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Comparison of Isoelectronic Aluminum-Nitrogen and Silicon-Carbon Double Bonds Using Valence Bond Methods

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Dimethyl-aluminum amide ($(CH_3)_2AlNH_2$) is a postulated intermediate in the reaction between trimethyl aluminum ($(CH_3)_3Al$) and ammonia to form aluminum nitride. Results of geometry optimization calculations for $(CH_3)_2AlNH_2$, H_2AlNH_2 and isoelectronic H_2SiCH_2(silaethylene) are presented. Each of these has a planar equilibrium skeleton with C_{2v} symmetry. Geometry optimizations were carried out using Generalized Valence Bond Perfect-Pairing (GVB-PP) wave functions. Al-N bond distances of 1.78 and 1.80 Å are predicted for the dihydro- and dimethyl-aluminum amides, respectively, slightly longer than the optimized Si-C bond distance in silaethylene (1.74 Å). Al-N bond distances in these compounds are fitted into a phenomenological correlation established by Haaland which relates the covalent:dative character of such a bond to the bond distance. We compare the Al-N and Si-C bonds in the shapes of the GVB-PP orbitals representing them and in their predicted dipole moments.

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Comparison Of Isoelectronic Aluminum Nitrogen And Silicon Carbon Double Bonds Using Valence Bond Methods

Peipei Pang

Comparison Of Isoelectronic Aluminum Nitrogen And Silicon Carbon Double Bonds Using Valence Bond Methods: **Comparison of Isoelectronic Aluminum-Nitrogen and Silicon-Carbon Double Bonds Using Valence Bond Methods** Mary M. Lyman,Leonard V. Interrante,Charles H. Patterson,Richard P. Messmer,RENSSELAER POLYTECHNIC INST TROY N Y DEPT OF CHEMISTRY.,1990 Dimethyl aluminum amide CH3 2AlNH2 is a postulated intermediate in the reaction between trimethyl aluminum CH3 3Al and ammonia to form aluminum nitride Results of geometry optimization calculations for CH3 2AlNH2 H2AlNH2 and isoelectronic H2SiCH2 silaethylene are presented Each of these has a planar equilibrium skeleton with C 2v symmetry Geometry optimizations were carried out using Generalized Valence Bond Perfect Pairing GVB PP wave functions Al Nitrogen bond distances of 1 78 and 1 80 A are predicted for the dihydro and dimethyl aluminum amides respectively slightly longer than the optimized Silicon Carbon bond distance in silaethylene 1 74 A Al N bond distances in these compounds are fitted into a phenomenological correlation established by Haaland which relates the covalent dative character of such a bond to the bond distance We compare the Al N and Si C bonds in the shapes of the GVB PP orbitals representing them and in their predicted dipole moments aw Government Reports Announcements & Index ,1990 **ACS Directory of Graduate Research 1993** American Chemical Society. Committee on Professional Training,1993 **Government reports annual index** ,199? □□□□ ,2000 □□□□ ,2001 **Binary Fluorides** Donald T. Hawkins,2012-12-06 Coverage For some time we have contemplated a comprehensive review of the structures and force fields of the binary fluorides This bibliography of 1498 references marks the first step of that effort We are pub lishing this material now rather than waiting until the review is complete some two years hence because we believe that the information already accumulated will be of immediate use to a broad spectrum of researchers Anyone ambitious enough to read through all the articles on binary fluorides will find that the struc tures and force fields of many of these molecules are at present unknown For example it has not been clearly established to which point group s the lanthanide trifluorides should be assigned There remain interesting problems relating to the role of Jahn Teller and pseudo Jahn Teller distortions in some of the transition metal fluorides such as VF MoF ReF and ReF to name only a few One s s 6 7 also finds fascinating examples of large amplitude motions or pseudorotations as they are often called in such molecules as XeF 6 I F 7 and PF 5 For those binary fluorides whose equilibrium geometries are precisely known there still exists the problem of accurately determining the harmonic force field In a few cases most notably the Group VA trifluorides there has been some attempt made at extracting the cubic and quartic contributions to the force field **Zhongguo ke xue** ,2002 **Chemical Abstracts** ,2002 *Journal of the American Chemical Society* American Chemical Society,1974 Proceedings of the Society are included in v 1 59 1879 1937

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