Table 1. Crystal data and structure refinement for compound 10—ccdc-936572.

| | | |
|---|---|---|
| Identification code | compound 10—ccdc-936572 | |
| Empirical formula | C17 H37 Al2 N3 | |
| Formula weight | 337.46 | |
| Temperature | 149(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/n | |
| Unit cell dimensions | a = 11.2028(4) Å | α= 90°. |
| | b = 17.9524(6) Å | β= 112.398(2)°. |
| | c = 11.7448(4) Å | γ = 90°. |
| Volume | 2183.88(13) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.026 $Mg/m^3$ | |
| Absorption coefficient | 0.135 $mm^{-1}$ | |
| F(000) | 744 | |
| Crystal size | 0.30 x 0.25 x 0.20 $mm^3$ | |
| Theta range for data collection | 2.94 to 28.74°. | |
| Index ranges | -15<=h<=15, -24<=k<=24, -15<=l<=15 | |
| Reflections collected | 31678 | |
| Independent reflections | 5646 [R(int) = 0.0363] | |
| Completeness to theta = 28.74° | 99.7 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.973 and 0.960 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5646 / 0 / 209 | |
| Goodness-of-fit on $F^2$ | 1.035 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0356, wR2 = 0.0910 | |
| R indices (all data) | R1 = 0.0490, wR2 = 0.0990 | |
| Largest diff. peak and hole | 0.278 and -0.209 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei292_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 2185(1) | 8590(1) | 9630(1) | 23(1) |
| Al(2) | 3539(1) | 10177(1) | 6119(1) | 24(1) |
| N(1) | 1836(1) | 8587(1) | 11207(1) | 25(1) |
| N(2) | 2352(1) | 9637(1) | 9858(1) | 20(1) |
| N(3) | 2675(1) | 10433(1) | 7322(1) | 23(1) |
| C(1) | 1208(1) | 7938(1) | 11589(1) | 32(1) |
| C(2) | 1382(2) | 8025(1) | 12934(2) | 54(1) |
| C(3) | -220(1) | 7897(1) | 10772(2) | 41(1) |
| C(4) | 1891(1) | 7238(1) | 11420(2) | 45(1) |
| C(5) | 1288(1) | 9342(1) | 11273(1) | 26(1) |
| C(6) | 1967(1) | 9888(1) | 10772(1) | 22(1) |
| C(7) | 2331(1) | 10615(1) | 11060(1) | 25(1) |
| C(8) | 2978(1) | 10830(1) | 10284(1) | 25(1) |
| C(9) | 2977(1) | 10226(1) | 9561(1) | 21(1) |
| C(10) | 701(1) | 8267(1) | 8182(1) | 38(1) |
| C(11) | 3836(1) | 8094(1) | 9923(1) | 35(1) |
| C(12) | 3522(1) | 10153(1) | 8591(1) | 22(1) |
| C(13) | 1389(1) | 10073(1) | 6908(1) | 38(1) |
| C(14) | 2501(1) | 11251(1) | 7350(1) | 34(1) |
| C(15) | 5119(1) | 10801(1) | 6711(1) | 34(1) |
| C(16) | 2226(1) | 10431(1) | 4485(1) | 36(1) |
| C(17) | 3886(2) | 9098(1) | 6347(2) | 44(1) |

Table 3. Bond lengths [Å] and angles [°] for pei292_0m.

| | |
|---|---|
| Al(1)-N(2) | 1.8971(10) |
| Al(1)-C(10) | 1.9588(14) |
| Al(1)-C(11) | 1.9616(14) |
| Al(1)-N(1) | 2.0337(11) |
| Al(2)-C(17) | 1.9734(15) |
| Al(2)-C(16) | 1.9760(14) |
| Al(2)-C(15) | 1.9827(14) |
| Al(2)-N(3) | 2.0466(11) |
| N(1)-C(5) | 1.5011(16) |
| N(1)-C(1) | 1.5159(16) |
| N(2)-C(6) | 1.3764(15) |
| N(2)-C(9) | 1.3840(15) |
| N(3)-C(13) | 1.4813(16) |
| N(3)-C(14) | 1.4842(17) |
| N(3)-C(12) | 1.5154(14) |
| C(1)-C(4) | 1.522(2) |
| C(1)-C(3) | 1.5221(19) |
| C(1)-C(2) | 1.524(2) |
| C(5)-C(6) | 1.4929(16) |
| C(6)-C(7) | 1.3714(17) |
| C(7)-C(8) | 1.4168(17) |
| C(8)-C(9) | 1.3773(17) |
| C(9)-C(12) | 1.4890(16) |

| | |
|---|---|
| N(2)-Al(1)-C(10) | 114.91(6) |
| N(2)-Al(1)-C(11) | 112.93(5) |
| C(10)-Al(1)-C(11) | 116.70(7) |
| N(2)-Al(1)-N(1) | 85.26(4) |
| C(10)-Al(1)-N(1) | 113.31(6) |
| C(11)-Al(1)-N(1) | 109.54(6) |
| C(17)-Al(2)-C(16) | 113.20(7) |
| C(17)-Al(2)-C(15) | 113.77(7) |
| C(16)-Al(2)-C(15) | 116.42(6) |
| C(17)-Al(2)-N(3) | 104.28(6) |

| | |
|---|---|
| C(16)-Al(2)-N(3) | 104.24(5) |
| C(15)-Al(2)-N(3) | 103.02(5) |
| C(5)-N(1)-C(1) | 115.71(10) |
| C(5)-N(1)-Al(1) | 105.60(7) |
| C(1)-N(1)-Al(1) | 122.95(9) |
| C(6)-N(2)-C(9) | 106.60(9) |
| C(6)-N(2)-Al(1) | 112.98(8) |
| C(9)-N(2)-Al(1) | 138.89(8) |
| C(13)-N(3)-C(14) | 108.65(11) |
| C(13)-N(3)-C(12) | 110.16(10) |
| C(14)-N(3)-C(12) | 110.17(10) |
| C(13)-N(3)-Al(2) | 109.41(8) |
| C(14)-N(3)-Al(2) | 109.72(8) |
| C(12)-N(3)-Al(2) | 108.72(7) |
| N(1)-C(1)-C(4) | 106.42(11) |
| N(1)-C(1)-C(3) | 110.20(10) |
| C(4)-C(1)-C(3) | 109.73(13) |
| N(1)-C(1)-C(2) | 109.70(12) |
| C(4)-C(1)-C(2) | 110.41(13) |
| C(3)-C(1)-C(2) | 110.32(13) |
| C(6)-C(5)-N(1) | 106.99(10) |
| C(7)-C(6)-N(2) | 110.57(10) |
| C(7)-C(6)-C(5) | 132.59(11) |
| N(2)-C(6)-C(5) | 116.83(10) |
| C(6)-C(7)-C(8) | 106.15(11) |
| C(9)-C(8)-C(7) | 107.53(11) |
| C(8)-C(9)-N(2) | 109.15(10) |
| C(8)-C(9)-C(12) | 129.58(11) |
| N(2)-C(9)-C(12) | 121.27(10) |
| C(9)-C(12)-N(3) | 115.93(9) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei292_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 22(1) | 20(1) | 24(1) | -2(1) | 6(1) | -2(1) |
| Al(2) | 25(1) | 28(1) | 20(1) | 0(1) | 8(1) | 1(1) |
| N(1) | 20(1) | 25(1) | 26(1) | 5(1) | 6(1) | -1(1) |
| N(2) | 22(1) | 21(1) | 18(1) | 0(1) | 7(1) | -1(1) |
| N(3) | 20(1) | 29(1) | 20(1) | 4(1) | 6(1) | 2(1) |
| C(1) | 25(1) | 30(1) | 39(1) | 14(1) | 11(1) | 0(1) |
| C(2) | 60(1) | 61(1) | 44(1) | 22(1) | 23(1) | -6(1) |
| C(3) | 26(1) | 33(1) | 61(1) | 13(1) | 14(1) | -3(1) |
| C(4) | 32(1) | 30(1) | 70(1) | 19(1) | 16(1) | 4(1) |
| C(5) | 28(1) | 27(1) | 25(1) | 1(1) | 12(1) | 0(1) |
| C(6) | 22(1) | 25(1) | 19(1) | 1(1) | 8(1) | 0(1) |
| C(7) | 30(1) | 24(1) | 20(1) | -2(1) | 9(1) | 0(1) |
| C(8) | 28(1) | 22(1) | 22(1) | -1(1) | 7(1) | -3(1) |
| C(9) | 20(1) | 24(1) | 19(1) | 2(1) | 5(1) | -1(1) |
| C(10) | 39(1) | 33(1) | 33(1) | -5(1) | 2(1) | -8(1) |
| C(11) | 32(1) | 30(1) | 46(1) | -4(1) | 16(1) | 2(1) |
| C(12) | 20(1) | 27(1) | 19(1) | 3(1) | 6(1) | 2(1) |
| C(13) | 22(1) | 62(1) | 26(1) | 4(1) | 6(1) | -8(1) |
| C(14) | 42(1) | 32(1) | 31(1) | 8(1) | 17(1) | 13(1) |
| C(15) | 25(1) | 46(1) | 31(1) | 2(1) | 12(1) | -2(1) |
| C(16) | 34(1) | 49(1) | 23(1) | 2(1) | 8(1) | -5(1) |
| C(17) | 62(1) | 34(1) | 39(1) | -1(1) | 24(1) | 10(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei292_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 2675 | 8612 | 11778 | 30 |
| H(2A) | 2302 | 8080 | 13444 | 81 |
| H(2B) | 1042 | 7583 | 13198 | 81 |
| H(2C) | 914 | 8468 | 13024 | 81 |
| H(3A) | -657 | 8346 | 10888 | 61 |
| H(3B) | -604 | 7457 | 10993 | 61 |
| H(3C) | -319 | 7860 | 9908 | 61 |
| H(4A) | 1752 | 7183 | 10548 | 67 |
| H(4B) | 1543 | 6803 | 11691 | 67 |
| H(4C) | 2818 | 7280 | 11910 | 67 |
| H(5A) | 348 | 9350 | 10779 | 31 |
| H(5B) | 1431 | 9466 | 12136 | 31 |
| H(7) | 2181 | 10914 | 11659 | 30 |
| H(8) | 3344 | 11305 | 10265 | 30 |
| H(10A) | -43 | 8586 | 8082 | 58 |
| H(10B) | 491 | 7749 | 8293 | 58 |
| H(10C) | 913 | 8305 | 7448 | 58 |
| H(11A) | 4138 | 8229 | 9270 | 53 |
| H(11B) | 3719 | 7553 | 9925 | 53 |
| H(11C) | 4475 | 8251 | 10722 | 53 |
| H(12A) | 3715 | 9620 | 8522 | 27 |
| H(12B) | 4351 | 10426 | 8866 | 27 |
| H(13A) | 982 | 10186 | 7494 | 56 |
| H(13B) | 1488 | 9533 | 6864 | 56 |
| H(13C) | 846 | 10263 | 6092 | 56 |
| H(14A) | 1994 | 11430 | 6517 | 51 |
| H(14B) | 3348 | 11495 | 7657 | 51 |
| H(14C) | 2048 | 11369 | 7895 | 51 |
| H(15A) | 5657 | 10677 | 6247 | 50 |
| H(15B) | 5604 | 10705 | 7589 | 50 |

| | | | | |
|---|---|---|---|---|
| H(15C) | 4876 | 11328 | 6590 | 50 |
| H(16A) | 2632 | 10450 | 3879 | 54 |
| H(16B) | 1850 | 10919 | 4526 | 54 |
| H(16C) | 1546 | 10052 | 4239 | 54 |
| H(17A) | 3096 | 8838 | 6286 | 66 |
| H(17B) | 4562 | 9008 | 7160 | 66 |
| H(17C) | 4174 | 8914 | 5708 | 66 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 11—ccdc-936573.

| | | |
|---|---|---|
| Identification code | compound 11—ccdc-936573 | |
| Empirical formula | C21 H34 Al N3 O | |
| Formula weight | 371.49 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 8.525(2) Å | α= 65.054(12)°. |
| | b = 11.534(2) Å | β= 86.170(15)°. |
| | c = 12.736(3) Å | γ = 75.424(15)°. |
| Volume | 1097.9(4) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.124 $Mg/m^3$ | |
| Absorption coefficient | 0.106 $mm^{-1}$ | |
| F(000) | 404 | |
| Crystal size | 0.35 x 0.20 x 0.15 $mm^3$ | |
| Theta range for data collection | 2.01 to 28.85°. | |
| Index ranges | -10<=h<=11, -15<=k<=15, -17<=l<=17 | |
| Reflections collected | 17542 | |
| Independent reflections | 5679 [R(int) = 0.0571] | |
| Completeness to theta = 28.85° | 98.5 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.984 and 0.975 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5679 / 0 / 243 | |
| Goodness-of-fit on $F^2$ | 1.012 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0538, wR2 = 0.1421 | |
| R indices (all data) | R1 = 0.0955, wR2 = 0.1634 | |
| Largest diff. peak and hole | 0.258 and -0.288 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei366_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 7505(1) | 5891(1) | 1900(1) | 46(1) |
| N(1) | 8487(2) | 6696(1) | 542(1) | 38(1) |
| N(2) | 9993(2) | 4550(1) | 2258(1) | 40(1) |
| N(3) | 5312(2) | 7454(2) | 513(1) | 44(1) |
| O(1) | 7404(2) | 6647(1) | 2823(1) | 56(1) |
| C(6) | 10089(2) | 6314(2) | 346(2) | 40(1) |
| C(9) | 7814(2) | 7856(2) | -385(2) | 42(1) |
| C(5) | 11066(2) | 5121(2) | 1306(2) | 46(1) |
| C(14) | 6945(2) | 7780(2) | 2957(2) | 44(1) |
| C(7) | 10425(2) | 7211(2) | -712(2) | 49(1) |
| C(10) | 6113(2) | 8500(2) | -233(2) | 47(1) |
| C(15) | 7889(2) | 8702(2) | 2544(2) | 51(1) |
| C(8) | 8969(2) | 8190(2) | -1175(2) | 50(1) |
| C(13) | 6324(2) | 4515(2) | 2362(2) | 54(1) |
| C(19) | 5558(2) | 7991(2) | 3566(2) | 55(1) |
| C(1) | 10876(2) | 3819(2) | 3444(2) | 52(1) |
| C(11) | 4899(2) | 6815(2) | -178(2) | 55(1) |
| C(16) | 7401(3) | 9831(2) | 2747(2) | 66(1) |
| C(12) | 3813(2) | 8025(2) | 949(2) | 61(1) |
| C(4) | 11331(3) | 4776(2) | 3809(2) | 66(1) |
| C(2) | 12388(3) | 2781(2) | 3421(2) | 72(1) |
| C(18) | 5121(3) | 9154(3) | 3724(2) | 73(1) |
| C(21) | 9401(3) | 8500(3) | 1901(2) | 71(1) |
| C(17) | 6038(4) | 10063(3) | 3323(2) | 77(1) |
| C(3) | 9687(3) | 3152(3) | 4295(2) | 78(1) |
| C(20) | 4589(3) | 6978(3) | 4050(2) | 82(1) |

Table 3. Bond lengths [Å] and angles [°] for pei366_0m.

| | |
|---|---|
| Al(1)-O(1) | 1.7211(14) |
| Al(1)-N(1) | 1.8438(15) |
| Al(1)-C(13) | 1.953(2) |
| Al(1)-N(2) | 2.2321(16) |
| Al(1)-N(3) | 2.4337(17) |
| N(1)-C(6) | 1.366(2) |
| N(1)-C(9) | 1.373(2) |
| N(2)-C(5) | 1.490(2) |
| N(2)-C(1) | 1.522(2) |
| N(3)-C(11) | 1.470(2) |
| N(3)-C(12) | 1.471(2) |
| N(3)-C(10) | 1.479(2) |
| O(1)-C(14) | 1.347(2) |
| C(6)-C(7) | 1.375(3) |
| C(6)-C(5) | 1.491(3) |
| C(9)-C(8) | 1.364(3) |
| C(9)-C(10) | 1.495(2) |
| C(14)-C(19) | 1.397(3) |
| C(14)-C(15) | 1.399(3) |
| C(7)-C(8) | 1.412(3) |
| C(15)-C(16) | 1.390(3) |
| C(15)-C(21) | 1.501(3) |
| C(19)-C(18) | 1.395(3) |
| C(19)-C(20) | 1.496(3) |
| C(1)-C(4) | 1.504(3) |
| C(1)-C(3) | 1.529(3) |
| C(1)-C(2) | 1.530(3) |
| C(16)-C(17) | 1.362(4) |
| C(18)-C(17) | 1.371(4) |

| | |
|---|---|
| O(1)-Al(1)-N(1) | 112.84(7) |
| O(1)-Al(1)-C(13) | 115.46(8) |
| N(1)-Al(1)-C(13) | 131.09(8) |
| O(1)-Al(1)-N(2) | 104.03(7) |

| | |
|---|---|
| N(1)-Al(1)-N(2) | 78.67(6) |
| C(13)-Al(1)-N(2) | 96.65(8) |
| O(1)-Al(1)-N(3) | 99.42(7) |
| N(1)-Al(1)-N(3) | 74.26(6) |
| C(13)-Al(1)-N(3) | 90.64(7) |
| N(2)-Al(1)-N(3) | 149.42(6) |
| C(6)-N(1)-C(9) | 107.85(14) |
| C(6)-N(1)-Al(1) | 124.98(12) |
| C(9)-N(1)-Al(1) | 126.75(12) |
| C(5)-N(2)-C(1) | 112.97(14) |
| C(5)-N(2)-Al(1) | 110.01(10) |
| C(1)-N(2)-Al(1) | 124.73(11) |
| C(11)-N(3)-C(12) | 108.86(15) |
| C(11)-N(3)-C(10) | 108.70(15) |
| C(12)-N(3)-C(10) | 110.31(15) |
| C(11)-N(3)-Al(1) | 107.98(11) |
| C(12)-N(3)-Al(1) | 118.71(12) |
| C(10)-N(3)-Al(1) | 101.80(10) |
| C(14)-O(1)-Al(1) | 146.78(13) |
| N(1)-C(6)-C(7) | 108.92(16) |
| N(1)-C(6)-C(5) | 115.88(15) |
| C(7)-C(6)-C(5) | 135.09(16) |
| C(8)-C(9)-N(1) | 109.20(16) |
| C(8)-C(9)-C(10) | 135.99(17) |
| N(1)-C(9)-C(10) | 114.38(16) |
| N(2)-C(5)-C(6) | 109.87(14) |
| O(1)-C(14)-C(19) | 119.01(19) |
| O(1)-C(14)-C(15) | 120.43(17) |
| C(19)-C(14)-C(15) | 120.48(19) |
| C(6)-C(7)-C(8) | 106.95(16) |
| N(3)-C(10)-C(9) | 108.16(14) |
| C(16)-C(15)-C(14) | 118.2(2) |
| C(16)-C(15)-C(21) | 119.7(2) |
| C(14)-C(15)-C(21) | 122.02(18) |
| C(9)-C(8)-C(7) | 107.07(16) |
| C(18)-C(19)-C(14) | 118.4(2) |

| | |
|---|---|
| C(18)-C(19)-C(20) | 121.2(2) |
| C(14)-C(19)-C(20) | 120.4(2) |
| C(4)-C(1)-N(2) | 110.24(17) |
| C(4)-C(1)-C(3) | 108.88(19) |
| N(2)-C(1)-C(3) | 106.73(16) |
| C(4)-C(1)-C(2) | 110.37(18) |
| N(2)-C(1)-C(2) | 110.44(16) |
| C(3)-C(1)-C(2) | 110.10(19) |
| C(17)-C(16)-C(15) | 122.1(2) |
| C(17)-C(18)-C(19) | 121.5(2) |
| C(16)-C(17)-C(18) | 119.3(2) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei366_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 45(1) | 54(1) | 51(1) | -31(1) | 17(1) | -22(1) |
| N(1) | 29(1) | 43(1) | 43(1) | -21(1) | 3(1) | -8(1) |
| N(2) | 35(1) | 48(1) | 41(1) | -22(1) | 2(1) | -9(1) |
| N(3) | 33(1) | 49(1) | 54(1) | -26(1) | 3(1) | -9(1) |
| O(1) | 63(1) | 60(1) | 60(1) | -38(1) | 18(1) | -23(1) |
| C(6) | 31(1) | 52(1) | 44(1) | -27(1) | 6(1) | -14(1) |
| C(9) | 40(1) | 44(1) | 46(1) | -20(1) | 0(1) | -13(1) |
| C(5) | 30(1) | 65(1) | 45(1) | -27(1) | 4(1) | -8(1) |
| C(14) | 47(1) | 52(1) | 38(1) | -25(1) | 1(1) | -8(1) |
| C(7) | 39(1) | 64(1) | 51(1) | -27(1) | 12(1) | -22(1) |
| C(10) | 42(1) | 43(1) | 53(1) | -18(1) | -3(1) | -6(1) |
| C(15) | 52(1) | 53(1) | 51(1) | -26(1) | -5(1) | -9(1) |
| C(8) | 54(1) | 49(1) | 47(1) | -15(1) | 3(1) | -23(1) |
| C(13) | 46(1) | 55(1) | 62(1) | -25(1) | 8(1) | -18(1) |
| C(19) | 49(1) | 71(1) | 41(1) | -26(1) | 3(1) | -5(1) |
| C(1) | 50(1) | 60(1) | 41(1) | -20(1) | -5(1) | -8(1) |
| C(11) | 42(1) | 62(1) | 68(1) | -33(1) | -4(1) | -14(1) |
| C(16) | 84(2) | 49(1) | 63(1) | -26(1) | -14(1) | -8(1) |
| C(12) | 42(1) | 64(1) | 74(1) | -34(1) | 10(1) | -4(1) |
| C(4) | 61(1) | 90(2) | 57(1) | -43(1) | -6(1) | -12(1) |
| C(2) | 64(1) | 72(2) | 68(1) | -30(1) | -22(1) | 12(1) |
| C(18) | 64(2) | 88(2) | 54(1) | -37(1) | 0(1) | 18(1) |
| C(21) | 63(1) | 80(2) | 86(2) | -41(1) | 19(1) | -35(1) |
| C(17) | 98(2) | 57(2) | 70(2) | -37(1) | -13(1) | 12(1) |
| C(3) | 79(2) | 92(2) | 49(1) | -9(1) | -1(1) | -32(1) |
| C(20) | 67(2) | 115(2) | 64(1) | -38(2) | 24(1) | -29(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei366_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 9774 | 3842 | 2096 | 49 |
| H(5A) | 11603 | 4457 | 1011 | 56 |
| H(5B) | 11917 | 5362 | 1606 | 56 |
| H(7) | 11443 | 7178 | -1066 | 59 |
| H(10A) | 6117 | 9105 | 133 | 56 |
| H(10B) | 5520 | 9018 | -995 | 56 |
| H(8) | 8821 | 8939 | -1899 | 60 |
| H(13A) | 5186 | 4879 | 2467 | 80 |
| H(13B) | 6809 | 3785 | 3092 | 80 |
| H(13C) | 6384 | 4191 | 1758 | 80 |
| H(11A) | 4185 | 7477 | -844 | 82 |
| H(11B) | 4341 | 6134 | 302 | 82 |
| H(11C) | 5893 | 6409 | -454 | 82 |
| H(16) | 8038 | 10460 | 2476 | 79 |
| H(12A) | 3050 | 8637 | 295 | 91 |
| H(12B) | 4067 | 8501 | 1370 | 91 |
| H(12C) | 3322 | 7317 | 1471 | 91 |
| H(4A) | 10363 | 5470 | 3766 | 98 |
| H(4B) | 12139 | 5173 | 3293 | 98 |
| H(4C) | 11787 | 4309 | 4608 | 98 |
| H(2A) | 12863 | 2242 | 4210 | 108 |
| H(2B) | 13183 | 3222 | 2927 | 108 |
| H(2C) | 12088 | 2215 | 3113 | 108 |
| H(18) | 4165 | 9321 | 4120 | 88 |
| H(21A) | 9115 | 8515 | 1162 | 107 |
| H(21B) | 10134 | 7646 | 2369 | 107 |
| H(21C) | 9941 | 9207 | 1754 | 107 |
| H(17) | 5727 | 10846 | 3445 | 92 |
| H(3A) | 8707 | 3821 | 4283 | 118 |
| H(3B) | 10196 | 2690 | 5078 | 118 |

| | | | | |
|---|---|---|---|---|
| H(3C) | 9394 | 2516 | 4069 | 118 |
| H(20A) | 5167 | 6233 | 4739 | 123 |
| H(20B) | 4437 | 6668 | 3466 | 123 |
| H(20C) | 3529 | 7371 | 4263 | 123 |

Table 1. Crystal data and structure refinement for compound 12—ccdc-936574.

| | | |
|---|---|---|
| Identification code | compound 12—ccdc-936574 | |
| Empirical formula | C24 H38 Al N3 O | |
| Formula weight | 411.55 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/n | |
| Unit cell dimensions | a = 9.340(4) Å | α= 90°. |
| | b = 21.360(8) Å | β= 107.88(2)°. |
| | c = 12.639(5) Å | γ = 90°. |
| Volume | 2399.9(16) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.139 $Mg/m^3$ | |
| Absorption coefficient | 0.103 $mm^{-1}$ | |
| F(000) | 896 | |
| Crystal size | 0.30 x 0.20 x 0.18 $mm^3$ | |
| Theta range for data collection | 1.91 to 28.89°. | |
| Index ranges | -12<=h<=12, -28<=k<=28, -17<=l<=17 | |
| Reflections collected | 40805 | |
| Independent reflections | 6223 [R(int) = 0.1532] | |
| Completeness to theta = 28.89° | 98.6 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.982 and 0.976 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6223 / 0 / 270 | |
| Goodness-of-fit on $F^2$ | 0.975 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0723, wR2 = 0.1836 | |
| R indices (all data) | R1 = 0.1432, wR2 = 0.2293 | |
| Largest diff. peak and hole | 0.560 and -0.426 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei358_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 2271(1) | 1304(1) | 3733(1) | 45(1) |
| N(1) | 4019(2) | 1059(1) | 3347(2) | 44(1) |
| N(2) | 1769(3) | 252(1) | 3323(2) | 53(1) |
| N(3) | 3560(2) | 3157(1) | 4412(2) | 47(1) |
| O(1) | 2911(2) | 2180(1) | 3857(2) | 55(1) |
| C(16) | 3901(3) | 2589(1) | 4140(2) | 41(1) |
| C(9) | 5523(3) | 2446(1) | 4164(2) | 39(1) |
| C(8) | 5406(3) | 2058(1) | 3084(2) | 43(1) |
| C(10) | 6392(3) | 3061(1) | 4184(2) | 40(1) |
| C(11) | 7142(3) | 3357(1) | 5175(2) | 48(1) |
| C(17) | 2048(3) | 3380(1) | 4410(2) | 51(1) |
| C(7) | 5189(3) | 1359(1) | 3101(2) | 43(1) |
| C(15) | 6405(3) | 3358(1) | 3207(2) | 48(1) |
| C(5) | 5554(3) | 329(1) | 2979(2) | 55(1) |
| C(13) | 7827(3) | 4218(1) | 4216(3) | 54(1) |
| C(3) | 3297(3) | -12(1) | 3650(3) | 56(1) |
| C(12) | 7858(3) | 3932(1) | 5195(2) | 54(1) |
| C(6) | 6136(3) | 928(1) | 2872(2) | 52(1) |
| C(14) | 7101(3) | 3931(1) | 3225(2) | 53(1) |
| C(21) | 6227(3) | 2044(1) | 5212(2) | 49(1) |
| C(4) | 4296(3) | 423(1) | 3285(2) | 49(1) |
| C(22) | 7852(4) | 1853(2) | 5376(3) | 64(1) |
| C(23) | 301(3) | 1545(2) | 2679(3) | 63(1) |
| C(24) | 2460(4) | 1205(2) | 5326(2) | 67(1) |
| C(18) | 1455(4) | 2985(2) | 5189(3) | 70(1) |
| C(2) | 1046(4) | 142(2) | 2130(3) | 67(1) |
| C(20) | 2268(4) | 4056(1) | 4835(3) | 69(1) |
| C(19) | 990(4) | 3369(2) | 3228(3) | 70(1) |
| C(1) | 841(4) | -50(2) | 3929(3) | 74(1) |

Table 3. Bond lengths [Å] and angles [°] for pei358_0m.

| | |
|---|---|
| Al(1)-N(1) | 1.915(2) |
| Al(1)-O(1) | 1.956(2) |
| Al(1)-C(24) | 1.977(3) |
| Al(1)-C(23) | 1.980(3) |
| Al(1)-N(2) | 2.321(3) |
| N(1)-C(7) | 1.383(3) |
| N(1)-C(4) | 1.389(3) |
| N(2)-C(2) | 1.469(4) |
| N(2)-C(1) | 1.470(4) |
| N(2)-C(3) | 1.471(4) |
| N(3)-C(16) | 1.326(3) |
| N(3)-C(17) | 1.491(3) |
| N(3)-H(3) | 0.9999 |
| O(1)-C(16) | 1.243(3) |
| C(16)-C(9) | 1.538(3) |
| C(9)-C(10) | 1.541(3) |
| C(9)-C(21) | 1.545(3) |
| C(9)-C(8) | 1.571(3) |
| C(8)-C(7) | 1.507(3) |
| C(8)-H(8A) | 0.9900 |
| C(8)-H(8B) | 0.9900 |
| C(10)-C(11) | 1.385(4) |
| C(10)-C(15) | 1.392(3) |
| C(11)-C(12) | 1.396(4) |
| C(11)-H(11) | 0.9500 |
| C(17)-C(19) | 1.517(4) |
| C(17)-C(18) | 1.524(4) |
| C(17)-C(20) | 1.531(4) |
| C(7)-C(6) | 1.368(4) |
| C(15)-C(14) | 1.383(4) |
| C(15)-H(15) | 0.9500 |
| C(5)-C(4) | 1.360(4) |
| C(5)-C(6) | 1.413(4) |
| C(5)-H(5) | 0.9500 |

| | |
|---|---|
| C(13)-C(12) | 1.371(4) |
| C(13)-C(14) | 1.372(4) |
| C(13)-H(13) | 0.9500 |
| C(3)-C(4) | 1.487(4) |
| C(3)-H(3A) | 0.9900 |
| C(3)-H(3B) | 0.9900 |
| C(12)-H(12) | 0.9500 |
| C(6)-H(6) | 0.9500 |
| C(14)-H(14) | 0.9500 |
| C(21)-C(22) | 1.523(4) |
| C(21)-H(21A) | 0.9900 |
| C(21)-H(21B) | 0.9900 |
| C(22)-H(22A) | 0.9800 |
| C(22)-H(22B) | 0.9800 |
| C(22)-H(22C) | 0.9800 |
| C(23)-H(23A) | 0.9800 |
| C(23)-H(23B) | 0.9800 |
| C(23)-H(23C) | 0.9800 |
| C(24)-H(24A) | 0.9800 |
| C(24)-H(24B) | 0.9800 |
| C(24)-H(24C) | 0.9800 |
| C(18)-H(18A) | 0.9800 |
| C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 |
| C(2)-H(2A) | 0.9800 |
| C(2)-H(2B) | 0.9800 |
| C(2)-H(2C) | 0.9800 |
| C(20)-H(20A) | 0.9800 |
| C(20)-H(20B) | 0.9800 |
| C(20)-H(20C) | 0.9800 |
| C(19)-H(19A) | 0.9800 |
| C(19)-H(19B) | 0.9800 |
| C(19)-H(19C) | 0.9800 |
| C(1)-H(1A) | 0.9800 |
| C(1)-H(1B) | 0.9800 |
| C(1)-H(1C) | 0.9800 |

| | |
|---|---|
| N(1)-Al(1)-O(1) | 91.03(9) |
| N(1)-Al(1)-C(24) | 114.42(13) |
| O(1)-Al(1)-C(24) | 95.22(12) |
| N(1)-Al(1)-C(23) | 126.04(12) |
| O(1)-Al(1)-C(23) | 90.19(11) |
| C(24)-Al(1)-C(23) | 119.16(15) |
| N(1)-Al(1)-N(2) | 78.94(9) |
| O(1)-Al(1)-N(2) | 168.42(9) |
| C(24)-Al(1)-N(2) | 94.21(11) |
| C(23)-Al(1)-N(2) | 91.08(12) |
| C(7)-N(1)-C(4) | 105.5(2) |
| C(7)-N(1)-Al(1) | 136.47(18) |
| C(4)-N(1)-Al(1) | 117.98(18) |
| C(2)-N(2)-C(1) | 107.8(3) |
| C(2)-N(2)-C(3) | 109.1(2) |
| C(1)-N(2)-C(3) | 111.2(2) |
| C(2)-N(2)-Al(1) | 112.50(18) |
| C(1)-N(2)-Al(1) | 114.78(19) |
| C(3)-N(2)-Al(1) | 101.35(16) |
| C(16)-N(3)-C(17) | 126.5(2) |
| C(16)-N(3)-H(3) | 106.7 |
| C(17)-N(3)-H(3) | 126.6 |
| C(16)-O(1)-Al(1) | 151.45(19) |
| O(1)-C(16)-N(3) | 120.2(2) |
| O(1)-C(16)-C(9) | 120.5(2) |
| N(3)-C(16)-C(9) | 119.4(2) |
| C(16)-C(9)-C(10) | 110.0(2) |
| C(16)-C(9)-C(21) | 106.5(2) |
| C(10)-C(9)-C(21) | 112.1(2) |
| C(16)-C(9)-C(8) | 106.4(2) |
| C(10)-C(9)-C(8) | 111.08(19) |
| C(21)-C(9)-C(8) | 110.5(2) |
| C(7)-C(8)-C(9) | 118.9(2) |
| C(7)-C(8)-H(8A) | 107.6 |
| C(9)-C(8)-H(8A) | 107.6 |

| | |
|---|---|
| C(7)-C(8)-H(8B) | 107.6 |
| C(9)-C(8)-H(8B) | 107.6 |
| H(8A)-C(8)-H(8B) | 107.0 |
| C(11)-C(10)-C(15) | 117.1(2) |
| C(11)-C(10)-C(9) | 121.4(2) |
| C(15)-C(10)-C(9) | 121.4(2) |
| C(10)-C(11)-C(12) | 121.6(3) |
| C(10)-C(11)-H(11) | 119.2 |
| C(12)-C(11)-H(11) | 119.2 |
| N(3)-C(17)-C(19) | 109.1(2) |
| N(3)-C(17)-C(18) | 110.8(2) |
| C(19)-C(17)-C(18) | 111.8(3) |
| N(3)-C(17)-C(20) | 106.0(2) |
| C(19)-C(17)-C(20) | 109.7(3) |
| C(18)-C(17)-C(20) | 109.4(3) |
| C(6)-C(7)-N(1) | 110.0(2) |
| C(6)-C(7)-C(8) | 124.4(2) |
| N(1)-C(7)-C(8) | 125.6(2) |
| C(14)-C(15)-C(10) | 121.4(3) |
| C(14)-C(15)-H(15) | 119.3 |
| C(10)-C(15)-H(15) | 119.3 |
| C(4)-C(5)-C(6) | 106.5(2) |
| C(4)-C(5)-H(5) | 126.7 |
| C(6)-C(5)-H(5) | 126.7 |
| C(12)-C(13)-C(14) | 119.5(3) |
| C(12)-C(13)-H(13) | 120.3 |
| C(14)-C(13)-H(13) | 120.3 |
| N(2)-C(3)-C(4) | 108.6(2) |
| N(2)-C(3)-H(3A) | 110.0 |
| C(4)-C(3)-H(3A) | 110.0 |
| N(2)-C(3)-H(3B) | 110.0 |
| C(4)-C(3)-H(3B) | 110.0 |
| H(3A)-C(3)-H(3B) | 108.3 |
| C(13)-C(12)-C(11) | 119.9(3) |
| C(13)-C(12)-H(12) | 120.0 |
| C(11)-C(12)-H(12) | 120.0 |

| | |
|---|---|
| C(7)-C(6)-C(5) | 107.3(2) |
| C(7)-C(6)-H(6) | 126.4 |
| C(5)-C(6)-H(6) | 126.4 |
| C(13)-C(14)-C(15) | 120.6(3) |
| C(13)-C(14)-H(14) | 119.7 |
| C(15)-C(14)-H(14) | 119.7 |
| C(22)-C(21)-C(9) | 114.1(2) |
| C(22)-C(21)-H(21A) | 108.7 |
| C(9)-C(21)-H(21A) | 108.7 |
| C(22)-C(21)-H(21B) | 108.7 |
| C(9)-C(21)-H(21B) | 108.7 |
| H(21A)-C(21)-H(21B) | 107.6 |
| C(5)-C(4)-N(1) | 110.6(2) |
| C(5)-C(4)-C(3) | 132.4(3) |
| N(1)-C(4)-C(3) | 116.7(2) |
| C(21)-C(22)-H(22A) | 109.5 |
| C(21)-C(22)-H(22B) | 109.5 |
| H(22A)-C(22)-H(22B) | 109.5 |
| C(21)-C(22)-H(22C) | 109.5 |
| H(22A)-C(22)-H(22C) | 109.5 |
| H(22B)-C(22)-H(22C) | 109.5 |
| Al(1)-C(23)-H(23A) | 109.5 |
| Al(1)-C(23)-H(23B) | 109.5 |
| H(23A)-C(23)-H(23B) | 109.5 |
| Al(1)-C(23)-H(23C) | 109.5 |
| H(23A)-C(23)-H(23C) | 109.5 |
| H(23B)-C(23)-H(23C) | 109.5 |
| Al(1)-C(24)-H(24A) | 109.5 |
| Al(1)-C(24)-H(24B) | 109.5 |
| H(24A)-C(24)-H(24B) | 109.5 |
| Al(1)-C(24)-H(24C) | 109.5 |
| H(24A)-C(24)-H(24C) | 109.5 |
| H(24B)-C(24)-H(24C) | 109.5 |
| C(17)-C(18)-H(18A) | 109.5 |
| C(17)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |

| | |
|---|---|
| C(17)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| N(2)-C(2)-H(2A) | 109.5 |
| N(2)-C(2)-H(2B) | 109.5 |
| H(2A)-C(2)-H(2B) | 109.5 |
| N(2)-C(2)-H(2C) | 109.5 |
| H(2A)-C(2)-H(2C) | 109.5 |
| H(2B)-C(2)-H(2C) | 109.5 |
| C(17)-C(20)-H(20A) | 109.5 |
| C(17)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(17)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(17)-C(19)-H(19A) | 109.5 |
| C(17)-C(19)-H(19B) | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 |
| C(17)-C(19)-H(19C) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 |
| N(2)-C(1)-H(1A) | 109.5 |
| N(2)-C(1)-H(1B) | 109.5 |
| H(1A)-C(1)-H(1B) | 109.5 |
| N(2)-C(1)-H(1C) | 109.5 |
| H(1A)-C(1)-H(1C) | 109.5 |
| H(1B)-C(1)-H(1C) | 109.5 |

---

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei358_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 42(1) | 47(1) | 49(1) | 0(1) | 19(1) | -2(1) |
| N(1) | 46(1) | 38(1) | 50(1) | -3(1) | 18(1) | -2(1) |
| N(2) | 57(2) | 49(1) | 56(1) | 1(1) | 24(1) | -9(1) |
| N(3) | 38(1) | 46(1) | 59(1) | -6(1) | 19(1) | 1(1) |
| O(1) | 41(1) | 45(1) | 80(1) | -7(1) | 20(1) | -3(1) |
| C(16) | 41(2) | 40(1) | 45(1) | 1(1) | 16(1) | -1(1) |
| C(9) | 37(1) | 39(1) | 42(1) | 2(1) | 13(1) | 0(1) |
| C(8) | 43(2) | 43(1) | 47(1) | -2(1) | 18(1) | -2(1) |
| C(10) | 33(1) | 40(1) | 48(1) | 0(1) | 13(1) | 0(1) |
| C(11) | 46(2) | 48(2) | 49(1) | -4(1) | 16(1) | 0(1) |
| C(17) | 44(2) | 48(2) | 65(2) | -6(1) | 22(1) | 4(1) |
| C(7) | 42(2) | 44(1) | 44(1) | -4(1) | 14(1) | -1(1) |
| C(15) | 48(2) | 48(2) | 46(1) | -1(1) | 14(1) | -2(1) |
| C(5) | 62(2) | 38(1) | 68(2) | -3(1) | 27(2) | 8(1) |
| C(13) | 44(2) | 41(1) | 78(2) | -7(1) | 22(2) | -3(1) |
| C(3) | 61(2) | 42(2) | 67(2) | 1(1) | 25(2) | 0(1) |
| C(12) | 49(2) | 52(2) | 64(2) | -15(1) | 19(1) | -4(1) |
| C(6) | 48(2) | 50(2) | 63(2) | -4(1) | 27(1) | 0(1) |
| C(14) | 53(2) | 47(2) | 62(2) | 10(1) | 22(1) | 2(1) |
| C(21) | 53(2) | 48(2) | 42(1) | 3(1) | 10(1) | -2(1) |
| C(4) | 58(2) | 38(1) | 55(2) | -2(1) | 20(1) | -2(1) |
| C(22) | 54(2) | 58(2) | 68(2) | 4(2) | 0(2) | 10(2) |
| C(23) | 46(2) | 56(2) | 81(2) | -1(2) | 13(2) | -6(1) |
| C(24) | 86(3) | 62(2) | 58(2) | -1(2) | 29(2) | -1(2) |
| C(18) | 64(2) | 67(2) | 94(2) | -2(2) | 50(2) | 3(2) |
| C(2) | 73(2) | 62(2) | 65(2) | -7(2) | 20(2) | -13(2) |
| C(20) | 66(2) | 49(2) | 97(2) | -11(2) | 33(2) | 6(2) |
| C(19) | 58(2) | 68(2) | 75(2) | -6(2) | 8(2) | 16(2) |
| C(1) | 73(2) | 68(2) | 92(2) | 7(2) | 42(2) | -14(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei358_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 4529 | 3393 | 4686 | 56 |
| H(8A) | 4558 | 2232 | 2477 | 52 |
| H(8B) | 6335 | 2136 | 2882 | 52 |
| H(11) | 7169 | 3163 | 5858 | 57 |
| H(15) | 5927 | 3162 | 2513 | 57 |
| H(5) | 5961 | -63 | 2860 | 66 |
| H(13) | 8304 | 4611 | 4225 | 65 |
| H(3A) | 3285 | -427 | 3298 | 67 |
| H(3B) | 3673 | -67 | 4467 | 67 |
| H(12) | 8366 | 4125 | 5885 | 65 |
| H(6) | 7020 | 1015 | 2677 | 62 |
| H(14) | 7076 | 4128 | 2546 | 64 |
| H(21A) | 6182 | 2283 | 5873 | 59 |
| H(21B) | 5613 | 1661 | 5165 | 59 |
| H(22A) | 8464 | 2228 | 5400 | 97 |
| H(22B) | 7898 | 1585 | 4758 | 97 |
| H(22C) | 8239 | 1623 | 6077 | 97 |
| H(23A) | -431 | 1210 | 2640 | 94 |
| H(23B) | 408 | 1612 | 1940 | 94 |
| H(23C) | -51 | 1932 | 2934 | 94 |
| H(24A) | 2937 | 1579 | 5734 | 101 |
| H(24B) | 3078 | 837 | 5622 | 101 |
| H(24C) | 1459 | 1151 | 5410 | 101 |
| H(18A) | 2241 | 2940 | 5906 | 104 |
| H(18B) | 1167 | 2570 | 4860 | 104 |
| H(18C) | 575 | 3190 | 5302 | 104 |
| H(2A) | 1022 | -309 | 1979 | 100 |
| H(2B) | 1618 | 355 | 1703 | 100 |
| H(2C) | 16 | 305 | 1912 | 100 |
| H(20A) | 2730 | 4302 | 4373 | 103 |

| | | | | |
|---|---|---|---|---|
| H(20B) | 2925 | 4060 | 5607 | 103 |
| H(20C) | 1290 | 4237 | 4798 | 103 |
| H(19A) | 848 | 2936 | 2960 | 105 |
| H(19B) | 1421 | 3617 | 2749 | 105 |
| H(19C) | 16 | 3547 | 3213 | 105 |
| H(1A) | 1359 | -27 | 4730 | 111 |
| H(1B) | 677 | -490 | 3703 | 111 |
| H(1C) | -130 | 165 | 3758 | 111 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 3.

| | | |
|---|---|---|
| Identification code | compound 3—ccdc-936565 | |
| Empirical formula | C12 H22 Al Cl2 N3 | |
| Formula weight | 306.21 | |
| Temperature | 149(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 12.5365(4) Å | α= 90°. |
| | b = 13.4673(4) Å | β= 112.575(2)°. |
| | c = 10.0304(3) Å | γ = 90°. |
| Volume | 1563.70(8) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.301 $Mg/m^3$ | |
| Absorption coefficient | 0.459 $mm^{-1}$ | |
| F(000) | 648 | |
| Crystal size | ? x ? x ? $mm^3$ | |
| Theta range for data collection | 1.76 to 28.28°. | |
| Index ranges | -16<=h<=16, -17<=k<=17, -13<=l<=13 | |
| Reflections collected | 21774 | |
| Independent reflections | 3884 [R(int) = 0.0361] | |
| Completeness to theta = 28.28° | 99.9 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3884 / 0 / 168 | |
| Goodness-of-fit on $F^2$ | 1.052 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0330, wR2 = 0.0862 | |
| R indices (all data) | R1 = 0.0420, wR2 = 0.0939 | |
| Largest diff. peak and hole | 0.484 and -0.291 e.$Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei1081_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cl(1) | 566(1) | 8960(1) | 8039(1) | 32(1) |
| Cl(2) | 2014(1) | 11038(1) | 10264(1) | 34(1) |
| Al(1) | 2173(1) | 9603(1) | 9421(1) | 22(1) |
| N(1) | 3426(1) | 8804(1) | 9751(1) | 25(1) |
| N(2) | 2296(1) | 8827(1) | 11404(1) | 27(1) |
| N(3) | 2941(1) | 10266(1) | 7960(1) | 24(1) |
| C(1) | 3033(2) | 11254(1) | 5888(2) | 42(1) |
| C(2) | 1663(1) | 9826(1) | 5438(2) | 33(1) |
| C(3) | 1336(2) | 11377(1) | 6595(2) | 40(1) |
| C(4) | 2246(1) | 10673(1) | 6462(2) | 30(1) |
| C(5) | 3983(1) | 9679(1) | 8022(2) | 28(1) |
| C(6) | 4231(1) | 8887(1) | 9152(2) | 26(1) |
| C(7) | 5047(1) | 8158(1) | 9719(2) | 31(1) |
| C(8) | 4715(1) | 7602(1) | 10712(2) | 32(1) |
| C(9) | 3712(1) | 8022(1) | 10693(2) | 29(1) |
| C(10) | 2820(1) | 7840(1) | 11325(2) | 33(1) |
| C(11) | 1187(2) | 8676(1) | 11593(2) | 37(1) |
| C(12) | 3100(2) | 9353(1) | 12696(2) | 37(1) |

Table 3. Bond lengths [Å] and angles [°] for pei1081_0m.

| | |
|---|---|
| Cl(1)-Al(1) | 2.1418(6) |
| Cl(2)-Al(1) | 2.1485(5) |
| Al(1)-N(1) | 1.8266(13) |
| Al(1)-N(2) | 2.2006(13) |
| Al(1)-N(3) | 2.2249(12) |
| N(1)-C(6) | 1.3623(18) |
| N(1)-C(9) | 1.3680(19) |
| N(2)-C(12) | 1.481(2) |
| N(2)-C(11) | 1.4867(19) |
| N(2)-C(10) | 1.4977(19) |
| N(3)-C(5) | 1.5073(19) |
| N(3)-C(4) | 1.5206(19) |
| C(1)-C(4) | 1.533(2) |
| C(2)-C(4) | 1.521(2) |
| C(3)-C(4) | 1.528(2) |
| C(5)-C(6) | 1.500(2) |
| C(6)-C(7) | 1.374(2) |
| C(7)-C(8) | 1.430(2) |
| C(8)-C(9) | 1.372(2) |
| C(9)-C(10) | 1.502(2) |

| | |
|---|---|
| N(1)-Al(1)-Cl(1) | 114.15(5) |
| N(1)-Al(1)-Cl(2) | 131.42(5) |
| Cl(1)-Al(1)-Cl(2) | 114.33(2) |
| N(1)-Al(1)-N(2) | 78.42(5) |
| Cl(1)-Al(1)-N(2) | 96.58(4) |
| Cl(2)-Al(1)-N(2) | 93.23(4) |
| N(1)-Al(1)-N(3) | 78.26(5) |
| Cl(1)-Al(1)-N(3) | 105.86(4) |
| Cl(2)-Al(1)-N(3) | 91.58(4) |
| N(2)-Al(1)-N(3) | 152.66(5) |
| C(6)-N(1)-C(9) | 108.99(12) |
| C(6)-N(1)-Al(1) | 127.07(10) |
| C(9)-N(1)-Al(1) | 123.93(10) |

| | |
|---|---|
| C(12)-N(2)-C(11) | 108.03(12) |
| C(12)-N(2)-C(10) | 107.80(13) |
| C(11)-N(2)-C(10) | 109.67(12) |
| C(12)-N(2)-Al(1) | 110.53(10) |
| C(11)-N(2)-Al(1) | 115.85(10) |
| C(10)-N(2)-Al(1) | 104.68(9) |
| C(5)-N(3)-C(4) | 112.86(11) |
| C(5)-N(3)-Al(1) | 110.46(9) |
| C(4)-N(3)-Al(1) | 124.52(9) |
| N(3)-C(4)-C(2) | 109.95(12) |
| N(3)-C(4)-C(3) | 107.52(12) |
| C(2)-C(4)-C(3) | 110.07(14) |
| N(3)-C(4)-C(1) | 110.34(13) |
| C(2)-C(4)-C(1) | 109.93(13) |
| C(3)-C(4)-C(1) | 108.99(14) |
| C(6)-C(5)-N(3) | 109.23(11) |
| N(1)-C(6)-C(7) | 108.63(13) |
| N(1)-C(6)-C(5) | 114.66(12) |
| C(7)-C(6)-C(5) | 136.60(13) |
| C(6)-C(7)-C(8) | 106.99(13) |
| C(9)-C(8)-C(7) | 106.55(14) |
| N(1)-C(9)-C(8) | 108.83(13) |
| N(1)-C(9)-C(10) | 112.15(12) |
| C(8)-C(9)-C(10) | 138.90(15) |
| N(2)-C(10)-C(9) | 106.92(12) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei1081_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Cl(1) | 24(1) | 36(1) | 31(1) | 3(1) | 7(1) | -4(1) |
| Cl(2) | 44(1) | 26(1) | 41(1) | -4(1) | 26(1) | 0(1) |
| Al(1) | 21(1) | 24(1) | 23(1) | 0(1) | 10(1) | 2(1) |
| N(1) | 23(1) | 31(1) | 23(1) | 1(1) | 11(1) | 4(1) |
| N(2) | 26(1) | 32(1) | 26(1) | 4(1) | 14(1) | 3(1) |
| N(3) | 26(1) | 26(1) | 22(1) | -2(1) | 11(1) | -4(1) |
| C(1) | 54(1) | 41(1) | 34(1) | 4(1) | 21(1) | -15(1) |
| C(2) | 35(1) | 38(1) | 22(1) | 1(1) | 8(1) | -6(1) |
| C(3) | 49(1) | 34(1) | 37(1) | 10(1) | 16(1) | 8(1) |
| C(4) | 36(1) | 29(1) | 25(1) | 3(1) | 12(1) | -5(1) |
| C(5) | 26(1) | 39(1) | 23(1) | -5(1) | 14(1) | -4(1) |
| C(6) | 21(1) | 33(1) | 23(1) | -10(1) | 10(1) | -3(1) |
| C(7) | 23(1) | 39(1) | 30(1) | -13(1) | 9(1) | 3(1) |
| C(8) | 28(1) | 33(1) | 30(1) | -3(1) | 6(1) | 8(1) |
| C(9) | 28(1) | 30(1) | 26(1) | 1(1) | 10(1) | 6(1) |
| C(10) | 35(1) | 31(1) | 33(1) | 10(1) | 16(1) | 8(1) |
| C(11) | 33(1) | 45(1) | 40(1) | 10(1) | 23(1) | 3(1) |
| C(12) | 38(1) | 51(1) | 24(1) | -1(1) | 14(1) | 0(1) |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 4.

| | | |
|---|---|---|
| Identification code | compound 4—ccdc-936566 | |
| Empirical formula | C14 H26 Al Cl2 N3 | |
| Formula weight | 334.26 | |
| Temperature | 149(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | C c | |
| Unit cell dimensions | a = 13.7242(4) Å | α= 90°. |
| | b = 14.8920(4) Å | β= 100.6970(10)°. |
| | c = 17.5053(5) Å | γ = 90°. |
| Volume | 3515.57(17) $Å^3$ | |
| Z | 8 | |
| Density (calculated) | 1.263 $Mg/m^3$ | |
| Absorption coefficient | 0.414 $mm^{-1}$ | |
| F(000) | 1424 | |
| Crystal size | 0.45 x 0.35 x 0.30 $mm^3$ | |
| Theta range for data collection | 2.04 to 28.28°. | |
| Index ranges | -18<=h<=17, -16<=k<=19, -23<=l<=23 | |
| Reflections collected | 20383 | |
| Independent reflections | 8321 [R(int) = 0.0222] | |
| Completeness to theta = 28.28° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.883 and 0.840 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 8321 / 2 / 373 | |
| Goodness-of-fit on $F^2$ | 1.030 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0267, wR2 = 0.0656 | |
| R indices (all data) | R1 = 0.0303, wR2 = 0.0674 | |
| Absolute structure parameter | 0.09(3) | |
| Largest diff. peak and hole | 0.249 and -0.163 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei76_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 5546(1) | 8422(1) | 8594(1) | 21(1) |
| Al(2) | 575(1) | 8995(1) | 8505(1) | 22(1) |
| C(1) | -435(2) | 9439(1) | 6308(1) | 32(1) |
| C(2) | -1116(2) | 10924(1) | 6605(1) | 35(1) |
| C(3) | -1674(1) | 9538(1) | 7198(1) | 33(1) |
| C(4) | -796(1) | 9996(1) | 6934(1) | 25(1) |
| C(5) | 878(1) | 10634(1) | 7498(1) | 29(1) |
| C(6) | 1747(1) | 10447(1) | 8126(1) | 24(1) |
| C(7) | 2667(1) | 10832(1) | 8371(1) | 29(1) |
| C(8) | 3195(1) | 10254(1) | 8955(1) | 30(1) |
| C(9) | 2569(1) | 9555(1) | 9043(1) | 26(1) |
| C(10) | 2611(1) | 8775(1) | 9580(1) | 32(1) |
| C(11) | 1445(2) | 7658(1) | 10023(1) | 35(1) |
| C(12) | 2335(2) | 7070(2) | 10364(1) | 53(1) |
| C(13) | 1197(2) | 8263(2) | 10673(1) | 45(1) |
| C(14) | 568(2) | 7075(1) | 9690(1) | 47(1) |
| C(15) | 4059(2) | 10538(1) | 6787(1) | 38(1) |
| C(16) | 5779(2) | 10411(1) | 7534(1) | 34(1) |
| C(17) | 5161(2) | 9329(1) | 6462(1) | 36(1) |
| C(18) | 4883(1) | 9883(1) | 7123(1) | 29(1) |
| C(19) | 3621(1) | 8768(1) | 7417(1) | 29(1) |
| C(20) | 3546(1) | 7974(1) | 7929(1) | 24(1) |
| C(21) | 2857(1) | 7326(1) | 7968(1) | 26(1) |
| C(22) | 3292(1) | 6702(1) | 8555(1) | 25(1) |
| C(23) | 4231(1) | 7018(1) | 8847(1) | 24(1) |
| C(24) | 5040(1) | 6774(1) | 9504(1) | 28(1) |
| C(25) | 6763(1) | 7238(1) | 10122(1) | 25(1) |
| C(26) | 6442(2) | 7770(1) | 10783(1) | 34(1) |
| C(27) | 7695(1) | 7646(1) | 9913(1) | 32(1) |
| C(28) | 6964(1) | 6258(1) | 10382(1) | 32(1) |
| Cl(1) | 6654(1) | 8080(1) | 7929(1) | 30(1) |

| | | | | |
|---|---|---|---|---|
| Cl(2) | 5889(1) | 9514(1) | 9401(1) | 32(1) |
| Cl(3) | 204(1) | 7837(1) | 7782(1) | 30(1) |
| Cl(4) | -501(1) | 9335(1) | 9206(1) | 30(1) |
| N(1) | 1694(1) | 9670(1) | 8537(1) | 23(1) |
| N(2) | 15(1) | 10082(1) | 7652(1) | 21(1) |
| N(3) | 1676(1) | 8232(1) | 9360(1) | 26(1) |
| N(4) | 4556(1) | 9278(1) | 7731(1) | 24(1) |
| N(5) | 4383(1) | 7790(1) | 8464(1) | 22(1) |
| N(6) | 5965(1) | 7258(1) | 9396(1) | 21(1) |

Table 3. Bond lengths [Å] and angles [°] for pei76_0m.

| | |
|---|---|
| Al(1)-N(5) | 1.8303(15) |
| Al(1)-Cl(1) | 2.1411(6) |
| Al(1)-Cl(2) | 2.1482(6) |
| Al(1)-N(4) | 2.2354(14) |
| Al(1)-N(6) | 2.2358(14) |
| Al(2)-N(1) | 1.8269(15) |
| Al(2)-Cl(3) | 2.1442(6) |
| Al(2)-Cl(4) | 2.1493(6) |
| Al(2)-N(3) | 2.2312(15) |
| Al(2)-N(2) | 2.2384(14) |
| C(1)-C(4) | 1.528(2) |
| C(2)-C(4) | 1.530(2) |
| C(3)-C(4) | 1.528(2) |
| C(4)-N(2) | 1.523(2) |
| C(5)-C(6) | 1.491(3) |
| C(5)-N(2) | 1.507(2) |
| C(6)-N(1) | 1.372(2) |
| C(6)-C(7) | 1.380(2) |
| C(7)-C(8) | 1.427(3) |
| C(8)-C(9) | 1.376(3) |
| C(9)-N(1) | 1.365(2) |
| C(9)-C(10) | 1.490(2) |
| C(10)-N(3) | 1.504(2) |
| C(11)-C(14) | 1.511(3) |
| C(11)-N(3) | 1.521(2) |
| C(11)-C(12) | 1.532(3) |
| C(11)-C(13) | 1.539(3) |
| C(15)-C(18) | 1.526(3) |
| C(16)-C(18) | 1.522(3) |
| C(17)-C(18) | 1.527(2) |
| C(18)-N(4) | 1.524(2) |
| C(19)-C(20) | 1.500(2) |
| C(19)-N(4) | 1.504(2) |
| C(20)-C(21) | 1.361(2) |

| | |
|---|---|
| C(20)-N(5) | 1.368(2) |
| C(21)-C(22) | 1.431(3) |
| C(22)-C(23) | 1.379(2) |
| C(23)-N(5) | 1.366(2) |
| C(23)-C(24) | 1.488(2) |
| C(24)-N(6) | 1.503(2) |
| C(25)-N(6) | 1.517(2) |
| C(25)-C(27) | 1.523(3) |
| C(25)-C(26) | 1.533(2) |
| C(25)-C(28) | 1.537(2) |

| | |
|---|---|
| N(5)-Al(1)-Cl(1) | 120.09(5) |
| N(5)-Al(1)-Cl(2) | 123.37(5) |
| Cl(1)-Al(1)-Cl(2) | 116.54(3) |
| N(5)-Al(1)-N(4) | 78.58(6) |
| Cl(1)-Al(1)-N(4) | 99.92(4) |
| Cl(2)-Al(1)-N(4) | 92.52(4) |
| N(5)-Al(1)-N(6) | 78.27(6) |
| Cl(1)-Al(1)-N(6) | 91.79(4) |
| Cl(2)-Al(1)-N(6) | 100.05(4) |
| N(4)-Al(1)-N(6) | 156.85(5) |
| N(1)-Al(2)-Cl(3) | 124.50(5) |
| N(1)-Al(2)-Cl(4) | 121.07(5) |
| Cl(3)-Al(2)-Cl(4) | 114.42(3) |
| N(1)-Al(2)-N(3) | 78.42(6) |
| Cl(3)-Al(2)-N(3) | 92.48(4) |
| Cl(4)-Al(2)-N(3) | 100.84(4) |
| N(1)-Al(2)-N(2) | 78.78(6) |
| Cl(3)-Al(2)-N(2) | 99.96(4) |
| Cl(4)-Al(2)-N(2) | 91.36(4) |
| N(3)-Al(2)-N(2) | 157.19(6) |
| N(2)-C(4)-C(1) | 110.62(14) |
| N(2)-C(4)-C(3) | 106.43(13) |
| C(1)-C(4)-C(3) | 110.73(15) |
| N(2)-C(4)-C(2) | 110.46(14) |
| C(1)-C(4)-C(2) | 109.26(14) |

| | |
|---|---|
| C(3)-C(4)-C(2) | 109.30(15) |
| C(6)-C(5)-N(2) | 108.31(13) |
| N(1)-C(6)-C(7) | 108.80(15) |
| N(1)-C(6)-C(5) | 115.52(14) |
| C(7)-C(6)-C(5) | 135.43(15) |
| C(6)-C(7)-C(8) | 106.63(16) |
| C(9)-C(8)-C(7) | 106.95(16) |
| N(1)-C(9)-C(8) | 108.99(15) |
| N(1)-C(9)-C(10) | 115.66(15) |
| C(8)-C(9)-C(10) | 135.18(17) |
| C(9)-C(10)-N(3) | 109.11(14) |
| C(14)-C(11)-N(3) | 107.02(16) |
| C(14)-C(11)-C(12) | 109.96(18) |
| N(3)-C(11)-C(12) | 110.74(16) |
| C(14)-C(11)-C(13) | 110.63(18) |
| N(3)-C(11)-C(13) | 109.97(15) |
| C(12)-C(11)-C(13) | 108.52(17) |
| C(16)-C(18)-N(4) | 107.00(14) |
| C(16)-C(18)-C(15) | 109.13(15) |
| N(4)-C(18)-C(15) | 110.67(15) |
| C(16)-C(18)-C(17) | 110.14(16) |
| N(4)-C(18)-C(17) | 110.93(14) |
| C(15)-C(18)-C(17) | 108.94(16) |
| C(20)-C(19)-N(4) | 109.21(14) |
| C(21)-C(20)-N(5) | 109.15(15) |
| C(21)-C(20)-C(19) | 135.57(16) |
| N(5)-C(20)-C(19) | 115.10(15) |
| C(20)-C(21)-C(22) | 107.14(15) |
| C(23)-C(22)-C(21) | 106.30(15) |
| N(5)-C(23)-C(22) | 108.86(15) |
| N(5)-C(23)-C(24) | 115.15(14) |
| C(22)-C(23)-C(24) | 135.67(15) |
| C(23)-C(24)-N(6) | 108.15(13) |
| N(6)-C(25)-C(27) | 107.33(13) |
| N(6)-C(25)-C(26) | 111.04(14) |
| C(27)-C(25)-C(26) | 110.31(15) |

| | |
|---|---|
| N(6)-C(25)-C(28) | 109.27(13) |
| C(27)-C(25)-C(28) | 109.72(15) |
| C(26)-C(25)-C(28) | 109.15(15) |
| C(9)-N(1)-C(6) | 108.63(14) |
| C(9)-N(1)-Al(2) | 125.77(11) |
| C(6)-N(1)-Al(2) | 125.08(12) |
| C(5)-N(2)-C(4) | 112.09(12) |
| C(5)-N(2)-Al(2) | 109.27(10) |
| C(4)-N(2)-Al(2) | 126.78(10) |
| C(10)-N(3)-C(11) | 113.30(14) |
| C(10)-N(3)-Al(2) | 109.67(10) |
| C(11)-N(3)-Al(2) | 125.94(12) |
| C(19)-N(4)-C(18) | 112.69(13) |
| C(19)-N(4)-Al(1) | 109.21(10) |
| C(18)-N(4)-Al(1) | 126.03(11) |
| C(23)-N(5)-C(20) | 108.55(14) |
| C(23)-N(5)-Al(1) | 125.48(11) |
| C(20)-N(5)-Al(1) | 125.81(11) |
| C(24)-N(6)-C(25) | 112.29(12) |
| C(24)-N(6)-Al(1) | 109.06(10) |
| C(25)-N(6)-Al(1) | 127.11(10) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei76_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 21(1) | 19(1) | 22(1) | -4(1) | 4(1) | -2(1) |
| Al(2) | 25(1) | 18(1) | 24(1) | 0(1) | 9(1) | -1(1) |
| C(1) | 35(1) | 34(1) | 26(1) | -4(1) | 6(1) | 4(1) |
| C(2) | 38(1) | 36(1) | 31(1) | 6(1) | 7(1) | 13(1) |
| C(3) | 24(1) | 40(1) | 33(1) | -4(1) | 4(1) | 0(1) |
| C(4) | 26(1) | 27(1) | 20(1) | -2(1) | 2(1) | 4(1) |
| C(5) | 31(1) | 24(1) | 32(1) | 8(1) | 6(1) | -4(1) |
| C(6) | 28(1) | 20(1) | 27(1) | 0(1) | 9(1) | -2(1) |
| C(7) | 28(1) | 24(1) | 39(1) | -6(1) | 13(1) | -3(1) |
| C(8) | 22(1) | 30(1) | 38(1) | -11(1) | 6(1) | 0(1) |
| C(9) | 26(1) | 27(1) | 26(1) | -5(1) | 5(1) | 4(1) |
| C(10) | 33(1) | 34(1) | 25(1) | 0(1) | -1(1) | 8(1) |
| C(11) | 56(1) | 28(1) | 25(1) | 9(1) | 18(1) | 13(1) |
| C(12) | 80(2) | 51(1) | 34(1) | 19(1) | 22(1) | 36(1) |
| C(13) | 66(2) | 47(1) | 26(1) | 4(1) | 21(1) | 17(1) |
| C(14) | 77(2) | 27(1) | 44(1) | 12(1) | 26(1) | 0(1) |
| C(15) | 48(1) | 33(1) | 32(1) | 8(1) | 8(1) | 10(1) |
| C(16) | 40(1) | 24(1) | 38(1) | 4(1) | 9(1) | -2(1) |
| C(17) | 51(1) | 33(1) | 27(1) | 1(1) | 15(1) | 5(1) |
| C(18) | 38(1) | 23(1) | 27(1) | 4(1) | 11(1) | 4(1) |
| C(19) | 25(1) | 33(1) | 26(1) | 3(1) | -2(1) | 1(1) |
| C(20) | 24(1) | 26(1) | 21(1) | -4(1) | 2(1) | 3(1) |
| C(21) | 21(1) | 35(1) | 22(1) | -9(1) | 2(1) | -1(1) |
| C(22) | 25(1) | 26(1) | 26(1) | -6(1) | 7(1) | -5(1) |
| C(23) | 24(1) | 23(1) | 23(1) | -2(1) | 4(1) | -2(1) |
| C(24) | 30(1) | 26(1) | 28(1) | 6(1) | 2(1) | -7(1) |
| C(25) | 25(1) | 30(1) | 20(1) | -4(1) | -1(1) | -1(1) |
| C(26) | 41(1) | 38(1) | 23(1) | -8(1) | 5(1) | -1(1) |
| C(27) | 25(1) | 39(1) | 30(1) | -5(1) | -2(1) | -4(1) |
| C(28) | 33(1) | 34(1) | 27(1) | 4(1) | 0(1) | 5(1) |
| Cl(1) | 31(1) | 25(1) | 36(1) | 5(1) | 16(1) | 5(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl(2) | 39(1) | 23(1) | 32(1) | -9(1) | -4(1) | 2(1) |
| Cl(3) | 34(1) | 18(1) | 36(1) | -5(1) | 3(1) | 1(1) |
| Cl(4) | 36(1) | 26(1) | 33(1) | 4(1) | 18(1) | 5(1) |
| N(1) | 24(1) | 20(1) | 25(1) | 2(1) | 3(1) | 0(1) |
| N(2) | 24(1) | 18(1) | 20(1) | 0(1) | 5(1) | 1(1) |
| N(3) | 36(1) | 22(1) | 21(1) | 3(1) | 10(1) | 9(1) |
| N(4) | 27(1) | 23(1) | 20(1) | 0(1) | 3(1) | 2(1) |
| N(5) | 21(1) | 22(1) | 23(1) | 0(1) | 1(1) | -2(1) |
| N(6) | 22(1) | 22(1) | 18(1) | -3(1) | 2(1) | -2(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei76_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 94 | 9764 | 6119 | 47 |
| H(1B) | -987 | 9334 | 5875 | 47 |
| H(1C) | -180 | 8862 | 6529 | 47 |
| H(2A) | -1281 | 11305 | 7020 | 52 |
| H(2B) | -1698 | 10864 | 6190 | 52 |
| H(2C) | -572 | 11199 | 6395 | 52 |
| H(3A) | -2230 | 9497 | 6759 | 49 |
| H(3B) | -1874 | 9891 | 7616 | 49 |
| H(3C) | -1479 | 8934 | 7390 | 49 |
| H(5A) | 1036 | 10474 | 6986 | 35 |
| H(5B) | 709 | 11281 | 7493 | 35 |
| H(7) | 2902 | 11376 | 8187 | 35 |
| H(8) | 3853 | 10337 | 9231 | 36 |
| H(10A) | 2676 | 8990 | 10122 | 38 |
| H(10B) | 3194 | 8397 | 9545 | 38 |
| H(12A) | 2910 | 7452 | 10554 | 80 |
| H(12B) | 2490 | 6667 | 9960 | 80 |
| H(12C) | 2175 | 6713 | 10795 | 80 |
| H(13A) | 676 | 8689 | 10453 | 68 |
| H(13B) | 1791 | 8594 | 10916 | 68 |
| H(13C) | 965 | 7892 | 11066 | 68 |
| H(14A) | 733 | 6708 | 9267 | 71 |
| H(14B) | -4 | 7456 | 9489 | 71 |
| H(14C) | 408 | 6682 | 10098 | 71 |
| H(15A) | 3481 | 10201 | 6520 | 56 |
| H(15B) | 4294 | 10940 | 6417 | 56 |
| H(15C) | 3872 | 10893 | 7209 | 56 |
| H(16A) | 6019 | 10803 | 7159 | 51 |
| H(16B) | 6306 | 9994 | 7759 | 51 |
| H(16C) | 5588 | 10777 | 7948 | 51 |

| | | | | |
|---|---|---|---|---|
| H(17A) | 5654 | 8876 | 6676 | 54 |
| H(17B) | 5439 | 9724 | 6109 | 54 |
| H(17C) | 4568 | 9030 | 6175 | 54 |
| H(19A) | 3038 | 9164 | 7403 | 35 |
| H(19B) | 3632 | 8564 | 6881 | 35 |
| H(21) | 2209 | 7294 | 7662 | 31 |
| H(22) | 2992 | 6175 | 8712 | 31 |
| H(24A) | 5152 | 6117 | 9511 | 34 |
| H(24B) | 4857 | 6951 | 10004 | 34 |
| H(26A) | 6248 | 8378 | 10603 | 51 |
| H(26B) | 6995 | 7802 | 11226 | 51 |
| H(26C) | 5878 | 7469 | 10944 | 51 |
| H(27A) | 7881 | 7311 | 9480 | 49 |
| H(27B) | 8237 | 7617 | 10364 | 49 |
| H(27C) | 7568 | 8275 | 9759 | 49 |
| H(28A) | 7532 | 6236 | 10814 | 48 |
| H(28B) | 7111 | 5903 | 9946 | 48 |
| H(28C) | 6378 | 6011 | 10553 | 48 |
| H(2) | -278 | 10472 | 7958 | 31 |
| H(3) | 1878 | 7797 | 9042 | 39 |
| H(4) | 4330 | 9696 | 8052 | 35 |
| H(6) | 6223 | 6861 | 9075 | 32 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 5—ccdc936567.

| | | |
|---|---|---|
| Identification code | compound 5—ccdc936567 | |
| Empirical formula | C19 H30 Al Cl N4 | |
| Formula weight | 376.90 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 8.8099(5) Å | α= 87.190(4)°. |
| | b = 9.5732(5) Å | β= 86.082(4)°. |
| | c = 12.5602(7) Å | γ = 76.421(3)°. |
| Volume | 1026.70(10) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.219 $Mg/m^3$ | |
| Absorption coefficient | 0.238 $mm^{-1}$ | |
| F(000) | 404 | |
| Crystal size | 0.45 x 0.30 x 0.30 $mm^3$ | |
| Theta range for data collection | 1.63 to 28.78°. | |
| Index ranges | -11<=h<=11, -12<=k<=12, -17<=l<=16 | |
| Reflections collected | 20205 | |
| Independent reflections | 5299 [R(int) = 0.0467] | |
| Completeness to theta = 28.78° | 99.4 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.931 and 0.918 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5299 / 0 / 232 | |
| Goodness-of-fit on $F^2$ | 1.011 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0470, wR2 = 0.1188 | |
| R indices (all data) | R1 = 0.0767, wR2 = 0.1345 | |
| Largest diff. peak and hole | 0.263 and -0.271 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei294_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 3524(1) | 786(1) | 2582(1) | 37(1) |
| Cl(1) | 5221(1) | -934(1) | 3314(1) | 57(1) |
| N(1) | 3737(2) | 1599(2) | 1251(1) | 38(1) |
| N(2) | 2838(2) | -781(2) | 1547(1) | 41(1) |
| N(3) | 4898(2) | 2441(2) | 2862(1) | 44(1) |
| N(4) | 1806(2) | 1511(2) | 3478(1) | 42(1) |
| C(1) | 1660(3) | -1677(2) | 1884(2) | 52(1) |
| C(2) | 56(3) | -686(3) | 2082(2) | 68(1) |
| C(3) | 1617(3) | -2746(3) | 1024(2) | 73(1) |
| C(4) | 2174(3) | -2491(3) | 2915(2) | 71(1) |
| C(5) | 2666(3) | -161(2) | 437(2) | 49(1) |
| C(6) | 3251(2) | 1181(2) | 338(1) | 41(1) |
| C(7) | 3336(3) | 2198(2) | -452(2) | 55(1) |
| C(8) | 3874(3) | 3298(2) | 8(2) | 57(1) |
| C(9) | 4103(2) | 2906(2) | 1056(2) | 44(1) |
| C(10) | 4394(3) | 3591(2) | 2043(2) | 53(1) |
| C(11) | 4595(3) | 3047(3) | 3938(2) | 69(1) |
| C(12) | 6597(3) | 1837(3) | 2687(2) | 62(1) |
| C(13) | 1820(3) | 995(3) | 4594(2) | 62(1) |
| C(14) | 630(2) | 2731(2) | 3253(2) | 41(1) |
| C(15) | 333(2) | 3216(2) | 2204(2) | 48(1) |
| C(16) | -805(3) | 4443(2) | 1967(2) | 60(1) |
| C(17) | -1704(3) | 5218(3) | 2755(3) | 74(1) |
| C(18) | -1458(3) | 4756(3) | 3790(3) | 80(1) |
| C(19) | -323(3) | 3531(3) | 4051(2) | 64(1) |

Table 3. Bond lengths [Å] and angles [°] for pei294_0m.

| | |
|---|---|
| Al(1)-N(1) | 1.8254(15) |
| Al(1)-N(4) | 1.8412(16) |
| Al(1)-Cl(1) | 2.1621(7) |
| Al(1)-N(2) | 2.2425(16) |
| Al(1)-N(3) | 2.2612(16) |
| N(1)-C(6) | 1.361(2) |
| N(1)-C(9) | 1.370(2) |
| N(2)-C(5) | 1.491(2) |
| N(2)-C(1) | 1.522(2) |
| N(3)-C(12) | 1.478(3) |
| N(3)-C(11) | 1.480(3) |
| N(3)-C(10) | 1.480(3) |
| N(4)-C(14) | 1.399(2) |
| N(4)-C(13) | 1.463(2) |
| C(1)-C(2) | 1.518(3) |
| C(1)-C(4) | 1.517(3) |
| C(1)-C(3) | 1.532(3) |
| C(5)-C(6) | 1.489(3) |
| C(6)-C(7) | 1.367(3) |
| C(7)-C(8) | 1.414(3) |
| C(8)-C(9) | 1.366(3) |
| C(9)-C(10) | 1.495(3) |
| C(14)-C(19) | 1.398(3) |
| C(14)-C(15) | 1.396(3) |
| C(15)-C(16) | 1.389(3) |
| C(16)-C(17) | 1.360(4) |
| C(17)-C(18) | 1.367(4) |
| C(18)-C(19) | 1.393(4) |

| | |
|---|---|
| N(1)-Al(1)-N(4) | 120.36(7) |
| N(1)-Al(1)-Cl(1) | 126.10(6) |
| N(4)-Al(1)-Cl(1) | 113.39(6) |
| N(1)-Al(1)-N(2) | 78.15(6) |
| N(4)-Al(1)-N(2) | 106.80(7) |

| | |
|---|---|
| Cl(1)-Al(1)-N(2) | 90.63(5) |
| N(1)-Al(1)-N(3) | 77.24(6) |
| N(4)-Al(1)-N(3) | 97.55(7) |
| Cl(1)-Al(1)-N(3) | 92.73(5) |
| N(2)-Al(1)-N(3) | 151.73(6) |
| C(6)-N(1)-C(9) | 108.72(16) |
| C(6)-N(1)-Al(1) | 125.77(13) |
| C(9)-N(1)-Al(1) | 124.16(13) |
| C(5)-N(2)-C(1) | 113.14(15) |
| C(5)-N(2)-Al(1) | 109.52(11) |
| C(1)-N(2)-Al(1) | 124.83(12) |
| C(12)-N(3)-C(11) | 108.54(18) |
| C(12)-N(3)-C(10) | 108.92(17) |
| C(11)-N(3)-C(10) | 109.76(18) |
| C(12)-N(3)-Al(1) | 111.09(13) |
| C(11)-N(3)-Al(1) | 113.94(13) |
| C(10)-N(3)-Al(1) | 104.45(11) |
| C(14)-N(4)-C(13) | 115.30(16) |
| C(14)-N(4)-Al(1) | 125.08(12) |
| C(13)-N(4)-Al(1) | 118.16(14) |
| C(2)-C(1)-C(4) | 109.4(2) |
| C(2)-C(1)-N(2) | 109.25(17) |
| C(4)-C(1)-N(2) | 107.55(17) |
| C(2)-C(1)-C(3) | 110.5(2) |
| C(4)-C(1)-C(3) | 109.63(19) |
| N(2)-C(1)-C(3) | 110.51(18) |
| C(6)-C(5)-N(2) | 109.62(15) |
| N(1)-C(6)-C(7) | 108.79(18) |
| N(1)-C(6)-C(5) | 115.62(16) |
| C(7)-C(6)-C(5) | 135.42(18) |
| C(6)-C(7)-C(8) | 106.85(18) |
| C(9)-C(8)-C(7) | 107.41(18) |
| C(8)-C(9)-N(1) | 108.20(18) |
| C(8)-C(9)-C(10) | 137.48(18) |
| N(1)-C(9)-C(10) | 113.50(16) |
| N(3)-C(10)-C(9) | 108.18(16) |

| | |
|---|---|
| C(19)-C(14)-N(4) | 122.69(19) |
| C(19)-C(14)-C(15) | 115.88(19) |
| N(4)-C(14)-C(15) | 121.42(16) |
| C(16)-C(15)-C(14) | 122.2(2) |
| C(17)-C(16)-C(15) | 121.0(2) |
| C(16)-C(17)-C(18) | 118.2(2) |
| C(17)-C(18)-C(19) | 122.0(2) |
| C(18)-C(19)-C(14) | 120.7(2) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei294_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 36(1) | 41(1) | 33(1) | 2(1) | -1(1) | -5(1) |
| Cl(1) | 57(1) | 54(1) | 56(1) | 6(1) | -18(1) | -1(1) |
| N(1) | 42(1) | 37(1) | 34(1) | -1(1) | 2(1) | -9(1) |
| N(2) | 39(1) | 39(1) | 43(1) | -2(1) | -2(1) | -8(1) |
| N(3) | 42(1) | 52(1) | 40(1) | -7(1) | 1(1) | -15(1) |
| N(4) | 42(1) | 51(1) | 32(1) | 0(1) | 2(1) | -10(1) |
| C(1) | 52(1) | 47(1) | 59(1) | -8(1) | 2(1) | -18(1) |
| C(2) | 45(1) | 75(2) | 86(2) | -18(1) | 5(1) | -20(1) |
| C(3) | 82(2) | 60(1) | 85(2) | -19(1) | 2(1) | -32(1) |
| C(4) | 88(2) | 58(1) | 73(2) | 11(1) | 0(1) | -33(1) |
| C(5) | 55(1) | 55(1) | 38(1) | -7(1) | -6(1) | -14(1) |
| C(6) | 39(1) | 47(1) | 34(1) | -2(1) | 0(1) | -3(1) |
| C(7) | 58(1) | 64(1) | 38(1) | 6(1) | -4(1) | -7(1) |
| C(8) | 64(1) | 50(1) | 52(1) | 15(1) | 2(1) | -11(1) |
| C(9) | 44(1) | 40(1) | 46(1) | 2(1) | 5(1) | -9(1) |
| C(10) | 58(1) | 43(1) | 60(1) | -4(1) | 4(1) | -19(1) |
| C(11) | 77(2) | 85(2) | 53(1) | -25(1) | 4(1) | -35(1) |
| C(12) | 41(1) | 74(2) | 73(2) | -6(1) | -2(1) | -20(1) |
| C(13) | 66(2) | 78(2) | 40(1) | 6(1) | 7(1) | -16(1) |
| C(14) | 33(1) | 46(1) | 47(1) | -10(1) | 3(1) | -13(1) |
| C(15) | 37(1) | 49(1) | 55(1) | -1(1) | 2(1) | -6(1) |
| C(16) | 47(1) | 55(1) | 78(2) | 12(1) | -4(1) | -9(1) |
| C(17) | 59(2) | 51(1) | 106(2) | -11(1) | -3(2) | 1(1) |
| C(18) | 62(2) | 74(2) | 96(2) | -44(2) | 11(2) | 3(1) |
| C(19) | 56(1) | 76(2) | 57(1) | -24(1) | 0(1) | -7(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei294_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 3847 | -1459 | 1539 | 50 |
| H(2A) | -251 | -120 | 1428 | 101 |
| H(2B) | 92 | -38 | 2655 | 101 |
| H(2C) | -708 | -1261 | 2291 | 101 |
| H(3A) | 2678 | -3315 | 856 | 109 |
| H(3B) | 1198 | -2220 | 379 | 109 |
| H(3C) | 946 | -3389 | 1288 | 109 |
| H(4A) | 2162 | -1805 | 3471 | 107 |
| H(4B) | 3235 | -3087 | 2799 | 107 |
| H(4C) | 1456 | -3106 | 3140 | 107 |
| H(5A) | 3268 | -865 | -76 | 58 |
| H(5B) | 1552 | 56 | 268 | 58 |
| H(7) | 3082 | 2171 | -1173 | 65 |
| H(8) | 4045 | 4152 | -346 | 68 |
| H(10A) | 5217 | 4133 | 1886 | 63 |
| H(10B) | 3426 | 4270 | 2305 | 63 |
| H(11A) | 5207 | 3770 | 3996 | 103 |
| H(11B) | 4899 | 2276 | 4479 | 103 |
| H(11C) | 3479 | 3497 | 4052 | 103 |
| H(12A) | 7156 | 2607 | 2711 | 92 |
| H(12B) | 6812 | 1400 | 1987 | 92 |
| H(12C) | 6951 | 1105 | 3245 | 92 |
| H(13A) | 803 | 794 | 4819 | 93 |
| H(13B) | 2023 | 1732 | 5043 | 93 |
| H(13C) | 2642 | 113 | 4668 | 93 |
| H(15) | 930 | 2690 | 1634 | 58 |
| H(16) | -958 | 4745 | 1242 | 73 |
| H(17) | -2482 | 6058 | 2592 | 89 |
| H(18) | -2079 | 5287 | 4348 | 95 |
| H(19) | -195 | 3235 | 4778 | 76 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 6—ccdc-936568.

| | | |
|---|---|---|
| Identification code | compound 6—ccdc-936568 | |
| Empirical formula | C21 H34 Al Cl N4 | |
| Formula weight | 404.95 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 11.5583(7) Å | α= 98.218(5)°. |
| | b = 11.9274(8) Å | β= 104.901(5)°. |
| | c = 18.6239(16) Å | γ = 107.932(4)°. |
| Volume | 2290.7(3) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.174 $Mg/m^3$ | |
| Absorption coefficient | 0.218 $mm^{-1}$ | |
| F(000) | 872 | |
| Crystal size | 0.35 x 0.30 x 0.25 $mm^3$ | |
| Theta range for data collection | 1.17 to 28.88°. | |
| Index ranges | -15<=h<=15, -13<=k<=16, -25<=l<=25 | |
| Reflections collected | 34113 | |
| Independent reflections | 11899 [R(int) = 0.0533] | |
| Completeness to theta = 28.88° | 98.8 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.947 and 0.927 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 11899 / 0 / 501 | |
| Goodness-of-fit on $F^2$ | 1.003 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0495, wR2 = 0.1224 | |
| R indices (all data) | R1 = 0.0999, wR2 = 0.1508 | |
| Largest diff. peak and hole | 0.273 and -0.205 e.$Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for bi1531_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cl(1) | 3965(1) | 2861(1) | 2543(1) | 55(1) |
| Cl(2) | 7840(1) | 4025(1) | 3749(1) | 62(1) |
| Al(1) | 4107(1) | 1249(1) | 1918(1) | 43(1) |
| Al(2) | 8068(1) | 5498(1) | 3172(1) | 49(1) |
| N(1) | 5547(2) | 1295(1) | 1669(1) | 44(1) |
| N(2) | 3773(2) | 1901(1) | 829(1) | 44(1) |
| N(3) | 5472(2) | 1162(2) | 3034(1) | 47(1) |
| N(4) | 2694(2) | -111(1) | 1732(1) | 44(1) |
| N(5) | 7033(2) | 5275(2) | 2201(1) | 46(1) |
| N(6) | 6237(2) | 5706(2) | 3354(1) | 47(1) |
| N(7) | 9056(2) | 4684(2) | 2456(1) | 58(1) |
| N(8) | 9298(2) | 6938(2) | 3768(1) | 54(1) |
| C(1) | 2483(2) | 1746(2) | 280(1) | 51(1) |
| C(2) | 2643(2) | 2383(2) | -364(1) | 73(1) |
| C(3) | 1798(2) | 2308(2) | 740(2) | 69(1) |
| C(4) | 1707(2) | 394(2) | -62(1) | 62(1) |
| C(5) | 4644(2) | 1603(2) | 424(1) | 52(1) |
| C(6) | 5763(2) | 1544(2) | 1012(1) | 45(1) |
| C(7) | 6980(2) | 1628(2) | 1046(1) | 54(1) |
| C(8) | 7537(2) | 1404(2) | 1759(1) | 57(1) |
| C(9) | 6635(2) | 1205(2) | 2124(1) | 48(1) |
| C(10) | 6540(2) | 865(2) | 2851(1) | 56(1) |
| C(11) | 5084(2) | 620(2) | 3659(1) | 57(1) |
| C(12) | 4199(3) | 1202(3) | 3895(2) | 80(1) |
| C(13) | 4362(2) | -744(2) | 3352(1) | 70(1) |
| C(14) | 6259(3) | 879(3) | 4353(1) | 81(1) |
| C(15) | 2522(2) | -1279(2) | 1357(1) | 45(1) |
| C(16) | 3551(2) | -1573(2) | 1253(1) | 59(1) |
| C(17) | 3409(3) | -2735(2) | 903(2) | 75(1) |
| C(18) | 2217(3) | -3638(2) | 627(2) | 83(1) |
| C(19) | 1193(3) | -3373(2) | 713(2) | 84(1) |

| | | | | |
|---|---|---|---|---|
| C(20) | 1321(2) | -2220(2) | 1074(1) | 67(1) |
| C(21) | 1593(2) | -12(2) | 1951(1) | 60(1) |
| C(22) | 6140(2) | 6397(2) | 4071(1) | 59(1) |
| C(23) | 4733(2) | 6159(3) | 4009(2) | 82(1) |
| C(24) | 6857(2) | 7744(2) | 4201(1) | 72(1) |
| C(25) | 6744(3) | 5942(3) | 4738(1) | 87(1) |
| C(26) | 5476(2) | 5897(2) | 2637(1) | 54(1) |
| C(27) | 5866(2) | 5406(2) | 1999(1) | 46(1) |
| C(28) | 5367(2) | 5103(2) | 1217(1) | 56(1) |
| C(29) | 6271(2) | 4784(2) | 928(1) | 60(1) |
| C(30) | 7280(2) | 4908(2) | 1546(1) | 50(1) |
| C(31) | 8567(2) | 4821(2) | 1662(1) | 65(1) |
| C(32) | 10478(2) | 4875(3) | 2703(2) | 78(1) |
| C(33) | 11266(2) | 6229(3) | 2839(2) | 91(1) |
| C(34) | 10775(3) | 4454(3) | 3440(2) | 102(1) |
| C(35) | 10796(3) | 4122(3) | 2091(2) | 107(1) |
| C(36) | 9505(2) | 8062(2) | 3587(1) | 49(1) |
| C(37) | 8823(2) | 8161(2) | 2879(1) | 58(1) |
| C(38) | 8950(2) | 9262(2) | 2702(1) | 65(1) |
| C(39) | 9785(3) | 10322(2) | 3212(2) | 72(1) |
| C(40) | 10486(3) | 10253(2) | 3897(2) | 83(1) |
| C(41) | 10379(2) | 9159(2) | 4094(2) | 73(1) |
| C(42) | 10096(2) | 6972(2) | 4533(1) | 78(1) |

Table 3. Bond lengths [Å] and angles [°] for bi1531_0m.

| | |
|---|---|
| Cl(1)-Al(1) | 2.1748(8) |
| Cl(2)-Al(2) | 2.1710(9) |
| Al(1)-N(4) | 1.8259(16) |
| Al(1)-N(1) | 1.8273(17) |
| Al(1)-N(2) | 2.2584(17) |
| Al(1)-N(3) | 2.3018(17) |
| Al(2)-N(5) | 1.8240(17) |
| Al(2)-N(8) | 1.8275(17) |
| Al(2)-N(7) | 2.264(2) |
| Al(2)-N(6) | 2.3064(18) |
| N(1)-C(6) | 1.366(2) |
| N(1)-C(9) | 1.369(2) |
| N(2)-C(5) | 1.496(3) |
| N(2)-C(1) | 1.515(2) |
| N(3)-C(10) | 1.489(3) |
| N(3)-C(11) | 1.509(3) |
| N(4)-C(15) | 1.395(2) |
| N(4)-C(21) | 1.465(3) |
| N(5)-C(30) | 1.367(3) |
| N(5)-C(27) | 1.367(2) |
| N(6)-C(26) | 1.488(3) |
| N(6)-C(22) | 1.515(3) |
| N(7)-C(31) | 1.492(3) |
| N(7)-C(32) | 1.522(3) |
| N(8)-C(36) | 1.393(3) |
| N(8)-C(42) | 1.472(3) |
| C(1)-C(3) | 1.524(3) |
| C(1)-C(4) | 1.526(3) |
| C(1)-C(2) | 1.528(3) |
| C(5)-C(6) | 1.492(3) |
| C(6)-C(7) | 1.363(3) |
| C(7)-C(8) | 1.421(3) |
| C(8)-C(9) | 1.365(3) |
| C(9)-C(10) | 1.489(3) |

| | |
|---|---|
| C(11)-C(12) | 1.518(3) |
| C(11)-C(13) | 1.524(3) |
| C(11)-C(14) | 1.528(3) |
| C(15)-C(16) | 1.390(3) |
| C(15)-C(20) | 1.400(3) |
| C(16)-C(17) | 1.386(3) |
| C(17)-C(18) | 1.373(4) |
| C(18)-C(19) | 1.357(4) |
| C(19)-C(20) | 1.387(4) |
| C(22)-C(24) | 1.515(3) |
| C(22)-C(25) | 1.518(3) |
| C(22)-C(23) | 1.533(3) |
| C(26)-C(27) | 1.483(3) |
| C(27)-C(28) | 1.368(3) |
| C(28)-C(29) | 1.414(3) |
| C(29)-C(30) | 1.364(3) |
| C(30)-C(31) | 1.486(3) |
| C(32)-C(34) | 1.520(4) |
| C(32)-C(35) | 1.539(4) |
| C(32)-C(33) | 1.536(4) |
| C(36)-C(37) | 1.394(3) |
| C(36)-C(41) | 1.402(3) |
| C(37)-C(38) | 1.372(3) |
| C(38)-C(39) | 1.366(3) |
| C(39)-C(40) | 1.353(4) |
| C(40)-C(41) | 1.383(4) |

| | |
|---|---|
| N(4)-Al(1)-N(1) | 125.46(8) |
| N(4)-Al(1)-Cl(1) | 112.71(6) |
| N(1)-Al(1)-Cl(1) | 121.76(6) |
| N(4)-Al(1)-N(2) | 104.70(7) |
| N(1)-Al(1)-N(2) | 78.24(7) |
| Cl(1)-Al(1)-N(2) | 90.90(5) |
| N(4)-Al(1)-N(3) | 102.39(7) |
| N(1)-Al(1)-N(3) | 76.85(7) |
| Cl(1)-Al(1)-N(3) | 89.07(5) |

| | |
|---|---|
| N(2)-Al(1)-N(3) | 150.59(6) |
| N(5)-Al(2)-N(8) | 125.31(8) |
| N(5)-Al(2)-Cl(2) | 120.89(6) |
| N(8)-Al(2)-Cl(2) | 113.72(6) |
| N(5)-Al(2)-N(7) | 77.99(8) |
| N(8)-Al(2)-N(7) | 104.84(8) |
| Cl(2)-Al(2)-N(7) | 90.92(6) |
| N(5)-Al(2)-N(6) | 76.66(7) |
| N(8)-Al(2)-N(6) | 101.52(7) |
| Cl(2)-Al(2)-N(6) | 89.81(5) |
| N(7)-Al(2)-N(6) | 150.82(7) |
| C(6)-N(1)-C(9) | 107.92(16) |
| C(6)-N(1)-Al(1) | 124.92(13) |
| C(9)-N(1)-Al(1) | 126.88(14) |
| C(5)-N(2)-C(1) | 112.46(15) |
| C(5)-N(2)-Al(1) | 107.43(12) |
| C(1)-N(2)-Al(1) | 126.22(12) |
| C(10)-N(3)-C(11) | 113.79(16) |
| C(10)-N(3)-Al(1) | 108.11(12) |
| C(11)-N(3)-Al(1) | 126.27(13) |
| C(15)-N(4)-C(21) | 114.49(16) |
| C(15)-N(4)-Al(1) | 125.72(13) |
| C(21)-N(4)-Al(1) | 119.73(13) |
| C(30)-N(5)-C(27) | 108.08(17) |
| C(30)-N(5)-Al(2) | 125.34(14) |
| C(27)-N(5)-Al(2) | 126.55(14) |
| C(26)-N(6)-C(22) | 113.17(16) |
| C(26)-N(6)-Al(2) | 108.15(12) |
| C(22)-N(6)-Al(2) | 126.69(12) |
| C(31)-N(7)-C(32) | 112.95(19) |
| C(31)-N(7)-Al(2) | 107.36(13) |
| C(32)-N(7)-Al(2) | 125.23(16) |
| C(36)-N(8)-C(42) | 115.02(17) |
| C(36)-N(8)-Al(2) | 125.54(13) |
| C(42)-N(8)-Al(2) | 119.26(15) |
| N(2)-C(1)-C(3) | 107.21(16) |

| | |
|---|---|
| N(2)-C(1)-C(4) | 109.24(17) |
| C(3)-C(1)-C(4) | 110.06(19) |
| N(2)-C(1)-C(2) | 111.19(17) |
| C(3)-C(1)-C(2) | 109.6(2) |
| C(4)-C(1)-C(2) | 109.55(18) |
| C(6)-C(5)-N(2) | 107.81(16) |
| C(7)-C(6)-N(1) | 109.48(18) |
| C(7)-C(6)-C(5) | 135.18(19) |
| N(1)-C(6)-C(5) | 115.26(17) |
| C(6)-C(7)-C(8) | 106.56(19) |
| C(9)-C(8)-C(7) | 107.15(19) |
| C(8)-C(9)-N(1) | 108.88(19) |
| C(8)-C(9)-C(10) | 136.0(2) |
| N(1)-C(9)-C(10) | 115.03(18) |
| N(3)-C(10)-C(9) | 108.51(16) |
| N(3)-C(11)-C(12) | 107.68(18) |
| N(3)-C(11)-C(13) | 109.59(17) |
| C(12)-C(11)-C(13) | 109.2(2) |
| N(3)-C(11)-C(14) | 110.76(19) |
| C(12)-C(11)-C(14) | 109.2(2) |
| C(13)-C(11)-C(14) | 110.4(2) |
| C(16)-C(15)-N(4) | 121.21(17) |
| C(16)-C(15)-C(20) | 116.20(19) |
| N(4)-C(15)-C(20) | 122.6(2) |
| C(17)-C(16)-C(15) | 122.3(2) |
| C(18)-C(17)-C(16) | 120.2(3) |
| C(19)-C(18)-C(17) | 118.8(2) |
| C(18)-C(19)-C(20) | 121.8(2) |
| C(19)-C(20)-C(15) | 120.8(2) |
| N(6)-C(22)-C(24) | 110.06(19) |
| N(6)-C(22)-C(25) | 107.47(19) |
| C(24)-C(22)-C(25) | 109.7(2) |
| N(6)-C(22)-C(23) | 110.71(18) |
| C(24)-C(22)-C(23) | 109.9(2) |
| C(25)-C(22)-C(23) | 108.9(2) |
| C(27)-C(26)-N(6) | 107.93(16) |

| | |
|---|---|
| N(5)-C(27)-C(28) | 108.76(19) |
| N(5)-C(27)-C(26) | 115.98(16) |
| C(28)-C(27)-C(26) | 135.1(2) |
| C(27)-C(28)-C(29) | 107.15(19) |
| C(30)-C(29)-C(28) | 106.85(19) |
| C(29)-C(30)-N(5) | 109.2(2) |
| C(29)-C(30)-C(31) | 135.6(2) |
| N(5)-C(30)-C(31) | 115.11(18) |
| C(30)-C(31)-N(7) | 108.44(18) |
| C(34)-C(32)-N(7) | 107.0(2) |
| C(34)-C(32)-C(35) | 109.2(3) |
| N(7)-C(32)-C(35) | 110.9(2) |
| C(34)-C(32)-C(33) | 110.6(3) |
| N(7)-C(32)-C(33) | 109.3(2) |
| C(35)-C(32)-C(33) | 109.7(2) |
| N(8)-C(36)-C(37) | 121.08(18) |
| N(8)-C(36)-C(41) | 123.4(2) |
| C(37)-C(36)-C(41) | 115.5(2) |
| C(38)-C(37)-C(36) | 122.4(2) |
| C(39)-C(38)-C(37) | 121.1(2) |
| C(40)-C(39)-C(38) | 117.9(2) |
| C(39)-C(40)-C(41) | 122.4(2) |
| C(40)-C(41)-C(36) | 120.7(2) |

---

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for bi1531_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Cl(1) | 62(1) | 44(1) | 54(1) | 3(1) | 15(1) | 21(1) |
| Cl(2) | 62(1) | 56(1) | 66(1) | 25(1) | 12(1) | 20(1) |
| Al(1) | 42(1) | 37(1) | 48(1) | 6(1) | 16(1) | 12(1) |
| Al(2) | 46(1) | 45(1) | 43(1) | 10(1) | 2(1) | 12(1) |
| N(1) | 42(1) | 45(1) | 46(1) | 13(1) | 14(1) | 16(1) |
| N(2) | 43(1) | 41(1) | 44(1) | 10(1) | 11(1) | 15(1) |
| N(3) | 50(1) | 44(1) | 44(1) | 12(1) | 12(1) | 15(1) |
| N(4) | 42(1) | 40(1) | 49(1) | 9(1) | 17(1) | 12(1) |
| N(5) | 49(1) | 44(1) | 39(1) | 3(1) | 8(1) | 16(1) |
| N(6) | 47(1) | 46(1) | 41(1) | 5(1) | 8(1) | 16(1) |
| N(7) | 54(1) | 53(1) | 72(1) | 17(1) | 23(1) | 22(1) |
| N(8) | 47(1) | 53(1) | 46(1) | 9(1) | -4(1) | 10(1) |
| C(1) | 48(1) | 55(1) | 48(1) | 14(1) | 8(1) | 20(1) |
| C(2) | 70(2) | 80(2) | 62(2) | 33(1) | 6(1) | 23(1) |
| C(3) | 61(1) | 75(2) | 75(2) | 15(1) | 12(1) | 39(1) |
| C(4) | 50(1) | 60(1) | 63(1) | 8(1) | 6(1) | 15(1) |
| C(5) | 53(1) | 56(1) | 46(1) | 15(1) | 20(1) | 17(1) |
| C(6) | 48(1) | 39(1) | 48(1) | 9(1) | 20(1) | 14(1) |
| C(7) | 55(1) | 52(1) | 62(1) | 17(1) | 30(1) | 20(1) |
| C(8) | 46(1) | 57(1) | 75(2) | 18(1) | 23(1) | 26(1) |
| C(9) | 44(1) | 46(1) | 55(1) | 13(1) | 12(1) | 18(1) |
| C(10) | 52(1) | 60(1) | 59(1) | 22(1) | 12(1) | 24(1) |
| C(11) | 62(1) | 60(1) | 42(1) | 18(1) | 12(1) | 16(1) |
| C(12) | 102(2) | 98(2) | 60(2) | 29(2) | 42(2) | 43(2) |
| C(13) | 74(2) | 65(2) | 61(2) | 27(1) | 16(1) | 13(1) |
| C(14) | 83(2) | 89(2) | 51(1) | 25(1) | 3(1) | 15(2) |
| C(15) | 51(1) | 40(1) | 38(1) | 11(1) | 13(1) | 10(1) |
| C(16) | 62(1) | 42(1) | 72(2) | 10(1) | 30(1) | 13(1) |
| C(17) | 96(2) | 52(1) | 86(2) | 14(1) | 49(2) | 26(1) |
| C(18) | 113(2) | 43(1) | 85(2) | 0(1) | 45(2) | 12(2) |
| C(19) | 83(2) | 50(2) | 88(2) | -6(1) | 22(2) | -4(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(20) | 57(1) | 51(1) | 74(2) | 5(1) | 14(1) | 5(1) |
| C(21) | 48(1) | 62(1) | 69(2) | 12(1) | 24(1) | 16(1) |
| C(22) | 58(1) | 67(2) | 50(1) | 5(1) | 20(1) | 24(1) |
| C(23) | 70(2) | 96(2) | 80(2) | 6(2) | 34(1) | 25(2) |
| C(24) | 71(2) | 69(2) | 61(2) | -11(1) | 18(1) | 22(1) |
| C(25) | 108(2) | 116(2) | 46(1) | 20(2) | 27(1) | 50(2) |
| C(26) | 52(1) | 54(1) | 50(1) | 6(1) | 6(1) | 24(1) |
| C(27) | 47(1) | 41(1) | 43(1) | 7(1) | 4(1) | 14(1) |
| C(28) | 66(1) | 47(1) | 42(1) | 12(1) | -2(1) | 18(1) |
| C(29) | 84(2) | 50(1) | 37(1) | 11(1) | 13(1) | 19(1) |
| C(30) | 65(1) | 41(1) | 43(1) | 8(1) | 19(1) | 15(1) |
| C(31) | 69(2) | 64(2) | 63(2) | 11(1) | 30(1) | 22(1) |
| C(32) | 55(1) | 80(2) | 109(2) | 29(2) | 32(2) | 31(1) |
| C(33) | 53(1) | 83(2) | 127(3) | 24(2) | 26(2) | 16(1) |
| C(34) | 64(2) | 123(3) | 135(3) | 60(2) | 26(2) | 50(2) |
| C(35) | 84(2) | 101(2) | 159(3) | 25(2) | 63(2) | 48(2) |
| C(36) | 41(1) | 47(1) | 50(1) | 4(1) | 9(1) | 12(1) |
| C(37) | 60(1) | 49(1) | 50(1) | 7(1) | 6(1) | 11(1) |
| C(38) | 68(2) | 57(1) | 62(1) | 16(1) | 13(1) | 17(1) |
| C(39) | 79(2) | 49(1) | 80(2) | 14(1) | 20(1) | 19(1) |
| C(40) | 84(2) | 50(1) | 81(2) | -4(1) | 2(2) | 8(1) |
| C(41) | 66(2) | 57(2) | 64(2) | 2(1) | -6(1) | 9(1) |
| C(42) | 69(2) | 74(2) | 61(2) | 16(1) | -15(1) | 15(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for bi1531_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 4193 | 2806 | 1057 | 53 |
| H(3) | 5829 | 2023 | 3222 | 56 |
| H(6) | 5852 | 4882 | 3317 | 56 |
| H(7B) | 8629 | 3858 | 2430 | 70 |
| H(2A) | 2987 | 1958 | -696 | 110 |
| H(2B) | 3237 | 3224 | -143 | 110 |
| H(2C) | 1808 | 2375 | -664 | 110 |
| H(3A) | 2307 | 3173 | 960 | 104 |
| H(3B) | 1697 | 1899 | 1152 | 104 |
| H(3C) | 952 | 2213 | 403 | 104 |
| H(4A) | 1654 | -22 | 352 | 93 |
| H(4B) | 2130 | 51 | -380 | 93 |
| H(4C) | 841 | 287 | -376 | 93 |
| H(5A) | 4183 | 813 | 44 | 62 |
| H(5B) | 4938 | 2236 | 153 | 62 |
| H(7) | 7378 | 1802 | 667 | 64 |
| H(8) | 8379 | 1395 | 1947 | 68 |
| H(10A) | 6370 | -14 | 2794 | 67 |
| H(10B) | 7356 | 1319 | 3271 | 67 |
| H(12A) | 3438 | 1030 | 3453 | 121 |
| H(12B) | 4651 | 2082 | 4081 | 121 |
| H(12C) | 3934 | 870 | 4304 | 121 |
| H(13A) | 4926 | -1123 | 3193 | 104 |
| H(13B) | 3606 | -896 | 2912 | 104 |
| H(13C) | 4090 | -1091 | 3754 | 104 |
| H(14A) | 6728 | 1757 | 4533 | 121 |
| H(14B) | 6820 | 482 | 4207 | 121 |
| H(14C) | 5983 | 564 | 4763 | 121 |
| H(16) | 4380 | -956 | 1428 | 70 |
| H(17) | 4139 | -2908 | 855 | 90 |

| | | | | |
|---|---|---|---|---|
| H(18) | 2112 | -4434 | 380 | 100 |
| H(19) | 366 | -3994 | 522 | 101 |
| H(20) | 585 | -2068 | 1130 | 80 |
| H(21A) | 1390 | -563 | 2281 | 90 |
| H(21B) | 850 | -233 | 1490 | 90 |
| H(21C) | 1802 | 824 | 2227 | 90 |
| H(23A) | 4687 | 6542 | 4498 | 124 |
| H(23B) | 4261 | 5282 | 3887 | 124 |
| H(23C) | 4352 | 6502 | 3603 | 124 |
| H(24A) | 7767 | 7895 | 4273 | 107 |
| H(24B) | 6771 | 8185 | 4658 | 107 |
| H(24C) | 6498 | 8025 | 3755 | 107 |
| H(25A) | 7653 | 6116 | 4793 | 131 |
| H(25B) | 6301 | 5064 | 4642 | 131 |
| H(25C) | 6669 | 6353 | 5209 | 131 |
| H(26A) | 4548 | 5472 | 2541 | 64 |
| H(26B) | 5642 | 6774 | 2683 | 64 |
| H(28) | 4564 | 5107 | 924 | 68 |
| H(29) | 6190 | 4531 | 405 | 72 |
| H(31A) | 9163 | 5563 | 1590 | 78 |
| H(31B) | 8506 | 4113 | 1285 | 78 |
| H(33A) | 12183 | 6365 | 3037 | 136 |
| H(33B) | 11033 | 6709 | 3212 | 136 |
| H(33C) | 11085 | 6477 | 2355 | 136 |
| H(34A) | 10213 | 3609 | 3352 | 152 |
| H(34B) | 10630 | 4968 | 3841 | 152 |
| H(34C) | 11673 | 4514 | 3600 | 152 |
| H(35A) | 10199 | 3278 | 1948 | 160 |
| H(35B) | 11677 | 4149 | 2297 | 160 |
| H(35C) | 10714 | 4459 | 1638 | 160 |
| H(37) | 8250 | 7441 | 2505 | 69 |
| H(38) | 8449 | 9287 | 2217 | 78 |
| H(39) | 9870 | 11084 | 3089 | 86 |
| H(40) | 11073 | 10983 | 4256 | 100 |
| H(41) | 10902 | 9151 | 4577 | 87 |
| H(42A) | 9956 | 7513 | 4923 | 117 |

| | | | | |
|---|---|---|---|---|
| H(42B) | 11003 | 7273 | 4566 | 117 |
| H(42C) | 9860 | 6152 | 4620 | 117 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 7—ccdc-936569.

| | | |
|---|---|---|
| Identification code | compound 7—ccdc-936569 | |
| Empirical formula | C28 H40 Al N3 O2 | |
| Formula weight | 477.61 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 9.6058(17) Å | α= 90°. |
| | b = 27.908(5) Å | β= 104.168(12)°. |
| | c = 10.519(2) Å | γ = 90°. |
| Volume | 2734.2(9) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.160 $Mg/m^3$ | |
| Absorption coefficient | 0.102 $mm^{-1}$ | |
| F(000) | 1032 | |
| Crystal size | 0.45 x 0.35 x 0.30 $mm^3$ | |
| Theta range for data collection | 2.19 to 28.28°. | |
| Index ranges | -12<=h<=12, -37<=k<=37, -14<=l<=13 | |
| Reflections collected | 32096 | |
| Independent reflections | 6685 [R(int) = 0.0699] | |
| Completeness to theta = 28.28° | 98.6 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.970 and 0.958 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6685 / 0 / 315 | |
| Goodness-of-fit on $F^2$ | 1.004 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0607, wR2 = 0.1808 | |
| R indices (all data) | R1 = 0.1055, wR2 = 0.2063 | |
| Largest diff. peak and hole | 0.679 and -0.322 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for bi155_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 4948(1) | 1038(1) | 3928(1) | 43(1) |
| N(1) | 5347(2) | 852(1) | 5647(2) | 43(1) |
| N(2) | 6281(2) | 414(1) | 3834(2) | 44(1) |
| N(3) | 3727(2) | 1608(1) | 4985(2) | 52(1) |
| O(1) | 3474(2) | 809(1) | 2820(1) | 48(1) |
| O(2) | 5844(2) | 1489(1) | 3329(1) | 48(1) |
| C(15) | 2673(2) | 889(1) | 1593(2) | 41(1) |
| C(6) | 6275(2) | 486(1) | 6142(2) | 45(1) |
| C(20) | 1379(2) | 640(1) | 1161(2) | 45(1) |
| C(22) | 6492(2) | 1896(1) | 3854(2) | 41(1) |
| C(16) | 3070(3) | 1212(1) | 746(2) | 51(1) |
| C(5) | 6979(3) | 249(1) | 5194(2) | 52(1) |
| C(11) | 2396(3) | 1887(1) | 4399(2) | 51(1) |
| C(19) | 518(2) | 726(1) | -81(2) | 54(1) |
| C(18) | 894(3) | 1055(1) | -925(2) | 54(1) |
| C(9) | 4904(3) | 1056(1) | 6664(2) | 50(1) |
| C(23) | 7349(2) | 1914(1) | 5123(2) | 52(1) |
| C(27) | 6330(3) | 2310(1) | 3121(2) | 56(1) |
| C(17) | 2184(3) | 1295(1) | -494(2) | 56(1) |
| C(24) | 7956(3) | 2342(1) | 5642(2) | 61(1) |
| C(10) | 3837(3) | 1444(1) | 6344(2) | 60(1) |
| C(1) | 7249(3) | 379(1) | 2908(3) | 57(1) |
| C(8) | 5541(3) | 817(1) | 7797(2) | 62(1) |
| C(7) | 6403(3) | 456(1) | 7464(2) | 58(1) |
| C(26) | 6936(3) | 2738(1) | 3664(3) | 65(1) |
| C(25) | 7756(3) | 2760(1) | 4932(3) | 61(1) |
| C(4) | 6313(4) | 483(1) | 1539(3) | 79(1) |
| C(28) | 8396(4) | 3230(1) | 5526(4) | 98(1) |
| C(3) | 8456(3) | 747(1) | 3290(3) | 77(1) |
| C(2) | 7888(4) | -127(1) | 2941(3) | 78(1) |
| C(21) | -90(3) | 1160(1) | -2266(3) | 82(1) |

| | | | | |
|---|---|---|---|---|
| C(14) | 2563(4) | 2101(1) | 3141(3) | 86(1) |
| C(13) | 1161(3) | 1522(1) | 4070(3) | 83(1) |
| C(12) | 2065(4) | 2260(1) | 5320(4) | 90(1) |

Table 3. Bond lengths [Å] and angles [°] for bi155_0m.

| | |
|---|---|
| Al(1)-O(1) | 1.7215(14) |
| Al(1)-O(2) | 1.7277(16) |
| Al(1)-N(1) | 1.8294(18) |
| Al(1)-N(2) | 2.177(2) |
| Al(1)-N(3) | 2.406(2) |
| N(1)-C(9) | 1.368(3) |
| N(1)-C(6) | 1.373(3) |
| N(2)-C(1) | 1.506(3) |
| N(2)-C(5) | 1.496(3) |
| N(3)-C(10) | 1.480(3) |
| N(3)-C(11) | 1.494(3) |
| O(1)-C(15) | 1.350(2) |
| O(2)-C(22) | 1.349(2) |
| C(15)-C(16) | 1.384(3) |
| C(15)-C(20) | 1.399(3) |
| C(6)-C(7) | 1.368(3) |
| C(6)-C(5) | 1.488(4) |
| C(20)-C(19) | 1.385(3) |
| C(22)-C(27) | 1.377(3) |
| C(22)-C(23) | 1.387(3) |
| C(16)-C(17) | 1.391(3) |
| C(11)-C(14) | 1.497(4) |
| C(11)-C(12) | 1.509(4) |
| C(11)-C(13) | 1.536(4) |
| C(19)-C(18) | 1.385(4) |
| C(18)-C(17) | 1.385(4) |
| C(18)-C(21) | 1.522(3) |
| C(9)-C(8) | 1.371(3) |
| C(9)-C(10) | 1.473(3) |
| C(23)-C(24) | 1.381(3) |
| C(27)-C(26) | 1.388(3) |
| C(24)-C(25) | 1.373(4) |
| C(1)-C(4) | 1.528(3) |
| C(1)-C(2) | 1.536(4) |

| | |
|---|---|
| C(1)-C(3) | 1.528(4) |
| C(8)-C(7) | 1.401(4) |
| C(26)-C(25) | 1.374(4) |
| C(25)-C(28) | 1.519(4) |

| | |
|---|---|
| O(1)-Al(1)-O(2) | 115.12(8) |
| O(1)-Al(1)-N(1) | 120.15(9) |
| O(2)-Al(1)-N(1) | 124.35(8) |
| O(1)-Al(1)-N(2) | 93.88(7) |
| O(2)-Al(1)-N(2) | 102.38(8) |
| N(1)-Al(1)-N(2) | 80.49(8) |
| O(1)-Al(1)-N(3) | 98.39(8) |
| O(2)-Al(1)-N(3) | 91.68(8) |
| N(1)-Al(1)-N(3) | 74.84(8) |
| N(2)-Al(1)-N(3) | 155.33(7) |
| C(9)-N(1)-C(6) | 108.07(17) |
| C(9)-N(1)-Al(1) | 128.70(15) |
| C(6)-N(1)-Al(1) | 123.06(16) |
| C(1)-N(2)-C(5) | 113.28(18) |
| C(1)-N(2)-Al(1) | 123.05(14) |
| C(5)-N(2)-Al(1) | 109.49(14) |
| C(10)-N(3)-C(11) | 114.3(2) |
| C(10)-N(3)-Al(1) | 108.26(14) |
| C(11)-N(3)-Al(1) | 128.16(14) |
| C(15)-O(1)-Al(1) | 140.06(14) |
| C(22)-O(2)-Al(1) | 133.33(14) |
| O(1)-C(15)-C(16) | 122.81(18) |
| O(1)-C(15)-C(20) | 118.7(2) |
| C(16)-C(15)-C(20) | 118.47(18) |
| C(7)-C(6)-N(1) | 108.6(2) |
| C(7)-C(6)-C(5) | 135.4(2) |
| N(1)-C(6)-C(5) | 115.80(18) |
| C(19)-C(20)-C(15) | 119.8(2) |
| O(2)-C(22)-C(27) | 120.07(18) |
| O(2)-C(22)-C(23) | 121.99(19) |
| C(27)-C(22)-C(23) | 117.9(2) |

| | |
|---|---|
| C(15)-C(16)-C(17) | 120.7(2) |
| C(6)-C(5)-N(2) | 109.49(17) |
| N(3)-C(11)-C(14) | 107.9(2) |
| N(3)-C(11)-C(12) | 112.8(2) |
| C(14)-C(11)-C(12) | 112.1(3) |
| N(3)-C(11)-C(13) | 106.5(2) |
| C(14)-C(11)-C(13) | 108.1(2) |
| C(12)-C(11)-C(13) | 109.3(3) |
| C(18)-C(19)-C(20) | 122.1(2) |
| C(17)-C(18)-C(19) | 117.61(19) |
| C(17)-C(18)-C(21) | 120.9(2) |
| C(19)-C(18)-C(21) | 121.5(2) |
| N(1)-C(9)-C(8) | 108.6(2) |
| N(1)-C(9)-C(10) | 117.32(18) |
| C(8)-C(9)-C(10) | 133.9(2) |
| C(24)-C(23)-C(22) | 120.3(2) |
| C(22)-C(27)-C(26) | 120.8(2) |
| C(18)-C(17)-C(16) | 121.3(2) |
| C(25)-C(24)-C(23) | 122.0(2) |
| C(9)-C(10)-N(3) | 109.3(2) |
| N(2)-C(1)-C(4) | 106.5(2) |
| N(2)-C(1)-C(2) | 110.7(2) |
| C(4)-C(1)-C(2) | 109.6(2) |
| N(2)-C(1)-C(3) | 109.5(2) |
| C(4)-C(1)-C(3) | 110.7(3) |
| C(2)-C(1)-C(3) | 109.8(2) |
| C(9)-C(8)-C(7) | 107.3(2) |
| C(6)-C(7)-C(8) | 107.43(19) |
| C(25)-C(26)-C(27) | 121.3(2) |
| C(26)-C(25)-C(24) | 117.5(2) |
| C(26)-C(25)-C(28) | 121.0(3) |
| C(24)-C(25)-C(28) | 121.5(2) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for bi155_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 48(1) | 41(1) | 36(1) | 6(1) | 4(1) | -10(1) |
| N(1) | 50(1) | 40(1) | 37(1) | 3(1) | 8(1) | 0(1) |
| N(2) | 44(1) | 40(1) | 48(1) | -1(1) | 10(1) | -5(1) |
| N(3) | 64(1) | 52(1) | 42(1) | 4(1) | 15(1) | 10(1) |
| O(1) | 50(1) | 49(1) | 37(1) | 2(1) | -1(1) | -8(1) |
| O(2) | 61(1) | 42(1) | 43(1) | -1(1) | 14(1) | -13(1) |
| C(15) | 44(1) | 40(1) | 38(1) | -5(1) | 5(1) | 3(1) |
| C(6) | 45(1) | 40(1) | 45(1) | 6(1) | 1(1) | -5(1) |
| C(20) | 41(1) | 44(1) | 49(1) | -2(1) | 8(1) | 1(1) |
| C(22) | 41(1) | 41(1) | 43(1) | 1(1) | 13(1) | -7(1) |
| C(16) | 53(1) | 54(1) | 44(1) | 0(1) | 8(1) | -8(1) |
| C(5) | 52(1) | 45(1) | 56(1) | 5(1) | 6(1) | 5(1) |
| C(11) | 51(1) | 54(1) | 49(1) | 0(1) | 12(1) | 5(1) |
| C(19) | 42(1) | 60(2) | 53(1) | -10(1) | -1(1) | 2(1) |
| C(18) | 55(1) | 62(2) | 39(1) | -4(1) | 1(1) | 14(1) |
| C(9) | 61(1) | 50(1) | 36(1) | 1(1) | 9(1) | -3(1) |
| C(23) | 55(1) | 52(1) | 45(1) | 7(1) | 4(1) | -4(1) |
| C(27) | 63(1) | 53(1) | 46(1) | 11(1) | 4(1) | -16(1) |
| C(17) | 68(1) | 60(2) | 41(1) | 5(1) | 15(1) | 3(1) |
| C(24) | 58(1) | 69(2) | 50(1) | -4(1) | 3(1) | -17(1) |
| C(10) | 75(2) | 67(2) | 40(1) | 1(1) | 19(1) | 11(1) |
| C(1) | 56(1) | 57(2) | 63(1) | -3(1) | 25(1) | 1(1) |
| C(8) | 82(2) | 66(2) | 35(1) | 5(1) | 9(1) | 2(1) |
| C(7) | 66(1) | 56(2) | 45(1) | 14(1) | -1(1) | 0(1) |
| C(26) | 77(2) | 45(1) | 70(2) | 10(1) | 14(1) | -13(1) |
| C(25) | 63(2) | 55(2) | 65(2) | -12(1) | 19(1) | -17(1) |
| C(4) | 91(2) | 102(2) | 51(2) | 0(1) | 31(2) | 15(2) |
| C(28) | 127(3) | 72(2) | 95(2) | -23(2) | 23(2) | -46(2) |
| C(3) | 60(2) | 74(2) | 108(2) | 2(2) | 40(2) | -9(1) |
| C(2) | 83(2) | 66(2) | 93(2) | -8(2) | 37(2) | 14(2) |
| C(21) | 78(2) | 106(3) | 50(1) | 5(1) | -9(1) | 14(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(14) | 95(2) | 93(2) | 74(2) | 32(2) | 25(2) | 33(2) |
| C(13) | 59(2) | 104(3) | 85(2) | -12(2) | 13(2) | -9(2) |
| C(12) | 105(3) | 72(2) | 92(2) | -7(2) | 24(2) | 23(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for bi155_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2D) | 5606 | 176 | 3531 | 53 |
| H(3D) | 4399 | 1855 | 5142 | 63 |
| H(20) | 1092 | 412 | 1717 | 55 |
| H(16) | 3958 | 1378 | 1013 | 61 |
| H(5A) | 6889 | -103 | 5252 | 62 |
| H(5B) | 8013 | 331 | 5411 | 62 |
| H(19) | -357 | 555 | -362 | 65 |
| H(23) | 7520 | 1630 | 5637 | 63 |
| H(27) | 5796 | 2304 | 2232 | 67 |
| H(17) | 2470 | 1522 | -1055 | 67 |
| H(24) | 8529 | 2347 | 6517 | 73 |
| H(10A) | 4130 | 1714 | 6962 | 72 |
| H(10B) | 2891 | 1327 | 6429 | 72 |
| H(8) | 5421 | 884 | 8649 | 74 |
| H(7) | 6971 | 232 | 8049 | 70 |
| H(26) | 6781 | 3022 | 3149 | 78 |
| H(4A) | 6048 | 822 | 1473 | 118 |
| H(4B) | 5443 | 286 | 1382 | 118 |
| H(4C) | 6849 | 406 | 883 | 118 |
| H(28A) | 9422 | 3187 | 5928 | 148 |
| H(28B) | 7909 | 3333 | 6196 | 148 |
| H(28C) | 8272 | 3474 | 4838 | 148 |
| H(3A) | 9067 | 666 | 4155 | 116 |
| H(3B) | 8043 | 1067 | 3322 | 116 |
| H(3C) | 9033 | 744 | 2640 | 116 |
| H(2A) | 7116 | -365 | 2824 | 117 |
| H(2B) | 8574 | -179 | 3787 | 117 |
| H(2C) | 8382 | -160 | 2234 | 117 |
| H(21A) | -1093 | 1138 | -2216 | 124 |
| H(21B) | 88 | 926 | -2903 | 124 |

| | | | | |
|---|---|---|---|---|
| H(21C) | 103 | 1483 | -2543 | 124 |
| H(14A) | 2770 | 1847 | 2571 | 130 |
| H(14B) | 3356 | 2332 | 3327 | 130 |
| H(14C) | 1673 | 2265 | 2702 | 130 |
| H(13A) | 1087 | 1357 | 4873 | 125 |
| H(13B) | 1351 | 1288 | 3440 | 125 |
| H(13C) | 259 | 1689 | 3689 | 125 |
| H(12A) | 2852 | 2493 | 5535 | 134 |
| H(12B) | 1957 | 2105 | 6126 | 134 |
| H(12C) | 1171 | 2426 | 4898 | 134 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 8—ccdc-936570.

| | | |
|---|---|---|
| Identification code | compound 8—ccdc-936570 | |
| Empirical formula | C20 H42 Al N5 | |
| Formula weight | 379.57 | |
| Temperature | 150(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 33.541(4) Å | α= 90°. |
| | b = 10.5578(13) Å | β= 102.422(8)°. |
| | c = 28.080(4) Å | γ = 90°. |
| Volume | 9711(2) $Å^3$ | |
| Z | 16 | |
| Density (calculated) | 1.038 $Mg/m^3$ | |
| Absorption coefficient | 0.096 $mm^{-1}$ | |
| F(000) | 3264 | |
| Crystal size | 0.25 x 0.20 x 0.20 $mm^3$ | |
| Theta range for data collection | 1.87 to 28.76°. | |
| Index ranges | -45<=h<=45, -14<=k<=14, -37<=l<=28 | |
| Reflections collected | 136674 | |
| Independent reflections | 25097 [R(int) = 0.2407] | |
| Completeness to theta = 28.76° | 99.4 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.927 and 0.913 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 25097 / 0 / 981 | |
| Goodness-of-fit on $F^2$ | 0.876 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0711, wR2 = 0.1619 | |
| R indices (all data) | R1 = 0.1817, wR2 = 0.2140 | |
| Largest diff. peak and hole | 0.675 and -0.537 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei368_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 3758(1) | 6947(1) | 3016(1) | 27(1) |
| Al(4) | 3836(1) | 8157(1) | 603(1) | 28(1) |
| Al(2) | 1222(1) | 1837(1) | 1226(1) | 27(1) |
| Al(3) | 1188(1) | 1902(1) | 8684(1) | 26(1) |
| N(1) | 3682(1) | 5815(2) | 3499(1) | 30(1) |
| N(4) | 3327(1) | 7701(2) | 2631(1) | 31(1) |
| N(5) | 3884(1) | 5754(2) | 2523(1) | 32(1) |
| N(2) | 4164(1) | 7722(2) | 3447(1) | 33(1) |
| N(3) | 3320(1) | 3701(2) | 2740(1) | 40(1) |
| N(6) | 1426(1) | 3155(2) | 1651(1) | 30(1) |
| N(20) | 4294(1) | 7969(2) | 380(1) | 33(1) |
| N(11) | 1246(1) | 724(2) | 9187(1) | 26(1) |
| N(14) | 1632(1) | 2605(2) | 8532(1) | 31(1) |
| N(10) | 1616(1) | 1820(2) | 790(1) | 33(1) |
| N(15) | 1047(1) | 792(2) | 8106(1) | 30(1) |
| N(7) | 1301(1) | 735(2) | 1732(1) | 31(1) |
| N(17) | 3720(1) | 9291(2) | 1038(1) | 32(1) |
| N(16) | 3640(1) | 6845(2) | 934(1) | 33(1) |
| N(13) | 1539(1) | -1412(2) | 8589(1) | 35(1) |
| N(19) | 3464(1) | 8057(2) | -48(1) | 35(1) |
| N(12) | 797(1) | 2713(2) | 8921(1) | 31(1) |
| N(9) | 774(1) | 2079(2) | 758(1) | 32(1) |
| N(8) | 1678(1) | 4804(3) | 821(1) | 45(1) |
| N(18) | 3475(1) | 5108(3) | -6(1) | 55(1) |
| C(6) | 3973(1) | 5990(3) | 3918(1) | 34(1) |
| C(13) | 2987(1) | 8461(3) | 2732(1) | 37(1) |
| C(9) | 3478(1) | 4707(3) | 3551(1) | 36(1) |
| C(5) | 4253(1) | 7113(3) | 3927(1) | 40(1) |
| C(8) | 3638(1) | 4201(3) | 4000(1) | 45(1) |
| C(17) | 4295(1) | 5202(3) | 2505(1) | 39(1) |
| C(1) | 4397(1) | 8895(3) | 3416(1) | 44(1) |

| | | | | |
|---|---|---|---|---|
| C(10) | 3154(1) | 4237(3) | 3146(1) | 41(1) |
| C(15) | 2881(1) | 9518(3) | 2358(2) | 50(1) |
| C(18) | 4489(1) | 4710(3) | 3007(2) | 52(1) |
| C(11) | 3526(1) | 2500(3) | 2892(2) | 62(1) |
| C(4) | 4275(1) | 9397(3) | 2900(1) | 50(1) |
| C(2) | 4292(1) | 9920(3) | 3761(2) | 55(1) |
| C(7) | 3956(1) | 5019(3) | 4239(1) | 43(1) |
| C(14) | 3114(1) | 9026(4) | 3237(2) | 62(1) |
| C(19) | 4229(1) | 4129(4) | 2131(2) | 57(1) |
| C(20) | 4552(1) | 6245(4) | 2348(2) | 59(1) |
| C(3) | 4856(1) | 8655(4) | 3543(2) | 58(1) |
| C(12) | 2988(1) | 3507(4) | 2314(2) | 62(1) |
| C(16) | 2611(1) | 7631(4) | 2708(2) | 72(1) |
| C(26) | 1580(1) | 2703(3) | 2109(1) | 32(1) |
| C(25) | 1505(1) | 1321(3) | 2193(1) | 39(1) |
| C(27) | 1791(1) | 3651(3) | 2391(1) | 40(1) |
| C(30) | 1428(1) | 5136(3) | 1177(1) | 41(1) |
| C(28) | 1765(1) | 4739(3) | 2089(1) | 39(1) |
| C(29) | 1542(1) | 4407(3) | 1642(1) | 36(1) |
| C(21) | 1148(1) | -560(3) | 1774(1) | 37(1) |
| C(24) | 996(1) | -1083(3) | 1260(1) | 48(1) |
| C(23) | 791(1) | -580(3) | 2032(2) | 54(1) |
| C(22) | 1483(1) | -1442(3) | 2050(2) | 54(1) |
| C(31) | 2087(1) | 5335(4) | 976(2) | 66(1) |
| C(32) | 1480(2) | 5292(4) | 343(2) | 76(1) |
| C(34) | 337(1) | 2777(3) | 1286(1) | 45(1) |
| C(37) | 2048(1) | 1302(3) | 903(1) | 41(1) |
| C(38) | 2274(1) | 1868(3) | 1380(1) | 49(1) |
| C(33) | 354(1) | 2439(3) | 770(1) | 38(1) |
| C(39) | 2027(1) | -138(3) | 940(2) | 57(1) |
| C(36) | 227(1) | 3582(4) | 436(2) | 57(1) |
| C(40) | 2247(1) | 1669(4) | 481(2) | 66(1) |
| C(35) | 62(1) | 1337(4) | 591(2) | 71(1) |
| C(46) | 975(1) | 957(3) | 9479(1) | 29(1) |
| C(53) | 1989(1) | 3246(3) | 8825(1) | 31(1) |
| C(48) | 1298(1) | -851(3) | 9732(1) | 37(1) |

| | | | | |
|---|---|---|---|---|
| C(49) | 1442(1) | -399(2) | 9344(1) | 31(1) |
| C(41) | 583(1) | 3933(3) | 8791(1) | 34(1) |
| C(47) | 1000(1) | 13(3) | 9822(1) | 36(1) |
| C(42) | 720(1) | 4935(3) | 9188(1) | 40(1) |
| C(50) | 1737(1) | -948(3) | 9077(1) | 32(1) |
| C(44) | 698(1) | 4424(3) | 8328(1) | 42(1) |
| C(43) | 120(1) | 3768(3) | 8703(1) | 45(1) |
| C(45) | 708(1) | 2108(3) | 9354(1) | 40(1) |
| C(52) | 1845(1) | -1691(3) | 8302(1) | 50(1) |
| C(54) | 1893(1) | 3711(6) | 9289(2) | 105(2) |
| C(51) | 1302(1) | -2550(3) | 8637(2) | 56(1) |
| C(55) | 2090(2) | 4399(4) | 8561(2) | 105(2) |
| C(56) | 2348(1) | 2390(5) | 8916(3) | 139(3) |
| C(57) | 633(1) | 304(3) | 7852(1) | 40(1) |
| C(60) | 691(1) | -717(4) | 7491(2) | 60(1) |
| C(59) | 426(1) | -236(4) | 8241(2) | 54(1) |
| C(58) | 384(1) | 1398(3) | 7590(2) | 57(1) |
| C(66) | 3439(1) | 7326(3) | 1270(1) | 35(1) |
| C(67) | 3209(1) | 6388(3) | 1421(1) | 42(1) |
| C(65) | 3497(1) | 8730(3) | 1382(1) | 40(1) |
| C(63) | 4228(1) | 10595(3) | 1603(2) | 53(1) |
| C(68) | 3272(1) | 5274(3) | 1161(1) | 45(1) |
| C(70) | 3691(1) | 4830(3) | 500(2) | 51(1) |
| C(61) | 3872(1) | 10586(3) | 1162(1) | 40(1) |
| C(69) | 3534(1) | 5583(3) | 865(1) | 39(1) |
| C(64) | 4021(1) | 11120(3) | 725(2) | 53(1) |
| C(62) | 3531(1) | 11454(3) | 1263(2) | 56(1) |
| C(71) | 3076(1) | 4490(5) | -98(2) | 87(2) |
| C(72) | 3711(2) | 4644(5) | -350(2) | 91(2) |
| C(73) | 3028(1) | 8514(4) | -192(1) | 52(1) |
| C(76) | 3021(1) | 9943(4) | -120(2) | 71(1) |
| C(75) | 2872(1) | 8181(5) | -724(2) | 68(1) |
| C(74) | 2780(1) | 7842(5) | 135(2) | 72(1) |
| C(78) | 4726(1) | 7244(3) | 1131(1) | 46(1) |
| C(77) | 4718(1) | 7684(3) | 615(1) | 42(1) |
| C(80) | 4877(1) | 6633(5) | 330(2) | 83(2) |

| | | | | |
|---|---|---|---|---|
| C(79) | 4985(1) | 8873(5) | 638(2) | 87(2) |

Table 3. Bond lengths [Å] and angles [°] for pei368_0m.

| | |
|---|---|
| Al(1)-N(4) | 1.793(2) |
| Al(1)-N(2) | 1.813(3) |
| Al(1)-N(1) | 1.867(3) |
| Al(1)-N(5) | 1.984(3) |
| Al(4)-N(20) | 1.792(2) |
| Al(4)-N(17) | 1.811(3) |
| Al(4)-N(16) | 1.864(3) |
| Al(4)-N(19) | 1.983(3) |
| Al(2)-N(9) | 1.788(3) |
| Al(2)-N(7) | 1.811(3) |
| Al(2)-N(6) | 1.866(3) |
| Al(2)-N(10) | 1.984(3) |
| Al(3)-N(14) | 1.795(2) |
| Al(3)-N(12) | 1.809(2) |
| Al(3)-N(11) | 1.863(3) |
| Al(3)-N(15) | 1.975(3) |
| N(1)-C(6) | 1.372(4) |
| N(1)-C(9) | 1.378(3) |
| N(4)-C(13) | 1.472(4) |
| N(5)-C(17) | 1.507(4) |
| N(2)-C(5) | 1.465(4) |
| N(2)-C(1) | 1.477(4) |
| N(3)-C(12) | 1.462(4) |
| N(3)-C(11) | 1.465(4) |
| N(3)-C(10) | 1.484(4) |
| N(6)-C(26) | 1.365(4) |
| N(6)-C(29) | 1.379(4) |
| N(20)-C(77) | 1.465(4) |
| N(11)-C(46) | 1.370(4) |
| N(11)-C(49) | 1.379(3) |
| N(14)-C(53) | 1.464(4) |
| N(10)-C(37) | 1.517(3) |
| N(15)-C(57) | 1.509(4) |
| N(7)-C(25) | 1.466(4) |

| | |
|---|---|
| N(7)-C(21) | 1.475(4) |
| N(17)-C(65) | 1.468(4) |
| N(17)-C(61) | 1.474(4) |
| N(16)-C(66) | 1.371(4) |
| N(16)-C(69) | 1.382(4) |
| N(13)-C(51) | 1.463(4) |
| N(13)-C(52) | 1.464(4) |
| N(13)-C(50) | 1.474(4) |
| N(19)-C(73) | 1.510(4) |
| N(12)-C(45) | 1.460(4) |
| N(12)-C(41) | 1.480(3) |
| N(9)-C(33) | 1.468(3) |
| N(8)-C(32) | 1.458(5) |
| N(8)-C(31) | 1.461(4) |
| N(8)-C(30) | 1.477(4) |
| N(18)-C(72) | 1.458(5) |
| N(18)-C(71) | 1.463(5) |
| N(18)-C(70) | 1.478(5) |
| C(6)-C(7) | 1.373(4) |
| C(6)-C(5) | 1.509(4) |
| C(13)-C(14) | 1.513(5) |
| C(13)-C(15) | 1.519(4) |
| C(13)-C(16) | 1.525(4) |
| C(9)-C(8) | 1.368(5) |
| C(9)-C(10) | 1.481(5) |
| C(8)-C(7) | 1.425(5) |
| C(17)-C(18) | 1.513(5) |
| C(17)-C(20) | 1.520(5) |
| C(17)-C(19) | 1.528(5) |
| C(1)-C(4) | 1.515(5) |
| C(1)-C(3) | 1.526(5) |
| C(1)-C(2) | 1.543(5) |
| C(26)-C(27) | 1.373(4) |
| C(26)-C(25) | 1.508(4) |
| C(27)-C(28) | 1.420(5) |
| C(30)-C(29) | 1.493(5) |

| | |
|---|---|
| C(28)-C(29) | 1.361(5) |
| C(21)-C(24) | 1.525(5) |
| C(21)-C(23) | 1.526(5) |
| C(21)-C(22) | 1.537(4) |
| C(34)-C(33) | 1.506(5) |
| C(37)-C(38) | 1.513(5) |
| C(37)-C(39) | 1.526(5) |
| C(37)-C(40) | 1.530(5) |
| C(33)-C(36) | 1.531(5) |
| C(33)-C(35) | 1.534(5) |
| C(46)-C(47) | 1.375(4) |
| C(46)-C(45) | 1.506(4) |
| C(53)-C(56) | 1.481(5) |
| C(53)-C(54) | 1.492(5) |
| C(53)-C(55) | 1.502(5) |
| C(48)-C(49) | 1.369(4) |
| C(48)-C(47) | 1.414(4) |
| C(49)-C(50) | 1.483(4) |
| C(41)-C(44) | 1.526(5) |
| C(41)-C(43) | 1.531(4) |
| C(41)-C(42) | 1.532(4) |
| C(57)-C(58) | 1.518(4) |
| C(57)-C(60) | 1.520(5) |
| C(57)-C(59) | 1.527(5) |
| C(66)-C(67) | 1.377(4) |
| C(66)-C(65) | 1.518(4) |
| C(67)-C(68) | 1.424(5) |
| C(63)-C(61) | 1.527(5) |
| C(68)-C(69) | 1.372(5) |
| C(70)-C(69) | 1.481(5) |
| C(61)-C(64) | 1.530(5) |
| C(61)-C(62) | 1.538(4) |
| C(73)-C(75) | 1.515(5) |
| C(73)-C(76) | 1.523(5) |
| C(73)-C(74) | 1.536(5) |
| C(78)-C(77) | 1.518(5) |

| | |
|---|---|
| C(77)-C(80) | 1.529(5) |
| C(77)-C(79) | 1.534(5) |
| | |
| N(4)-Al(1)-N(2) | 126.53(12) |
| N(4)-Al(1)-N(1) | 120.27(11) |
| N(2)-Al(1)-N(1) | 90.18(12) |
| N(4)-Al(1)-N(5) | 97.30(12) |
| N(2)-Al(1)-N(5) | 120.66(11) |
| N(1)-Al(1)-N(5) | 100.58(11) |
| N(20)-Al(4)-N(17) | 129.27(12) |
| N(20)-Al(4)-N(16) | 120.83(11) |
| N(17)-Al(4)-N(16) | 90.36(12) |
| N(20)-Al(4)-N(19) | 95.10(12) |
| N(17)-Al(4)-N(19) | 118.30(11) |
| N(16)-Al(4)-N(19) | 101.56(12) |
| N(9)-Al(2)-N(7) | 128.70(12) |
| N(9)-Al(2)-N(6) | 119.85(11) |
| N(7)-Al(2)-N(6) | 90.28(12) |
| N(9)-Al(2)-N(10) | 96.55(12) |
| N(7)-Al(2)-N(10) | 118.31(11) |
| N(6)-Al(2)-N(10) | 101.62(11) |
| N(14)-Al(3)-N(12) | 126.57(12) |
| N(14)-Al(3)-N(11) | 119.92(11) |
| N(12)-Al(3)-N(11) | 90.17(11) |
| N(14)-Al(3)-N(15) | 96.61(11) |
| N(12)-Al(3)-N(15) | 121.25(11) |
| N(11)-Al(3)-N(15) | 101.24(11) |
| C(6)-N(1)-C(9) | 107.5(3) |
| C(6)-N(1)-Al(1) | 110.79(19) |
| C(9)-N(1)-Al(1) | 140.3(2) |
| C(13)-N(4)-Al(1) | 133.1(2) |
| C(17)-N(5)-Al(1) | 127.13(19) |
| C(5)-N(2)-C(1) | 114.7(2) |
| C(5)-N(2)-Al(1) | 113.09(18) |
| C(1)-N(2)-Al(1) | 132.0(2) |
| C(12)-N(3)-C(11) | 110.3(3) |

| | |
|---|---|
| C(12)-N(3)-C(10) | 109.6(3) |
| C(11)-N(3)-C(10) | 109.7(3) |
| C(26)-N(6)-C(29) | 107.6(3) |
| C(26)-N(6)-Al(2) | 110.80(19) |
| C(29)-N(6)-Al(2) | 140.2(2) |
| C(77)-N(20)-Al(4) | 133.6(2) |
| C(46)-N(11)-C(49) | 107.2(2) |
| C(46)-N(11)-Al(3) | 111.02(18) |
| C(49)-N(11)-Al(3) | 141.3(2) |
| C(53)-N(14)-Al(3) | 132.7(2) |
| C(37)-N(10)-Al(2) | 127.4(2) |
| C(57)-N(15)-Al(3) | 128.6(2) |
| C(25)-N(7)-C(21) | 115.1(2) |
| C(25)-N(7)-Al(2) | 112.60(18) |
| C(21)-N(7)-Al(2) | 131.6(2) |
| C(65)-N(17)-C(61) | 114.7(3) |
| C(65)-N(17)-Al(4) | 112.97(19) |
| C(61)-N(17)-Al(4) | 131.3(2) |
| C(66)-N(16)-C(69) | 107.7(3) |
| C(66)-N(16)-Al(4) | 110.19(19) |
| C(69)-N(16)-Al(4) | 139.0(2) |
| C(51)-N(13)-C(52) | 110.2(3) |
| C(51)-N(13)-C(50) | 109.4(3) |
| C(52)-N(13)-C(50) | 110.5(2) |
| C(73)-N(19)-Al(4) | 127.6(2) |
| C(45)-N(12)-C(41) | 114.2(2) |
| C(45)-N(12)-Al(3) | 113.15(18) |
| C(41)-N(12)-Al(3) | 132.2(2) |
| C(33)-N(9)-Al(2) | 132.8(2) |
| C(32)-N(8)-C(31) | 110.6(3) |
| C(32)-N(8)-C(30) | 109.0(3) |
| C(31)-N(8)-C(30) | 110.0(3) |
| C(72)-N(18)-C(71) | 109.9(3) |
| C(72)-N(18)-C(70) | 110.2(4) |
| C(71)-N(18)-C(70) | 108.8(3) |
| N(1)-C(6)-C(7) | 109.9(3) |

| | |
|---|---|
| N(1)-C(6)-C(5) | 116.5(3) |
| C(7)-C(6)-C(5) | 133.5(3) |
| N(4)-C(13)-C(14) | 108.8(3) |
| N(4)-C(13)-C(15) | 110.2(3) |
| C(14)-C(13)-C(15) | 109.5(3) |
| N(4)-C(13)-C(16) | 110.2(3) |
| C(14)-C(13)-C(16) | 109.3(3) |
| C(15)-C(13)-C(16) | 108.8(3) |
| C(8)-C(9)-N(1) | 109.0(3) |
| C(8)-C(9)-C(10) | 130.9(3) |
| N(1)-C(9)-C(10) | 120.1(3) |
| N(2)-C(5)-C(6) | 109.1(3) |
| C(9)-C(8)-C(7) | 107.6(3) |
| N(5)-C(17)-C(18) | 108.3(3) |
| N(5)-C(17)-C(20) | 108.0(3) |
| C(18)-C(17)-C(20) | 111.2(3) |
| N(5)-C(17)-C(19) | 108.1(2) |
| C(18)-C(17)-C(19) | 110.8(3) |
| C(20)-C(17)-C(19) | 110.3(3) |
| N(2)-C(1)-C(4) | 108.3(3) |
| N(2)-C(1)-C(3) | 111.5(3) |
| C(4)-C(1)-C(3) | 109.4(3) |
| N(2)-C(1)-C(2) | 110.8(3) |
| C(4)-C(1)-C(2) | 107.7(3) |
| C(3)-C(1)-C(2) | 109.0(3) |
| C(9)-C(10)-N(3) | 112.6(3) |
| C(6)-C(7)-C(8) | 106.0(3) |
| N(6)-C(26)-C(27) | 109.4(3) |
| N(6)-C(26)-C(25) | 116.3(3) |
| C(27)-C(26)-C(25) | 134.3(3) |
| N(7)-C(25)-C(26) | 109.4(3) |
| C(26)-C(27)-C(28) | 106.7(3) |
| N(8)-C(30)-C(29) | 113.2(3) |
| C(29)-C(28)-C(27) | 107.1(3) |
| C(28)-C(29)-N(6) | 109.3(3) |
| C(28)-C(29)-C(30) | 131.3(3) |

| | |
|---|---|
| N(6)-C(29)-C(30) | 119.4(3) |
| N(7)-C(21)-C(24) | 108.1(3) |
| N(7)-C(21)-C(23) | 111.9(2) |
| C(24)-C(21)-C(23) | 108.0(3) |
| N(7)-C(21)-C(22) | 111.9(3) |
| C(24)-C(21)-C(22) | 108.4(3) |
| C(23)-C(21)-C(22) | 108.4(3) |
| C(38)-C(37)-N(10) | 108.4(3) |
| C(38)-C(37)-C(39) | 110.7(3) |
| N(10)-C(37)-C(39) | 108.6(3) |
| C(38)-C(37)-C(40) | 111.5(3) |
| N(10)-C(37)-C(40) | 107.7(3) |
| C(39)-C(37)-C(40) | 109.9(3) |
| N(9)-C(33)-C(34) | 108.6(3) |
| N(9)-C(33)-C(36) | 109.5(3) |
| C(34)-C(33)-C(36) | 109.8(3) |
| N(9)-C(33)-C(35) | 110.2(3) |
| C(34)-C(33)-C(35) | 109.9(3) |
| C(36)-C(33)-C(35) | 108.9(3) |
| N(11)-C(46)-C(47) | 109.9(2) |
| N(11)-C(46)-C(45) | 116.3(3) |
| C(47)-C(46)-C(45) | 133.7(3) |
| N(14)-C(53)-C(56) | 110.5(3) |
| N(14)-C(53)-C(54) | 109.8(3) |
| C(56)-C(53)-C(54) | 111.8(4) |
| N(14)-C(53)-C(55) | 110.0(3) |
| C(56)-C(53)-C(55) | 108.5(4) |
| C(54)-C(53)-C(55) | 106.2(4) |
| C(49)-C(48)-C(47) | 107.5(3) |
| C(48)-C(49)-N(11) | 109.1(3) |
| C(48)-C(49)-C(50) | 130.9(3) |
| N(11)-C(49)-C(50) | 119.9(3) |
| N(12)-C(41)-C(44) | 107.9(2) |
| N(12)-C(41)-C(43) | 111.2(2) |
| C(44)-C(41)-C(43) | 109.4(3) |
| N(12)-C(41)-C(42) | 111.7(3) |

| | |
|---|---|
| C(44)-C(41)-C(42) | 107.1(3) |
| C(43)-C(41)-C(42) | 109.3(3) |
| C(46)-C(47)-C(48) | 106.3(3) |
| N(13)-C(50)-C(49) | 112.5(2) |
| N(12)-C(45)-C(46) | 109.3(2) |
| N(15)-C(57)-C(58) | 108.9(3) |
| N(15)-C(57)-C(60) | 108.7(3) |
| C(58)-C(57)-C(60) | 110.7(3) |
| N(15)-C(57)-C(59) | 107.6(3) |
| C(58)-C(57)-C(59) | 110.1(3) |
| C(60)-C(57)-C(59) | 110.8(3) |
| N(16)-C(66)-C(67) | 109.6(3) |
| N(16)-C(66)-C(65) | 116.4(3) |
| C(67)-C(66)-C(65) | 133.9(3) |
| C(66)-C(67)-C(68) | 106.3(3) |
| N(17)-C(65)-C(66) | 108.6(3) |
| C(69)-C(68)-C(67) | 107.5(3) |
| N(18)-C(70)-C(69) | 112.7(3) |
| N(17)-C(61)-C(63) | 111.5(3) |
| N(17)-C(61)-C(64) | 107.9(3) |
| C(63)-C(61)-C(64) | 108.3(3) |
| N(17)-C(61)-C(62) | 111.4(3) |
| C(63)-C(61)-C(62) | 109.3(3) |
| C(64)-C(61)-C(62) | 108.3(3) |
| C(68)-C(69)-N(16) | 108.8(3) |
| C(68)-C(69)-C(70) | 131.4(3) |
| N(16)-C(69)-C(70) | 119.7(3) |
| N(19)-C(73)-C(75) | 107.2(3) |
| N(19)-C(73)-C(76) | 108.7(3) |
| C(75)-C(73)-C(76) | 110.4(4) |
| N(19)-C(73)-C(74) | 108.0(3) |
| C(75)-C(73)-C(74) | 111.5(3) |
| C(76)-C(73)-C(74) | 110.8(3) |
| N(20)-C(77)-C(78) | 107.8(2) |
| N(20)-C(77)-C(80) | 109.2(3) |
| C(78)-C(77)-C(80) | 110.0(3) |

| | |
|---|---|
| N(20)-C(77)-C(79) | 110.6(3) |
| C(78)-C(77)-C(79) | 108.7(3) |
| C(80)-C(77)-C(79) | 110.6(4) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei368_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 28(1) | 27(1) | 26(1) | -2(1) | 7(1) | -4(1) |
| Al(4) | 27(1) | 31(1) | 26(1) | 1(1) | 5(1) | 2(1) |
| Al(2) | 29(1) | 26(1) | 26(1) | -1(1) | 5(1) | 4(1) |
| Al(3) | 26(1) | 27(1) | 25(1) | 1(1) | 5(1) | 4(1) |
| N(1) | 33(1) | 29(1) | 28(2) | 0(1) | 5(1) | -2(1) |
| N(4) | 34(1) | 35(1) | 26(2) | 0(1) | 9(1) | 2(1) |
| N(5) | 32(1) | 35(1) | 29(2) | 0(1) | 5(1) | -1(1) |
| N(2) | 34(1) | 38(1) | 28(2) | -1(1) | 6(1) | -9(1) |
| N(3) | 48(2) | 33(1) | 39(2) | -9(1) | 6(1) | -6(1) |
| N(6) | 35(1) | 29(1) | 26(2) | 2(1) | 5(1) | 1(1) |
| N(20) | 30(1) | 43(1) | 26(2) | 6(1) | 3(1) | 6(1) |
| N(11) | 28(1) | 26(1) | 24(2) | 0(1) | 5(1) | 4(1) |
| N(14) | 34(1) | 33(1) | 25(2) | -3(1) | 6(1) | -2(1) |
| N(10) | 29(1) | 40(1) | 28(2) | -2(1) | 5(1) | 5(1) |
| N(15) | 30(1) | 33(1) | 27(2) | 3(1) | 4(1) | 2(1) |
| N(7) | 37(1) | 25(1) | 30(2) | 0(1) | 4(1) | 1(1) |
| N(17) | 38(1) | 31(1) | 30(2) | -2(1) | 10(1) | -2(1) |
| N(16) | 36(1) | 34(1) | 31(2) | -2(1) | 10(1) | -1(1) |
| N(13) | 41(1) | 29(1) | 35(2) | -7(1) | 7(1) | 3(1) |
| N(19) | 26(1) | 47(2) | 30(2) | -2(1) | 3(1) | 5(1) |
| N(12) | 37(1) | 33(1) | 26(2) | 8(1) | 12(1) | 9(1) |
| N(9) | 31(1) | 36(1) | 29(2) | -4(1) | 7(1) | 7(1) |
| N(8) | 60(2) | 44(2) | 32(2) | 7(1) | 11(2) | -4(1) |
| N(18) | 75(2) | 59(2) | 38(2) | -16(2) | 25(2) | -21(2) |
| C(6) | 37(2) | 38(2) | 27(2) | 0(1) | 8(1) | 3(1) |
| C(13) | 38(2) | 35(2) | 40(2) | 3(2) | 15(2) | 5(1) |
| C(9) | 46(2) | 28(2) | 36(2) | 2(1) | 14(2) | -2(1) |
| C(5) | 39(2) | 48(2) | 29(2) | -3(2) | 0(1) | -5(1) |
| C(8) | 66(2) | 28(2) | 45(3) | 9(2) | 17(2) | 0(2) |
| C(17) | 33(2) | 47(2) | 38(2) | -8(2) | 11(2) | 3(1) |
| C(1) | 46(2) | 47(2) | 41(3) | -8(2) | 14(2) | -21(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(10) | 42(2) | 34(2) | 49(3) | 0(2) | 13(2) | -10(1) |
| C(15) | 63(2) | 39(2) | 50(3) | 8(2) | 18(2) | 13(2) |
| C(18) | 41(2) | 61(2) | 51(3) | 0(2) | 5(2) | 16(2) |
| C(11) | 78(3) | 33(2) | 77(4) | -9(2) | 19(2) | -4(2) |
| C(4) | 64(2) | 41(2) | 50(3) | 0(2) | 22(2) | -23(2) |
| C(2) | 70(2) | 46(2) | 55(3) | -17(2) | 24(2) | -28(2) |
| C(7) | 56(2) | 40(2) | 32(2) | 5(2) | 6(2) | 8(2) |
| C(14) | 74(3) | 72(3) | 46(3) | 4(2) | 24(2) | 30(2) |
| C(19) | 54(2) | 60(2) | 59(3) | -26(2) | 16(2) | 8(2) |
| C(20) | 53(2) | 66(2) | 66(3) | -9(2) | 33(2) | -7(2) |
| C(3) | 44(2) | 73(3) | 60(3) | -10(2) | 13(2) | -27(2) |
| C(12) | 62(2) | 68(2) | 54(3) | -13(2) | 5(2) | -25(2) |
| C(16) | 41(2) | 56(2) | 126(5) | 20(3) | 31(2) | 4(2) |
| C(26) | 35(2) | 35(2) | 27(2) | 0(1) | 8(1) | 0(1) |
| C(25) | 46(2) | 38(2) | 32(2) | 4(2) | 4(2) | -2(1) |
| C(27) | 41(2) | 52(2) | 26(2) | -7(2) | 5(2) | -8(2) |
| C(30) | 54(2) | 30(2) | 39(2) | 3(2) | 7(2) | 0(1) |
| C(28) | 49(2) | 36(2) | 34(2) | -7(2) | 11(2) | -12(1) |
| C(29) | 44(2) | 29(2) | 37(2) | -4(1) | 10(2) | -1(1) |
| C(21) | 49(2) | 25(1) | 37(2) | 1(1) | 8(2) | 1(1) |
| C(24) | 59(2) | 30(2) | 51(3) | 1(2) | 4(2) | -1(2) |
| C(23) | 65(2) | 41(2) | 59(3) | 5(2) | 24(2) | -6(2) |
| C(22) | 71(2) | 33(2) | 53(3) | 12(2) | 2(2) | 8(2) |
| C(31) | 67(3) | 70(3) | 68(3) | 7(2) | 27(2) | -21(2) |
| C(32) | 115(4) | 72(3) | 40(3) | 19(2) | 12(3) | 4(3) |
| C(34) | 43(2) | 57(2) | 38(3) | 6(2) | 15(2) | 19(2) |
| C(37) | 31(2) | 56(2) | 39(2) | -3(2) | 10(2) | 9(1) |
| C(38) | 34(2) | 60(2) | 50(3) | -13(2) | 1(2) | 7(2) |
| C(33) | 28(2) | 50(2) | 36(2) | -3(2) | 5(1) | 9(1) |
| C(39) | 44(2) | 58(2) | 63(3) | -13(2) | 0(2) | 21(2) |
| C(36) | 51(2) | 83(3) | 40(3) | 15(2) | 15(2) | 34(2) |
| C(40) | 44(2) | 109(3) | 51(3) | -2(3) | 24(2) | 10(2) |
| C(35) | 35(2) | 89(3) | 87(4) | -32(3) | 10(2) | -6(2) |
| C(46) | 31(1) | 31(2) | 25(2) | -2(1) | 6(1) | 0(1) |
| C(53) | 32(1) | 30(1) | 33(2) | -6(1) | 10(1) | -3(1) |
| C(48) | 48(2) | 29(2) | 32(2) | 8(1) | 5(2) | 3(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(49) | 36(2) | 25(1) | 29(2) | 1(1) | 3(1) | 1(1) |
| C(41) | 36(2) | 35(2) | 31(2) | 4(1) | 6(1) | 12(1) |
| C(47) | 49(2) | 30(2) | 31(2) | 1(1) | 13(2) | 0(1) |
| C(42) | 44(2) | 38(2) | 38(2) | -1(2) | 8(2) | 8(1) |
| C(50) | 35(2) | 24(1) | 36(2) | 0(1) | 5(1) | 5(1) |
| C(44) | 54(2) | 35(2) | 35(2) | 13(2) | 10(2) | 13(1) |
| C(43) | 38(2) | 46(2) | 49(3) | 3(2) | 3(2) | 14(1) |
| C(45) | 41(2) | 42(2) | 41(2) | 8(2) | 17(2) | 11(1) |
| C(52) | 55(2) | 52(2) | 43(3) | -9(2) | 12(2) | 14(2) |
| C(54) | 75(3) | 198(6) | 43(3) | -47(4) | 18(2) | -61(3) |
| C(51) | 70(2) | 30(2) | 62(3) | -8(2) | 2(2) | -11(2) |
| C(55) | 121(4) | 81(3) | 96(5) | 18(3) | -17(3) | -64(3) |
| C(56) | 41(2) | 90(4) | 250(8) | -96(4) | -44(3) | 23(2) |
| C(57) | 34(2) | 43(2) | 38(2) | -4(2) | -3(2) | -1(1) |
| C(60) | 58(2) | 63(2) | 53(3) | -26(2) | -6(2) | 3(2) |
| C(59) | 38(2) | 67(2) | 58(3) | -1(2) | 8(2) | -16(2) |
| C(58) | 50(2) | 67(2) | 44(3) | -2(2) | -11(2) | 8(2) |
| C(66) | 32(2) | 41(2) | 30(2) | 0(2) | 4(1) | -3(1) |
| C(67) | 40(2) | 57(2) | 29(2) | -2(2) | 10(2) | -12(2) |
| C(65) | 46(2) | 42(2) | 36(2) | -4(2) | 16(2) | 0(1) |
| C(63) | 61(2) | 45(2) | 51(3) | -7(2) | 6(2) | -14(2) |
| C(68) | 51(2) | 48(2) | 35(2) | -3(2) | 7(2) | -17(2) |
| C(70) | 69(2) | 34(2) | 56(3) | -7(2) | 26(2) | -8(2) |
| C(61) | 49(2) | 32(2) | 40(2) | -1(2) | 13(2) | 1(1) |
| C(69) | 45(2) | 35(2) | 37(2) | 1(2) | 10(2) | -3(1) |
| C(64) | 71(2) | 38(2) | 53(3) | 1(2) | 26(2) | -5(2) |
| C(62) | 72(2) | 38(2) | 59(3) | -8(2) | 20(2) | 6(2) |
| C(71) | 95(3) | 104(4) | 59(4) | -25(3) | 9(3) | -51(3) |
| C(72) | 136(4) | 88(3) | 65(4) | -25(3) | 57(3) | -12(3) |
| C(73) | 27(2) | 98(3) | 28(2) | 3(2) | 3(1) | 15(2) |
| C(76) | 61(2) | 99(3) | 53(3) | 8(2) | 14(2) | 48(2) |
| C(75) | 34(2) | 130(4) | 34(3) | -6(2) | -4(2) | 15(2) |
| C(74) | 31(2) | 141(4) | 44(3) | 4(3) | 9(2) | 6(2) |
| C(78) | 41(2) | 58(2) | 33(2) | 7(2) | 0(2) | 17(2) |
| C(77) | 30(2) | 65(2) | 33(2) | 14(2) | 7(1) | 12(2) |
| C(80) | 62(2) | 141(4) | 44(3) | 8(3) | 11(2) | 66(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(79) | 39(2) | 130(4) | 85(4) | 49(3) | -4(2) | -23(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for pei368_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(4) | 3317 | 7594 | 2318 | 37 |
| H(5A) | 3715 | 5069 | 2525 | 39 |
| H(5B) | 3794 | 6145 | 2226 | 39 |
| H(20) | 4257 | 8070 | 63 | 40 |
| H(14) | 1636 | 2555 | 8221 | 37 |
| H(10A) | 1485 | 1406 | 512 | 39 |
| H(10B) | 1640 | 2651 | 701 | 39 |
| H(15A) | 1148 | 1198 | 7867 | 36 |
| H(15B) | 1205 | 80 | 8186 | 36 |
| H(19A) | 3599 | 8458 | -258 | 42 |
| H(19B) | 3455 | 7213 | -132 | 42 |
| H(9) | 814 | 1959 | 461 | 38 |
| H(5C) | 4211 | 7723 | 4179 | 48 |
| H(5D) | 4541 | 6830 | 4009 | 48 |
| H(8) | 3552 | 3441 | 4129 | 54 |
| H(10C) | 2966 | 4942 | 3020 | 49 |
| H(10D) | 2994 | 3576 | 3271 | 49 |
| H(15C) | 3121 | 10053 | 2369 | 75 |
| H(15D) | 2659 | 10031 | 2434 | 75 |
| H(15E) | 2794 | 9151 | 2032 | 75 |
| H(18A) | 4535 | 5415 | 3239 | 78 |
| H(18B) | 4751 | 4308 | 2999 | 78 |
| H(18C) | 4308 | 4087 | 3109 | 78 |
| H(11A) | 3330 | 1897 | 2977 | 94 |
| H(11B) | 3748 | 2644 | 3177 | 94 |
| H(11C) | 3639 | 2155 | 2625 | 94 |
| H(4A) | 4352 | 8783 | 2674 | 76 |
| H(4B) | 4416 | 10202 | 2876 | 76 |
| H(4C) | 3979 | 9533 | 2815 | 76 |
| H(2A) | 3995 | 10034 | 3698 | 83 |

| | | | | |
|---|---|---|---|---|
| H(2B) | 4422 | 10721 | 3704 | 83 |
| H(2C) | 4392 | 9655 | 4100 | 83 |
| H(7) | 4123 | 4915 | 4556 | 52 |
| H(14A) | 3191 | 8344 | 3476 | 93 |
| H(14B) | 2886 | 9507 | 3313 | 93 |
| H(14C) | 3348 | 9591 | 3249 | 93 |
| H(19C) | 4045 | 3495 | 2223 | 86 |
| H(19D) | 4491 | 3733 | 2122 | 86 |
| H(19E) | 4107 | 4470 | 1808 | 86 |
| H(20A) | 4405 | 6614 | 2040 | 88 |
| H(20B) | 4812 | 5890 | 2304 | 88 |
| H(20C) | 4606 | 6904 | 2600 | 88 |
| H(3A) | 4942 | 8453 | 3890 | 87 |
| H(3B) | 5000 | 9415 | 3470 | 87 |
| H(3C) | 4922 | 7943 | 3349 | 87 |
| H(12A) | 3098 | 3162 | 2045 | 94 |
| H(12B) | 2853 | 4318 | 2215 | 94 |
| H(12C) | 2789 | 2910 | 2397 | 94 |
| H(16A) | 2541 | 7213 | 2389 | 108 |
| H(16B) | 2382 | 8157 | 2754 | 108 |
| H(16C) | 2670 | 6989 | 2966 | 108 |
| H(25A) | 1767 | 887 | 2322 | 47 |
| H(25B) | 1332 | 1235 | 2436 | 47 |
| H(27) | 1927 | 3591 | 2724 | 48 |
| H(30A) | 1137 | 4975 | 1028 | 50 |
| H(30B) | 1458 | 6052 | 1251 | 50 |
| H(28) | 1881 | 5546 | 2181 | 47 |
| H(24A) | 783 | -527 | 1078 | 72 |
| H(24B) | 885 | -1935 | 1280 | 72 |
| H(24C) | 1224 | -1124 | 1093 | 72 |
| H(23A) | 881 | -245 | 2363 | 80 |
| H(23B) | 695 | -1452 | 2047 | 80 |
| H(23C) | 568 | -55 | 1850 | 80 |
| H(22A) | 1720 | -1411 | 1897 | 81 |
| H(22B) | 1379 | -2311 | 2038 | 81 |
| H(22C) | 1565 | -1166 | 2390 | 81 |

| | | | | |
|---|---|---|---|---|
| H(31A) | 2256 | 5067 | 750 | 99 |
| H(31B) | 2210 | 5033 | 1305 | 99 |
| H(31C) | 2071 | 6262 | 978 | 99 |
| H(32A) | 1454 | 6214 | 361 | 115 |
| H(32B) | 1209 | 4912 | 242 | 115 |
| H(32C) | 1645 | 5078 | 106 | 115 |
| H(34A) | 425 | 2049 | 1499 | 67 |
| H(34B) | 56 | 3004 | 1300 | 67 |
| H(34C) | 517 | 3498 | 1394 | 67 |
| H(38A) | 2272 | 2794 | 1354 | 73 |
| H(38B) | 2556 | 1563 | 1453 | 73 |
| H(38C) | 2139 | 1614 | 1642 | 73 |
| H(39A) | 1903 | -367 | 1213 | 85 |
| H(39B) | 2304 | -490 | 994 | 85 |
| H(39C) | 1862 | -481 | 637 | 85 |
| H(36A) | 408 | 4296 | 551 | 86 |
| H(36B) | -55 | 3817 | 442 | 86 |
| H(36C) | 245 | 3364 | 102 | 86 |
| H(40A) | 2084 | 1333 | 175 | 99 |
| H(40B) | 2523 | 1315 | 537 | 99 |
| H(40C) | 2261 | 2594 | 460 | 99 |
| H(35A) | 75 | 1123 | 255 | 106 |
| H(35B) | -217 | 1585 | 602 | 106 |
| H(35C) | 142 | 598 | 801 | 106 |
| H(48) | 1382 | -1606 | 9908 | 44 |
| H(47) | 848 | -46 | 10070 | 43 |
| H(42A) | 648 | 4657 | 9491 | 60 |
| H(42B) | 584 | 5740 | 9083 | 60 |
| H(42C) | 1016 | 5048 | 9242 | 60 |
| H(50A) | 1942 | -295 | 9044 | 38 |
| H(50B) | 1884 | -1658 | 9270 | 38 |
| H(44A) | 995 | 4499 | 8380 | 62 |
| H(44B) | 573 | 5256 | 8245 | 62 |
| H(44C) | 599 | 3832 | 8059 | 62 |
| H(43A) | 34 | 3091 | 8464 | 68 |
| H(43B) | -14 | 4562 | 8577 | 68 |

| | | | | |
|---|---|---|---|---|
| H(43C) | 43 | 3546 | 9010 | 68 |
| H(45A) | 417 | 1856 | 9291 | 48 |
| H(45B) | 760 | 2710 | 9630 | 48 |
| H(52A) | 2035 | -2334 | 8470 | 74 |
| H(52B) | 1996 | -917 | 8263 | 74 |
| H(52C) | 1708 | -2009 | 7980 | 74 |
| H(54A) | 1651 | 4256 | 9215 | 157 |
| H(54B) | 2125 | 4196 | 9472 | 157 |
| H(54C) | 1839 | 2988 | 9485 | 157 |
| H(51A) | 1485 | -3213 | 8803 | 84 |
| H(51B) | 1165 | -2847 | 8313 | 84 |
| H(51C) | 1097 | -2351 | 8828 | 84 |
| H(55A) | 2189 | 4137 | 8272 | 158 |
| H(55B) | 2303 | 4889 | 8778 | 158 |
| H(55C) | 1845 | 4922 | 8462 | 158 |
| H(56A) | 2295 | 1671 | 9115 | 208 |
| H(56B) | 2589 | 2854 | 9090 | 208 |
| H(56C) | 2396 | 2081 | 8604 | 208 |
| H(60A) | 831 | -356 | 7250 | 91 |
| H(60B) | 424 | -1045 | 7325 | 91 |
| H(60C) | 855 | -1408 | 7666 | 91 |
| H(59A) | 602 | -880 | 8431 | 82 |
| H(59B) | 165 | -622 | 8084 | 82 |
| H(59C) | 377 | 446 | 8459 | 82 |
| H(58A) | 331 | 2012 | 7831 | 85 |
| H(58B) | 124 | 1078 | 7399 | 85 |
| H(58C) | 537 | 1811 | 7373 | 85 |
| H(67) | 3042 | 6468 | 1653 | 50 |
| H(65A) | 3229 | 9148 | 1350 | 48 |
| H(65B) | 3654 | 8849 | 1721 | 48 |
| H(63A) | 4137 | 10270 | 1889 | 80 |
| H(63B) | 4329 | 11463 | 1668 | 80 |
| H(63C) | 4448 | 10057 | 1537 | 80 |
| H(68) | 3155 | 4466 | 1187 | 54 |
| H(70A) | 3986 | 5011 | 533 | 61 |
| H(70B) | 3662 | 3918 | 566 | 61 |

| | | | | |
|---|---|---|---|---|
| H(64A) | 4233 | 10564 | 649 | 79 |
| H(64B) | 4134 | 11969 | 803 | 79 |
| H(64C) | 3792 | 11167 | 442 | 79 |
| H(62A) | 3297 | 11428 | 985 | 83 |
| H(62B) | 3633 | 12325 | 1312 | 83 |
| H(62C) | 3445 | 11163 | 1557 | 83 |
| H(71A) | 2923 | 4708 | -426 | 131 |
| H(71B) | 2923 | 4778 | 143 | 131 |
| H(71C) | 3112 | 3570 | -73 | 131 |
| H(72A) | 3753 | 3729 | -306 | 136 |
| H(72B) | 3976 | 5074 | -290 | 136 |
| H(72C) | 3562 | 4817 | -684 | 136 |
| H(76A) | 3127 | 10145 | 225 | 106 |
| H(76B) | 2741 | 10254 | -221 | 106 |
| H(76C) | 3193 | 10351 | -318 | 106 |
| H(75A) | 2595 | 8511 | -836 | 101 |
| H(75B) | 2870 | 7258 | -763 | 101 |
| H(75C) | 3052 | 8557 | -918 | 101 |
| H(74A) | 2898 | 8037 | 477 | 108 |
| H(74B) | 2788 | 6925 | 84 | 108 |
| H(74C) | 2496 | 8135 | 52 | 108 |
| H(78A) | 4602 | 7895 | 1303 | 68 |
| H(78B) | 5009 | 7100 | 1303 | 68 |
| H(78C) | 4571 | 6454 | 1121 | 68 |
| H(80A) | 4701 | 5888 | 313 | 124 |
| H(80B) | 5156 | 6406 | 496 | 124 |
| H(80C) | 4877 | 6930 | 0 | 124 |
| H(79A) | 4983 | 9165 | 307 | 131 |
| H(79B) | 5265 | 8672 | 806 | 131 |
| H(79C) | 4876 | 9541 | 817 | 131 |

Electronic Supplementary Material (ESI) for Dalton Transactions

Table 1. Crystal data and structure refinement for compound 9—ccdc-936571.

| | | |
|---|---|---|
| Identification code | compound 9—ccdc-936571 | |
| Empirical formula | C14 H28 Al N3 | |
| Formula weight | 265.37 | |
| Temperature | 149(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 11.6676(11) Å | α= 90°. |
| | b = 11.1033(9) Å | β= 99.842(4)°. |
| | c = 12.7218(11) Å | γ = 90°. |
| Volume | 1623.8(2) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.085 $Mg/m^3$ | |
| Absorption coefficient | 0.115 $mm^{-1}$ | |
| F(000) | 584 | |
| Crystal size | 0.40 x 0.30 x 0.30 $mm^3$ | |
| Theta range for data collection | 1.77 to 28.73°. | |
| Index ranges | -15<=h<=15, -14<=k<=14, -17<=l<=17 | |
| Reflections collected | 24380 | |
| Independent reflections | 4194 [R(int) = 0.0288] | |
| Completeness to theta = 28.73° | 99.9 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9660 and 0.9590 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4194 / 0 / 170 | |
| Goodness-of-fit on $F^2$ | 1.038 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0398, wR2 = 0.1091 | |
| R indices (all data) | R1 = 0.0484, wR2 = 0.1164 | |
| Largest diff. peak and hole | 0.441 and -0.172 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for pei50_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Al(1) | 7729(1) | 6210(1) | 445(1) | 33(1) |
| N(1) | 7395(1) | 8392(1) | -18(1) | 38(1) |
| N(2) | 6376(1) | 6657(1) | 947(1) | 30(1) |
| N(3) | 7021(1) | 4415(1) | 814(1) | 29(1) |
| C(1) | 9188(1) | 6517(1) | 1440(1) | 44(1) |
| C(2) | 7801(1) | 5834(1) | -1057(1) | 38(1) |
| C(3) | 8418(2) | 9153(2) | -17(1) | 54(1) |
| C(4) | 6631(1) | 8474(1) | -1065(1) | 46(1) |
| C(5) | 6731(1) | 8796(1) | 813(1) | 41(1) |
| C(6) | 5949(1) | 7800(1) | 1026(1) | 36(1) |
| C(7) | 4892(1) | 7727(1) | 1366(1) | 42(1) |
| C(8) | 4668(1) | 6486(1) | 1514(1) | 37(1) |
| C(9) | 5602(1) | 5866(1) | 1248(1) | 30(1) |
| C(10) | 5944(1) | 4571(1) | 1293(1) | 32(1) |
| C(11) | 7780(1) | 3397(1) | 1309(1) | 37(1) |
| C(12) | 8294(1) | 3711(2) | 2460(1) | 50(1) |
| C(13) | 7089(2) | 2221(1) | 1284(1) | 50(1) |
| C(14) | 8739(1) | 3230(2) | 646(1) | 53(1) |

Table 3. Bond lengths [Å] and angles [°] for pei50_0m.

| | |
|---|---|
| Al(1)-N(2) | 1.8678(11) |
| Al(1)-C(1) | 1.9698(13) |
| Al(1)-C(2) | 1.9716(13) |
| Al(1)-N(3) | 2.2382(11) |
| N(1)-C(3) | 1.4628(19) |
| N(1)-C(4) | 1.4743(17) |
| N(1)-C(5) | 1.4827(17) |
| N(2)-C(9) | 1.3612(15) |
| N(2)-C(6) | 1.3727(16) |
| N(3)-C(10) | 1.4979(14) |
| N(3)-C(11) | 1.5057(16) |
| C(5)-C(6) | 1.4884(19) |
| C(6)-C(7) | 1.3777(19) |
| C(7)-C(8) | 1.421(2) |
| C(8)-C(9) | 1.3793(17) |
| C(9)-C(10) | 1.4906(18) |
| C(11)-C(14) | 1.5225(19) |
| C(11)-C(12) | 1.5255(19) |
| C(11)-C(13) | 1.531(2) |

| | |
|---|---|
| N(2)-Al(1)-C(1) | 114.99(6) |
| N(2)-Al(1)-C(2) | 124.45(5) |
| C(1)-Al(1)-C(2) | 118.96(6) |
| N(2)-Al(1)-N(3) | 78.55(4) |
| C(1)-Al(1)-N(3) | 109.16(5) |
| C(2)-Al(1)-N(3) | 95.34(5) |
| C(3)-N(1)-C(4) | 109.42(11) |
| C(3)-N(1)-C(5) | 110.52(11) |
| C(4)-N(1)-C(5) | 108.46(12) |
| C(9)-N(2)-C(6) | 108.00(10) |
| C(9)-N(2)-Al(1) | 124.40(9) |
| C(6)-N(2)-Al(1) | 127.52(9) |
| C(10)-N(3)-C(11) | 113.05(9) |
| C(10)-N(3)-Al(1) | 110.33(7) |

| | |
|---|---|
| C(11)-N(3)-Al(1) | 123.01(8) |
| N(1)-C(5)-C(6) | 108.39(11) |
| N(2)-C(6)-C(7) | 108.96(12) |
| N(2)-C(6)-C(5) | 115.61(11) |
| C(7)-C(6)-C(5) | 135.24(13) |
| C(6)-C(7)-C(8) | 107.02(12) |
| C(9)-C(8)-C(7) | 106.31(12) |
| N(2)-C(9)-C(8) | 109.70(12) |
| N(2)-C(9)-C(10) | 116.58(10) |
| C(8)-C(9)-C(10) | 133.59(11) |
| C(9)-C(10)-N(3) | 109.49(9) |
| N(3)-C(11)-C(14) | 107.14(11) |
| N(3)-C(11)-C(12) | 109.63(11) |
| C(14)-C(11)-C(12) | 110.74(13) |
| N(3)-C(11)-C(13) | 111.18(11) |
| C(14)-C(11)-C(13) | 108.62(12) |
| C(12)-C(11)-C(13) | 109.50(12) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pei50_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Al(1) | 27(1) | 48(1) | 25(1) | -5(1) | 5(1) | -5(1) |
| N(1) | 49(1) | 37(1) | 28(1) | 0(1) | 7(1) | -5(1) |
| N(2) | 32(1) | 33(1) | 25(1) | 0(1) | 5(1) | 0(1) |
| N(3) | 30(1) | 33(1) | 23(1) | 1(1) | 4(1) | 0(1) |
| C(1) | 32(1) | 54(1) | 44(1) | -3(1) | 0(1) | -9(1) |
| C(2) | 46(1) | 42(1) | 31(1) | -3(1) | 15(1) | -6(1) |
| C(3) | 66(1) | 47(1) | 53(1) | 2(1) | 14(1) | -17(1) |
| C(4) | 64(1) | 43(1) | 31(1) | 5(1) | 4(1) | 2(1) |
| C(5) | 60(1) | 32(1) | 32(1) | -3(1) | 10(1) | -1(1) |
| C(6) | 46(1) | 34(1) | 27(1) | -3(1) | 7(1) | 5(1) |
| C(7) | 45(1) | 47(1) | 35(1) | -6(1) | 11(1) | 11(1) |
| C(8) | 33(1) | 52(1) | 28(1) | -5(1) | 9(1) | 1(1) |
| C(9) | 29(1) | 40(1) | 21(1) | -1(1) | 4(1) | -1(1) |
| C(10) | 30(1) | 38(1) | 30(1) | 5(1) | 8(1) | -3(1) |
| C(11) | 39(1) | 35(1) | 36(1) | 2(1) | 6(1) | 6(1) |
| C(12) | 53(1) | 53(1) | 40(1) | 5(1) | -8(1) | 12(1) |
| C(13) | 66(1) | 35(1) | 49(1) | 6(1) | 13(1) | 2(1) |
| C(14) | 51(1) | 47(1) | 66(1) | 3(1) | 23(1) | 16(1) |

Electronic Supplementary Material (ESI) for Dalton Transactions

**Supporting information**

# Aluminum Complexes Incorporating Symmetrical and Asymmetrical Tridentate Pincer Type Pyrrolyl Ligands [$C_4H_2NH(2\text{-}CH_2NH^tBu)(5\text{-}CH_2NR_1R_2)$] : Synthesis, Characterization and Reactivity Study

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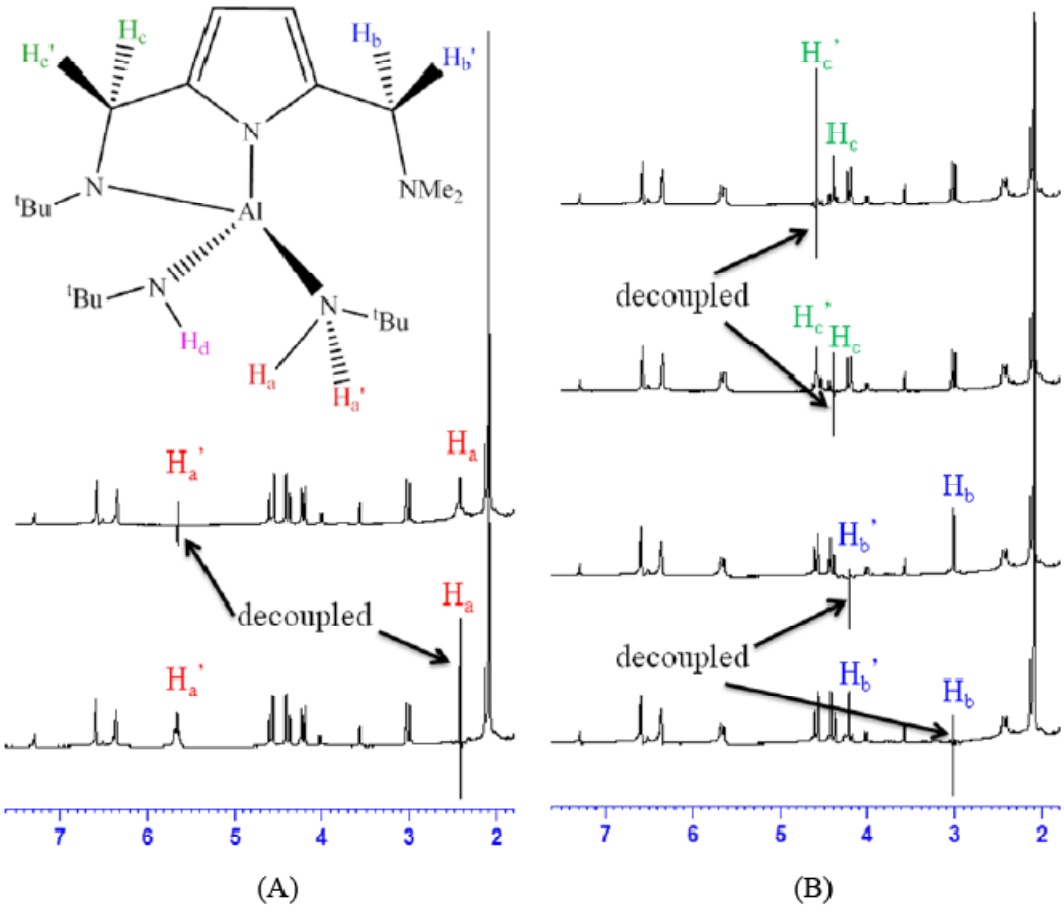


Homonuclear decoupling of $^1H$ NMR spectra of compound **8** in $C_6D_6$ using 300 MHz NMR spectrometer. (A) Homonuclear decoupling of $H_a$ and $H_b$; (B) Homonuclear decoupling of $H_c$, $H_d$, $H_e$, and $H_f$.