

Intramolecular Migration of Coordinated Pt(II) from the N7 Site to the Exocyclic Amino Group in 9-Methyladenine

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Supporting Information (Tables 1-7, total of 8 pages)

Table 1. Crystal data and structure refinement for trans-[Pt(NH₃)₂(9-made-N6)(9-made-N7)](NO₃)₂·2H₂O.

Empirical formula	C ₁₂ H ₂₄ N ₁₄ O ₈ Pt
Formula weight	687.54
Temperature	294(2) K
Wavelength	0.71069 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.113(5) Å alpha = 90.09(4) deg b = 12.579(6) Å beta = 96.93(3) deg c = 8.238(3) Å gamma = 110.60(3) deg
Volume	1165.2(9) Å ³
Z	2
Calculated density	1.960 Mg/m ³
Absorption coefficient	6.091 mm ⁻¹
F(000)	672
Crystal size	0.16 x 0.12 x 0.12 mm
Theta range for data collection	1.73 to 25.00 deg.
Index ranges	0 ≤ h ≤ 14, -14 ≤ k ≤ 13, -9 ≤ l ≤ 9
Reflections collected / unique	4320 / 4108 [R(int) = 0.0328]
Completeness to 2theta = 25.00	100.0%
Max. and min. transmission	0.5285 and 0.4424
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4108 / 6 / 334
Goodness-of-fit on F ²	1.029

Final R indices [$I > 2\sigma(I)$] $R_1 = 0.0388$, $wR_2 = 0.0715$
 R indices (all data) $R_1 = 0.0817$, $wR_2 = 0.0812$
 Largest diff. peak and hole 0.885 and -1.075 e. \AA^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for trans-[Pt(NH₃)₂(9-made-N6)(9-made-N7)](NO₃)₂·2H₂O. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Pt	6502(1)	3632(1)	3431(1)	39(1)
O(1)	6006(6)	3597(7)	8491(8)	77(2)
O(2)	4682(8)	4165(9)	7283(10)	117(3)
O(3)	4346(7)	3151(8)	9384(10)	109(3)
O(4)	918(8)	2183(8)	5601(12)	122(4)
O(5)	2571(9)	2518(8)	4666(13)	121(3)
O(6)	2046(8)	1275(8)	6383(14)	130(4)
O(7)	8147(6)	1705(7)	747(11)	82(2)
O(8)	9618(12)	621(14)	2493(18)	179(5)
N(1A)	4379(7)	1200(6)	6457(9)	48(2)
N(1B)	10886(6)	4933(6)	2805(8)	49(2)
N(3A)	5277(7)	41(6)	7916(9)	53(2)
N(3B)	10575(6)	6407(6)	1145(9)	52(2)
N(6A)	5228(6)	2551(6)	4583(9)	45(2)
N(6B)	9421(6)	3566(6)	3933(8)	48(2)
N(7A)	7387(6)	1717(6)	5344(9)	51(2)
N(7B)	7743(6)	4781(6)	2271(8)	41(2)
N(9B)	8498(6)	6261(6)	784(9)	48(2)
N(9A)	7229(7)	337(6)	7162(9)	51(2)
N(10)	6228(6)	2438(6)	1608(8)	54(2)
N(11)	6762(6)	4871(6)	5217(8)	51(2)
N(12)	5020(8)	3660(8)	8426(10)	69(2)
N(13)	1802(9)	1982(8)	5543(13)	76(3)
C(2A)	4414(8)	405(7)	7542(11)	53(2)
C(2B)	11217(8)	5845(8)	1903(11)	52(2)
C(4B)	9423(7)	5933(7)	1377(10)	39(2)
C(4A)	6195(8)	554(7)	7078(10)	44(2)
C(5A)	6281(7)	1392(6)	5932(9)	39(2)
C(5B)	8952(7)	4991(7)	2310(9)	38(2)
C(6A)	5316(7)	1781(7)	5594(10)	41(2)
C(6B)	9724(7)	4466(7)	3049(9)	39(2)
C(8B)	7514(8)	5547(8)	1337(10)	53(2)
C(8A)	7895(8)	1068(7)	6110(11)	54(2)
C(9A)	7557(9)	-478(8)	8176(11)	67(3)
C(9B)	8545(9)	7206(8)	-292(13)	76(3)

Table 3. Bond lengths [Å] and angles [deg] for trans-[Pt(NH₃)₂(9-made-N₆)(9-made-N₇)](NO₃)₂·2H₂O.

Pt-N(6A)	2.003(7)
Pt-N(7B)	2.021(7)
Pt-N(10)	2.035(7)
Pt-N(11)	2.057(7)
O(1)-N(12)	1.219(9)
O(2)-N(12)	1.246(9)
O(3)-N(12)	1.219(10)
O(4)-N(13)	1.190(10)
O(5)-N(13)	1.252(11)
O(6)-N(13)	1.223(11)
O(7)-H(71)	0.80(2)
O(7)-H(72)	0.81(2)
O(8)-H(81)	0.82(2)
O(8)-H(82)	0.81(2)
N(1A)-C(2A)	1.351(10)
N(1A)-C(6A)	1.393(10)
N(1A)-H(1A)	0.86(9)
N(1B)-C(2B)	1.334(10)
N(1B)-C(6B)	1.361(10)
N(3A)-C(2A)	1.288(10)
N(3A)-C(4A)	1.345(10)
N(3B)-C(2B)	1.328(10)
N(3B)-C(4B)	1.349(10)
N(6A)-C(6A)	1.303(9)
N(6A)-H(6A)	0.90(8)
N(6B)-C(6B)	1.312(9)
N(6B)-H(6B1)	0.8600
N(6B)-H(6B2)	0.8600
N(7A)-C(8A)	1.305(10)
N(7A)-C(5A)	1.403(10)
N(7B)-C(8B)	1.318(10)
N(7B)-C(5B)	1.391(9)
N(9B)-C(8B)	1.347(10)
N(9B)-C(4B)	1.364(9)
N(9B)-C(9B)	1.473(9)
N(9A)-C(4A)	1.366(10)
N(9A)-C(8A)	1.377(10)
N(9A)-C(9A)	1.456(10)
N(10)-H(10A)	0.8900
N(10)-H(10B)	0.8900
N(10)-H(10C)	0.8900
N(11)-H(11A)	0.8900
N(11)-H(11B)	0.8900
N(11)-H(11C)	0.8900
C(2A)-H(2A)	0.9300
C(2B)-H(2B)	0.9300
C(4B)-C(5B)	1.398(10)
C(4A)-C(5A)	1.401(10)
C(5A)-C(6A)	1.417(11)
C(5B)-C(6B)	1.407(10)
C(8B)-H(8B)	0.9300
C(8A)-H(8A)	0.9300
C(9A)-H(9A1)	0.9600
C(9A)-H(9A2)	0.9600
C(9A)-H(9A3)	0.9600
C(9B)-H(9B1)	0.9600
C(9B)-H(9B2)	0.9600
C(9B)-H(9B3)	0.9600

N(6A) - Pt - N(7B)	177.0 (3)
N(6A) - Pt - N(10)	91.3 (3)
N(7B) - Pt - N(10)	90.5 (3)
N(6A) - Pt - N(11)	89.6 (3)
N(7B) - Pt - N(11)	88.6 (3)
N(10) - Pt - N(11)	178.1 (3)
H(71) - O(7) - H(72)	107 (4)
H(81) - O(8) - H(82)	105 (4)
C(2A) - N(1A) - C(6A)	124.0 (8)
C(2A) - N(1A) - H(1A)	113 (6)
C(6A) - N(1A) - H(1A)	122 (6)
C(2B) - N(1B) - C(6B)	118.8 (7)
C(2A) - N(3A) - C(4A)	111.7 (7)
C(2B) - N(3B) - C(4B)	110.9 (7)
C(6A) - N(6A) - Pt	128.2 (6)
C(6A) - N(6A) - H(6A)	119 (6)
Pt - N(6A) - H(6A)	113 (6)
C(6B) - N(6B) - H(6B1)	120.0
C(6B) - N(6B) - H(6B2)	120.0
H(6B1) - N(6B) - H(6B2)	120.0
C(8A) - N(7A) - C(5A)	103.1 (7)
C(8B) - N(7B) - C(5B)	106.2 (7)
C(8B) - N(7B) - Pt	123.1 (6)
C(5B) - N(7B) - Pt	130.7 (5)
C(8B) - N(9B) - C(4B)	107.5 (7)
C(8B) - N(9B) - C(9B)	125.7 (7)
C(4B) - N(9B) - C(9B)	126.8 (7)
C(4A) - N(9A) - C(8A)	105.3 (7)
C(4A) - N(9A) - C(9A)	127.0 (8)
C(8A) - N(9A) - C(9A)	127.7 (8)
Pt - N(10) - H(10A)	109.5
Pt - N(10) - H(10B)	109.5
H(10A) - N(10) - H(10B)	109.5
Pt - N(10) - H(10C)	109.5
H(10A) - N(10) - H(10C)	109.5
H(10B) - N(10) - H(10C)	109.5
Pt - N(11) - H(11A)	109.5
Pt - N(11) - H(11B)	109.5
H(11A) - N(11) - H(11B)	109.5
Pt - N(11) - H(11C)	109.5
H(11A) - N(11) - H(11C)	109.5
H(11B) - N(11) - H(11C)	109.5
O(3) - N(12) - O(1)	120.0 (9)
O(3) - N(12) - O(2)	120.9 (9)
O(1) - N(12) - O(2)	118.7 (9)
O(4) - N(13) - O(6)	122.5 (11)
O(4) - N(13) - O(5)	122.0 (11)
O(6) - N(13) - O(5)	115.4 (10)
N(3A) - C(2A) - N(1A)	126.7 (8)
N(3A) - C(2A) - H(2A)	116.7
N(1A) - C(2A) - H(2A)	116.7
N(3B) - C(2B) - N(1B)	130.0 (8)
N(3B) - C(2B) - H(2B)	115.0
N(1B) - C(2B) - H(2B)	115.0
N(3B) - C(4B) - N(9B)	128.2 (8)
N(3B) - C(4B) - C(5B)	125.4 (8)
N(9B) - C(4B) - C(5B)	106.5 (7)
N(3A) - C(4A) - N(9A)	126.2 (8)
N(3A) - C(4A) - C(5A)	127.6 (8)
N(9A) - C(4A) - C(5A)	106.2 (7)

C(4A) - C(5A) - N(7A)	110.1(7)
C(4A) - C(5A) - C(6A)	118.4(7)
N(7A) - C(5A) - C(6A)	131.5(7)
N(7B) - C(5B) - C(4B)	107.8(7)
N(7B) - C(5B) - C(6B)	133.9(7)
C(4B) - C(5B) - C(6B)	118.3(7)
N(6A) - C(6A) - N(1A)	120.7(7)
N(6A) - C(6A) - C(5A)	127.6(8)
N(1A) - C(6A) - C(5A)	111.6(7)
N(6B) - C(6B) - N(1B)	117.5(7)
N(6B) - C(6B) - C(5B)	125.9(8)
N(1B) - C(6B) - C(5B)	116.6(7)
N(7B) - C(8B) - N(9B)	112.0(8)
N(7B) - C(8B) - H(8B)	124.0
N(9B) - C(8B) - H(8B)	124.0
N(7A) - C(8A) - N(9A)	115.3(8)
N(7A) - C(8A) - H(8A)	122.4
N(9A) - C(8A) - H(8A)	122.4
N(9A) - C(9A) - H(9A1)	109.5
N(9A) - C(9A) - H(9A2)	109.5
H(9A1) - C(9A) - H(9A2)	109.5
N(9A) - C(9A) - H(9A3)	109.5
H(9A1) - C(9A) - H(9A3)	109.5
H(9A2) - C(9A) - H(9A3)	109.5
N(9B) - C(9B) - H(9B1)	109.5
N(9B) - C(9B) - H(9B2)	109.5
H(9B1) - C(9B) - H(9B2)	109.5
N(9B) - C(9B) - H(9B3)	109.5
H(9B1) - C(9B) - H(9B3)	109.5
H(9B2) - C(9B) - H(9B3)	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for trans-[Pt(NH₃)₂(9-made-N6)(9-made-N7)](NO₃)₂·2H₂O.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Pt	33(1)	43(1)	44(1)	15(1)	8(1)	18(1)
O(1)	52(4)	128(7)	67(5)	25(4)	17(4)	47(5)
O(2)	131(8)	193(10)	97(6)	72(6)	57(6)	128(8)
O(3)	82(6)	172(9)	113(7)	74(7)	52(5)	81(6)
O(4)	93(7)	154(9)	158(9)	32(7)	22(6)	89(7)
O(5)	100(7)	107(8)	168(10)	23(7)	43(7)	44(6)
O(6)	85(7)	99(7)	226(12)	55(8)	35(7)	53(6)
O(7)	69(5)	79(6)	97(6)	13(5)	30(5)	19(4)
O(8)	110(10)	190(13)	218(13)	106(11)	16(9)	32(8)
N(1A)	48(5)	48(5)	58(5)	18(4)	26(4)	22(4)
N(1B)	32(4)	65(5)	51(5)	14(4)	8(3)	16(4)
N(3A)	62(5)	47(5)	57(5)	15(4)	22(4)	22(4)
N(3B)	39(4)	52(5)	61(5)	5(4)	12(4)	10(4)
N(6A)	36(4)	52(5)	52(5)	23(4)	6(4)	21(4)
N(6B)	43(4)	49(5)	59(5)	13(4)	6(4)	26(4)
N(7A)	45(5)	54(5)	59(5)	13(4)	14(4)	20(4)
N(7B)	39(4)	48(4)	40(4)	6(3)	4(3)	21(4)
N(9B)	45(4)	51(5)	60(5)	23(4)	21(4)	30(4)

N(9A)	54(5)	47(5)	57(5)	13(4)	12(4)	25(4)
N(10)	65(5)	53(5)	54(5)	17(4)	14(4)	30(4)
N(11)	53(5)	58(5)	45(4)	6(4)	6(4)	25(4)
N(12)	64(6)	105(8)	57(6)	7(5)	11(5)	51(6)
N(13)	71(7)	57(6)	110(8)	2(6)	19(6)	31(6)
C(2A)	48(6)	43(6)	64(6)	9(5)	19(5)	9(5)
C(2B)	29(5)	57(6)	68(6)	-1(5)	7(5)	13(5)
C(4B)	34(5)	37(5)	44(5)	-3(4)	3(4)	11(4)
C(4A)	46(5)	47(5)	41(5)	2(4)	7(4)	17(5)
C(5A)	43(5)	33(5)	42(5)	4(4)	5(4)	15(4)
C(5B)	37(5)	37(5)	41(5)	3(4)	6(4)	12(4)
C(6A)	42(5)	36(5)	46(5)	5(4)	13(4)	14(4)
C(6B)	41(5)	37(5)	38(5)	2(4)	1(4)	14(4)
C(8B)	46(6)	71(7)	50(6)	18(5)	10(5)	27(5)
C(8A)	44(6)	54(6)	71(7)	10(5)	9(5)	24(5)
C(9A)	83(8)	58(6)	71(7)	17(5)	-1(6)	43(6)
C(9B)	75(8)	68(7)	107(9)	57(6)	40(7)	44(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for trans-[Pt(NH₃)₂(9-made-N6)(9-made-N7)](NO₃)₂·2H₂O.

	x	y	z	U(eq)
H(71)	8590(8)	1430(9)	1230(14)	123
H(72)	8560(8)	2300(6)	400(14)	123
H(81)	9270(17)	0(9)	2800(2)	268
H(82)	10170(14)	930(16)	3200(19)	268
H(1A)	3750(8)	1370(8)	6430(11)	72
H(6A)	4510(8)	2610(7)	4310(10)	68
H(6B1)	9949	3293	4333	58
H(6B2)	8695	3248	4112	58
H(10A)	5615	1820	1767	81
H(10B)	6877	2259	1612	81
H(10C)	6074	2714	648	81
H(11A)	6139	4676	5773	76
H(11B)	6841	5529	4754	76
H(11C)	7417	4946	5897	76
H(2A)	3746	88	8074	64
H(2B)	12022	6132	1787	62
H(8B)	6761	5590	1089	64
H(8A)	8653	1097	5956	65
H(9A1)	7399	-394	9274	100
H(9A2)	8389	-342	8181	100
H(9A3)	7100	-1235	7743	100
H(9B1)	7756	7212	-591	113
H(9B2)	8874	7110	-1260	113
H(9B3)	9036	7913	275	113

Table 6. Torsion angles [deg] for trans-[Pt(NH₃)₂(9-made-N6)(9-made-N7)](NO₃)₂·2H₂O.

N(7B) - Pt - N(6A) - C(6A)	-150(5)
N(10) - Pt - N(6A) - C(6A)	84.5(8)
N(11) - Pt - N(6A) - C(6A)	-97.2(8)
N(6A) - Pt - N(7B) - C(8B)	-28(6)
N(10) - Pt - N(7B) - C(8B)	97.7(7)
N(11) - Pt - N(7B) - C(8B)	-80.6(7)
N(6A) - Pt - N(7B) - C(5B)	149(5)
N(10) - Pt - N(7B) - C(5B)	-85.7(7)
N(11) - Pt - N(7B) - C(5B)	95.9(7)
C(4A) - N(3A) - C(2A) - N(1A)	0.0(14)
C(6A) - N(1A) - C(2A) - N(3A)	-1.9(15)
C(4B) - N(3B) - C(2B) - N(1B)	-0.1(14)
C(6B) - N(1B) - C(2B) - N(3B)	-0.6(15)
C(2B) - N(3B) - C(4B) - N(9B)	-179.4(8)
C(2B) - N(3B) - C(4B) - C(5B)	1.1(12)
C(8B) - N(9B) - C(4B) - N(3B)	-179.6(8)
C(9B) - N(9B) - C(4B) - N(3B)	1.6(15)
C(8B) - N(9B) - C(4B) - C(5B)	0.0(9)
C(9B) - N(9B) - C(4B) - C(5B)	-178.8(8)
C(2A) - N(3A) - C(4A) - N(9A)	-178.2(8)
C(2A) - N(3A) - C(4A) - C(5A)	0.5(13)
C(8A) - N(9A) - C(4A) - N(3A)	-179.5(8)
C(9A) - N(9A) - C(4A) - N(3A)	-0.7(15)
C(8A) - N(9A) - C(4A) - C(5A)	1.6(9)
C(9A) - N(9A) - C(4A) - C(5A)	-179.5(8)
N(3A) - C(4A) - C(5A) - N(7A)	179.4(8)
N(9A) - C(4A) - C(5A) - N(7A)	-1.7(10)
N(3A) - C(4A) - C(5A) - C(6A)	0.9(13)
N(9A) - C(4A) - C(5A) - C(6A)	179.8(7)
C(8A) - N(7A) - C(5A) - C(4A)	1.1(9)
C(8A) - N(7A) - C(5A) - C(6A)	179.3(9)
C(8B) - N(7B) - C(5B) - C(4B)	1.2(9)
Pt - N(7B) - C(5B) - C(4B)	-175.8(5)
C(8B) - N(7B) - C(5B) - C(6B)	-178.4(9)
Pt - N(7B) - C(5B) - C(6B)	4.6(14)
N(3B) - C(4B) - C(5B) - N(7B)	178.9(8)
N(9B) - C(4B) - C(5B) - N(7B)	-0.7(9)
N(3B) - C(4B) - C(5B) - C(6B)	-1.4(12)
N(9B) - C(4B) - C(5B) - C(6B)	179.0(7)
Pt - N(6A) - C(6A) - N(1A)	171.4(6)
Pt - N(6A) - C(6A) - C(5A)	-10.9(14)
C(2A) - N(1A) - C(6A) - N(6A)	-179.0(9)
C(2A) - N(1A) - C(6A) - C(5A)	3.0(12)
C(4A) - C(5A) - C(6A) - N(6A)	179.7(8)
N(7A) - C(5A) - C(6A) - N(6A)	1.6(15)
C(4A) - C(5A) - C(6A) - N(1A)	-2.5(11)
N(7A) - C(5A) - C(6A) - N(1A)	179.4(8)
C(2B) - N(1B) - C(6B) - N(6B)	179.6(8)
C(2B) - N(1B) - C(6B) - C(5B)	0.3(12)
N(7B) - C(5B) - C(6B) - N(6B)	1.0(15)
C(4B) - C(5B) - C(6B) - N(6B)	-178.6(8)
N(7B) - C(5B) - C(6B) - N(1B)	-179.8(8)
C(4B) - C(5B) - C(6B) - N(1B)	0.6(11)
C(5B) - N(7B) - C(8B) - N(9B)	-1.2(10)
Pt - N(7B) - C(8B) - N(9B)	176.1(5)
C(4B) - N(9B) - C(8B) - N(7B)	0.8(10)

C (9B) -N(9B) -C (8B) -N(7B)	179.6 (8)
C (5A) -N(7A) -C (8A) -N(9A)	0.0 (10)
C (4A) -N(9A) -C (8A) -N(7A)	-1.0 (11)
C (9A) -N(9A) -C (8A) -N(7A)	-179.9 (8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen-bonds for trans-[Pt(NH₃)₂ (9-made-N6) (9-made-N7)] (NO₃)₂·2H₂O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7) -H(71) ...O(8)	0.80 (2)	2.06 (2)	2.864 (14)	176 (11)
O(7) -H(72) ...N(3B) #1	0.81 (2)	2.12 (4)	2.911 (10)	164 (12)
O(8) -H(81) ...O(6) #2	0.82 (2)	1.99 (8)	2.772 (16)	159 (23)
O(8) -H(82) ...O(4) #3	0.81 (2)	2.40 (14)	3.12 (2)	148 (24)
N(1A) -H(1A) ...O(6)	0.86 (9)	2.02 (9)	2.855 (11)	163 (9)
N(6A) -H(6A) ...O(5)	0.90 (8)	2.36 (9)	3.213 (11)	157 (7)
N(6B) -H(6B2) ...N(7A)	0.86	2.34	3.082 (10)	144.0
N(6B) -H(6B1) ...O(4) #3	0.86	2.30	3.134 (10)	164.5
N(10) -H(10A) ...N(3A) #2	0.89	2.24	3.063 (10)	154.2
N(10) -H(10B) ...O(7)	0.89	2.09	2.942 (10)	159.5
N(10) -H(10C) ...O(1) #4	0.89	2.10	2.985 (9)	169.8
N(11) -H(11A) ...O(2)	0.89	2.19	3.082 (10)	176.1
N(11) -H(11B) ...O(5) #5	0.89	2.34	3.091 (12)	142.8
N(11) -H(11C) ...N(1B) #6	0.89	2.15	3.037 (9)	170.7

Symmetry transformations used to generate equivalent atoms:

#1 -x+2, -y+1, -z #2 -x+1, -y, -z+1 #3 x+1, y, z
 #4 x, y, z-1 #5 -x+1, -y+1, -z+1 #6 -x+2, -y+1, -z+1