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Addition/Correction

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Correction to "Pyridine Ligand Rotation in Self-Assembled Trigonal Prisms. Evidence for Intracage Solvent Vapor Bubbles"

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The solvent vapor bubble formation inside a self-assembled molecular cage reported as a result of UFF molecular dynamics simulations cannot be reproduced using the current version of the TINK[1] code. It is only observed with a code version containing two programming errors that affect results for the highly positively charged molecular cage with counterions, and all other results obtained with the TINK code appear correct. The errors are the following: (i) The charge equilibration procedure that was used iteratively to estimate the atomic charges did not converge to the requested total charge of 0 *e* but to a total charge of +12 *e*. (ii) In certain instances the pair listing algorithm omitted some interactions and doubled others. The erroneous result suggested a possible explanation of experimental observations, but more recent results showed that the cage is filled with solvent,[2] in agreement with correctly performed UFF molecular simulations.

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REFERENCES

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(2) Givelet, C. C.; Dron, P. I.; Wen, J.; Magnera, T. F.; Zamadar, M.; Čépe, K.; Fujiwara, H.; Shi, Y.; Tuchband, M. R.; Clark, N.; Zbořil, R.; Michl, J. *J. Am. Chem. Soc.* **2016**, DOI: 10.1021/jacs.5b12050.

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