

Supporting Information

Table S1. Crystal data and structure refinement for $[\text{Pt}(\text{C}^2, \text{O}^5\text{-Asc})(\text{en})] \cdot 2\text{H}_2\text{O}$

Empirical formula	$\text{C}_8\text{H}_{18}\text{N}_2\text{O}_8\text{Pt}$	
Formula weight	465.33	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2_1	
Unit cell dimensions	$a = 6.1374(4)$ Å	$a = 90^\circ$
	$b = 16.0713(10)$ Å	$b = 107.206(2)^\circ$
	$c = 6.7618(3)$ Å	$c = 90^\circ$
Volume	$637.11(6)$ Å ³	
Z	2	
Density (calculated)	2.426 Mg/m ³	
Absorption coefficient	11.051 mm ⁻¹	
F(000)	444	
Crystal size	0.28 x 0.16 x 0.15 mm ³	
Theta range for data collection	3.15 to 29.58°	
Index ranges	-8 < h < 7, -20 < k < 20, 0 < l < 9	
Reflections collected	11336	
Independent reflections	3236 [R(int) = 0.037]	
Completeness to theta = 29.58°	91.4 %	
Absorption correction	Empirical, sadabs	
Max. and min. transmission	0.2880 and 0.1479	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3236 / 1 / 172	
Goodness-of-fit on F ²	1.061	
Final R indices [I > 2sigma(I)]	R1 = 0.0183, wR2 = 0.0395	
R indices (all data)	R1 = 0.0203, wR2 = 0.0399	
Absolute structure parameter	0.037(8)	
Largest diff. peak and hole	0.813 and -1.203 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Pt}(\text{C}^2, \text{O}^5\text{-Asc})(\text{en})].2\text{H}_2\text{O}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1222(1)	2(1)	1544(1)	15(1)
O(1)	1467(5)	2033(2)	-1240(5)	30(1)
O(2)	1021(5)	328(2)	-2800(4)	23(1)
O(3)	-3441(5)	-244(2)	-2099(5)	25(1)
O(4)	-1682(5)	1782(2)	-339(5)	23(1)
O(5)	-432(5)	738(2)	3079(5)	20(1)
O(6)	-3504(6)	1402(3)	5113(5)	40(1)
N(1)	2584(6)	-704(2)	4208(5)	22(1)
N(2)	2985(6)	-821(2)	276(6)	22(1)
C(1)	77(6)	1527(3)	-1009(6)	19(1)
C(2)	-7(6)	620(3)	-1353(6)	17(1)
C(3)	-2289(8)	369(3)	-1369(7)	21(1)
C(4)	-3096(6)	1068(3)	-243(6)	19(1)
C(5)	-2771(6)	889(3)	2052(6)	19(1)
C(6)	-3617(7)	1606(3)	3053(7)	26(1)
C(1')	3364(8)	-1515(3)	3578(7)	28(1)
C(2')	4540(7)	-1341(3)	1943(7)	27(1)
O(1S)	-505(6)	-1431(2)	-3427(6)	39(1)
O(2S)	2293(5)	2017(2)	-5074(5)	31(1)

Table S3. Bond lengths [Å] and angles [°] for [Pt(C²,O⁵-Asc)(en)].2H₂O.

Pt(1)-O(5)	2.032(3)
Pt(1)-N(2)	2.052(3)
Pt(1)-N(1)	2.083(3)
Pt(1)-C(2)	2.126(4)
Pt(1)-C(3)	2.522(4)
O(1)-C(1)	1.221(5)
O(2)-C(2)	1.393(5)
O(3)-C(3)	1.228(5)
O(4)-C(1)	1.352(5)
O(4)-C(4)	1.451(5)
O(5)-C(5)	1.418(4)
O(6)-C(6)	1.412(5)
N(1)-C(1')	1.494(6)
N(2)-C(2')	1.498(5)
C(1)-C(2)	1.475(6)
C(2)-C(3)	1.455(6)
C(3)-C(4)	1.520(6)
C(4)-C(5)	1.532(6)
C(5)-C(6)	1.504(6)
C(1')-C(2')	1.515(7)
O(5)-Pt(1)-N(2)	173.77(12)
O(5)-Pt(1)-N(1)	90.52(13)
N(2)-Pt(1)-N(1)	83.31(14)
O(5)-Pt(1)-C(2)	95.98(14)
N(2)-Pt(1)-C(2)	90.18(15)
N(1)-Pt(1)-C(2)	173.45(14)
O(5)-Pt(1)-C(3)	79.77(12)
N(2)-Pt(1)-C(3)	105.00(14)
N(1)-Pt(1)-C(3)	146.55(14)
C(2)-Pt(1)-C(3)	35.19(15)
C(1)-O(4)-C(4)	108.9(3)
C(5)-O(5)-Pt(1)	115.8(2)
C(1')-N(1)-Pt(1)	108.0(3)

C(2')-N(2)-Pt(1)	110.0(3)
O(1)-C(1)-O(4)	119.9(4)
O(1)-C(1)-C(2)	129.1(4)
O(4)-C(1)-C(2)	111.0(3)
O(2)-C(2)-C(3)	122.4(4)
O(2)-C(2)-C(1)	116.2(3)
C(3)-C(2)-C(1)	105.3(3)
O(2)-C(2)-Pt(1)	112.3(2)
C(3)-C(2)-Pt(1)	87.4(3)
C(1)-C(2)-Pt(1)	109.3(3)
O(3)-C(3)-C(2)	131.6(4)
O(3)-C(3)-C(4)	124.1(4)
C(2)-C(3)-C(4)	104.3(4)
O(3)-C(3)-Pt(1)	112.5(3)
C(2)-C(3)-Pt(1)	57.4(2)
C(4)-C(3)-Pt(1)	96.4(3)
O(4)-C(4)-C(3)	105.9(3)
O(4)-C(4)-C(5)	107.1(3)
C(3)-C(4)-C(5)	113.8(3)
O(5)-C(5)-C(6)	110.2(3)
O(5)-C(5)-C(4)	109.7(3)
C(6)-C(5)-C(4)	110.7(3)
O(6)-C(6)-C(5)	110.1(4)
N(1)-C(1')-C(2')	108.0(4)
N(2)-C(2')-C(1')	108.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Pt}(\text{C}^2, \text{O}^5\text{-Asc})(\text{en})].2\text{H}_2\text{O}$.

The anisotropic displacement factor exponent takes the form:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	15(1)	15(1)	15(1)	0(1)	3(1)	2(1)
O(1)	34(2)	25(2)	33(2)	1(1)	12(1)	-7(1)
O(2)	29(1)	25(2)	15(1)	3(1)	10(1)	11(1)
O(3)	23(1)	24(2)	24(2)	-4(1)	1(1)	-7(1)
O(4)	27(1)	19(2)	25(2)	1(1)	11(1)	3(1)
O(5)	18(1)	23(2)	19(1)	-2(1)	3(1)	6(1)
O(6)	39(2)	63(3)	16(2)	7(2)	7(1)	24(2)
N(1)	25(2)	20(2)	20(2)	2(1)	4(1)	2(1)
N(2)	21(2)	21(2)	24(2)	-1(1)	6(1)	4(1)
C(1)	23(2)	20(2)	15(2)	4(1)	7(1)	3(2)
C(2)	19(2)	17(2)	16(2)	3(1)	4(1)	2(1)
C(3)	25(2)	23(2)	15(2)	3(2)	5(2)	5(2)
C(4)	14(2)	23(2)	20(2)	2(2)	5(1)	1(1)
C(5)	15(2)	21(2)	19(2)	2(2)	4(1)	1(1)
C(6)	22(2)	34(3)	24(2)	4(2)	8(2)	10(2)
C(1')	34(2)	16(2)	31(2)	4(2)	7(2)	7(2)
C(2')	26(2)	21(2)	35(2)	3(2)	8(2)	11(2)
O(1S)	35(2)	28(2)	53(2)	-11(2)	12(2)	-5(1)
O(2S)	28(2)	29(2)	38(2)	-1(1)	14(1)	-3(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Pt}(\text{C}^2, \text{O}^5\text{-Asc})(\text{en})].2\text{H}_2\text{O}$.

	x	y	z	U(eq)
H(2)	244	460	-3967	34
H(6)	-2179	1300	5771	60
H(1A)	3767	-434	5080	26
H(1B)	1520	-791	4858	26
H(2A)	1997	-1152	-637	27
H(2B)	3808	-540	-407	27
H(4)	-4701	1196	-946	23
H(5)	-3647	390	2163	22
H(6A)	-2691	2094	3044	31
H(6B)	-5180	1734	2275	31
H(1'A)	2070	-1881	3026	33
H(1'B)	4414	-1784	4766	33
H(2'A)	5962	-1048	2553	33
H(2'B)	4882	-1860	1365	33
H(1S)	-1312	-1973	-4017	58
H(2S)	2078	2008	-3575	58
H(1S')	-1452	-1077	-3018	46