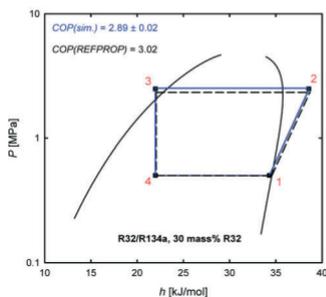


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Refrigeration Cycle Design for Refrigerant Mixtures by Molecular Simulation

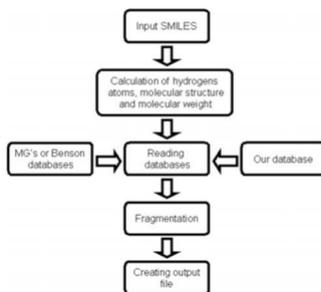
William R. Smith Magda Francová,
Marian Kowalski and Ivo Nezbeda



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Tool for Group Contribution Methods – Computational Fragmentation

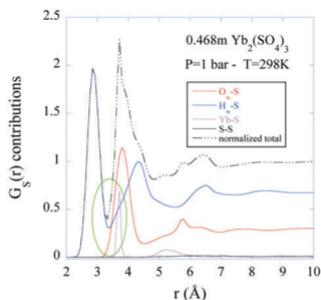
Zdeňka Kolská and Pavel Petrus



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Solvation and Ion Pair Association in Aqueous Metal Sulfates: Interpretation of NDIS Raw Data by Isobaric–Isothermal Molecular Dynamics Simulation

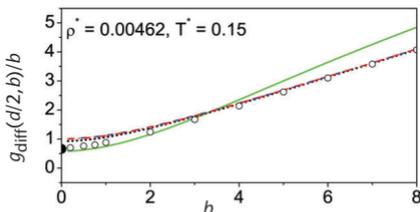
Ariel A. Chialvo and J. Michael Simonson



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A Modified Poisson–Boltzmann Study of the Singlet Ion Distribution at Contact with the Electrode for a Planar Electric Double Layer

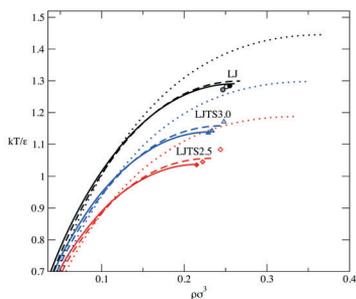
Whashington Silvestre-Alcantara,
Lutful B. Bhuiyan, Christopher W. Outhwaite and Douglas Henderson



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The Effect of Truncation and Shift on Virial Coefficients of Lennard-Jones Potentials

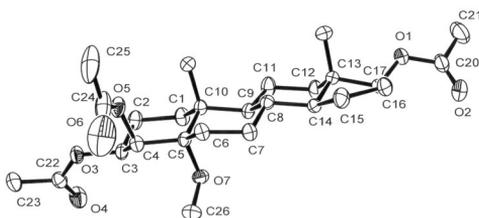
Katherine R. S. Shaul, Andrew J. Schultz and David A. Kofke



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Methanolysis of 3β-Substituted 4,5-Epoxyandrostanes Catalysed by Tetracyanoethylene

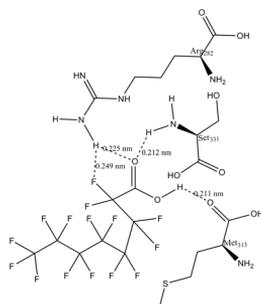
Cavit Uyanik, Aslihan Malay, Hayal B. Sonmez, Loic Queudrue and James R. Hanson



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3D-QSAR Study of the Endocrine Disrupting Effect of Perfluorooctane Sulfonates (PFOS) and Perfluorooctanoic Acid (PFOA) on Human Estrogen, Androgen and Thyroid Receptors

Yan Cheng, Hui-ming Chen, Wen-lian Yu, Yuan Cui, Li-li Zhou and Xin Zhou



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Self-Association of Copolymers with Various Composition Profiles

Jitka Kuldová, Peter Kořovan, Zuzana Limpouchová, Karel Procházka and Oleg V. Borisov

