Electronic Supplementary Information for Dalton Transactions

SUPPORTING INFORMATION

$[NO_3 \subset \{(en)Pt(2,2'\text{-}bpz)\}_3]NO_3(SO_4)_2$: Snapshot of nitrate insertion into a cationic Pt_3 metallacycle or simply a packing effect?

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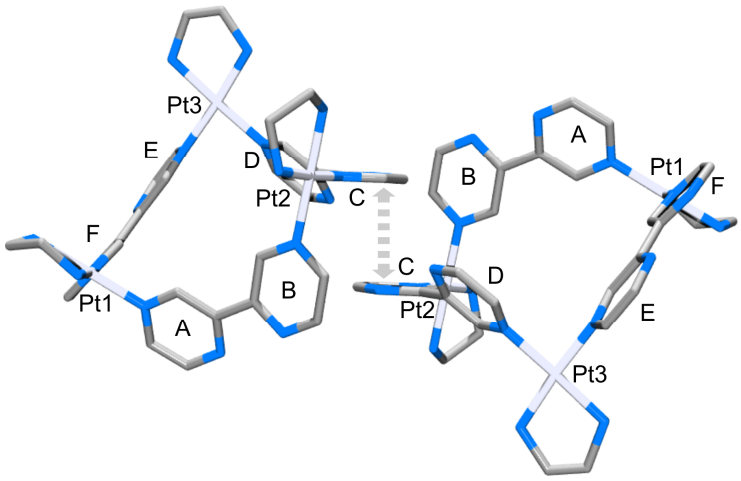

Figure SI1: Detail of the π–π staking (C-rings, 3.3 Å) connecting both cations of **3** within the unit cell. Water molecules and counter anions were omitted for clarity.

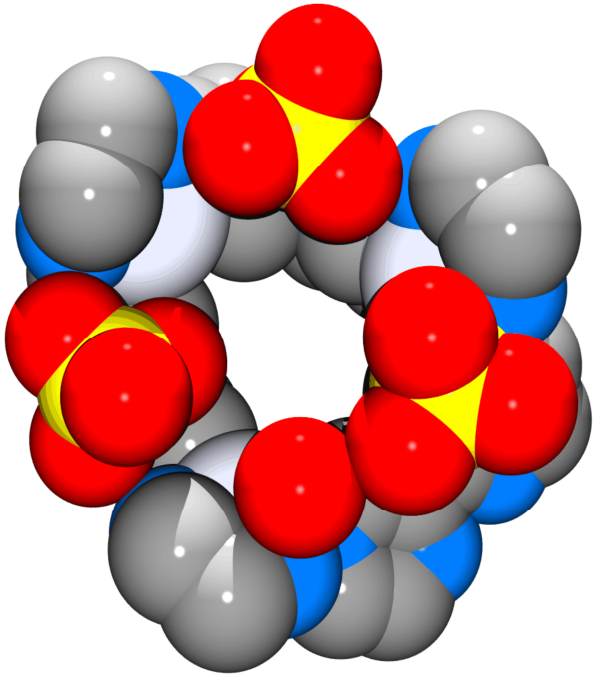

Figure SI2: Lower view (space filling) of the cation **3** with detail of binding of three sulfate anions and a water molecule in its basis.

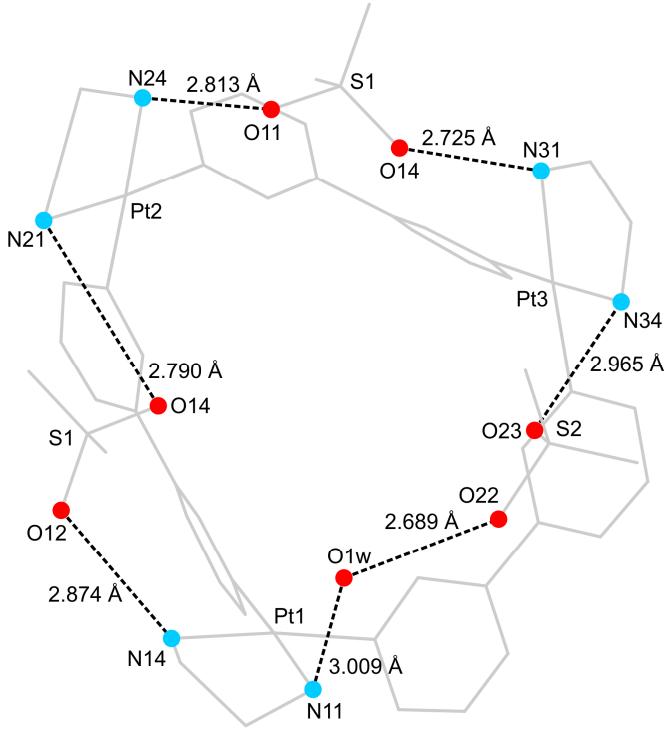

Figure SI3: Schematic representation of hydrogen bonding involving the sulfate anions inserted between enPt^{II} entities in **3**.

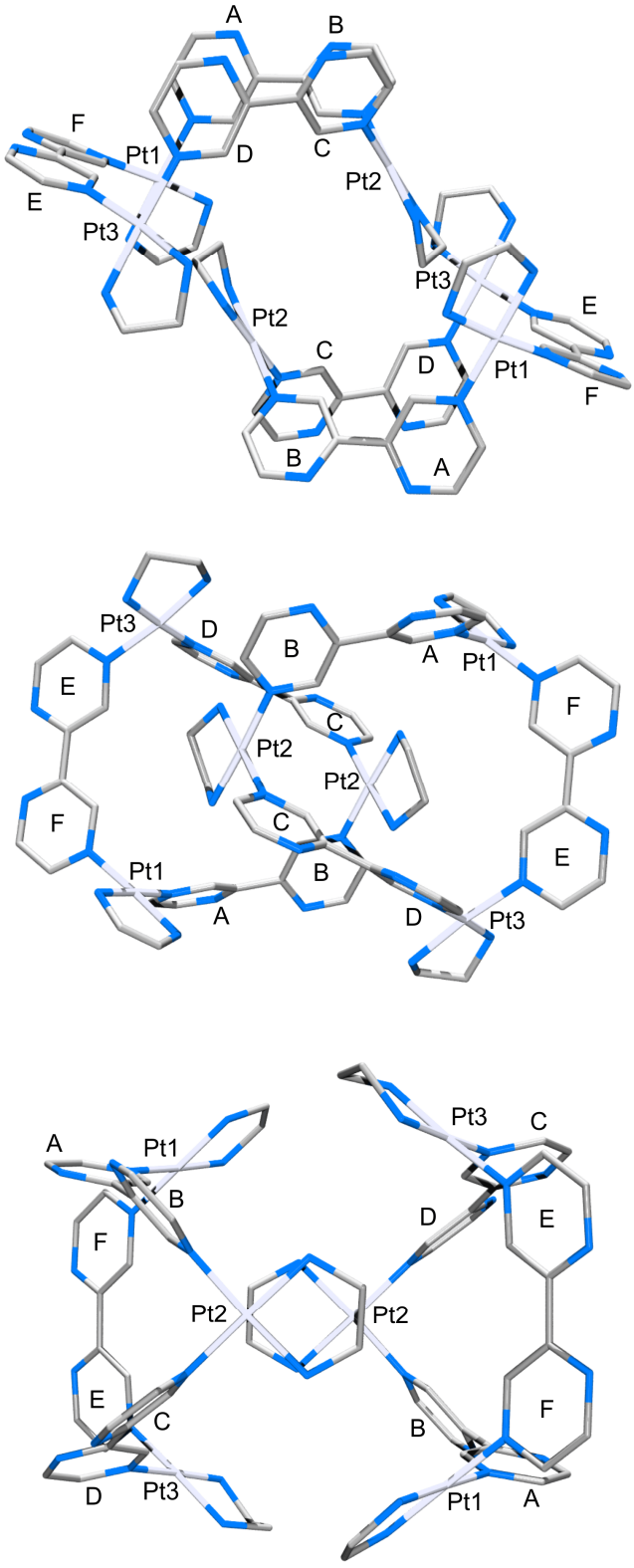

Figure SI4: Three different views of the mutual interaction between two cations of **3**.

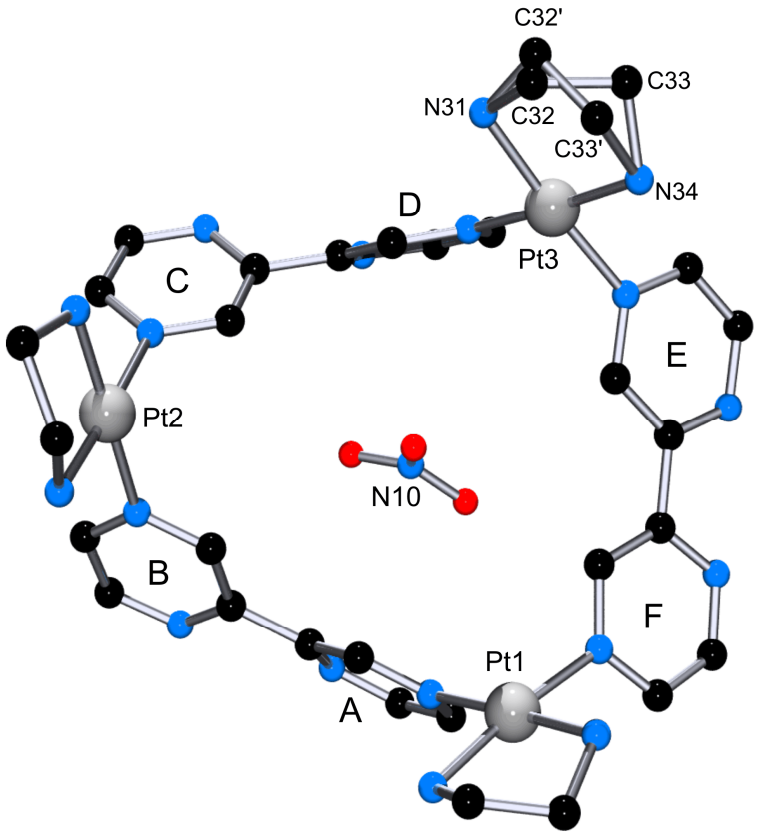

Figure SI-5: Views of cations **3** showing the two different conformations (δ and λ pucker) of the ethylendiamine ring at Pt3.

Table SI-1: Selected bond distances (Å) and angles (°) for compound **3**.

Pt1-N11, 2.008(7)	N11-Pt1-N14, 84.1(3)	$Pt1N_4$ / Pt_3 plane, 64.8
Pt1-N14, 2.021(6)	N11-Pt1-N4A, 177.6(3)	$Pt2N_4$ / Pt_3 plane, 67.9
Pt2-N21, 2.018(7)	N14-Pt1-N4A, 93.6(3)	$Pt3N_4$ / Pt_3 plane, 65.5
Pt2-N24, 2.017(6)	N11-Pt1-N4F, 91.2(3)	Pt1···Pt2, 7.9600(5)
Pt3-N31, 2.034(7)	N14-Pt1-N4F, 173.8(3)	Pt2···Pt3, 7.9112(5)
Pt3-N34, 2.030(8)	N4A-Pt1-N4F, 91.2(3)	Pt3···Pt1, 7.886(5)
Pt1-N4A, 2.024(7)	N4C-Pt2-N21, 176.5(2)	N1a···N1d, 6.827(11)
Pt1-N4F, 2.039(6)	N4C-Pt2-N24, 92.4(2)	N1b···N1c, 6.440(10)
Pt2-N4B, 2.022(6)	N21-Pt2-N24, 84.1(3)	N1a···N1b, 2.726(10)
Pt2-N4C, 2.012(6)	N4C-Pt2-N4B, 88.7(2)	N1c···N1d, 2.842(10)
Pt3-N4D, 2.029(7)	N21-Pt2-N4B, 94.8(3)	N1e···N1f, 2.694(10)
Pt3-N4E, 2.018(7)	N24-Pt2-N4B, 178.9(3)	N(A) / N(B), 26.2
	N4E-Pt3-N4D, 90.9(3)	N(C) / N(D), 42.4
	N4E-Pt3-N34, 91.3(3)	N(E) / N(F), 9.0
	N4D-Pt3-N34, 177.7(3)	
	N4E-Pt3-N31, 175.5(3)	
	N4D-Pt3-N31, 93.4(3)	
	N34-Pt3-N31, 84.4(3)	

Table SI-2: Hydrogen bonding distances (Å) for compound **3**.

N11···O6w[x, y, z+1], 2.920(10)	O2w···O41, 2.895(16)
N11···O1w[–x+2, –y+1, –z+1], 3.010(9)	O3w···O12, 2.786 (10)
N11···O7w[x, y, z+1], 3.081(13)	O4w···N1a[–x+1, –y+1, –z+1], 2.935(10)
N14···O12[–x+2, –y+1, –z+1], 2.874(9)	O4w···O3w[–x+2, –y, –z+1], 2.746(12)
N14···O2w[x, y+1, z], 2.948(9)	O4w···O2w, 2.786(11)
N21···O23, 3.210(15)	O4w···O5w, 2.874(13)
N21···O14[–x+2, –y+1, –z+1], 2.790(10)	O5w···O32[–x+1, –y+1, –z+1], 2.977(12)
N24···O11, 2.812(9)	O6w···O21, 2.699(15)
N24···O1w, 2.881(9)	O8w···O23[–x+2, –y+1, –z], 3.057(18)
N31···O41, 3.009(16)	O9w···O13w, 3.01(2)
N31···O14, 2.725(10)	O10w···O6w, 2.806(18)
N34···O23 [–x+2, –y+1, –z+1], 2.965(16)	O10w···O8w[–x+2, –y+1, –z], 2.800(18)
N34···O10w [–x+2, –y+1, –z+1], 2.867(13)	O11w···O24, 2.555(17)
O1w···O22, 2.689(13)	O11w··O43[–x+1, –y+1, –z+1], 2.66(2)
O1w···O5w, 2.789(9)	O12w···O42, 2.54(3)
O2w···O13, 2.667(10)	O12w···O11w[x, y–1, z+1], 2.91(2)