Probing Local Structures of Siliceous Zeolite Frameworks by Solid-State NMR and First-Principles Calculations of ^{29}Si-O-^{29}Si Scalar Couplings[a]

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ERRATUM

In Table 3, columns 5 and 6 of our manuscript Cadars, *et al*., *Phys. Chem. Chem. Phys*., *11*, 1825 (2009), the $^{2}J(^{29}\text{Si-O-}^{29}\text{Si})$ coupling constants calculated for the DFT-optimized structures of ZSM-12 were mislabeled and out of sequence with respect to those of the ^{29}Si-O-^{29}Si site-pairs listed in column 1. Consequently, Table 3 has been revised to correct these labeling discrepancies and should read as follows:

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Table 3. Experimental and calculated $^{2}J(^{29}\text{Si-O-}^{29}\text{Si})$ coupling constants measured for siliceous zeolite ZSM-12.

Site Pair	J_{exp} (Hz) [a]	J_{calc} (Hz) [b] PXRD	NMR-refined	DFT-opt from PXRD	DFT-opt from NMR-refined
3-1	10	11.4	9.2	6.8	6.9
3-7	10	14.8	9.3	8.5	7.9
3-5	14	13.1	14.1	11.8	11.2
6-7	19	14.8	13.6	13.6	12.3
4-5	15	13.0	11.9	11.1	10.6
4-2	12	12.5	12.7	9.5	9.7
6-5	11	14.5	13.0	9.3	9.4
1-2	16	15.3	13.2	12.0	11.7
	u [c]	1.05	1.13	1.38	1.58
	v (Hz) [c]	-1.1	-0.4	-0.9	-2.5
	R^2	0.25	0.45	0.90	0.84
	χ^2 [d]	14.6	13.0	21.4	27.5

[a] *J*-coupling values are estimated from the 2D deconvolution of the refocused-INADEQUATE ^{29}Si{^{29}Si} spectrum shown in Fig. 5, with estimated uncertainties of ± 2 Hz.

[b] Values calculated for SiH-terminated clusters extracted from the powder-XRD and CSA-refined structures (3rd and 4th columns, respectively), using the cc-PV5Z basis set on coupled ^{29}Si atoms and 6-31G* basis sets with added (3df, 3pd) diffuse functions on other atoms (so-called "cc-PV5Z / diffuse" LDBS).

[c] From best fits to the expression: $J_{exp} = u*J_{calc} + v$.

[d] Calculated using eqn (1)

The entries in columns 1, 2, 3, and 4, the entries in the rows of all columns associated with the calculated u, v, R^2, χ^2 values, and the footnotes are correct and remain unchanged. In addition, the DFT calculations and results summarized in Figure 6 are correctly labeled, so that the subsequent analyses, discussions, and conclusions of the paper remain unaffected and unchanged.