Supplementary information for

Water-Exchange Rates of Lanthanide Ions in an Ionic Liquid

Zhijin Lin,[a] Megan L. Shelby,[b] Dugan Hayes,[b] Kelly A. Fransted,[b] Lin X. Chen,[b] and Matthew J. Allen[a,]*

[a] Department of Chemistry, Wayne State University, 5101 Cass Avenue, Detroit, MI 48202, USA. E-mail: mallen@chem.wayne.edu; Fax: 1 313 577 8822;

[b] Chemical Science and Engineering Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, USA.

Experimental Procedures

Lanthanide(III) triflates were purchased from Sigma-Aldrich and dried at 0.38 Torr and 80 ºC for 12 h before use. 1-Ethyl-3-methylimidazolium ethylsulfate was purchased from Alfa Aesar and dried at 0.38 Torr and 80 ºC for 12 h before use. Tb_4O_7 was purchased from Alfa Aesar and used as received. ^{17}O-enriched water (10 or 35–40%) was provided by Cambridge Isotope Laboratories, Inc. Variable-temperature ^{17}O-NMR measurements were performed to calculate water-exchange rates, and luminescence-decay measurements were used to determine the water-coordination numbers.

The Tb L_3-edge XANES were collected at beamline 12BM at the Advanced Photon Source of Argonne National Laboratory. The X-ray absorption spectra at the terbium L_3-edge was collected for $Tb(OTf)_3$ in water/EMIES (1:19, v/v) as well as for solid powders of $Tb(OTf)_3$ and Tb_4O_7 diluted with powdered boron nitride, which is inert and X-ray transparent at the energies of interest. These powders serve as references for the oxidation state of the dissolved terbium because Tb^{4+} and Tb^{3+} have distinct XANES features. The L_3 edges were collected at 90° from the incident beam in fluorescence detection mode using a Canberra 13-element germanium solid-state detector array with the fluorescence energy window set to collect the terbium Lα emission. X-ray absorption fine structure data processing was performed with the Athena package (Bruce Ravel, NIST).[1]

Inductively coupled plasma optical emission spectroscopy (ICP-OES) measurements were performed on a HORIBA Jobin Yvon *ULTIMA* or PerkinElmer Optima 7000 DV spectrometer. Samples for ICP-OES were diluted with nitric acid (2% v/v, aqueous), and standards were prepared by serial dilution of commercially available Gd, Tb, Dy, Ho, and Er standards.

Luminescence-emission and luminescence-decay measurements of $Eu(OTf)_3$ or $Tb(OTf)_3$ in H_2O/1-ethyl-3-methylimidazolium ethylsulfate (EMIES) (1:19, v/v) and D_2O/EMIES (1:19, v/v) were acquired separately using a HORIBA Jobin Yvon Fluoromax-4 spectrofluorometer. For luminescence-decay measurements of $Eu(OTf)_3$, the following parameters were used: excitation wavelength (395 nm), emission wavelength (591 nm), excitation and emission slit widths (5 nm), flash count (100), initial delay (0.001 ms), maximum delay (1 ms), and delay increment (0.02 ms). For luminescence-decay measurements of $Tb(OTf)_3$, the following parameters were used: excitation wavelength (487 nm), emission wavelengths (544 nm), excitation and emission

slit widths (5 nm), flash count (100), initial delay (0.001 ms), maximum delay (2 ms), and delay increment (0.02 ms). The number of coordinated water molecules was determined using the method reported by Horrocks and coworkers.[2]

Variable-temperature ^{17}O-NMR measurements of lanthanide triflates [$Gd(OTf)_3$, $Tb(OTf)_3$, $Dy(OTf)_3$, $Ho(OTf)_3$, and $Er(OTf)_3$] and their diamagnetic reference [$Y(OTf)_3$] were performed in H_2O/EMIES (1:19, v/v) using a Varian-500S (67.78 MHz) spectrometer in the Lumingen Instrumentation Center at Wayne State University. ^{17}O-labled water (10% or 35–40% enrichment) was used in the measurements to improve the signal-to-noise ratios of the ^{17}O-NMR spectra. Reduced line widths of the bulk water peak at half height ($\Delta\upsilon_{1/2}$) in the presence of lanthanide ions and the diamagnetic reference were measured from 5 to 70 ºC in increments of 5 to 10 ºC to calculate the transverse relaxation ($\Delta\upsilon_{1/2}\pi = \frac{1}{T_2} - \frac{1}{T_{2A}}$). The water-coordination number of $Gd(OTf)_3$ in H_2O/EMIES (1:19, v/v) was set to 1.63 based on the luminescence-decay measurements of $Eu(OTf)_3$ in the same solvent. The water-coordination numbers of other lanthanide triflates were fixed to 1.65 based on the luminescence-decay measurements of $Tb(OTf)_3$ in the same solvent. The selection of $Eu(OTf)_3$ or $Tb(OTf)_3$ for water-coordination numbers was based on the lowest ionic radius difference between the ions. The concentrations of lanthanide ions were measured using ICP-OES. Finally, the reduced transverse relaxation rates of each studied lanthanide ion versus absolute temperature in H_2O/EMIES (1:19, v/v) were plotted and fitted using origin software (8.0951 B951) following a previously published procedure to solve the for water-exchange rates.[3]

Briefly, the water-exchange rate was fitted by measuring the transverse relaxation rates of water as a function of temperature for each lanthanide ion in H_2O/EMIES (1:19, v/v) according to eq's 1, 2, 3, and 4.

$$\frac{1}{T_{2r}} = \left(\frac{1}{T_2} - \frac{1}{T_{2A}}\right)\left(\frac{[H_2O]}{q[Ln]}\right) = \frac{1}{T_{2m} + \tau_m} \qquad (1)$$

$$\frac{1}{T_{2m}} \cong \frac{S(S+1)}{3}\left(\frac{A}{\hbar}\right)^2 (T_{1e}^{-1} + \tau_m^{-1})^{-1} \qquad (2)$$

$$\frac{1}{T_{1e}} \cong \frac{1}{T_{1e}^{298}} \exp\left(\frac{\Delta E_{T_{1e}}}{R}\left(\frac{1}{T} - \frac{1}{298K}\right)\right) \qquad (3)$$

$$\frac{1}{\tau_m} \cong \frac{1}{\tau_m^{298}} \frac{T}{298K} \exp\left(\frac{\Delta H}{R}\left(\frac{1}{298K} - \frac{1}{T}\right)\right) \qquad (4)$$

In eq 1, $\frac{1}{T_{2r}}$ is the reduced transverse relaxation rate of water; $\frac{1}{T_2}$ is the transverse relaxation rate of water for paramagnetic lanthanide ions, while $\frac{1}{T_{2A}}$ is the transverse relaxation rate of water for the diamagnetic reference [$Y(OTf)_3$ was used as diamagnetic reference in this study due to its similar ionic radius to the lanthanide ions studied.]; q is the water-coordination number of lanthanide in H_2O/EMIES (1:19, v/v); [H_2O] and [Ln] are the concentration of water and lanthanide, respectively; T_{2m} is the transverse relaxation time of bound water in the paramagnetic sample; and τ_m is the residency lifetime of bound water. T_{2m} can be expressed by eq 2. In eq 2, S is the electron spin quantum number of Ln^{3+}; $\frac{A}{\hbar}$ is the hyperfine coupling constant between the Ln^{3+} and the oxygen nucleus, and these values were adopted by previous reported values (Table S1);[3] and T_{1e} is the electron relaxation time that is assumed to vary as a function of temperature based on eq's 3 and 4. In eq 3, T_{1e}^{298} is the electron relaxation time at 298 K; $\Delta E_{T_{1e}}$ is the activation energy for $1/T_{1e}$ and was fixed to 2.5×10^{-11} J/mol; T is the absolute temperature; and R is the ideal gas constant. In eq 4, τ_m^{298} is the residency life time of a bound water molecule at 298 K, and ΔH is the enthalpy associated with the exchange process.

Table S1. A/ħ for different lanthanide ions[4]

Ln^{3+}	A/ħ (10^{-6} rad/s)
Gd^{3+}	–3.80
Tb^{3+}	–3.89
Dy^{3+}	–3.74
Ho^{3+}	–3.77
Er^{3+}	–4.17

Luminescence-Decay Rate Data and Calculated *q* Values

	rate for $Eu(OTf)_3$ (ms^{-1})	rate for $Tb(OTf)_3$ (ms^{-1})
H_2O/EMIES (1:19, v/v)	2.38 ± 0.02	0.790 ± 0.006
D_2O/EMIES (1:19, v/v)	0.599 ± 0.006	0.401 ± 0.002

	$Eu(OTf)_3$	$Tb(OTf)_3$
q	1.6	1.6

q values were calculated using the equation in reference 2. The specific forms are listed below:

For Eu^{3+}: $q = 1.11(\tau_{H_2O}^{-1} - \tau_{D_2O}^{-1} - 0.31)$;

For Tb^{3+}: $q = 4.2(\tau_{H_2O}^{-1} - \tau_{D_2O}^{-1})$;

$\tau_{H_2O}^{-1}$ and $\tau_{D_2O}^{-1}$ are the luminescence-decay rates of lanthanide ions in H_2O and D_2O, respectively.

^{17}O-NMR Data

$Gd(OTf)_3$ in H_2O/EMIES_Trial 1

Temperature (ºC)	Linewidth at half height (Hz)	
	Gd^{3+}	Y^{3+}
15	4128	2410
20	4165	1964
30	3948	1433
40	3336	1009
50	2740	740
60	2070	546
70	1434	432

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (10/10/2013 15:29:17)*

Parameters

		Value	Standard Error
1overT2P	T1e298	4.26971E-7	8.31507E-8
	taum298	1.70197E-7	7.17026E-9
	deltaH	35075.46794	1552.43679
	deltaE	2.5E-11	0
	q	1.63	0
	Gd	0.00352	0

Iterations Performed = 8
Total Iterations in Session = 8
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

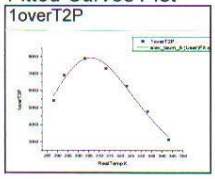
Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	65729.92999
Residual Sum of Squares	262919.71998
Adj. R-Square	0.97561
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot

1overT2P



$Gd(OTf)_3$ in H_2O/EMIES_Trial 2

Temperature (ºC)	Linewidth at half height (Hz)	
	Gd^{3+}	Y^{3+}
15	4196	2612
20	3995	2191
30	3947	1504
40	3425	1014
50	3024	741
60	2143	567
70	1302	432

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/20/2014 14:12:37)*

Parameters

		Value	Standard Error
1overT2P	T1e298	8.79721E-8	9.18903E-9
	taum298	2.37436E-7	1.95863E-8
	deltaH	47042.99122	2997.44853
	deltaE	2.5E-11	0
	q	1.63	0
	Gd	0.00521	0

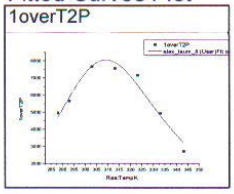
Iterations Performed = 11
Total Iterations in Session = 11
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	210909.34066
Residual Sum of Squares	843637.36265
Adj. R-Square	0.93471
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Gd(OTf)_3$ in H_2O/EMIES_Trial 3

Temperature (ºC)	Linewidth at half height (Hz)	
	Gd^{3+}	Y^{3+}
15	4409	2844
20	3872	2243
30	3951	1454
40	3147	1058
50	2457	781
60	1869	588
70	1268	443

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/20/2014 14:15:19)*

Parameters

		Value	Standard Error
1overT2P	T1e298	1.35504E-7	2.41055E-8
	taum298	1.95353E-7	1.93297E-8
	deltaH	44885.63994	3753.90545
	deltaE	2.5E-11	0
	q	1.63	0
	Gd	0.00407	0

Iterations Performed = 7
Total Iterations in Session = 7
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

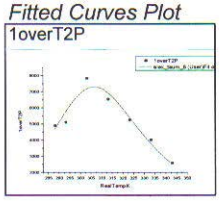
Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	275647.05476
Residual Sum of Squares	1.10259E6
Adj. R-Square	0.90343
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot

1overT2P



$Tb(OTf)_3$ in H_2O/EMIES_Trial 1

Temperature (ºC)	Linewidth at half height (Hz)	
	Tb^{3+}	Y^{3+}
15	3417	2704
20	2700	2227
25	2101	1712
30	1738	1431
40	1166	985
50	855	746
60	626	561
70	484	435

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/20/2014 14:57:33)*

Parameters

		Value	Standard Error
1overT2P	T1e298	6E-8	0
	taum298	1.03118E-8	3.85269E-10
	deltaH	45932.79844	3206.4636
	deltaE	2.5E-11	0
	q	1.65	0
	Tb	0.00397	0

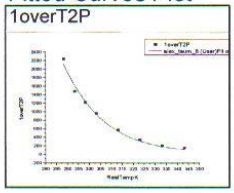
Iterations Performed = 6
Total Iterations in Session = 6
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	8
Degrees of Freedom	6
Reduced Chi-Sqr	7155.72932
Residual Sum of Squares	42934.37592
Adj. R-Square	0.9865
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Tb(OTf)_3$ in H_2O/EMIES_Trial 2

Temperature (ºC)	Linewidth at half height (Hz)	
	Tb^{3+}	Y^{3+}
5	5463	4178
10	4560	3617
15	3517	2802
20	2884	2244
30	1888	1510
40	1261	1059
50	886	777

1

Nonlinear Curve Fit (alex_taum_8 (User)) (4/16/2014 15:48:03)

Parameters

		Value	Standard Error
1overT2P	T1e298	9E-8	0
	taum298	9.35628E-9	5.30272E-10
	deltaH	41270.86692	2636.55162
	deltaE	2.5E-11	0
	q	1.65	0
	Tb	0.0047	0

Iterations Performed = 6
Total Iterations in Session = 6
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

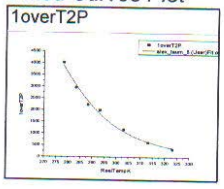
Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	5
Reduced Chi-Sqr	18984.74243
Residual Sum of Squares	94923.71217
Adj. R-Square	0.989
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot

1overT2P



$Tb(OTf)_3$ in H_2O/EMIES_Trial 3

Temperature (ºC)	Linewidth at half height (Hz)	
	Tb^{3+}	Y^{3+}
15	3637	2757
20	2984	2233
30	1947	1483
40	1337	1045
50	941	760
60	700	571
70	533	442

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/20/2014 15:57:14)*

Parameters

		Value	Standard Error
1overT2P	T1e298	9E-8	0
	taum298	1.26832E-8	1.91145E-10
	deltaH	35790.20387	1064.38225
	deltaE	2.5E-11	0
	q	1.65	0
	Tb	0.0046	0

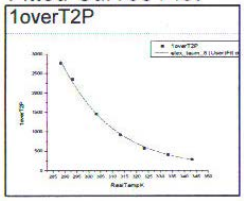
Iterations Performed = 4
Total Iterations in Session = 4
Fit converged - Chi-sqr no longer changed.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	5
Reduced Chi-Sqr	2342.56875
Residual Sum of Squares	11712.84373
Adj. R-Square	0.99757
Fit Status	Succeeded(101)

Fit Status Code :
101 : Fit converged

Fitted Curves Plot



$Tb(OTf)_3$ in H_2O/EMIES_Trial 4

Temperature (ºC)	Linewidth at half height (Hz)	
	Tb^{3+}	Y^{3+}
15	3407	2931
20	2740	2329
30	2331	1900
40	1855	1599
50	1280	1098
60	959	813
70	683	606

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/20/2014 15:14:25)*

Parameters

		Value	Standard Error
1overT2P	T1e298	9E-8	0
	taum298	7.40187E-9	1.59356E-10
	deltaH	29031.5069	1436.33912
	deltaE	2.5E-11	0
	q	1.65	0
	Tb	0.00417	0

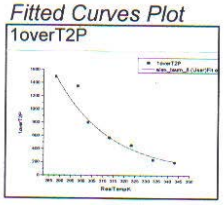
Iterations Performed = 5
Total Iterations in Session = 5
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	5
Reduced Chi-Sqr	1858.48044
Residual Sum of Squares	9292.40219
Adj. R-Square	0.99268
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Dy(OTf)_3$ in H_2O/EMIES_Trial 1

Temperature (°C)	Linewidth at half height (Hz)	
	Dy^{3+}	Y^{3+}
15	3474	2757
20	2908	2233
30	1797	1483
40	1239	1045
50	886	760
60	655	571
70	493	442

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/23/2014 19:48:44)*

Parameters

		Value	Standard Error
1overT2P	T1e298	4.38487E-8	2.67429E-8
	taum298	1.97969E-8	7.48666E-9
	deltaH	54256.51253	16233.32243
	deltaE	2.5E-11	0
	q	1.65	0
	Dy	0.0046	0

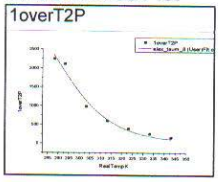
Iterations Performed = 9
Total Iterations in Session = 9
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	22005.74019
Residual Sum of Squares	88022.96076
Adj. R-Square	0.97119
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Dy(OTf)_3$ in H_2O/EMIES_Trial 2

Temperature (ºC)	Linewidth at half height (Hz)	
	Dy^{3+}	Y^{3+}
15	3131	2703
20	2633	2227
25	2055	1712
30	1748	1431
40	1192	985
50	853	746
60	628	561
70	472	434

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (8/12/2013 15:04:12)*

Parameters

		Value	Standard Error
1overT2P	T1e298	1.66457E-8	6.86318E-10
	taum298	3.62926E-8	4.34465E-9
	deltaH	62208.40188	4282.65049
	deltaE	2.5E-11	0
	q	1.65	0
	Dy	0.0042	0

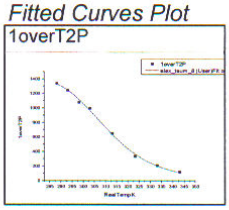
Iterations Performed = 6
Total Iterations in Session = 6
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	8
Degrees of Freedom	5
Reduced Chi-Sqr	862.9925
Residual Sum of Squares	4314.9625
Adj. R-Square	0.9963
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Dy(OTf)_3$ in H_2O/EMIES_Trial 3

Temperature (°C)	Linewidth at half height (Hz)	
	Dy^{3+}	Y^{3+}
15	3113	2754
20	2558	2206
30	1735	1454
50	871	757
60	644	565
70	489	434

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/23/2014 19:50:18)*

Parameters

		Value	Standard Error
1overT2P	T1e298	1.21411E-8	8.04749E-10
	taum298	3.15739E-8	7.47723E-9
	deltaH	57083.60132	6652.05691
	deltaE	2.5E-11	0
	q	1.65	0
	Dy	0.0047	0

Iterations Performed = 5
Total Iterations in Session = 5
Fit converged - Chi-sqr no longer changed.
Some parameter values were fixed.

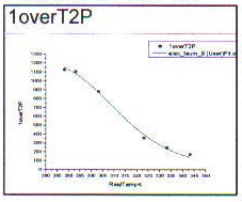
Statistics

	1overT2P
Number of Points	6
Degrees of Freedom	3
Reduced Chi-Sqr	1267.88008
Residual Sum of Squares	3803.64023
Adj. R-Square	0.99342
Fit Status	Succeeded(101)

Fit Status Code :
101 : Fit converged

Fitted Curves Plot

1overT2P



$Ho(OTf)_3$ in H_2O/EMIES_Trial 1

Temperature (ºC)	Linewidth at half height (Hz)	
	Ho^{3+}	Y^{3+}
15	3155	2702
20	2594	2266
30	1940	1769
40	1669	1477
50	1134	1031
60	837	757
70	607	558

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (4/18/2014 13:22:47*

Parameters

		Value	Standard Error
1overT2P	T1e298	3.75434E-8	1.45628E-8
	taum298	1.93417E-8	4.93209E-9
	deltaH	46134.93133	8768.43068
	deltaE	2.5E-11	0
	q	1.65	0
	Ho	0.00448	0

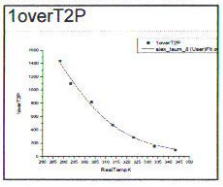
Iterations Performed = 10
Total Iterations in Session = 10
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	2885.23565
Residual Sum of Squares	11540.94262
Adj. R-Square	0.98898
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Ho(OTf)_3$ in H_2O/EMIES_Trial 2

Temperature (ºC)	Linewidth at half height (Hz)	
	Ho^{3+}	Y^{3+}
20	2481	2206
30	1674	1454
40	1149	1070
50	819	757
60	610	565
70	470	434

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/23/2014 19:56:55)*

Parameters

		Value	Standard Error
1overT2P	T1e298	1.83889E-8	1.16703E-8
	taum298	2.13722E-8	1.80651E-8
	deltaH	60119.86167	29256.48609
	deltaE	2.5E-11	0
	q	1.65	0
	Ho	0.0045	0

Iterations Performed = 6
Total Iterations in Session = 6
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

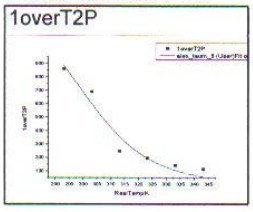
Statistics

	1overT2P
Number of Points	6
Degrees of Freedom	3
Reduced Chi-Sqr	8468.71591
Residual Sum of Squares	25406.14772
Adj. R-Square	0.91662
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot

1overT2P



$Ho(OTf)_3$ in H_2O/EMIES_Trial 3

Temperature (ºC)	Linewidth at half height (Hz)	
	Ho^{3+}	Y^{3+}
20	2465	2145
30	1587	1444
40	1153	1042
50	809	749
60	594	572
70	469	442

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (1/23/2014 19:58:05)*

Parameters

		Value	Standard Error
1overT2P	T1e298	1.28243E-8	1.12984E-9
	taum298	2.55447E-8	4.82698E-9
	deltaH	58866.43619	5754.42141
	deltaE	2.5E-11	0
	q	1.65	0
	Ho	0.0045	0

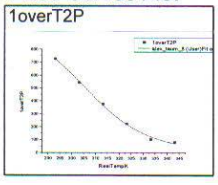
Iterations Performed = 7
Total Iterations in Session = 7
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

Statistics

	1overT2P
Number of Points	6
Degrees of Freedom	3
Reduced Chi-Sqr	271.61149
Residual Sum of Squares	814.83447
Adj. R-Square	0.99587
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Er(OTf)_3$ in H_2O/EMIES_Trial 1

Temperature (°C)	Linewidth at half height (Hz)	
	Er^{3+}	Y^{3+}
15	3295	2862
25	2040	1738
30	1707	1506
40	1152	1038
50	816	750
60	610	562
70	463	444

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (4/18/2014 13:38:59*

Parameters

		Value	Standard Error
1overT2P	T1e298	4.35855E-8	1.03711E-8
	taum298	2.41928E-8	4.3206E-9
	deltaH	56550.64723	8359.14399
	deltaE	2.5E-11	0
	q	1.65	0
	Er	0.00448	0

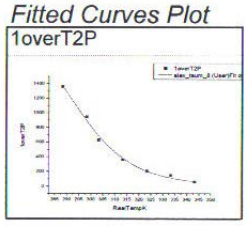
Iterations Performed = 7
Total Iterations in Session = 7
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	4
Reduced Chi-Sqr	2048.66142
Residual Sum of Squares	8194.64569
Adj. R-Square	0.99104
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Er(OTf)_3$ in H_2O/EMIES_Trial 2

Temperature (°C)	Linewidth at half height (Hz)	
	Er^{3+}	Y^{3+}
15	3145	2844
20	2511	2243
30	1651	1454
40	1123	1058
50	806	781
60	609	588
70	464	443

1 Nonlinear Curve Fit (alex_taum_8 (User)) (4/18/2014 14:10:47

Parameters

		Value	Standard Error
1overT2P	T1e298	7E-8	0
	taum298	1.6983E-8	9.61401E-10
	deltaH	71740.7672	7460.53738
	deltaE	2.5E-11	0
	q	1.65	0
	Er	0.00492	0

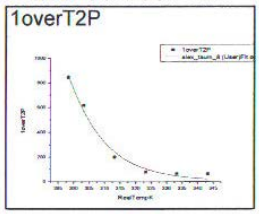
Iterations Performed = 4
Total Iterations in Session = 4
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

Statistics

	1overT2P
Number of Points	6
Degrees of Freedom	4
Reduced Chi-Sqr	1835.18236
Residual Sum of Squares	7340.72945
Adj. R-Square	0.98369
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot



$Er(OTf)_3$ in H_2O/EMIES_Trial 3

Temperature (°C)	Linewidth at half height (Hz)	
	Er^{3+}	Y^{3+}
15	3102	2612
20	2449	2191
30	1632	1503
40	1132	1015
50	863	741
60	614	567
70	468	433

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (4/18/2014 13:54:09)*

Parameters

		Value	Standard Error
1overT2P	T1e298	9E-8	0
	taum298	1.68693E-8	2.66764E-9
	deltaH	51490.97875	12725.87356
	deltaE	2.5E-11	0
	q	1.65	0
	Er	0.00415	0

Iterations Performed = 14
Total Iterations in Session = 14
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.
Some input data points are missing.

Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	5
Reduced Chi-Sqr	32812.99585
Residual Sum of Squares	164064.97923
Adj. R-Square	0.86723
Fit Status	Succeeded(100)

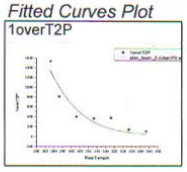
Fit Status Code :
100 : Fit converged

ANOVA

		DF	Sum of Squares	Mean Square	F Value	Prob>F
1overT2P	Regression	2	3.34336E6	1.67168E6	50.94567	8.38067E-4
	Residual	5	164064.97923	32812.99585		
	Uncorrected Total	7	3.50743E6			
	Corrected Total	6	1.4828E6			

Fitted Curves Plot

1overT2P



$Er(OTf)_3$ in H_2O/EMIES_Trial 4

Temperature (°C)	Linewidth at half height (Hz)	
	Er^{3+}	Y^{3+}
20	2529	2161
25	2040	1803
30	1688	1465
35	1376	1256
40	1121	1072
45	972	884
50	833	768

1 *Nonlinear Curve Fit (alex_taum_8 (User)) (4/18/2014 14:20:10*

Parameters

		Value	Standard Error
1overT2P	T1e298	9E-8	0
	taum298	1.63732E-8	1.21545E-9
	deltaH	56836.33027	8181.8336
	deltaE	2.5E-11	0
	q	1.65	0
	Er	0.0046	0

Iterations Performed = 5
Total Iterations in Session = 5
Fit converged - tolerance criterion satisfied.
Some parameter values were fixed.

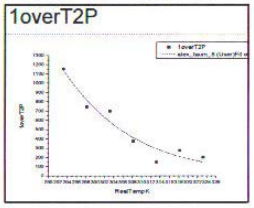
Statistics

	1overT2P
Number of Points	7
Degrees of Freedom	5
Reduced Chi-Sqr	9677.5094
Residual Sum of Squares	48387.547
Adj. R-Square	0.92753
Fit Status	Succeeded(100)

Fit Status Code :
100 : Fit converged

Fitted Curves Plot

1overT2P



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