ADDITIONS AND CORRECTIONS

2007, Volume 111A

Gabriel da Silva and Joseph W. Bozzelli* : Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide

Page 12026. Entropy values calculated using the ROTATOR program in Table 3 were not corrected for loss of symmetry in methyl rotors. Table 3 in the original manuscript should read as given below.

From the above table we find that there is now good agreement between the ROTATOR and Ayala and Schlegel entropies for the CH_3OO radical (all ca. 64−65 cal mol^{-1} K^{-1}). For $CH_3OOOOCH_3$, the Ayala and Schlegel entropies (ca. 86 cal mol^{-1} K^{-1}) are between the ROTATOR values obtained when treating all internal rotors and only the two methyl internal rotors. We now recommend use of the Ayala and Schlegel "best-fit" entropy (86.61 kcal mol^{-1}). The $CH_3OOOOCH_3$ entropy in Table 4 should therefore be 86.61 cal mol^{-1} K^{-1}, and the $C/H_3/O$ group entropy in Table 11 should be 29.64 cal mol^{-1} K^{-1}.

We thank Prof. David Golden for alerting us to this oversight.

TABLE 3: Entropies (cal mol^{-1} K^{-1}) for $CH_3OOOOCH_3$ and Its Radicals, Calculated Using Different Internal Rotor Treatments, at the B3LYP/cc-pVTZ+d Level of Theory[a]

	$CH_3OOOOCH_3$	CH_3OOOO	CH_3OOO	CH_3OO	CH_3O
RRHO[b]	83.53	95.66	71.37	64.30	**56.64**
Methyl Rotor(s)[c]	83.76	94.40	71.77	64.68	
All Rotors[d]	89.40	**94.58**	**73.71**	**64.68**	
Ayala and Schlegel (T)[e]	85.69		−11.60	64.09	
Ayala and Schlegel (PG)[e]	86.70		−11.60	64.52	
Ayala and Schlegel (BF)[e]	**86.61**			64.51	

[a] Recommended values are listed in bold. ROTATOR entropies for $CH_3OOOOCH_3$ corrected by $-R$ ln 9 and CH_3OOOO, CH_3OOO, and CH_3OO corrected by $-R$ ln 3 for loss of methyl rotor symmetry. [b] All vibrational modes treated as frequencies using the rigid-rotor-harmonic-oscillator (RRHO) approximation. [c] Methyl internal rotors treated using the ROTATOR program. [d] All internal rotors treated using the ROTATOR program. [e] RRHO entropies, corrected according to the formalism of Ayala and Schlegel as implemented in Gaussian 03, using the corrections of Truhlar (T), Pitzer and Gwinn (PG), and the "best fit" (BF) values.[26]

10.1021/jp801491d
Published on Web 04/03/2008