CORRIGENDA

M. Flock, C. Marschner* 4635–4642

Silyl Anions or Silylenoids?—A DFT Study of Silyllithium Compounds with π-Donating Substituents

Chem. Eur. J., **2005**, *11*

DOI: 10.1002/chem.200401353

On page 4640 the energies needed for the dissociation of the lithium silylenoids $XMe(H_3Si)SiLi{\cdot}(OMe_2)_3$ with $X = NH_2$, PH_2, OH, SH, F, and Cl into their fragments silylene $Me(H_3Si)Si$ and $XLi{\cdot}(OMe_2)_3$ were discussed. Owing to erroneous absolute energies for the lithium halides, the respective α-elimination reaction for X = F and Cl was reported to be exothermic. By using the correct absolute energies, the respective reactions are endothermic with energies of 154.6 and 89.5 $kJ\,mol^{-1}$ (see Table 1). Accordingly, the dissociation energies decrease in the order $X = NH_2 > OH > PH_2 > F > SH > Cl$ and the absolute energy of the silylene $Me(H_3Si)Si$ is 620.585913 hartree. The authors apologize for the oversight and thank Prof. S. Feng, D. Feng, and R. Li for calling attention to this mistake.

Table 1. Zero-point vibration corrected absolute and relative energies for the α-elimination of the silylenoids $XMe(H_3Si)SiLi{\cdot}(OMe_2)_3$ obtained at the B3LYP/6-31+G* level.

X	$X(H_3Si)MeSiLi$	XLi	ΔE [$kJ\,mol^{-1}$]
F	−1193.00413	−572.35935	154.6
Cl	−1553.34936	−932.72936	89.5