CORRIGENDA

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In the paper by Rotzinger in *Chem. Eur. J.* **2007**, *13*, 800–811, the energies for the A mechanism in Table 6, computed at the CAS/SCF(12/11)PCM geometries/frequencies and MCQDPT2(12/11)PCM energies level, are 5.42 kJ mol^{-1} too high because of an error in the MCQDPT2(12/11) calculation on the reactant $[UO_2(OH_2)_5]^{2+}$, which was performed with seven 1s oxygen molecular orbitals as frozen cores instead of eight. This error does not affect the conclusions. The corrected values in Table 6 are italicized. The author apologizes for this error.

Table 6. Experimental and computed thermodynamic activation parameters.[a]

Mechanism	ΔE^{+} (ΔE)	ΔH^{+} (ΔH)	ΔS^{+} (ΔS)	ΔG^{+} (ΔG)	$\Delta V_{cav}{}^{+}$ (ΔV_{cav})
experimental data[b]		26	−40	38	
CAS-SCF(12/11)-SCRF geometries/frequencies, and MCQDPT2(12/11)-PCM energies[c,d]					
D	50.1 (44.3)	48.4 (46.2)	2.7 (11.4)	47.6 (42.8)	6.9 (8.7)
D	49.6 (45.2[e])	48.2[e] (47.3[e])	−0.3[e] (8.3[e])	48.3[e] (44.9[e])	6.3[e] (8.2[e])
A	31.3 (29.5)	27.2 (27.7)	−17.7 (−0.4)	32.4 (27.8)	−4.1 (−3.6)
A	27.9 (26.9[e])	23.6[e] (25.0[e])	−11.6[e] (7.7[e])	27.0[e] (22.7[e])	−3.9[e] (−3.7[e])
CAS-SCF(12/11)-PCM geometries/frequencies, and MCQDPT2(12/11)-PCM energies[c,d]					
D	52.6 (47.9)	50.0 (48.7)	−24.0 (−14.9)	57.1 (53.2)	3.1 (3.6)
D	55.3[f] (48.4[f])	52.7[f] (49.2[f])		59.8[f] (53.7[f])	
A	*25.6* (*20.5*)	*22.9* (*20.2*)	*−23.4* (*−2.4*)	*29.9* (*20.9*)	*−2.4* (*−2.9*)
A	*29.6*[f] (*25.5*[f])	*27.0*[f] (*25.2*[f])		*33.9*[f] (*25.9*[f])	
HF-CPCM geometries/MP2-CPCM energies[c,g]					
D	59.2 (54.5)	[h]	[h]	[h]	4.9 (3.6)
A	18.7 (15.8)	[h]	[h]	[h]	−3.0 (−3.4)
CPDM geometries/CPMD energies[c,i]					
D				45.2 (36.4)[j]	
A				28.0 (26.8)[j]	

[a] Units: energies: kJ mol^{-1}, entropy: J K^{-1}, volume: cm^3 mol^{-1}. [b] From reference [1]. [c] In parenthesis: parameters for the corresponding intermediate. [d] This work. [e] 6-31G(d,p) basis set for H_2O. [f] Corrected for the BSSE. [g] From reference [5]. [h] The vibrational frequencies were not computed. [i] From reference [10]. [j] ΔA^{+} (ΔA), Helmholz free energy at 27 °C.

