 113.03(16) |
| C(11)-C(5)-C(4) | 111.03(16) |
| C(6)-S(1)-C(9) | 92.49(13) |
| C(7)-C(6)-C(3) | 128.4(3) |
| C(7)-C(6)-S(1) | 111.4(3) |
| C(3)-C(6)-S(1) | 120.23(12) |
| C(6)-C(7)-C(8) | 113.5(4) |
| C(6)-C(7)-H(7A) | 123.3 |
| C(8)-C(7)-H(7A) | 123.3 |
| C(9)-C(8)-C(7) | 111.1(3) |
| C(9)-C(8)-H(8A) | 124.4 |
| C(7)-C(8)-H(8A) | 124.4 |
| C(8)-C(9)-S(1) | 111.6(2) |
| C(8)-C(9)-H(9) | 124.2 |
| S(1)-C(9)-H(9) | 124.2 |
| C(6A)-S(1A)-C(9A) | 93.8(4) |
| C(7A)-C(6A)-C(3) | 119.0(5) |
| C(7A)-C(6A)-S(1A) | 111.1(5) |
| C(3)-C(6A)-S(1A) | 129.9(3) |
| C(6A)-C(7A)-C(8A) | 112.8(7) |
| C(6A)-C(7A)-H(7AA) | 123.6 |
| C(8A)-C(7A)-H(7AA) | 123.6 |
| C(9A)-C(8A)-C(7A) | 110.8(8) |
| C(9A)-C(8A)-H(8AA) | 124.6 |
| C(7A)-C(8A)-H(8AA) | 124.6 |
| C(8A)-C(9A)-S(1A) | 111.2(7) |
| C(8A)-C(9A)-H(9A) | 124.4 |
| S(1A)-C(9A)-H(9A) | 124.4 |
| C(5)-C(10)-H(10A) | 109.5 |
| C(5)-C(10)-H(10B) | 109.5 |
| H(10A)-C(10)-H(10B) | 109.5 |
| C(5)-C(10)-H(10C) | 109.5 |
| H(10A)-C(10)-H(10C) | 109.5 |
| H(10B)-C(10)-H(10C) | 109.5 |
| C(5)-C(11)-H(11A) | 109.5 |

| | |
|---|---|
| C(5)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 |
| C(5)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| O(3)-C(12)-C(13) | 125.19(14) |
| O(3)-C(12)-C(16) | 114.26(14) |
| C(13)-C(12)-C(16) | 120.55(14) |
| C(12)-C(13)-C(14) | 122.48(15) |
| C(12)-C(13)-H(13A) | 118.8 |
| C(14)-C(13)-H(13A) | 118.8 |
| N(2)-C(14)-O(4) | 115.51(14) |
| N(2)-C(14)-C(13) | 128.20(15) |
| O(4)-C(14)-C(13) | 116.27(14) |
| O(4)-C(15)-C(20) | 105.95(14) |
| O(4)-C(15)-H(15A) | 110.5 |
| C(20)-C(15)-H(15A) | 110.5 |
| O(4)-C(15)-H(15B) | 110.5 |
| C(20)-C(15)-H(15B) | 110.5 |
| H(15A)-C(15)-H(15B) | 108.7 |
| C(19)-S(2)-C(16) | 91.67(8) |
| C(17)-C(16)-C(12) | 130.55(15) |
| C(17)-C(16)-S(2) | 110.99(12) |
| C(12)-C(16)-S(2) | 118.43(12) |
| C(16)-C(17)-C(18) | 112.65(15) |
| C(16)-C(17)-H(17A) | 123.7 |
| C(18)-C(17)-H(17A) | 123.7 |
| C(19)-C(18)-C(17) | 112.64(15) |
| C(19)-C(18)-H(18A) | 123.7 |
| C(17)-C(18)-H(18A) | 123.7 |
| C(18)-C(19)-S(2) | 112.04(13) |
| C(18)-C(19)-H(19) | 124.0 |
| S(2)-C(19)-H(19) | 124.0 |
| N(2)-C(20)-C(22) | 109.61(14) |
| N(2)-C(20)-C(21) | 110.11(14) |
| C(22)-C(20)-C(21) | 111.00(16) |

| | |
|---|---|
| N(2)-C(20)-C(15) | 102.00(13) |
| C(22)-C(20)-C(15) | 111.74(16) |
| C(21)-C(20)-C(15) | 112.01(15) |
| C(20)-C(21)-H(21A) | 109.5 |
| C(20)-C(21)-H(21B) | 109.5 |
| H(21A)-C(21)-H(21B) | 109.5 |
| C(20)-C(21)-H(21C) | 109.5 |
| H(21A)-C(21)-H(21C) | 109.5 |
| H(21B)-C(21)-H(21C) | 109.5 |
| C(20)-C(22)-H(22A) | 109.5 |
| C(20)-C(22)-H(22B) | 109.5 |
| H(22A)-C(22)-H(22B) | 109.5 |
| C(20)-C(22)-H(22C) | 109.5 |
| H(22A)-C(22)-H(22C) | 109.5 |
| H(22B)-C(22)-H(22C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d1835_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 20(1) | 19(1) | 18(1) | 5(1) | 6(1) | 1(1) |
| O(1) | 24(1) | 20(1) | 18(1) | 2(1) | 7(1) | 2(1) |
| O(2) | 36(1) | 25(1) | 22(1) | 1(1) | 10(1) | 10(1) |
| O(3) | 21(1) | 24(1) | 19(1) | 7(1) | 2(1) | -2(1) |
| O(4) | 16(1) | 30(1) | 31(1) | 8(1) | 2(1) | -2(1) |
| N(1) | 19(1) | 23(1) | 16(1) | 1(1) | 6(1) | 1(1) |
| N(2) | 18(1) | 18(1) | 23(1) | 2(1) | 7(1) | -2(1) |
| C(1) | 17(1) | 21(1) | 21(1) | -1(1) | 5(1) | 0(1) |
| C(2) | 23(1) | 20(1) | 19(1) | 5(1) | 6(1) | 1(1) |
| C(3) | 16(1) | 20(1) | 17(1) | 1(1) | 4(1) | -4(1) |
| C(4) | 42(1) | 35(1) | 21(1) | -2(1) | 10(1) | 10(1) |
| C(5) | 24(1) | 30(1) | 18(1) | 0(1) | 9(1) | 5(1) |
| S(1) | 28(1) | 20(1) | 25(1) | -5(1) | 13(1) | 0(1) |
| C(6) | 22(1) | 23(1) | 17(1) | -2(1) | 6(1) | -7(1) |
| C(7) | 24(2) | 18(2) | 8(2) | 5(1) | 2(2) | -1(1) |
| C(8) | 39(2) | 22(2) | 17(1) | -2(1) | 6(1) | -8(1) |
| C(9) | 39(2) | 28(2) | 15(1) | -2(1) | 11(1) | -9(1) |
| S(1A) | 35(2) | 21(2) | 15(2) | 11(1) | -5(2) | -2(1) |
| C(6A) | 22(1) | 23(1) | 17(1) | -2(1) | 6(1) | -7(1) |
| C(7A) | 33(4) | 25(4) | 13(4) | 7(3) | 8(3) | -8(3) |
| C(8A) | 33(4) | 21(4) | 16(4) | 2(3) | 10(3) | -3(3) |
| C(9A) | 34(4) | 29(4) | 13(3) | -1(4) | 9(3) | -7(4) |
| C(10) | 38(1) | 48(1) | 19(1) | -1(1) | 6(1) | 13(1) |
| C(11) | 32(1) | 50(1) | 40(1) | 0(1) | 21(1) | -2(1) |
| C(12) | 22(1) | 16(1) | 17(1) | 0(1) | 7(1) | 0(1) |
| C(13) | 20(1) | 20(1) | 21(1) | 6(1) | 4(1) | 1(1) |
| C(14) | 18(1) | 19(1) | 21(1) | -1(1) | 4(1) | 2(1) |
| C(15) | 20(1) | 40(1) | 38(1) | 9(1) | 9(1) | -5(1) |
| S(2) | 21(1) | 27(1) | 22(1) | 4(1) | 3(1) | -5(1) |
| C(16) | 19(1) | 19(1) | 18(1) | -2(1) | 6(1) | 0(1) |
| C(17) | 20(1) | 21(1) | 25(1) | 4(1) | 7(1) | 1(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(18) | 29(1) | 21(1) | 31(1) | 6(1) | 11(1) | -2(1) |
| C(19) | 26(1) | 26(1) | 31(1) | 1(1) | 10(1) | -8(1) |
| C(20) | 18(1) | 20(1) | 30(1) | 1(1) | 10(1) | -3(1) |
| C(21) | 29(1) | 51(1) | 32(1) | -1(1) | 16(1) | -2(1) |
| C(22) | 31(1) | 22(1) | 74(2) | -6(1) | 19(1) | -5(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d1835_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 5152 | 7221 | 6020 | 25 |
| H(4A) | 4022 | 7548 | 8524 | 39 |
| H(4B) | 5679 | 7707 | 8693 | 39 |
| H(7A) | 4955 | 7125 | 4620 | 20 |
| H(8A) | 5613 | 6872 | 3266 | 32 |
| H(9) | 7071 | 5529 | 3339 | 32 |
| H(7AA) | 7276 | 4854 | 5184 | 28 |
| H(8AA) | 7505 | 5167 | 3720 | 27 |
| H(9A) | 6110 | 6469 | 3110 | 30 |
| H(10A) | 7115 | 6450 | 9312 | 53 |
| H(10B) | 6430 | 5480 | 9377 | 53 |
| H(10C) | 5945 | 6341 | 9826 | 53 |
| H(11A) | 3925 | 5188 | 8543 | 58 |
| H(11B) | 3052 | 6003 | 8015 | 58 |
| H(11C) | 3457 | 6026 | 9030 | 58 |
| H(13A) | 7976 | 3215 | 9674 | 25 |
| H(15A) | 11409 | 4300 | 8675 | 39 |
| H(15B) | 11233 | 5116 | 9294 | 39 |
| H(17A) | 6576 | 2045 | 9968 | 26 |
| H(18A) | 4533 | 1102 | 10012 | 32 |
| H(19) | 2437 | 1570 | 8981 | 32 |
| H(21A) | 9137 | 5125 | 6852 | 54 |
| H(21B) | 9947 | 4222 | 7239 | 54 |
| H(21C) | 10785 | 5152 | 7265 | 54 |
| H(22A) | 8802 | 6371 | 7836 | 62 |
| H(22B) | 10448 | 6396 | 8258 | 62 |
| H(22C) | 9384 | 6241 | 8838 | 62 |

Table 6. Torsion angles [°] for d1835_a.

| | |
|---|---|
| C(5)-N(1)-C(1)-O(2) | 3.3(2) |
| Ni(1)-N(1)-C(1)-O(2) | -178.81(11) |
| C(5)-N(1)-C(1)-C(2) | -175.09(16) |
| Ni(1)-N(1)-C(1)-C(2) | 2.8(2) |
| C(4)-O(2)-C(1)-N(1) | 10.3(2) |
| C(4)-O(2)-C(1)-C(2) | -171.16(15) |
| N(1)-C(1)-C(2)-C(3) | -1.6(3) |
| O(2)-C(1)-C(2)-C(3) | -179.88(15) |
| Ni(1)-O(1)-C(3)-C(2) | 4.6(2) |
| Ni(1)-O(1)-C(3)-C(6A) | -176.68(10) |
| Ni(1)-O(1)-C(3)-C(6) | -176.68(10) |
| C(1)-C(2)-C(3)-O(1) | -2.5(3) |
| C(1)-C(2)-C(3)-C(6A) | 178.81(15) |
| C(1)-C(2)-C(3)-C(6) | 178.81(15) |
| C(1)-O(2)-C(4)-C(5) | -18.61(18) |
| C(1)-N(1)-C(5)-C(10) | -134.54(16) |
| Ni(1)-N(1)-C(5)-C(10) | 47.7(2) |
| C(1)-N(1)-C(5)-C(11) | 102.73(17) |
| Ni(1)-N(1)-C(5)-C(11) | -75.05(18) |
| C(1)-N(1)-C(5)-C(4) | -14.36(18) |
| Ni(1)-N(1)-C(5)-C(4) | 167.87(12) |
| O(2)-C(4)-C(5)-N(1) | 19.60(18) |
| O(2)-C(4)-C(5)-C(10) | 138.21(15) |
| O(2)-C(4)-C(5)-C(11) | -95.97(17) |
| O(1)-C(3)-C(6)-C(7) | 170.8(6) |
| C(2)-C(3)-C(6)-C(7) | -10.4(6) |
| O(1)-C(3)-C(6)-S(1) | -10.4(2) |
| C(2)-C(3)-C(6)-S(1) | 168.45(14) |
| C(9)-S(1)-C(6)-C(7) | 1.1(5) |
| C(9)-S(1)-C(6)-C(3) | -177.93(17) |
| C(3)-C(6)-C(7)-C(8) | 177.4(4) |
| S(1)-C(6)-C(7)-C(8) | -1.5(9) |
| C(6)-C(7)-C(8)-C(9) | 1.2(9) |
| C(7)-C(8)-C(9)-S(1) | -0.4(6) |

| | |
|---|---|
| C(6)-S(1)-C(9)-C(8) | -0.4(3) |
| O(1)-C(3)-C(6A)-C(7A) | -9.5(11) |
| C(2)-C(3)-C(6A)-C(7A) | 169.3(11) |
| O(1)-C(3)-C(6A)-S(1A) | 169.5(5) |
| C(2)-C(3)-C(6A)-S(1A) | -11.7(6) |
| C(9A)-S(1A)-C(6A)-C(7A) | -3.8(13) |
| C(9A)-S(1A)-C(6A)-C(3) | 177.1(5) |
| C(3)-C(6A)-C(7A)-C(8A) | -175.4(11) |
| S(1A)-C(6A)-C(7A)-C(8A) | 5(2) |
| C(6A)-C(7A)-C(8A)-C(9A) | -4(2) |
| C(7A)-C(8A)-C(9A)-S(1A) | 1.6(19) |
| C(6A)-S(1A)-C(9A)-C(8A) | 1.2(13) |
| Ni(1)-O(3)-C(12)-C(13) | 1.7(2) |
| Ni(1)-O(3)-C(12)-C(16) | -177.34(10) |
| O(3)-C(12)-C(13)-C(14) | -7.9(3) |
| C(16)-C(12)-C(13)-C(14) | 171.15(15) |
| C(20)-N(2)-C(14)-O(4) | -0.06(19) |
| Ni(1)-N(2)-C(14)-O(4) | -176.40(10) |
| C(20)-N(2)-C(14)-C(13) | -178.51(16) |
| Ni(1)-N(2)-C(14)-C(13) | 5.2(2) |
| C(15)-O(4)-C(14)-N(2) | -1.2(2) |
| C(15)-O(4)-C(14)-C(13) | 177.47(15) |
| C(12)-C(13)-C(14)-N(2) | 4.1(3) |
| C(12)-C(13)-C(14)-O(4) | -174.35(15) |
| C(14)-O(4)-C(15)-C(20) | 1.81(19) |
| O(3)-C(12)-C(16)-C(17) | 176.04(16) |
| C(13)-C(12)-C(16)-C(17) | -3.1(3) |
| O(3)-C(12)-C(16)-S(2) | -2.07(19) |
| C(13)-C(12)-C(16)-S(2) | 178.80(12) |
| C(19)-S(2)-C(16)-C(17) | 0.26(13) |
| C(19)-S(2)-C(16)-C(12) | 178.72(13) |
| C(12)-C(16)-C(17)-C(18) | -178.36(16) |
| S(2)-C(16)-C(17)-C(18) | -0.14(18) |
| C(16)-C(17)-C(18)-C(19) | -0.1(2) |
| C(17)-C(18)-C(19)-S(2) | 0.3(2) |
| C(16)-S(2)-C(19)-C(18) | -0.32(15) |

| | |
|---|---|
| C(14)-N(2)-C(20)-C(22) | -117.38(17) |
| Ni(1)-N(2)-C(20)-C(22) | 58.73(19) |
| C(14)-N(2)-C(20)-C(21) | 120.24(16) |
| Ni(1)-N(2)-C(20)-C(21) | -63.65(18) |
| C(14)-N(2)-C(20)-C(15) | 1.16(18) |
| Ni(1)-N(2)-C(20)-C(15) | 177.27(12) |
| O(4)-C(15)-C(20)-N(2) | -1.77(18) |
| O(4)-C(15)-C(20)-C(22) | 115.24(17) |
| O(4)-C(15)-C(20)-C(21) | -119.49(16) |

Symmetry transformations used to generate equivalent atoms:

## Complex 3f.

Table 1. Crystal data and structure refinement for d18101_a.

| | | |
|---|---|---|
| Identification code | d18101_a | |
| Empirical formula | C28 H26 N4 Ni O4 | |
| Formula weight | 541.24 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 6.9179(6) Å | α= 103.140(3)°. |
| | b = 9.6038(10) Å | β= 94.606(3)°. |
| | c = 20.210(2) Å | γ = 98.490(3)°. |
| Volume | 1284.2(2) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.400 $Mg/m^3$ | |
| Absorption coefficient | 0.797 $mm^{-1}$ | |
| F(000) | 564 | |
| Crystal size | 0.250 x 0.080 x 0.050 $mm^3$ | |
| Theta range for data collection | 2.084 to 27.673°. | |
| Index ranges | -9<=h<=9, -12<=k<=12, -26<=l<=26 | |
| Reflections collected | 52010 | |
| Independent reflections | 5966 [R(int) = 0.0449] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.7090 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5966 / 0 / 338 | |
| Goodness-of-fit on $F^2$ | 1.024 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0305, wR2 = 0.0640 | |
| R indices (all data) | R1 = 0.0448, wR2 = 0.0692 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.361 and -0.294 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d18101_a. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 2238(1) | 3694(1) | 2491(1) | 17(1) |
| O(1) | 3714(2) | 3389(1) | 3281(1) | 21(1) |
| O(2) | -941(2) | 5443(1) | 4004(1) | 26(1) |
| O(3) | 2711(2) | 4588(1) | 1743(1) | 20(1) |
| O(4) | 665(2) | 124(1) | 877(1) | 27(1) |
| N(1) | 487(2) | 4690(1) | 3057(1) | 17(1) |
| N(2) | 9216(3) | 614(2) | 5901(1) | 45(1) |
| N(3) | 1378(2) | 1800(2) | 1877(1) | 18(1) |
| N(4) | 3811(2) | 8964(2) | -878(1) | 33(1) |
| C(1) | 3260(2) | 3560(2) | 3903(1) | 18(1) |
| C(2) | 1758(2) | 4245(2) | 4141(1) | 21(1) |
| C(3) | 490(2) | 4782(2) | 3710(1) | 19(1) |
| C(4) | -2085(3) | 5866(2) | 3471(1) | 22(1) |
| C(5) | -1226(2) | 5268(2) | 2803(1) | 19(1) |
| C(6) | 4532(2) | 2938(2) | 4358(1) | 19(1) |
| C(7) | 4058(3) | 2776(2) | 4997(1) | 28(1) |
| C(8) | 5252(3) | 2166(2) | 5392(1) | 32(1) |
| C(9) | 6935(3) | 1708(2) | 5156(1) | 26(1) |
| C(10) | 7421(3) | 1845(2) | 4517(1) | 31(1) |
| C(11) | 6209(3) | 2451(2) | 4125(1) | 27(1) |
| C(12) | 8201(3) | 1088(2) | 5573(1) | 32(1) |
| C(13) | -2636(3) | 4021(2) | 2315(1) | 24(1) |
| C(14) | -556(3) | 6468(2) | 2449(1) | 30(1) |
| C(15) | 2356(2) | 3994(2) | 1089(1) | 18(1) |
| C(16) | 1677(3) | 2549(2) | 807(1) | 22(1) |
| C(17) | 1262(2) | 1536(2) | 1214(1) | 20(1) |
| C(18) | -13(3) | -623(2) | 1387(1) | 26(1) |
| C(19) | 897(3) | 399(2) | 2077(1) | 22(1) |
| C(20) | 2725(2) | 5045(2) | 644(1) | 17(1) |
| C(21) | 3469(3) | 6498(2) | 955(1) | 24(1) |
| C(22) | 3777(3) | 7520(2) | 571(1) | 26(1) |

| | | | | |
|---|---|---|---|---|
| C(23) | 3343(2) | 7089(2) | -138(1) | 21(1) |
| C(24) | 2625(3) | 5639(2) | -455(1) | 25(1) |
| C(25) | 2319(3) | 4633(2) | -66(1) | 22(1) |
| C(26) | 3618(3) | 8147(2) | -547(1) | 25(1) |
| C(27) | -553(3) | 540(2) | 2609(1) | 29(1) |
| C(28) | 2818(3) | -8(2) | 2344(1) | 28(1) |

Table 3. Bond lengths [Å] and angles [°] for d18101_a.

| | |
|---|---|
| Ni(1)-O(1) | 1.9276(11) |
| Ni(1)-O(3) | 1.9282(11) |
| Ni(1)-N(3) | 1.9338(14) |
| Ni(1)-N(1) | 1.9381(13) |
| O(1)-C(1) | 1.2998(19) |
| O(2)-C(3) | 1.3580(19) |
| O(2)-C(4) | 1.452(2) |
| O(3)-C(15) | 1.3020(19) |
| O(4)-C(17) | 1.358(2) |
| O(4)-C(18) | 1.453(2) |
| N(1)-C(3) | 1.303(2) |
| N(1)-C(5) | 1.484(2) |
| N(2)-C(12) | 1.138(2) |
| N(3)-C(17) | 1.300(2) |
| N(3)-C(19) | 1.490(2) |
| N(4)-C(26) | 1.143(2) |
| C(1)-C(2) | 1.372(2) |
| C(1)-C(6) | 1.500(2) |
| C(2)-C(3) | 1.417(2) |
| C(2)-H(2A) | 0.9500 |
| C(4)-C(5) | 1.544(2) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(13) | 1.524(2) |
| C(5)-C(14) | 1.524(2) |
| C(6)-C(11) | 1.391(2) |
| C(6)-C(7) | 1.395(2) |
| C(7)-C(8) | 1.383(2) |
| C(7)-H(7A) | 0.9500 |
| C(8)-C(9) | 1.387(3) |
| C(8)-H(8A) | 0.9500 |
| C(9)-C(10) | 1.389(3) |
| C(9)-C(12) | 1.448(2) |
| C(10)-C(11) | 1.385(2) |

| | |
|---|---|
| C(10)-H(10A) | 0.9500 |
| C(11)-H(11A) | 0.9500 |
| C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 |
| C(13)-H(13C) | 0.9800 |
| C(14)-H(14A) | 0.9800 |
| C(14)-H(14B) | 0.9800 |
| C(14)-H(14C) | 0.9800 |
| C(15)-C(16) | 1.370(2) |
| C(15)-C(20) | 1.505(2) |
| C(16)-C(17) | 1.422(2) |
| C(16)-H(16A) | 0.9500 |
| C(18)-C(19) | 1.535(2) |
| C(18)-H(18A) | 0.9900 |
| C(18)-H(18B) | 0.9900 |
| C(19)-C(27) | 1.526(2) |
| C(19)-C(28) | 1.532(2) |
| C(20)-C(25) | 1.394(2) |
| C(20)-C(21) | 1.394(2) |
| C(21)-C(22) | 1.385(2) |
| C(21)-H(21A) | 0.9500 |
| C(22)-C(23) | 1.393(2) |
| C(22)-H(22A) | 0.9500 |
| C(23)-C(24) | 1.391(2) |
| C(23)-C(26) | 1.449(2) |
| C(24)-C(25) | 1.380(2) |
| C(24)-H(24A) | 0.9500 |
| C(25)-H(25A) | 0.9500 |
| C(27)-H(27A) | 0.9800 |
| C(27)-H(27B) | 0.9800 |
| C(27)-H(27C) | 0.9800 |
| C(28)-H(28A) | 0.9800 |
| C(28)-H(28B) | 0.9800 |
| C(28)-H(28C) | 0.9800 |

| | |
|---|---|
| O(1)-Ni(1)-O(3) | 138.36(5) |

| | |
|---|---|
| O(1)-Ni(1)-N(3) | 106.42(5) |
| O(3)-Ni(1)-N(3) | 92.11(5) |
| O(1)-Ni(1)-N(1) | 91.51(5) |
| O(3)-Ni(1)-N(1) | 109.82(5) |
| N(3)-Ni(1)-N(1) | 122.31(6) |
| C(1)-O(1)-Ni(1) | 128.54(10) |
| C(3)-O(2)-C(4) | 107.37(12) |
| C(15)-O(3)-Ni(1) | 128.22(11) |
| C(17)-O(4)-C(18) | 105.98(13) |
| C(3)-N(1)-C(5) | 109.54(13) |
| C(3)-N(1)-Ni(1) | 124.34(11) |
| C(5)-N(1)-Ni(1) | 125.57(10) |
| C(17)-N(3)-C(19) | 108.75(14) |
| C(17)-N(3)-Ni(1) | 124.74(12) |
| C(19)-N(3)-Ni(1) | 126.34(10) |
| O(1)-C(1)-C(2) | 124.30(15) |
| O(1)-C(1)-C(6) | 114.30(14) |
| C(2)-C(1)-C(6) | 121.40(14) |
| C(1)-C(2)-C(3) | 122.01(15) |
| C(1)-C(2)-H(2A) | 119.0 |
| C(3)-C(2)-H(2A) | 119.0 |
| N(1)-C(3)-O(2) | 115.18(14) |
| N(1)-C(3)-C(2) | 128.11(15) |
| O(2)-C(3)-C(2) | 116.69(14) |
| O(2)-C(4)-C(5) | 105.45(13) |
| O(2)-C(4)-H(4A) | 110.7 |
| C(5)-C(4)-H(4A) | 110.7 |
| O(2)-C(4)-H(4B) | 110.7 |
| C(5)-C(4)-H(4B) | 110.7 |
| H(4A)-C(4)-H(4B) | 108.8 |
| N(1)-C(5)-C(13) | 108.50(13) |
| N(1)-C(5)-C(14) | 110.64(14) |
| C(13)-C(5)-C(14) | 111.05(14) |
| N(1)-C(5)-C(4) | 102.09(12) |
| C(13)-C(5)-C(4) | 112.68(14) |
| C(14)-C(5)-C(4) | 111.50(14) |

| | |
|---|---|
| C(11)-C(6)-C(7) | 118.45(15) |
| C(11)-C(6)-C(1) | 119.00(15) |
| C(7)-C(6)-C(1) | 122.51(15) |
| C(8)-C(7)-C(6) | 120.49(17) |
| C(8)-C(7)-H(7A) | 119.8 |
| C(6)-C(7)-H(7A) | 119.8 |
| C(7)-C(8)-C(9) | 120.23(17) |
| C(7)-C(8)-H(8A) | 119.9 |
| C(9)-C(8)-H(8A) | 119.9 |
| C(8)-C(9)-C(10) | 120.15(16) |
| C(8)-C(9)-C(12) | 120.29(17) |
| C(10)-C(9)-C(12) | 119.56(18) |
| C(11)-C(10)-C(9) | 119.11(17) |
| C(11)-C(10)-H(10A) | 120.4 |
| C(9)-C(10)-H(10A) | 120.4 |
| C(10)-C(11)-C(6) | 121.54(17) |
| C(10)-C(11)-H(11A) | 119.2 |
| C(6)-C(11)-H(11A) | 119.2 |
| N(2)-C(12)-C(9) | 179.1(2) |
| C(5)-C(13)-H(13A) | 109.5 |
| C(5)-C(13)-H(13B) | 109.5 |
| H(13A)-C(13)-H(13B) | 109.5 |
| C(5)-C(13)-H(13C) | 109.5 |
| H(13A)-C(13)-H(13C) | 109.5 |
| H(13B)-C(13)-H(13C) | 109.5 |
| C(5)-C(14)-H(14A) | 109.5 |
| C(5)-C(14)-H(14B) | 109.5 |
| H(14A)-C(14)-H(14B) | 109.5 |
| C(5)-C(14)-H(14C) | 109.5 |
| H(14A)-C(14)-H(14C) | 109.5 |
| H(14B)-C(14)-H(14C) | 109.5 |
| O(3)-C(15)-C(16) | 124.83(15) |
| O(3)-C(15)-C(20) | 114.22(14) |
| C(16)-C(15)-C(20) | 120.95(14) |
| C(15)-C(16)-C(17) | 122.33(15) |
| C(15)-C(16)-H(16A) | 118.8 |

| | |
|---|---|
| C(17)-C(16)-H(16A) | 118.8 |
| N(3)-C(17)-O(4) | 115.35(15) |
| N(3)-C(17)-C(16) | 127.60(15) |
| O(4)-C(17)-C(16) | 117.06(14) |
| O(4)-C(18)-C(19) | 104.82(13) |
| O(4)-C(18)-H(18A) | 110.8 |
| C(19)-C(18)-H(18A) | 110.8 |
| O(4)-C(18)-H(18B) | 110.8 |
| C(19)-C(18)-H(18B) | 110.8 |
| H(18A)-C(18)-H(18B) | 108.9 |
| N(3)-C(19)-C(27) | 109.86(13) |
| N(3)-C(19)-C(28) | 108.39(14) |
| C(27)-C(19)-C(28) | 112.17(15) |
| N(3)-C(19)-C(18) | 101.08(13) |
| C(27)-C(19)-C(18) | 112.82(15) |
| C(28)-C(19)-C(18) | 111.88(14) |
| C(25)-C(20)-C(21) | 118.36(15) |
| C(25)-C(20)-C(15) | 122.79(15) |
| C(21)-C(20)-C(15) | 118.84(14) |
| C(22)-C(21)-C(20) | 121.25(16) |
| C(22)-C(21)-H(21A) | 119.4 |
| C(20)-C(21)-H(21A) | 119.4 |
| C(21)-C(22)-C(23) | 119.50(16) |
| C(21)-C(22)-H(22A) | 120.2 |
| C(23)-C(22)-H(22A) | 120.2 |
| C(24)-C(23)-C(22) | 119.83(15) |
| C(24)-C(23)-C(26) | 119.83(16) |
| C(22)-C(23)-C(26) | 120.34(16) |
| C(25)-C(24)-C(23) | 120.08(16) |
| C(25)-C(24)-H(24A) | 120.0 |
| C(23)-C(24)-H(24A) | 120.0 |
| C(24)-C(25)-C(20) | 120.97(16) |
| C(24)-C(25)-H(25A) | 119.5 |
| C(20)-C(25)-H(25A) | 119.5 |
| N(4)-C(26)-C(23) | 178.8(2) |
| C(19)-C(27)-H(27A) | 109.5 |

| | |
|---|---|
| C(19)-C(27)-H(27B) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 |
| C(19)-C(27)-H(27C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 |
| C(19)-C(28)-H(28A) | 109.5 |
| C(19)-C(28)-H(28B) | 109.5 |
| H(28A)-C(28)-H(28B) | 109.5 |
| C(19)-C(28)-H(28C) | 109.5 |
| H(28A)-C(28)-H(28C) | 109.5 |
| H(28B)-C(28)-H(28C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d18101_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 20(1) | 21(1) | 13(1) | 6(1) | 3(1) | 5(1) |
| O(1) | 20(1) | 29(1) | 15(1) | 9(1) | 3(1) | 6(1) |
| O(2) | 32(1) | 35(1) | 18(1) | 9(1) | 9(1) | 18(1) |
| O(3) | 23(1) | 22(1) | 14(1) | 6(1) | 2(1) | 3(1) |
| O(4) | 42(1) | 18(1) | 19(1) | 4(1) | 3(1) | 3(1) |
| N(1) | 18(1) | 18(1) | 16(1) | 6(1) | 1(1) | 4(1) |
| N(2) | 57(1) | 45(1) | 36(1) | 12(1) | -10(1) | 20(1) |
| N(3) | 22(1) | 19(1) | 17(1) | 7(1) | 4(1) | 5(1) |
| N(4) | 40(1) | 31(1) | 32(1) | 16(1) | 1(1) | 2(1) |
| C(1) | 18(1) | 18(1) | 15(1) | 5(1) | 0(1) | -2(1) |
| C(2) | 27(1) | 24(1) | 13(1) | 5(1) | 3(1) | 6(1) |
| C(3) | 20(1) | 17(1) | 18(1) | 3(1) | 4(1) | 2(1) |
| C(4) | 22(1) | 25(1) | 21(1) | 6(1) | 3(1) | 8(1) |
| C(5) | 20(1) | 19(1) | 19(1) | 7(1) | 5(1) | 8(1) |
| C(6) | 21(1) | 18(1) | 17(1) | 5(1) | -1(1) | 0(1) |
| C(7) | 34(1) | 36(1) | 18(1) | 8(1) | 5(1) | 15(1) |
| C(8) | 47(1) | 39(1) | 16(1) | 10(1) | 2(1) | 17(1) |
| C(9) | 31(1) | 21(1) | 24(1) | 6(1) | -7(1) | 4(1) |
| C(10) | 26(1) | 38(1) | 32(1) | 16(1) | 3(1) | 10(1) |
| C(11) | 25(1) | 38(1) | 23(1) | 16(1) | 5(1) | 7(1) |
| C(12) | 38(1) | 30(1) | 26(1) | 7(1) | -6(1) | 7(1) |
| C(13) | 22(1) | 30(1) | 20(1) | 6(1) | 1(1) | 6(1) |
| C(14) | 37(1) | 26(1) | 34(1) | 17(1) | 13(1) | 13(1) |
| C(15) | 15(1) | 24(1) | 16(1) | 8(1) | 4(1) | 7(1) |
| C(16) | 29(1) | 24(1) | 14(1) | 7(1) | 3(1) | 6(1) |
| C(17) | 21(1) | 19(1) | 20(1) | 4(1) | 2(1) | 5(1) |
| C(18) | 32(1) | 19(1) | 26(1) | 9(1) | 4(1) | 3(1) |
| C(19) | 29(1) | 16(1) | 22(1) | 8(1) | 5(1) | 5(1) |
| C(20) | 15(1) | 22(1) | 17(1) | 7(1) | 4(1) | 6(1) |
| C(21) | 34(1) | 24(1) | 16(1) | 5(1) | 5(1) | 7(1) |
| C(22) | 35(1) | 19(1) | 25(1) | 6(1) | 7(1) | 5(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(23) | 21(1) | 24(1) | 23(1) | 13(1) | 6(1) | 7(1) |
| C(24) | 27(1) | 31(1) | 17(1) | 10(1) | 1(1) | 2(1) |
| C(25) | 26(1) | 22(1) | 18(1) | 5(1) | 1(1) | 1(1) |
| C(26) | 26(1) | 26(1) | 24(1) | 9(1) | 3(1) | 4(1) |
| C(27) | 37(1) | 22(1) | 31(1) | 12(1) | 14(1) | 5(1) |
| C(28) | 35(1) | 24(1) | 29(1) | 10(1) | 1(1) | 9(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d18101_a.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 1561 | 4364 | 4609 | 25 |
| H(4A) | -1955 | 6936 | 3566 | 27 |
| H(4B) | -3494 | 5443 | 3438 | 27 |
| H(7A) | 2907 | 3086 | 5162 | 34 |
| H(8A) | 4919 | 2061 | 5827 | 39 |
| H(10A) | 8568 | 1527 | 4352 | 37 |
| H(11A) | 6532 | 2536 | 3686 | 33 |
| H(13A) | -1939 | 3556 | 1945 | 36 |
| H(13B) | -3737 | 4396 | 2121 | 36 |
| H(13C) | -3140 | 3308 | 2565 | 36 |
| H(14A) | 116 | 6076 | 2057 | 44 |
| H(14B) | 349 | 7254 | 2772 | 44 |
| H(14C) | -1704 | 6843 | 2289 | 44 |
| H(16A) | 1476 | 2212 | 323 | 26 |
| H(18A) | 442 | -1569 | 1327 | 31 |
| H(18B) | -1467 | -790 | 1355 | 31 |
| H(21A) | 3771 | 6793 | 1438 | 29 |
| H(22A) | 4281 | 8506 | 790 | 31 |
| H(24A) | 2346 | 5341 | -939 | 30 |
| H(25A) | 1824 | 3646 | -287 | 27 |
| H(27A) | 55 | 1277 | 3022 | 43 |
| H(27B) | -904 | -395 | 2725 | 43 |
| H(27C) | -1742 | 828 | 2422 | 43 |
| H(28A) | 3414 | 717 | 2762 | 43 |
| H(28B) | 3730 | -39 | 1996 | 43 |
| H(28C) | 2540 | -964 | 2445 | 43 |

Table 6. Torsion angles [°] for d18101_a.

| | |
|---|---|
| Ni(1)-O(1)-C(1)-C(2) | -12.0(2) |
| Ni(1)-O(1)-C(1)-C(6) | 168.05(10) |
| O(1)-C(1)-C(2)-C(3) | 2.8(3) |
| C(6)-C(1)-C(2)-C(3) | -177.19(15) |
| C(5)-N(1)-C(3)-O(2) | -3.9(2) |
| Ni(1)-N(1)-C(3)-O(2) | -175.78(10) |
| C(5)-N(1)-C(3)-C(2) | 174.19(16) |
| Ni(1)-N(1)-C(3)-C(2) | 2.3(3) |
| C(4)-O(2)-C(3)-N(1) | -0.13(19) |
| C(4)-O(2)-C(3)-C(2) | -178.45(14) |
| C(1)-C(2)-C(3)-N(1) | 2.1(3) |
| C(1)-C(2)-C(3)-O(2) | -179.86(15) |
| C(3)-O(2)-C(4)-C(5) | 3.86(17) |
| C(3)-N(1)-C(5)-C(13) | -113.34(15) |
| Ni(1)-N(1)-C(5)-C(13) | 58.42(17) |
| C(3)-N(1)-C(5)-C(14) | 124.60(15) |
| Ni(1)-N(1)-C(5)-C(14) | -63.65(17) |
| C(3)-N(1)-C(5)-C(4) | 5.84(17) |
| Ni(1)-N(1)-C(5)-C(4) | 177.59(11) |
| O(2)-C(4)-C(5)-N(1) | -5.69(16) |
| O(2)-C(4)-C(5)-C(13) | 110.49(15) |
| O(2)-C(4)-C(5)-C(14) | -123.84(15) |
| O(1)-C(1)-C(6)-C(11) | 9.5(2) |
| C(2)-C(1)-C(6)-C(11) | -170.44(16) |
| O(1)-C(1)-C(6)-C(7) | -167.93(16) |
| C(2)-C(1)-C(6)-C(7) | 12.1(3) |
| C(11)-C(6)-C(7)-C(8) | 1.1(3) |
| C(1)-C(6)-C(7)-C(8) | 178.53(17) |
| C(6)-C(7)-C(8)-C(9) | -0.1(3) |
| C(7)-C(8)-C(9)-C(10) | -0.7(3) |
| C(7)-C(8)-C(9)-C(12) | 179.14(18) |
| C(8)-C(9)-C(10)-C(11) | 0.4(3) |
| C(12)-C(9)-C(10)-C(11) | -179.43(18) |
| C(9)-C(10)-C(11)-C(6) | 0.7(3) |

| | |
|---|---|
| C(7)-C(6)-C(11)-C(10) | -1.4(3) |
| C(1)-C(6)-C(11)-C(10) | -178.92(17) |
| Ni(1)-O(3)-C(15)-C(16) | -4.7(2) |
| Ni(1)-O(3)-C(15)-C(20) | 174.33(10) |
| O(3)-C(15)-C(16)-C(17) | 0.8(3) |
| C(20)-C(15)-C(16)-C(17) | -178.20(15) |
| C(19)-N(3)-C(17)-O(4) | 2.9(2) |
| Ni(1)-N(3)-C(17)-O(4) | 178.54(10) |
| C(19)-N(3)-C(17)-C(16) | -177.30(16) |
| Ni(1)-N(3)-C(17)-C(16) | -1.7(3) |
| C(18)-O(4)-C(17)-N(3) | 10.38(19) |
| C(18)-O(4)-C(17)-C(16) | -169.41(15) |
| C(15)-C(16)-C(17)-N(3) | 2.6(3) |
| C(15)-C(16)-C(17)-O(4) | -177.61(15) |
| C(17)-O(4)-C(18)-C(19) | -18.45(17) |
| C(17)-N(3)-C(19)-C(27) | -133.33(15) |
| Ni(1)-N(3)-C(19)-C(27) | 51.15(18) |
| C(17)-N(3)-C(19)-C(28) | 103.79(16) |
| Ni(1)-N(3)-C(19)-C(28) | -71.72(17) |
| C(17)-N(3)-C(19)-C(18) | -13.94(17) |
| Ni(1)-N(3)-C(19)-C(18) | 170.55(11) |
| O(4)-C(18)-C(19)-N(3) | 19.24(16) |
| O(4)-C(18)-C(19)-C(27) | 136.50(14) |
| O(4)-C(18)-C(19)-C(28) | -95.91(16) |
| O(3)-C(15)-C(20)-C(25) | -176.03(15) |
| C(16)-C(15)-C(20)-C(25) | 3.0(2) |
| O(3)-C(15)-C(20)-C(21) | 2.7(2) |
| C(16)-C(15)-C(20)-C(21) | -178.23(16) |
| C(25)-C(20)-C(21)-C(22) | 0.9(3) |
| C(15)-C(20)-C(21)-C(22) | -177.92(15) |
| C(20)-C(21)-C(22)-C(23) | -0.2(3) |
| C(21)-C(22)-C(23)-C(24) | -0.7(3) |
| C(21)-C(22)-C(23)-C(26) | 178.78(16) |
| C(22)-C(23)-C(24)-C(25) | 0.9(3) |
| C(26)-C(23)-C(24)-C(25) | -178.57(16) |
| C(23)-C(24)-C(25)-C(20) | -0.2(3) |

| | |
|---|---|
| C(21)-C(20)-C(25)-C(24) | -0.6(3) |
| C(15)-C(20)-C(25)-C(24) | 178.09(15) |

Symmetry transformations used to generate equivalent atoms:

## Complex 3g.

Table 1. Crystal data and structure refinement for d18100.

| | | |
|---|---|---|
| Identification code | d18100 | |
| Empirical formula | C16 H18 F6 N2 Ni O4 | |
| Formula weight | 475.03 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | Pbca | |
| Unit cell dimensions | a = 11.1193(4) Å | α= 90°. |
| | b = 18.3316(8) Å | β= 90°. |
| | c = 19.0410(8) Å | γ = 90°. |
| Volume | 3881.2(3) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.626 $Mg/m^3$ | |
| Absorption coefficient | 1.081 $mm^{-1}$ | |
| F(000) | 1936 | |
| Crystal size | 0.300 x 0.150 x 0.050 $mm^3$ | |
| Theta range for data collection | 2.139 to 27.524°. | |
| Index ranges | -12<=h<=14, -22<=k<=23, -24<=l<=23 | |
| Reflections collected | 26354 | |
| Independent reflections | 4427 [R(int) = 0.0721] | |
| Completeness to theta = 25.242° | 99.5 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.6878 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4427 / 51 / 294 | |
| Goodness-of-fit on $F^2$ | 0.993 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0386, wR2 = 0.0679 | |
| R indices (all data) | R1 = 0.0735, wR2 = 0.0789 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.331 and -0.279 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for d18100. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ni(1) | 3836(1) | 1647(1) | 3739(1) | 21(1) |
| F(1) | 1433(1) | 3392(1) | 2715(1) | 62(1) |
| F(2) | 2749(2) | 3755(1) | 1982(1) | 46(1) |
| F(3) | 2985(2) | 3985(1) | 3068(1) | 56(1) |
| F(4) | 1856(16) | -57(12) | 5584(4) | 67(3) |
| F(5) | 2786(12) | -663(5) | 4825(14) | 73(3) |
| F(6) | 1230(9) | -33(11) | 4551(9) | 49(3) |
| F(4A) | 1117(9) | 50(13) | 4702(11) | 61(4) |
| F(5A) | 2170(20) | -243(12) | 5582(4) | 77(4) |
| F(6A) | 2652(15) | -593(6) | 4547(10) | 64(3) |
| O(1) | 3127(2) | 2516(1) | 3360(1) | 28(1) |
| O(2) | 5009(2) | 1493(1) | 1706(1) | 44(1) |
| O(3) | 2909(1) | 867(1) | 4150(1) | 26(1) |
| O(4) | 5154(2) | 1710(1) | 5750(1) | 33(1) |
| N(1) | 4551(2) | 1383(1) | 2844(1) | 22(1) |
| N(2) | 4672(2) | 1844(1) | 4613(1) | 22(1) |
| C(1) | 3266(2) | 2761(1) | 2733(1) | 24(1) |
| C(2) | 3882(2) | 2458(1) | 2196(1) | 28(1) |
| C(3) | 4473(2) | 1773(1) | 2276(1) | 26(1) |
| C(4) | 5378(3) | 754(2) | 1888(2) | 51(1) |
| C(5) | 5296(2) | 727(1) | 2687(1) | 27(1) |
| C(6) | 2611(2) | 3477(2) | 2619(2) | 33(1) |
| C(7) | 6502(2) | 818(2) | 3044(2) | 53(1) |
| C(8) | 4675(3) | 35(2) | 2936(2) | 44(1) |
| C(9) | 3013(2) | 626(1) | 4779(1) | 24(1) |
| C(10) | 3733(2) | 877(1) | 5301(1) | 28(1) |
| C(11) | 4519(2) | 1482(1) | 5193(1) | 24(1) |
| C(12) | 5993(2) | 2253(2) | 5485(1) | 32(1) |
| C(13) | 5487(2) | 2473(1) | 4771(2) | 27(1) |
| C(14) | 2228(2) | -38(2) | 4922(1) | 35(1) |
| C(15) | 6445(3) | 2539(2) | 4210(2) | 44(1) |

| | | | | |
|---|---|---|---|---|
| C(16) | 4728(3) | 3167(2) | 4819(2) | 42(1) |

Table 3. Bond lengths [Å] and angles [°] for d18100.

| | |
|---|---|
| Ni(1)-O(1) | 1.9185(17) |
| Ni(1)-O(3) | 1.9284(16) |
| Ni(1)-N(2) | 1.940(2) |
| Ni(1)-N(1) | 1.941(2) |
| F(1)-C(6) | 1.331(3) |
| F(2)-C(6) | 1.326(3) |
| F(3)-C(6) | 1.330(3) |
| F(4)-C(14) | 1.327(6) |
| F(5)-C(14) | 1.316(6) |
| F(6)-C(14) | 1.315(6) |
| F(4A)-C(14) | 1.314(6) |
| F(5A)-C(14) | 1.314(6) |
| F(6A)-C(14) | 1.329(6) |
| O(1)-C(1) | 1.285(3) |
| O(2)-C(3) | 1.341(3) |
| O(2)-C(4) | 1.457(3) |
| O(3)-C(9) | 1.281(3) |
| O(4)-C(11) | 1.339(3) |
| O(4)-C(12) | 1.455(3) |
| N(1)-C(3) | 1.301(3) |
| N(1)-C(5) | 1.491(3) |
| N(2)-C(11) | 1.300(3) |
| N(2)-C(13) | 1.497(3) |
| C(1)-C(2) | 1.351(3) |
| C(1)-C(6) | 1.516(3) |
| C(2)-C(3) | 1.424(3) |
| C(2)-H(2A) | 0.9500 |
| C(4)-C(5) | 1.525(4) |
| C(4)-H(4A) | 0.9900 |
| C(4)-H(4B) | 0.9900 |
| C(5)-C(7) | 1.513(4) |
| C(5)-C(8) | 1.520(4) |
| C(7)-H(7A) | 0.9800 |
| C(7)-H(7B) | 0.9800 |

| | |
|---|---|
| C(7)-H(7C) | 0.9800 |
| C(8)-H(8A) | 0.9800 |
| C(8)-H(8B) | 0.9800 |
| C(8)-H(8C) | 0.9800 |
| C(9)-C(10) | 1.357(3) |
| C(9)-C(14) | 1.522(4) |
| C(10)-C(11) | 1.427(4) |
| C(10)-H(10A) | 0.9500 |
| C(12)-C(13) | 1.527(4) |
| C(12)-H(12A) | 0.9900 |
| C(12)-H(12B) | 0.9900 |
| C(13)-C(15) | 1.513(4) |
| C(13)-C(16) | 1.530(4) |
| C(15)-H(15A) | 0.9800 |
| C(15)-H(15B) | 0.9800 |
| C(15)-H(15C) | 0.9800 |
| C(16)-H(16A) | 0.9800 |
| C(16)-H(16B) | 0.9800 |
| C(16)-H(16C) | 0.9800 |

| | |
|---|---|
| O(1)-Ni(1)-O(3) | 123.24(7) |
| O(1)-Ni(1)-N(2) | 111.40(8) |
| O(3)-Ni(1)-N(2) | 92.62(8) |
| O(1)-Ni(1)-N(1) | 92.58(8) |
| O(3)-Ni(1)-N(1) | 113.00(8) |
| N(2)-Ni(1)-N(1) | 127.11(8) |
| C(1)-O(1)-Ni(1) | 126.23(16) |
| C(3)-O(2)-C(4) | 106.7(2) |
| C(9)-O(3)-Ni(1) | 125.91(16) |
| C(11)-O(4)-C(12) | 106.14(19) |
| C(3)-N(1)-C(5) | 108.3(2) |
| C(3)-N(1)-Ni(1) | 124.48(17) |
| C(5)-N(1)-Ni(1) | 127.24(17) |
| C(11)-N(2)-C(13) | 107.6(2) |
| C(11)-N(2)-Ni(1) | 124.88(17) |
| C(13)-N(2)-Ni(1) | 127.24(17) |

| | |
|---|---|
| O(1)-C(1)-C(2) | 128.3(2) |
| O(1)-C(1)-C(6) | 112.2(2) |
| C(2)-C(1)-C(6) | 119.5(2) |
| C(1)-C(2)-C(3) | 121.1(2) |
| C(1)-C(2)-H(2A) | 119.5 |
| C(3)-C(2)-H(2A) | 119.5 |
| N(1)-C(3)-O(2) | 115.7(2) |
| N(1)-C(3)-C(2) | 127.2(2) |
| O(2)-C(3)-C(2) | 117.1(2) |
| O(2)-C(4)-C(5) | 104.6(2) |
| O(2)-C(4)-H(4A) | 110.8 |
| C(5)-C(4)-H(4A) | 110.8 |
| O(2)-C(4)-H(4B) | 110.8 |
| C(5)-C(4)-H(4B) | 110.8 |
| H(4A)-C(4)-H(4B) | 108.9 |
| N(1)-C(5)-C(7) | 108.3(2) |
| N(1)-C(5)-C(8) | 111.0(2) |
| C(7)-C(5)-C(8) | 110.8(3) |
| N(1)-C(5)-C(4) | 102.0(2) |
| C(7)-C(5)-C(4) | 113.0(3) |
| C(8)-C(5)-C(4) | 111.4(3) |
| F(2)-C(6)-F(3) | 106.4(2) |
| F(2)-C(6)-F(1) | 106.5(2) |
| F(3)-C(6)-F(1) | 107.6(2) |
| F(2)-C(6)-C(1) | 114.1(2) |
| F(3)-C(6)-C(1) | 111.4(2) |
| F(1)-C(6)-C(1) | 110.6(2) |
| C(5)-C(7)-H(7A) | 109.5 |
| C(5)-C(7)-H(7B) | 109.5 |
| H(7A)-C(7)-H(7B) | 109.5 |
| C(5)-C(7)-H(7C) | 109.5 |
| H(7A)-C(7)-H(7C) | 109.5 |
| H(7B)-C(7)-H(7C) | 109.5 |
| C(5)-C(8)-H(8A) | 109.5 |
| C(5)-C(8)-H(8B) | 109.5 |
| H(8A)-C(8)-H(8B) | 109.5 |

| | |
|---|---|
| C(5)-C(8)-H(8C) | 109.5 |
| H(8A)-C(8)-H(8C) | 109.5 |
| H(8B)-C(8)-H(8C) | 109.5 |
| O(3)-C(9)-C(10) | 128.4(2) |
| O(3)-C(9)-C(14) | 113.0(2) |
| C(10)-C(9)-C(14) | 118.6(2) |
| C(9)-C(10)-C(11) | 121.3(2) |
| C(9)-C(10)-H(10A) | 119.4 |
| C(11)-C(10)-H(10A) | 119.4 |
| N(2)-C(11)-O(4) | 116.4(2) |
| N(2)-C(11)-C(10) | 126.8(2) |
| O(4)-C(11)-C(10) | 116.8(2) |
| O(4)-C(12)-C(13) | 104.61(19) |
| O(4)-C(12)-H(12A) | 110.8 |
| C(13)-C(12)-H(12A) | 110.8 |
| O(4)-C(12)-H(12B) | 110.8 |
| C(13)-C(12)-H(12B) | 110.8 |
| H(12A)-C(12)-H(12B) | 108.9 |
| N(2)-C(13)-C(15) | 110.3(2) |
| N(2)-C(13)-C(12) | 101.5(2) |
| C(15)-C(13)-C(12) | 113.0(2) |
| N(2)-C(13)-C(16) | 108.6(2) |
| C(15)-C(13)-C(16) | 111.4(3) |
| C(12)-C(13)-C(16) | 111.7(2) |
| F(5A)-C(14)-F(4A) | 107.2(11) |
| F(6)-C(14)-F(5) | 109.2(11) |
| F(6)-C(14)-F(4) | 104.3(10) |
| F(5)-C(14)-F(4) | 104.9(8) |
| F(5A)-C(14)-F(6A) | 108.1(8) |
| F(4A)-C(14)-F(6A) | 104.9(11) |
| F(5A)-C(14)-C(9) | 115.2(9) |
| F(4A)-C(14)-C(9) | 112.6(10) |
| F(6)-C(14)-C(9) | 112.5(9) |
| F(5)-C(14)-C(9) | 113.6(6) |
| F(4)-C(14)-C(9) | 111.7(9) |
| F(6A)-C(14)-C(9) | 108.2(7) |

| | |
|---|---|
| C(13)-C(15)-H(15A) | 109.5 |
| C(13)-C(15)-H(15B) | 109.5 |
| H(15A)-C(15)-H(15B) | 109.5 |
| C(13)-C(15)-H(15C) | 109.5 |
| H(15A)-C(15)-H(15C) | 109.5 |
| H(15B)-C(15)-H(15C) | 109.5 |
| C(13)-C(16)-H(16A) | 109.5 |
| C(13)-C(16)-H(16B) | 109.5 |
| H(16A)-C(16)-H(16B) | 109.5 |
| C(13)-C(16)-H(16C) | 109.5 |
| H(16A)-C(16)-H(16C) | 109.5 |
| H(16B)-C(16)-H(16C) | 109.5 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d18100. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Ni(1) | 24(1) | 24(1) | 15(1) | 3(1) | 1(1) | -2(1) |
| F(1) | 33(1) | 52(1) | 103(2) | 30(1) | 10(1) | 15(1) |
| F(2) | 65(1) | 36(1) | 38(1) | 16(1) | -4(1) | 4(1) |
| F(3) | 87(1) | 31(1) | 51(1) | -9(1) | -12(1) | 13(1) |
| F(4) | 68(6) | 89(9) | 43(4) | 23(3) | 12(3) | -35(5) |
| F(5) | 49(3) | 22(2) | 149(9) | 22(4) | 22(6) | 6(2) |
| F(6) | 45(4) | 57(6) | 46(4) | 25(4) | -14(4) | -30(4) |
| F(4A) | 29(3) | 58(5) | 96(9) | 25(6) | 7(4) | -5(3) |
| F(5A) | 105(10) | 77(7) | 51(4) | 45(4) | -21(4) | -45(6) |
| F(6A) | 80(5) | 21(3) | 91(7) | -3(3) | 24(5) | -11(3) |
| O(1) | 31(1) | 30(1) | 24(1) | 5(1) | 6(1) | 7(1) |
| O(2) | 68(1) | 37(1) | 26(1) | 1(1) | 19(1) | 9(1) |
| O(3) | 26(1) | 30(1) | 23(1) | 6(1) | -2(1) | -7(1) |
| O(4) | 35(1) | 44(1) | 21(1) | -6(1) | -7(1) | 0(1) |
| N(1) | 23(1) | 22(1) | 22(1) | 0(1) | 2(1) | 0(1) |
| N(2) | 21(1) | 21(1) | 24(1) | -2(1) | -1(1) | 0(1) |
| C(1) | 23(1) | 26(1) | 24(1) | 6(1) | -2(1) | -5(1) |
| C(2) | 36(1) | 28(1) | 19(1) | 6(1) | 2(1) | -2(1) |
| C(3) | 30(1) | 29(2) | 21(1) | -1(1) | 6(1) | -4(1) |
| C(4) | 72(2) | 39(2) | 42(2) | -3(2) | 17(2) | 11(2) |
| C(5) | 24(1) | 24(1) | 32(2) | -3(1) | 6(1) | 2(1) |
| C(6) | 36(2) | 28(2) | 35(2) | 6(1) | 0(1) | 1(1) |
| C(7) | 26(2) | 50(2) | 83(3) | -23(2) | -6(2) | 10(1) |
| C(8) | 37(2) | 29(2) | 64(2) | 1(2) | 9(2) | -1(1) |
| C(9) | 24(1) | 21(1) | 27(2) | 5(1) | 6(1) | 4(1) |
| C(10) | 35(1) | 31(1) | 17(1) | 6(1) | 0(1) | 4(1) |
| C(11) | 26(1) | 27(1) | 18(1) | -4(1) | -1(1) | 8(1) |
| C(12) | 29(1) | 35(2) | 34(2) | -11(1) | -7(1) | 0(1) |
| C(13) | 25(1) | 27(1) | 29(2) | -8(1) | -2(1) | -5(1) |
| C(14) | 36(2) | 31(2) | 38(2) | 9(1) | 4(1) | -2(1) |
| C(15) | 39(2) | 55(2) | 39(2) | -11(2) | 7(1) | -24(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(16) | 44(2) | 27(2) | 54(2) | -7(1) | -9(2) | -1(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for d18100.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 3923 | 2705 | 1758 | 33 |
| H(4A) | 6211 | 658 | 1729 | 61 |
| H(4B) | 4835 | 390 | 1672 | 61 |
| H(7A) | 7009 | 394 | 2942 | 79 |
| H(7B) | 6384 | 859 | 3552 | 79 |
| H(7C) | 6895 | 1261 | 2868 | 79 |
| H(8A) | 5150 | -390 | 2794 | 65 |
| H(8B) | 3873 | 5 | 2724 | 65 |
| H(8C) | 4601 | 45 | 3448 | 65 |
| H(10A) | 3714 | 645 | 5747 | 33 |
| H(12A) | 6810 | 2044 | 5436 | 39 |
| H(12B) | 6033 | 2679 | 5805 | 39 |
| H(15A) | 6992 | 2939 | 4330 | 67 |
| H(15B) | 6064 | 2639 | 3756 | 67 |
| H(15C) | 6899 | 2082 | 4182 | 67 |
| H(16A) | 5252 | 3585 | 4917 | 62 |
| H(16B) | 4138 | 3116 | 5198 | 62 |
| H(16C) | 4308 | 3246 | 4373 | 62 |

Table 6. Torsion angles [°] for d18100.

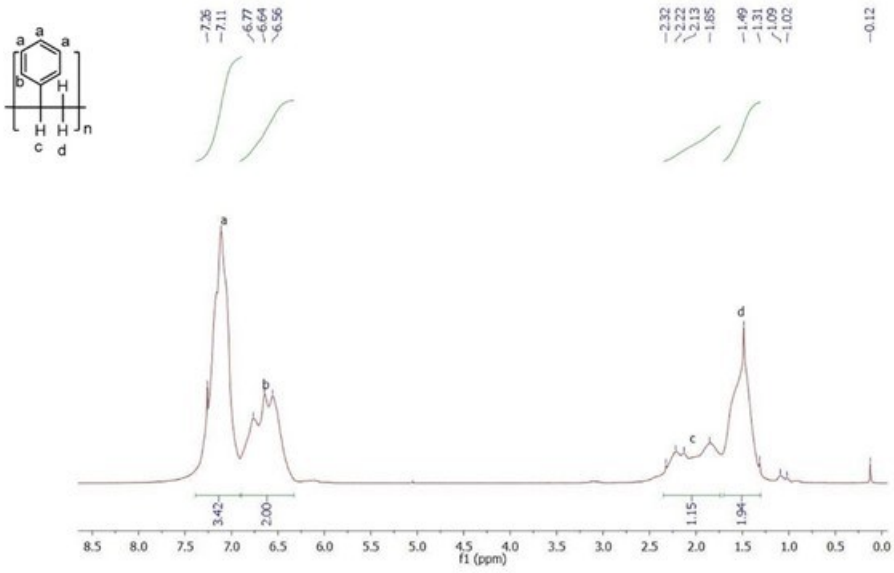
| | |
|---|---|
| Ni(1)-O(1)-C(1)-C(2) | 3.2(4) |
| Ni(1)-O(1)-C(1)-C(6) | -177.88(16) |
| O(1)-C(1)-C(2)-C(3) | 1.1(4) |
| C(6)-C(1)-C(2)-C(3) | -177.8(2) |
| C(5)-N(1)-C(3)-O(2) | 2.6(3) |
| Ni(1)-N(1)-C(3)-O(2) | -178.83(16) |
| C(5)-N(1)-C(3)-C(2) | -177.6(2) |
| Ni(1)-N(1)-C(3)-C(2) | 1.0(4) |
| C(4)-O(2)-C(3)-N(1) | 8.4(3) |
| C(4)-O(2)-C(3)-C(2) | -171.4(2) |
| C(1)-C(2)-C(3)-N(1) | -3.3(4) |
| C(1)-C(2)-C(3)-O(2) | 176.5(2) |
| C(3)-O(2)-C(4)-C(5) | -15.2(3) |
| C(3)-N(1)-C(5)-C(7) | 107.7(3) |
| Ni(1)-N(1)-C(5)-C(7) | -70.8(3) |
| C(3)-N(1)-C(5)-C(8) | -130.5(2) |
| Ni(1)-N(1)-C(5)-C(8) | 51.0(3) |
| C(3)-N(1)-C(5)-C(4) | -11.8(3) |
| Ni(1)-N(1)-C(5)-C(4) | 169.76(19) |
| O(2)-C(4)-C(5)-N(1) | 15.9(3) |
| O(2)-C(4)-C(5)-C(7) | -100.1(3) |
| O(2)-C(4)-C(5)-C(8) | 134.4(2) |
| O(1)-C(1)-C(6)-F(2) | 178.9(2) |
| C(2)-C(1)-C(6)-F(2) | -2.1(3) |
| O(1)-C(1)-C(6)-F(3) | 58.5(3) |
| C(2)-C(1)-C(6)-F(3) | -122.5(3) |
| O(1)-C(1)-C(6)-F(1) | -61.1(3) |
| C(2)-C(1)-C(6)-F(1) | 117.9(3) |
| Ni(1)-O(3)-C(9)-C(10) | 3.7(4) |
| Ni(1)-O(3)-C(9)-C(14) | -174.84(15) |
| O(3)-C(9)-C(10)-C(11) | -0.5(4) |
| C(14)-C(9)-C(10)-C(11) | 178.0(2) |
| C(13)-N(2)-C(11)-O(4) | -4.4(3) |
| Ni(1)-N(2)-C(11)-O(4) | -178.36(15) |

| | |
|---|---|
| C(13)-N(2)-C(11)-C(10) | 174.5(2) |
| Ni(1)-N(2)-C(11)-C(10) | 0.6(4) |
| C(12)-O(4)-C(11)-N(2) | -8.7(3) |
| C(12)-O(4)-C(11)-C(10) | 172.3(2) |
| C(9)-C(10)-C(11)-N(2) | -1.8(4) |
| C(9)-C(10)-C(11)-O(4) | 177.1(2) |
| C(11)-O(4)-C(12)-C(13) | 17.4(3) |
| C(11)-N(2)-C(13)-C(15) | 134.6(2) |
| Ni(1)-N(2)-C(13)-C(15) | -51.7(3) |
| C(11)-N(2)-C(13)-C(12) | 14.7(2) |
| Ni(1)-N(2)-C(13)-C(12) | -171.62(16) |
| C(11)-N(2)-C(13)-C(16) | -103.1(3) |
| Ni(1)-N(2)-C(13)-C(16) | 70.6(3) |
| O(4)-C(12)-C(13)-N(2) | -19.0(2) |
| O(4)-C(12)-C(13)-C(15) | -137.0(2) |
| O(4)-C(12)-C(13)-C(16) | 96.5(2) |
| O(3)-C(9)-C(14)-F(5A) | -170.8(13) |
| C(10)-C(9)-C(14)-F(5A) | 10.5(13) |
| O(3)-C(9)-C(14)-F(4A) | -47.4(12) |
| C(10)-C(9)-C(14)-F(4A) | 133.9(12) |
| O(3)-C(9)-C(14)-F(6) | -30.9(10) |
| C(10)-C(9)-C(14)-F(6) | 150.4(10) |
| O(3)-C(9)-C(14)-F(5) | 93.8(13) |
| C(10)-C(9)-C(14)-F(5) | -84.9(13) |
| O(3)-C(9)-C(14)-F(4) | -147.8(10) |
| C(10)-C(9)-C(14)-F(4) | 33.5(10) |
| O(3)-C(9)-C(14)-F(6A) | 68.1(10) |
| C(10)-C(9)-C(14)-F(6A) | -110.6(10) |

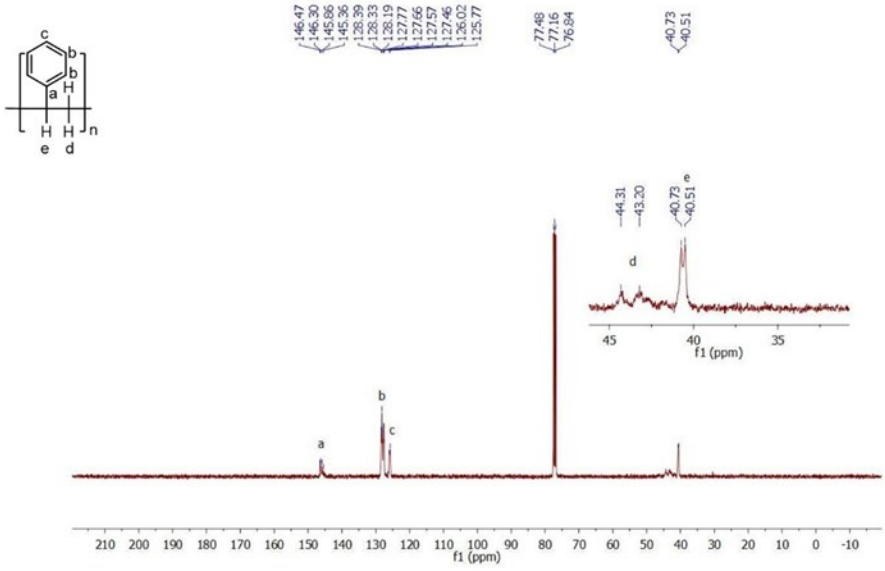
Symmetry transformations used to generate equivalent atoms:

**Poly-styrene Characterisation**.[14]

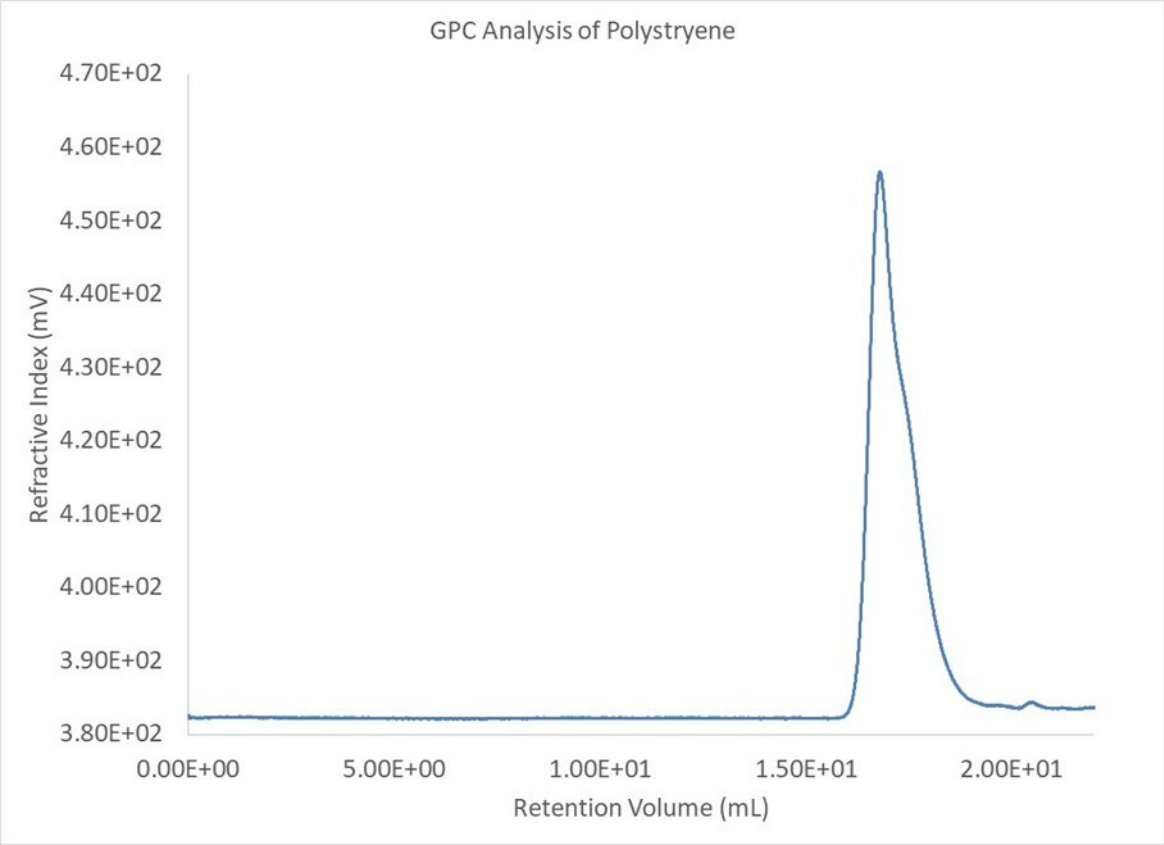
$^{1}$H NMR.



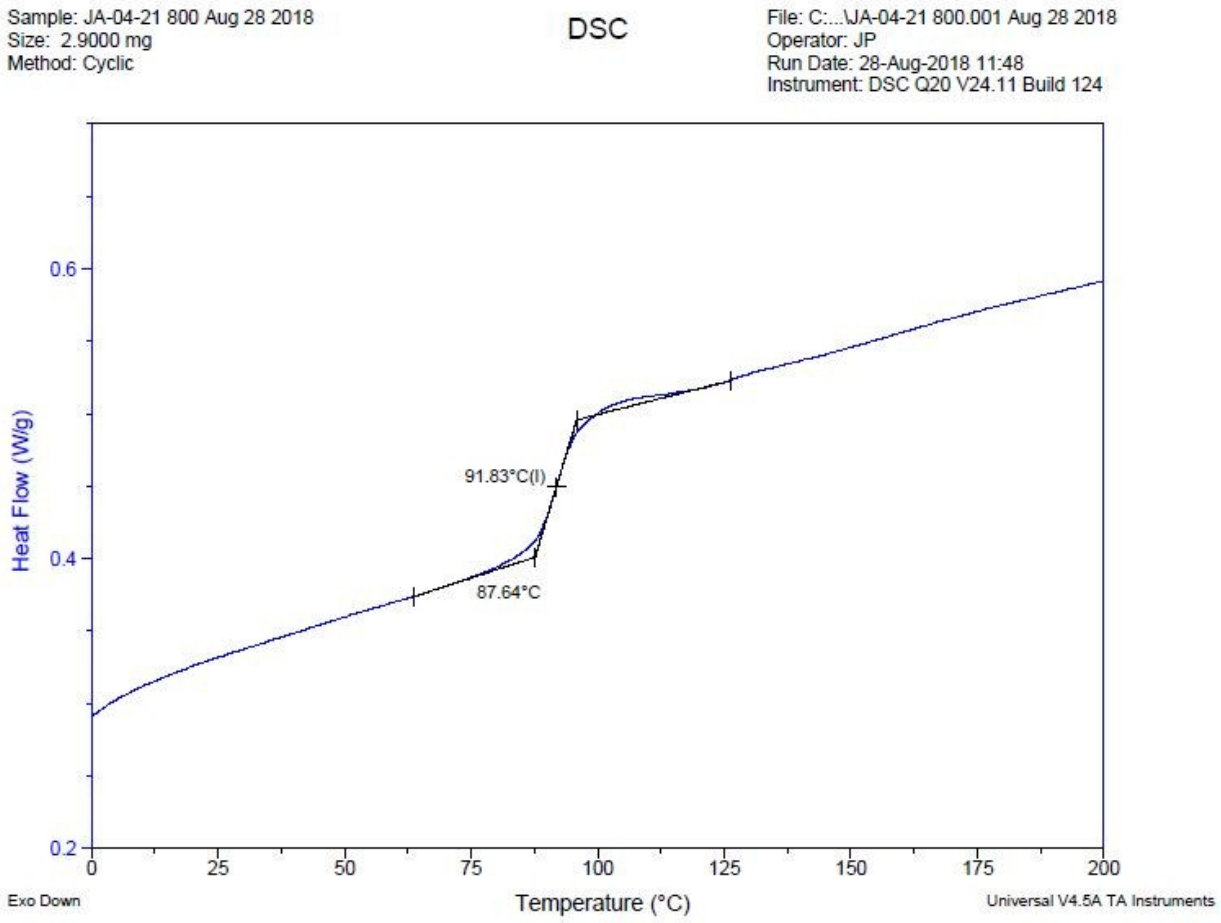

$^{13}$C{$^{1}$H} NMR.



GPC analysis of polystyrene.



DSC of polystyrene.



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