



Corrigendum

Corrigendum to “Understanding reactions with O₂ for ⁹⁰Sr measurements by ICP-MS with collision reaction cell” by Favre et al. [Int. J. Mass Spectrom. 289 (2010) 177]

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In his Letter Schofield found a discrepancy of 357 kJ mol⁻¹ between his and our [1] values calculated for $\Delta H_{f298K}(SrO_2^+)$. Indeed he estimated $\Delta H_{f298K}(SrO_2^+) = 496 \pm 45$ kJ mol⁻¹, while our value would be 853 kJ mol⁻¹—we actually wrote 846 kJ mol⁻¹ in the abstract and in the text for $\Delta H_f(SrO_2^+)$. He concluded that our value is in error, since if true it would have significant implications not only for strontium but for trends of its fellow alkaline earth elements in the periodic table. Our calculation was actually done in the course of an essentially experimental work, part of Favre's Ph.D. thesis. He calculated $\Delta H_f(SrO_2^+)$ as follows (Eq. (c) and Reaction (4) in Ref. [1])

$$\Delta H_f(SrO_2^+) = \Delta H_{fDFT} + \Delta H_f(Sr^+)_{exp} + \Delta H_f(O_2)_{exp}$$

where ΔH_{fDFT} is the enthalpy of Reaction (c) (Table 1). A first reason of the discrepancy evidenced in Schofield's Letter could be in the different definitions of $\Delta H_f(SrO_2^+)$, typically in the reference state. It is probably not the case, since we indeed found again the 357 kJ mol⁻¹ discrepancy – actually 356 kJ mol⁻¹ – using another thermodynamic cycle from Schofield's values in Ref. [2] he cited in his Letter to support his calculations. We now explain this alternative thermodynamic cycle, beginning with the reason why we considered it.

Favre's Ph.D. thesis was essentially an experimental mass spectrometry work, where he did not observe the formation of SrO₂⁺ in conditions where he obtained ZrO₂⁺, and he used this difference in chemical reactivities for separating Sr⁺ from Zr⁺ by mass spectrometry using O₂(g) in the reaction cell of the mass spectrometer. This is a strong indication that SrO₂⁺ is not stable, namely that Reaction (c) is not much possible: its energy change cannot be very negative.

Table 1

Enthalpies of reaction (first column kJ mol⁻¹) reported by Schofield (two first lines [2]) and calculated from these values (last line).

549	Sr = Sr ⁺ + e ⁻	IP(Sr)	Table 2	(a)
326	Sr + O ₂ = SrO ₂ ⁺ + e ⁻	(3)	Table 3	(b)
-223	Sr ⁺ + O ₂ = SrO ₂ ⁺			(c) = (b) – (a)

In his letter Schofield did not compare his calculations with such experimental data; but he reported values, from which we calculated the enthalpy of this reaction of formation of SrO₂⁺ (Table 1) that was not observed namely, for Reaction (c) (= (b) – (a) in Table 1 from Ref. [2]) we calculated -223 kJ mol⁻¹ from values reported by Schofield [2], while our DFT value is +133 kJ mol⁻¹ (Table 5 in Ref. [1]): the discrepancy between our [1] and Schofield [2] values is 356 kJ mol⁻¹, virtually the same (357 kJ mol⁻¹) value calculated by Schofield in his letter under discussion.

This note is to recognize and confirm this inconsistency; but we are not very sure the problem can only be in our DFT calculations as Schofield's concluded: as explained in the present Erratum, the formation of SrO₂⁺ via Reaction (c) is predicted to be quite easy when using Schofield's reported value, in contradiction with experimental observations, while our value is positive enough to be consistent with this experimental observation. Now we completely agree that our value needs confirmation, since it was essentially obtained by (B3LYP) DFT quantum calculations, even though our other DFT values agree with available experimental data as pointed in our original paper [1].

References

- [1] G. Favre, R. Brennetot, F. Chartier, P. Vitorge, Int. J. Mass Spectrom. 265 (2007) 15–22.
- [2] K. Schofield, J. Phys. Chem. A 110 (2006) 6938.

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