Table 4. C_1 and C_3 parameter values of the tetrad effect variations for the reactions (4-2) and (4-1) determined in the least-squares fittings using the improved RSPET equation (21).

	C_1 and C_3 parameters of tetrad effect variations[1)]	
Reaction (4-2) for $[LnEDTA\cdot(H_2O)_3]^-_{(aq)}$	$C_1/10^{-1}$	$C_3/10^{-2}$
ΔH_r(hyc) (kJ/mol)	+(0.16±0.06)	+(0.34±0.19)
ΔS_r(hyc) (J/mol/K)	+(0.46±0.30)	+(0.85±0.96)
ΔG_r(hyc) (kJ/mol)	+ (0.03±0.03) [+(0.02±0.11)]	+ (0.09±0.11) [+ (0.09±0.34)]
Reaction (4-1) for $[LnEDTA\cdot(H_2O)_2]^-_{(aq)}$	$C_1/10^{-1}$	$C_3/10^{-2}$
ΔH_r(hyc) (kJ/mol)	– (0.08±0.03)	–(0.15±0.10)
ΔS_r(hyc) (J/mol/K)	+ (0.07±0.14)	+(0.36±0.47)
ΔG_r(hyc) (kJ/mol)	– (0.10±0.06) [–(0.10±0.05)]	–(0.26±0.19) [–(0.26±0.17)]

1) ΔH_r(hyc), ΔS_r(hyc) , and ΔG_r(hyc) values are based on the experimental ΔH_r data for Ln(III)-EDTA formations by Mackey et al. (1962) combined with the ΔG_r data by Kawabe (2013a), together with the hydration change corrections for light $Ln^{3+}_{(aq)}$ by Kawabe (1999a). They are listed in Part A of Table 2, and fitted to the RSPET equation of (21).

2) The C_1 and C_3 values in the square brackets are calculated according to eq. (26). They are in good agreements with the values by the direct least-squares fittings.

Table 5. C_1 and C_3 parameter values determined by the least-squares fittings of the data of $\Delta\Delta H^0$, $\Delta\Delta S^0$, and $\Delta\Delta G^0$ for hydration change reactions for Ln-EDTA of (3) to the improved RSPET equation (21), along with their one-S.D. errors. They are compared with those calculated from the results of Table 4.

	Regression of the data[1)] by the improved RSPET equation (21)		Differences[2)] by the results of Table 4	
Reaction (3) that $[LnEDTA(H_2O)_3]^-_{(aq)} = [LnEDTA(H_2O)_2]^-_{(aq)} + H_2O_{(l)}$	$C_1/10^{-1}$	$C_3/10^{-2}$	$C_1/10^{-1}$	$C_3/10^{-2}$
$\Delta\Delta H^0_r$ (kJ/mol)	− (0.25±0.08)	− (0.49±0.25)	− (0.24±0.07)	− (0.49±0.21)
$\Delta\Delta S^0_r$ (J/mol/K)	− (0.39±0.20)	− (0.48±0.63)	− (0.39±0.33)	− (0.49±1.07)
$\Delta\Delta G^0_r$ (kJ/mol)	− (0.13±0.03) [− (0.13±0.05)]	− (0.35±0.11) [− (0.35±0.24)]	− (0.13±0.07)	− (0.35±0.22)

1) $\Delta\Delta H^0$, $\Delta\Delta S^0$, and $\Delta\Delta G^0$ for hydration change reactions for Ln-EDTA of (3) are calculated from the experimental ΔH_r data for Ln(III)-EDTA formations by Mackey et al. (1962) combined with the ΔG_r data by Kawabe (2013a). Such sets of $\Delta\Delta H^0_r$, $\Delta\Delta S^0_r$, and $\Delta\Delta G^0_r$ are individually fitted to the improved RSPET equation (21). The C_1 and C_3 values in the square brackets are those calculated as differences according to eq. (26).

2) Calculated as differences in C_1 and C_3 between the reactions of (4-2) and (4-1), which are listed in Table 3.

Table 6. Changes of Racah (E^1 and E^3) parameters for Nd^{3+} determined in the least-squares fittings of the enthalpy data to the improved RSPET equation[1)]

Change of aqueous Nd^{3+} species	ΔCN	ΔE^1 (cm^{-1})	ΔE^3 ((cm^{-1})
ΔH_r(hyc) for the reaction (4-2): $Nd^{3+}{}_{(octa,aq)} \rightarrow [Nd \cdot EDTA(H_2O)_3]^{-}{}_{(aq)}$	+1 (8→ 9)	+(39±14)	+(8±4)
ΔH_r(hyc) for the reaction (4-1): $Nd^{3+}{}_{(octa,aq)} \rightarrow [Nd \cdot EDTA(H_2O)_2]^{-}{}_{(aq)}$	0 (8→8)	−(19±7)	− (4±2)
$\Delta\Delta H^0_r$ for the reaction (3): $[NdEDTA(H_2O)_3]^{-}(aq) \rightarrow [Nd \cdot EDTA(H_2O)_2]^{-}(aq)$	−1 (9→8)	− (58±18) [− (58±17)][2)]	− (12±6) [− (12±4)] [2)]

1) Calculations are based on eq. (22) and 1 kJ/mol=83.5935 cm^{-1}, together with and the results listed in Tables 4 and 5.

2) The values in the square brackets are the simple differences in $\Delta E^1(Nd^{3+})$ or $\Delta E^3(Nd^{3+})$ between the reactions of (4-1) and (4-2). They are in good agreements with the values in the direct least-squares fittings without square brackets.

Table 7. The proportionally constant of κ given by the ratio of ΔS_r(tetrad) and ΔH_r(tetrad)[1).

	$\kappa(E^1)/(1/K)$	$\kappa(E^3)/(1/K)$
Light Ln(III)-EDTA complex formation[2) ΔH_r(hyc) and ΔS_r(hyc) for the reaction (4-2)	(**2.9±2.2**)$\times10^{-3}$	(**2.5±4.6**)$\times10^{-3}$
Heavy Ln(III)-EDTA complex formation[2) ΔH_r(hyc) and ΔS_r(hyc) for the reaction (4-1)	−(0.9±1.7)$\times10^{-3}$	− (2.4±3.5)$\times10^{-3}$
$[LnEDTA(H_2O)_3]^-(aq)$ $=[LnEDTA(H_2O)_2]^-(aq)+H_2O(l)$ $\Delta\Delta H^0_r$ and $\Delta\Delta S^0_r$ for the reaction (3)[3)	(1.6±0.9)$\times10^{-3}$	(1.0±1.4)$\times10^{-3}$

1) $\kappa(E^1)=C_1(\Delta S_r)/C_1(\Delta H_r)$ and $\kappa(E^3)=C_3(\Delta S_r)/C_3(\Delta H_r)$. The values in bold indicate that they are close to $\kappa\approx3\text{x}10^{-3}$ (1/K) , which gives rise to no significant tetrad effect in ΔG_r even though both ΔH_r and ΔS_r show similar tetrad effects at normal temperatures.

2) C_1 and C_3 parameters of the tetrad effect variations of ΔH_r(hyc) and ΔS_r(hyc) for the reactions (4-2) and (4-1) are listed Table 4.

3) C_1 and C_3 parameters for the tetrad effect variations for $\Delta\Delta H_r$ and $\Delta\Delta S_r$ for the reaction (3) are listed in Table 5.