

Supporting Information

A Comparative Study on the Binding Interaction of Nd(III) with D-Proline and DL- Proline in Absence and Presence of Zn(II) using 4f-4f Transition Spectra as an Absorption Probe

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Table S1 Transition energies and intraconfigurational $U^{(\lambda)}$ matrix elements for Nd(III)

Transition	Approximate (cm ⁻¹)	ν	$[U^{(2)}]^2$	$[U^{(4)}]^2$	$[U^{(6)}]^2$
$^4I_{9/2} \rightarrow ^4F_{3/2}$	11232	0		0.2299	0.0547
$^4I_{9/2} \rightarrow ^4F_{5/2}$	12277	0.0009		0.2361	0.3973
$^4I_{9/2} \rightarrow ^2H_{9/2}$	12527	0.0062		0.0076	0.4249
$^4I_{9/2} \rightarrow ^4S_{3/2}$	13113	0		0.0027	0.0381
$^4I_{9/2} \rightarrow ^4F_{7/2}$	13268	0.0010		0.0420	0.0355
$^4I_{9/2} \rightarrow ^4G_{5/2}$	16897	0.8968		0.04091	0.0547
$^4I_{9/2} \rightarrow ^2G_{7/2}$	17044	0.0755		0.1848	0.0136
$^4I_{9/2} \rightarrow ^2K_{3/2}$	18803	0.0068		0.0002	0.0407
$^4I_{9/2} \rightarrow ^4G_{7/2}$	18823	0.051		0.1569	0.0080
$^4I_{9/2} \rightarrow ^4G_{9/2}$	19260	0.0046		0.0611	0

Table S2

Observed and computed values of energies in cm^{-1} for Nd(III); Nd(III):D-Proline (1:1); Nd(III):D-Proline:Zn(II) (1:1:1) and Nd(III):DL-Proline (1:1); Nd(III):DL-Proline:Zn(II) (1:1:1) in absence and presence of Zn(II) in different aquated organic solvents at 298 K

System	$^4\text{I}_{9/2} \rightarrow ^4\text{G}_{7/2}$		$^4\text{I}_{9/2} \rightarrow ^4\text{G}_{5/2}$		$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{7/2}$		$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{5/2}$		$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{3/2}$		r.m.s
	E _{obs}	E _{cal}	E _{obs}	E _{cal}	E _{obs}	E _{cal}	E _{obs}	E _{obs}	E _{obs}	E _{cal}	
1. H ₂ O											
Nd(III)	19168.47	19173.73	17394.33	17409.81	13509.13	13466.71	12591.60	12627.26	11560.29	11552.67	25.96
Nd(III):D-Proline	19168.10	19173.81	17393.12	17408.88	13508.22	13466.50	12591.60	12626.93	11560.69	11552.13	25.86
Nd(III):D-Proline:Zn(II)	19166.63	19173.48	17393.42	17408.06	13508.04	13466.42	12591.13	12626.75	11560.83	11551.62	25.48
Nd(III):DL-Proline	19167.37	19173.55	17394.33	17409.11	13508.58	13466.56	12591.29	12627.05	11560.69	11552.23	25.97
Nd(III):DL-Proline:Zn(II)	19166.27	19173.51	17394.03	17407.44	13507.85	13466.26	12590.49	12626.52	11560.43	11551.25	25.84
2. CH ₃ CN											
Nd(III)	19183.92	19178.30	17394.93	17417.59	13509.32	13466.13	12591.13	12627.92	11560.83	11557.36	27.48
Nd(III):D-Proline	19180.61	19177.58	17392.82	17414.37	13509.13	13466.03	12590.34	12627.31	11560.69	11555.49	27.29
Nd(III):D-Proline:Zn(II)	19178.40	19177.14	17391.30	17411.69	13508.95	13465.91	12589.70	12626.75	11560.03	11553.94	27.13
Nd(III):DL-Proline	19180.61	19177.55	17392.82	17414.37	13509.50	13466.08	12589.54	12627.35	11560.56	11555.49	27.49
Nd(III):DL-Proline:Zn(II)	19179.87	19177.48	17391.30	17412.74	13509.50	13466.00	12589.70	12626.99	11560.16	11554.58	27.49
3. CH ₃ OH											
Nd(III)	19163.70	19174.00	17388.28	17395.64	13506.94	13465.10	12586.69	12623.42	11552.95	11544.62	25.80
Nd(III):D-Proline	19163.33	19173.88	17387.68	17396.10	13507.85	13465.20	12585.74	12623.59	11554.42	11544.88	26.55
Nd(III):D-Proline:Zn(II)	19161.86	19173.89	17384.65	17392.13	13509.40	13464.81	12584.95	12622.56	11553.08	11542.63	26.46
Nd(III):DL-Proline	19164.43	19173.94	17388.88	17399.43	13506.94	13465.36	12587.48	12624.33	11556.82	11546.73	26.04
Nd(III):DL-Proline:Zn(II)	19161.86	19173.80	17383.75	17392.80	13507.13	13464.95	12585.26	12622.80	11554.28	11543.01	26.61
4. Dioxane											
Nd(III)	19160.76	19174.23	17366.24	17383.91	13507.31	13464.74	12584.16	12620.94	11555.08	11538.14	28.09
Nd(III):D-Proline	19160.03	19174.36	17361.11	17379.45	13507.31	13464.55	12583.52	12619.95	11553.21	11535.68	28.30
Nd(III):D-Proline:Zn(II)	19159.66	19174.79	17357.49	17378.60	13505.12	13463.98	12582.73	12619.35	11556.95	11535.14	28.93
Nd(III):DL-Proline	19160.03	19174.40	17360.51	17380.09	13506.76	13464.50	12583.68	12620.03	11554.82	11536.02	28.46
Nd(III):DL-Proline:Zn(II)	19159.66	19174.79	17355.99	17375.55	13506.58	13464.10	12582.26	12618.85	11552.95	11533.50	28.75
5. DMF											
Nd(III)	19150.48	19212.74	17272.35	17214.13	13374.17	13415.32	12500.63	12550.27	11546.14	11439.58	67.50
Nd(III):D-Proline	19149.75	19212.08	17272.35	17214.64	13376.49	13415.96	12500.94	12550.88	11545.48	11439.91	66.95
Nd(III):D-Proline:Zn(II)	19151.58	19213.01	17272.95	17214.56	13373.81	13415.29	12501.25	12550.31	11545.34	11439.84	66.99
Nd(III):DL-Proline	19149.75	19212.31	17272.35	17213.84	13375.06	13415.62	12501.09	12550.47	11545.21	11439.44	67.24
Nd(III):DL-Proline:Zn(II)	19150.85	19212.26	17272.35	17216.17	13376.85	13416.10	12501.25	12551.26	11546.41	11440.80	66.52