

Supporting Information

Blue and White light electroluminescence in a multilayer OLED using a new Aluminium complex

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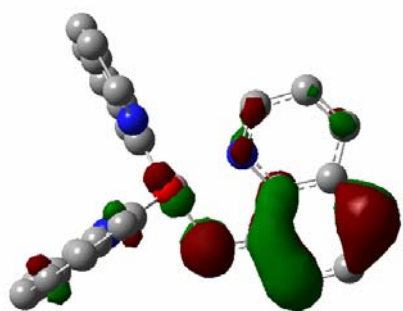
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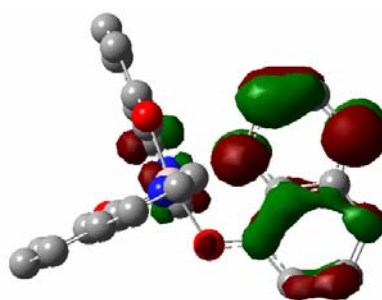
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- 1. HOMO and LUMO distribution in Alq3**
- 2. ¹H NMR of 1**
- 3. Cyclic voltammogram of 1 in dichloromethane with ferrocene as internal standard.**
- 4. Emission and excitation spectra of 1 in thin film.**
- 5. PL decays of 1 in solution (chloroform) and as thin film.**
- 6. Crystal data and structure refinement for 1**

1. HOMO and LUMO distribution in Alq3



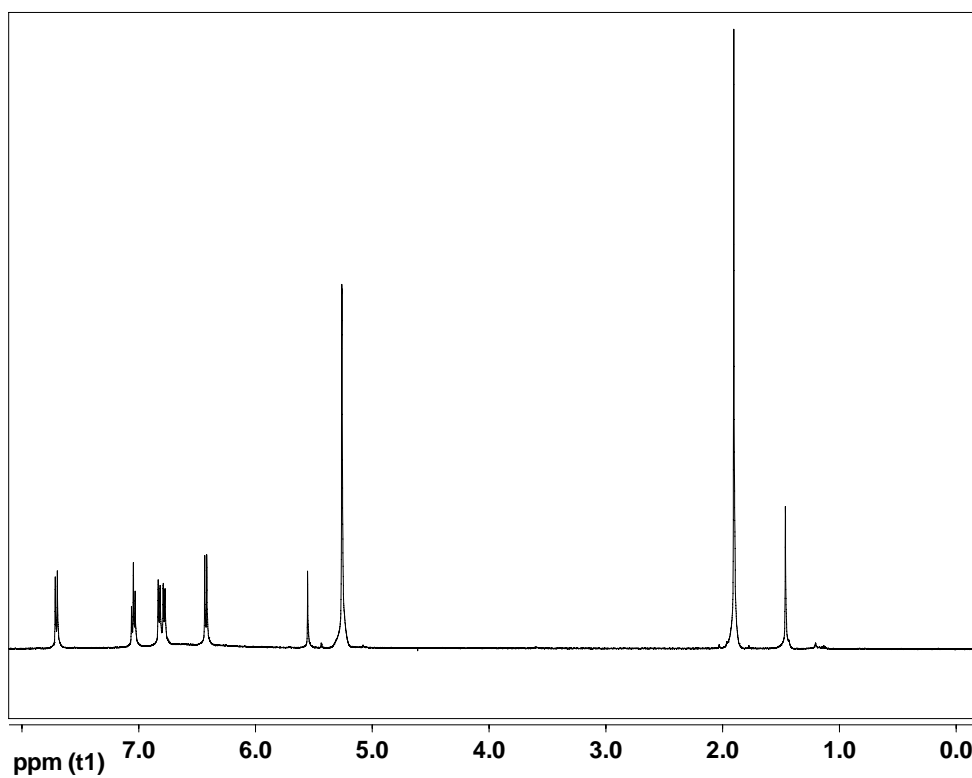
HOMO of Alq3



LUMO of Alq3

HOMO and LUMO distribution in Alq3

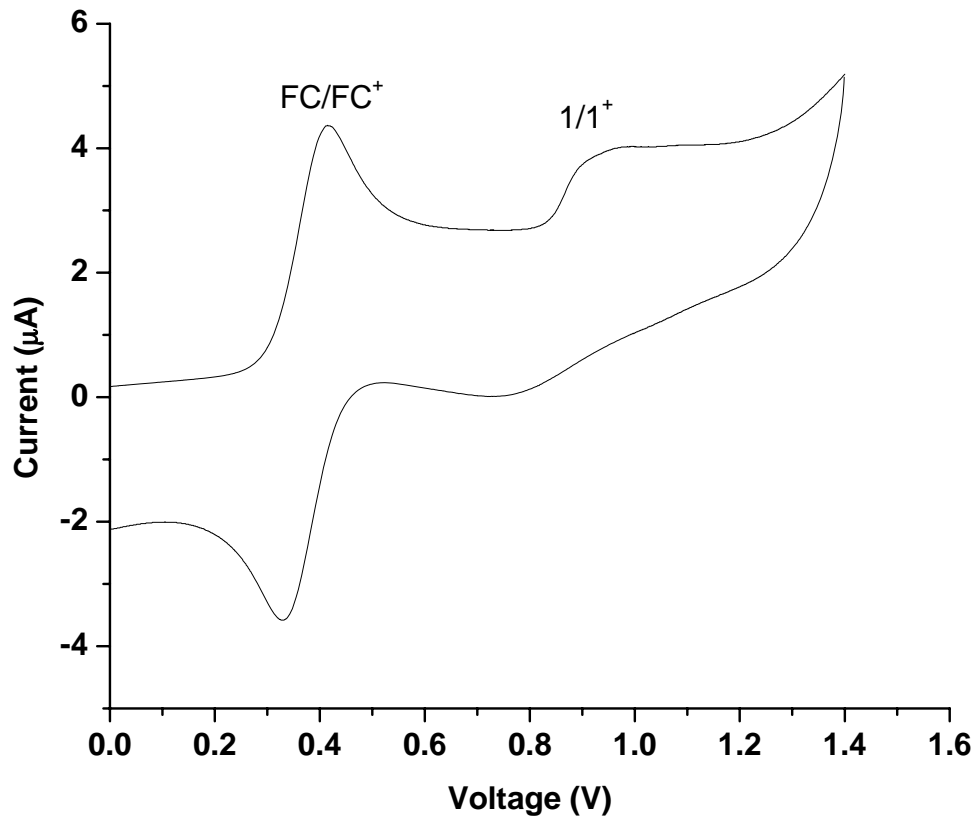
2: ¹H NMR of 1



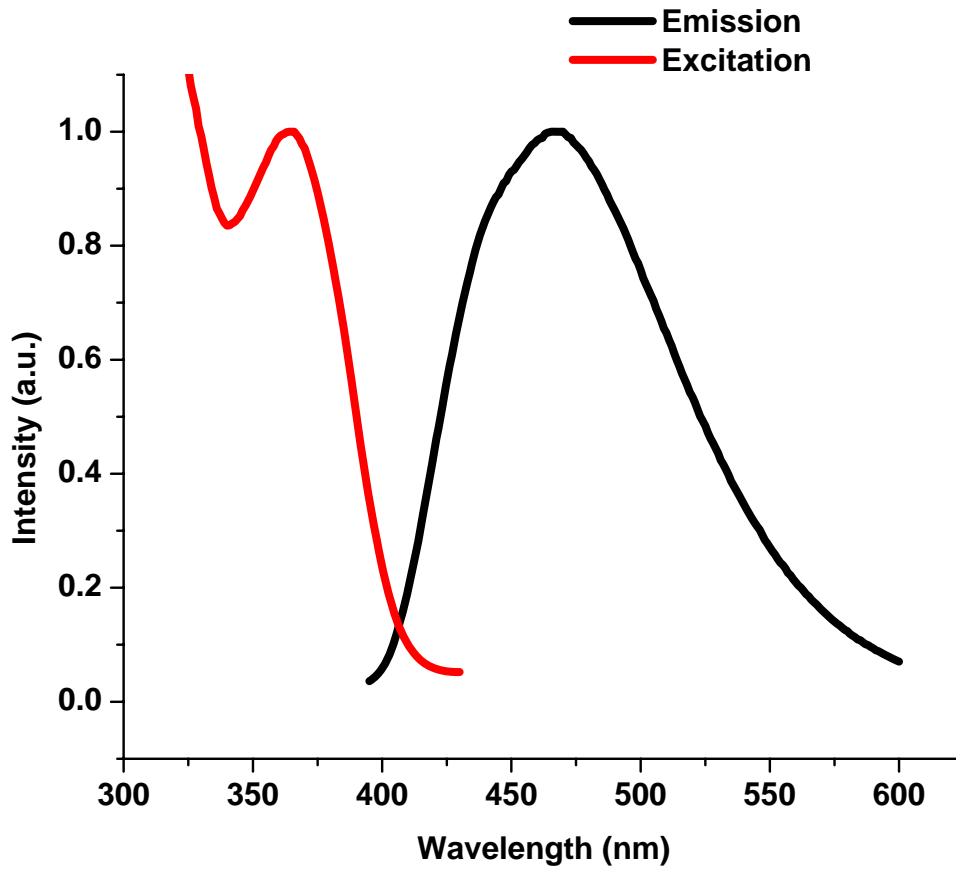
¹H NMR (500MHz, CD₂Cl₂)

7.71 (d, 2H, J= 9 Hz), 7.05 (dd, 2H), 6.82 (d, 2H, J=8 Hz), 6.78 (d, 2H, 7 Hz) 6.43 (d, 2H, J = 9 Hz) 5.55 (s, 1H) 1.90 (s, 6H).

3. Cyclic voltammogram of **1** in dichloromethane with ferrocene as internal standard.



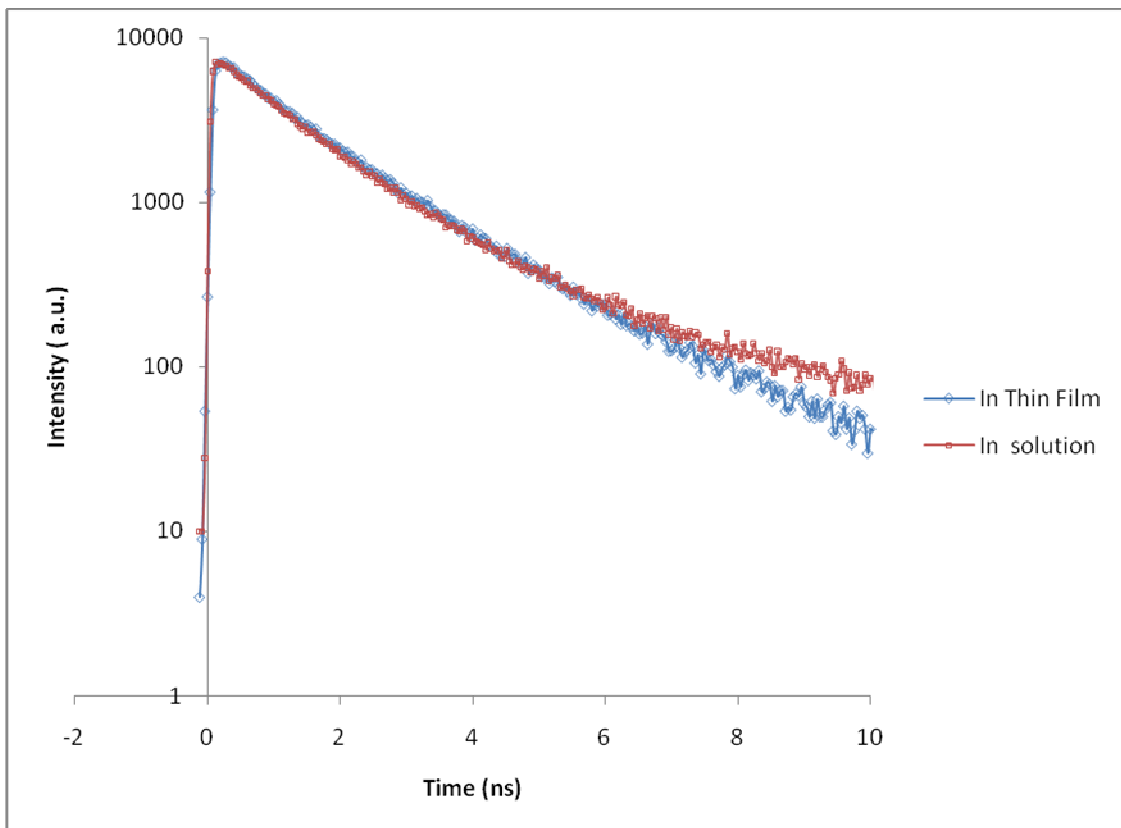
4. Emission and excitation spectra of 1 in thin film.



5. PL decays at the emission maximum of 1 in solution (chloroform) and as thin film. The results of bi-exponential fits, lifetimes (amplitudes), average lifetime and chi-square are as follows:

Solution : 1.192 ns (0.887), 3.567 ns (0.113); average lifetime = 1.462 ns; chi-square = 1.025

Thin film: 1.082 ns (0.663) and 2.231 ns (0.337); average lifetime = 1.469 ns; chi-square = 1.198



6. Crystallographic data and structure refinement for 1 (Deposition number CCDC 790272)

Table 1. Crystal data and structure refinement for 1

Identification code	tifr005
Empirical formula	C ₂₃ H ₂₁ Al N ₄ O ₄
Formula weight	444.42
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 2 ₁ /n
Unit cell dimensions	a = 10.6984(13) Å alpha = 90 deg. b = 13.6505(11) Å beta = 100.553(10) deg. c = 14.4382(16) Å gamma = 90 deg.
Volume	2072.9(4) Å ³
Z, Calculated density	4, 1.424 Mg/m ³
Absorption coefficient	0.138 mm ⁻¹
F(000)	928
Crystal size	0.23 x 0.17 x 0.13 mm
Theta range for data collection	3.01 to 25.00 deg.
Limiting indices	-12 ≤ h ≤ 12, -16 ≤ k ≤ 15, -17 ≤ l ≤ 17
Reflections collected / unique	16628 / 3648 [R(int) = 0.0259]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9823 and 0.9690
Refinement method	Full-matrix least-squares on F ²

Data / restraints / parameters 3648 / 0 / 307

Goodness-of-fit on F^2 1.007

Final R indices [$I > 2\sigma(I)$] $R_1 = 0.0278$, $wR_2 = 0.0718$

R indices (all data) $R_1 = 0.0406$, $wR_2 = 0.0739$

Largest diff. peak and hole 0.179 and -0.242 e. \AA^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for tifr005.

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

	x	y	z	U(eq)
Al(1)	5328(1)	2482(1)	4596(1)	18(1)
O(1)	4327(1)	3409(1)	5046(1)	20(1)
O(2)	6406(1)	1524(1)	4315(1)	21(1)
O(3)	5460(1)	3312(1)	3570(1)	22(1)
O(4)	3896(1)	1853(1)	3872(1)	21(1)
N(1)	4995(1)	1699(1)	5779(1)	19(1)
N(2)	6192(1)	277(1)	5779(1)	27(1)
N(3)	7028(1)	3154(1)	5220(1)	19(1)
N(4)	6349(1)	4627(1)	5757(1)	24(1)
C(1)	3841(1)	3168(1)	5807(1)	20(1)
C(2)	3091(2)	3782(1)	6230(1)	25(1)
C(3)	2615(2)	3459(1)	7021(1)	30(1)
C(4)	2877(2)	2545(1)	7385(1)	31(1)
C(5)	3671(2)	1915(1)	6989(1)	25(1)
C(6)	4162(1)	2237(1)	6207(1)	20(1)
C(7)	4054(2)	959(1)	7330(1)	31(1)
C(8)	4853(2)	427(1)	6919(1)	30(1)
C(9)	5347(2)	811(1)	6138(1)	22(1)
C(10)	7655(2)	1685(1)	4580(1)	21(1)
C(11)	8591(2)	1049(1)	4420(1)	25(1)
C(12)	9878(2)	1310(1)	4676(1)	29(1)
C(13)	10242(2)	2200(1)	5070(1)	31(1)
C(14)	9305(2)	2862(1)	5259(1)	25(1)
C(15)	8027(1)	2582(1)	5047(1)	19(1)
C(16)	9546(2)	3826(1)	5629(1)	31(1)
C(17)	8574(2)	4404(1)	5772(1)	29(1)
C(18)	7297(2)	4051(1)	5574(1)	20(1)
C(19)	4948(2)	4256(1)	2188(1)	30(1)
C(20)	4611(2)	3493(1)	2842(1)	22(1)
C(21)	3444(2)	3012(1)	2643(1)	27(1)
C(22)	3145(2)	2211(1)	3147(1)	22(1)
C(23)	1901(2)	1697(1)	2858(1)	32(1)

Table 3. Bond lengths [Å] and angles [deg] for tifr005.

Al(1)-O(2)	1.8375(10)
Al(1)-O(1)	1.8505(10)
Al(1)-O(3)	1.8901(10)
Al(1)-O(4)	1.8954(11)
Al(1)-N(3)	2.0878(13)
Al(1)-N(1)	2.1000(12)
O(1)-C(1)	1.3400(16)
O(2)-C(10)	1.3394(18)
O(3)-C(20)	1.2809(17)
O(4)-C(22)	1.2937(17)
N(1)-C(9)	1.3444(17)
N(1)-C(6)	1.3847(18)
N(2)-C(9)	1.338(2)
N(2)-H(2N)	0.903(17)
N(2)-H(2NA)	0.869(17)
N(3)-C(18)	1.3376(17)
N(3)-C(15)	1.3826(18)
N(4)-C(18)	1.3473(19)
N(4)-H(4N)	0.858(16)
N(4)-H(4NA)	0.865(17)
C(1)-C(2)	1.377(2)
C(1)-C(6)	1.4121(19)
C(2)-C(3)	1.403(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.363(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.403(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.400(2)
C(5)-C(7)	1.428(2)
C(7)-C(8)	1.340(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.430(2)
C(8)-H(8)	0.9500
C(10)-C(11)	1.376(2)
C(10)-C(15)	1.420(2)
C(11)-C(12)	1.405(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.367(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.413(2)
C(13)-H(13)	0.9500

C(14)-C(15)	1.399(2)
C(14)-C(16)	1.425(2)
C(16)-C(17)	1.351(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.427(2)
C(17)-H(17)	0.9500
C(19)-C(20)	1.494(2)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.393(2)
C(21)-C(22)	1.382(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.495(2)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
O(2)-Al(1)-O(1)	172.31(5)
O(2)-Al(1)-O(3)	96.54(5)
O(1)-Al(1)-O(3)	89.83(4)
O(2)-Al(1)-O(4)	91.82(5)
O(1)-Al(1)-O(4)	92.44(5)
O(3)-Al(1)-O(4)	90.47(5)
O(2)-Al(1)-N(3)	82.89(5)
O(1)-Al(1)-N(3)	93.57(5)
O(3)-Al(1)-N(3)	83.72(5)
O(4)-Al(1)-N(3)	171.62(5)
O(2)-Al(1)-N(1)	91.36(5)
O(1)-Al(1)-N(1)	82.33(4)
O(3)-Al(1)-N(1)	172.08(5)
O(4)-Al(1)-N(1)	88.72(5)
N(3)-Al(1)-N(1)	97.86(5)
C(1)-O(1)-Al(1)	117.24(8)
C(10)-O(2)-Al(1)	116.97(8)
C(20)-O(3)-Al(1)	127.95(10)
C(22)-O(4)-Al(1)	126.47(9)
C(9)-N(1)-C(6)	117.62(12)
C(9)-N(1)-Al(1)	134.04(10)
C(6)-N(1)-Al(1)	108.19(8)
C(9)-N(2)-H(2N)	116.3(10)
C(9)-N(2)-H(2NA)	118.8(11)
H(2N)-N(2)-H(2NA)	118.2(15)
C(18)-N(3)-C(15)	117.78(13)
C(18)-N(3)-Al(1)	132.60(10)
C(15)-N(3)-Al(1)	108.35(9)

C(18)-N(4)-H(4N)	115.3(11)
C(18)-N(4)-H(4NA)	117.4(10)
H(4N)-N(4)-H(4NA)	120.3(15)
O(1)-C(1)-C(2)	124.03(13)
O(1)-C(1)-C(6)	116.96(12)
C(2)-C(1)-C(6)	118.98(13)
C(1)-C(2)-C(3)	119.81(14)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(4)-C(3)-C(2)	121.45(15)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	120.05(14)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	118.73(13)
C(6)-C(5)-C(7)	116.05(14)
C(4)-C(5)-C(7)	125.20(14)
N(1)-C(6)-C(5)	124.08(13)
N(1)-C(6)-C(1)	115.05(12)
C(5)-C(6)-C(1)	120.86(13)
C(8)-C(7)-C(5)	120.52(14)
C(8)-C(7)-H(7)	119.7
C(5)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	120.58(14)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
N(2)-C(9)-N(1)	120.26(14)
N(2)-C(9)-C(8)	118.62(13)
N(1)-C(9)-C(8)	121.10(14)
O(2)-C(10)-C(11)	124.56(13)
O(2)-C(10)-C(15)	117.08(13)
C(11)-C(10)-C(15)	118.35(14)
C(10)-C(11)-C(12)	120.32(14)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	121.65(15)
C(13)-C(12)-H(12)	119.2
C(11)-C(12)-H(12)	119.2
C(12)-C(13)-C(14)	119.43(16)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	118.82(14)
C(15)-C(14)-C(16)	115.90(14)
C(13)-C(14)-C(16)	125.25(15)
N(3)-C(15)-C(14)	124.27(13)

N(3)-C(15)-C(10)	114.50(13)
C(14)-C(15)-C(10)	121.16(13)
C(17)-C(16)-C(14)	120.32(15)
C(17)-C(16)-H(16)	119.8
C(14)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	120.51(14)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
N(3)-C(18)-N(4)	119.48(14)
N(3)-C(18)-C(17)	121.13(14)
N(4)-C(18)-C(17)	119.39(13)
C(20)-C(19)-H(19A)	109.5
C(20)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(20)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(3)-C(20)-C(21)	123.54(13)
O(3)-C(20)-C(19)	115.85(13)
C(21)-C(20)-C(19)	120.60(13)
C(22)-C(21)-C(20)	123.32(14)
C(22)-C(21)-H(21)	118.3
C(20)-C(21)-H(21)	118.3
O(4)-C(22)-C(21)	123.73(14)
O(4)-C(22)-C(23)	115.94(13)
C(21)-C(22)-C(23)	120.33(13)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for tifr005.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Al(1)	19(1)	16(1)	18(1)	1(1)	2(1)	1(1)
O(1)	22(1)	18(1)	21(1)	2(1)	6(1)	1(1)
O(2)	22(1)	19(1)	22(1)	-2(1)	3(1)	1(1)
O(3)	25(1)	21(1)	19(1)	2(1)	4(1)	-1(1)
O(4)	23(1)	19(1)	21(1)	3(1)	0(1)	0(1)
N(1)	21(1)	16(1)	18(1)	0(1)	1(1)	-1(1)
N(2)	34(1)	16(1)	30(1)	6(1)	4(1)	3(1)
N(3)	21(1)	16(1)	18(1)	2(1)	3(1)	2(1)
N(4)	26(1)	15(1)	32(1)	-2(1)	4(1)	0(1)
C(1)	18(1)	21(1)	20(1)	-1(1)	1(1)	-5(1)
C(2)	24(1)	24(1)	26(1)	-2(1)	3(1)	2(1)
C(3)	29(1)	35(1)	27(1)	-8(1)	9(1)	0(1)
C(4)	36(1)	38(1)	20(1)	-4(1)	12(1)	-8(1)
C(5)	30(1)	26(1)	20(1)	-2(1)	4(1)	-8(1)
C(6)	20(1)	20(1)	17(1)	-3(1)	1(1)	-6(1)
C(7)	46(1)	28(1)	20(1)	4(1)	8(1)	-9(1)
C(8)	45(1)	20(1)	24(1)	6(1)	2(1)	-3(1)
C(9)	26(1)	18(1)	20(1)	0(1)	-4(1)	-4(1)
C(10)	23(1)	22(1)	16(1)	4(1)	5(1)	2(1)
C(11)	33(1)	22(1)	22(1)	1(1)	8(1)	6(1)
C(12)	29(1)	32(1)	28(1)	3(1)	11(1)	11(1)
C(13)	21(1)	37(1)	34(1)	5(1)	7(1)	3(1)
C(14)	23(1)	28(1)	24(1)	2(1)	5(1)	1(1)
C(15)	22(1)	21(1)	16(1)	4(1)	4(1)	3(1)
C(16)	22(1)	32(1)	38(1)	0(1)	1(1)	-6(1)
C(17)	29(1)	23(1)	32(1)	-3(1)	1(1)	-4(1)
C(18)	26(1)	18(1)	17(1)	2(1)	2(1)	0(1)
C(19)	38(1)	28(1)	24(1)	7(1)	6(1)	0(1)
C(20)	29(1)	20(1)	17(1)	-1(1)	5(1)	6(1)
C(21)	28(1)	30(1)	20(1)	5(1)	-2(1)	3(1)
C(22)	22(1)	24(1)	20(1)	-3(1)	2(1)	3(1)
C(23)	26(1)	39(1)	28(1)	2(1)	-1(1)	-6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for tifr005.

	x	y	z	U(eq)
H(2)	2897	4422	5987	30
H(3)	2099	3887	7308	36
H(4)	2521	2335	7908	37
H(7)	3740	698	7853	37
H(8)	5093	-211	7148	36
H(11)	8365	431	4136	30
H(12)	10512	856	4572	34
H(13)	11116	2371	5214	37
H(16)	10394	4063	5775	37
H(17)	8742	5050	6007	34
H(19A)	5125	4877	2529	45
H(19B)	4236	4345	1662	45
H(19C)	5703	4048	1946	45
H(21)	2824	3245	2135	32
H(23A)	2051	996	2783	48
H(23B)	1455	1968	2259	48
H(23C)	1380	1791	3343	48
H(2N)	6374(16)	483(12)	5224(12)	33(5)
H(4N)	6510(15)	5244(12)	5780(10)	27(4)
H(2NA)	6253(15)	-345(13)	5907(11)	30(5)
H(4NA)	5579(17)	4421(11)	5576(11)	26(5)

Table 6. Torsion angles [deg] for tifr005.

O(2)-Al(1)-O(1)-C(1)	-38.3(4)
O(3)-Al(1)-O(1)-C(1)	175.65(10)
O(4)-Al(1)-O(1)-C(1)	85.19(10)
N(3)-Al(1)-O(1)-C(1)	-100.65(10)
N(1)-Al(1)-O(1)-C(1)	-3.19(9)
O(1)-Al(1)-O(2)-C(10)	-64.8(4)
O(3)-Al(1)-O(2)-C(10)	80.93(9)
O(4)-Al(1)-O(2)-C(10)	171.61(9)
N(3)-Al(1)-O(2)-C(10)	-1.87(9)
N(1)-Al(1)-O(2)-C(10)	-99.63(9)
O(2)-Al(1)-O(3)-C(20)	109.83(11)
O(1)-Al(1)-O(3)-C(20)	-74.49(11)
O(4)-Al(1)-O(3)-C(20)	17.95(11)
N(3)-Al(1)-O(3)-C(20)	-168.10(11)
N(1)-Al(1)-O(3)-C(20)	-66.1(4)
O(2)-Al(1)-O(4)-C(22)	-119.38(11)
O(1)-Al(1)-O(4)-C(22)	67.03(12)
O(3)-Al(1)-O(4)-C(22)	-22.82(12)
N(3)-Al(1)-O(4)-C(22)	-68.8(3)
N(1)-Al(1)-O(4)-C(22)	149.30(12)
O(2)-Al(1)-N(1)-C(9)	-4.95(14)
O(1)-Al(1)-N(1)-C(9)	179.47(14)
O(3)-Al(1)-N(1)-C(9)	171.0(3)
O(4)-Al(1)-N(1)-C(9)	86.84(14)
N(3)-Al(1)-N(1)-C(9)	-87.96(14)
O(2)-Al(1)-N(1)-C(6)	179.89(9)
O(1)-Al(1)-N(1)-C(6)	4.32(9)
O(3)-Al(1)-N(1)-C(6)	-4.1(4)
O(4)-Al(1)-N(1)-C(6)	-88.32(9)
N(3)-Al(1)-N(1)-C(6)	96.89(9)
O(2)-Al(1)-N(3)-C(18)	170.21(13)
O(1)-Al(1)-N(3)-C(18)	-16.65(13)
O(3)-Al(1)-N(3)-C(18)	72.78(13)
O(4)-Al(1)-N(3)-C(18)	119.1(3)
N(1)-Al(1)-N(3)-C(18)	-99.40(13)
O(2)-Al(1)-N(3)-C(15)	3.77(8)
O(1)-Al(1)-N(3)-C(15)	176.91(8)
O(3)-Al(1)-N(3)-C(15)	-93.65(9)
O(4)-Al(1)-N(3)-C(15)	-47.3(3)
N(1)-Al(1)-N(3)-C(15)	94.17(9)
Al(1)-O(1)-C(1)-C(2)	179.24(11)
Al(1)-O(1)-C(1)-C(6)	1.41(16)

O(1)-C(1)-C(2)-C(3)	179.38(13)
C(6)-C(1)-C(2)-C(3)	-2.8(2)
C(1)-C(2)-C(3)-C(4)	0.0(2)
C(2)-C(3)-C(4)-C(5)	2.1(2)
C(3)-C(4)-C(5)-C(6)	-1.2(2)
C(3)-C(4)-C(5)-C(7)	177.37(16)
C(9)-N(1)-C(6)-C(5)	0.2(2)
Al(1)-N(1)-C(6)-C(5)	176.32(12)
C(9)-N(1)-C(6)-C(1)	179.19(12)
Al(1)-N(1)-C(6)-C(1)	-4.74(14)
C(4)-C(5)-C(6)-N(1)	177.23(13)
C(7)-C(5)-C(6)-N(1)	-1.5(2)
C(4)-C(5)-C(6)-C(1)	-1.7(2)
C(7)-C(5)-C(6)-C(1)	179.63(14)
O(1)-C(1)-C(6)-N(1)	2.65(19)
C(2)-C(1)-C(6)-N(1)	-175.30(13)
O(1)-C(1)-C(6)-C(5)	-178.38(13)
C(2)-C(1)-C(6)-C(5)	3.7(2)
C(6)-C(5)-C(7)-C(8)	1.0(2)
C(4)-C(5)-C(7)-C(8)	-177.67(15)
C(5)-C(7)-C(8)-C(9)	0.7(2)
C(6)-N(1)-C(9)-N(2)	-177.11(13)
Al(1)-N(1)-C(9)-N(2)	8.1(2)
C(6)-N(1)-C(9)-C(8)	1.5(2)
Al(1)-N(1)-C(9)-C(8)	-173.27(11)
C(7)-C(8)-C(9)-N(2)	176.62(15)
C(7)-C(8)-C(9)-N(1)	-2.1(2)
Al(1)-O(2)-C(10)-C(11)	-179.51(11)
Al(1)-O(2)-C(10)-C(15)	-0.44(15)
O(2)-C(10)-C(11)-C(12)	176.16(12)
C(15)-C(10)-C(11)-C(12)	-2.9(2)
C(10)-C(11)-C(12)-C(13)	-1.3(2)
C(11)-C(12)-C(13)-C(14)	2.5(2)
C(12)-C(13)-C(14)-C(15)	0.7(2)
C(12)-C(13)-C(14)-C(16)	-177.18(15)
C(18)-N(3)-C(15)-C(14)	3.2(2)
Al(1)-N(3)-C(15)-C(14)	171.94(11)
C(18)-N(3)-C(15)-C(10)	-173.67(12)
Al(1)-N(3)-C(15)-C(10)	-4.92(14)
C(13)-C(14)-C(15)-N(3)	178.38(12)
C(16)-C(14)-C(15)-N(3)	-3.6(2)
C(13)-C(14)-C(15)-C(10)	-5.0(2)
C(16)-C(14)-C(15)-C(10)	173.08(13)
O(2)-C(10)-C(15)-N(3)	3.90(17)
C(11)-C(10)-C(15)-N(3)	-176.96(12)
O(2)-C(10)-C(15)-C(14)	-173.06(12)

C(11)-C(10)-C(15)-C(14)	6.1(2)
C(15)-C(14)-C(16)-C(17)	1.2(2)
C(13)-C(14)-C(16)-C(17)	179.13(15)
C(14)-C(16)-C(17)-C(18)	1.3(2)
C(15)-N(3)-C(18)-N(4)	-179.59(12)
Al(1)-N(3)-C(18)-N(4)	15.0(2)
C(15)-N(3)-C(18)-C(17)	-0.41(19)
Al(1)-N(3)-C(18)-C(17)	-165.84(10)
C(16)-C(17)-C(18)-N(3)	-1.8(2)
C(16)-C(17)-C(18)-N(4)	177.43(14)
Al(1)-O(3)-C(20)-C(21)	-6.6(2)
Al(1)-O(3)-C(20)-C(19)	174.38(9)
O(3)-C(20)-C(21)-C(22)	-8.0(2)
C(19)-C(20)-C(21)-C(22)	170.95(14)
Al(1)-O(4)-C(22)-C(21)	16.9(2)
Al(1)-O(4)-C(22)-C(23)	-164.00(10)
C(20)-C(21)-C(22)-O(4)	2.6(2)
C(20)-C(21)-C(22)-C(23)	-176.56(14)

Symmetry transformations used to generate equivalent atoms: