

Correspondence

**Reply to the Comment on "Application of the COSMO-SAC-BP
Solvation Model to Predictions of Normal Boiling
Temperatures for Environmentally Significant Substances"**

S. Wang, S.-T. Lin, J. Chang, W. A. Goddard, and S. I. Sandler

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Reply to the Comment on "Application of the COSMO-SAC-BP Solvation Model to Predictions of Normal Boiling Temperatures for Environmentally Significant Substances"

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Sir: In his comment, Dr. Klamt states "we want to point out, that in Reference 19 there is no remark on nitriles at all. We also cannot remember to have made similar statements on nitrile groups anywhere else. Instead, we generally achieve very good results for nitriles when using our original COSMO-RS method as implemented in the COSMOtherm program."

We thank Dr. Klamt for pointing out our mistake in citing Eckert and Klamt¹ (which is referenced as Reference 19 in his comment) rather than Klamt,² which is the COSMO-RS method paper to which he refers to. In this latter paper, he made the following statement referring to cyano compounds—and, therefore, to nitriles, which are organic cyano compounds:

"(ii) The errors from the underlying semiempirical Hamiltonian have to be overcome. For example, the AM1 Hamiltonian as well as other semiempirical Hamiltonians give wrong partial dipole moments for several electronically sophisticated functional groups like nitro or cyano. This causes considerable errors in the screening energies of molecules containing these groups. We have therefore left out such problematic groups in our test set."

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Dr. Klamt has referenced other problems in his methods with nitrogen-containing compounds elsewhere. For example, in ref 3, he states

"Unfortunately this term failed to adequately describe the acceptor behavior of nitrogen in neutral amines, especially if they are multiply substituted with methyl, ethyl, or even more bulky groups. Problems with a correct description of amines in CSMs are well-known.^{8,33}"

Because the COSMOtherm program and its subsequent modifications are not publicly available, we cannot verify his assertion that his program satisfactorily addresses nitrile compounds. Therefore, we must rely on the statements that Dr. Klamt has made in print that it does not.

Literature Cited

- (1) Eckert, F.; Klamt, A. Fast Solvent Screening Via Quantum Chemistry: Cosmo-Rs Approach. *AIChE J.* **2002**, *48*, 369.
- (2) Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena. *J. Phys. Chem.* **1995**, *99*, 2224.
- (3) Klamt, A.; Jonas, V.; Burger, T.; Lohrenz, J. Refinement and Parametrization of COSMO-RS. *J. Phys. Chem. A* **1998**, *102*, 5074.

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