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Erratum

RECP calculations for reactions of H_2 with Pt, Os, Ir, and Re – a systematic comparison

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The title article describes quantum chemical studies on the insertion of rhenium, osmium, iridium, and platinum atoms into the hydrogen molecule. This Erratum concerns the results found for osmium exclusively. An error has been found in the Effective Core Potential (ECP) that we used for this metal. This lead to an unphysical migration of electron density from the valence into the outer core area of the osmium atom.

In the following, we report results for the gas-phase reaction

$$\mathrm{Os} + \mathrm{H}_2 \rightleftharpoons \mathrm{OsH}_2 \tag{1}$$

as calculated with the corrected ECP. In all other respects, we have closely followed the procedures described in the title article.

Table 1 of this Erratum should be substituted for Table 3 in the title article. We note a significant improvement of the atomic excitation energies. The present Table 2 should be substituted for Table 9 in the title article. The qualitative orbital occupation patterns for OsH_2, as listed in Table 10 of the title article, do not change upon correction of the ECP.

The corrected results, both for energies and geometries, are more in line with periodic trends when compared to results for the metals Re, Ir, and Pt.

Table 1. Low-lying terms of the osmium atom. Relative energies in kcal/mol. For the ^3P term, only the *j*-component with highest energy is experimentally assigned, and therefore only an upper limit can be inferred from experiment

Term	Occupation	E_{CI}	$E_{exp.}$
^5D	d^6s^2	0	0
^5F	d^7s^1	15	17
^3P	d^7s^1	24	<52
^3F	d^7s^1	31	28
^3H	d^6s^2	43	34
^7D	$d^5s^2p^1$	56	68
^7P	$d^6s^1p^1$	64	—

Table 2. Geometries and energies for OsH_2. Distances in Ångströms, angles in degrees, and relative energies in kcal/mol

State	Dissoc. *E*	Transition *R*	Transition ϕ	Transition *E*	Minimum *R*	Minimum ϕ	Minimum *E*
$^5A_1$	0	1.74	25	+ 33	1.70	152	−7
$^3B_1$	24	—	—	—	1.59	95	−15
$^3A_1$	31	—	—	—	1.62	107	−5