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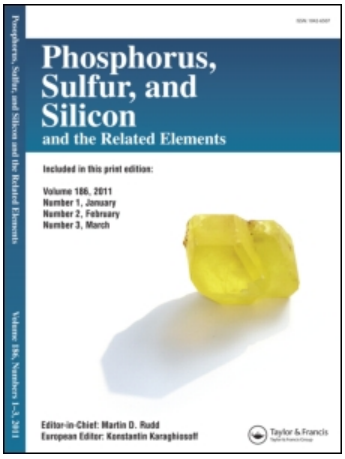

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Chalcogeno Methylene Phosphoranes 2,4,6-*t*Bu<*sub*>3</*sub*>C_6H_2-P(=X)=C($Sime_3$)$_2$, X = O, S, Se Crystal Structure, ^{31}P CP Mas NMR and IGLO Calculations

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CHALCOGENO METHYLENE PHOSPHORANES $2,4,6\text{-}t\text{Bu}_3C_6H_2\text{–}P(=X)=C(SiMe_3)_2$, X = O, S, Se CRYSTAL STRUCTURE, ^{31}P CP MAS NMR AND IGLO CALCULATIONS

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Chalcogeno methylene phosphoranes $2,4,6\text{-}t\text{Bu}_3C_6H_2P(=X)=C(SiMe_3)_2$ with X = O, S or Se were synthesized and their crystal structures characterized by means of X-ray structure analysis. ^{31}P CP MAS NMR measurements and IGLO calculations of model compounds $C_6H_5P(=X)(=CH_2)$ allow to study the influence of the chalcogeno substituent X on the principal values of the nuclear magnetic shielding tensor σ_{ii}.

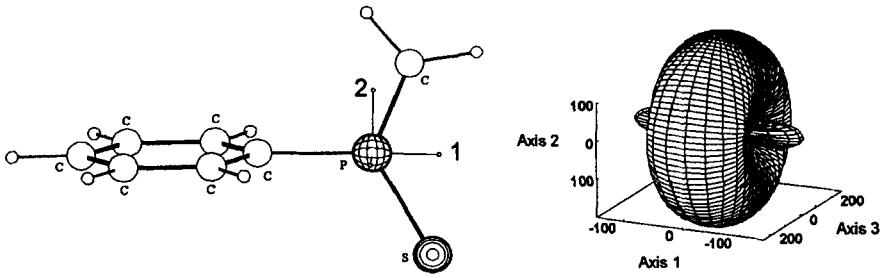

FIGURE 1 Orientation of the principal axes 1, 2 and 3 in the molecular framework of $C_6H_5P(=S)(=CH_2)$ with the corresponding ^{31}P tensor ovaloid

IGLO calculations for the model compounds $C_6H_5P(=X)(=CH_2)$ reflect the experimentally observed trends in σ_{ii} for X = O to Se in a satisfactory manner. The IGLO calculations allow also the assignment of the principal axes in the molecular framework and a discussion what reasons account for the changed assignment of axes 2 and 3.