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SUPPLEMENTARY MATERIAL TO

New rhodium(III)–ED3AP complex: Crystal structure, characterization and computational chemistry

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TABLE S-I. Crystal data and structure refinement for complex *trans*(O_5)-Na[Rh(ED3AP)]·3H_2O

Empirical formula	$C_{11}H_{20}N_2NaO_{11}Rh$
Formula weight	482.19
T / K	100(2)
Radiation	Mo-Kα (λ = 0.71073 Å)
Crystal system, space group	orthorhombic, $P2_12_12_1$
a, b, c / Å	8.7006(3), 11.2207(6), 16.8707(9)
α, β, γ / °	90, 90, 90
V / Å^3	1647.03(14)
Z	4
F(000)	976
$D_{calc.}$ / Mg m^{-3}	1.945
θ / °	6-20
μ / mm^{-1}	1.13
Crystal size, mm; color; shape	0.32×0.27×0.08; yellow; prism
Index ranges	h = −11→12, k = −15→14, l = −23→22
T_{min}, T_{max}	0.738, 0.910
No. of collected, independent and observed [$I > 2\sigma(I)$] reflections	26443, 4556, 4326
R_{int}	0.029
θ_{min}; θ_{max} / °	3.4; 29.6
Refinement method on F^2	Full-matrix least-squares on F^2
Reflections/restraints/parameters	4556/9/295
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.017, wR2 = 0.0363

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TABLE S-I. Continued

Hydrogen site location	Difference Fourrier map. Only H-atom coordinates refined
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0148P)^2 + 0.5898P]$, where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$; $\Delta\rho_{min}$ / e Å^{-3}	0.46; -0.49

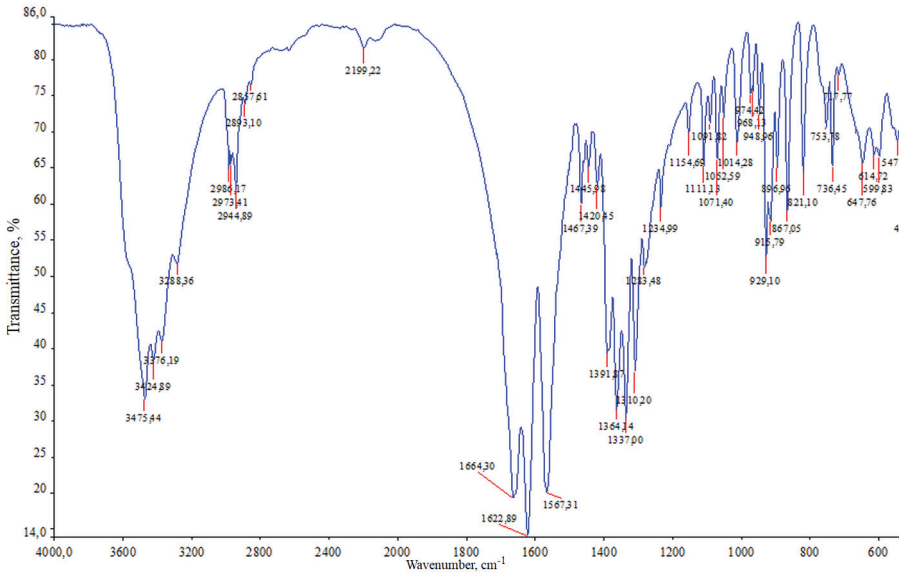


Fig. S-1. IR spectrum of *trans*(O_5)-Na[Rh(ED3AP)]·3H_2O complex

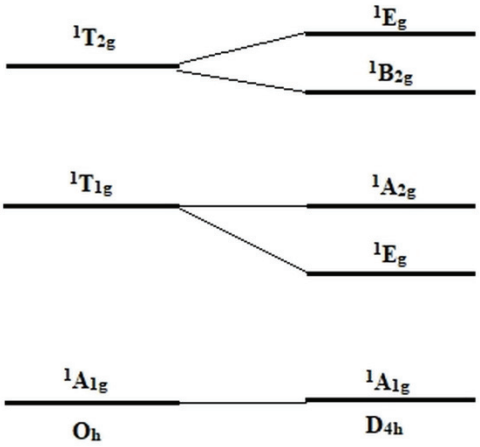
TABLE S-II. Selected bond distances and angles for *trans*(O_5)-Na[Rh(ED3AP)]·3H_2O

M-L bond lengths, Å			
Rh(1)-N(1)	2.011(2)	Rh(1)-O(3)	2.053(2)
Rh(1)-N(2)	2.023(2)	Rh(1)-O(5)	2.006(2)
Rh(1)-O(1)	1.999(2)	Rh(1)-O(7)	2.043(2)
Valence angles, °			
N(1)-Rh(1)-O(7)	175.12(7)	O(5)-Rh(1)-O(3)	90.21(7)
N(2)-Rh(1)-O(3)	167.88(7)	O(5)-Rh(1)-O(7)	89.53(7)
N(2)-Rh(1)-O(7)	93.83(7)	O(7)-Rh(1)-O(3)	97.03(7)
O(1)-Rh(1)-N(1)	85.59(7)	N(1)-Rh(1)-O(7)	175.12(7)
O(1)-Rh(1)-N(2)	96.43(7)	N(2)-Rh(1)-O(3)	167.88(7)
O(1)-Rh(1)-O(3)	88.97(7)	N(2)-Rh(1)-O(7)	93.83(7)
O(1)-Rh(1)-O(5)	178.99(7)	O(1)-Rh(1)-N(1)	85.59(7)
O(1)-Rh(1)-O(7)	89.99(7)	O(5)-Rh(1)-N(2)	84.49(7)
O(5)-Rh(1)-N(1)	94.86(7)	O(5)-Rh(1)-O(3)	90.21(7)
O(5)-Rh(1)-N(2)	84.49(7)		

TABLE S-III. Average bond distances of $[Rh(ED3AP)]^-$ isomers

$[Rh(ED3AP)]^-$	X-ray *trans*(O_5)	B3LYP optimized *trans*(O_5)	B3LYP optimized *trans*(O_5O_6)
average (Rh-N)	2.017	2.055	2.049
average (Rh-O)[a]	2.002	2.036	2.043
average (Rh-O)[b]	2.048	2.062	2.081

[a]average length of Rh-O axial oxygen
[b]average length of Rh-O equatorial oxygen



Scheme S-1. Therm splitting of d^6 complexes in Oh and D_{4h} symmetry.