Berichtigungen

In der Zuschrift „Silynes (RC≡SiR′) and Disilynes (RSi≡SiR′): Why Are Less Bonds Worth Energetically More?“ von S. Shaik et al. (*Angew. Chem.* **2001**, *113*, 4146–4150; *Angew. Chem. Int. Ed.* **2001**, *40*, 4023–4026) enthält Tabelle 2 falsche Zahlenwerte. Die korrigierte Version der Tabelle ist hier wiedergegeben.

Tabelle 2. In situ bond energies for the linear and *trans*-bent isomers of HCSiH (**1**), HSiSiH (**2**), and HCCH (**3**) in the linear (**L**) and *trans*-bent (**B**) isomers.[a]

		Bond energies [kcal mol^{-1}]					
		HCSiH		HSiSiH		HCCH	
	Type	**1L**	**1B**	**2L**	**2B**	**3L**	**3B**[b]
1	$D(\pi_{out})$	57.7	56.5	45.5	34.0	88.2	74.1
2	$D(\pi_{in})$	57.7	∼35[c]	45.5	∼27[c]	88.2	∼44[c]
3	$D_{2\pi}$	∼105[c]	∼71[c]	∼80[c]	∼56[c]	169.8	∼110[c]
4	ΔE_σ[d]	−42.1		−53.0		−33.9	

[a] Calculated using the VB procedure described in ref. [17] with the 6-311G* basis set. The $D(\pi_{out})$ values are calculated with the BOVB method.[18] [b] The H-C-C angle was fixed at 124.6° (as in **2B**) and all other geometrical parameters were optimized. [c] These are estimated BOVB bond energies which were calculated by adding dynamic correlation increments obtained for the out-of-plane π bonds. For these cases BOVB calculations are too CPU-time demanding. [d] $\Delta E_\sigma = E_\sigma(\mathbf{B}) - E_\sigma(\mathbf{L})$. Obtained by comparing the total energy of the corresponding σ frames with all the π electrons uncoupled (Figure 3).

