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SCREENING RESULTS ON THE TOXICITY OF NUMEROUS FLUORO ORGANIC COMPOUNDS

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Predictions on the toxicity of organic fluorine compounds, based on chemical structural elements, can be rather unreliable. As a matter of fact, closely related substances may possess strikingly different toxic properties. On the grounds of working safety with new chemicals, we were interested in setting up a quick and simple pre-screening test using NRMI-mice which affords preliminary data on acute inhalation toxicities of volatile fluorine compounds. We now report on experimental procedure, evaluation and results of such tests and - a point of much importance - the correlation between the pre-screening data and those obtained from some more elaborate LC_{50} studies (4 h). We determined, besides others, the following pre-screening data (1 h)(in parantheses: values given in ppm):

C_2F_5I (>10.000), ICF_2CF_2I (50-100), $CF_2Cl-CFClI$ (50-100), $CCl_2Br-CClBrH$ (100-300), $CF_3-CFI-CF_3$ (1.000-2.000), $CF_3CFI-CF_2Cl$ (50-100), C_4F_9I (>10.000), $C_6F_{13}Br$ (>10.000), $C_2F_5CH_2CH_2I$ (100-500), $C_3F_7CH_2CH_2I$ (250-500), $C_4F_9CH_2CH_2I$ (1.000-5.000), $CF_2Cl-CF=CF_2$ (<90), $(CF_3)_2C=CH_2$ (500-1.000), $BrCF_2CF_2-CH=CH_2$ (>10.000), $CF_3CCl=CClCF_3$ (50-100), $C_4F_9CH=CH_2$ (>7.000), $C_6F_{13}CH=CH_2$ (>10.000), $CF_2=C(CF_3)-C(CF_3)=CF_2$ (100-300), CF_3CH_2OH (>2.500), $C_6F_{13}SOCl$ (<50), $C_2F_5CH_2COCl$ (100-300), $CH_3CH(OCF_2CF_2H)COCl$ (250-500), $C_6F_{13}CH_2CH_2SH$ (2.500-5.000).

Our results prove that it is possible to predict the order of LC_{50} values with surprising accuracy and little experimental effort.

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PREPARATION, STABILITY AND SYNTHETIC CONVERSIONS OF FLUORO-METHYLENE YLIDE

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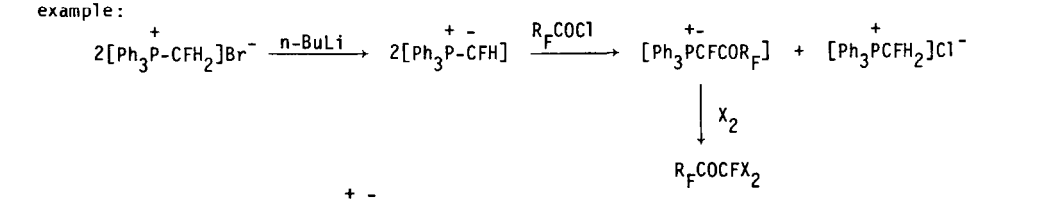
Previous routes to $[Ph_3\overset{+}{P}-\overset{-}{C}FH]$ employed either expensive or hazardous reagents. In contrast to these earlier methods, we have now found that the precursor to this ylide can be easily prepared in high yield from Ph_3P and $CFBr_3$. The resultant fluoromethylene ylide can, via transylidation reactions, be easily converted to new phosphonium intermediates, which can be cleaved to give functionalized fluorinated derivatives. For example:



The preparation of $[Ph_3\overset{+}{P}-\overset{-}{C}FH]$ will be presented, as well as the acylation, halogenation, arylation and pyrolysis of this ylide and its derivatives.