Supporting Information for M. K. Beyer, R. B. Metz:
Salt-bridge transition state for the charge separation $Co(H_2O)_4^{2+}$ -> $CoOH(H_2O)_2^{+}$ + H_3O^{+}

Cartesian coordinates of optimized structures:

Saltbridge Transition State of $Co(H_2O)_4^{2+}$:

O	-1.925545	-0.317639	-0.026641
Co	-0.209163	-0.004485	-0.061873
O	1.317284	-1.364461	0.086651
O	0.911485	1.678751	0.033854
H	-2.541136	-0.399130	0.706296
H	1.519734	1.904920	0.748887
H	0.636951	2.504286	-0.386002
H	2.100448	-1.393694	-0.477389
H	1.114695	-2.274226	0.341355
H	-3.762523	-0.739523	-2.015647
O	-4.284743	-0.903598	-2.831534
H	-4.714878	-1.784360	-2.848509
H	-4.908768	-0.178886	-3.047017

$CoOH(H_2O)_2^{+}$:

Co	-0.190615	-0.013035	-0.070979
O	-1.907924	-0.322816	-0.058307
O	0.931846	1.668496	0.033114
H	-2.533812	-0.399985	0.666330
H	1.530521	1.896613	0.755570
H	0.664779	2.492722	-0.394066
O	1.330983	-1.375215	0.104627
H	2.121863	-1.408353	-0.448322
H	1.123110	-2.283489	0.360390

H_3O^{+}:

O	-0.034273	0.059361	-0.026702
H	-0.080092	0.138729	0.948455
H	0.883344	0.100923	-0.367415
H	-0.529073	-0.714538	-0.367419

Summary of thermochemistry output in Gaussian98:

Saltbridge Transition State of $Co(H_2O)_4^{2+}$:

	(Hartree/Particle)
Zero-point correction=	0.097579
Thermal correction to Energy=	0.109983
Thermal correction to Enthalpy=	0.110927
Thermal correction to Gibbs Free Energy=	0.055779
Sum of electronic and zero-point Energies=	-451.021340
Sum of electronic and thermal Energies=	-451.008936
Sum of electronic and thermal Enthalpies=	-451.007992
Sum of electronic and thermal Free Energies=	-451.063140

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	69.016	37.410	116.069
ELECTRONIC	0.000	0.000	2.755
TRANSLATIONAL	0.889	2.981	40.523
ROTATIONAL	0.889	2.981	29.374
VIBRATIONAL	67.238	31.448	43.417

$CoOH(H_2O)_2^+$:

	(Hartree/Particle)
Zero-point correction=	0.062075
Thermal correction to Energy=	0.070764
Thermal correction to Enthalpy=	0.071708
Thermal correction to Gibbs Free Energy=	0.027713
Sum of electronic and zero-point Energies=	-374.381873
Sum of electronic and thermal Energies=	-374.373184
Sum of electronic and thermal Enthalpies=	-374.372240
Sum of electronic and thermal Free Energies=	-374.416235

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	44.405	27.413	92.596
ELECTRONIC	0.000	0.000	2.755
TRANSLATIONAL	0.889	2.981	40.055
ROTATIONAL	0.889	2.981	26.200
VIBRATIONAL	42.628	21.451	23.587

H_3O^+:

	(Hartree/Particle)
Zero-point correction=	0.034255
Thermal correction to Energy=	0.037166
Thermal correction to Enthalpy=	0.038110
Thermal correction to Gibbs Free Energy=	0.015117
Sum of electronic and zero-point Energies=	-76.702547
Sum of electronic and thermal Energies=	-76.699636
Sum of electronic and thermal Enthalpies=	-76.698692
Sum of electronic and thermal Free Energies=	-76.721684

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	23.322	6.664	48.392
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	34.771
ROTATIONAL	0.889	2.981	13.417
VIBRATIONAL	21.544	0.702	0.204