Molecule Atom	Surface Atom	A	r_0	C
HA	Br	3034.0	0.244	0.15
HA	K	550736.6	0.137	0.19
CA	Br	173793.6	0.215	0.16
CA	K	1862.4	0.318	0.12
CT	Br	1846.2	0.345	0.11
CT	K	1936.6	0.276	0.11
HC	Br	1056.9	0.263	0.13
HC	K	559764.9	0.154	0.13
YC	Br	1002.4	0.243	0.05
YC	K	1117.2	0.326	1.60
YN	Br	1776.4	0.324	4.70
YN	K	4580.0	0.282	78.05

Buckingham potential parameters for the interaction of the organic species with the KBr (001) surface, with functional form $E(r) = Aexp(r/r_0) - C$ in eV. The organic atom names correspond to the types given in the force field of Cornell *et al* [58] and the additional nitrile potentials given in Ref. 59.