

ADDITIONS AND CORRECTIONS

2009, Volume 113A

S. Joseph and A. J. C. Varandas*: Accurate Double Many-Body Expansion Potential Energy Surface for the Lowest Singlet State of Methylene

Page 4175. We have detected misprints in the frequencies (ω_1 , ω_2 , ω_3) of the linear barrier (C–H–H) given in Table 3 (columns 5, 6, 7). The correct values are: 4565i, 1371i, 915 (BHL); 4341i, 1454i, 1117 (RKHS); 2624i, 1232i, 1515 (DMBE). The relative energy of the CH + H channel extracted from ref 13 and the R_1/a_0 value from ref 47 given in Table 3 are also misprinted, with the correct values being -3.86 kcal mol⁻¹ and $3.27a_0$, respectively.

10.1021/jp910270q

Published on Web 11/13/2009