

After equilibration the obtained structures are analyzed by clustering [2, 4]. It allows us to visualize the relationship between the idealized crystal structures and the obtained crystal structures in a classification tree. In dependence of the conditions we observe structural changes in the different polymorphs in accordance with the experimental phase diagram. At high pressure we find the structures VII and VIII stable, at low pressure ice I.

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 [2] Hofmann, D.W.M.; Kuleshova, L. N., *Data Mining in Crystallography*, Structure and Bonding, 2010, 134. [3] Hofmann, D. W. M.; Kuleshova, L.N.; D'Aguzzo, B.; *Chem. Phys. Lett.*, 2007, 448, 138. [4] Hofmann, D. W. M.; Kuleshova, L.N.; Hofmann, F.; D'Aguzzo, B.; *Chem. Phys. Lett.*, 2009, 475, 149.

Keywords: molecular dynamics, reactive force field, cluster analysis

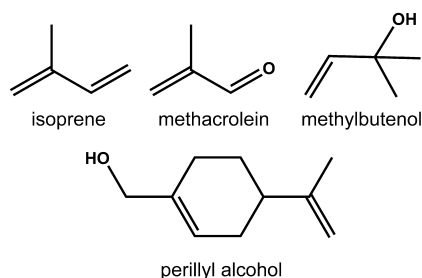
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Simulation of the interaction of terpenes and their oxidation products with ice. Sonja M. Hammer^a, Christian Czech^a, Boris Bonn^b, Martin U. Schmidt^a.

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Local structures and energies are calculated for the interactions of atmospherically relevant volatile organic compounds (isoprene, methacrolein, methylbutenol, perillyl alcohol) with ice I_h by force-field methods.



Ice I_h is the stable ice polymorph at atmospheric conditions.^[1] When ice (snow/hail/graupel) begins to form in the troposphere, volatile organic compounds will be adsorbed at the surface or incorporated into the crystals.

For all compounds, the interactions were calculated for an adsorption at the (0001) surface of ice as well as for an absorption into the ice bulk as point defect. For methacrolein the interaction with a small-angle grain boundary as a 2D-lattice defect was also considered. For all calculations a modified Dreiding force field was used.^[2] Results:^[3]

For all investigated compounds the adsorption on the (0001) surface is energetically preferred (enthalpies between -15 and -56 kJ mol⁻¹). The adsorption of isoprene at the ice surface is based on van der Waals interactions only. The methacrolein molecule forms two hydrogen bonds with water molecules of the ice surface. The alcohols could either be adsorbed on top of the surface, or, with similar adsorption enthalpies, be incorporated into the surface (replacing one water molecule). In all cases the alcohols form three hydrogen bonds between the OH-group and the water molecules of the ice surface. The absorption into the ice crystal is energetically unfavourable for all compounds. The fraction of adsorbed molecules is calculated with Boltzmann statistic. All molecules are mainly adsorbed on the surface. Only methylbutenol is also incorporated into the ice crystals in significant amounts.

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Keywords: force field method, ice, terpenes

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Experimental and Computational Study of (E)-4-Methyl-2-[[tris(hydroxymethyl)-methyl]iminomethyl]phenolate. Gonca Özdemir Tari^a, Hasan Tanak^a, Mustafa Macit^c, Ferda Erşahin^b, Şamil Işık^a. ^aDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey, ^bGerze Sinop Vocational School, Sinop University, Sinop, Turkey, ^cDepartment of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.

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Schiff bases can be classified by their photochromic and thermochromic properties [Cohen et al., 1964]. In general, Schiff bases based on salicylic aldehyde display two possible tautomeric forms, the iminomethyl-phenol (OH) and the aminomethylene-cyclohexa-2,4-dienone (NH) forms. Depending on the tautomers, two types of intramolecular hydrogen bonds are observed in Schiff bases: O—H···N in the former and N—H···O in the latter tautomer. Another form of the Schiff base compounds is also regarded to be zwitterionic showing an ionic intramolecular hydrogen bond (N⁺—H···O⁻) and this form is rarely seen in the solid state. The NH form of Schiff bases in the solid state can be regarded as a resonance hybrid of two canonical structures, the aminomethylene-cyclohexa-2,4-dienone and the zwitterionic form [Ogawa, *et al.*, 2003].

The crystal and molecular structure of the title compound, C₁₂H₁₇NO₄, has been synthesized and x-ray single-crystal structure determination has been performed. The title molecule exists in a zwitterionic form with a strong intramolecular N⁺—H···O⁻ hydrogen bond between the NH⁺ and the phenolate O⁻. In the crystal structure, molecules are linked together by intermolecular C—H···O and O—H···O interactions

Geometric optimization based on x-ray diffraction technique and quantum mechanical calculations were performed. The calculated geometric parameters were compared to the

corresponding x-ray determination results of the compound. The x-ray crystallographic data have been compared with computational methods.

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Keywords: X-ray diffraction, Computational Methods.