Supplementary Material (ESI) for Dalton Transactions

Synthesis and NMR characterization of the *cis* and *trans* isomers of $[Pt^{II}(N^9\text{-adeH})_2(pz)_2]$ and X-ray crystallography of the *trans* isomer

Karel D. Klika,*[a,b] Henri Kivelä,[a] Vladimir V. Ovcharenko,[a]
Ville Nieminen,[c] Reijo Sillanpää[d] and Jorma Arpalahti[a]

[a] *Department of Chemistry, University of Turku, Vatselankatu 2, FIN-20014 Turku, Finland. E-mail: klikakd@yahoo.co.uk,* [b] *The UNSW Analytical Centre, Chemical Sciences Building (F10), University of New South Wales, Sydney, Australia NSW 2052,* [c] *Laboratory of Industrial Chemistry, Process Chemistry Centre, Åbo Akademi University, Piispankatu 8, FIN-20500 Turku, Finland,* [d] *Department of Chemistry, University of Jyväskylä, Survontie 9, FIN-40014 Jyväskylä, Finland*

Electronic Supplementary Information:

Tables of NMR and MS data for **1**–**3** and the free ligands;

the X-ray structure of *trans*-$[Pt^{II}(N^9\text{-adeH})_2(pz)_2](NO_3)_4\cdot H_2O$ (**2**);

X-ray structure tables including cif file and atomic coordinates;

Cartesian coordinates of the optimized structures of **2** and **3** (also available as separate files).

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Table 1 ^{195}Pt, ^{13}C, and ^{15}N chemical shifts[a] (δ, ppm) for compounds **1**–**3** and the free ligands

	Pt[b]	C-2	C-4	C-5	C-6	C-8	Cα	Cβ	N-1	N-3	N-6	N-7	N-9	N–Pt	Nγ
pyrazine	–	–	–	–	–	–	147.63		–	–	–	–	–	–62.06	
adenine[c]	–	154.68[d]	no	118.8	156.9	143.1[d]	–	–	Not measured.					–	–
adenine[e]	–	152.29	150.2	118.3	155.6	138.9	–	–	–145.0	–155.1	–301.1	–139.7	–223.1	–	–
1	–2450	–	–	–	–	–	149.35	152.17	–	–	–	–	–	–168.7	–42.8
2[f]	–2387, –2423 (5:1)	148.76	157.65	118.65	152.69	151.57	150.32	151.02	–210.6	–155.4	no	–171.7	–234.4	–166.5	–46.6
3[f]	–2412, –2381 (3:1)	150.22	157.59	117.50	152.55	151.49	149.04	151.57	–210.1	–153.9	no	–181.7	–242.5	–160.4	–47.4
2[g]	Not measured.	151.42	158.0	120.7	155.7	151.63	150.12	150.68	Not measured.						
3[g]	–2400, –2370 (8:1)	153.92	158.56	121.95	157.84	151.85	150.13	151.01	–158.9 ↔ –156.2		no	–151.7	–249.6	–152.6	–49.1

Legend: no, not observed. [a] Spectra acquired in D_2O or H_2O/D_2O mixtures at 25 °C and referenced internally to TSP for carbon (0 ppm) and externally to nitromethane for nitrogen (0 ppm) and $[PtCl_4]^{2-}$ for platinum (–1625 ppm); for ^{13}C and ^{15}N, shifts given to one decimal place indicate that they were acquired indirectly or are very broad signals in directly-measured spectra. [b] Two platinum signals were observed for **2** and **3** with the respective ratio given in parentheses. [c] Acquired in D_2O/DMSO-d_6 (*ca.* 2:1). [d] In D_2O: 155.4 (C-2); 143.9 (C-8). [e] Acquired in DMSO-d_6. [f] Spectra of the tetraprotonated species. [g] Spectra of the neutral complexes.

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Table 2 ^{1}H NMR data[a] (δ, ppm; J, Hz) for compounds **1**–**3** and the free ligands and MS (% RA) for compounds **1**–**3**

	H-2, H-8	Hα, Hβ	NH_2s	$J_{\alpha,\beta}$[b]	$J_{\alpha,\alpha}$, $J_{\beta,\beta}$[b]	Prominent ions[c] from ESI$^+$/FAB$^+$-MS with RAs and tentative assignments; ^{1}H NMR in other solvents; other comments
pyrazine	–	8.654, s	–	–	–	–
adenine	8.222, s; 8.174, s	–	no	–	–	In D_2O/DMSO-d_6 (*ca.* 2:1): 8.229 (s, H-2), 8.208 (s, H-8); H-6s and H-9 not observed. In DMSO-d_6: 12.828, (v b s, H-9); 7.088 (2H, b s, H-6s); 8.114 (s, H-2), 8.098 (s, H-8).
1	–	9.053, m; 8.839, m	–	3.40, 1.23	0.00, –0.68	ESI$^+$: 583[d] (3.65, [Pt(pz)$_3$TSP]); 576 (0.43, [Pt(pz)$_4$]·NO_3); 503 (12.9, [Pt(pz)$_2$TSP]); 496 (3.83, [Pt(pz)$_3$]·NO_3); 423 (9.33, [Pt(pz)TSP]); 416 (46.0, [Pt(pz)$_2$]·NO_3).
2[e]	8.368, s; 8.509, s	8.772, m; 8.602, m	no	3.45, 1.22	–0.01, –0.65	FAB$^+$: 623.1402 ([^{194}Pt(ade)$_2$(pz)$_2$] + H); 624.1428 ([^{195}Pt(ade)$_2$(pz)$_2$] + H). calc: 623.1387 (78.0, [^{194}Pt(ade)$_2$(pz)$_2$] + H); 624.1408 (100, [^{195}Pt(ade)$_2$(pz)$_2$] + H). ESI$^+$: 685! (1.35, [Pt^{III}(ade)$_2$(pz)$_2$]·NO_3); 623[e] (8.87, [Pt(ade)$_2$(pz)$_2$] + H); 543 (12.0, [Pt(ade)$_2$(pz)] + H); 463 (10.7, [Pt(ade)$_2$] + H); 408 (26.9, [Pt(ade)(pz)]).
3[e]	8.459, s; 8.582, s	9.145, m; 8.841, m	no	3.41, 1.24	–0.11, –0.63	FAB$^+$: 623.1390 (83.1, [^{194}Pt(ade)$_2$(pz)$_2$] + H); 624.1412 (100, [^{195}Pt(ade)$_2$(pz)$_2$] + H); 625 (91.0); 626 (25.4); 627 (21.4); 628 (5.96); 543 (6.44, [Pt(ade)$_2$(pz)] + H). calc: 623.1387 (78.0, [^{194}Pt(ade)$_2$(pz)$_2$] + H); 624.1408 (100, [^{195}Pt(ade)$_2$(pz)$_2$] + H); 625 (82.8); 626 (18.0); 627 (19.2); 628 (4.51).
2[f]	8.267, s; 8.279, s	8.694, m; 8.562, m	7.17 b s	3.46, 1.23	–0.11, –0.62	MS not measured. For a sample of tetraprotonated **2** examined under quality conditions ($\upsilon_{½,TSP}$ = 0.21 Hz), $^{6}J_{H2,H8}$ was observable (J = 0.18 Hz) by the multiplicity of H-2. Though H-8 remained as a "singlet" due to its linewidth ($\upsilon_{½,H8}$, 0.44; $\upsilon_{½,H2}$, 0.26 Hz), its shape was correctly simulated by Perch.[1] For adenine (N^9 tautomer), a value of 0.15 Hz was calculated[2] for $^{6}J_{H2,H8}$.
3[f]	8.282, s; 8.082, s	9.079, m; 8.811, m	6.50 b s	3.41, 1.21	–0.02, –0.61	ESI$^+$: 1267 (3.65, {[Pt(ade)$_2$(pz)$_2$]}$_2$ + Na); 1187 (2.42, [Pt(ade)$_2$(pz)$_2$] + [Pt(ade)$_2$(pz)] + Na); 1110 (3.08, [Pt(ade)$_2$(pz)$_2$] + [Pt(ade)(pz)$_2$]); 645 (95.2, [Pt(ade)$_2$(pz)$_2$] + Na); 565 (48.1, [Pt(ade)$_2$(pz)] + Na); 485 (40.0, [Pt(ade)$_2$] + Na); 408 (18.1, [Pt(ade)(pz)]).

Legend: b, broad; m, multiplet; no, not observed; s, singlet. [a] NMR spectra acquired in D_2O or H_2O/D_2O mixtures at 25 °C and referenced to TSP (0 ppm). [b] Couplings extracted using Perch simulation.[1] The signs of the couplings were assumed based on the number of intervening bonds, *i.e.* if n is even, ^{n}J was entered as a negative value prior to initiation of the iteration; if n is odd, ^{n}J was entered as a positive value. [c] All ions provided patterns consistent with the natural isotopic distribution of platinum and only ions of the ^{194}Pt and/or ^{195}Pt isotopomers (except in one case) are reported as nominal values relative to the highest mass ligand when it is the base peak; corresponding Na^+ (H^+) adducts also present at weaker intensities for each H^+ (Na^+) adduct; TSP = d_4-trimethylsilyl propanoate. [d] Results confirmed by FAB$^+$ analysis and HRMS on the ^{194}Pt and ^{195}Pt isotopomers. [e] Spectra of the tetraprotonated species. [f] Spectra of the neutral complexes.

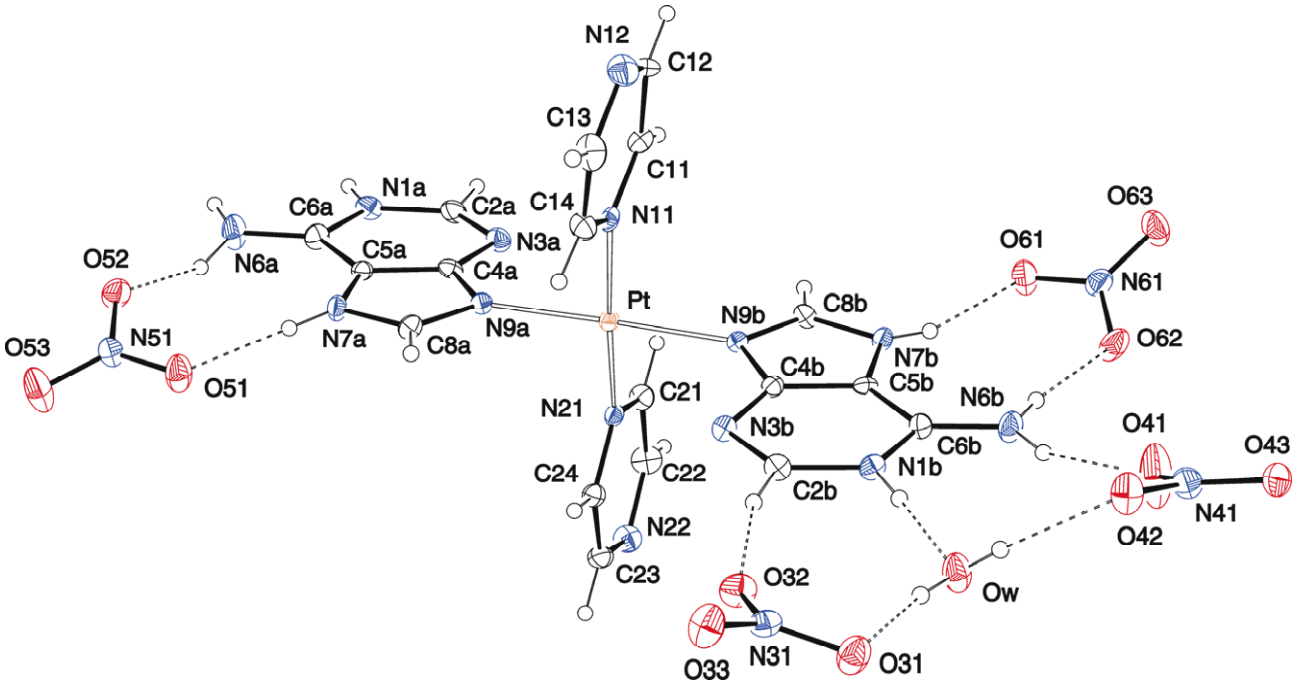

Fig. ESI1 The X-ray structure of *trans*-[Pt^{II}(N^9-adeH)$_2$(pz)$_2$](NO$_3$)$_4$·H$_2$O (**2**).

Table 1. Crystal data and structure refinement for **2**.

Identification code arpa1u

Empirical formula C18 H22 N18 O13 Pt

Formula weight 893.63

Temperature 173(2) K

Wavelength 0.71073 A

Crystal system, space group Monoclinic, P 21/c

Unit cell dimensions a = 10.8863(2) A alpha = 90 deg.
b = 11.0417(3) A beta = 95.512(2) deg.
c = 24.5202(7) A gamma = 90 deg.

Volume 2933.78(13) A^3

Z, 4

Calculated density 2.023 Mg/m^3

Absorption coefficient 4.881 mm^-1

F(000) 1752

Crystal size 0.16 x 0.14 x 0.12 mm

Theta range for data collection 2.39 to 26.37 deg.

Limiting indices -13<=h<=11, -12<=k<=13, -24<=l<=30

Reflections collected / unique 18581 / 5988 [R(int) = 0.0513]

Completeness to theta = 26.37 99.6 %

Absorption correction Empirical (SHELXA)

Max. and min. transmission 0.557 and 0.448

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 5988 / 0 / 493

Goodness-of-fit on F^2 1.070

Final R indices [I>2sigma(I)] R1 = 0.0348, wR2 = 0.0643

R indices (all data) R1 = 0.0457, wR2 = 0.0686

Largest diff. peak and hole 0.637 and -0.660 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pt	-98(1)	8595(1)	1186(1)	18(1)
OW	4422(4)	7349(5)	-1196(2)	41(1)
N(1A)	-3566(4)	9925(4)	2600(2)	26(1)
C(2A)	-2345(5)	9632(5)	2670(2)	28(1)
N(3A)	-1670(4)	9340(4)	2279(2)	27(1)
C(4A)	-2313(4)	9384(5)	1780(2)	21(1)
C(5A)	-3528(4)	9717(5)	1665(2)	20(1)
C(6A)	-4237(5)	10001(5)	2099(2)	26(1)
N(6A)	-5403(4)	10298(6)	2052(2)	40(1)
N(7A)	-3794(4)	9664(4)	1108(2)	25(1)
C(8A)	-2774(4)	9303(5)	897(2)	23(1)
N(9A)	-1844(3)	9109(4)	1293(2)	19(1)
N(1B)	3373(4)	7527(4)	-271(2)	23(1)
C(2B)	2175(5)	7896(5)	-333(2)	23(1)
N(3B)	1495(3)	8130(4)	66(2)	21(1)
C(4B)	2114(4)	7958(4)	569(2)	19(1)
C(5B)	3338(4)	7613(4)	665(2)	19(1)
N(6B)	5164(4)	6969(5)	253(2)	31(1)
C(6B)	4024(4)	7356(5)	225(2)	24(1)
N(7B)	3596(4)	7568(4)	1228(2)	21(1)
C(8B)	2566(4)	7873(5)	1444(2)	21(1)
N(9B)	1646(3)	8112(4)	1066(2)	20(1)
N(11)	-603(3)	6864(4)	1036(2)	21(1)
N(12)	-1141(4)	4432(4)	856(2)	36(1)
C(11)	-442(4)	6055(5)	1445(2)	24(1)
C(12)	-722(5)	4849(5)	1347(2)	27(1)
C(13)	-1302(5)	5253(6)	457(3)	37(2)
C(14)	-1053(4)	6467(5)	542(2)	28(1)
N(21)	478(3)	10288(4)	1362(2)	21(1)
N(22)	1364(4)	12596(4)	1603(2)	33(1)
C(21)	942(5)	10579(5)	1876(2)	26(1)
C(22)	1369(5)	11730(5)	1985(2)	35(1)
C(23)	902(5)	12284(5)	1104(2)	28(1)
C(24)	461(4)	11127(5)	974(2)	23(1)
N(31)	1925(4)	7563(4)	-2131(2)	30(1)
O(31)	3037(3)	7463(4)	-2219(2)	40(1)
O(32)	1668(4)	7915(4)	-1670(2)	37(1)
O(33)	1094(4)	7309(4)	-2497(2)	44(1)
N(41)	6840(4)	5390(5)	-933(2)	33(1)
O(41)	6714(4)	5982(6)	-517(2)	74(2)
O(42)	5942(3)	5321(4)	-1298(2)	40(1)
O(43)	7818(3)	4858(4)	-995(2)	36(1)
N(51)	-6680(4)	10764(5)	584(2)	31(1)
O(51)	-5704(3)	10456(4)	385(2)	41(1)
O(52)	-6824(3)	10515(4)	1069(2)	37(1)
O(53)	-7501(4)	11277(5)	286(2)	58(2)
N(61)	6375(4)	6247(5)	1722(2)	33(1)
O(61)	5488(3)	6782(4)	1923(2)	40(1)
O(62)	6631(3)	6539(5)	1251(2)	48(1)
O(63)	6972(4)	5489(5)	1998(2)	49(1)

Table 3. Bond lengths [A] and angles [deg] for **2**.

Pt-N(21) 2.006(4)
Pt-N(11) 2.013(4)
Pt-N(9B) 2.020(4)
Pt-N(9A) 2.025(4)
OW-H(1OW) 0.84(7)
OW-H(2OW) 0.73(7)
N(1A)-C(2A) 1.363(7)
N(1A)-C(6A) 1.369(7)
N(1A)-H(1A) 0.84(6)
C(2A)-N(3A) 1.304(7)
C(2A)-H(2A) 0.94(6)
N(3A)-C(4A) 1.352(6)
C(4A)-C(5A) 1.376(7)
C(4A)-N(9A) 1.376(6)
C(5A)-N(7A) 1.370(6)
C(5A)-C(6A) 1.409(7)
C(6A)-N(6A) 1.306(7)
N(6A)-H(6A1) 0.98(7)
N(6A)-H(6A2) 0.83(6)
N(7A)-C(8A) 1.330(6)
N(7A)-H(7A) 0.87(6)
C(8A)-N(9A) 1.349(6)
C(8A)-H(8A) 0.94(5)
N(1B)-C(6B) 1.361(7)
N(1B)-C(2B) 1.361(6)
N(1B)-H(1B) 0.81(6)
C(2B)-N(3B) 1.308(6)
C(2B)-H(2B) 0.98(5)
N(3B)-C(4B) 1.362(6)
C(4B)-N(9B) 1.375(6)
C(4B)-C(5B) 1.385(6)
C(5B)-N(7B) 1.382(6)
C(5B)-C(6B) 1.400(7)
N(6B)-C(6B) 1.308(7)
N(6B)-H(6B1) 0.75(6)
N(6B)-H(6B2) 0.82(6)
N(7B)-C(8B) 1.330(6)
N(7B)-H(7B) 0.76(5)
C(8B)-N(9B) 1.325(6)
C(8B)-H(8B) 0.87(5)
N(11)-C(14) 1.337(7)
N(11)-C(11) 1.342(7)
N(12)-C(12) 1.328(7)
N(12)-C(13) 1.331(8)
C(11)-C(12) 1.383(7)
C(11)-H(11) 0.9500
C(12)-H(12) 0.9500
C(13)-C(14) 1.379(8)
C(13)-H(13) 0.9500
C(14)-H(14) 0.9500
N(21)-C(24) 1.327(6)
N(21)-C(21) 1.351(6)
N(22)-C(23) 1.325(7)
N(22)-C(22) 1.337(7)
C(21)-C(22) 1.370(8)
C(21)-H(21) 0.9500
C(22)-H(22) 0.9500
C(23)-C(24) 1.390(7)
C(23)-H(23) 0.9500
C(24)-H(24) 0.9500
N(31)-O(33) 1.243(6)
N(31)-O(32) 1.252(6)

N(31)-O(31) 1.255(6)
N(41)-O(41) 1.231(6)
N(41)-O(43) 1.238(6)
N(41)-O(42) 1.263(6)
N(51)-O(53) 1.236(6)
N(51)-O(52) 1.247(6)
N(51)-O(51) 1.257(5)
N(61)-O(63) 1.223(6)
N(61)-O(62) 1.256(6)
N(61)-O(61) 1.271(6)

N(21)-Pt-N(11) 177.02(16)
N(21)-Pt-N(9B) 89.91(16)
N(11)-Pt-N(9B) 88.10(16)
N(21)-Pt-N(9A) 89.38(16)
N(11)-Pt-N(9A) 92.65(16)
N(9B)-Pt-N(9A) 178.65(17)
H(1OW)-OW-H(2OW) 113(7)
C(2A)-N(1A)-C(6A) 123.8(4)
C(2A)-N(1A)-H(1A) 118(4)
C(6A)-N(1A)-H(1A) 118(4)
N(3A)-C(2A)-N(1A) 125.3(5)
N(3A)-C(2A)-H(2A) 121(3)
N(1A)-C(2A)-H(2A) 113(3)
C(2A)-N(3A)-C(4A) 112.2(4)
N(3A)-C(4A)-C(5A) 126.8(5)
N(3A)-C(4A)-N(9A) 125.1(4)
C(5A)-C(4A)-N(9A) 108.1(4)
N(7A)-C(5A)-C(4A) 107.5(4)
N(7A)-C(5A)-C(6A) 133.2(5)
C(4A)-C(5A)-C(6A) 119.3(5)
N(6A)-C(6A)-N(1A) 121.6(5)
N(6A)-C(6A)-C(5A) 126.0(5)
N(1A)-C(6A)-C(5A) 112.4(4)
C(6A)-N(6A)-H(6A1) 118(4)
C(6A)-N(6A)-H(6A2) 120(5)
H(6A1)-N(6A)-H(6A2) 122(6)
C(8A)-N(7A)-C(5A) 107.1(4)
C(8A)-N(7A)-H(7A) 116(4)
C(5A)-N(7A)-H(7A) 136(4)
N(7A)-C(8A)-N(9A) 111.5(5)
N(7A)-C(8A)-H(8A) 125(3)
N(9A)-C(8A)-H(8A) 124(3)
C(8A)-N(9A)-C(4A) 105.9(4)
C(8A)-N(9A)-Pt 126.9(3)
C(4A)-N(9A)-Pt 127.2(3)
C(6B)-N(1B)-C(2B) 123.5(4)
C(6B)-N(1B)-H(1B) 118(4)
C(2B)-N(1B)-H(1B) 118(4)
N(3B)-C(2B)-N(1B) 125.5(5)
N(3B)-C(2B)-H(2B) 123(3)
N(1B)-C(2B)-H(2B) 112(3)
C(2B)-N(3B)-C(4B) 112.6(4)
N(3B)-C(4B)-N(9B) 126.3(4)
N(3B)-C(4B)-C(5B) 125.2(4)
N(9B)-C(4B)-C(5B) 108.5(4)
N(7B)-C(5B)-C(4B) 106.2(4)
N(7B)-C(5B)-C(6B) 133.7(5)
C(4B)-C(5B)-C(6B) 120.0(5)
C(6B)-N(6B)-H(6B1) 120(5)
C(6B)-N(6B)-H(6B2) 124(4)
H(6B1)-N(6B)-H(6B2) 116(6)
N(6B)-C(6B)-N(1B) 120.2(5)
N(6B)-C(6B)-C(5B) 126.7(5)
N(1B)-C(6B)-C(5B) 113.0(4)

C(8B)-N(7B)-C(5B) 106.9(4)
C(8B)-N(7B)-H(7B) 131(4)
C(5B)-N(7B)-H(7B) 122(4)
N(9B)-C(8B)-N(7B) 112.4(5)
N(9B)-C(8B)-H(8B) 128(3)
N(7B)-C(8B)-H(8B) 120(3)
C(8B)-N(9B)-C(4B) 106.0(4)
C(8B)-N(9B)-Pt 127.4(3)
C(4B)-N(9B)-Pt 126.5(3)
C(14)-N(11)-C(11) 118.0(5)
C(14)-N(11)-Pt 123.1(4)
C(11)-N(11)-Pt 118.8(3)
C(12)-N(12)-C(13) 116.0(5)
N(11)-C(11)-C(12) 120.0(5)
N(11)-C(11)-H(11) 120.0
C(12)-C(11)-H(11) 120.0
N(12)-C(12)-C(11) 122.9(5)
N(12)-C(12)-H(12) 118.6
C(11)-C(12)-H(12) 118.6
N(12)-C(13)-C(14) 122.8(6)
N(12)-C(13)-H(13) 118.6
C(14)-C(13)-H(13) 118.6
N(11)-C(14)-C(13) 120.3(5)
N(11)-C(14)-H(14) 119.8
C(13)-C(14)-H(14) 119.8
C(24)-N(21)-C(21) 118.8(5)
C(24)-N(21)-Pt 120.9(4)
C(21)-N(21)-Pt 120.3(4)
C(23)-N(22)-C(22) 115.9(5)
N(21)-C(21)-C(22) 119.4(5)
N(21)-C(21)-H(21) 120.3
C(22)-C(21)-H(21) 120.3
N(22)-C(22)-C(21) 123.3(5)
N(22)-C(22)-H(22) 118.4
C(21)-C(22)-H(22) 118.4
N(22)-C(23)-C(24) 122.9(5)
N(22)-C(23)-H(23) 118.6
C(24)-C(23)-H(23) 118.6
N(21)-C(24)-C(23) 119.8(5)
N(21)-C(24)-H(24) 120.1
C(23)-C(24)-H(24) 120.1
O(33)-N(31)-O(32) 120.8(5)
O(33)-N(31)-O(31) 120.3(5)
O(32)-N(31)-O(31) 119.0(5)
O(41)-N(41)-O(43) 121.2(5)
O(41)-N(41)-O(42) 118.7(5)
O(43)-N(41)-O(42) 120.1(5)
O(53)-N(51)-O(52) 121.0(4)
O(53)-N(51)-O(51) 119.0(5)
O(52)-N(51)-O(51) 119.9(4)
O(63)-N(61)-O(62) 122.0(5)
O(63)-N(61)-O(61) 119.2(5)
O(62)-N(61)-O(61) 118.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pt	17(1)	18(1)	19(1)	0(1)	5(1)	1(1)
OW	34(2)	61(4)	26(2)	-2(2)	5(2)	15(2)
N(1A)	34(3)	29(3)	19(2)	1(2)	10(2)	5(2)
C(2A)	33(3)	31(3)	20(3)	8(2)	6(2)	5(2)
N(3A)	27(2)	33(3)	20(2)	5(2)	2(2)	5(2)
C(4A)	28(3)	20(3)	16(3)	4(2)	3(2)	3(2)
C(5A)	21(2)	17(3)	22(3)	2(2)	4(2)	1(2)
C(6A)	27(3)	30(3)	22(3)	-2(2)	8(2)	1(2)
N(6A)	28(3)	70(4)	23(3)	6(3)	13(2)	17(3)
N(7A)	17(2)	33(3)	26(3)	0(2)	4(2)	5(2)
C(8A)	23(2)	27(3)	19(3)	-4(2)	5(2)	0(2)
N(9A)	20(2)	20(2)	17(2)	-2(2)	3(2)	1(2)
N(1B)	26(2)	27(3)	18(2)	-3(2)	7(2)	1(2)
C(2B)	28(3)	26(3)	15(3)	-4(2)	1(2)	1(2)
N(3B)	21(2)	23(2)	18(2)	-5(2)	2(2)	-2(2)
C(4B)	19(2)	15(3)	23(3)	-1(2)	5(2)	-1(2)
C(5B)	24(2)	17(3)	15(2)	2(2)	6(2)	-3(2)
N(6B)	25(2)	47(3)	24(3)	2(3)	9(2)	6(2)
C(6B)	22(2)	23(3)	29(3)	1(2)	5(2)	2(2)
N(7B)	16(2)	27(3)	21(2)	1(2)	3(2)	1(2)
C(8B)	24(3)	25(3)	16(3)	-2(2)	1(2)	4(2)
N(9B)	18(2)	19(2)	23(2)	2(2)	6(2)	0(2)
N(11)	15(2)	24(2)	26(2)	-3(2)	6(2)	0(2)
N(12)	39(3)	27(3)	41(3)	-5(2)	0(2)	0(2)
C(11)	24(3)	26(3)	24(3)	-3(2)	6(2)	-3(2)
C(12)	32(3)	18(3)	32(3)	9(2)	5(2)	0(2)
C(13)	35(3)	41(4)	34(3)	-10(3)	-5(3)	0(3)
C(14)	29(3)	28(3)	28(3)	1(3)	0(2)	0(2)
N(21)	16(2)	26(3)	21(2)	3(2)	5(2)	2(2)
N(22)	37(3)	29(3)	33(3)	-6(2)	5(2)	-2(2)
C(21)	28(3)	29(3)	22(3)	-2(2)	0(2)	-1(2)
C(22)	41(3)	35(4)	27(3)	-7(3)	3(2)	-2(3)
C(23)	31(3)	24(3)	32(3)	5(2)	12(2)	3(2)
C(24)	25(3)	22(3)	23(3)	-1(2)	9(2)	4(2)
N(31)	34(3)	25(3)	30(3)	2(2)	5(2)	-5(2)
O(31)	33(2)	57(3)	30(2)	-1(2)	8(2)	0(2)
O(32)	47(2)	41(3)	23(2)	-4(2)	12(2)	1(2)
O(33)	35(2)	64(3)	32(2)	-12(2)	-4(2)	-4(2)
N(41)	35(3)	40(3)	24(3)	4(2)	7(2)	7(2)
O(41)	53(3)	132(5)	34(3)	-37(3)	-5(2)	40(3)
O(42)	35(2)	57(3)	27(2)	-9(2)	1(2)	7(2)
O(43)	33(2)	36(3)	40(2)	-1(2)	12(2)	7(2)
N(51)	27(2)	35(3)	30(3)	0(2)	1(2)	4(2)
O(51)	29(2)	65(3)	31(2)	-1(2)	8(2)	13(2)
O(52)	31(2)	52(3)	27(2)	9(2)	5(2)	-2(2)
O(53)	47(3)	102(4)	27(2)	14(3)	11(2)	40(3)
N(61)	25(2)	43(3)	31(3)	8(2)	0(2)	-4(2)
O(61)	32(2)	57(3)	32(2)	3(2)	4(2)	14(2)
O(62)	30(2)	84(4)	31(2)	21(2)	7(2)	-1(2)
O(63)	43(2)	67(3)	39(3)	21(2)	7(2)	24(2)

Table 5. Torsion angles [deg] for **2**.

C(6A)-N(1A)-C(2A)-N(3A)	-2.9(9)
N(1A)-C(2A)-N(3A)-C(4A)	1.5(8)
C(2A)-N(3A)-C(4A)-C(5A)	1.5(8)
C(2A)-N(3A)-C(4A)-N(9A)	-179.3(5)
N(3A)-C(4A)-C(5A)-N(7A)	178.4(5)
N(9A)-C(4A)-C(5A)-N(7A)	-0.9(6)
N(3A)-C(4A)-C(5A)-C(6A)	-3.0(8)
N(9A)-C(4A)-C(5A)-C(6A)	177.6(5)
C(2A)-N(1A)-C(6A)-N(6A)	-179.2(6)
C(2A)-N(1A)-C(6A)-C(5A)	1.2(8)
N(7A)-C(5A)-C(6A)-N(6A)	0.0(10)
C(4A)-C(5A)-C(6A)-N(6A)	-178.1(6)
N(7A)-C(5A)-C(6A)-N(1A)	179.6(5)
C(4A)-C(5A)-C(6A)-N(1A)	1.5(7)
C(4A)-C(5A)-N(7A)-C(8A)	0.4(6)

cif file for **2**

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I/sigma threshold for reflections = 5.000
Delta(U)/lambda**2 = 0.000
Highest even order spherical harmonic = 6
Highest odd order spherical harmonic = 3
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'HKL Denzo and Scalepack (Otwinowski & Minor 1997)'
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_computing_molecular_graphics 'Ortep-3 for Windows (Farrugia, 1997)'
_computing_publication_material
'WinGX publication routines (Farrugia, 1999)'

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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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Pt Pt -0.009800(16) 0.859508(18) 0.118596(8) 0.01792(6) Uani 1 1 d . . .
OW O 0.4422(4) 0.7349(5) -0.11961(18) 0.0405(12) Uani 1 1 d . . .
H1OW H 0.392(6) 0.742(6) -0.148(3) 0.049 Uiso 1 1 d . . .
H2OW H 0.483(6) 0.683(7) -0.121(3) 0.049 Uiso 1 1 d . . .
N1A N -0.3566(4) 0.9925(4) 0.25998(19) 0.0264(10) Uani 1 1 d . . .
H1A H -0.393(5) 1.007(5) 0.288(2) 0.032 Uiso 1 1 d . . .
C2A C -0.2345(5) 0.9632(5) 0.2670(2) 0.0280(13) Uani 1 1 d . . .
H2A H -0.204(5) 0.957(5) 0.304(2) 0.034 Uiso 1 1 d . . .

N3A N -0.1670(4) 0.9340(4) 0.22790(18) 0.0270(10) Uani 1 1 d . . .
C4A C -0.2313(4) 0.9384(5) 0.1780(2) 0.0211(11) Uani 1 1 d . . .
C5A C -0.3528(4) 0.9717(5) 0.1665(2) 0.0197(11) Uani 1 1 d . . .
C6A C -0.4237(5) 1.0001(5) 0.2099(2) 0.0257(12) Uani 1 1 d . . .
N6A N -0.5403(4) 1.0298(6) 0.2052(2) 0.0400(14) Uani 1 1 d . . .
H6A1 H -0.579(5) 1.049(6) 0.168(3) 0.048 Uiso 1 1 d . . .
H6A2 H -0.579(6) 1.032(6) 0.233(3) 0.048 Uiso 1 1 d . . .
N7A N -0.3794(4) 0.9664(4) 0.11077(19) 0.0251(10) Uani 1 1 d . . .
H7A H -0.440(5) 0.990(5) 0.087(2) 0.030 Uiso 1 1 d . . .
C8A C -0.2774(4) 0.9303(5) 0.0897(2) 0.0226(11) Uani 1 1 d . . .
H8A H -0.271(4) 0.917(5) 0.052(2) 0.027 Uiso 1 1 d . . .
N9A N -0.1844(3) 0.9109(4) 0.12926(16) 0.0193(9) Uani 1 1 d . . .
N1B N 0.3373(4) 0.7527(4) -0.02714(18) 0.0234(10) Uani 1 1 d . . .
H1B H 0.374(5) 0.747(5) -0.054(2) 0.028 Uiso 1 1 d . . .
C2B C 0.2175(5) 0.7896(5) -0.0333(2) 0.0232(11) Uani 1 1 d . . .
H2B H 0.187(4) 0.798(5) -0.072(2) 0.028 Uiso 1 1 d . . .
N3B N 0.1495(3) 0.8130(4) 0.00659(17) 0.0207(9) Uani 1 1 d . . .
C4B C 0.2114(4) 0.7958(4) 0.0569(2) 0.0187(10) Uani 1 1 d . . .
C5B C 0.3338(4) 0.7613(4) 0.06652(19) 0.0187(10) Uani 1 1 d . . .
N6B N 0.5164(4) 0.6969(5) 0.0253(2) 0.0314(12) Uani 1 1 d . . .
H6B1 H 0.550(5) 0.681(6) 0.053(3) 0.038 Uiso 1 1 d . . .
H6B2 H 0.555(5) 0.684(6) -0.002(3) 0.038 Uiso 1 1 d . . .
C6B C 0.4024(4) 0.7356(5) 0.0225(2) 0.0245(12) Uani 1 1 d . . .
N7B N 0.3596(4) 0.7568(4) 0.12277(18) 0.0213(10) Uani 1 1 d . . .
H7B H 0.423(5) 0.738(5) 0.136(2) 0.026 Uiso 1 1 d . . .
C8B C 0.2566(4) 0.7873(5) 0.1444(2) 0.0214(11) Uani 1 1 d . . .
H8B H 0.256(5) 0.791(5) 0.180(2) 0.026 Uiso 1 1 d . . .
N9B N 0.1646(3) 0.8112(4) 0.10657(17) 0.0199(9) Uani 1 1 d . . .
N11 N -0.0603(3) 0.6864(4) 0.10361(17) 0.0211(9) Uani 1 1 d . . .
N12 N -0.1141(4) 0.4432(4) 0.0856(2) 0.0358(12) Uani 1 1 d . . .
C11 C -0.0442(4) 0.6055(5) 0.1445(2) 0.0244(12) Uani 1 1 d . . .
H11 H -0.0135 0.6311 0.1802 0.029 Uiso 1 1 calc R . .
C12 C -0.0722(5) 0.4849(5) 0.1347(2) 0.0272(12) Uani 1 1 d . . .
H12 H -0.0610 0.4293 0.1643 0.033 Uiso 1 1 calc R . .
C13 C -0.1302(5) 0.5253(6) 0.0457(3) 0.0371(15) Uani 1 1 d . . .
H13 H -0.1600 0.4991 0.0100 0.045 Uiso 1 1 calc R . .
C14 C -0.1053(4) 0.6467(5) 0.0542(2) 0.0282(12) Uani 1 1 d . . .
H14 H -0.1203 0.7024 0.0248 0.034 Uiso 1 1 calc R . .
N21 N 0.0478(3) 1.0288(4) 0.13620(17) 0.0207(9) Uani 1 1 d . . .
N22 N 0.1364(4) 1.2596(4) 0.1603(2) 0.0328(11) Uani 1 1 d . . .
C21 C 0.0942(5) 1.0579(5) 0.1876(2) 0.0264(12) Uani 1 1 d . . .
H21 H 0.0972 0.9991 0.2160 0.032 Uiso 1 1 calc R . .
C22 C 0.1369(5) 1.1730(5) 0.1985(2) 0.0345(14) Uani 1 1 d . . .
H22 H 0.1683 1.1922 0.2349 0.041 Uiso 1 1 calc R . .
C23 C 0.0902(5) 1.2284(5) 0.1104(2) 0.0283(12) Uani 1 1 d . . .
H23 H 0.0870 1.2876 0.0822 0.034 Uiso 1 1 calc R . .
C24 C 0.0461(4) 1.1127(5) 0.0974(2) 0.0225(11) Uani 1 1 d . . .
H24 H 0.0148 1.0938 0.0609 0.027 Uiso 1 1 calc R . .
N31 N 0.1925(4) 0.7563(4) -0.21312(19) 0.0298(11) Uani 1 1 d . . .
O31 O 0.3037(3) 0.7463(4) -0.22191(16) 0.0398(11) Uani 1 1 d . . .
O32 O 0.1668(4) 0.7915(4) -0.16699(16) 0.0365(10) Uani 1 1 d . . .
O33 O 0.1094(4) 0.7309(4) -0.24969(17) 0.0443(11) Uani 1 1 d . . .
N41 N 0.6840(4) 0.5390(5) -0.09333(19) 0.0327(11) Uani 1 1 d . . .
O41 O 0.6714(4) 0.5982(6) -0.05168(19) 0.0735(19) Uani 1 1 d . . .
O42 O 0.5942(3) 0.5321(4) -0.12984(16) 0.0398(11) Uani 1 1 d . . .
O43 O 0.7818(3) 0.4858(4) -0.09946(16) 0.0358(10) Uani 1 1 d . . .
N51 N -0.6680(4) 1.0764(5) 0.05835(19) 0.0307(11) Uani 1 1 d . . .
O51 O -0.5704(3) 1.0456(4) 0.03849(16) 0.0414(11) Uani 1 1 d . . .
O52 O -0.6824(3) 1.0515(4) 0.10693(16) 0.0369(10) Uani 1 1 d . . .
O53 O -0.7501(4) 1.1277(5) 0.02856(17) 0.0583(15) Uani 1 1 d . . .
N61 N 0.6375(4) 0.6247(5) 0.1722(2) 0.0332(12) Uani 1 1 d . . .
O61 O 0.5488(3) 0.6782(4) 0.19233(16) 0.0404(11) Uani 1 1 d . . .
O62 O 0.6631(3) 0.6539(5) 0.12513(17) 0.0479(12) Uani 1 1 d . . .
O63 O 0.6972(4) 0.5489(5) 0.19978(18) 0.0494(13) Uani 1 1 d . . .

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OW 0.034(2) 0.061(4) 0.026(2) -0.002(2) 0.0050(18) 0.015(2)
N1A 0.034(3) 0.029(3) 0.019(2) 0.001(2) 0.0103(19) 0.005(2)
C2A 0.033(3) 0.031(3) 0.020(3) 0.008(2) 0.006(2) 0.005(2)
N3A 0.027(2) 0.033(3) 0.020(2) 0.005(2) 0.0021(18) 0.005(2)
C4A 0.028(3) 0.020(3) 0.016(3) 0.004(2) 0.003(2) 0.003(2)
C5A 0.021(2) 0.017(3) 0.022(3) 0.002(2) 0.004(2) 0.0009(19)
C6A 0.027(3) 0.030(3) 0.022(3) -0.002(2) 0.008(2) 0.001(2)
N6A 0.028(3) 0.070(4) 0.023(3) 0.006(3) 0.013(2) 0.017(3)
N7A 0.017(2) 0.033(3) 0.026(3) 0.000(2) 0.0036(17) 0.0049(19)
C8A 0.023(2) 0.027(3) 0.019(3) -0.004(2) 0.005(2) 0.000(2)
N9A 0.020(2) 0.020(2) 0.017(2) -0.0016(18) 0.0029(16) 0.0005(17)
N1B 0.026(2) 0.027(3) 0.018(2) -0.003(2) 0.0073(18) 0.0009(19)
C2B 0.028(3) 0.026(3) 0.015(3) -0.004(2) 0.001(2) 0.001(2)
N3B 0.021(2) 0.023(2) 0.018(2) -0.0045(19) 0.0016(16) -0.0016(17)
C4B 0.019(2) 0.015(3) 0.023(3) -0.001(2) 0.0047(19) -0.0007(19)
C5B 0.024(2) 0.017(3) 0.015(2) 0.002(2) 0.0061(19) -0.003(2)
N6B 0.025(2) 0.047(3) 0.024(3) 0.002(3) 0.009(2) 0.006(2)
C6B 0.022(2) 0.023(3) 0.029(3) 0.001(2) 0.005(2) 0.002(2)
N7B 0.016(2) 0.027(3) 0.021(2) 0.001(2) 0.0032(17) 0.0012(18)
C8B 0.024(3) 0.025(3) 0.016(3) -0.002(2) 0.001(2) 0.004(2)
N9B 0.018(2) 0.019(2) 0.023(2) 0.0019(19) 0.0055(17) -0.0001(17)
N11 0.0146(19) 0.024(2) 0.026(2) -0.003(2) 0.0062(17) 0.0004(17)
N12 0.039(3) 0.027(3) 0.041(3) -0.005(2) 0.000(2) 0.000(2)
C11 0.024(3) 0.026(3) 0.024(3) -0.003(2) 0.006(2) -0.003(2)
C12 0.032(3) 0.018(3) 0.032(3) 0.009(2) 0.005(2) 0.000(2)
C13 0.035(3) 0.041(4) 0.034(3) -0.010(3) -0.005(3) 0.000(3)
C14 0.029(3) 0.028(3) 0.028(3) 0.001(3) 0.000(2) 0.000(2)
N21 0.016(2) 0.026(3) 0.021(2) 0.0027(19) 0.0047(16) 0.0015(17)
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N31 0.034(3) 0.025(3) 0.030(3) 0.002(2) 0.005(2) -0.005(2)
O31 0.033(2) 0.057(3) 0.030(2) -0.001(2) 0.0078(17) 0.000(2)
O32 0.047(2) 0.041(3) 0.023(2) -0.0038(19) 0.0115(18) 0.0009(19)
O33 0.035(2) 0.064(3) 0.032(2) -0.012(2) -0.0035(18) -0.004(2)
N41 0.035(3) 0.040(3) 0.024(3) 0.004(2) 0.007(2) 0.007(2)
O41 0.053(3) 0.132(5) 0.034(3) -0.037(3) -0.005(2) 0.040(3)
O42 0.035(2) 0.057(3) 0.027(2) -0.009(2) 0.0010(17) 0.007(2)
O43 0.033(2) 0.036(3) 0.040(2) -0.001(2) 0.0120(18) 0.0074(18)
N51 0.027(2) 0.035(3) 0.030(3) 0.000(2) 0.001(2) 0.004(2)
O51 0.029(2) 0.065(3) 0.031(2) -0.001(2) 0.0077(17) 0.013(2)
O52 0.031(2) 0.052(3) 0.027(2) 0.009(2) 0.0054(16) -0.0024(19)
O53 0.047(3) 0.102(4) 0.027(2) 0.014(3) 0.0105(19) 0.040(3)
N61 0.025(2) 0.043(3) 0.031(3) 0.008(2) 0.000(2) -0.004(2)
O61 0.032(2) 0.057(3) 0.032(2) 0.003(2) 0.0040(17) 0.014(2)
O62 0.030(2) 0.084(4) 0.031(2) 0.021(2) 0.0066(17) -0.001(2)
O63 0.043(2) 0.067(3) 0.039(3) 0.021(2) 0.007(2) 0.024(2)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Pt N11 2.013(4) . ?
Pt N9B 2.020(4) . ?
Pt N9A 2.025(4) . ?
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OW H2OW 0.73(7) . ?
N1A C2A 1.363(7) . ?
N1A C6A 1.369(7) . ?
N1A H1A 0.84(6) . ?
C2A N3A 1.304(7) . ?
C2A H2A 0.94(6) . ?
N3A C4A 1.352(6) . ?
C4A C5A 1.376(7) . ?
C4A N9A 1.376(6) . ?
C5A N7A 1.370(6) . ?
C5A C6A 1.409(7) . ?
C6A N6A 1.306(7) . ?
N6A H6A1 0.98(7) . ?
N6A H6A2 0.83(6) . ?
N7A C8A 1.330(6) . ?
N7A H7A 0.87(6) . ?
C8A N9A 1.349(6) . ?
C8A H8A 0.94(5) . ?
N1B C6B 1.361(7) . ?
N1B C2B 1.361(6) . ?
N1B H1B 0.81(6) . ?
C2B N3B 1.308(6) . ?
C2B H2B 0.98(5) . ?
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C4B C5B 1.385(6) . ?
C5B N7B 1.382(6) . ?
C5B C6B 1.400(7) . ?
N6B C6B 1.308(7) . ?
N6B H6B1 0.75(6) . ?
N6B H6B2 0.82(6) . ?
N7B C8B 1.330(6) . ?
N7B H7B 0.76(5) . ?
C8B N9B 1.325(6) . ?
C8B H8B 0.87(5) . ?
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N11 C11 1.342(7) . ?
N12 C12 1.328(7) . ?
N12 C13 1.331(8) . ?
C11 C12 1.383(7) . ?
C11 H11 0.9500 . ?
C12 H12 0.9500 . ?
C13 C14 1.379(8) . ?
C13 H13 0.9500 . ?
C14 H14 0.9500 . ?
N21 C24 1.327(6) . ?
N21 C21 1.351(6) . ?
N22 C23 1.325(7) . ?
N22 C22 1.337(7) . ?
C21 C22 1.370(8) . ?

C21 H21 0.9500 . ?
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C24 H24 0.9500 . ?
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N31 O31 1.255(6) . ?
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H1OW OW H2OW 113(7) . . ?
C2A N1A C6A 123.8(4) . . ?
C2A N1A H1A 118(4) . . ?
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C4A C5A C6A 119.3(5) . . ?
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N6A C6A C5A 126.0(5) . . ?
N1A C6A C5A 112.4(4) . . ?
C6A N6A H6A1 118(4) . . ?
C6A N6A H6A2 120(5) . . ?
H6A1 N6A H6A2 122(6) . . ?
C8A N7A C5A 107.1(4) . . ?
C8A N7A H7A 116(4) . . ?
C5A N7A H7A 136(4) . . ?
N7A C8A N9A 111.5(5) . . ?
N7A C8A H8A 125(3) . . ?
N9A C8A H8A 124(3) . . ?
C8A N9A C4A 105.9(4) . . ?
C8A N9A Pt 126.9(3) . . ?
C4A N9A Pt 127.2(3) . . ?
C6B N1B C2B 123.5(4) . . ?
C6B N1B H1B 118(4) . . ?
C2B N1B H1B 118(4) . . ?
N3B C2B N1B 125.5(5) . . ?

N3B C2B H2B 123(3) . . ?
N1B C2B H2B 112(3) . . ?
C2B N3B C4B 112.6(4) . . ?
N3B C4B N9B 126.3(4) . . ?
N3B C4B C5B 125.2(4) . . ?
N9B C4B C5B 108.5(4) . . ?
N7B C5B C4B 106.2(4) . . ?
N7B C5B C6B 133.7(5) . . ?
C4B C5B C6B 120.0(5) . . ?
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N6B C6B N1B 120.2(5) . . ?
N6B C6B C5B 126.7(5) . . ?
N1B C6B C5B 113.0(4) . . ?
C8B N7B C5B 106.9(4) . . ?
C8B N7B H7B 131(4) . . ?
C5B N7B H7B 122(4) . . ?
N9B C8B N7B 112.4(5) . . ?
N9B C8B H8B 128(3) . . ?
N7B C8B H8B 120(3) . . ?
C8B N9B C4B 106.0(4) . . ?
C8B N9B Pt 127.4(3) . . ?
C4B N9B Pt 126.5(3) . . ?
C14 N11 C11 118.0(5) . . ?
C14 N11 Pt 123.1(4) . . ?
C11 N11 Pt 118.8(3) . . ?
C12 N12 C13 116.0(5) . . ?
N11 C11 C12 120.0(5) . . ?
N11 C11 H11 120.0 . . ?
C12 C11 H11 120.0 . . ?
N12 C12 C11 122.9(5) . . ?
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N12 C13 C14 122.8(6) . . ?
N12 C13 H13 118.6 . . ?
C14 C13 H13 118.6 . . ?
N11 C14 C13 120.3(5) . . ?
N11 C14 H14 119.8 . . ?
C13 C14 H14 119.8 . . ?
C24 N21 C21 118.8(5) . . ?
C24 N21 Pt 120.9(4) . . ?
C21 N21 Pt 120.3(4) . . ?
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N21 C21 C22 119.4(5) . . ?
N21 C21 H21 120.3 . . ?
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Supplementary Material (ESI) for Dalton Transactions

Atomic coordinates of **3**, *head-to-head* conformer:

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N1      -1.612539887    0.655478807   -0.686839593 XXX  ND     n
N   0.000
C2      -2.394973489   -0.306388052   -1.272956772 XXX  ND     c
C   0.000
C3      -3.305125994    0.369820584   -2.091148700 XXX  ND     c
C   0.000
N4      -3.105542059    1.729127696   -2.017639899 XXX  ND     n
N   0.000
C5      -2.098698172    1.840949461   -1.179488144 XXX  ND     c
C   0.000
C6      -4.214382771   -0.420592906   -2.812185787 XXX  ND     c
C   0.000
N7      -4.166925498   -1.751787313   -2.674492843 XXX  ND     n
N   0.000
C8      -3.260087966   -2.273216115   -1.838865516 XXX  ND     c
C   0.000
N9      -2.351753291   -1.639908735   -1.103743383 XXX  ND     n
N   0.000
N10     -5.156039999    0.120976933   -3.624433555 XXX  ND     n
N   0.000
H11     -5.080100908    1.093802494   -3.865933344 XXX  ND     h
H   0.000
H12     -5.655263517   -0.496920257   -4.240801898 XXX  ND     h
H   0.000
H13     -1.671896590    2.787016595   -0.881560530 XXX  ND     h
H   0.000
H14     -3.273823940   -3.355594162   -1.754947570 XXX  ND     h
H   0.000
N15      2.244294141    1.542696248   -2.831589392 XXX  ND     n
N   0.000
C16      1.300884447    1.650188533   -1.922518043 XXX  ND     c
C   0.000
N17      1.255965075    0.630181265   -1.003811070 XXX  ND     n
N   0.000
C18      2.271630186   -0.216344960   -1.378044901 XXX  ND     c
C   0.000
C19      2.868975399    0.361912725   -2.502557005 XXX  ND     c
C   0.000
C20      3.940603389   -0.336553252   -3.080423361 XXX  ND     c
C   0.000
N21      4.327611464   -1.495989702   -2.534926569 XXX  ND     n
N   0.000
C22      3.675548982   -1.936110343   -1.450981504 XXX  ND     c
C   0.000
N23      2.656749486   -1.372877652   -0.811005364 XXX  ND     n
N   0.000
N24     -3.115981004   -0.459201498    4.197307023 XXX  ND     n
N   0.000
C25     -3.083578192   -1.229952407    3.114391583 XXX  ND     c
C   0.000
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C26     -2.211085771   -1.003427512    2.055456849 XXX  ND     c
C   0.000
N27     -1.347474837    0.022843283    2.101768970 XXX  ND     n
N   0.000
C28     -1.374900391    0.811063170    3.187158261 XXX  ND     c
C   0.000
C29     -2.261998599    0.561901466    4.222743420 XXX  ND     c
C   0.000
PT30    -0.028206823    0.353626502    0.528125796 XXX  ND     pt
Pt  0.000
N31      1.606118244    0.029330297    1.753174513 XXX  ND     n
N   0.000
C32      1.891159118   -1.197353166    2.209350534 XXX  ND     c
C   0.000
C33      3.006293947   -1.411754444    3.007215118 XXX  ND     c
C   0.000
N34      3.846689418   -0.435425993    3.336536852 XXX  ND     n
N   0.000
C35      3.569339757    0.772999850    2.853338551 XXX  ND     c
C   0.000
C36      2.456524957    1.018693046    2.062599450 XXX  ND     c
C   0.000
N37      4.616636509    0.141293639   -4.157069987 XXX  ND     n
N   0.000
H38      4.209535672    0.900479303   -4.675700775 XXX  ND     h
H   0.000
H39      5.242092738   -0.487821294   -4.630862715 XXX  ND     h
H   0.000
H40      0.598182728    2.467581263   -1.887233069 XXX  ND     h
H   0.000
H41      4.032373981   -2.879130380   -1.047700016 XXX  ND     h
H   0.000
H42     -3.775177743   -2.062991699    3.072522292 XXX  ND     h
H   0.000
H43     -2.203396233   -1.615062476    1.159187815 XXX  ND     h
H   0.000
H44     -0.685055408    1.641949658    3.215451137 XXX  ND     h
H   0.000
H45     -2.279308898    1.208228386    5.092535847 XXX  ND     h
H   0.000
H46      1.232940923   -2.001085395    1.916685733 XXX  ND     h
H   0.000
H47      3.224894170   -2.406808252    3.375978971 XXX  ND     h
H   0.000
H48      4.251952561    1.578857293    3.096022134 XXX  ND     h
H   0.000
H49      2.241887298    1.998796882    1.662297010 XXX  ND     h
H   0.000
end
end
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Atomic coordinates of **3**, *head-to-tail* conformer:

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N1      -0.930734288   -0.452005645    1.332638387 XXX  ND     n
N   0.000
C2      -1.318051267    0.279947036    2.425248133 XXX  ND     c
C   0.000
C3      -2.425215322   -0.380435806    2.967323034 XXX  ND     c
C   0.000
N4      -2.731022157   -1.499974301    2.229047472 XXX  ND     n
N   0.000
C5      -1.825952764   -1.492191882    1.275073836 XXX  ND     c
C   0.000
C6      -3.015459992    0.199877086    4.101176541 XXX  ND     c
C   0.000
N7      -2.500832318    1.336973480    4.590210015 XXX  ND     n
N   0.000
C8      -1.431593163    1.863676788    3.982277392 XXX  ND     c
C   0.000
N9      -0.779180097    1.412466194    2.914617104 XXX  ND     n
N   0.000
N10     -4.080650997   -0.359871746    4.727709629 XXX  ND     n
N   0.000
H11     -4.569226878   -1.110216884    4.269921675 XXX  ND     h
H   0.000
H12     -4.560121337    0.185693920    5.423359039 XXX  ND     h
H   0.000
H13     -1.769972414   -2.230395254    0.489399067 XXX  ND     h
H   0.000
H14     -1.053084433    2.781957787    4.421462739 XXX  ND     h
H   0.000
N15     -2.732554454    1.487917027   -2.228878393 XXX  ND     n
N   0.000
C16     -1.830358911    1.477584408   -1.272178105 XXX  ND     c
C   0.000
N17     -0.927494983    0.444148150   -1.336613399 XXX  ND     n
N   0.000
C18     -1.304110089   -0.277486139   -2.440076786 XXX  ND     c
C   0.000
C19     -2.414990799    0.379367229   -2.978363779 XXX  ND     c
C   0.000
C20     -2.997594231   -0.193991591   -4.119655798 XXX  ND     c
C   0.000
N21     -2.469943450   -1.319242993   -4.621918164 XXX  ND     n
N   0.000
C22     -1.398715948   -1.843754704   -4.015992157 XXX  ND     c
C   0.000
N23     -0.754599670   -1.400203208   -2.940117962 XXX  ND     n
N   0.000
N24      3.915422906   -1.245471749    3.239790809 XXX  ND     n
N   0.000
C25      3.752373533   -1.907858387    2.095809111 XXX  ND     c
C   0.000
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C26      2.787506905   -1.554432174    1.166084792 XXX  ND     c
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N27      1.964751436   -0.517733680    1.389717522 XXX  ND     n
N   0.000
C28      2.106903263    0.150447504    2.545650015 XXX  ND     c
C   0.000
C29      3.089735770   -0.225574547    3.454746465 XXX  ND     c
C   0.000
PT30     0.512208185   -0.004160131    0.000067949 XXX  ND     pt
Pt  0.000
N31      1.974243389    0.515361023   -1.376779829 XXX  ND     n
N   0.000
C32      2.114273191   -0.131879155   -2.545174793 XXX  ND     c
C   0.000
C33      3.104961623    0.253493068   -3.441688375 XXX  ND     c
C   0.000
N34      3.941562390    1.259092766   -3.203038729 XXX  ND     n
N   0.000
C35      3.780984416    1.899443558   -2.046387292 XXX  ND     c
C   0.000
C36      2.807646109    1.539242888   -1.128135738 XXX  ND     c
C   0.000
N37     -4.064274636    0.363958009   -4.742485737 XXX  ND     n
N   0.000
H38     -4.560953436    1.102891839   -4.276159642 XXX  ND     h
H   0.000
H39     -4.537177601   -0.178142812   -5.444358444 XXX  ND     h
H   0.000
H40     -1.783324219    2.207034825   -0.477739682 XXX  ND     h
H   0.000
H41     -1.009173810   -2.752411699   -4.465520390 XXX  ND     h
H   0.000
H42      4.407408978   -2.750336982    1.906528328 XXX  ND     h
H   0.000
H43      2.658394519   -2.098591468    0.241316054 XXX  ND     h
H   0.000
H44      1.404826917    0.954216388    2.737134323 XXX  ND     h
H   0.000
H45      3.201890598    0.321929892    4.383399472 XXX  ND     h
H   0.000
H46      1.407854455   -0.928206576   -2.753934986 XXX  ND     h
H   0.000
H47      3.214009925   -0.274488055   -4.381742712 XXX  ND     h
H   0.000
H48      4.445066747    2.729980842   -1.836834799 XXX  ND     h
H   0.000
H49      2.679807346    2.068354845   -0.193359469 XXX  ND     h
H   0.000
end
end
```

Atomic coordinates of **2**, *head-to-head* conformer:

```
N1      -0.000301732    1.246368537   -4.206637155 XXX  ND     n
N   0.000
C2      -0.000179851    1.592885120   -2.935491156 XXX  ND     c
C   0.000
N3      -0.000187850    0.551311568   -2.044160926 XXX  ND     n
N   0.000
C4      -0.000330081   -0.570772680   -2.829451204 XXX  ND     c
C   0.000
C5      -0.000387905   -0.128666804   -4.156255923 XXX  ND     c
C   0.000
C6      -0.000484294   -1.121953327   -5.150336536 XXX  ND     c
C   0.000
N7      -0.000489661   -2.408567392   -4.778675312 XXX  ND     n
N   0.000
C8      -0.000417130   -2.695242658   -3.468902497 XXX  ND     c
C   0.000
N9      -0.000335005   -1.857747477   -2.438029762 XXX  ND     n
N   0.000
N10     -4.797370920    0.228070675    0.000632889 XXX  ND     n
N   0.000
C11     -3.998123569   -0.835207338    0.001235594 XXX  ND     c
C   0.000
C12     -2.613496146   -0.729486257    0.001104815 XXX  ND     c
C   0.000
N13     -2.033428188    0.479624886    0.000314857 XXX  ND     n
N   0.000
C14     -2.824539682    1.560476172   -0.000294221 XXX  ND     c
C   0.000
C15     -4.204187029    1.418842014   -0.000119019 XXX  ND     c
C   0.000
PT16     0.000087193    0.568628550   -0.000002150 XXX  ND     pt
Pt  0.000
N17      2.033592801    0.479374610   -0.000319470 XXX  ND     n
N   0.000
C18      2.613503151   -0.729812469   -0.000488313 XXX  ND     c
C   0.000
C19      3.998116030   -0.835718515   -0.000683150 XXX  ND     c
C   0.000
N20      4.797504069    0.227454099   -0.000714519 XXX  ND     n
N   0.000
C21      4.204476978    1.418303703   -0.000555867 XXX  ND     c
C   0.000
C22      2.824848122    1.560120262   -0.000361542 XXX  ND     c
C   0.000
N23      0.000357654    0.551355848    2.044159468 XXX  ND     n
N   0.000
C24      0.000163410   -0.570708383    2.829482068 XXX  ND     c
C   0.000
C25      0.000372704   -0.128565624    4.156276211 XXX  ND     c
C   0.000
```

```
N26      0.000671548    1.246471775    4.206616202 XXX  ND     n
N   0.000
C27      0.000645566    1.592950619    2.935460573 XXX  ND     c
C   0.000
C28      0.000117235   -1.121822447    5.150382725 XXX  ND     c
C   0.000
N29     -0.000291871   -2.408450335    4.778737645 XXX  ND     n
N   0.000
C30     -0.000468872   -2.695159960    3.468975511 XXX  ND     c
C   0.000
N31     -0.000276870   -1.857685230    2.438081107 XXX  ND     n
N   0.000
N32     -0.000540485   -0.821665910   -6.469275049 XXX  ND     n
N   0.000
N33      0.000230520   -0.821524906    6.469319118 XXX  ND     n
N   0.000
H34     -0.000477282    0.136969466   -6.766079364 XXX  ND     h
H   0.000
H35     -0.000619985   -1.566392692   -7.142479894 XXX  ND     h
H   0.000
H36      0.000563474    0.137110371    6.766122503 XXX  ND     h
H   0.000
H37      0.000012176   -1.566253564    7.142522604 XXX  ND     h
H   0.000
H38     -0.000088184    2.619162667   -2.597670267 XXX  ND     h
H   0.000
H39     -0.000421554   -3.753757167   -3.226955399 XXX  ND     h
H   0.000
H40     -4.464378193   -1.813151807    0.001857018 XXX  ND     h
H   0.000
H41     -1.960324430   -1.590798173    0.001681575 XXX  ND     h
H   0.000
H42     -2.345203145    2.528114653   -0.000932145 XXX  ND     h
H   0.000
H43     -4.840026937    2.296239017   -0.000602374 XXX  ND     h
H   0.000
H44      1.960218174   -1.591039143   -0.000484647 XXX  ND     h
H   0.000
H45      4.464241433   -1.813724820   -0.000818616 XXX  ND     h
H   0.000
H46      4.840433454    2.295616273   -0.000589426 XXX  ND     h
H   0.000
H47      2.345640343    2.527822530   -0.000236594 XXX  ND     h
H   0.000
H48      0.000836006    2.619214078    2.597608666 XXX  ND     h
H   0.000
H49     -0.000821481   -3.753679621    3.227051543 XXX  ND     h
H   0.000
end
end
```

Atomic coordinates of **2**, *head-to-tail* conformer:

```
N1      -0.104016320    3.742420061   -2.018782687 XXX  ND     n
N   0.000
C2      -0.106242021    2.429688880   -1.912023752 XXX  ND     c
C   0.000
N3      -0.030896000    1.946041641   -0.629576729 XXX  ND     n
N   0.000
C4       0.027407226    3.068195644    0.153645478 XXX  ND     c
C   0.000
C5      -0.019635199    4.164660714   -0.712776505 XXX  ND     c
C   0.000
C6       0.026523828    5.437817880   -0.120577895 XXX  ND     c
C   0.000
N7       0.111583801    5.528105617    1.214512292 XXX  ND     n
N   0.000
C8       0.149366016    4.397543544    1.929904481 XXX  ND     c
C   0.000
N9       0.113476621    3.140583197    1.495355546 XXX  ND     n
N   0.000
N10     -4.827914750   -0.018647907    0.023078412 XXX  ND     n
N   0.000
C11     -4.127761754   -0.918859989   -0.662344167 XXX  ND     c
C   0.000
C12     -2.740084805   -0.931916255   -0.677249338 XXX  ND     c
C   0.000
N13     -2.051468856   -0.008001430    0.010582524 XXX  ND     n
N   0.000
C14     -2.741094778    0.910663160    0.704278611 XXX  ND     c
C   0.000
C15     -4.128582459    0.887115006    0.702102592 XXX  ND     c
C   0.000
PT16    -0.016603048    0.000179292    0.001457610 XXX  ND     pt
Pt  0.000
N17      2.018076834    0.007236432   -0.008903809 XXX  ND     n
N   0.000
C18      2.704288381   -0.886713561   -0.737591607 XXX  ND     c
C   0.000
C19      4.091888858   -0.864474598   -0.736495736 XXX  ND     c
C   0.000
N20      4.793496528    0.013709466   -0.024284225 XXX  ND     n
N   0.000
C21      4.095617196    0.888418342    0.695707186 XXX  ND     c
C   0.000
C22      2.707887925    0.904334620    0.712423314 XXX  ND     c
C   0.000
N23     -0.005466692   -1.945701039    0.632349915 XXX  ND     n
N   0.000
C24      0.024840233   -3.066433025   -0.154248100 XXX  ND     c
C   0.000
C25      0.018232535   -4.164358735    0.711509623 XXX  ND     c
C   0.000
```

```
N26     -0.014404946   -3.744288384    2.020513034 XXX  ND     n
N   0.000
C27     -0.026936469   -2.431398996    1.916030626 XXX  ND     c
C   0.000
C28      0.045233331   -5.436332568    0.115612528 XXX  ND     c
C   0.000
N29      0.074872564   -5.523986160   -1.222082663 XXX  ND     n
N   0.000
C30      0.078286925   -4.392112197   -1.936448349 XXX  ND     c
C   0.000
N31      0.055150237   -3.136009629   -1.498505541 XXX  ND     n
N   0.000
N32     -0.011404600    6.574317010   -0.850721554 XXX  ND     n
N   0.000
N33      0.042302747   -6.574192016    0.844594332 XXX  ND     n
N   0.000
H34     -0.074918811    6.526490246   -1.851332413 XXX  ND     h
H   0.000
H35      0.024738906    7.461515550   -0.381942549 XXX  ND     h
H   0.000
H36      0.020818569   -6.528312188    1.847086620 XXX  ND     h
H   0.000
H37      0.062292471   -7.460472401    0.373114331 XXX  ND     h
H   0.000
H38     -0.163145187    1.760219404   -2.757604433 XXX  ND     h
H   0.000
H39      0.219090685    4.530347730    3.005271449 XXX  ND     h
H   0.000
H40     -4.680746071   -1.662802751   -1.223373854 XXX  ND     h
H   0.000
H41     -2.170071998   -1.665825568   -1.230419259 XXX  ND     h
H   0.000
H42     -2.172157095    1.649596455    1.251403966 XXX  ND     h
H   0.000
H43     -4.682215104    1.626920100    1.267943971 XXX  ND     h
H   0.000
H44      2.131954486   -1.605131703   -1.309397649 XXX  ND     h
H   0.000
H45      4.643772262   -1.583138285   -1.330576030 XXX  ND     h
H   0.000
H46      4.650640179    1.609728184    1.283624392 XXX  ND     h
H   0.000
H47      2.137988629    1.619958334    1.290610388 XXX  ND     h
H   0.000
H48     -0.052807777   -1.763399357    2.764271194 XXX  ND     h
H   0.000
H49      0.103480670   -4.522847672   -3.014045246 XXX  ND     h
H   0.000
end
end
```

References

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