MedeA Forcefields Bundle: Access to the Most Accurate Forcefields

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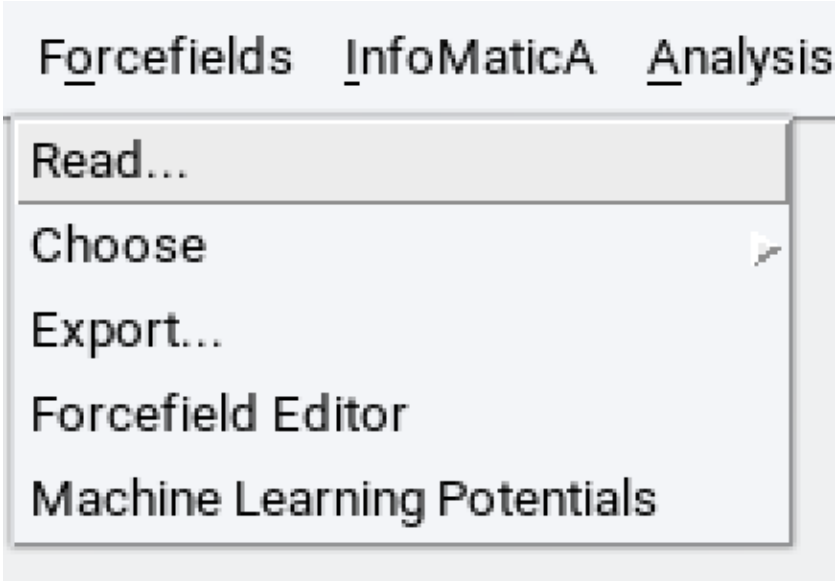
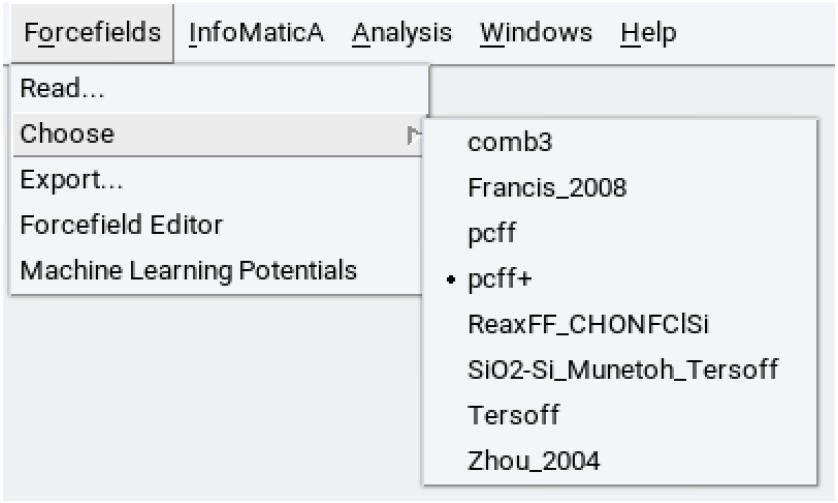
This section explains the basics of the interatomic potentials (force fields or forcefields) supported in the *MedeA* environment. For Forcefields >> Machine Learning Potentials, please see MedeA MLPG: Data Manager for more details.

1 Selecting a Forcefield



To select a specific forcefield, read in a forcefield file from Forcefields >> Read... .

One forcefield file can contain different versions, and most likely you want to use the default version.



You can select or verify using a specific variant via Forcefield >> Choose. In this case you want to make sure that you use the additions from Materials Design to pcff:

The initial selection comprises forcefields for:

Organic molecules and polymers

- pcff.frc
- pcff+.frc
- oplsaa.frc
- oplsaa_extended.frc
- oplsaa+.frc
- compass.frc
- compass+.frc (published part)
- gaff.frc
- AUA.frc
- AUA+.frc
- trappe+.frc
- small_molecules+solids.frc

Inorganic compounds

- inorganic.frc
- cvff_aug.frc (augmented)
- bks.frc
- nacl.frc
- clayff.frc
- clayff-dioctahedral.frc
- clayff-trioctahedral.frc
- comb3.frc
- Si-O_JCP2016-comb3.frc
- AlO_eam_coul.frc
- CeThUNpPuAmCmO_eam_coul.frc
- TaO_eam_coul.frc
- LiS_morse_coul.frc

Semiconductors

- Tersoff.frc
- SiO2-Si_Munetoh_2007_Tersoff.frc

- StillingerWeber.frc
- ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc
- REBO.frc

Metallic systems

- Zhou_2004.frc
- Ni_EAM.frc
- ZrH_v4.frc
- md-eam.frc
- EAM_Adams.frc
- AlMg_Adams_1997.frc
- AlCu_Cai_1996.frc
- FeNiCr_Bonny_2011.frc
- AlCo_Mishin_2013.frc
- AlNi_Mishin_2009.frc
- AlTi_Mishin_2003.frc
- MEAM.frc
- AlSiMgCuFe_MEAM.frc
- AuSi_MEAM.frc
- CH_MEAM.frc
- Cu_MEAM.frc
- FeC_MEAM.frc
- FeTiC_MEAM.frc
- Ni_MEAM.frc
- SiC_MEAM.frc
- W_MEAM.frc

Nist Interatomic Potentials Repository

- Ag-ATVF^Ag.frc
- Ag-YM^Ag.frc
- Al-Fe-MIM^Al-Fe.frc
- Al-LEA^Al-LEA.frc
- Al-MDSL^MDSL.frc
- Al-MIM^Al1.frc
- Al-Mg-LOARH^mg-al-set.frc
- Al-Mg-MIM^Al-Mg.frc
- Al-Pb-LWS^alpb-setfl.frc
- Al-Sm-Mendelev-2014^Al90Sm10_MendelevM_2014.frc
- Al-YM2^Al03.frc
- Al-YM^Al99.frc Au-ATVF^Au.frc
- Au-GRS05^Au-Grochola-JCP05.frc
- Co-PM12^Co_PurjaPun_2012.frc
- Cu-ATVF^Cu.frc
- Cu-Ag-HW^cu_ag_ymwu.frc
- Cu-Ag^CuAg.frc
- Cu-MIM^Cu1.frc
- Cu-MIM^Mendelev_Cu2_2012.frc
- Cu-YM^Cu01.frc
- Cu-Zr^Cu-Zr.frc
- Cu-Zr^Cu-Zr_2.frc
- Fe-ATVF^Fe.frc
- Fe-Cu-Ni-GB^FeCuNi.frc
- Fe-MIM2^Fe_2.frc
- Fe-MIM^Fe_5.frc

- Fe-Ni-Cr-GB-2013^FeNiCr_Bonny_2013_ptDef.frc
- Fe-Ni-Cr-GB^FeNiCr.frc
- Fe-Ni-GB^Fe-Ni.frc
- Fe-P-MIM^Fe-P.frc
- FeC-GJA^Fe-C_Hepburn_Ackland.frc
- Mg-MIM^Mg.frc
- Na-MIM^Na_MendelevM_2014.frc
- Nb-FPW^Nb.frc
- Nb-Ti-Al-Farkas-1996^Farkas_Nb-Ti-Al_1996.frc
- Ni-ATVF^Ni.frc
- Ni-Al-B2^NiAl02.frc
- Ni-Al-Co-YM13^Mishin-Al-Co-2013.frc
- Ni-Al-Co-YM13^Mishin-Ni-Al-Co-2013.frc
- Ni-Al-Co-YM13^Mishin-Ni-Co-2013.frc
- Ni-Al-H-AMB^NiAlH_jea.frc
- Ni-Al-Ni3Al^NiAl.frc
- Ni-Al-YM09^Mishin-Ni-Al-2009.frc
- Ni-MIM-2012^Ni1_Mendelev_2012.frc
- Ni-YM^Ni99.frc
- Ni-Zr-MIM-2012^Ni-Zr_Mendelev_2012.frc
- Ni-Zr-MIM-2014^Ni-Zr_Mendelev_2014.frc
- PdAgH-Hale-2013^PdAgH_HybridPd3Ag.frc
- PdAgH-Hale-2013^PdAgH_MorsePd3Ag.frc
- Ru-MIM^Ru.frc
- Ta-LSAL^newPP1_47-setfl.frc
- Ta-Ravelo-2013^Ta1_Ravelo_2013.frc
- Ta-Ravelo-2013^Ta2_Ravelo_2013.frc
- Ti-Al-RRZ03^Zope-Ti-Al-2003.frc
- Ti-GJA^Ti.frc
- U-Mo-Xe-SKS13^U_Mo_Xe.2013.frc
- V-Fe-MIM^V-Fe.frc
- W-ATVF^W.frc
- Zr-MIM2^Zr_2.frc
- Zr-MIM2^Zr_3.frc
- Zr-MIM^Zr_1.frc

Noble gases

- argon_rahman.frc

ReaxFF forcefields

- AlLiSiO.frc
- AuOH.frc
- BaZrYOH.frc
- CeO.frc
- CHO.frc
- CHON.frc
- CHONFClSi.frc
- CHONSFPtClNi.frc
- CHONSMoNi.frc
- clay_zeolite_water.frc
- CuClOH.frc
- CuOH.frc
- epoxy.frc
- FeCrOS.frc

- FeOHCl.frc
- Generic.frc
- HONB.frc
- LiC.frc
- LiMnO.frc
- LiPFCHO.frc
- LiSCFO.frc
- LiSiCHOF.frc
- MoS.frc
- PdCHO.frc
- protein_water.frc
- PtCH.frc
- PtNiCHO.frc
- PtO.frc
- TiOH.frc
- VCHO.frc
- ZnOH.frc

Mesoscale forcefields

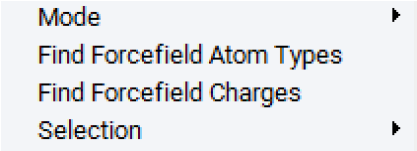
- Martini.frc
- Martini-3.0.frc
- SPICA.frc

Machine Learning Potentials (MLPs)

- Cu-SNAP.frc
- Cu_Zuo_JPCA2020.frc
- Cu-SNAP.frc
- Ge_Zuo_JPCA2020.frc
- InP_JCPA2020.frc
- Li3N-SNAP.frc
- Li_Zuo_JPCA2020.frc
- Mo_Zuo_JPCA2020.frc
- Ni_Zuo_JPCA2020.frc
- Si_Zuo_JPCA2020.frc
- Mo-SNAP.frc
- NbMoTaW-SNAP.frc
- Ni-SNAP.frc
- NiMo-SNAP.frc
- Ta06A.frc
- WBe_Wood_PRB2019.frc
- W_2940_2017_2.frc

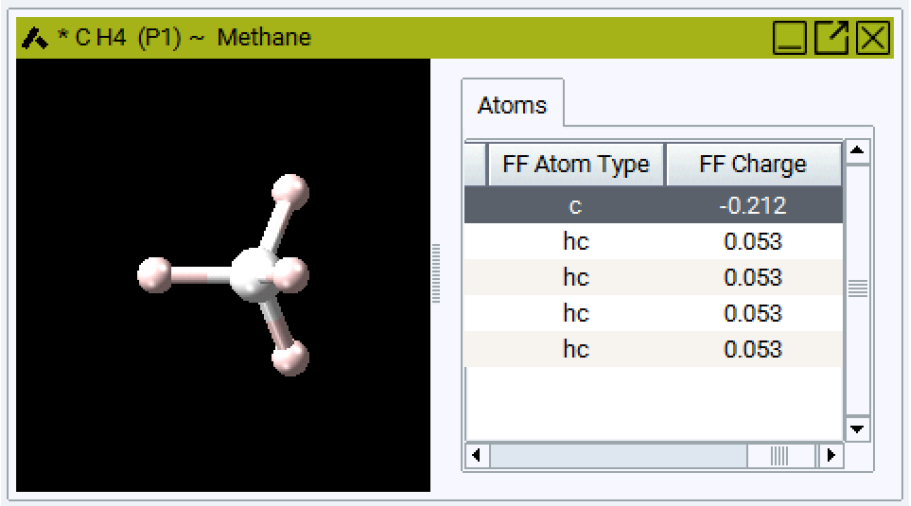
2 Assigning Forcefield Parameters and Charges

Right-click in your model window and use Find Forcefield Atom types and Find Forcefield Charges to perform the automatic atom type and partial charge assignment.



Note that when using covalent forcefields, it is important to ensure that appropriate bonds and bond orders - single, double, partial-double, and triple - have been set in order for correct atom types to be assigned using the forcefield's atom template definitions. Failure to use correct bond orders generally results in atoms with incorrect chemical valence, which can give the misleading impression that a forcefield cannot be used for a given molecule. Therefore, if attempts at atom type assignment result in a warning message indicating that the atom type assignment resulted in unknown atom types, you should first ensure that the chemical structures of the molecules in the model are correct.

You may inspect the assignment by clicking on the Spreadsheet Icon  , where atom types are listed in the *FF Atom Type* column (with '?' used to denote any unassigned types). If necessary, the spreadsheet also allows you to change charges and assign any atom type for a selected atom or group of atoms.



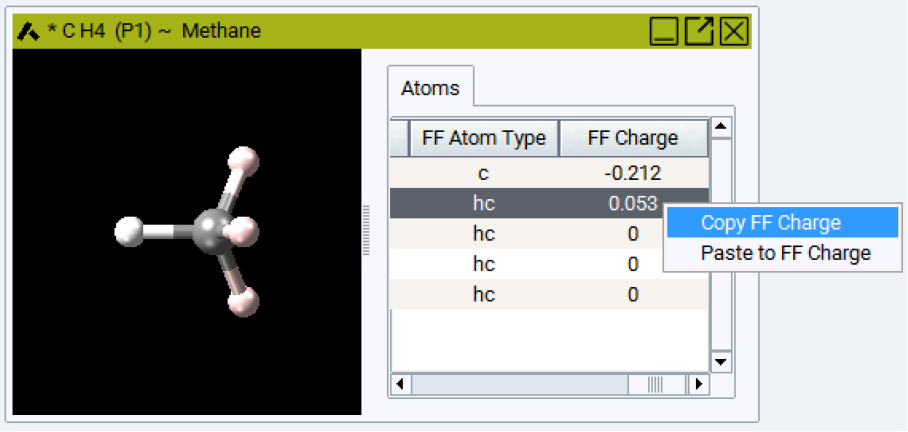
You can skip the automatic assignment and set all forcefield related values by hand (e.g. to match a publication). In this case, open the spreadsheet and you won't see the columns *FF Atom Type* and *FF Charge*. Insert them by right-clicking in the heading of the spreadsheet and select new columns *FF Atom Type* and *FF Charge*.

You can arrange and sort the atoms in the model and assign atom types to groups by selecting more than one field: The selected fields are highlighted in blue, the active field is white. In the example below you can choose one atom type for all four H atoms in Methane.

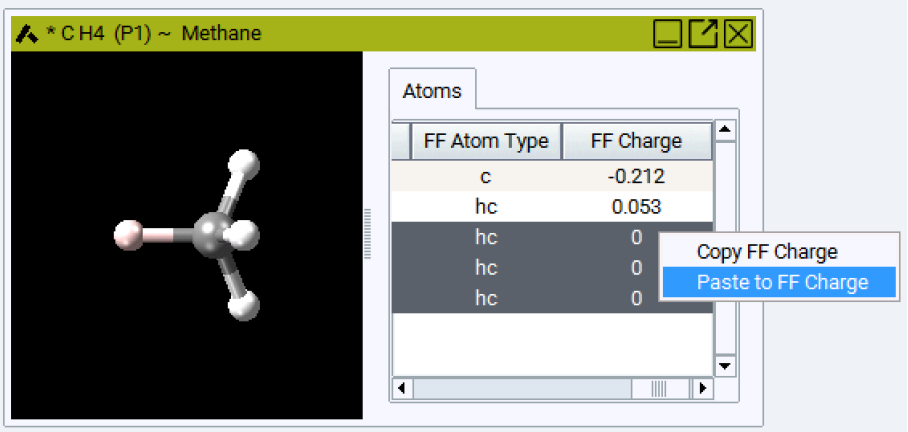
Setting charges is similar:

1. Enter charge for the first atom. Click into field and copy with right-click >> Copy FF charge

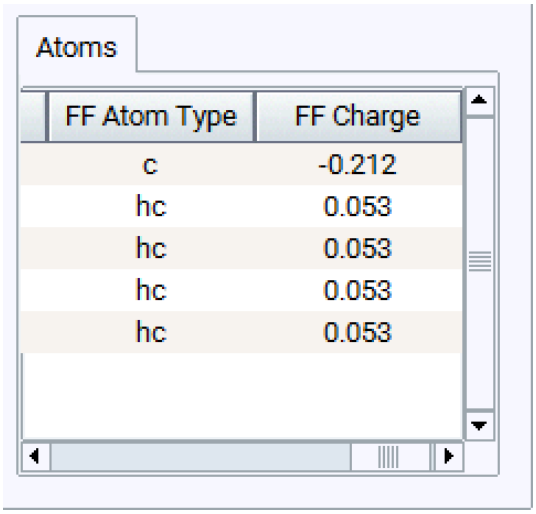
DOCUMENTATION



2. Select remaining atoms with mouse and paste with right-click >> Paste to FF charge



3. Charge values are copied into the selection



When using mesoscale systems the forcefield bead types cannot be changed independently. A mesoscale system is built with beads from a particular mesoscale forcefield. Therefore, the forcefield bead type is automatically set at build time. It can be inspected by labeling with Bead labels in the viewer or by clicking on the Spreadsheet Icon for periodic systems, where bead types are listed in the *Bead Type* column.

3 Forcefield Overview

3.1 Organic Molecules and Polymers

We recommend and support the use of pcff+ for all atom molecular dynamics, energy minimization, and related simulations. OPLS-AA, AUA and TraPPE are supplied to use with *MedeA GIBBS* for computationally efficient configurational space sampling and the use of extended atoms.

All the forcefields for organic systems require topological information (such as bonds and bond orders) to determine the atom type and charge for each atom. These forcefields cannot describe the creation or the breaking of bonds.

pcff+.frc:

A significant extension to the *pcff.frc* included with the LAMMPS distribution (see, for example, Sun, Mumby, Maple & Hagler [1]). *pcff+.frc* preserves the 'cff-series' ab-initio based parameters for valence interactions (as used in cff91.frc, cff93.frc and pcff.frc). This is supplemented by a substantial refinement of nonbonded parameters based on high quality experimental data for small molecule liquids and gases, together with new parameterizations for selected compounds such as thiophenes. Details are given in the References section at the end of the file.

Ag	Ag	Silver metal
Al	Al	Aluminium metal
Au	Au	Gold metal
Br	Br	bromine ion
Cl	Cl	chlorine ion
Cr	Cr	Chromium metal
Cu	Cu	Copper metal
Fe	Fe	Iron metal
K	K	Potassium metal
Li	Li	Lithium metal
Mo	Mo	Molybdenum metal
Na	Na	Sodium metal
Ni	Ni	Nickel metal
Pb	Pb	Lead metal
Pd	Pd	Palladium metal
Pt	Pt	Platinum metal
Sn	Sn	Tin metal
W	W	Tungsten metal
Ar	ar	Argon
Al	az	aluminium atom in zeolites
Br	br	bromine atom
C	c	generic SP3 carbon
C	c+	C in guanidinium group
C	c-	C in charged carboxylate
C	c1	sp3 carbon with 1 H 3 heavies
C	c2	sp3 carbon with 2 H's, 2 Heavy's
C	c3	sp3 carbon with 3 hHs 1 heavy
C	c3h	sp3 carbon in 3-membered ring with hydrogens
C	c3m	sp3 carbon in 3-membered ring
C	c4h	sp3 carbon in 4-membered ring with hydrogens
C	c4m	sp3 carbon in 4-membered ring

Continued on next page

[1] Huai Sun, Stephen J. Mumby, Jon R. Maple, and Arnold T. Hagler, "An Ab Initio CFF93 All-Atom Force Field for Polycarbonates," Journal of the American Chemical Society 116, no. 7 (1994): 2978-2987.

Table 1 – continued from previous page

C	c5	sp2 aromatic carbon in 5-membered ring
C	c=	non aromatic end doubly bonded carbon
C	c=1	non aromatic, next to end doubly bonded carbon
C	c=2	non aromatic doubly bonded carbon
C	c_0	carbonyl carbon of aldehydes, ketones
C	c_1	carbonyl carbon of acid, ester, amide
C	c_2	carbonyl carbon of carbamate, urea
C	c_a	general amino acid alpha carbon (sp3)
Ca	ca+	calcium ion
C	cg	sp3 alpha carbon in glycine
C	ci	sp2 aromatic carbon in charged imidazole ring (His+)
Cl	cl	chlorine atom
C	co	sp3 carbon in acetals
C	coh	sp3 carbon in acetals with hydrogen
C	cp	sp2 aromatic carbon
C	cr	C in neutral arginine
C	cs	sp2 aromatic carbon in 5 membered ring next to S
C	ct	sp carbon involved in a triple bond
C	cz	carbonyl carbon of carbonate
D	dw	deuterium in heivy water
F	f	fluorine atom
H	h	generic hydrogen bound to C, Si,or H
H	h*	hydrogen bonded to nitrogen, Oxygen
H	h+	charged hydrogen in cations
H	hb	hydrogen atom in bridging hydroxyl group
H	hc	hydrogen bonded to carbon
He	he	Helium
H	hi	Hydrogen in charged imidazole ring
H	hn	hydrogen bonded to nitrogen
H	hn2	amino hydrogen
H	ho	hydrogen bonded to oxygen
H	ho2	hydroxyl hydrogen
H	hoa	hydrogen atom in terminal hydroxyl group on aluminium
H	hos	hydrogen atom in terminal hydroxyl group on silicon
H	hp	hydrogen bonded to phosphorus
H	hs	hydrogen bonded to sulfur
H	hsi	silane hydrogen
H	hw	hydrogen in water
I	i	iodine atom
Kr	kr	Krypton
N	n	generic sp2 nitrogen (in amids))
N	n+	sp3 nitrogen in protonated amines
N	n1	sp2 nitrogen in charged arginine
N	n2	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
N	n3m	sp3 nitrogen in 3- membered ring
N	n3n	sp2 nitrogen in 3- membered ring
N	n4	sp3 nitrogen in protonated amines
N	n4m	sp3 nitrogen in 4- membered ring
N	n4n	sp2 nitrogen in 4- membered ring
N	n=	non aromatic end doubly bonded nitrogen
N	n=1	non aromatic, next to end doubly bonded carbon
N	n=2	non aromatic doubly bonded nitrogen
N	n_2	nitrogen of urethane
N	na	sp3 nitrogen in amines

Continued on next page

Table 1 – continued from previous page

N	nb	sp2 nitrogen in aromatic amines
Ne	ne	Neon
N	nh	sp2 nitrogen in 5 or 6 membered ring
N	nh+	protonated nitrogen in 6 membered ring
N	nho	sp2 nitrogen in 6 membered ring next to a carbonyl
N	ni	nitrogen in charged imidazole ring
N	nn	sp2 nitrogen in aromatic amines
N	np	sp2 nitrogen in 5- or 6- membered ring
N	npc	sp2 nitrogen in 5- or 6- membered ring and with a heavy atom
N	nr	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
N	nt	sp nitrogen involved in a triple bond
N	nz	sp3 nitrogen bonded to two atoms
O	o	generic SP3 oxygen
O	o*	oxygen in water
O	o-	partial double oxygen
O	o3e	sp3 oxygen in three membered ring
O	o4e	sp3 oxygen in four membered ring
O	o=	oxygen double bonded to O, C, S, N, P
O	o_1	oxygen in carbonyl group
O	o_2	ester oxygen
O	oah	oxygen atom in terminal hydroxyl group on aluminium
O	oas	oxygen atom between aluminium and silicon
O	ob	oxygen atom in bridging hydroxyl group
O	oc	sp3 oxygen in ether or acetals
O	oe	sp3 oxygen in ester
O	oh	oxygen bonded to hydrogen
O	oo	oxygen in carbonyl group, carbonate only
O	op	sp2 aromatic in 5 membered ring
O	osh	oxygen atom in terminal hydroxyl group on silicon
O	osi	siloxane oxygen
O	oss	oxygen atom between two silicons
O	oz	ester oxygen in carbonate
P	p	general phosphorous atom
P	p=	phosphazene phosphorous atom
S	s	sp3 sulfur
S	s'	S in thioketone group
S	s-	partial double sulfur
S	s1	sp3 sulfur involved in (S-S) group of disulfides
S	s3e	sulfur in three membered ring
S	s4e	sulfur in four membered ring
S	sc	sp3 sulfur in methionines (C-S-C) group
S	sf	S in sulfonate group
S	sh	sp3 sulfur in sulfhydryl (-SH) group (e.g. cysteine)
Si	si	silicon atom
Si	sio	siloxane silicon
S	sp	sulfur in an aromatic ring (e.g. thiophene)
Si	sz	silicon atom in zeolites
Xe	xe	Xenon
As	as	Arsenic in AsR3
B	b3n	sp2 boron in hexagonal boron nitride
Br	brh	bromine in HBr molecule
C	c0	sp3 carbon with 0 H, 4 heavies
C	c0x	sp3 carbon with 0 H, 4 fluorines
C	c1o	carbon in CO

Continued on next page

Table 1 – continued from previous page

C	c2=	carbon in CO2 and CS2
C	c3as	sp3 carbon in methyl arsines
C	c3h1	sp3 carbon in 3-membered ring with one hydrogen
C	c3si	sp3 carbon with 3 hydrogens and Si
C	c3o-	carbon in carbonate anion
C	c41o	carbon, sp3, in methanol
C	c43o	carbon, sp3 in secondary alcohols
C	c4h1	sp3 carbon in 4-membered ring with one hydrogen
C	c4o	alpha carbon
C	c0oe	alpha carbon in ether containing tertiary alkyl group, e.g. -C-O-C-R3
C	c1oe	alpha carbon in ether containing secondary alkyl group, e.g. -C-O-CH-R2
C	c2oe	alpha carbon in ether containing primary alkyl group, -C-O-CH2-R
C	c2oz	alpha carbon in carbonates -O(O)C-O-CH2-R
C	c3oe	alpha carbon in methyl containing ethers -C-O-CH3
C	c3oz	alpha carbon in methyl-containing carbonates -O(O)C-O-CH3
C	c4oe	alpha carbon in general ethers -C-O-C- (legacy)
C	c5h	sp3 carbon in 5-membered ring
C	c5h1	sp3 carbon in 5-membered ring with one hydrogen
Cl	cl4	chlorine in ClO4- anion
Cl	clh	chlorine in HCl molecule
C	cpc	alpha/ipso carbon in aromatic ethers -C-O-C-
Cs	Cs+	cesium ion
F	ff	fluorine atom in perfluorinated aliphatics
F	ffp	fluorine atom in perfluorinated aromatics
F	F	fluorine ion
Ge	ge4	generic germanium with four bonds attached
H	h1h	hydrogen in H2
H	h_1p	hydrogen in NH4+
H	hbr	hydrogen in HBr molecule
H	hcl	hydrogen in HCl molecule
H	hhi	hydrogen in HI molecule
H	ho-	hydrogen in hydroxide ion OH-
I	I	iodine ion
I	ih	iodine in HI molecule
K	K+	potassium ion
Li	Li+	lithium ion
N	n1o	nitrogen in NO
N	n2o	nitrogen in NO2
N	n2-	nitrogen in amide/imide anion
N	n3b	sp2 nitrogen in hexagonal boron nitride
N	n4o	nitrogen in amine oxides
N	n_3	nitrogen in primary or secondary amide
N	n_3-	nitrogen in NO3- nitrate ion
N	n_30	nitrogen in tertiary amide
N	n_31	nitrogen in secondary amide
N	n_32	nitrogen in primary amide
N	n_4	nitrogen in NH4+
N	n_4c	nitrogen in NR4+
N	na0	sp3 nitrogen in tertiary aliphatic amines
N	na1	sp3 nitrogen in secondary aliphatic amines
N	na2	sp3 nitrogen in primary aliphatic amines (same as na)

Continued on next page

Table 1 – continued from previous page

N	nbo	sp2 nitrogen in aromatic nitro compounds
Na	Na+	sodium ion
O	o=n	oxygen double bonded to N in aromatic nitro group
O	o1=	oxygen in NO2 and SO2
O	o1=*	oxygen in CO2
O	o1c	oxygen in CO
O	o1c-	oxygen in carbonate anion
O	o1n	oxygen in NO
O	o1n4	oxygen in amine oxides
O	o1o	oxygen in O2
O	o1s-	oxygen in sulfate or sulfonate anion
O	o1n-	oxygen in nitrate ion
O	o2s-	ether oxygen in sulfate anion
O	o_1h	oxygen in carbonyl group of aldehydes
O	o_1r	oxygen in ClO4- anion
O	o_2c	oxygen in carboxylic acids
O	oc	sp3 oxygen in ether or acetals
O	oh-	oxygen in hydroxide ion OH-
P	p6-	phosphorous in phosphate
P	ph3	phosphorous in phosphine
Rb	Rb+	rubidium ion
S	s1=	sulfur in CS2
S	s2=	sulfur in SO2
S	se-	sulfur in sulfate anion

oplsaa+.frc

Based on Jorgensen, Maxwell & Tirado-Rives [2] (oplsaa), supplemented with inclusion of additional parameters derived by various groups (oplsaa_extended), and original work by Materials Design (oplsaa+).

Ar	Ar	Argon atom
C	C	Carbonyl carbon in amides, esters
C	CA	Aromatic carbon
C	CAh1	Aromatic carbon pyridine atom 2
C	CAh2	Aromatic carbon pyridine atom 3
C	CAh3	Aromatic carbon pyridine atom 4
C	CAh4	Aromatic carbon pyrimidine atom 3
C	CAh5	Aromatic carbon pyrimidine atom 4
C	CAh6	Aromatic carbon pyridazine atom 2
C	CAh7	Aromatic carbon pyridazine atom 3
C	CAh8	Aromatic carbon pyrazine
C	CAh9	Aromatic carbon pyrazole
C	CAh0	Aromatic carbon isoxazole
C	CAi1	Aromatic carbon indole atom 4
C	CAi2	Aromatic carbon indole atom 5
C	CAi3	Aromatic carbon indole atom 6
C	CAi4	Aromatic carbon indole atom 7
C	CB	Aromatic carbon indole atom 9
C	CM	sp2 aliphatic carbon
C	CN	aromatic carbon indole atom 8

Continued on next page

[2] William L Jorgensen, David S Maxwell, and Julian Tirado-Rives, "Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids," Journal of the American Chemical Society 118, no. 45 (January 1996): 11225-11236.

Table 2 – continued from previous page

C	CO	Acetal carbon ROCOR
C	CQ	pyrimidine N-C-N aromatic carbon
C	CR	Aromatic carbon imidazole
C	CRh1	Aromatic carbon oxazole
C	CS	Generic 5-membered ring carbon
C	CSh1	Aromatic carbon pyrrole
C	CSh2	Aromatic carbon furan
C	CSh3	Aromatic carbon indole atom 3
C	CT	sp3 aliphatic carbon
C	CT1	sp3 alpha carbon in nitriles
C	CTEX	Exocyclic sp3 aliphatic carbon in cyclic amine
C	CTfn	Perfluoroalkane carbon
C	CTf4	Tetrafluoromethane carbon
C	CU	Aromatic carbon pyrazole
C	CUh1	Aromatic carbon isoxazole
C	CV	Aromatic carbon imidazole
C	CVh1	Aromatic carbon oxazole
C	CW	sp2 aliphatic carbon
C	CWh1	Aromatic carbon pyrrole
C	CWh2	Aromatic carbon furan
C	CWh3	Aromatic carbon pyrazole
C	CWh4	Aromatic carbon isoxazole
C	CWh5	Aromatic carbon imidazole
C	CWh6	Aromatic carbon oxazole
C	CWh7	Aromatic carbon indole atom 2
C	CZ	sp alkyl nitrile carbon
C	CZ1	sp aryl nitrile carbon
F	F	Fluorine in perfluorinated hydrocarbons
H	H	Amide or amine H(N) hydrogen
H	HA	Aromatic hydrogen
H	HC	Hydrogen bonded to carbon
H	HC1	Hydrogen bonded to carbon in methanol
H	HC2	Hydrogen bonded to carbon in alkenes RH-C= and H2-C=
H	HC3	Hydrogen bonded to carbon in ethers
H	HC4	Hydrogen bonded to carbon next to NR2, NO2, or nitrile
H	HC5	alpha alkoxy H in esters
H	HC6	H on alpha carbon of aldehyde and ketone
He	He	Helium atom
H	HEX4	Amine hydrogen in 4-membered cyclic amine (azetidine)
H	HEX5	Amine hydrogen in 5-membered cyclic amine (pyrrolidine)
H	HEX6	Amine hydrogen in 6-membered cyclic amine (piperidine)
H	HW	Hydrogen in TIP3P water
H	HO	Hydrogen bonded to O
H	HS	Hydrogen bonded to S in thiols
Kr	Kr	Krypton atom
N	N	Nitrogen in amides
N	N1	Nitrogen in primary amides
N	N2	Nitrogen in secondary amides
N	N3	Nitrogen in tertiary amides
Ne	Ne	Neon atom
N	NA	Nitrogen in pyrrole
N	NAh2	N-H Nitrogen in pyrazole
N	NAh3	N-H Nitrogen in imidazole
N	NAh4	N-H Nitrogen in indole (atom 1)

Continued on next page

Table 2 – continued from previous page

N	NB	Nitrogen in pyrazole
N	NBh1	Nitrogen in isoxazole
N	NBh2	Nitrogen in imidazole
N	NBh3	Nitrogen in oxazole
N	NC	Nitrogen in pyridine and diazenes
N	NO	Nitrogen in nitroalkane
N	NT0	Nitrogen in ammonia
N	NT	Nitrogen in primary amines
N	NT2	Nitrogen in secondary amines
N	NT3	Nitrogen in tertiary amines
N	NZ	Nitrogen in nitriles
O	O	Oxygen in amides
O	O1	Oxygen in carboxylate esters
O	O2	Oxygen in aldehydes
O	O3	Oxygen in ketones
O	O4	Oxygen in carboxylic acids RCOOH
O	OH	Oxygen in hydroxyl (OH) group
O	OH2	Oxygen in hydroxyl (OH) group (diols)
O	OH3	Oxygen in hydroxyl (OH) group (triols)
O	OH4	Oxygen in hydroxyl (OH) group (RCOOH)
O	OH5	Oxygen in hydroxyl (OH) group (phenol)
O	ON	Oxygen in nitro group
O	OS	Oxygen in ethers, including acetals
O	OS1	Alkoxy oxygen in esters
O	OW	Oxygen in TIP3P water
S	S	Sulfur in sulfides and disulfides
S	SH	Sulfur in thiols
S	SH1	Sulfur in H2S
Xe	Xe	Xenon atom
C	C1i	aliphatic carbon bonded to N in R4N+
C	C2i	aliphatic carbon bonded to C1i in R4N+
C	CTi	sp3 aliphatic carbon in ionic liquid
F	Fi	Fluorine in ionic liquid anion
H	H1	Hydrogen bonded to C1 in R4N+ cation
N	N2i	Nitrogen bonded to S in triflimide anion
N	N4i	Nitrogen in R4N+ cation
O	OYi	Oxygen bonded to S in triflate
S	SY6i	Sulfur in bis triflimide

Trappe+.frc

Martin [3] , Kamath [4] , Stubbs [5] , Wick [6] , Chen [7] , Wick [8] , Martin [9] , Lubna [10] , Maerzke [11]

C	C	Aliphatic
C	CHx-aliphatic	Aliphatic
C	CH4-TraPPE-UA	Molecule CH4-TraPPE-UA
C	CH3-TraPPE-UA	Group CH3-TraPPE-UA-
C	CH2-TraPPE-UA	Group CH2-TraPPE-UA-
C	CH-TraPPE-UA	Group CH-TraPPE-UA-
C	C-TraPPE-UA	Group C-TraPPE-UA-
C	CH2-olef-TraPPE-UA	Group CH2-olef-TraPPE-UA=
C	CH-olef-TraPPE-UA	Group CH-olef-TraPPE-UA=
C	C-olef-TraPPE-UA	Group C-olef-TraPPE-UA=
C	CH-EA-TraPPE-UA	Group CH-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	CH-(EA)-TraPPE-UA	Group CH-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-EA-TraPPE-UA	Group C-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-(EA)-TraPPE-UA	Group C-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon
C	C-l-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon linking two rings in condensed units (naphthalene, indane, phenanthrene,..)
C	C-d-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon linking two rings in diphenyl
C	CH-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon with one hydrogen
C	CH-aldehyde-TraPPE-UA	C connected to O in aldehydes TraPPE-UA
C	CH-(aldehyde)-TraPPE-UA	C connected to O in aldehydes TraPPE-UA
C	C-ketone-TraPPE-UA	C connected to O in ketones TraPPE-UA
C	C-(ketone)-TraPPE-UA	C connected to O in ketones TraPPE-UA

Continued on next page

[3] MG Martin and IJ Siepmann, "Transferable Models for Phase Equilibria 1. United-Atom Description of N-Alkanes," Journal of Physical Chemistry B 102 (1998): 2569.
[4] Ganesh Kamath, Feng Cao, and Jeffrey J Potoff, "An Improved Force Field for the Prediction of the Vapor-Liquid Equilibria for Carboxylic Acids," *Journal of Physical Chemistry B* 108, no. 37 (September 2004): 14130-14136.
[5] John M Stubbs, Jeffrey J Potoff, and J Ilja Siepmann, "Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes," *Journal of Physical Chemistry B* 108, no. 45 (November 2004): 17596-17605.
[6] Collin D Wick, John M Stubbs, Neeraj Rai, and J Ilja Siepmann, "Transferable Potentials for Phase Equilibria. 7. Primary, Secondary, and Tertiary Amines, Nitroalkanes and Nitrobenzene, Nitriles, Amides, Pyridine, and Pyrimidine," *Journal of Physical Chemistry B* 109, no. 40 (October 2005): 18974-18982.
[7] Bin Chen, Jeffrey J Potoff, and J Ilja Siepmann, "Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols," *Journal of Physical Chemistry B* 105, no. 15 (April 2001): 3093-3104.
[8] Collin D Wick, Marcus G Martin, and J Ilja Siepmann, "Transferable Potentials for Phase Equilibria. 4. United-Atom Description of Linear and Branched Alkenes and Alkylbenzenes," *Journal of Physical Chemistry B* 104, no. 33 (August 2000): 8008-8016.
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[11] Katie A Maerzke, Nathan E Schultz, Richard B Ross, and J Ilja Siepmann, "TraPPE-UA Force Field for Acrylates and Monte Carlo Simulations for Their Mixtures with Alkanes and Alcohols," *Journal of Physical Chemistry B* 113, no. 18 (May 7, 2009): 6415-6425.

Table 3 – continued from previous page

C	CH2-cyc5-TraPPE-UA	Group CH2- in a 5-membered cyclic non-aromatic ring
C	CH2-cyc6-TraPPE-UA	Group CH2- in a 6-membered cyclic non-aromatic ring
C	CH-cyc-TraPPE-UA	Group CH- in a 5- or 6-membered cyclic non-aromatic ring
C	C-cyc-TraPPE-UA	Group C- in a 5- or 6-membered cyclic non-aromatic ring
H	H-OH-TraPPE-UA	Hydrogen bonded to O in OH groups
H	H(-OH)-TraPPE-UA	Hydrogen bonded to O in OH groups
H	HA	Aromatic hydrogen
H	UnitedH	ghost H (used also for aromatic in this version)
H	H-SH-TraPPE-UA	H bonded with S in thiols
H	H-pyrrole-TraPPE-UA	H bonded with N in pyrrole
N	N-pyridine-TraPPE-UA	Nitrogen in pyridine
N	N-pyrrole-TraPPE-UA	Nitrogen in pyrrole
N	N-arom-TraPPE-UA	Nitrogen in aromatic rings
O	O-OH-TraPPE-UA	Oxygen in hydroxyl (O-OH-TraPPE-UA) group
O	O(-OH)-TraPPE-UA	Oxygen in hydroxyl (O-OH-TraPPE-UA) group
O	O-ROR-TraPPE-UA	Oxygen in ethers
O	O(ROR)-TraPPE-UA	Oxygen in ethers
O	O-aldehydeketone-TraPPE-UA	Oxygen in aldehydes and ketones TraPPE-UA
O	O-(aldehydeketone)-TraPPE-UA	Oxygen in aldehydes and ketones TraPPE-UA
S	S	Sulfur
S	S-thiol-TraPPE-UA	Sulfur in thiols
S	S-sulfide-TraPPE-UA	Sulfur in sulfides
S	S-disulfide-TraPPE-UA	Sulfur in disulfides
S	S-thiophene-TraPPE-UA	Sulfur in thiophene

compass+.frc - The Published Part of COMPASS

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated, as the forcefield is not maintained. [12] Contains the collection of compass parameters in their original published form. compass+.frc includes subsequently published corrections.

[12] H Sun, "COMPASS: an Ab Initio Force-Field Optimized for Condensed-Phase -Overview with Details on Alkane and Benzene Compounds," *Journal of Physical Chemistry B* 102, no. 38 (September 1998): 7338-7364.

Cvff.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [13]

Cff91.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [14]

Cff93.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [15]

3.2 Inorganic Compounds

We don't make overall recommendations for inorganic forcefields, because the local coordination of inorganic systems varies widely, and the transferability of forcefield terms cannot be assumed from one compound to another. The scope and applicability of forcefields for inorganics are best discerned through reference to their original derivation. These forcefields don't require bonds.

inorganic.frc

Compiled by Woodley, Battle, Gale & Catlow [16], Xia [17] for use in inorganic crystal structure prediction.

Ag	Ag1+	
Ag	Ag3+	
Al	Al3+	
Ba	Ba2+	
Ca	Ca2+	
Cd	Cd2+	
Ce	Ce4+	
Co	Co2+	
Co	Co3+	
Cr	Cr3+	
Cu	Cu1+	
Fe	Fe2+	
Fe	Fe3+	
Ge	Ge4+	
K	K1+	
La	La3+	
Mg	Mg2+	

Continued on next page

[13] Jö rg-R diger Hill, Clive M Freeman, and Lalitha Subramanian, "Use of Force Fields in Materials Modeling," in Reviews in Computational Chemistry, ed. by Kenny B Lipkowitz and Donald B Boyd, vol. 16, (Hoboken, NJ, USA: John Wiley & Sons, Inc., 2000), 141-216.

[14] J R Maple, M J Hwang, T P Stockfisch, U Dinur, M Waldman, et al., "Derivation of Class II Force Fields. I. Methodology and Quantum Force Field for the Alkyl Functional Group and Alkane Molecules," Journal of Computational Chemistry 15, no. 2 (February 1994): 162-182; M J Hwang, T P Stockfisch, and A T Hagler, "Derivation of Class II Force Fields. 2. Derivation and Characterization of a Class II Force Field, CFF93, for the Alkyl Functional Group and Alkane Molecules," Journal of the American Chemical Society 116, no. 6 (1994): 2515-2525.

[15] J R Maple, M J Hwang, T P Stockfisch, U Dinur, M Waldman, et al., "Derivation of Class II Force Fields. I. Methodology and Quantum Force Field for the Alkyl Functional Group and Alkane Molecules," Journal of Computational Chemistry 15, no. 2 (February 1994): 162-182; M J Hwang, T P Stockfisch, and A T Hagler, "Derivation of Class II Force Fields. 2. Derivation and Characterization of a Class II Force Field, CFF93, for the Alkyl Functional Group and Alkane Molecules," Journal of the American Chemical Society 116, no. 6 (1994): 2515-2525.

[16] S.M. Woodley, P.D. Battle, J D Gale, and C Richard A Catlow, "The Prediction of Inorganic Crystal Structures Using a Genetic Algorithm and Energy Minimisation," Physical Chemistry Chemical Physics 1, no. 10 (1999): 2535-2542.

[17] Xin Xia, "Computational Modelling Study of Yttria-Stabilized Zirconia," (University College London, 2010).

Table 4 – continued from previous page

Mn	Mn2+	
Mn	Mn4+	
Na	Na1+	
Nb	Nb5+	
Ni	Ni2+	
O	O2-	
O	O12-	
O	O22-	
Pb	Pb1+	
Po	Po4+	
Pr	Pr3+	
Rb	Rb1+	
Si	Si4+	
Sn	Sn4+	
Sr	Sr2+	
Ta	Ta2+	
Tl	Tl3+	
Ti	Ti3+	
Ti	Ti4+	
U	U2+	
V	V2+	
V	V3+	
V	V4+	
Y	Y3+	
Zn	Zn2+	
Zr	Zr2+	

bks.frc

Derived by van Beest, Kramer & van Santen [18] to provide a description of structural and vibrational properties for framework structure materials based on two-body (i.e. without explicit angle terms).

Al	Al	
O	O	
P	P	
Si	Si	

CVFF_aug.frc

This forcefield was developed by Behnam Vessal using a methodology similar to that employed by van Beest, to create a broad two-body (i.e. without explicit angle terms) description of framework structured materials able to support extra framework atoms. [19]

H	h	Hydrogen bonded to C. Masses from CRC 1973/74 pages B-250.
H	d	General Deuterium
H	hn	Hydrogen bonded to N
H	ho	Hydrogen bonded to O

Continued on next page

[18] B W H van Beest, G J Kramer, and R A van Santen, "Force Fields for Silicas and Aluminophosphates Based on Ab Initio Calculations," Physical Review Letters 64, no. 16 (April 1990): 1955-1958.

[19] Jö rg-R diger Hill, Clive M Freeman, and Lalitha Subramanian, "Use of Force Fields in Materials Modeling," in Reviews in Computational Chemistry, ed. by Kenny B Lipkowitz and Donald B Boyd, vol. 16, (Hoboken, NJ, USA: John Wiley & Sons, Inc., 2000), 141-216.

Table 5 – continued from previous page

H	hp	Hydrogen bonded to P
H	hs	Hydrogen bonded to S
H	h*	Hydrogen in water molecule
H	h$	Hydrogen atom for automatic parameter assignment
L	lp	Lone Pair
L	lp	Lone Pair
H	h+	Charged hydrogen in cations
H	hc	Hydrogen bonded to carbon
H	hi	Hydrogen in charged imidazole ring
H	hw	Hydrogen in water
D	dw	Deuterium in heivy water
C	c	Sp3 aliphatic carbon
C	cg	Sp3 alpha carbon in glycine
C	c'	Sp2 carbon in carbonyl (C=O) group
C	c*	Carbon in carbonyl group, non_amides
C	c"	Carbon in carbonyl group, non_amides
C	cp	Sp2 aromatic carbon (partial double bonds)
C	cr	Carbon in guanidinium group (HN=C(NH2)2)
C	c+	C in guanidinium group
C	c-	Carbon in charged carboxylate (COO-) group
C	ca	General amino acid alpha carbon (sp3)
C	c3	Sp3 carbon in methyl (CH3) group
C	cn	Sp3 Carbon bonded to N
C	c2	Sp3 carbon bonded to 2 H's, 2 heavy atoms
C	c1	Sp3 carbon bonded to 1 H, 3 Heavy atoms
C	c5	Sp2 aromatic carbon in five membered ring
C	cs	Sp2 carbon involved in thiophene
C	c=	Non aromatic end doubly bonded carbon
C	c=1	Non aromatic, next to end doubly bonded carbon
C	c=2	Non aromatic doubly bonded carbon
C	ct	Sp carbon involved in triple bond
C	ci	Sp2 aromatic carbon in charged imidazole ring (His+)
C	c$	Carbon atom for automatic parameter assignment
C	co	Sp3 carbon in acetals
C	c3m	Sp3 carbon in 3-membered ring
C	c4m	Sp3 carbon in 4-membered ring
C	coh	Sp3 carbon in acetals with hydrogen
C	c3h	Sp3 carbon in 3-membered ring with hydrogens
C	c4h	Sp3 carbon in 4-membered ring with hydrogens
C	ci	Sp2 aromatic carbon in charged imidazole ring (His+)
N	n	Sp2 nitrogen with 1 H, 2 heavy atoms (amide group)
N	no	Sp2 nitrogen in nitro group
N	n2	Sp2 nitrogen (NH2 in the guanidinium group (HN=C(NH2)2))
N	np	Sp2 aromatic nitrogen (partial double bonds)
N	n3	Sp3 nitrogen with three substituents
N	n4	Sp3 nitrogen with four substituents
N	n=	Non aromatic end double bonded nitrogen
N	n=1	Non aromatic, next to end doubly bonded carbon
N	n=2	Non aromatic doubly bonded nitrogen
N	nt	Sp nitrogen involved in triple bond
N	nz	Sp nitrogen in N2
N	n1	Sp2 nitrogen in charged arginine
N	ni	Sp2 nitrogen in a charged imidazole ring (HIS+)
N	n$	Nitrogen atom for automatic parameter assignment

Continued on next page

Table 5 – continued from previous page

N	na	Sp3 nitrogen in amines
N	n3m	Sp3 nitrogen in 3- membered ring
N	n4m	Sp3 nitrogen in 4- membered ring
N	n3n	Sp2 nitrogen in 3- membered ring
N	n4n	Sp2 nitrogen in 4- membered ring
N	nb	sp2 nitrogen in aromatic amines
N	nn	sp2 nitrogen in aromatic amines
N	npc	sp2 nitrogen in 5- or 6- membered ring bonded to a heavy atom
N	nh	sp2 nitrogen in 5-or 6- membered ring with hydrogen attached
N	nho	sp2 nitrogen in 6- membered ring next to a carbonyl group and with a hydrogen
N	nh+	protonated nitrogen in 6- membered ring with hydrogen attached
N	n+	sp3 nitrogen in protonated amines
N	nr	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
O	o’	Oxygen in carbonyl (C=O) group
O	o	sp3 oxygen in ether or ester groups
O	o-	Oxygen in charged carboxylate (COO-) group
O	oh	Oxygen in hydroxyl (OH) group
O	o*	Oxygen in water molecule
O	op	Oxygen in aromatic rings. e.g. furan
O	of	Oxygen in
O	o$	Oxygen atom for automatic parameter assignment
O	oc	sp3 oxygen in ether or acetals
O	oe	sp3 oxygen in ester
O	o3e	sp3 oxygen in three membered ring
O	o4e	sp3 oxygen in four membered ring
S	s	Sulfur in methionine (C-S-C) group
S	s1	Sulfur involved in S-S disulfide bond
S	sh	Sulfur in sulfhydryl (-SH) group
S	sp	Sulfur in thiophene
S	s’	Sulfur in thioketone (>C=S) group
S	s$	Sulfur atom for automatic parameter assignment
S	sc	sp3 sulfur in methionines (C-S-C) group
S	s3e	Sulfur in three membered ring
S	s4e	Sulfur in four membered ring
S	s-	Sulfur bonded to something then bonded to another partial double O or S
P	p	General phosphorous atom
P	p$	Phosphorous atom for automatic parameter assignment
Ca	ca+	Calcium ion - Ca++, mass = mass of Ca - 2*electron mass.
F	f	Fluorine bonded to a carbon
Cl	cl	Chlorine bonded to a carbon
Br	br	Bromine bonded to a carbon
I	i	Covalently bound Iodine
Si	si	Silicon atom (General)
H	nu	NULL atom for relative free energy
Cl	Cl	Chloride ion Cl-
Br	Br	Bromide ion Br-
Na	Na	Sodium metal
Ar	ar	Argon
Si	sz	Silicon atom in zeolites
Si	sy	Tetrahedral Silicon atom in Clays

Continued on next page

Table 5 – continued from previous page

O	oz	Oxygen atom in zeolites
O	oy	Oxygen atom in Clays
Al	az	Tetrahedral Aluminum atom in zeolites
Al	ay	Octahedral Aluminum atom in Clays
Al	ayt	Tetrahedral Aluminum atom to be used with oy
P	pz	Phosphorous atom in zeolites
P	py	Phosphorous atom to be used with oy
Ga	ga	Gallium atom in zeolites
Ge	ge	Germanium atom in zeolites
Ti	tioc	Titanium (Octahedral) in zeolites
Ti	ti4c	Titanium (Octahedral) to be used with oy
Ti	titd	Titanium (Tetrahedral) in zeolites
Li	li+	Lithium ion in zeolites
Li	lic+	Lithium ion to be used with oy in Clays
Li	lioh	Lithium ion in water to be used with o*
Na	na+	Sodium ion in zeolites
Na	nac+	Sodium ion in Clays
Na	naoh	Sodium ion in water to be used with o*
K	k+	Potassium ion in zeolites
K	koh	Potassium ion in water to be used with o*
Rb	rb+	Rubidium ion in zeolites
Cs	cs+	Cesium ion in zeolites
N	nh4+	United atom type for ammonium ion to be used with oy
Mg	mg2+	Magnesium ion in zeolites
Mg	mg2c	Octahedral Magnesium ion in Clays
Mn	mn4c	Manganese (IV) ion to be used with oy in Clays
Mn	mn3c	Manganese (III) ion to be used with oy in Clays
Co	co2c	Cobalt (II) ion to be used with oy in Clays
Ni	ni2c	Nickel (II) ion to be used with oy in Clays
Ca	ca2+	Calcium ion in zeolites
Ca	ca2c	Calcium ion to be used with oy in Clays
Sr	sr2c	Strontium ion to be used with oy in Clays
Ba	ba2+	Barium ion in zeolites
Cu	cu2+	Copper(II) ion in zeolites
Fe	fe2c	Octahedral Fe(II) ion in clays
F	f-	Fluoride ion in zeolites
Be	beoh	Beryllium (II) in water to be used with o*
F	foh	Fluoride ion in water to be used with o*
Cl	cl-	Chloride ion in zeolites
Cl	cloh	Chloride ion in water to be used with o*
Cl	cly-	Chloride ion to be used with oy in Clays
Br	br-	Bromide ion in zeolites
I	i-	Iodide ion in zeolites
S	so4	Sulfur in sulphate ion to be used with oz
S	so4y	Sulfur in sulphate ion to be used with oy in Clays
H	hocl	Hydrogen in hydroxyl group in Clays
Pd	pd2+	Palladium(II)
V	vy	Tetrahedral Vanadium to be used with oy
Al	al	Aluminium metal
Na	Na	Sodium metal
Pt	Pt	Platinum metal
Pd	Pd	Palladium metal
Au	Au	Gold metal
Ag	Ag	Silver metal

Continued on next page

Table 5 – continued from previous page

Sn	Sn	Tin metal
K	K	Potassium metal
Li	Li	Lithium metal
Mo	Mo	Molybdenum metal
Fe	Fe	Iron metal
W	W	Tungsten metal
Ni	Ni	Nickel metal
Cr	Cr	Chromium metal
Cu	Cu	Copper metal
Pb	Pb	Lead metal

Nacl.fr

This forcefield provides an illustration of the incorporation of a general inorganic forcefield description in the *MedeA* environment framework.

Na	Na1+	sodium atom
Cl	Cl1-	chlorine atom

Clayff.frc

Also applies to clayff-dioctahedral.frc and clayff-trioctahedral.frc.

H	h*	water hydrogen
H	ho	H hydroxyl hydrogen
O	o*	water oxygen
O	oh	hydroxyl oxygen
O	ob	Basal bridging oxygen
O	oa	Apical bridging oxygen
Si	st	Silicon in SiO2
Al	ao	Aluminium in the octahedral sheet
Al	at	Aluminium in Zeolites
Mg	mgo	Magnesium in the octahedral sheet
Ca	cao	Calcium in the octahedral sheet
Fe	feo	iron in the octahedral sheet
Li	lio	Lithium in the octahedral sheet
O	obss	bridging oxygen with double substitution
O	obts	bridging oxygen with tetrahedral substitution
O	obos	bridging oxygen with octahedral substitution
O	ohs	hydroxyl oxygen with substitution
Ca	cah	hydroxide calcium
Mg	mgh	hydroxide magnesium
Na	Na	Sodium ion
K	K	Potassium ion
Cs	Cs	Cs+ ion
Ca	Ca	Ca2+ ion
Ba	Ba	Ba2+ ion
Cl	Cl	Cl- ion

AlO_eam_coul.frc TaO_eam_coul.frc CeThUNpPuAmCmO_eam_coul.frc

These forcefields are known as the Streitz-Mintmire or charge-transfer ionic (CTIP) potentials [20] which combine EAM and Coulomb (charges described via Slater type orbitals instead of point charges) forcefields along with variable charge equilibration.

AlO_eam_coul.frc

Al	Al	
O1	O1	

TaO_eam_coul.frc

Ta	Ta	
O2	O2	

CeThUNpPuAmCmO_eam_coul.frc

Ce	Ce	
Th	Th	
U	U	
Np	Np	
Pu	Pu	
Am	Am	
Cm	Cm	
O	O	

comb3.frc Si-O_JCP2016-comb3.frc

The 3rd generation charge-optimized many-body (COMB3) [21] forcefields are improvements over the previous generations of COMB forcefields. COMB3 contains an advanced bond order term for describing complex chemical reactions (bond breaking and formation), Coulomb with charge density described with Slater-type orbitals, and variable charge equilibration (atomic charges automatically assigned based on atomic surroundings).

[20] F. H. Streitz and J. W. Mintmire, “Electrostatic potentials for metal-oxide surfaces and interfaces” Phys. Rev. B 50, 11996
[21] T. Liang, T.-R. Shan, Y.-T. Cheng, B. D. Devine, M. Noordhoek, Y. Li, Z. Lu, S. R. Phillpot, and S. B. Sinnott, Mat. Sci. & Eng: R 74, 255-279 (2013).

comb3.frc

Ti	Ti	Titanium
H	H	Hydrogen
C	C	Carbon
N	N	Nitrogen
O	O	Oxygen
Cu	Cu	Copper
Zn	Zn	Zinc
Zr	Zr	Zirconium
Si	Si	Silicon
Ti	Ti	Titanium
Al	Al	Aluminum
Ni	Ni	Nickel
Mo	Mo	Molybdenum
S	S	Sulfur
Pt	Pt	Platinum
Au	Au	Gold

Si-O_JCP2016-comb3.frc

O	O	Oxygen
Si	Si	Silicon

3.3 Semiconductors

Forcefields for semiconductor materials. These forcefields don't require bonds.

StillingerWeber.frc ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc

Stilllinger-Weber forcefields that allow for the simulation of various crystalline and amorphous solids. This forcefield uses an explicit angular term to assess nearest neighbor coordination (to include three-body forces) based on the local environment of simulated atoms [22].

StillingerWeber.frc

Cd	Cd	cadmium
Ga	Ga	gallium
N	N	nitrogen
Si	Si	silicon
Te	Te	tellurium

[22] Frank H Stillinger and Thomas A Weber, "Computer Simulation of Local Order in Condensed Phases of Silicon," Physical Review B 31, no. 8 (1985): 5262-5271; A. Bò rò and A. Serra, "On the Atomic Structures, Mobility and Interactions of Extended Defects in GaN: Dislocations, Tilt and Twin Boundaries," Philosophical Magazine 86, no. 15 (2006): 2159-2192.

ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc

Cd	Cd	cadmium
Zn	Zn	zinc
Te	Te	tellurium
Se	Se	selenium
Hg	Hg	mercury
S	S	sulfur

Tersoff.frc SiO2-Si_Munetoh_2007_Tersoff.frc

Tersoff forcefields that allow for the simulation of various crystalline and amorphous solids. This forcefield uses a bond order term to assess nearest neighbor coordination (to include three-body forces) based on the local environment of simulated atoms. [23]

Tersoff.frc

C	C	carbon
Ga	Ga	gallium
Ge	Ge	germanium
N	N	nitrogen
Si	Si	silicon, final parameters
Si	Si(B)	silicon, original parameters
Si	Si(C)	silicon, second set of parameters
O	O	oxygen atom

SiO2-Si_Munetoh_2007_Tersoff.frc

Si	Si	silicon, final parameters
O	O	oxygen atom

REBO.frc

1st generation reactive bond order (REBO) [24] forcefield closely related to Tersoff forcefields. It allows for simulations of Si with Cl, with Ar described via Moliere forcefield.

Si	Si	silicon
Cl	Cl	chlorine
Ar	Ar	argon

[23] J Tersoff, "New Empirical Approach for the Structure and Energy of Covalent Systems," Physical Review B 37, no. 12 (1988): 6991-7000; J Tersoff, "Empirical Interatomic Potential for Silicon with Improved Elastic Properties," Physical Review B 38, no. 14 (1988): 9902-9905; J Tersoff, "Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems," Physical Review B 39, no. 8 (1989): 5566-5568; J Tersoff, "Erratum: Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems," Physical Review B 41, no. 5 (1990): 3248-3248; "Modelling of Compound Semiconductors: Analytical Bond-Order Potential for Gallium, Nitrogen and Gallium Nitride," Journal of Physics: Condensed Matter 15, no. 32 (2003): 5649.

[24] D. W. Brenner Phys. Rev. B 42, 9458 (1990); D. Humbird and D. B. Graves, J. Chem. Phys. 120, 2405 (2004)

3.4 Metallic

The forcefields in this section don't require bonds during atom type assignment and allow to study of metallic systems using the EAM (embedded atom model) description pioneered by Mike Baskes and others.

As noted above, the variability in local coordination inherent in inorganic systems (as opposed to organic systems) dictates that the creation of transferable forcefield descriptions is challenging for such systems. Hence, for each of the inorganic and metallic forcefield descriptions we recommend that the original references are consulted in order to assess the applicability of these descriptions to a particular system.

Zhou_2004.frc

This forcefield provides support for the following set of atoms and alloys composed of mixtures of these atoms. Zhou [25], with additions from Francis [26]

Ag	Ag	silver
Al	Al	aluminum
Au	Au	gold
Co	Co	cobalt
Cu	Cu	copper
Fe	Fe	iron
Mg	Mg	magnesium
Mo	Mo	molybdenum
Ni	Ni	nickel
Pb	Pb	lead
Pd	Pd	palladium
Pt	Pt	platinum
Ta	Ta	tantalum
Ti	Ti	titanium
W	W	tungsten
Zr	Zr	zirconium

EAM_Adams.frc

Li, Siegel, Adams, and Liu: [27]

Al	Al	aluminum
Au	Au	gold
Cu	Cu	copper
Ni	Ni	nickel
Pd	Pd	palladium
Pt	Pt	platinum
Ta	Ta	tantalum

[25] X Zhou, R Johnson, and H Wadley, "Misfit-Energy-Increasing Dislocations in Vapor-Deposited CoFe/NiFe Multilayers," Physical Review B 69, no. 14 (April 2004).
[26] M F Francis, M N Neurock, X W Zhou, J J Quan, H N G Wadley, et al., "Atomic Assembly of Cu/Ta Multilayers: Surface Roughness, Grain Structure, Misfit Dislocations, and Amorphization," Journal of Applied Physics 104, no. 3 (2008): 034310.
[27] Youhong Li, Donald J Siegel, James Adams, and Xiang-Yang Liu, "Embedded-Atom-Method Tantalum Potential Developed by the Force-Matching Method," Physical Review B 67, no. 12 (2003).

Ni_EAM.frc

Mishin [28] , Ackland [29]

Ni	Ni	Nickel

ZrH_v4.frc

Mendelev [30]

H	H	hydrogen
Zr	Zr	zirconium

md-eam.frc

Updated pair interaction function

Zr	Zr	zirconium
Sn	Sn	tin
Cu	Cu	copper

FeNiCr_Bonny_2011.frc

EAM forcefield for alloys containing Fe, Ni, and Cr [31]

Fe	Fe	iron
Ni	Ni	nickel
Cr	Cr	chromium

AlCo_Mishin_2013.frc AlNi_Mishin_2009.frc AlTi_Mishin_2003.frc AlCu_Cai_1996.frc AlMg_Adams_1997.frc

EAM forcefields (eam/alloy format) for alloys containing Al/Co [32], Al/Ni [33], Al/Ti [34], Al/Cu [35], and Al/Mg [36].

[28] Yuri Mishin and Diana Farkas, “Atomistic Simulation of Point Defects and Diffusion in B2 NiAl Part1: Point Defect Energetics,” Philosophical Magazine A 75, no. 1 (1997): 169-185; Yuri Mishin and Diana Farkas, “Atomistic Simulation of Point Defects and Diffusion in B2 NiAl Part2: Diffusion Mechanisms,” Philosophical Magazine A 75, no. 1 (1997): 187-199.
[29] G J Ackland, G Tichy, V Vitek, and M W Finnis, “Simple N-Body Potentials for the Noble Metals and Nickel,” Philosophical Magazine A 56, no. 6 (December 1987): 735-756.
[30] M I Mendelev and G J Ackland, “Development of an Interatomic Potential for the Simulation of Phase Transformations in Zirconium,” Philosophical Magazine A 87, no. 5 (May 2007): 349-359.
[31] G. Bonny, D. Terentyev, R.C. Pasianot, S. Poncò , and A. Bakaev, “Interatomic potential to study plasticity in stainless steels: the FeNiCr model alloy.” Modelling and simulation in materials science and engineering, 19, 085008 (2011)
[32] Purja Pun, G. P., Yamakov, V., and Mishin, Y. (2015). Interatomic potential for the ternary Ni-Al-Co system and application to atomistic modeling of the B2-L1 0 martensitic transformation. Modelling Simul. Mater. Sci. Eng., 23(6), 065006
[33] G.P. Purja Pun and Y. Mishin, “Development of an interatomic potential for the Ni-Al system,” Phil. Mag. 89, 3245 (2009).
[34] R.R. Zope and Y. Mishin, “Interatomic potentials for atomistic simulations of the Ti-Al system,” Phys. Rev. B 68, 024102 (2003)
[35] X.-Y. Liu, C.-L. Liu, and L.J. Borucki, “A new investigation of copper’s role in enhancing Al-Cu interconnect electromigration resistance from an atomistic view,” Acta Mat. 47, 3227-3231 (1999)
[36] X.-Y. Liu, P.P. Ohotnicky, J.B. Adams, C. Lane Rohrer, R.W. Hyland, Jr., “Anisotropic surface segregation in Al-Mg alloys,” Surf. Sci. 373, 357-370 (1997)

Al	Al	aluminum
Co	Co	cobalt
Ni	Ni	nickel
Ti	Ti	titanium
Cu	Cu	copper
Mg	Mg	magnesium

AlSiMgCuFe_MEAM.frc AuSi_MEAM.frc CH_MEAM.frc Cu_MEAM.frc FeC_MEAM.frc FeTiC_MEAM.frc Ni_MEAM.frc SiC_MEAM.frc W_MEAM.frc..... MEAM.frc

Modified EAM (MEAM) forcefields include an additional angular term for a more accurate description of metals and alloys, including Al/Si/Mg/Cu/Fe [37], Au/Si [38], C/H [39], Fe/C [40], Fe/Ti/C [41], W [42], and Si/C, Cu, and Ni from the LAMMPS website. A generic MEAM.frc is also included to be used with custom MEAM forcefield parameter sets.

AlSiMgCuFe_MEAM.frc

Al	Al	aluminum
Si	Si	silicon
Mg	Mg	magnesium
Cu	Cu	copper
Fe	Fe	iron

AuSi_MEAM.frc

Au	Au	gold
Si	Si	silver

CH_MEAM.frc

C	C	carbon
H	H	hydrogen

FeC_MEAM.frc

Fe	Fe	iron
C	C	carbon

[37] B. Jelinek, S. Groh, M. Horstemeyer, J. Houze, S.G. Kim, G.J. Wagner, A. Moitra, and M.I. Baskes, "Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys," Phys. Rev. B 85, 245102 (2012)
[38] J. Godet, C. Furgeaud, L. Pizzagalli, M. Demkowicz, "Uniform tensile elongation in Au-Si core-shell nanowires", Extreme Mechanics Letters (2016)
[39] S. Nouranian, M.A. Tschopp, S.R. Gwaltney, M.I. Baskes, and M.F. Horstemeyer, "An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method," Physical Chemistry Chemical Physics 16, 6233 (2014).
[40] L.S.I. Liyanage, S.-G. Kim, J. Houze, S. Kim, M.A. Tschopp, M.I. Baskes, and M.F. Horstemeyer, "Structural, elastic, and thermal properties of cementite (Fe13C) calculated using a modified embedded atom method," Phys. Rev. B 89, 094102 (2014)
[41] Kim, H.-K., Jung, W.-S., and Lee, B.-J. (2009). Modified embedded-atom method interatomic potentials for the Fe-Ti-C and Fe-Ti-N ternary systems. Acta Materialia, 57(11), 3140-3147.
[42] Lee, Baskes, Kim, Cho. Phys. Rev. B, 64, 184102 (2001)

FeTiC_MEAM.frc

Fe	Fe	iron
Ti	Ti	titanium
C	C	carbon

W_MEAM.frc

W	W	tungsten

SiC_MEAM.frc

Si	Si	silicon
C	C	carbon

Ni_MEAM.frc

Ni	Ni	nickel

Cu_MEAM.frc

Cu	Cu	copper

3.5 NIST Interatomic Potentials Repository

Detailed descriptions are shown in the file selection dialog. These files are distributed with consent from Chandler A. Becker, the reviewer of this repository [43], http://www.ctcms.nist.gov/potentials.

3.6 ReaxFF Forcefields

Reactive Forcefields (ReaxFF) [44] is a family of well-established forcefields that simulate complex chemical reactions and charge transfer. It includes advanced bond terms over valence terms, shielded Coulomb, and variable charge equilibration.

AlLiSiO.frc

ReaxFF forcefield for Li in Si, SiO_x nanowires [57]

[43] Chandler A Becker, Francesca Tavazza, Zachary T Trautt, and Robert A Buarque de Macedo, "Considerations for Choosing and Using Force Fields and Interatomic Potentials in Materials Science and Engineering," *Current Opinion in Solid State and Materials Science* 17 (December 2013): 277-283.

[44] A.C.T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard, ReaxFF: A reactive force field for hydrocarbons, Journal of Physical Chemistry A 105, 9396-9409 (2001); Chenoweth, A.C.T. van Duin, and W.A. Goddard, ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation, Journal of Physical Chemistry A 112, 1040-1053 (2008)

[57] "Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF" Ostadhossein, Alireza and Cubuk, Ekin D. and Tritsaris, Georgios A. and Kaxiras, Efthimios and Zhang, Sulin and van Duin, Adri C. T. Phys. Chem. Chem. Phys., 2015,17, 3832-3840

Al	Al	aluminum
Li	Li	lithium
Si	Si	silicon
O	O	oxygen
H	H	hydrogen

AuOH.frc

ReaxFF forcefield for Au, AuO_x and water [45] from LAMMPS potentials repository

Au	Au	gold
O	O	oxygen
H	H	hydrogen

BaZrYOH.frc

ReaxFF forcefield for H diffusion in Y-Doped $BaZrO_3$ [58]

Ba	Ba	barium
C	C	carbon
H	H	hydrogen
O	O	oxygen
N	N	nitrogen
Y	Y	yttrium
Zr	Zr	zirconium

Warning: The following bond interactions are not included in this frc file:

- C - Zr
- C - Y
- C - Ba
- N - Zr
- N - Y
- N - Ba

CHO.frc

The well-established ReaxFF forcefield for combustion [46] simulations from LAMMPS potentials repository

C	C	carbon
O	O	oxygen
H	H	hydrogen

[45] Keith, J. A. et al. Phys Rev B 2010, 81, 235404
[58] "ReaxFF Reactive Force Field for the Y-Doped BaZrO3 Proton Conductor with Applications to Diffusion Rates for Multigranular Systems" Adri C. T. van Duin, Boris V. Merinov, Sang Soo Han, Claudio O. Dorso, and William A. Goddard III J. Phys. Chem. A 2008, 112, 11414–11422
[46] Chenoweth, A.C.T. van Duin, and W.A. Goddard, ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation, Journal of Physical Chemistry A 112, 1040-1053 (2008)

CHON.frc

The well-established ReaxFF forcefield for nitramines (RDX/HMX/TATB/PETN) [47] from LAMMPS potentials repository

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen

CHONSFPtClNi.frc

ReaxFF forcefield for fluorinated graphene [59]

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
F	F	fluorine
Cl	Cl	chlorine
Ni	Ni	nickel

Warning: The following bond interactions are not included in this frc file:

- N - Ni
- S - Cl
- S - Ni
- F - Cl
- F - Ni
- Cl - Ni

CHONSMoNi.frc

ReaxFF forcefield for combustion of coal char [60]

#elements C H O S Mo Ni N

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Mo	Mo	molybdenum
Ni	Ni	nickel

Warning: The following bond interactions are not included in this frc file:

[47] Strachan et al, Phys Rev Lett, 91, 098301 (2003)
[59] Singh, Phys Rev AB 87, 104114 (2013)
[60] "Combustion of an Illinois No. 6 coal char simulated using an atomistic char representation and the ReaxFF reactive force field" Fidel Castro-Marcano, Amar M. Kamat, Michael F. Russo Jr., Adri C.T. van Duin, Jonathan P. Mathews Combustion and Flame 159 (2012) 1272–1285

- S - Ni
- Mo - N
- Ni - N

CeO.frc

Reactive force field for CeO2 [61]

Ce	Ce	cerium
O	O	oxygen

CuClOH.frc

ReaxFF forcefield for aqueous chloride and copper chloride [62]

Cu	Cu	copper
O	O	oxygen
H	H	hydrogen
Cl	Cl	chlorine

CuOH.frc

ReaxFF forcefield for Cu, copper oxide, copper hydroxide and water interactions [63]

Cu	Cu	copper
C	C	carbon
O	O	oxygen
H	H	hydrogen

Warning: The following bond interactions are not included in this frc file:

- C - Cu

FeCrOS.frc

ReaxFF forcefield for Cr2O3 catalyst, butane, and Fe/Cr/O/S compounds [64]

[61] Broqvist et al. J. Phys. Chem. C 119(24), 13598-13609 (2015).
[62] Cu/O/H force field; van Duin et al., 2010 Cl parameters from Rahaman et al, 2010
[63] "Development and Validation of a ReaxFF Reactive Force Field for Cu Cation/Water Interactions and Copper Metal/Metal Oxide/Metal Hydroxide Condensed Phases" Adri C. T. van Duin, Vyacheslav S. Bryantsev, Mamadou S. Diallo, William A. Goddard, Obaidur Rahaman, Douglas J. Doren, David mand, and Kersti Hermansson J. Phys. Chem. A 2010, 114, 9507–9514
[64] "Development of a ReaxFF reactive force field for Fe/Cr/O/S and application to oxidation of butane over a pyrite-covered Cr2O3 catalyst." Shin, Y.K., Kwak, H., Vasenkov, A., Sengupta, D. and van Duin, A.C.T., ACS Catalysis 5, 7226-7236.

C	C	carbon
O	O	oxygen
H	H	hydrogen
Cr	Cr	chromium
Cu	Cu	copper
Al	Al	aluminum
Fe	Fe	iron
Ni	Ni	nickel
S	S	sulfur

Warning: The following bond interactions are not included in this frc file:

- C - Cu
- Fe - Cu
- Al - Cu
- Ni - Cu
- Ni - Cr
- Cu - S
- Cu - Cr

FeOCH.frc

ReaxFF forcefield for Fe/O/H (Fe, FeOx and water) with Cl [65]

C	C	carbon
O	O	oxygen
H	H	hydrogen
Fe	Fe	iron
Cl	Cl	chlorine

Warning: The following bond interactions are not included in this frc file:

- C - Cl

HONB.frc

ReaxFF forcefield for Ammonia Borane [48] from LAMMPS potentials repository

B	B	boron
O	O	oxygen
H	H	hydrogen
N	N	nitrogen

LiC.frc

ReaxFF forcefield for Li/C [66]

[65] "Development of a Reactive Force Field for Iron-Oxyhydroxide Systems" Masoud Aryanpour, Adri C. T. van Duin, and James D. Kubicki, J. Phys. Chem. A 114, 21, 6298-6307
[48] Weismiller, van Duin, Lee, Yetter, J Phys Chem A, 114, 5485-5492 (2010)
[66] "Reactive Force Field Study of Li/C Systems for Electrical Energy Storage" Muralikrishna Raju, P. Ganesh, R. C. Kent, and Adri C. T. van Duin, J. Chem. Theory Comput. 11, 5, 2156-2166

C	C	carbon
O	O	oxygen
H	H	hydrogen
Li	Li	lithium

Warning: The following bond interactions are not included in this frc file:

- O - C

LiMnO.frc

ReaxFF forcefield for LiMn2O4 and C/H/O/F [67]

C	C	carbon
O	O	oxygen
H	H	hydrogen
Li	Li	lithium
Mn	Mn	manganese
F	F	fluorine
P	P	phosphorus
Ni	Ni	nickel
Al	Al	aluminum

Warning: The following bond interactions are not included in this frc file:

- C - Ni
- C - Al
- H - Ni
- H - Al
- O - Ni
- O - Al
- Mn - Ni
- Mn - Al
- Li - Ni
- Li - Al
- F - Ni
- F - Al
- P - Ni
- P - Al
- Ni - Ni
- Ni - Al
- Al - Al

LiPFCHO.frc

ReaxFF forcefield for LiPF6/poly(propylene glycol) diacrylate solid electrolyte [68]

[67] "Chemical composition and formation mechanisms in the cathode-electrolyte interface layer of lithium manganese oxide batteries from reactive force field (ReaxFF) based molecular dynamics" Reddivari, S., Lastoskie, C., Wu, R. et al. Front. Energy (2017) 11: 365. https://doi.org/10.1007/s11708-017-0500-8

[68] "Salt concentration effects on mechanical properties of LiPF6/poly(propylene glycol) diacrylate solid electrolyte: Insights from reactive molecular dynamics simulations" Verners, O., Thijsse, B. J., van Duin, A. C. T., & Simone, A. Electrochimica Acta, 221, 115-123. DOI: 10.1016/j.electacta.2016.10.035

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Li	Li	lithium
Mo	Mo	molybdenum
F	F	fluorine
P	P	phosphorus
Ni	Ni	nickel
B	B	boron

Warning: The following bond interactions are not included in this frc file:

- S - F
- S - P
- S - N
- Mo - Li
- Mo - B
- Mo - F
- Mo - P
- Mo - N
- Ni - Li
- Ni - B
- Ni - F
- Ni - P
- Ni - N
- Li - B
- B - P
- B - N
- P - N

LiSCFO.frc

ReaxFF forcefield for LiS and Li/SWCNT with Teflon [69]

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Li	Li	lithium
Mo	Mo	molybdenum
F	F	fluorine
P	P	phosphorus
Ni	Ni	nickel
B	B	boron

Warning: The following bond interactions are not included in this frc file:

[69] "ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries" Md Mahbubul Islam, Vyacheslav S. Bryantsev, and Adri C. T. van Duin Journal of The Electrochemical Society, 161 (8) E3009-E3014 (2014)

- S - F
- S - P
- S - N
- Mo - Li
- Mo - B
- Mo - F
- Mo - P
- Mo - N
- Ni - Li
- Ni - B
- Ni - F
- Ni - P
- Ni - N
- Li - B
- B - P
- B - N
- P - N

LiSiCHOF.frc

ReaxFF forcefield for Si-based anode in LiB; contains parameters for C/H/O, Li2CO3, Li2O, and LiF [70]

C	C	carbon
O	O	oxygen
H	H	hydrogen
Si	Si	silicon
Li	Li	lithium
F	F	fluorine

MoS2.frc

ReaxFF forcefield for MoS2 [71]

C	C	carbon
O	O	oxygen
H	H	hydrogen
S	S	sulfur
Mo	Mo	molybdenum
Ni	Ni	nickel

Warning: The following bond interactions are not included in this frc file:

- S - Ni

[70] “Simulation Protocol for Prediction of a Solid-Electrolyte Interphase on the Silicon-based Anodes of a Lithium-Ion Battery: ReaxFF Reactive Force Field” Kang-Seop Yun, Sung Jin Pai, Byung Chul Yeo, Kwang-Ryeol Lee, Sun-Jae Kim, and Sang Soo Han, J. Phys. Chem. Lett. 8, 13, 2812-2818

[71] “ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS2)” Alireza Ostadhossein, Ali Rahnamoun, Yuanxi Wang, Peng Zhao, Sulin Zhang, Vincent H. Crespi, and Adri C. T. van Duin J. Phys. Chem. Lett. 2017, 8, 631-640

PdOCH.frc

ReaxFF forcefield for Pd nanoparticle catalysis with C/H/O [72]

C	C	carbon
O	O	oxygen
H	H	hydrogen
Pd	Pd	palladium

PtCH.frc

ReaxFF forcefield for Pt interacting with hydrocarbons and carbon platelets [73]

C	C	carbon
H	H	hydrogen
Pt	Pt	platinum

PtNiCHO.frc

ReaxFF forcefield for Pt-Ni Alloy Catalyst with C/H/O [74]

C	C	carbon
O	O	oxygen
H	H	hydrogen
Ni	Ni	nickel
Pt	Pt	platinum

PtO.frc

ReaxFF forcefield for Pt/O [75]

Pt	Pt	platinum
O	O	oxygen

TiOH.frc

ReaxFF forcefield for TiO2 and water interactions. Part of water branch [76]

[72] "Determining in situ phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential" Thomas P. Senftle, Adri C.T. van Duin, Michael J. Janik Catalysis Communications 52 (2014) 72-77

[73] "Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets" C.F. Sanz-Navarro, P.-O. Astrand, D. Chen, M. Eonning, A.C.T. van Duin, T. Jacob, and W.A. Goddard III J. Phys. Chem. A, 2008, 112 (7), pp 1392-1402

[74] "Development of a ReaxFF Reactive Force Field for the Pt-Ni Alloy Catalyst" Yun Kyung Shin, Lili Gai, Sumathy Raman, and Adri C. T. van Duin J. Phys. Chem. A 2016, 120, 8044-8055

[75] "Development of a ReaxFF potential for Pt-O systems describing the energetics and dynamics of Pt-oxide formation" Fantauzzi D, Bandlow J, Sabo L, Mueller JE, van Duin AC, Jacob T. Phys Chem Chem Phys. 2014 Nov 14;16(42):23118-33. doi: 10.1039/c4cp03111c.

[76] "Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems" Sung-Yup Kim, Nitin Kumar, Petter Persson, Jorge Sofo, Adri C. T. van Duin, and James D. Kubicki Langmuir, 2013, 29 (25), pp 7838-7846

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Ti	Ti	titanium
Mg	Mg	magnesium
F	F	fluorine
P	P	phosphorus
Na	Na	sodium
Cl	Cl	chlorine

Warning: The following bond interactions are not included in this frc file:

- C - Mg
- S - Mg
- S - P
- Mg - F
- P - F
- Na - F
- Ti - F
- Cl - F

VCHO.frc

ReaxFF forcefield for V, VOx and water [49] from LAMMPS potentials repository

V	V	vanadium
O	O	oxygen
H	H	hydrogen
C	C	carbon

ZnOH.frc

ReaxFF forcefield for Zn, ZnOx and water [50] from LAMMPS potentials repository

Zn	Zn	zinc
O	O	oxygen
H	H	hydrogen

clay_zeolite_water.frc

ReaxFF forcefield for Water in Smectite Clay-Zeolite Composites [77]

[49] Chenoweth et al, J Phys Chem C, 112, 14645-14654 (2008)
[50] mand, van Duin, Spangberg, Goddard and Hermansson, Surf Sci, 604, 741-752 (2010)
[77] “Dynamics of Confined Reactive Water in Smectite Clay-Zeolite Composites” Michael C. Pitman, and Adri C. T. van Duin, J. Am. Chem. Soc. 2012, 134, 3042-3053

C	C	carbon
O	O	oxygen
H	H	hydrogen
Fe	Fe	iron
Cl	Cl	chlorine
Si	Si	silicon
Al	Al	aluminum
Ca	Ca	calcium

Warning: The following bond interactions are not included in this frc file:

- C - Cl
- C - Ca
- Fe - Si
- Fe - Al
- Fe - Ca
- Cl - Si
- Cl - Al
- Cl - Ca

epoxy.frc

ReaxFF forcefield for describing the reactive crosslinking of polymers [78]

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Mg	Mg	magnesium
P	p	phosphorus
Na	Na	sodium
Cu	Cu	copper
Cl	Cl	chlorine

Warning: The following bond interactions are not included in this frc file:

- C - Mg
- S - Mg
- S - P
- S - Na
- S - Cu
- S - Cl
- Mg - Cu
- Mg - Cl
- P - Cu
- P - Cl
- Na - Cu
- Na - Cl

[78] "Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers" Aniruddh Vashisth, Chowdhury Ashraf, Weiwei Zhang, Charles E. Bakis, and Adri C. T. van Duin J. Phys. Chem. A 2018, 122, 6633-6642

protein_water.frc

ReaxFF forcefield for biomolecules in solution [79]

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
Mg	Mg	magnesium
P	p	phosphorus
Na	Na	sodium
Cu	Cu	copper
Cl	Cl	chlorine

Warning: The following bond interactions are not included in this frc file:

- C - Mg
- S - Mg
- S - P
- S - Na
- S - Cu
- S - Cl
- Mg - Cu
- Mg - Cl
- P - Cu
- P - Cl
- Na - Cu
- Na - Cl

3.7 Mesoscale Forcefields

Mesoscale forcefields are forcefields for simulations on time and length scales larger than the atomistic scale. In mesoscale simulations multiple atoms are collectively described as beads. The forcefields contain parameters for the interaction of these beads. How many atoms are represented by a bead varies between mesoscale forcefields. It can be just three or four heavy atoms, an entire functional group or even a monomer for polymer simulations.

With mesoscale forcefields time steps in dynamics simulations can be extended to ten or twenty femtoseconds. Therefore, it becomes possible to run simulations for microseconds and on systems with extents close to micrometers.

Martini.frc

Mesoscale forcefield for polymers and basic organic molecules [53]. The Martini forcefield was originally designed for the simulation of biomolecules. It has been parameterized in a systematic way, combining top-down and bottom-up strategies. The forcefield combines on average four heavy atoms and the attached hydrogens in one bead. Extensions to sugars, polymers, surfactants and nanoparticles are available. More information can be found on the Martini home page [55].

[79] "Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field" Susanna Monti, Alessandro Corozzi, Peter Fristrup, Kaushik L. Joshi, Yun Kyung Shin, Peter Oelschlaeger, Adri C. T. van Duin, and Vincenzo Barone Phys. Chem. Chem. Phys., 2013, 15, 15062

[53] Marrink, S. J., Risselada, H. J., Yefimov, S., Tieleman, D. P. and de Vries, A. H., J. Phys. Chem. B, 111, 7812-7824 (2007)

[55] http://cgmartini.nl/index.php/martini

C1	C1	Apolar-Degree of polarity: 1 (low)
C2	C2	Apolar-Degree of polarity: 2
C3	C3	Apolar-Degree of polarity: 3
C4	C4	Apolar-Degree of polarity: 4
C5	C5	Apolar-Degree of polarity: 5 (high)
N	N	Nonpolar-Hydrogen bonding capabilities: donor/acceptor
N0	N0	Nonpolar-Hydrogen bonding capabilities: none
Na	Na	Nonpolar-Hydrogen bonding capabilities: acceptor
Nd	Nd	Nonpolar-Hydrogen bonding capabilities: donor
P1	P1	Polar-Degree of polarity: 1 (low)
P2	P2	Polar-Degree of polarity: 2
P3	P3	Polar-Degree of polarity: 3
P4	P4	Polar-Degree of polarity: 4
P5	P5	Polar-Degree of polarity: 5 (high)
Q	Q	Charged-Hydrogen bonding capabilities: donor/acceptor
Q0	Q0	Charged-Hydrogen bonding capabilities: none
Qa	Qa	Charged-Hydrogen bonding capabilities: acceptor
Qd	Qd	Charged-Hydrogen bonding capabilities: donor
SC1	SC1	Apolar for ring structures-Degree of polarity: 1 (low)
SC2	SC2	Apolar for ring structures-Degree of polarity: 2
SC3	SC3	Apolar for ring structures-Degree of polarity: 3
SC4	SC4	Apolar for ring structures-Degree of polarity: 4
SC5	SC5	Apolar for ring structures-Degree of polarity: 5 (high)
SN	SN	Nonpolar for ring structures-Hydrogen bonding capabilities: donor/acceptor
SN0	N0	Nonpolar for ring structures-Hydrogen bonding capabilities: none
SNa	SNa	Nonpolar for ring structures-Hydrogen bonding capabilities: acceptor
SNd	SNd	Nonpolar for ring structures-Hydrogen bonding capabilities: donor
SP1	SP1	Polar for ring structures-Degree of polarity: 1 (low)
SP2	SP2	Polar for ring structures-Degree of polarity: 2
SP3	SP3	Polar for ring structures-Degree of polarity: 3
SP4	SP4	Polar for ring structures-Degree of polarity: 4
SP5	SP5	Polar for ring structures-Degree of polarity: 5 (high)
SQ	SQ	Charged for ring structures-Hydrogen bonding capabilities: donor/acceptor
SQ0	SQ0	Charged for ring structures-Hydrogen bonding capabilities: none
SQa	SQa	Charged for ring structures-Hydrogen bonding capabilities: acceptor
SQd	SQd	Charged for ring structures-Hydrogen bonding capabilities: donor

Martini-3.0.frc

The Martini 3.0 mesoscale forcefield is a reparameterization of the Martini model to address certain deficiencies of the original parameterization [54]. It is used in a wide range of applications in structural biology, biophysics, biomedicine, nanotechnology and materials design. The reparameterization has focused on reducing interactions of molecules which were too strong in the original version resulting in more accurate

[54] "Martini 3: a general purpose force field for coarse-grained molecular dynamics" P. C. T. Souza, R. Alessandri, J. Barnoud, S. Thallmair, I. Faustino, F. Grünewald, I. Patmanidis, H. Abdizadeh, B. M. H. Bruininks, T. A. Wassenaar, P. C. Kroon, J. Melcr, V. Nieto, V. Corradi, H. M. Khan, J. Domański, M. Javanainen, H. Martinez-Seara, N. Reuter, R. B. Best, I. Vattulainen, L. Monticelli, X. Periole, D. P. Tieleman, A. H. de Vries and S. J. Marrink, Nature Methods 18, 382-388 (2021)

simulations. In addition to the mapping of four heavy atoms to one bead in the original forcefield beads for three-to-one (small beads) and two-to-one (tiny beads) mappings have been introduced. Therefore, the number of bead types has increased significantly. More information can be found on the Martini home page [55].

P6	P6	Polar - degree of polarity: 6 (high)
P5	P5	Polar - degree of polarity: 5
P4	P4	Polar - degree of polarity: 4
P3	P3	Polar - degree of polarity: 3
P2	P2	Polar - degree of polarity: 2
P1	P1	Polar - degree of polarity: 1 (low)
N6	N6	Intermediate/non-polar - degree of polarity: 6 (high)
N5	N5	Intermediate/non-polar - degree of polarity: 5
N4	N4	Intermediate/non-polar - degree of polarity: 4
N3	N3	Intermediate/non-polar - degree of polarity: 3
N2	N2	Intermediate/non-polar - degree of polarity: 2
N1	N1	Intermediate/non-polar - degree of polarity: 1 (low)
C6	C6	Apolar - degree of polarity: 6 (high)
C5	C5	Apolar - degree of polarity: 5
C4	C4	Apolar - degree of polarity: 4
C3	C3	Apolar - degree of polarity: 3
C2	C2	Apolar - degree of polarity: 2
C1	C1	Apolar - degree of polarity: 1 (low)
X4	X4	Halo compound - polarity: 4 (high)
X3	X3	Halo compound - polarity: 3
X2	X2	Halo compound - polarity: 2
X1	X1	Halo compound - polarity: 1 (low)
P6d	P6d	Polar - degree of polarity: 6 (high), hydrogen bond donor
P5d	P5d	Polar - degree of polarity: 5, hydrogen bond donor
P4d	P4d	Polar - degree of polarity: 4, hydrogen bond donor
P3d	P3d	Polar - degree of polarity: 3, hydrogen bond donor
P2d	P2d	Polar - degree of polarity: 2, hydrogen bond donor
P1d	P1d	Polar - degree of polarity: 1 (low), hydrogen bond donor
N6d	N6d	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor
N5d	N5d	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor
N4d	N4d	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor
N3d	N3d	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor
N2d	N2d	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor
N1d	N1d	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor
P6a	P6a	Polar - degree of polarity: 6 (high), hydrogen bond acceptor
P5a	P5a	Polar - degree of polarity: 5, hydrogen bond acceptor
P4a	P4a	Polar - degree of polarity: 4, hydrogen bond acceptor
P3a	P3a	Polar - degree of polarity: 3, hydrogen bond acceptor
P2a	P2a	Polar - degree of polarity: 2, hydrogen bond acceptor
P1a	P1a	Polar - degree of polarity: 1 (low), hydrogen bond acceptor
N6a	N6a	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor
N5a	N5a	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor

Continued on next page

Table 7 – continued from previous page

N4a	N4a	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor
N3a	N3a	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor
N2a	N2a	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor
N1a	N1a	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor
C6v	C6v	Apolar - degree of polarity: 6 (high), electron acceptor
C5v	C5v	Apolar - degree of polarity: 5, electron acceptor
C4v	C4v	Apolar - degree of polarity: 4, electron acceptor
C3v	C3v	Apolar - degree of polarity: 3, electron acceptor
C2v	C2v	Apolar - degree of polarity: 2, electron acceptor
C1v	C1v	Apolar - degree of polarity: 1 (low), electron acceptor
X4v	X4v	Halo compound - polarity: 4 (high), electron acceptor
X3v	X3v	Halo compound - polarity: 3, electron acceptor
X2v	X2v	Halo compound - polarity: 2, electron acceptor
X1v	X1v	Halo compound - polarity: 1 (low), electron acceptor
C6e	C6e	Apolar - degree of polarity: 6 (high), electron donor
C5e	C5e	Apolar - degree of polarity: 5, electron donor
C4e	C4e	Apolar - degree of polarity: 4, electron donor
C3e	C3e	Apolar - degree of polarity: 3, electron donor
C2e	C2e	Apolar - degree of polarity: 2, electron donor
C1e	C1e	Apolar - degree of polarity: 1 (low), electron donor
X3e	X3e	Halo compound - polarity: 3, electron donor
X4e	X4e	Halo compound - polarity: 4 (high), electron donor
X2e	X2e	Halo compound - polarity: 2, electron donor
X1e	X1e	Halo compound - polarity: 1 (low), electron donor
D	D	Divalent ion
Q5	Q5	Monovalent ion - hardness: 5 (high)
Q4	Q4	Monovalent ion - hardness: 4
Q3	Q3	Monovalent ion - hardness: 3
Q2	Q2	Monovalent ion - hardness: 2
Q1	Q1	Monovalent ion - hardness: 1 (low)
Q5p	Q5p	Monovalent ion - hardness: 5 (high), hydrogen bond donor
Q4p	Q4p	Monovalent ion - hardness: 4, hydrogen bond donor
Q3p	Q3p	Monovalent ion - hardness: 3, hydrogen bond donor
Q2p	Q2p	Monovalent ion - hardness: 2, hydrogen bond donor
Q1p	Q1p	Monovalent ion - hardness: 1 (low), hydrogen bond donor
Q5n	Q5n	Monovalent ion - hardness: 5 (high), hydrogen bond acceptor
Q4n	Q4n	Monovalent ion - hardness: 4, hydrogen bond acceptor
Q3n	Q3n	Monovalent ion - hardness: 3, hydrogen bond acceptor
Q2n	Q2n	Monovalent ion - hardness: 2, hydrogen bond acceptor
Q1n	Q1n	Monovalent ion - hardness: 1 (low), hydrogen bond acceptor
P6q	P6q	Polar - degree of polarity: 6 (high), partial charge
P5q	P5q	Polar - degree of polarity: 5, partial charge
P4q	P4q	Polar - degree of polarity: 4, partial charge
P3q	P3q	Polar - degree of polarity: 3, partial charge
P2q	P2q	Polar - degree of polarity: 2, partial charge
P1q	P1q	Polar - degree of polarity: 1 (low), partial charge
N6q	N6q	Intermediate/non-polar - degree of polarity: 6 (high), partial charge
N5q	N5q	Intermediate/non-polar - degree of polarity: 5, partial charge
N4q	N4q	Intermediate/non-polar - degree of polarity: 4, partial charge

Continued on next page

Table 7 – continued from previous page

N3q	N3q	Intermediate/non-polar - degree of polarity: 3, partial charge
N2q	N2q	Intermediate/non-polar - degree of polarity: 2, partial charge
N1q	N1q	Intermediate/non-polar - degree of polarity: 1 (low), partial charge
C6q	C6q	Apolar - degree of polarity: 6 (high), partial charge
C5q	C5q	Apolar - degree of polarity: 5, partial charge
C4q	C4q	Apolar - degree of polarity: 4, partial charge
C3q	C3q	Apolar - degree of polarity: 3, partial charge
C2q	C2q	Apolar - degree of polarity: 2, partial charge
C1q	C1q	Apolar - degree of polarity: 1 (low), partial charge
X4q	X4q	Halo compound - polarity: 4 (high), partial charge
X3q	X3q	Halo compound - polarity: 3, partial charge
X2q	X2q	Halo compound - polarity: 2, partial charge
X1q	X1q	Halo compound - polarity: 1 (low), partial charge
P6dq	P6dq	Polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge
P5dq	P5dq	Polar - degree of polarity: 5, hydrogen bond donor, partial charge
P4dq	P4dq	Polar - degree of polarity: 4, hydrogen bond donor, partial charge
P3dq	P3dq	Polar - degree of polarity: 3, hydrogen bond donor, partial charge
P2dq	P2dq	Polar - degree of polarity: 2, hydrogen bond donor, partial charge
P1dq	P1dq	Polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge
N6dq	N6dq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge
N5dq	N5dq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, partial charge
N4dq	N4dq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, partial charge
N3dq	N3dq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, partial charge
N2dq	N2dq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, partial charge
N1dq	N1dq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge
P6aq	P6aq	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge
P5aq	P5aq	Polar - degree of polarity: 5, hydrogen bond acceptor, partial charge
P4aq	P4aq	Polar - degree of polarity: 4, hydrogen bond acceptor, partial charge
P3aq	P3aq	Polar - degree of polarity: 3, hydrogen bond acceptor, partial charge
P2aq	P2aq	Polar - degree of polarity: 2, hydrogen bond acceptor, partial charge
P1aq	P1aq	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge
N6aq	N6aq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge
N5aq	N5aq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, partial charge

Continued on next page

Table 7 – continued from previous page

N4aq	N4aq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, partial charge
N3aq	N3aq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, partial charge
N2aq	N2aq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, partial charge
N1aq	N1aq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge
C6vq	C6vq	Apolar - degree of polarity: 6 (high), partial charge, electron acceptor
C5vq	C5vq	Apolar - degree of polarity: 5, partial charge, electron acceptor
C4vq	C4vq	Apolar - degree of polarity: 4, partial charge, electron acceptor
C3vq	C3vq	Apolar - degree of polarity: 3, partial charge, electron acceptor
C2vq	C2vq	Apolar - degree of polarity: 2, partial charge, electron acceptor
C1vq	C1vq	Apolar - degree of polarity: 1 (low), partial charge, electron acceptor
X4vq	X4vq	Halo compound - polarity: 4 (high), partial charge, electron acceptor
X3vq	X3vq	Halo compound - polarity: 3, partial charge, electron acceptor
X2vq	X2vq	Halo compound - polarity: 2, partial charge, electron acceptor
X1vq	X1vq	Halo compound - polarity: 1 (low), partial charge, electron acceptor
C6eq	C6eq	Apolar - degree of polarity: 6 (high), electron donor, partial charge
C5eq	C5eq	Apolar - degree of polarity: 5, electron donor, partial charge
C4eq	C4eq	Apolar - degree of polarity: 4, electron donor, partial charge
C3eq	C3eq	Apolar - degree of polarity: 3, electron donor, partial charge
C2eq	C2eq	Apolar - degree of polarity: 2, electron donor, partial charge
C1eq	C1eq	Apolar - degree of polarity: 1 (low), electron donor, partial charge
X4eq	X4eq	Halo compound - polarity: 4 (high), electron donor, partial charge
X3eq	X3eq	Halo compound - polarity: 3, electron donor, partial charge
X2eq	X2eq	Halo compound - polarity: 2, electron donor, partial charge
X1eq	X1eq	Halo compound - polarity: 1 (low), electron donor, partial charge
P6h	P6h	Polar - degree of polarity: 6 (high), high self-interaction
P5h	P5h	Polar - degree of polarity: 5, high self-interaction
P4h	P4h	Polar - degree of polarity: 4, high self-interaction
P3h	P3h	Polar - degree of polarity: 3, high self-interaction
P2h	P2h	Polar - degree of polarity: 2, high self-interaction
P1h	P1h	Polar - degree of polarity: 1 (low), high self-interaction
N6h	N6h	Intermediate/non-polar - degree of polarity: 6 (high), high self-interaction
N5h	N5h	Intermediate/non-polar - degree of polarity: 5, high self-interaction
N4h	N4h	Intermediate/non-polar - degree of polarity: 4, high self-interaction
N3h	N3h	Intermediate/non-polar - degree of polarity: 3, high self-interaction
N2h	N2h	Intermediate/non-polar - degree of polarity: 2, high self-interaction
N1h	N1h	Intermediate/non-polar - degree of polarity: 1 (low), high self-interaction
C6h	C6h	Apolar - degree of polarity: 6 (high), high self-interaction

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Table 7 – continued from previous page

C5h	C5h	Apolar - degree of polarity: 5, high self-interaction
C4h	C4h	Apolar - degree of polarity: 4, high self-interaction
C3h	C3h	Apolar - degree of polarity: 3, high self-interaction
C2h	C2h	Apolar - degree of polarity: 2, high self-interaction
C1h	C1h	Apolar - degree of polarity: 1 (low), high self-interaction
X4h	X4h	Halo compound - polarity: 4 (high), high self-interaction
X3h	X3h	Halo compound - polarity: 3, high self-interaction
X2h	X2h	Halo compound - polarity: 2, high self-interaction
X1h	X1h	Halo compound - polarity: 1 (low), high self-interaction
P6dh	P6dh	Polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction
P5dh	P5dh	Polar - degree of polarity: 5, hydrogen bond donor, high self-interaction
P4dh	P4dh	Polar - degree of polarity: 4, hydrogen bond donor, high self-interaction
P3dh	P3dh	Polar - degree of polarity: 3, hydrogen bond donor, high self-interaction
P2dh	P2dh	Polar - degree of polarity: 2, hydrogen bond donor, high self-interaction
P1dh	P1dh	Polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction
N6dh	N6dh	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction
N5dh	N5dh	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, high self-interaction
N4dh	N4dh	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, high self-interaction
N3dh	N3dh	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, high self-interaction
N2dh	N2dh	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, high self-interaction
N1dh	N1dh	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction
P6ah	P6ah	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction
P5ah	P5ah	Polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction
P4ah	P4ah	Polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction
P3ah	P3ah	Polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction
P2ah	P2ah	Polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction
P1ah	P1ah	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction
N6ah	N6ah	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction
N5ah	N5ah	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction
N4ah	N4ah	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction
N3ah	N3ah	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction
N2ah	N2ah	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction

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Table 7 – continued from previous page

N1ah	N1ah	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction
C6vh	C6vh	Apolar - degree of polarity: 6 (high), high self-interaction, electron acceptor
C5vh	C5vh	Apolar - degree of polarity: 5, high self-interaction, electron acceptor
C4vh	C4vh	Apolar - degree of polarity: 4, high self-interaction, electron acceptor
C3vh	C3vh	Apolar - degree of polarity: 3, high self-interaction, electron acceptor
C2vh	C2vh	Apolar - degree of polarity: 2, high self-interaction, electron acceptor
C1vh	C1vh	Apolar - degree of polarity: 1 (low), high self-interaction, electron acceptor
X4vh	X4vh	Halo compound - polarity: 4 (high), high self-interaction, electron acceptor
X3vh	X3vh	Halo compound - polarity: 3, high self-interaction, electron acceptor
X2vh	X2vh	Halo compound - polarity: 2, high self-interaction, electron acceptor
X1vh	X1vh	Halo compound - polarity: 1 (low), high self-interaction, electron acceptor
C6eh	C6eh	Apolar - degree of polarity: 6 (high), electron donor, high self-interaction
C5eh	C5eh	Apolar - degree of polarity: 5, electron donor, high self-interaction
C4eh	C4eh	Apolar - degree of polarity: 4, electron donor, high self-interaction
C3eh	C3eh	Apolar - degree of polarity: 3, electron donor, high self-interaction
C2eh	C2eh	Apolar - degree of polarity: 2, electron donor, high self-interaction
C1eh	C1eh	Apolar - degree of polarity: 1 (low), electron donor, high self-interaction
X4eh	X4eh	Halo compound - polarity: 4 (high), electron donor, high self-interaction
X3eh	X3eh	Halo compound - polarity: 3, electron donor, high self-interaction
X2eh	X2eh	Halo compound - polarity: 2, electron donor, high self-interaction
X1eh	X1eh	Halo compound - polarity: 1 (low), electron donor, high self-interaction
P6r	P6r	Polar - degree of polarity: 6 (high), reduced self-interaction
P5r	P5r	Polar - degree of polarity: 5, reduced self-interaction
P4r	P4r	Polar - degree of polarity: 4, reduced self-interaction
P3r	P3r	Polar - degree of polarity: 3, reduced self-interaction
P2r	P2r	Polar - degree of polarity: 2, reduced self-interaction
P1r	P1r	Polar - degree of polarity: 1 (low), reduced self-interaction
N6r	N6r	Intermediate/non-polar - degree of polarity: 6 (high), reduced self-interaction
N5r	N5r	Intermediate/non-polar - degree of polarity: 5, reduced self-interaction
N4r	N4r	Intermediate/non-polar - degree of polarity: 4, reduced self-interaction

Continued on next page

Table 7 – continued from previous page

N3r	N3r	Intermediate/non-polar - degree of polarity: 3, reduced self-interaction
N2r	N2r	Intermediate/non-polar - degree of polarity: 2, reduced self-interaction
N1r	N1r	Intermediate/non-polar - degree of polarity: 1 (low), reduced self-interaction
C6r	C6r	Apolar - degree of polarity: 6 (high), reduced self-interaction
C5r	C5r	Apolar - degree of polarity: 5, reduced self-interaction
C4r	C4r	Apolar - degree of polarity: 4, reduced self-interaction
C3r	C3r	Apolar - degree of polarity: 3, reduced self-interaction
C2r	C2r	Apolar - degree of polarity: 2, reduced self-interaction
C1r	C1r	Apolar - degree of polarity: 1 (low), reduced self-interaction
X4r	X4r	Halo compound - polarity: 4 (high), reduced self-interaction
X3r	X3r	Halo compound - polarity: 3, reduced self-interaction
X2r	X2r	Halo compound - polarity: 2, reduced self-interaction
X1r	X1r	Halo compound - polarity: 1 (low), reduced self-interaction
P6dr	P6dr	Polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction
P5dr	P5dr	Polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction
P4dr	P4dr	Polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction
P3dr	P3dr	Polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction
P2dr	P2dr	Polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction
P1dr	P1dr	Polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction
N6dr	N6dr	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction
N5dr	N5dr	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction
N4dr	N4dr	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction
N3dr	N3dr	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction
N2dr	N2dr	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction
N1dr	N1dr	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction
P6ar	P6ar	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction
P5ar	P5ar	Polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction
P4ar	P4ar	Polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction
P3ar	P3ar	Polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction
P2ar	P2ar	Polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction
P1ar	P1ar	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction
N6ar	N6ar	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction

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N5ar	N5ar	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction
N4ar	N4ar	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction
N3ar	N3ar	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction
N2ar	N2ar	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction
N1ar	N1ar	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction
C6vr	C6vr	Apolar - degree of polarity: 6 (high), reduced self-interaction, electron acceptor
C5vr	C5vr	Apolar - degree of polarity: 5, reduced self-interaction, electron acceptor
C4vr	C4vr	Apolar - degree of polarity: 4, reduced self-interaction, electron acceptor
C3vr	C3vr	Apolar - degree of polarity: 3, reduced self-interaction, electron acceptor
C2vr	C2vr	Apolar - degree of polarity: 2, reduced self-interaction, electron acceptor
C1vr	C1vr	Apolar - degree of polarity: 1 (low), reduced self-interaction, electron acceptor
X4vr	X4vr	Halo compound - polarity: 4 (high), reduced self-interaction, electron acceptor
X3vr	X3vr	Halo compound - polarity: 3, reduced self-interaction, electron acceptor
X2vr	X2vr	Halo compound - polarity: 2, reduced self-interaction, electron acceptor
X1vr	X1vr	Halo compound - polarity: 1 (low), reduced self-interaction, electron acceptor
C6er	C6er	Apolar - degree of polarity: 6 (high), electron donor, reduced self-interaction
C5er	C5er	Apolar - degree of polarity: 5, electron donor, reduced self-interaction
C4er	C4er	Apolar - degree of polarity: 4, electron donor, reduced self-interaction
C3er	C3er	Apolar - degree of polarity: 3, electron donor, reduced self-interaction
C2er	C2er	Apolar - degree of polarity: 2, electron donor, reduced self-interaction
C1er	C1er	Apolar - degree of polarity: 1 (low), electron donor, reduced self-interaction
X4er	X4er	Halo compound - polarity: 4 (high), electron donor, reduced self-interaction
X3er	X3er	Halo compound - polarity: 3, electron donor, reduced self-interaction
X2er	X2er	Halo compound - polarity: 2, electron donor, reduced self-interaction
X1er	X1er	Halo compound - polarity: 1 (low), electron donor, reduced self-interaction
SP6	SP6	Polar - degree of polarity: 6 (high), small
SP5	SP5	Polar - degree of polarity: 5, small
SP4	SP4	Polar - degree of polarity: 4, small
SP3	SP3	Polar - degree of polarity: 3, small
SP2	SP2	Polar - degree of polarity: 2, small

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SP1	SP1	Polar - degree of polarity: 1 (low), small
SN6	SN6	Intermediate/non-polar - degree of polarity: 6 (high), small
SN5	SN5	Intermediate/non-polar - degree of polarity: 5, small
SN4	SN4	Intermediate/non-polar - degree of polarity: 4, small
SN3	SN3	Intermediate/non-polar - degree of polarity: 3, small
SN2	SN2	Intermediate/non-polar - degree of polarity: 2, small
SN1	SN1	Intermediate/non-polar - degree of polarity: 1 (low), small
SC6	SC6	Apolar - degree of polarity: 6 (high), small
SC5	SC5	Apolar - degree of polarity: 5, small
SC4	SC4	Apolar - degree of polarity: 4, small
SC3	SC3	Apolar - degree of polarity: 3, small
SC2	SC2	Apolar - degree of polarity: 2, small
SC1	SC1	Apolar - degree of polarity: 1 (low), small
SX4	SX4	Halo compound - polarity: 4 (high), small
SX3	SX3	Halo compound - polarity: 3, small
SX2	SX2	Halo compound - polarity: 2, small
SX1	SX1	Halo compound - polarity: 1 (low), small
SP6d	SP6d	Polar - degree of polarity: 6 (high), hydrogen bond donor, small
SP5d	SP5d	Polar - degree of polarity: 5, hydrogen bond donor, small
SP4d	SP4d	Polar - degree of polarity: 4, hydrogen bond donor, small
SP3d	SP3d	Polar - degree of polarity: 3, hydrogen bond donor, small
SP2d	SP2d	Polar - degree of polarity: 2, hydrogen bond donor, small
SP1d	SP1d	Polar - degree of polarity: 1 (low), hydrogen bond donor, small
SN6d	SN6d	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, small
SN5d	SN5d	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, small
SN4d	SN4d	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, small
SN3d	SN3d	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, small
SN2d	SN2d	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, small
SN1d	SN1d	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, small
SP6a	SP6a	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, small
SP5a	SP5a	Polar - degree of polarity: 5, hydrogen bond acceptor, small
SP4a	SP4a	Polar - degree of polarity: 4, hydrogen bond acceptor, small
SP3a	SP3a	Polar - degree of polarity: 3, hydrogen bond acceptor, small
SP2a	SP2a	Polar - degree of polarity: 2, hydrogen bond acceptor, small
SP1a	SP1a	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, small
SN6a	SN6a	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, small
SN5a	SN5a	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, small
SN4a	SN4a	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, small
SN3a	SN3a	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, small
SN2a	SN2a	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, small
SN1a	SN1a	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, small

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SC6v	SC6v	Apolar - degree of polarity: 6 (high), electron acceptor, small
SC5v	SC5v	Apolar - degree of polarity: 5, electron acceptor, small
SC4v	SC4v	Apolar - degree of polarity: 4, electron acceptor, small
SC3v	SC3v	Apolar - degree of polarity: 3, electron acceptor, small
SC2v	SC2v	Apolar - degree of polarity: 2, electron acceptor, small
SC1v	SC1v	Apolar - degree of polarity: 1 (low), electron acceptor, small
SX4v	SX4v	Halo compound - polarity: 4 (high), electron acceptor, small
SX3v	SX3v	Halo compound - polarity: 3, electron acceptor, small
SX2v	SX2v	Halo compound - polarity: 2, electron acceptor, small
SX1v	SX1v	Halo compound - polarity: 1 (low), electron acceptor, small
SC6e	SC6e	Apolar - degree of polarity: 6 (high), electron donor, small
SC5e	SC5e	Apolar - degree of polarity: 5, electron donor, small
SC4e	SC4e	Apolar - degree of polarity: 4, electron donor, small
SC3e	SC3e	Apolar - degree of polarity: 3, electron donor, small
SC2e	SC2e	Apolar - degree of polarity: 2, electron donor, small
SC1e	SC1e	Apolar - degree of polarity: 1 (low), electron donor, small
SX4e	SX4e	Halo compound - polarity: 4 (high), electron donor, small
SX3e	SX3e	Halo compound - polarity: 3, electron donor, small
SX2e	SX2e	Halo compound - polarity: 2, electron donor, small
SX1e	SX1e	Halo compound - polarity: 1 (low), electron donor, small
SD	SD	Divalent ion, small
SQ5	SQ5	Monovalent ion - hardness: 5 (high), small
SQ4	SQ4	Monovalent ion - hardness: 4, small
SQ3	SQ3	Monovalent ion - hardness: 3, small
SQ2	SQ2	Monovalent ion - hardness: 2, small
SQ1	SQ1	Monovalent ion - hardness: 1 (low), small
SQ5p	SQ5p	Monovalent ion - hardness: 5 (high), hydrogen bond donor, small
SQ4p	SQ4p	Monovalent ion - hardness: 4, hydrogen bond donor, small
SQ3p	SQ3p	Monovalent ion - hardness: 3, hydrogen bond donor, small
SQ2p	SQ2p	Monovalent ion - hardness: 2, hydrogen bond donor, small
SQ1p	SQ1p	Monovalent ion - hardness: 1 (low), hydrogen bond donor, small
SQ5n	SQ5n	Monovalent ion - hardness: 5 (high), hydrogen bond acceptor, small
SQ4n	SQ4n	Monovalent ion - hardness: 4, hydrogen bond acceptor, small
SQ3n	SQ3n	Monovalent ion - hardness: 3, hydrogen bond acceptor, small
SQ2n	SQ2n	Monovalent ion - hardness: 2, hydrogen bond acceptor, small
SQ1n	SQ1n	Monovalent ion - hardness: 1 (low), hydrogen bond acceptor, small
SP6q	SP6q	Polar - degree of polarity: 6 (high), partial charge, small
SP5q	SP5q	Polar - degree of polarity: 5, partial charge, small
SP4q	SP4q	Polar - degree of polarity: 4, partial charge, small
SP3q	SP3q	Polar - degree of polarity: 3, partial charge, small
SP2q	SP2q	Polar - degree of polarity: 2, partial charge, small
SP1q	SP1q	Polar - degree of polarity: 1 (low), partial charge, small
SN6q	SN6q	Intermediate/non-polar - degree of polarity: 6 (high), partial charge, small
SN5q	SN5q	Intermediate/non-polar - degree of polarity: 5, partial charge, small
SN4q	SN4q	Intermediate/non-polar - degree of polarity: 4, partial charge, small
SN3q	SN3q	Intermediate/non-polar - degree of polarity: 3, partial charge, small

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SN2q	SN2q	Intermediate/non-polar - degree of polarity: 2, partial charge, small
SN1q	SN1q	Intermediate/non-polar - degree of polarity: 1 (low), partial charge, small
SC6q	SC6q	Apolar - degree of polarity: 6 (high), partial charge, small
SC5q	SC5q	Apolar - degree of polarity: 5, partial charge, small
SC4q	SC4q	Apolar - degree of polarity: 4, partial charge, small
SC3q	SC3q	Apolar - degree of polarity: 3, partial charge, small
SC2q	SC2q	Apolar - degree of polarity: 2, partial charge, small
SC1q	SC1q	Apolar - degree of polarity: 1 (low), partial charge, small
SX4q	SX4q	Halo compound - polarity: 4 (high), partial charge, small
SX3q	SX3q	Halo compound - polarity: 3, partial charge, small
SX2q	SX2q	Halo compound - polarity: 2, partial charge, small
SX1q	SX1q	Halo compound - polarity: 1 (low), partial charge, small
SP6dq	SP6dq	Polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge, small
SP5dq	SP5dq	Polar - degree of polarity: 5, hydrogen bond donor, partial charge, small
SP4dq	SP4dq	Polar - degree of polarity: 4, hydrogen bond donor, partial charge, small
SP3dq	SP3dq	Polar - degree of polarity: 3, hydrogen bond donor, partial charge, small
SP2dq	SP2dq	Polar - degree of polarity: 2, hydrogen bond donor, partial charge, small
SP1dq	SP1dq	Polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge, small
SN6dq	SN6dq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge, small
SN5dq	SN5dq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, partial charge, small
SN4dq	SN4dq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, partial charge, small
SN3dq	SN3dq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, partial charge, small
SN2dq	SN2dq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, partial charge, small
SN1dq	SN1dq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge, small
SP6aq	SP6aq	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge, small
SP5aq	SP5aq	Polar - degree of polarity: 5, hydrogen bond acceptor, partial charge, small
SP4aq	SP4aq	Polar - degree of polarity: 4, hydrogen bond acceptor, partial charge, small
SP3aq	SP3aq	Polar - degree of polarity: 3, hydrogen bond acceptor, partial charge, small
SP2aq	SP2aq	Polar - degree of polarity: 2, hydrogen bond acceptor, partial charge, small
SP1aq	SP1aq	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge, small
SN6aq	SN6aq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge, small
SN5aq	SN5aq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, partial charge, small

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SN4aq	SN4aq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, partial charge, small
SN3aq	SN3aq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, partial charge, small
SN2aq	SN2aq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, partial charge, small
SN1aq	SN1aq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge, small
SC6vq	SC6vq	Apolar - degree of polarity: 6 (high), partial charge, electron acceptor, small
SC5vq	SC5vq	Apolar - degree of polarity: 5, partial charge, electron acceptor, small
SC4vq	SC4vq	Apolar - degree of polarity: 4, partial charge, electron acceptor, small
SC3vq	SC3vq	Apolar - degree of polarity: 3, partial charge, electron acceptor, small
SC2vq	SC2vq	Apolar - degree of polarity: 2, partial charge, electron acceptor, small
SC1vq	SC1vq	Apolar - degree of polarity: 1 (low), partial charge, electron acceptor, small
SX4vq	SX4vq	Halo compound - polarity: 4 (high), partial charge, electron acceptor, small
SX3vq	SX3vq	Halo compound - polarity: 3, partial charge, electron acceptor, small
SX2vq	SX2vq	Halo compound - polarity: 2, partial charge, electron acceptor, small
SX1vq	SX1vq	Halo compound - polarity: 1 (low), partial charge, electron acceptor, small
SC6eq	SC6eq	Apolar - degree of polarity: 6 (high), electron donor, partial charge, small
SC5eq	SC5eq	Apolar - degree of polarity: 5, electron donor, partial charge, small
SC4eq	SC4eq	Apolar - degree of polarity: 4, electron donor, partial charge, small
SC3eq	SC3eq	Apolar - degree of polarity: 3, electron donor, partial charge, small
SC2eq	SC2eq	Apolar - degree of polarity: 2, electron donor, partial charge, small
SC1eq	SC1eq	Apolar - degree of polarity: 1 (low), electron donor, partial charge, small
SX4eq	SX4eq	Halo compound - polarity: 4 (high), electron donor, partial charge, small
SX3eq	SX3eq	Halo compound - polarity: 3, electron donor, partial charge, small
SX2eq	SX2eq	Halo compound - polarity: 2, electron donor, partial charge, small
SX1eq	SX1eq	Halo compound - polarity: 1 (low), electron donor, partial charge, small
SP6h	SP6h	Polar - degree of polarity: 6 (high), high self-interaction, small
SP5h	SP5h	Polar - degree of polarity: 5, high self-interaction, small
SP4h	SP4h	Polar - degree of polarity: 4, high self-interaction, small
SP3h	SP3h	Polar - degree of polarity: 3, high self-interaction, small
SP2h	SP2h	Polar - degree of polarity: 2, high self-interaction, small
SP1h	SP1h	Polar - degree of polarity: 1 (low), high self-interaction, small

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SN6h	SN6h	Intermediate/non-polar - degree of polarity: 6 (high), high self-interaction, small
SN5h	SN5h	Intermediate/non-polar - degree of polarity: 5, high self-interaction, small
SN4h	SN4h	Intermediate/non-polar - degree of polarity: 4, high self-interaction, small
SN3h	SN3h	Intermediate/non-polar - degree of polarity: 3, high self-interaction, small
SN2h	SN2h	Intermediate/non-polar - degree of polarity: 2, high self-interaction, small
SN1h	SN1h	Intermediate/non-polar - degree of polarity: 1 (low), high self-interaction, small
SC6h	SC6h	Apolar - degree of polarity: 6 (high), high self-interaction, small
SC5h	SC5h	Apolar - degree of polarity: 5, high self-interaction, small
SC4h	SC4h	Apolar - degree of polarity: 4, high self-interaction, small
SC3h	SC3h	Apolar - degree of polarity: 3, high self-interaction, small
SC2h	SC2h	Apolar - degree of polarity: 2, high self-interaction, small
SC1h	SC1h	Apolar - degree of polarity: 1 (low), high self-interaction, small
SX4h	SX4h	Halo compound - polarity: 4 (high), high self-interaction, small
SX3h	SX3h	Halo compound - polarity: 3, high self-interaction, small
SX2h	SX2h	Halo compound - polarity: 2, high self-interaction, small
SX1h	SX1h	Halo compound - polarity: 1 (low), high self-interaction, small
SP6dh	SP6dh	Polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction, small
SP5dh	SP5dh	Polar - degree of polarity: 5, hydrogen bond donor, high self-interaction, small
SP4dh	SP4dh	Polar - degree of polarity: 4, hydrogen bond donor, high self-interaction, small
SP3dh	SP3dh	Polar - degree of polarity: 3, hydrogen bond donor, high self-interaction, small
SP2dh	SP2dh	Polar - degree of polarity: 2, hydrogen bond donor, high self-interaction, small
SP1dh	SP1dh	Polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction, small
SN6dh	SN6dh	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction, small
SN5dh	SN5dh	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, high self-interaction, small
SN4dh	SN4dh	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, high self-interaction, small
SN3dh	SN3dh	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, high self-interaction, small
SN2dh	SN2dh	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, high self-interaction, small
SN1dh	SN1dh	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction, small
SP6ah	SP6ah	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction, small
SP5ah	SP5ah	Polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction, small
SP4ah	SP4ah	Polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction, small
SP3ah	SP3ah	Polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction, small

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SP2ah	SP2ah	Polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction, small
SP1ah	SP1ah	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction, small
SN6ah	SN6ah	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction, small
SN5ah	SN5ah	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction, small
SN4ah	SN4ah	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction, small
SN3ah	SN3ah	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction, small
SN2ah	SN2ah	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction, small
SN1ah	SN1ah	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction, small
SC6vh	SC6vh	Apolar - degree of polarity: 6 (high), high self-interaction, electron acceptor, small
SC5vh	SC5vh	Apolar - degree of polarity: 5, high self-interaction, electron acceptor, small
SC4vh	SC4vh	Apolar - degree of polarity: 4, high self-interaction, electron acceptor, small
SC3vh	SC3vh	Apolar - degree of polarity: 3, high self-interaction, electron acceptor, small
SC2vh	SC2vh	Apolar - degree of polarity: 2, high self-interaction, electron acceptor, small
SC1vh	SC1vh	Apolar - degree of polarity: 1 (low), high self-interaction, electron acceptor, small
SX4vh	SX4vh	Halo compound - polarity: 4 (high), high self-interaction, electron acceptor, small
SX3vh	SX3vh	Halo compound - polarity: 3, high self-interaction, electron acceptor, small
SX2vh	SX2vh	Halo compound - polarity: 2, high self-interaction, electron acceptor, small
SX1vh	SX1vh	Halo compound - polarity: 1 (low), high self-interaction, electron acceptor, small
SC6eh	SC6eh	Apolar - degree of polarity: 6 (high), electron donor, high self-interaction, small
SC5eh	SC5eh	Apolar - degree of polarity: 5, electron donor, high self-interaction, small
SC4eh	SC4eh	Apolar - degree of polarity: 4, electron donor, high self-interaction, small
SC3eh	SC3eh	Apolar - degree of polarity: 3, electron donor, high self-interaction, small
SC2eh	SC2eh	Apolar - degree of polarity: 2, electron donor, high self-interaction, small
SC1eh	SC1eh	Apolar - degree of polarity: 1 (low), electron donor, high self-interaction, small
SX4eh	SX4eh	Halo compound - polarity: 4 (high), electron donor, high self-interaction, small
SX3eh	SX3eh	Halo compound - polarity: 3, electron donor, high self-interaction, small
SX2eh	SX2eh	Halo compound - polarity: 2, electron donor, high self-interaction, small

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SX1eh	SX1eh	Halo compound - polarity: 1 (low), electron donor, high self-interaction, small
SP6r	SP6r	Polar - degree of polarity: 6 (high), reduced self-interaction, small
SP5r	SP5r	Polar - degree of polarity: 5, reduced self-interaction, small
SP4r	SP4r	Polar - degree of polarity: 4, reduced self-interaction, small
SP3r	SP3r	Polar - degree of polarity: 3, reduced self-interaction, small
SP2r	SP2r	Polar - degree of polarity: 2, reduced self-interaction, small
SP1r	SP1r	Polar - degree of polarity: 1 (low), reduced self-interaction, small
SN6r	SN6r	Intermediate/non-polar - degree of polarity: 6 (high), reduced self-interaction, small
SN5r	SN5r	Intermediate/non-polar - degree of polarity: 5, reduced self-interaction, small
SN4r	SN4r	Intermediate/non-polar - degree of polarity: 4, reduced self-interaction, small
SN3r	SN3r	Intermediate/non-polar - degree of polarity: 3, reduced self-interaction, small
SN2r	SN2r	Intermediate/non-polar - degree of polarity: 2, reduced self-interaction, small
SN1r	SN1r	Intermediate/non-polar - degree of polarity: 1 (low), reduced self-interaction, small
SC6r	SC6r	Apolar - degree of polarity: 6 (high), reduced self-interaction, small
SC5r	SC5r	Apolar - degree of polarity: 5, reduced self-interaction, small
SC4r	SC4r	Apolar - degree of polarity: 4, reduced self-interaction, small
SC3r	SC3r	Apolar - degree of polarity: 3, reduced self-interaction, small
SC2r	SC2r	Apolar - degree of polarity: 2, reduced self-interaction, small
SC1r	SC1r	Apolar - degree of polarity: 1 (low), reduced self-interaction, small
SX4r	SX4r	Halo compound - polarity: 4 (high), reduced self-interaction, small
SX3r	SX3r	Halo compound - polarity: 3, reduced self-interaction, small
SX2r	SX2r	Halo compound - polarity: 2, reduced self-interaction, small
SX1r	SX1r	Halo compound - polarity: 1 (low), reduced self-interaction, small
SP6dr	SP6dr	Polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction, small
SP5dr	SP5dr	Polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction, small
SP4dr	SP4dr	Polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction, small
SP3dr	SP3dr	Polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction, small
SP2dr	SP2dr	Polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction, small
SP1dr	SP1dr	Polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction, small
SN6dr	SN6dr	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction, small
SN5dr	SN5dr	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction, small
SN4dr	SN4dr	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction, small

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SN3dr	SN3dr	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction, small
SN2dr	SN2dr	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction, small
SN1dr	SN1dr	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction, small
SP6ar	SP6ar	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction, small
SP5ar	SP5ar	Polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction, small
SP4ar	SP4ar	Polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction, small
SP3ar	SP3ar	Polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction, small
SP2ar	SP2ar	Polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction, small
SP1ar	SP1ar	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction, small
SN6ar	SN6ar	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction, small
SN5ar	SN5ar	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction, small
SN4ar	SN4ar	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction, small
SN3ar	SN3ar	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction, small
SN2ar	SN2ar	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction, small
SN1ar	SN1ar	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction, small
SC6vr	SC6vr	Apolar - degree of polarity: 6 (high), reduced self-interaction, electron acceptor, small
SC5vr	SC5vr	Apolar - degree of polarity: 5, reduced self-interaction, electron acceptor, small
SC4vr	SC4vr	Apolar - degree of polarity: 4, reduced self-interaction, electron acceptor, small
SC3vr	SC3vr	Apolar - degree of polarity: 3, reduced self-interaction, electron acceptor, small
SC2vr	SC2vr	Apolar - degree of polarity: 2, reduced self-interaction, electron acceptor, small
SC1vr	SC1vr	Apolar - degree of polarity: 1 (low), reduced self-interaction, electron acceptor, small
SX4vr	SX4vr	Halo compound - polarity: 4 (high), reduced self-interaction, electron acceptor, small
SX3vr	SX3vr	Halo compound - polarity: 3, reduced self-interaction, electron acceptor, small
SX2vr	SX2vr	Halo compound - polarity: 2, reduced self-interaction, electron acceptor, small
SX1vr	SX1vr	Halo compound - polarity: 1 (low), reduced self-interaction, electron acceptor, small
SC6er	SC6er	Apolar - degree of polarity: 6 (high), electron donor, reduced self-interaction, small
SC5er	SC5er	Apolar - degree of polarity: 5, electron donor, reduced self-interaction, small

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Table 7 – continued from previous page

SC4er	SC4er	Apolar - degree of polarity: 4, electron donor, reduced self-interaction, small
SC3er	SC3er	Apolar - degree of polarity: 3, electron donor, reduced self-interaction, small
SC2er	SC2er	Apolar - degree of polarity: 2, electron donor, reduced self-interaction, small
SC1er	SC1er	Apolar - degree of polarity: 1 (low), electron donor, reduced self-interaction, small
SX4er	SX4er	Halo compound - polarity: 4 (high), electron donor, reduced self-interaction, small
SX3er	SX3er	Halo compound - polarity: 3, electron donor, reduced self-interaction, small
SX2er	SX2er	Halo compound - polarity: 2, electron donor, reduced self-interaction, small
SX1er	SX1er	Halo compound - polarity: 1 (low), electron donor, reduced self-interaction, small
TP6	TP6	Polar - degree of polarity: 6 (high), tiny
TP5	TP5	Polar - degree of polarity: 5, tiny
TP4	TP4	Polar - degree of polarity: 4, tiny
TP3	TP3	Polar - degree of polarity: 3, tiny
TP2	TP2	Polar - degree of polarity: 2, tiny
TP1	TP1	Polar - degree of polarity: 1 (low), tiny
TN6	TN6	Intermediate/non-polar - degree of polarity: 6 (high), tiny
TN5	TN5	Intermediate/non-polar - degree of polarity: 5, tiny
TN4	TN4	Intermediate/non-polar - degree of polarity: 4, tiny
TN3	TN3	Intermediate/non-polar - degree of polarity: 3, tiny
TN2	TN2	Intermediate/non-polar - degree of polarity: 2, tiny
TN1	TN1	Intermediate/non-polar - degree of polarity: 1 (low), tiny
TC6	TC6	Apolar - degree of polarity: 6 (high), tiny
TC5	TC5	Apolar - degree of polarity: 5, tiny
TC4	TC4	Apolar - degree of polarity: 4, tiny
TC3	TC3	Apolar - degree of polarity: 3, tiny
TC2	TC2	Apolar - degree of polarity: 2, tiny
TC1	TC1	Apolar - degree of polarity: 1 (low), tiny
TX4	TX4	Halo compound - polarity: 4 (high), tiny
TX3	TX3	Halo compound - polarity: 3, tiny
TX2	TX2	Halo compound - polarity: 2, tiny
TX1	TX1	Halo compound - polarity: 1 (low), tiny
TP6d	TP6d	Polar - degree of polarity: 6 (high), hydrogen bond donor, tiny
TP5d	TP5d	Polar - degree of polarity: 5, hydrogen bond donor, tiny
TP4d	TP4d	Polar - degree of polarity: 4, hydrogen bond donor, tiny
TP3d	TP3d	Polar - degree of polarity: 3, hydrogen bond donor, tiny
TP2d	TP2d	Polar - degree of polarity: 2, hydrogen bond donor, tiny
TP1d	TP1d	Polar - degree of polarity: 1 (low), hydrogen bond donor, tiny
TN6d	TN6d	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, tiny
TN5d	TN5d	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, tiny
TN4d	TN4d	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, tiny
TN3d	TN3d	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, tiny
TN2d	TN2d	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, tiny

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TN1d	TN1d	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, tiny
TP6a	TP6a	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, tiny
TP5a	TP5a	Polar - degree of polarity: 5, hydrogen bond acceptor, tiny
TP4a	TP4a	Polar - degree of polarity: 4, hydrogen bond acceptor, tiny
TP3a	TP3a	Polar - degree of polarity: 3, hydrogen bond acceptor, tiny
TP2a	TP2a	Polar - degree of polarity: 2, hydrogen bond acceptor, tiny
TP1a	TP1a	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, tiny
TN6a	TN6a	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, tiny
TN5a	TN5a	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, tiny
TN4a	TN4a	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, tiny
TN3a	TN3a	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, tiny
TN2a	TN2a	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, tiny
TN1a	TN1a	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, tiny
TC6v	TC6v	Apolar - degree of polarity: 6 (high), electron acceptor, tiny
TC5v	TC5v	Apolar - degree of polarity: 5, electron acceptor, tiny
TC4v	TC4v	Apolar - degree of polarity: 4, electron acceptor, tiny
TC3v	TC3v	Apolar - degree of polarity: 3, electron acceptor, tiny
TC2v	TC2v	Apolar - degree of polarity: 2, electron acceptor, tiny
TC1v	TC1v	Apolar - degree of polarity: 1 (low), electron acceptor, tiny
TX4v	TX4v	Halo compound - polarity: 4 (high), electron acceptor, tiny
TX3v	TX3v	Halo compound - polarity: 3, electron acceptor, tiny
TX2v	TX2v	Halo compound - polarity: 2, electron acceptor, tiny
TX1v	TX1v	Halo compound - polarity: 1 (low), electron acceptor, tiny
TC6e	TC6e	Apolar - degree of polarity: 6 (high), electron donor, tiny
TC5e	TC5e	Apolar - degree of polarity: 5, electron donor, tiny
TC4e	TC4e	Apolar - degree of polarity: 4, electron donor, tiny
TC3e	TC3e	Apolar - degree of polarity: 3, electron donor, tiny
TC2e	TC2e	Apolar - degree of polarity: 2, electron donor, tiny
TC1e	TC1e	Apolar - degree of polarity: 1 (low), electron donor, tiny
TX4e	TX4e	Halo compound - polarity: 4 (high), electron donor, tiny
TX3e	TX3e	Halo compound - polarity: 3, electron donor, tiny
TX2e	TX2e	Halo compound - polarity: 2, electron donor, tiny
TX1e	TX1e	Halo compound - polarity: 1 (low), electron donor, tiny
TD	TD	Divalent ion, tiny
TQ5	TQ5	Monovalent ion - hardness: 5 (high), tiny
TQ4	TQ4	Monovalent ion - hardness: 4, tiny
TQ3	TQ3	Monovalent ion - hardness: 3, tiny
TQ2	TQ2	Monovalent ion - hardness: 2, tiny
TQ1	TQ1	Monovalent ion - hardness: 1 (low), tiny
TQ5p	TQ5p	Monovalent ion - hardness: 5 (high), hydrogen bond donor, tiny
TQ4p	TQ4p	Monovalent ion - hardness: 4, hydrogen bond donor, tiny
TQ3p	TQ3p	Monovalent ion - hardness: 3, hydrogen bond donor, tiny
TQ2p	TQ2p	Monovalent ion - hardness: 2, hydrogen bond donor, tiny
TQ1p	TQ1p	Monovalent ion - hardness: 1 (low), hydrogen bond donor, tiny

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TQ5n	TQ5n	Monovalent ion - hardness: 5 (high), hydrogen bond acceptor, tiny
TQ4n	TQ4n	Monovalent ion - hardness: 4, hydrogen bond acceptor, tiny
TQ3n	TQ3n	Monovalent ion - hardness: 3, hydrogen bond acceptor, tiny
TQ2n	TQ2n	Monovalent ion - hardness: 2, hydrogen bond acceptor, tiny
TQ1n	TQ1n	Monovalent ion - hardness: 1 (low), hydrogen bond acceptor, tiny
TP6q	TP6q	Polar - degree of polarity: 6 (high), partial charge, tiny
TP5q	TP5q	Polar - degree of polarity: 5, partial charge, tiny
TP4q	TP4q	Polar - degree of polarity: 4, partial charge, tiny
TP3q	TP3q	Polar - degree of polarity: 3, partial charge, tiny
TP2q	TP2q	Polar - degree of polarity: 2, partial charge, tiny
TP1q	TP1q	Polar - degree of polarity: 1 (low), partial charge, tiny
TN6q	TN6q	Intermediate/non-polar - degree of polarity: 6 (high), partial charge, tiny
TN5q	TN5q	Intermediate/non-polar - degree of polarity: 5, partial charge, tiny
TN4q	TN4q	Intermediate/non-polar - degree of polarity: 4, partial charge, tiny
TN3q	TN3q	Intermediate/non-polar - degree of polarity: 3, partial charge, tiny
TN2q	TN2q	Intermediate/non-polar - degree of polarity: 2, partial charge, tiny
TN1q	TN1q	Intermediate/non-polar - degree of polarity: 1 (low), partial charge, tiny
TC6q	TC6q	Apolar - degree of polarity: 6 (high), partial charge, tiny
TC5q	TC5q	Apolar - degree of polarity: 5, partial charge, tiny
TC4q	TC4q	Apolar - degree of polarity: 4, partial charge, tiny
TC3q	TC3q	Apolar - degree of polarity: 3, partial charge, tiny
TC2q	TC2q	Apolar - degree of polarity: 2, partial charge, tiny
TC1q	TC1q	Apolar - degree of polarity: 1 (low), partial charge, tiny
TX4q	TX4q	Halo compound - polarity: 4 (high), partial charge, tiny
TX3q	TX3q	Halo compound - polarity: 3, partial charge, tiny
TX2q	TX2q	Halo compound - polarity: 2, partial charge, tiny
TX1q	TX1q	Halo compound - polarity: 1 (low), partial charge, tiny
TP6dq	TP6dq	Polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge, tiny
TP5dq	TP5dq	Polar - degree of polarity: 5, hydrogen bond donor, partial charge, tiny
TP4dq	TP4dq	Polar - degree of polarity: 4, hydrogen bond donor, partial charge, tiny
TP3dq	TP3dq	Polar - degree of polarity: 3, hydrogen bond donor, partial charge, tiny
TP2dq	TP2dq	Polar - degree of polarity: 2, hydrogen bond donor, partial charge, tiny
TP1dq	TP1dq	Polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge, tiny
TN6dq	TN6dq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, partial charge, tiny
TN5dq	TN5dq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, partial charge, tiny
TN4dq	TN4dq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, partial charge, tiny
TN3dq	TN3dq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, partial charge, tiny

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TN2dq	TN2dq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, partial charge, tiny
TN1dq	TN1dq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, partial charge, tiny
TP6aq	TP6aq	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge, tiny
TP5aq	TP5aq	Polar - degree of polarity: 5, hydrogen bond acceptor, partial charge, tiny
TP4aq	TP4aq	Polar - degree of polarity: 4, hydrogen bond acceptor, partial charge, tiny
TP3aq	TP3aq	Polar - degree of polarity: 3, hydrogen bond acceptor, partial charge, tiny
TP2aq	TP2aq	Polar - degree of polarity: 2, hydrogen bond acceptor, partial charge, tiny
TP1aq	TP1aq	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge, tiny
TN6aq	TN6aq	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, partial charge, tiny
TN5aq	TN5aq	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, partial charge, tiny
TN4aq	TN4aq	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, partial charge, tiny
TN3aq	TN3aq	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, partial charge, tiny
TN2aq	TN2aq	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, partial charge, tiny
TN1aq	TN1aq	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, partial charge, tiny
TC6vq	TC6vq	Apolar - degree of polarity: 6 (high), partial charge, electron acceptor, tiny
TC5vq	TC5vq	Apolar - degree of polarity: 5, partial charge, electron acceptor, tiny
TC4vq	TC4vq	Apolar - degree of polarity: 4, partial charge, electron acceptor, tiny
TC3vq	TC3vq	Apolar - degree of polarity: 3, partial charge, electron acceptor, tiny
TC2vq	TC2vq	Apolar - degree of polarity: 2, partial charge, electron acceptor, tiny
TC1vq	TC1vq	Apolar - degree of polarity: 1 (low), partial charge, electron acceptor, tiny
TX4vq	TX4vq	Halo compound - polarity: 4 (high), partial charge, electron acceptor, tiny
TX3vq	TX3vq	Halo compound - polarity: 3, partial charge, electron acceptor, tiny
TX2vq	TX2vq	Halo compound - polarity: 2, partial charge, electron acceptor, tiny
TX1vq	TX1vq	Halo compound - polarity: 1 (low), partial charge, electron acceptor, tiny
TC6eq	TC6eq	Apolar - degree of polarity: 6 (high), electron donor, partial charge, tiny
TC5eq	TC5eq	Apolar - degree of polarity: 5, electron donor, partial charge, tiny
TC4eq	TC4eq	Apolar - degree of polarity: 4, electron donor, partial charge, tiny

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TC3eq	TC3eq	Apolar - degree of polarity: 3, electron donor, partial charge, tiny
TC2eq	TC2eq	Apolar - degree of polarity: 2, electron donor, partial charge, tiny
TC1eq	TC1eq	Apolar - degree of polarity: 1 (low), electron donor, partial charge, tiny
TX4eq	TX4eq	Halo compound - polarity: 4 (high), electron donor, partial charge, tiny
TX3eq	TX3eq	Halo compound - polarity: 3, electron donor, partial charge, tiny
TX2eq	TX2eq	Halo compound - polarity: 2, electron donor, partial charge, tiny
TX1eq	TX1eq	Halo compound - polarity: 1 (low), electron donor, partial charge, tiny
TP6h	TP6h	Polar - degree of polarity: 6 (high), high self-interaction, tiny
TP5h	TP5h	Polar - degree of polarity: 5, high self-interaction, tiny
TP4h	TP4h	Polar - degree of polarity: 4, high self-interaction, tiny
TP3h	TP3h	Polar - degree of polarity: 3, high self-interaction, tiny
TP2h	TP2h	Polar - degree of polarity: 2, high self-interaction, tiny
TP1h	TP1h	Polar - degree of polarity: 1 (low), high self-interaction, tiny
TN6h	TN6h	Intermediate/non-polar - degree of polarity: 6 (high), high self-interaction, tiny
TN5h	TN5h	Intermediate/non-polar - degree of polarity: 5, high self-interaction, tiny
TN4h	TN4h	Intermediate/non-polar - degree of polarity: 4, high self-interaction, tiny
TN3h	TN3h	Intermediate/non-polar - degree of polarity: 3, high self-interaction, tiny
TN2h	TN2h	Intermediate/non-polar - degree of polarity: 2, high self-interaction, tiny
TN1h	TN1h	Intermediate/non-polar - degree of polarity: 1 (low), high self-interaction, tiny
TC6h	TC6h	Apolar - degree of polarity: 6 (high), high self-interaction, tiny
TC5h	TC5h	Apolar - degree of polarity: 5, high self-interaction, tiny
TC4h	TC4h	Apolar - degree of polarity: 4, high self-interaction, tiny
TC3h	TC3h	Apolar - degree of polarity: 3, high self-interaction, tiny
TC2h	TC2h	Apolar - degree of polarity: 2, high self-interaction, tiny
TC1h	TC1h	Apolar - degree of polarity: 1 (low), high self-interaction, tiny
TX4h	TX4h	Halo compound - polarity: 4 (high), high self-interaction, tiny
TX3h	TX3h	Halo compound - polarity: 3, high self-interaction, tiny
TX2h	TX2h	Halo compound - polarity: 2, high self-interaction, tiny
TX1h	TX1h	Halo compound - polarity: 1 (low), high self-interaction, tiny
TP6dh	TP6dh	Polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction, tiny
TP5dh	TP5dh	Polar - degree of polarity: 5, hydrogen bond donor, high self-interaction, tiny
TP4dh	TP4dh	Polar - degree of polarity: 4, hydrogen bond donor, high self-interaction, tiny
TP3dh	TP3dh	Polar - degree of polarity: 3, hydrogen bond donor, high self-interaction, tiny
TP2dh	TP2dh	Polar - degree of polarity: 2, hydrogen bond donor, high self-interaction, tiny
TP1dh	TP1dh	Polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction, tiny

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TN6dh	TN6dh	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, high self-interaction, tiny
TN5dh	TN5dh	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, high self-interaction, tiny
TN4dh	TN4dh	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, high self-interaction, tiny
TN3dh	TN3dh	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, high self-interaction, tiny
TN2dh	TN2dh	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, high self-interaction, tiny
TN1dh	TN1dh	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, high self-interaction, tiny
TP6ah	TP6ah	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction, tiny
TP5ah	TP5ah	Polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction, tiny
TP4ah	TP4ah	Polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction, tiny
TP3ah	TP3ah	Polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction, tiny
TP2ah	TP2ah	Polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction, tiny
TP1ah	TP1ah	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction, tiny
TN6ah	TN6ah	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, high self-interaction, tiny
TN5ah	TN5ah	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, high self-interaction, tiny
TN4ah	TN4ah	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, high self-interaction, tiny
TN3ah	TN3ah	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, high self-interaction, tiny
TN2ah	TN2ah	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, high self-interaction, tiny
TN1ah	TN1ah	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, high self-interaction, tiny
TC6vh	TC6vh	Apolar - degree of polarity: 6 (high), high self-interaction, electron acceptor, tiny
TC5vh	TC5vh	Apolar - degree of polarity: 5, high self-interaction, electron acceptor, tiny
TC4vh	TC4vh	Apolar - degree of polarity: 4, high self-interaction, electron acceptor, tiny
TC3vh	TC3vh	Apolar - degree of polarity: 3, high self-interaction, electron acceptor, tiny
TC2vh	TC2vh	Apolar - degree of polarity: 2, high self-interaction, electron acceptor, tiny
TC1vh	TC1vh	Apolar - degree of polarity: 1 (low), high self-interaction, electron acceptor, tiny
TX4vh	TX4vh	Halo compound - polarity: 4 (high), high self-interaction, electron acceptor, tiny
TX3vh	TX3vh	Halo compound - polarity: 3, high self-interaction, electron acceptor, tiny
TX2vh	TX2vh	Halo compound - polarity: 2, high self-interaction, electron acceptor, tiny

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TX1vh	TX1vh	Halo compound - polarity: 1 (low), high self-interaction, electron acceptor, tiny
TC6eh	TC6eh	Apolar - degree of polarity: 6 (high), electron donor, high self-interaction, tiny
TC5eh	TC5eh	Apolar - degree of polarity: 5, electron donor, high self-interaction, tiny
TC4eh	TC4eh	Apolar - degree of polarity: 4, electron donor, high self-interaction, tiny
TC3eh	TC3eh	Apolar - degree of polarity: 3, electron donor, high self-interaction, tiny
TC2eh	TC2eh	Apolar - degree of polarity: 2, electron donor, high self-interaction, tiny
TC1eh	TC1eh	Apolar - degree of polarity: 1 (low), electron donor, high self-interaction, tiny
TX4eh	TX4eh	Halo compound - polarity: 4 (high), electron donor, high self-interaction, tiny
TX3eh	TX3eh	Halo compound - polarity: 3, electron donor, high self-interaction, tiny
TX2eh	TX2eh	Halo compound - polarity: 2, electron donor, high self-interaction, tiny
TX1eh	TX1eh	Halo compound - polarity: 1 (low), electron donor, high self-interaction, tiny
TP6r	TP6r	Polar - degree of polarity: 6 (high), reduced self-interaction, tiny
TP5r	TP5r	Polar - degree of polarity: 5, reduced self-interaction, tiny
TP4r	TP4r	Polar - degree of polarity: 4, reduced self-interaction, tiny
TP3r	TP3r	Polar - degree of polarity: 3, reduced self-interaction, tiny
TP2r	TP2r	Polar - degree of polarity: 2, reduced self-interaction, tiny
TP1r	TP1r	Polar - degree of polarity: 1 (low), reduced self-interaction, tiny
TN6r	TN6r	Intermediate/non-polar - degree of polarity: 6 (high), reduced self-interaction, tiny
TN5r	TN5r	Intermediate/non-polar - degree of polarity: 5, reduced self-interaction, tiny
TN4r	TN4r	Intermediate/non-polar - degree of polarity: 4, reduced self-interaction, tiny
TN3r	TN3r	Intermediate/non-polar - degree of polarity: 3, reduced self-interaction, tiny
TN2r	TN2r	Intermediate/non-polar - degree of polarity: 2, reduced self-interaction, tiny
TN1r	TN1r	Intermediate/non-polar - degree of polarity: 1 (low), reduced self-interaction, tiny
TC6r	TC6r	Apolar - degree of polarity: 6 (high), reduced self-interaction, tiny
TC5r	TC5r	Apolar - degree of polarity: 5, reduced self-interaction, tiny
TC4r	TC4r	Apolar - degree of polarity: 4, reduced self-interaction, tiny
TC3r	TC3r	Apolar - degree of polarity: 3, reduced self-interaction, tiny
TC2r	TC2r	Apolar - degree of polarity: 2, reduced self-interaction, tiny
TC1r	TC1r	Apolar - degree of polarity: 1 (low), reduced self-interaction, tiny
TX4r	TX4r	Halo compound - polarity: 4 (high), reduced self-interaction, tiny
TX3r	TX3r	Halo compound - polarity: 3, reduced self-interaction, tiny
TX2r	TX2r	Halo compound - polarity: 2, reduced self-interaction, tiny
TX1r	TX1r	Halo compound - polarity: 1 (low), reduced self-interaction, tiny

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TP6dr	TP6dr	Polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction, tiny
TP5dr	TP5dr	Polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction, tiny
TP4dr	TP4dr	Polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction, tiny
TP3dr	TP3dr	Polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction, tiny
TP2dr	TP2dr	Polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction, tiny
TP1dr	TP1dr	Polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction, tiny
TN6dr	TN6dr	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond donor, reduced self-interaction, tiny
TN5dr	TN5dr	Intermediate/non-polar - degree of polarity: 5, hydrogen bond donor, reduced self-interaction, tiny
TN4dr	TN4dr	Intermediate/non-polar - degree of polarity: 4, hydrogen bond donor, reduced self-interaction, tiny
TN3dr	TN3dr	Intermediate/non-polar - degree of polarity: 3, hydrogen bond donor, reduced self-interaction, tiny
TN2dr	TN2dr	Intermediate/non-polar - degree of polarity: 2, hydrogen bond donor, reduced self-interaction, tiny
TN1dr	TN1dr	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond donor, reduced self-interaction, tiny
TP6ar	TP6ar	Polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction, tiny
TP5ar	TP5ar	Polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction, tiny
TP4ar	TP4ar	Polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction, tiny
TP3ar	TP3ar	Polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction, tiny
TP2ar	TP2ar	Polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction, tiny
TP1ar	TP1ar	Polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction, tiny
TN6ar	TN6ar	Intermediate/non-polar - degree of polarity: 6 (high), hydrogen bond acceptor, reduced self-interaction, tiny
TN5ar	TN5ar	Intermediate/non-polar - degree of polarity: 5, hydrogen bond acceptor, reduced self-interaction, tiny
TN4ar	TN4ar	Intermediate/non-polar - degree of polarity: 4, hydrogen bond acceptor, reduced self-interaction, tiny
TN3ar	TN3ar	Intermediate/non-polar - degree of polarity: 3, hydrogen bond acceptor, reduced self-interaction, tiny
TN2ar	TN2ar	Intermediate/non-polar - degree of polarity: 2, hydrogen bond acceptor, reduced self-interaction, tiny
TN1ar	TN1ar	Intermediate/non-polar - degree of polarity: 1 (low), hydrogen bond acceptor, reduced self-interaction, tiny
TC6vr	TC6vr	Apolar - degree of polarity: 6 (high), reduced self-interaction, electron acceptor, tiny
TC5vr	TC5vr	Apolar - degree of polarity: 5, reduced self-interaction, electron acceptor, tiny
TC4vr	TC4vr	Apolar - degree of polarity: 4, reduced self-interaction, electron acceptor, tiny

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TC3vr	TC3vr	Apolar - degree of polarity: 3, reduced self-interaction, electron acceptor, tiny
TC2vr	TC2vr	Apolar - degree of polarity: 2, reduced self-interaction, electron acceptor, tiny
TC1vr	TC1vr	Apolar - degree of polarity: 1 (low), reduced self-interaction, electron acceptor, tiny
TX4vr	TX4vr	Halo compound - polarity: 4 (high), reduced self-interaction, electron acceptor, tiny
TX3vr	TX3vr	Halo compound - polarity: 3, reduced self-interaction, electron acceptor, tiny
TX2vr	TX2vr	Halo compound - polarity: 2, reduced self-interaction, electron acceptor, tiny
TX1vr	TX1vr	Halo compound - polarity: 1 (low), reduced self-interaction, electron acceptor, tiny
TC6er	TC6er	Apolar - degree of polarity: 6 (high), electron donor, reduced self-interaction, tiny
TC5er	TC5er	Apolar - degree of polarity: 5, electron donor, reduced self-interaction, tiny
TC4er	TC4er	Apolar - degree of polarity: 4, electron donor, reduced self-interaction, tiny
TC3er	TC3er	Apolar - degree of polarity: 3, electron donor, reduced self-interaction, tiny
TC2er	TC2er	Apolar - degree of polarity: 2, electron donor, reduced self-interaction, tiny
TC1er	TC1er	Apolar - degree of polarity: 1 (low), electron donor, reduced self-interaction, tiny
TX4er	TX4er	Halo compound - polarity: 4 (high), electron donor, reduced self-interaction, tiny
TX3er	TX3er	Halo compound - polarity: 3, electron donor, reduced self-interaction, tiny
TX2er	TX2er	Halo compound - polarity: 2, electron donor, reduced self-interaction, tiny
TX1er	TX1er	Halo compound - polarity: 1 (low), electron donor, reduced self-interaction, tiny
W	W	Water
SW	SW	Water, small
TW	TW	Water, tiny

SPICA.frc

Mesoscale forcefield for polymers and basic organic molecules [56]. SPICA stands for Surface Property fItting Coarse grAined model. This forcefield has been designed to reproduce thermodynamic quantities, such as surface/interfacial tension and density, as well as distribution functions obtained from all-atom molecular simulations based on the CHARMM force field. The SPICA forcefield is suitable to simulate bio-molecular systems and soft matter.

C2T	C2T	-CH-(CH3)2
CLA	CLA	Cl- (H2O)2
CM	CM	-CH2-CH2-CH2-
CM2	CM2	-CH2-CH2- (tail)
CM2R	CM2R	CH2-CH2- (ring)
CM4	CM4	-CH2-C(-)H-CH2-CH3 branched tail group
CMB	CMB	-CH2-CH=CH- (ring B/C)

Continued on next page

[56] http://www.spica-ff.org/

Table 8 – continued from previous page

CMD	CMD	-CH=CH-CH2-
CMD2	CMD2	-HC=CH- (cis)
CMDB	CMDB	-CH2-C=CH- (ring A/B)
CMO	CMO	-CH2-CH2-CH2- (the same as CM)
CMR	CMR	-CH-CH2-CH2- (ring B/C)
CMR5	CMR5	-CH2-CH2-CH- (ring D)
CT	CT	CH3-CH2-CH2-
CT2	CT2	CH3-CH2-
CTB	CTB	same composition with CT2, but shorter bond length with CMT, CMY and CM4
CTBA	CTBA	-C-CH3 (ring A/B)
CTBB	CTBB	-C-CH3 (ring C/D)
EO	EO	-CH2-O-CH2-
EOT	EOT	CH3-O-CH2-
EST1	EST1	-CH2CO2- in the sn-2 chain
EST2	EST2	-H2CO2- in the sn-1 chain
GL	GL	-CH2CH-CH2-
GL2	GL2	-CH2-CH-
NC	NC	-CH2CH2-N-(CH3)3
NC4	NC4	(CH3)3N+CH2
NH	NH	-CH2CH2-NH3
OA	OA	HOCH2-
OAB	OAB	-CH-OH (ring A)
OAD	OAD	>CH-OH
PEP	PEP	-CO-NH-
PH	PH	-PO4-
PHE	PHE	-PO4- for PE headgroup
PHS	PHS	-PO4- (sphingomyelin)
SO4	SO4	SO4-
SOD	SOD	Na+ (H2O)3
W	W	three water molecules

3.8 Machine Learning Potentials (MLPs)

Cu-SNAP.frc

SNAP potential for Cu [80]

Cu_Zuo_JPCA2020.frc

SNAP potential for Cu [81]

Ge_Zuo_JPCA2020.frc

SNAP potential for Ge [81]

[80] X. Li, C. Hu, C. Chen, Z. Deng, J. Luo, & S.P. Ong (2018). "Quantum-Accurate Spectral Neighbor Analysis Potential Models for Ni-Mo Binary Alloys and FCC Metals." arXiv:1806.04777

[81]

25. Zuo, C. Chen, X, Li, Z. Deng, Y. Chen, J. Behler, G. Csányi, A. V. Shapeev, A. P. Thompson, M. A. Wood, S. P. Ong, "Performance and Cost Assessment of Machine Learning Interatomic Potentials" J. Phys. Chem. A 124, 4, 731-745 (2020)

InP_JCPA2020.frc

SNAP potential for InP [81]

Li3N-SNAP.frc

SNAP potential for Li3N [83]

Li_Zuo_JPCA2020.frc

SNAP potential for Li [81]

Mo_Zuo_JPCA2020.frc

SNAP potential for Mo [81]

Ni_Zuo_JPCA2020.frc

SNAP potential for Ni [81]

Si_Zuo_JPCA2020.frc

SNAP potential for Si [81]

Mo-SNAP.frc

SNAP potential for Mo [84]

NbMoTaW-SNAP.frc

SNAP potential for Nb/Mo/Ta/W [85]

Ni-SNAP.frc

SNAP potential for Ni [89]

[83]

26. Deng, C. Chen, X. Li & S.P. Ong (2019). "An Electrostatic Spectral Neighbor Analysis Potential (eSNAP) for Lithium Nitride." arXiv:1901.08749

[84] Chen, C., Deng, Z., Tran, R., Tang, H., Chu, I. H., & Ong, S. P. (2017). Accurate force field for molybdenum by machine learning large materials data. Physical Review Materials, 1(4), 043603.

[85]

24. Li, C. Chen, H. Zheng & S.P. Ong (2019). "Complex Strengthening Mechanisms in the NbMoTaW Multi-Principal Element Alloy with Machine Learning Potentials", Cond. Mat Mat. Sci, https://arxiv.org/abs/1912.0178.

[89]

24. Li, C. Hu, C. Chen, Z. Deng, J. Luo, & S.P. Ong (2018). Quantum-Accurate Spectral Neighbor Analysis Potential Models for Ni-Mo Binary Alloys and FCC Metals. arXiv:1806.04777

DOCUMENTATION

NiMo-SNAP.frc

SNAP potential for Ni/Mo [89]

Ta06A.frc

SNAP potential for Ta [86]

WBe_Wood_PRB2019.frc

SNAP potential for W/Be [87]

W_2940_2017_2.frc

SNAP potential for W [88]

4 The Materials Design Forcefield Format - FRC

The advantages of the .frc format are as follows:

- **automated atom type assignment** using the templates section of the .frc file
- **wildcards**
- **atom type equivalences** for nonbonds, bonds, angles, torsions, etc.
- **versioning**: each parameter has its own version, so updates do not remove older parameters but override them
- **includes**: a user can modify a forcefield by including the original, adding parameters and, by using version numbers, override parameters in the original

The .frc format is much more compact and makes it easy to see and edit parameters. Wildcards are the ability to specify '*' for an atom type. For example, the AUA forcefield specifies angles as C-CH2-C, where the terminal C can be almost any type of C atom, -CH3, -CH2-, -CH<, olefinic, ketone, etc. When you enumerate the permutations, it grows to be a very large list, which must be explicitly enumerated in e.g. GIBBS' potparam.dat file.

With wildcards once specify one angle as *-CH2-*, where * matches any atom. More specific angles, like an alcohol *-C-O, including completely specific ones such as H-C-O take precedence in the obvious order. This also occurs in torsions, where typically the terminal atoms do not matter: *-CH2-CH2-*

For an example of the power of including forcefield files and version numbers, look at the oplsaa+.frc file, which includes the original oplsaa.frc, extensions published elsewhere (oplsaa-extended.frc), and adds some customs additions by Materials Design:

Include FF

!MD forcefield 1
#version oplsaa+.frc 1.0 12-Aug-2010
#define oplsaa+ default
!Ver Ref Function Label

[86] Thompson, Swiler, Trott, Foiles and Tucker, arxiv.org, 1409.3880 (2014)
[87] M.A. Wood, M.A. Cusentino, B.D. Wirth, and A.P. Thompson, "Data-driven material models for atomistic simulation", Physical Review B 99, 184305 (2019)
[88] Wood, M. A. and Thompson, A. P. "Quantum-Accurate Molecular Dynamics Potential for Tungsten" arXiv:1702.07042 [physics.comp-ph]

```
!—- — ———————————— ———
1.0 1 atom_types oplsaa oplsaa-extended oplsaa+
1.0 1 equivalence oplsaa oplsaa-extended oplsaa+
1.0 1 quadratic_bond oplsaa oplsaa-extended oplsaa+
1.0 1 quadratic_angle oplsaa oplsaa-extended oplsaa+
1.0 1 torsion_opls oplsaa oplsaa-extended oplsaa+
1.0 1 wilson_out_of_plane oplsaa oplsaa-extended oplsaa+
1.0 1 nonbond(12-6) oplsaa oplsaa-extended oplsaa+
1.0 1 bond_increments oplsaa oplsaa-extended oplsaa+
1.0 1 templates oplsaa
#include oplsaa_extended.frc
```

The first section is a definition of the OPLSAA+ forcefield, listing the functional forms and the sections of the file(s) that contain the parameters. In this case the forcefield uses the 'OPLSAA' section (which will come from oplsaa.frc via an include in oplsaa-extended.frc) and the 'oplsaa+' section (which is in this file). Next it includes the entire extended OPLS forcefield.

Atom Types

```
#atom_types oplsaa+ 200


> Atom type definitions for oplsaa+
> Masses from OPLSAA publications

!Ver Ref Type Mass Element Connections Comment
!—- — —- ———- ———————————————
! 1.0 1 CT 12.011000 C 4 sp3 aliphatic carbon

#equivalence oplsaa+ 200
@columns nonbond bond angle torsion oop bond_increment

! Equivalences
!———————————————
!Ver Ref Type NonB Bond Angle Torsion OOP BINCR
!—- — —- —- —- —— ——- —- ——
! 1.0 1 CT CT CT CT CT CT CT

#quadratic_bond oplsaa+ 200
> E = K2 * (R - R0)^2

!Ver Ref I J R0 K2
!—- — —- —- ——- ———
! 1.0 1 CT CT 1.5290 268.0000

#quadratic_angle oplsaa+ 200
> E = K2 * (Theta - Theta0)^2

!Ver Ref I J K Theta0 K2
```

```
!—- — —- —- —- ——— ———-
! 1.0 1 CT CT CT 112.7000 58.3500

#torsion_opls oplsaa+ 200
> E = SUM(n=1,4) { [V(n)/2] * [ 1 - ((-1)^n)cos(n*Phi + Phi0(n)) ] }
> with '1-4' interactions scaled by 0.5
@units V kcal/mol
@units Phi degree

!Ver Ref I J K L V1 Phi0 V2 Phi0 V3 Phi0 V4 Phi0
!————————————————————————————————
! 1.0 1 CT CT CT CT 1.7400 0.0 -0.1570 0.0 0.2790 0.0 0.0000 0.0

#wilson_out_of_plane oplsaa+ 200
> E = K * (Chi - Chi0)^2

!Ver Ref I J K L K Chi0
!—- — —- —- —- —- ———- —-
! 1.1 4 CT CT HC HC 0.0 0.0

#nonbond(12-6) oplsaa+ 200
> E = 4.0*eps(ij) [(r0(ij)*/r(ij))**12 - (r0(ij)*/r(ij))**6]
> where r0(ij)* = sqrt((r0(i)*)*(r0(j)*))
> eps(ij) = sqrt(eps(i) * eps(j))
@combination geometric
@type r0-eps
@units Sigma Ang
@units Epsilon kcal/mol

!Ver Ref I r0 eps
!—- — —- ——— ———
! 1.0 1 CT 3.50000 0.06600

#bond_increments oplsaa+ 200

!Ver Ref I J DeltaIJ DeltaJI
!—- — —- —- ———- ———-
! 1.0 1 CT CT 0.0000 0.0000

#reference 1
Additional Materials Design OPLSAA forcefield parameters
@Author D. Rigby
@Date 12-Aug-2010
#end
```

This section adds a new atom type for sp3 aliphatic carbon, 'CT'. Each section of the file has the name of the section optionally followed by an increment to version number, 200 in this case. This increment is added to the version numbers in the section, so the practical version number of the 'CT' atom type is 1.0+200 = 201.0. Assuming that the OPLSS/AA forcefield uses version numbers less than 200, the 'CT' atom type would override any 'CT' atom types in OPLSS/AA. This allows you to take similar forcefields and let one

override the other without modifying all the version numbers.

The next section defines equivalences, which simply say that when looking for the bond parameters for 'CAh1'use 'CA', but when looking for bond increase parameters, use a different value for 'CAh1', Thus we have a new atom type that is much like sp2 aromatic carbon, but the bond increments are different.

Equivalences

#equivalence oplsaa
@columns nonbond bond angle torsion oop bond_increment

! Equivalences
!————————————————————
!Ver Ref Type NonB Bond Angle Torsion OOP BINCR
!—- — —- —- —- —— ——- —- ——
1.0 1 Ar Ar Ar Ar Ar Ar Ar
1.1 4 C C C C C C C
1.0 1 CA CA CA CA CA CA CA
1.1 7 CAh1 CA CA CA CA CA CAh1

Having a higher version overrides the previous line, and now we can use specific bond increment parameters for our 'CAh1' atom type.

Bond Increments

#bond_increments oplsaa

!Ver Ref I J DeltaIJ DeltaJI
!—- — —- —- ——- ——-
1.0 1 CA CA 0.0000 0.0000
1.1 6 CA CZ1 0.0350 -0.0350
1.0 1 CA HA -0.1150 0.1150
1.1 9 CA OH5 0.1500 -0.1500
1.1 7 CAh1 CAh2 0.1460 -0.1460
1.1 7 CAh1 HA -0.0120 0.0120
1.1 7 CAh1 NC 0.3390 -0.3390

The last section of the example, the bond increment section, adds the bond parameters for our new 'CAh1' atom type. In addition, it adds or overrides some other bond parameters.

The final section concerns templates: It is by far the most complicated section, and unfortunately due to its nature cannot be versioned or added to. It must be taken as a whole unit because it specifies which atom type to assign to an atom in a structure, and hence is 'aware' of all the atom types in the forcefield and the relationship between them. Hence being monolithic.

If you need to modify the template section, copy the existing template section into the top level file and define this as the location of templates in the default section. Under normal circumstance you would inherit the template section from an included forcefield file and not touch it.

These extracts illustrate some of the important features. Each section defines how a local portion of the structure maps to an atom type. Each section is for an atom type and must contain the 'template:' line, which gives the topology.

Templates

#templates oplsaa

type: ?
! anything
template: (>*)
end_type

As usual, '*' is a wild card.

Parentheses around the template indicate that there may be other bonds to the atom that are not contemplated in the template; square brackets indicate that the template includes all bonds, and that extra bonds are not allowed. So the first template matches anything.

The '*' wildcard matches any element and the surrounding parentheses allow any number of bonds.

The atom type is '?' which is our shorthand for an atom for which there are no parameters. The next template is also quite simple: it matches any argon atom, regardless of whether it has bonds to it or not. If we wanted an explicit match for just argon atoms, i.e. without any bonds, we would surround the template with square brackets instead of a parenthesis.

Template for Ar

type: Ar
! Argon atom
    template: (>Ar)
end_type

For bonds we use '-' for single bonds, '=' for double bonds, ':' for aromatic bonds, and '#' for triple bonds; '~' matches any bond order, i.e. it is a wildcard.

Template for C in esters/acids

type:C
! Carbonyl carbon in carboxylate esters
template: (>C(-C)(-O(-C))(=O))
end_type

type:C
! Carbonyl carbon in carboxylic acids
template: (>C(=O)(-O(-H)))
end_type

Modifiers can narrow down the scope of wildcards: Allowed modifiers are hybridization, aromaticity, and elements:

Templates with wildcards

```
type:CA
! SP2 aromatic carbon
template:(>C(~*)(~*)(~*))
        atom_test:1
                hybridization: SP2
                aromaticity:AROMATIC
        end_test
end_type

type:CA
! This is used for aromatic carbons that fail the aromaticity test if
! the ring checker is unable to detect a ring with more than seven
! or eight sides. The NON_AROMATIC test is to eliminate the conflict
! with the above 'CA' definition.
template: [>C(-*)(:*)(:*)]
        atom_test:1
                hybridization:SP2
                aromaticity:NON_AROMATIC
        end_test
end_type

type:CAh1
! Aromatic carbon pyridine atom 2
template: (>C(:N))
end_type

type:CAh2
! Aromatic carbon pyridine atom 3
template: (>C(:C(:N)))
end_type
```

This template is quite specific for water. The square brackets both around the entire template and about the O and second H sees to that: there can be no other bonds anywhere.

Template with square brackets

```
type:HW
! TIP3P water hydrogen
template: [>H[-O[-H]]]
end_type
```

This template is less specific, but fits e.g. CO_2 and CS_2. It would also fit e.g. Ar-C-Ar and other nonsensical structures.

Template with square brackets and wildcards

```
type:c2=
! Carbon in =C= (e.g. CO2, CS2)
template: [>C[~*][~*]]
end_type
```

This is a key issue in forcefields: they know what they do match, but not what they don't!

With wildcards they tend to match many unintended things. So in the case of Ar-C-Ar, we would assign atom types just fine and (hopefully) still not be able to run because there would be missing Ar-C bond parameters and Ar-C-Ar angle parameters. On the other hand, if we had been lazy, and defined a set of generic bond parameters for 'C-*' and angle parameters for '*-C-*' we would be off and running . . . garbage! It might be reasonable to have a catch-all angle term like '*-C-*' since specific hybridization of the carbon atom (sp in this case) does roughly define the angle terms. But never a bond term like 'C-*'! That is not reasonable since the bond length and strength depends on the second atom. And it is very dangerous, though the code will let you be foolish.

This brings us to more restraint use of wildcards: Here we see explicit tests that limit the power of the wildcards. The atom numbers are in the order the atoms appear in the templates, so the carbon of interest must be sp2; the two atoms other than oxygen that are bonded to it must be a C or H and an O or N. In other words this will match -C-C(=O)-OH, or H-C(=O)-OH, or -C-C(=O)-NH2 but not -C-C(=O)-C-. The modifiers for wildcards can be hybridization, which elements, and whether it is aromatic. At the moment, the code for recognizing hybridization and aromaticity is only partially complete.

Templates

```
type:c3'
! Carbonyl carbon [one polar substituent such as O,N]
! e.g. amide, acid and ester
template: (>C (~O) (~*) (~*))
        atom_test:1
                hybridization:sp2
        end_test
        atom_test:3
                allowed_elements: C, H
        end_test
        atom_test:4
                allowed_elements: O, N
        end_test
end_type
```

The implementation in OPLS avoids the hybridization requirement and does not handle all cases, but goes through acids, esters, and, as shown amides:

Templates

```
type:C
! Carbonyl carbon in amides
template: (>C(-*)(=O)(-N(-*)(-*)))
        atom_test:2
                allowed_elements: C,H
        end_test
        atom_test:5
                allowed_elements: C,H
        end_test
        atom_test:6
                allowed_elements: C,H
        end_test
end_type
```

Though not shown in this example, templates can match next nearest neighbors, etc. For example, the template for a carbon attached to an azide (-N3 group) looks like this:

Templates

```
type: c4z
! Carbon, sp3, bonded to -N3 (azides)
template: (>C(-N(~N(~N)))(-*)(-*)(-*))
        atom_test:1
                hybridization:SP3
        end_test
end_type
```

The last section in the example is the precedence tree. An atom in a structure may match several templates, yielding different atom types. The precedence tree solves this ambiguity by providing a tree of atom types. The most specific match, i.e. the furthest from the trunk down a branch wins. The parentheses group the branches together but are admittedly rather hard to read.

Precedence tree

```
precedence:
(?
        (Ar)
        (C)
        (CA (CAh1 (CQ) (CAh6)) (CAh2 (CAh5) (CAh7) (CAh8)) (CAh3 (CAh4)) (CR)
        (CRh1)
        (CS (CAh9) (CSh1(CV)) (CSh2 (CAh0) (CVh1)) (CU) (CUh1) (CWh1 (CWh3)
        (CWh5)) (CWh2 (CWh4) (CWh6)) ) )
        (CM)
```

```
        (CO)
        (CT (CT1) (CTEX) (CTfn) (CTf4) )
        (CZ (CZ1) )
        (F)
        (H (HEX4) (HEX5) (HEX6) )
        (HC (HA (HC2)) (HC1) (HC2) (HC3) (HC4) (HC5) (HC6) )
        (He)
        (HO (HW) )
        (HS)
        (Kr)
        (N (N1) (N2) (N3))
        (NA (NAh2) (NAh3))
        (NB)
        (NBh1)
        (NBh2)
        (NBh3)
        (Ne)
        (NC)
        (NO)
        (NT)
        (NT0)
        (NT2 (NTC4) )
        (NT3)
        (NZ)
        (O)
        (O1)
        (O2)
        (O3)
        (O4)
        (OH (OH2 (OH3) ) (OH4) (OH5) (OW) )
        (ON)
        (OS (OS1) )
        (OW)
        (S)
        (SH)
        (SH1)
        (Xe)
)
end_precedence
```

Other groups such as AMBER do have some level of typing engines, but mostly the bio-organic community relies on the regularity of peptides, proteins and DNA to use systematic atom naming schemes and 'template libraries' to match the atom types. Thus a protein is built from peptide fragments that alcreated have the atom names and atom types assigned by hand. Since there are only twenty some amino acids, creating the fragment library is quite feasible. Proteins from the PDB also have systematic names for the atoms, so the template libraries match the atom types with the names. These are not, however, very general solutions.