Electronic supplementary information

Spectroscopic effects resulting from interacting singlet and triplet excited states: vibronic structure involving the O-H stretching mode in d-d absorption bands of $Ni(H_2O)_6^{2+}$

Christopher Dobe,[a] Emmanuel Gonzalez,[b] Philip L. W. Tregenna-Piggott,[a,x] Christian Reber[b*]

[a] Departement für Chemie und Biochimie, Universität Bern, CH-3012 Bern, Switzerland

[b] Département de chimie, Université de Montréal, Montréal QC H3C 3J7, Canada

[*] author for correspondence, christian.reber@umontreal.ca, tel. +1-514-343-7332

[x] Dedicated to the memory of our friend and colleague PLWTP

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Table ESI1 Anisotropic displacement parameters ($Å^2x10^3$) for $CsNi(H_2O)_6PO_4$. The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2 a^{*2}U^{11} + \ldots + 2 h k a^* b^* U^{12})$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	31(2)	77(2)	77(2)	-44(3)	0	0
O(2)	32(1)	32(1)	32(1)	-4(1)	-4(1)	-4(1)

Table ESI2 Hydrogen bonds for $CsNi(H_2O)_6PO_4$ (Å and °).

D-H…A	d(D-H)	d(H…A)	d(D…A)	D-H-A
O(1)-H…O(2)	0.72(5)	1.93(4)	2.644(2)	174(6)

Table ESI3. Ligand field and angular-overlap (AOM) parameters for $Ni(BrO_3)_2 \cdot 6H_2O$ and $Cs[Ni(H_2O)_6](PO_4)$

Parameter	$[Ni(H_2O)_6](BrO_3)_2$	$Cs[Ni(H_2O)_6](PO_4)$
B (cm^{-1})	950	950
C (cm^{-1})	3800	3800
Dq	6665	6330
e_σ (cm^{-1})	3520	3482
e_π (cm^{-1})	974	1029
^1E_g	14622	14608
$^3T_{1g}$ (^3F)	14343	14005
ζ (cm^{-1}) (ζ=-2 λ for Ni^{2+})	600	600
$E_g(^1E_g)$	15618	15445
$E_g(^3T_{1g})$	14054	13884
$A_{1g}(^3T_{1g})$	13632	13289
$T_{1g}(^3T_{1g})$	14104	13765
$T_{2g}(^3T_{1g})$	14850	14519