# Chalcogenides of the aminomethylphosphines derived from 1-methylpiperazine, 1-ethylpiperazine and morpholine: NMR, DFT and structural studies for determination of electronic and steric properties of the phosphines.

Autorzy

Radosław Starosta

Barbara Bażanów

W. Barszczewski

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Streszczenie

Chalcogenide derivatives of three aminomethylphosphines: P(CH2N(CH2CH2)2NCH3)3 (1), P(CH2N(CH2CH2)2NCH2CH3)3 (2) and P(CH2N(CH2CH2)2O)3 (3) were prepared: oxides--OP(CH2N(CH2CH2)2NCH3)3 (4), OP(CH2N(CH2CH2)2NCH2CH3)3 (5), OP(CH2N(CH2CH2)2O)3 (6), sulfides--SP(CH2N(CH2CH2)2NCH3)3 (7), SP(CH2N(CH2CH2)2NCH2CH3)3 (8), SP(CH2N(CH2CH2)2O)3 (9) and selenides--SeP(CH2N(CH2CH2)2NCH3)3 (10), SeP(CH2N(CH2CH2)2NCH2CH3)3 (11), SeP(CH2N(CH2CH2)2O)3 (12). The spectroscopic NMR analyses, DFT (B3LYP/6-31G**) calculations together with crystallographic studies of compounds 5, 6, 9 and 12 demonstrate that the structures and spectroscopic properties are strongly influenced by the chalcogen atom and not entirely contingent on aliphatic rings in the molecules. TEPs (Tolman's electronic parameters), estimated with DFT methods equal 2059.7 cm(-1) for 1, 2059.8 cm(-1) for 2 and 2061.2 cm(-1) for 3. These values are similar to TEPs estimated experimentally for other aminomethylphosphines. Phosphines 1, 2 and 3, despite very large Tolman cone angles show rather low influence of molecular geometry on their electronic properties: S4' (symmetric deformation coordinate) (59.8-64.8) and S4 (63.4-63.7) parameters are moderate. Suresh's steric effect (S(eff)) parameters for phosphines 1, 2 and 3 (2.70, 2.73 and 2.66, respectively) indicate minor electron-donating effect. Electronic effect (E(eff)) parameters (4.92, 5.21 and -0.40, respectively) can be easily modified by changing the substituents. 1J(SeP) coupling constants in the selenides are low (10: 707.5 11: 707.5 12: 709.8 Hz), but do not correlate with the TEP values in a way typical for aliphatic phosphines. The examined compounds do not show mutagenic properties and their potential toxicity is low, which is relevant in the context of their possible medical applications

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