4-Dimethylaminopyridinium carbamoylides as stable and non hazardous substitutes of arylsulfonyl and heteroaryl isocyanates

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Supplementary Data

The geometry of the sulfonylcarbamoylide **3a** was fully optimized using a molecular orbital *ab initio* method at the Hartree-Fock level of theory with the 6-31G** basis set. The *ab initio* calculations were carried out using the SPARTAN program v. 5.0 distributed by Wavefunction Inc. and installed on a Silicon Graphics *O2* workstation.

The optimized calculated values of the most relevant geometrical parameters [bond distances (Å) and angles (^{o})] are shown in Table 1.

The atomic charges were calculated using RHF/6-31G** optimized structure and the results are presented in Figure 2.

Table 1. Selected theoretical bond distances (Å) and bond angles (^{o}) for ylide **3a** [a)].

Bond	**(Å)**	**Angle**	**(^{o})**
C(1)-N(1)	1.516	N(1)-C(1)-O(1)	113.83
C(1)-O(1)	1.198	N(1)-C(1)-N(3)	109.15
C(1)-N(3)	1.298	O(1)-C(1)-N(3)	137.00
N(3)-S	1.623	C(1)-N(3)-S	120.14
S-O(2)	1.435	N(3)-S-O(2)	111.14
S-O(3)	1.434	N(3)-S-O(3)	105.58
N(1)-C(2)	1.339	O(2)-S-O(3)	118.89
C(2)-C(3)	1.359		
C(3)-C(4)	1.417		
C(4)-N(2)	1.340		

[a)] Numbering scheme show in Figure 2.

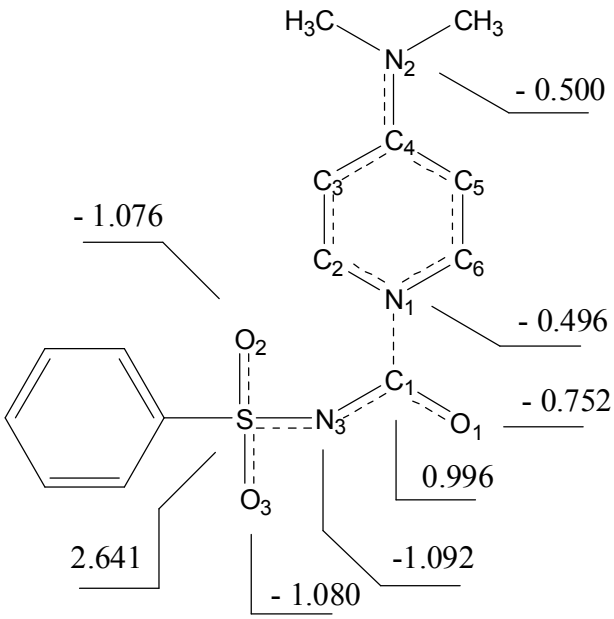

Figure 2. Molecular diagram of the ylide **3a** showing the natural atomic charges on selected atoms.

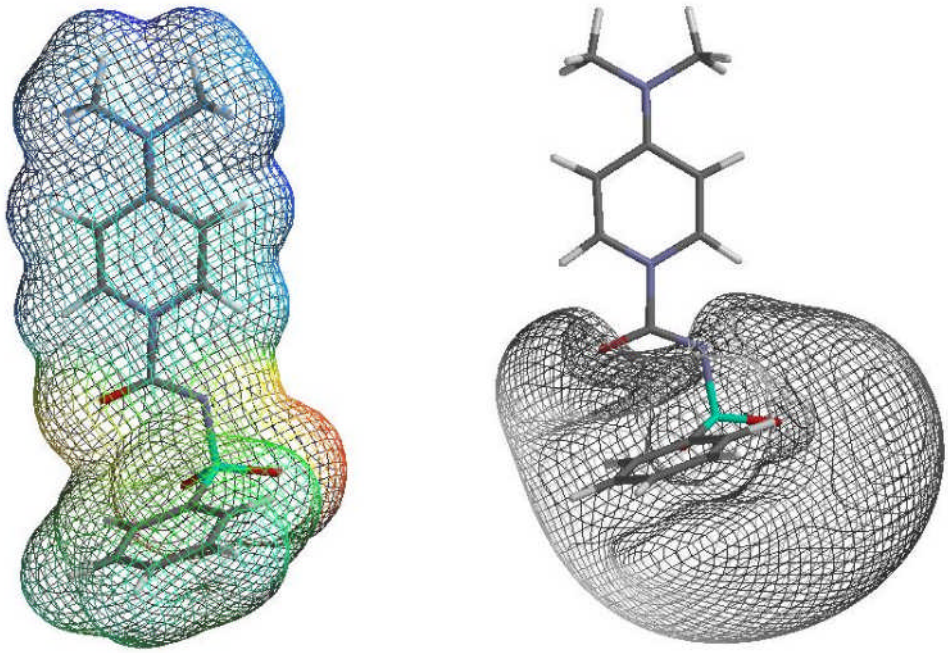

Figure 3. Absolute values of electrostatic potential mapped in colour onto the surface of electron density (*left*) and the electrostatic potential map of **3a** isocontoured at -20 kcal/mol (*right*).