Supplementary material: Parameters derived for halogenated compounds

TABLE 1: Force field parameters for halocompounds derivatives

Bonds	K_b (kcal mol^{-1} Å^{-2})[a]	r_0(Å)
CT-CL	367.0	1.791[b]
CT-BR	367.0	1.966[b]
CT-XC	379.1[c]	1.465
XC-XN	754.0[c]	1.134

[a]As bond force constant for CT-F.
[b]Averaged from different bromo- or chlorocompounds (Gaussian optimization).
[c]CT-XC and XC-XN force constants calculated through interpolation.

Angles	K_θ(Kcal mol^{-1} rad^{-2})[d]	θ_0(deg)[e]
CL-CT-H1	38.1	107.7
BR-CT-H1	38.1	106.0
CT-CT-BR	50.0	110.3
BR-CT-BR	77.7	113.1
BR-CT-H2	38.1	107.1
CT-CT-CL	50.0	110.3
H1-CT-XC	50.0	107.9
CT-XC-XN	140.0	179.5

[d]Assumed to be the same as bond angle constant in chloro analogues from Fox, T.; Thomas, B.E., IV; McCarrick, M.; Kollman, P.A. *J.Phys.Chem.* **1996**, *100*, 10779-10783. For acetonitrile as H1-CT-CT bond angle constant.
[e]Averaged from different bromocompounds (Gaussian optimization).

Dihedrals[f]	IDIVF	K_Φ(kcal mol^{-1} rad^{-1})	phase(deg)	periodicity
CL-CT-CT-CL	1	0.65	0.0	-3.
CL-CT-CT-CL	1	0.68	0.0	1.
X-CT-XC-X	3	0.00	0.0	1.

[f]This work.

Nonbonded parameters[g]	R*(Å)	ϵ(kcal mol^{-1})
CL	1.968	0.285
BR	2.0716	0.426
XN[h]	1.740	0.210

[g]This work. [h]Cyano nitrogen.