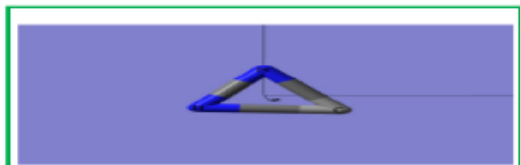
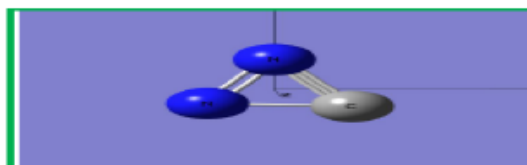




New Chemistry News



New News of Chem (NNC)



ChemNewsNew (CNN)

Editors' choice

CQC-Solvent Models

PCM(Polarizable Continuum Model)

FT-IR spectroscopy combined with DFT calculation to explore solvent effects of vinyl acetate

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Molecular and Biomolecular
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IEF-PCM

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TD-DFT, ADC, CC2

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PCM plus explicit water molecules

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COSMO(CONductor-like Screening MOdel)

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Prediction of Phospholipid-Water Partition Coefficients of Ionic Organic Chemicals Using the Mechanistic Model COSMOmic

Kai Bittermann, Simon Spycher, Satoshi Endo, Larissa Pohler, Uwe Huniar, Kai-Uwe Goss, and Andreas Klamt

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pKas / reduction potentials, H₂O, organic solvents, SMD

SMD(Solvent Model)

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COSMO	COnductor like Screening MOdel
RISM	Reference Interaction Site Model
RS	Real Solvents
SMD	Solvation Model based on Density
SMx	Solvent Model (x: version)
IEF	integral equation formalism

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