Environmentally Important Physico-Chemical Properties of Energetic Materials: Applications of Quantum-Chemical Calculations

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We will present recent advances of quantum-chemically based approximations (namely COSMO-RS) in the prediction of several environmentally important physico-chemical properties of energetic materials: vapor pressure, Henry's law constants, water solubility, octanol-water partition coefficients, and reduction and oxidation potentials. Since both solubility and redox properties play important roles in many environmental characteristics of energetic materials, this presentation focuses on the current status of the quantum-chemically based predictions of these two properties. Also, an approach for modeling the salinity effects will be discussed.

It is concluded that a combined approach employing a continuum model for the solvent along with statistical thermodynamics (this represents approximations of the COSMO-RS type) is a quite accurate prediction tool which on one hand avoids the empirically-based QSPR approximations, and on another hand, avoids the use of more computationally demanding techniques such as molecular dynamics and Monte Carlo approaches. An example of such predictions is presented in the Table below.

Vapor pressures, Henry's law constants, and octanol-water partition coefficients calculated with the COSMO-RS approach, and available experimental values for nitro- and amino-derivatives of toluene

Compound	Vapor Pressure, Log(kPa)		Henry's Law Constant, Log(atm·m^3·mol^{-1})		Water Solubility, Log(mg·L^{-1})		Octanol-Water Partition Coefficient Log(K_{ow})	
	COSMO-RS	Exp	COSMO-RS	Exp	COSMO-RS	Exp	COSMO-RS	Exp
TNT	-4.85	-5.97	-6.89	-7.68	2.36	2.06	2.76[b]	1.6
2-AmDNT	-9.03	–	-12.77	–	4.08	–	1.88	1.84
4-AmDNT	-6.22	-5.85	-10.22	-10.49	4.37	3.09	1.75	1.84
2,4-AmNT	-6.77	–	-11.64	–	4.73	–	0.45	–
2,6-AmNT	-6.89	–	-11.67	–	4.63	–	0.52	–
2,4,6AmT	-6.11	–	-8.14	–	5.01	–	-0.93	–
2,4DNT	-3.62	-4.71	-6.20	-7.27	2.80	2.30	2.32	1.98
2,6DNT	-3.42	-4.12	-6.08	-6.13	2.88	2.26	2.21	2.1
2NT	-1.68	-1.60	-4.68	-4.90	3.15	2.81	2.11	2.3
4NT	-1.97	-1.66	-4.96	-5.25	3.13	2.65	2.15	2.37
T	0.52	0.58	-2.39	-2.18	2.88	2.72	2.39	2.73
R	0.967	–	0.988	–	0.859	–	0.701	–
D	0.69	–	0.44	–	0.20	–	0.25	–
MUE	0.533	–	0.414	–	0.526	–	0.311	–