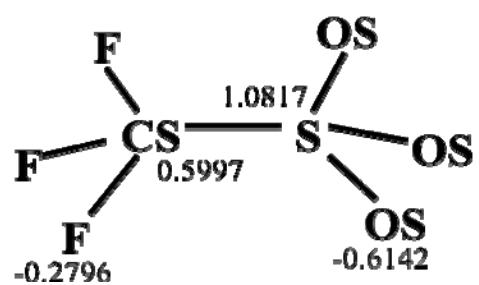
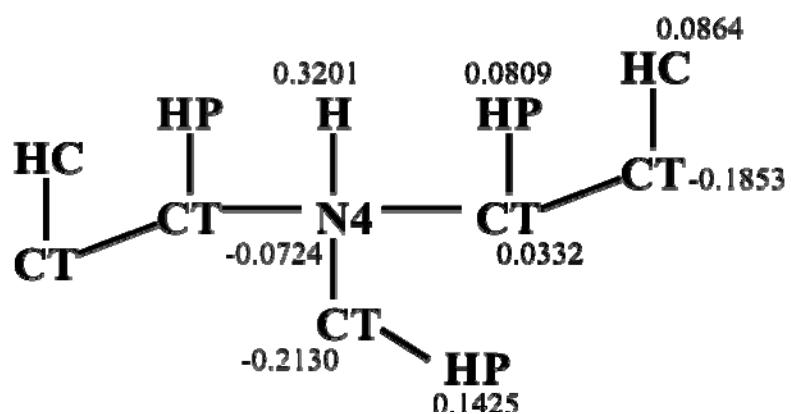


S. Figure 1 Partial Charges and Atom Types for the Molecular Models Used in this Work.



**S. Table 1. Potential Parameters for the Molecular Models Used in this Work.**

Atom type	$\sigma(\text{\AA})$	$\varepsilon(\text{kcal/mol})$
CT	3.475	0.1094
HP	1.960	0.0157
HC	2.650	0.0157
N4	3.296	0.1500
H	1.105	0.0157
CS	3.564	0.0894
F	3.350	0.0450
S	3.831	0.3400
OS	3.314	0.0960