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Index Abstracts

The homologous series of compounds, Me_3AlNH_2Bu' , $[Me_2AlNHBu']_2$ and $[Me_2AlNLi(THF)Bu']_2$ (shown) have been fully characterized. Thus, a direct comparison can be made of the spectroscopic and structural changes that occur on going across the series of an alkyl aluminum amine adduct, -amide, and -lithium amide. In the latter compound the lithium atom is essentially covalent and adopts an unusual T-shaped geometry. The question of π -bonding in this compound will be addressed.

Barium metal reacts with an oligoether thiol to form an organic solvent soluble dimeric metal *bis*(thiolate) compound, which gives crystalline BaS upon thermolysis at 220°C for two hours.

Many Lewis bases effectively trifluoromethylation catalyzed of F carbonyl compounds with trimethyl-By (trifluoromethyl)silane. using chiral Lewis bases as catalysts, asymtrifluoromethylation metric was achieved. The higher enantiomer excesses were observed on using trialkyl(trifluoromethyl) silanes bearing bulky alkyl groups on the silicon atom.





$$\begin{array}{c} O \\ A^{1} \\ H^{2} \\ H^{$$

D. A. Atwood and D. Rutherford

Unusual Structural Features in an Alkyl Aluminum Lithium Amide

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W. S. Rees, Jr. and G. Kräuter

Initial Preparation of a Barium *Bis*(oligoetherthiolate): An Intramolecularly-Stabilized Precursor for the Thermally Mild Formation of BaS

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T. Hagiwara, T. Kobayashi and T. Fuchikami

Lewis Base Catalyzed Trifluoromethylation of Carbonyl Compounds with Trialkyl (trifluoromethyl)silanes

The ²⁹Si NMR chemical shifts of the methyl chlorine silanes $(CH_3)_{3-n}$ -Cl_nSiX (n = 0..., 3) with X = H, CH_3 , C_2H_5 , CH_2Cl , $CHCl_2$ NH₂, N(H)CH₃, N(CH₃)₂, OH, OCH₃, OC₂H₅, OSiH₃, F, SiH₃, and Cl have been calculated using the IGLO (Individual Gauge for Localized Orbitals) method. The theoretical results are in good agreement with available experimental values.

From adventitious sources, singlecrystal samples of the first aromatically substituted cyclopentaarsines, $cyclo(C_6H_5As)_5$ and $cyclo(p-CH_3C_6-$ H₄As)₅, have been obtained and crystallographically characterized. In both cases, the structures are those expected of cyclopentane isolobal analogues, i.e., an essentially zero dihedral plane of four atoms with a fifth atom residing in a sharply angled flap plane. The flap angle is about 10° smaller for the phenyl- and *p*-tolylsubstituted rings than for two previously reported alkyl-substituted rings, but is 15-20° larger than the six-membered phenyl- and *p*-tolyl-substituted systems.

In the diphosphirane series, the substitution of one aryl group (2,4,6-tri-*tert*butyl-phenyl) by a chlorine atom leading to the *trans* P-chloro-diphosphirane via the *cis* isomer intermediate can be readily realized in chlorinated solvent under sonication or in the presence of gaseous hydrogen chloride in diethyl ether at room temperature. R. Wolff, H. Jancke and R. Radeglia

²⁹Si NMR Chemical Shifts and Reactivity Effects of the Series (CH₃)_{3-n}Cl_nSiX An *ab intio* Study **17–30**

A. L. Rheingold, O. M. Kekia and J. B. Strong

Structural Studies of *cyclo*pentaarsines. Crystallographic Characterization of *cyclo*- (PhAs)₅ and *cyclo*(*p*-TolAs)₅

31-35

M. Rifqui, G. Etemad-Moghadam, J. Berlan and M. Koenig

Substitution Reactions in a Diphosphirane Series: Evidence of "CIS" Isomer Intermediate



The solid state structures of 4-methyl-4-phosphatetracyclo[$3.3.0.0^{2.8}.0^{3.6}$]octane 4-sulfide (*trans*- **3a** and *cis*-**3b**) and 4-phenyl-4-phosphatetracyclo [$3.3.0.0^{2.8}.0^{3.6}$]octane 4-oxide (**5a**) were established by X-ray crystallography. Semi-empirical calculations at the PM3 level were used to estimate the relative energy of *trans*-**5a** and *cis*-**5b**.

Nucleophilic aromatic substitution (S_NAr) reactions of 4,5-dicyano- ^{NC} 2-fluoro-1-methylimidazole using disodium cyanamide or disodium malononitrile followed by methylation using dimethyl sulfate gave the 2-cyanimino and 2-dicyanomethylene pseudooxocarbon derivatives 4 and 6. The oxocarbon analog of 4 and 6, namely 4, 5-dicyano-1, 3-dimethyl-2imidazolone was synthesized by dimethylation of 4,5-dicyano-2imidazolone which, in turn, was synthesized from diaminomaleonitrile (DAMN) and triphosgene.

Oxidative addition of Br_2 to 1,3dimethyl-2(3H)-imidazoleselone results in a compound that can be viewed as a Se(II) bromide complex with a stabilized imidazolylidene ring as verified by X-ray crystallography. The structure consists of dimeric pairs containing nearly linear Br-Se-Br units bonded through carbon to planar imidazolylidene rings at torsion angles of 91.4° for NI-CI-Sel-Brl and 76.8° for N3-C6-Se2-Br4. Significant intermolecular contacts between dimeric units are seen through short Se-Se[3.494(1)Å] and Sel-Br4 bridging [3.509(1) Å].





T. M. Lane, A. C. Peterson, S. E. Cremer, D. W. Bennett and P. E. Fanwick

Structural Comparisons of Three Phosphatetracyclo[3.3.0.0^{2.8}.0^{3.6}] Octane Compounds

43-49

CH₃

CH

6

NC

NC

R. P. Subrayan and P. G. Rasmus-_{CN} sen

Nucleophilic Aromatic Substitution Reactions on 4, 5- Dicyano-2fluoro-1-methylimidazole: Syntheses and Properties of 4, 5-Dicyano-1, 3 dimethyl-2-imidazolone and its Pseudooxocarbon Derivatives

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D. J. Williams, D. Vanderveer, B. R. Crouse, R. R. Raye, T. Carter, K. S. Hagen and M. Brewer,

Spectroscopic Properties and Molecular Structure of 1, 3- Dimethyl-2-(Se,Se-di-bromoseleno)-2(3H)imidazolylidene.

The organothallium phosphorus adduct $(Me_3SiCH_2)_3TI \cdot P(SiMe_3)_3$ (1) (3) was prepared by combining $(Me_3Si CH_2)_3TI$ and $P(SiMe_3)_3$ at room temperature. The TI-P bond length in 1, previously unreported for compounds of this type, was found to be 2.922(3) Å.



R. A. Baldwin, R. L. Wells and P. S. White

67-71

Tin-119 and phosphorus-31 NMR spectra have been recorded for three tin tetrahalide complexes with tetraethyl propylenediphosphonate $SnX_4 \cdot L$, where $L = (EtO)_2 P(O)CH_2$ - $CHMeP(O)(OEt)_2, X = Cl$ (1); X = Br(2); X = 1(3). Each complex exists in solution in the form of only one isomer with two different phosphoryl units coordinated at tin. The crystal structure of $SnCl_4 \cdot L(1)$ shown has been determined. The complex has a monomeric 7-membered chelate structure with octahedral environment at tin.

The preparation and X-ray structure $ccl_{P(NHBU/2)}^{S}$ of new phosphonothioic amides is described.



E. V. Grigoriev, N. S. Yashina, V. S. Petrosyan, J. Lorberth, W. Massa and S. Wocadlo

Tin Tetrahalide Complexes with Tetraethyl Propylene-diphosphonate

73-78

CCl₃P(NHSiMe₃)₂

J. Příhoda, F. Kučera, D. Novotný and J. Marek

On the Reaction of Trichloromethylphosphonothioic Acid with Tertbutylamine and Hexamethyldisilazane