Supplementary Information

Establishing Cost-Effective Computational Models for the Prediction of Lanthanoid Binding in $[Ln(NO_3)]^{2+}$ (with Ln = La to Lu)

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Table S.1 contains the predicted Gibbs free energy of reaction for $[Ln(NO_3)]^{+2}$ calculated with CCSD(T)-FSI/cc-pVTZ-DK3, MP2-FSI/cc-pVTZ-DK3, CCSD(T)-FSII/cc-pwCVTZ-DK3, MP2-FSI/cc-pV∞Z, CCSD(T)-FSI/cc-pV∞Z-DK3, and CCSD(T)-FSII/cc-pCV∞Z-DK3.

Table S.2 contains the predicted Gibbs free energy of reaction for $[Ln(NO_3)]^{+2}$ calculated with the composite Method A and Method B, and the Target Method, CCSD(T)-FSII/cc-pwCV∞Z-DK3.

Table S.3 contains absolute and relative cost for target method and f-ccCA for $[Ln(NO_3)]^{+2}$ (with Ln = La, Ce, Sm, and Lu).

Table S.1: ΔG_{rxn} (kcal mol^{-1}) for $[Ln(NO_3)]^{+2}$ calculated with CCSD(T)-FSI/cc-pVTZ-DK3, MP2-FSI/cc-pVTZ-DK3, CCSD(T)-FSII/cc-pwCVTZ-DK3, MP2-FSI/cc-pV∞Z, CCSD(T)-FSI/cc-pV∞Z-DK3, and CCSD(T)-FSII/cc-pwCV∞Z-DK3.

	CCSD(T)-FSI /cc-pVTZ-DK3	**MP2-FSI /cc-pVTZ-DK3**	**CCSD(T)-FSII /cc-pwCVTZ-DK3**	**MP2-FSI /cc-pV∞Z-DK3**	**CCSD(T)-FSI /cc-pV∞Z-DK3**	**CCSD(T)-FSII /cc-pwCV∞Z-DK3**
La	-485.96	-483.15	-485.98	-474.77	-477.37	-478.62
Ce	-493.08	-490.13	-493.36	-482.78	-485.66	-485.78
Pr	-520.85	-534.33	-528.79	-526.40	-515.14	-522.59
Nd	-514.39	-554.46	-550.55	-546.08	-519.60	-544.21
Sm	-511.78	-509.87	-511.65	-503.00	-505.33	-505.80
Eu	-460.41	-453.94	-460.52	-446.69	-452.91	-452.52
Gd	-514.80	-512.99	-515.75	-506.32	-508.22	-508.19
Tb	-521.42	-520.16	-522.13	-513.82	-515.28	-514.87
Dy	-519.91	-519.69	-520.80	-513.25	-513.55	-514.33
Ho	-581.07	-594.73	-587.95	-586.20	-577.17	-581.12
Er	-581.45	-603.31	-594.51	-594.94	-581.13	-588.23
Tm	-571.60	-585.99	-578.23	-578.44	-567.72	-571.96
Yb	-525.38	-575.92	-517.27	-577.29	-526.38	-519.54
Lu	-536.44	-539.04	-537.38	-533.47	-530.64	-530.31

Table S.2: ΔG_{rxn} (kcal mol^{-1}) for $[Ln(NO_3)]^{+2}$ calculated with the composite Method A and Method B, and the Target Method, CCSD(T)-FSII/cc-pwCV∞Z-DK3

	Method A E_{ref}**[MP2] +** ΔE_{CC} **+** ΔE_{CV}	**Method B** E_{ref}**[CCSD(T)] +** ΔE_{CV}	**Target method CCSD(T)-FSII/cc-pwCV∞Z-DK3**
La	-478.52	-478.31	-478.62
Ce	-486.30	-486.23	-485.78
Pr	-522.84	-525.06	-522.59
Nd	-535.61	-549.20	-544.21
Sm	-504.59	-505.01	-505.80
Eu	-452.81	-452.57	-452.52
Gd	-508.40	-508.49	-508.19
Tb	-514.96	-515.16	-514.87
Dy	-513.67	-513.76	-514.33
Ho	-577.88	-582.51	-581.12
Er	-583.26	-591.30	-588.23
Tm	-569.67	-573.34	-571.96
Yb	-514.44	-514.07	-519.54
Lu	-530.75	-530.52	-530.31

Table S.3: Relative computational cost calculated with f-ccCA and the target method for $[Ln(NO_3)]^{+2}$ (with Ln = La, Ce, Sm, and Lu). [Relative computational cost is shown as a percentage and it is calculated as relative cost = (CPU units with f-ccCA)/(CPU units with target method) x 100]. Values shown in CPU units.

Ln	CCSD(T)-FSII /cc-pwCV∞Z-DK3+SO (target)	f-ccCA	Relative Cost
La	95.07	11.28	12%
Ce	61.96	14.20	23%
Sm	64.64	9.82	15%
Lu	77.89	10.39	13%