

metal-hydrogen systems. To study structure of liquid transition metal hydrogen alloys, we have performed in-situ energy-dispersive x-ray diffraction measurements at high pressures and high temperatures using a cubic-type multi-anvil press on BL14B1 at SPring-8 synchrotron facility. Pure metal wire was used as a starting material and LiAlH₄ was used as a hydrogen source. The x-ray diffraction measurements on liquid pure metals were also performed for comparison.

FeH_x is one of the most studied hydrides under high pressure. A solubility of hydrogen in iron is small at ambient conditions but iron and hydrogen react under high pressure and FeH_x (x≈0.8) is formed at 6.7GPa and 250°C [1]. The melting temperature of FeH_x has been reported by several groups and it is lower than that of pure iron by 500°C at 5 GPa [2], [3]. Our X-ray measurements confirmed the hydrogenation of iron and the decrease of the melting temperature. The pair correlation functions, which are obtained by Fourier transformation of structure factor, indicate that the Fe-Fe nearest neighbor distance in FeH_x is slightly longer than that in pure Fe [4]. Similar amount of elongations of the atomic distance were observed also in NiH_x and CoH_x. In spite of a suggestion of a large decrease of melting temperature in VH_x [5], we have not observed melting transition in our X-ray measurements for VH_x.

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Keywords: liquid, hydride, pressure

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Experimental and DFT studies of (E)-1-((3-iodophenylimino)methyl)naphthalene 2-ol

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The title compound, C₁₇H₁₂INO, crystallizes in a enol imine tautomeric form.

The title compound, (E)-1-((3-bromophenylimino)methyl)naphthalene-2-ol, has been synthesized and characterized by IR, UV, electronic spectroscopy, and X-ray single-crystal determination. The single crystal X-ray diffraction analysis of the title compound, C₁₇H₁₂BrNO, reveals that the crystal structure is stabilized in the solid state as an enol-imine tautomer, with a strong intramolecular O—H...N hydrogen bond. Molecular geometry from X-ray experiment of the title compound in the ground state have been compared using the density functional method (B3LYP) with 6-31G(d,p) basis set. To determine conformational flexibility, molecular energy profile of the title compound was obtained by DFT calculations with respect to two selected degrees of torsional freedom, which were varied from -180° to +180° in steps of 10°. Besides, molecular electrostatic potential (MEP), natural bond orbitals (NBO), frontier molecular orbitals (FMO), and thermodynamic properties were performed at B3LYP/6-31G(d,p) level of theory.

The C9-O1 and C7-N1 bond lengths verify the enol-imine tautomeric form. These distances agree with the literature [1]. The C1-I1 bond length in is also in a good agreement with the corresponding distances in the literature [2].

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Keywords: density functional theory(DFT), crystal and molecular structure studies, tautomerism

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Experimental and DFT computational study on hexaaquamagnesium(II) acesulfamate

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The parameters of unit cell are a=6.9404, b=8.5775, c=8.7200 α=68.564, β=78.640, γ=81.260 and Z=1. The crystal structure of the title compound, [Mg(H₂O)₆](C₄H₄NO₄S)₂, was determined at 296 K. The complex crystallizes in centrosymmetric triclinic space group P-1 and Mg^{II} atom is coordinated by six O atoms from six water molecules. The ligands in the Hexaaquamagnesium(II) Acesulfamate are linked with three dimension via O—H...O and O—H...N interactions. In this paper, the geometric parameters which are obtained from X-ray determination and theoretical parameters which are calculated by using density functional theory (B3LYP) with the 6-31G basis sets were compared. Experimental IR study, theoretical IR calculations, molecular electrostatic potential and frontier molecular orbital calculations were also put in this paper.

Keywords: acesulfame, X-ray, DFT

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Experimental and DFT studies of (2-Hydroxyethyl) trihenylphosphoniumchloride

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Triphenylphosphonium compounds and their various derivatives are key reagents in the Wittig reactions and are used to convert aldehydes and ketones into alkenes [1], specifically in applications ranging from the synthesis of simple alkenes to the construction of complex biologically active molecules in the pharmaceutical research [2]. They are also an important class of isoaromatic compounds and have widespread applications for their antimicrobial and anticancer activities [3].

In the crystal structure of the title compound, C₂₀H₂₀OOP⁺CP, the cations and anions are linked by intermolecular C—H...Cl and O—H...Cl hydrogen bonds into chains running parallel to the b axis. The compound crystallizes in the monoclinic, space group C2/c with unit cell dimensions a=14.1988(4), b=12.5743(3), c=19.7098(6), Mr=342.78 and Z=8.

The experimental geometry of (2-Hydroxyethyl)trihenyl