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Correction to "Force Field for Molecular Dynamics Computations in Flexible ZIF-8 Framework"

Bin Zheng, Marco Sant,* Pierfranco Demontis, and Giuseppe B. Suffritti J. Phys. Chem. C 2012, 116 (1), 933–938. DOI: 10.1021/jp209463a

T wo values in Table 1 should be substituted with the following ones:

| VDW interaction | |
|-------------------------|----------------|
| atom | σ (Å) 2.471 |
| H3 | 2.471 |
| partial charges q (e) | |
| atom | our model |
| C3 | -0.6042 |
| | |

Please note that all computations in the original paper were done using the values here reported; i.e., the mistakes were done in filling the table.

