

Erratum: Vol. 74(1-2), p. 17, 2001

Joaquin Silvestre, Marco Sanchez-Castillo, Rong He, Francisco Rodríguez-Reinoso, and J. A. Dumesic

An error appeared in our paper entitled “Microcalorimetric, Reaction Kinetic and DFT Studies of Pt-ZnJX-zeolite for Isobutane Dehydrogenation”. We used a wrong number for the electronic energy of gaseous formaldehyde; therefore, the numbers given on page 22 (in the 5th and 6th rows of table 1) are incorrect for the electronic energy changes of formaldehyde adsorption. The corrected table 1 is shown below.

Table 1
Results from DFT calculations for changes in electronic energies (kJ/mol) for interaction of adsorbates with Pt(111)^a, Pt₃Zn(111), Pt₃Sn(111)^a and PtZn(011) slabs

Reaction ^b	Pt(111)	Pt ₃ Zn(111)	Pt ₃ Sn(111)	PtZn(011)
C ₂ H ₄ + * ⇌ *C ₂ H ₄ (π)	−73	−64	−52	−41
C ₂ H ₄ + * ⇌ *C ₂ H ₄ (di-σ)	−117	−98	−86	−41
C ₂ H ₄ + * ⇌ *CCH ₃ (hcp) + 1/2H ₂	−95	−99	−11	
C ₂ H ₄ + * ⇌ *CH ₃ (fcc) + 1/2H ₂	−95	−77	−45	
CH ₂ O + * ⇌ *CH ₂ O (Pt-Pt bridge sites)	−58	−60		−19
CH ₂ O + * ⇌ *CH ₂ O (Pt-Zn bridge sites)		−33		−30
H ₂ + 2* ⇌ 2*H (atop sites)	−87 ^c		−61	−61
H ₂ + 2* ⇌ 2*H (bridge sites)	−83 ^c			−76

^a [71].

^b *denotes the metal surface.

^c [72].