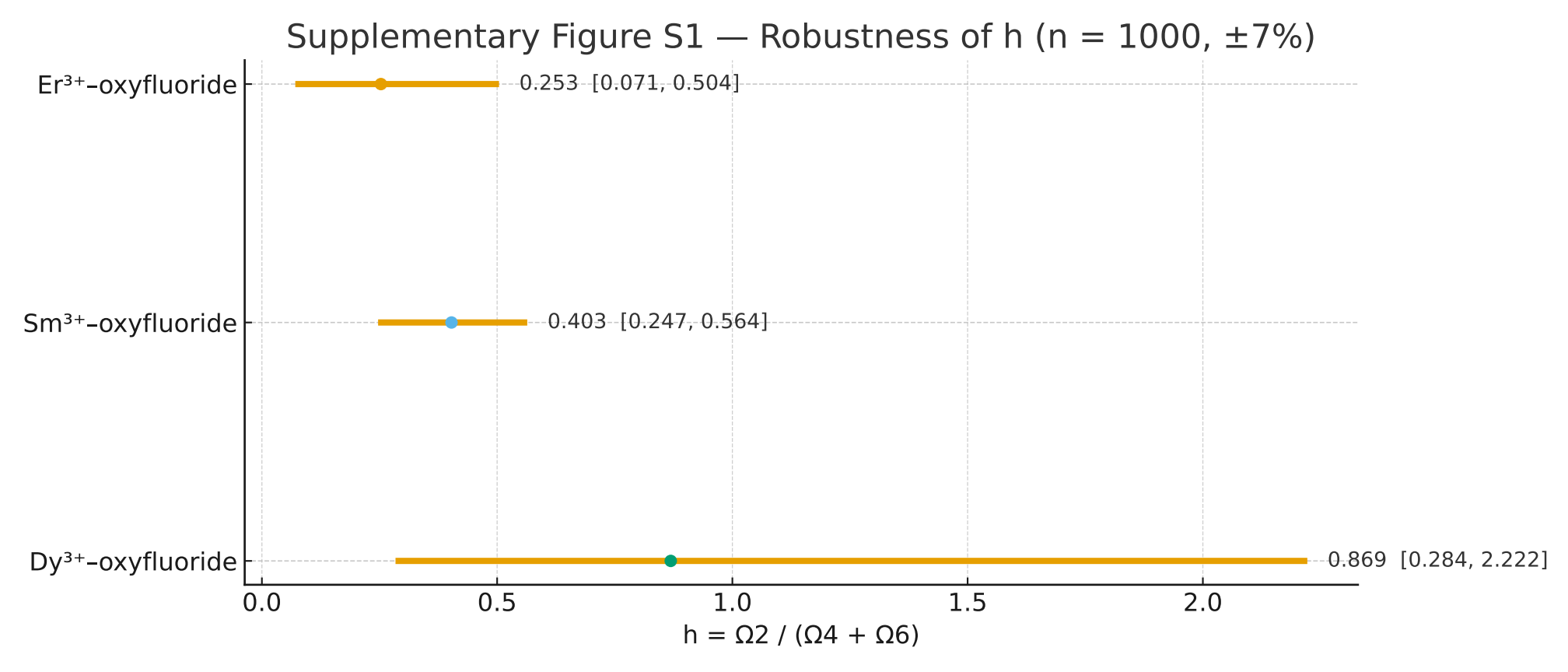
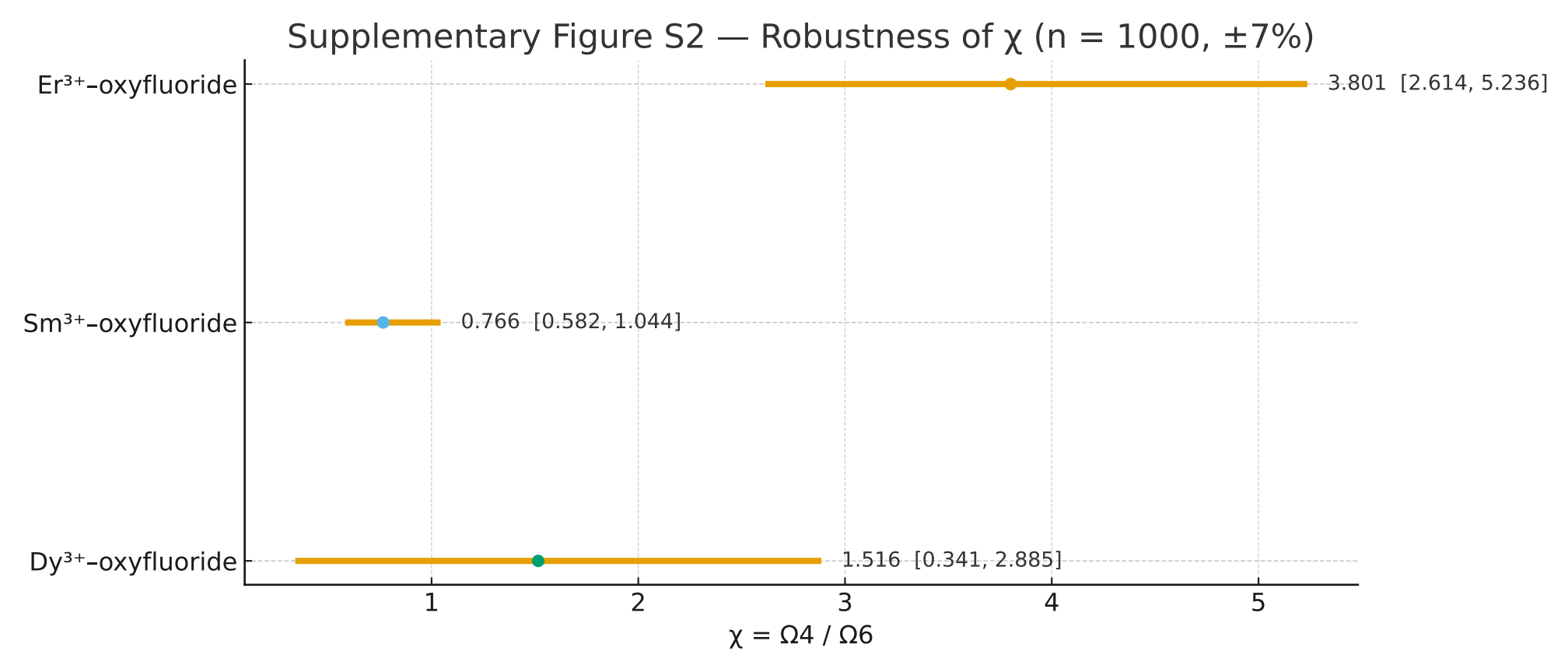

Supplementary Figure S1 — Robustness of h (n = 1000, ±7%)
Er³⁺–oxyfluoride
Sm³⁺–oxyfluoride
Dy³⁺–oxyfluoride
0.253 [0.071, 0.504]
0.403 [0.247, 0.564]
0.869 [0.284, 2.222]
0.0
0.5
1.0
1.5
2.0
h = Ω2 / (Ω4 + Ω6)


Supplementary Figure S2 — Robustness of χ (n = 1000, ±7%)
Er³⁺–oxyfluoride
Sm³⁺–oxyfluoride
Dy³⁺–oxyfluoride
3.801 [2.614, 5.236]
0.766 [0.582, 1.044]
1.516 [0.341, 2.885]
1
2
3
4
5
χ = Ω4 / Ω6

Supplementary Table S1 — Conditioning and robustness of inverse JO descriptors

Robustness intervals computed from n = 1000 Monte Carlo resamples with ±7% multiplicative jitter of S_{rel} and renormalization of the total; small baseline/window perturbations are modeled implicitly by the jitter.

Ion/Host	cond(3×3)	h (nominal)	h [2.5%,97.5%]	χ (nominal)	χ [2.5%,97.5%]	n
Er^{3+}–oxyfluoride	11.199	0.253	[0.071, 0.504]	3.801	[2.614, 5.236]	1000
Sm^{3+}–oxyfluoride	4.296	0.403	[0.247, 0.564]	0.766	[0.582, 1.044]	1000
Dy^{3+}–oxyfluoride	30.952	0.869	[0.284, 2.222]	1.516	[0.341, 2.885]	1000