Documentation

This file provides general information about the workings of the code, for those who want to make modifications. No guarantee that any of this is correct; it was compiled while reading through the program to understand what it is doing, not to check the program. Also, some of it was based on an abbreviated 1985 version of the program and may not apply to the full 1986 version.

General notes

The code uses Angstrom, picoseconds, atomic mass, and electron volt units. So it is frequently converting between eV and AMU A^2/ps^2. See ECONV in the variable name table.

Real*8 numerical precision is needed, or bcuint has notable round-off error. The same is almost certainly true for the other spline interpolation subroutines.

For the ideas behind the code, see Phys. Rev. B, Vol 42, pp 9458-9471 for formulae and their symbols. Also note, however

- The values found for AD, AXL, ... for V_A in param.f are grossly incompatible with those in Brenner's paper.
- Moreover, it appears that the potential V_A for CC in the program is made up of *three* of the exponential expressions as listed in the paper, (AD, AXL/ BD, BXL / CD, CXL), with expression A dominating for small r, being overtaken by C at 1.8, and B similar to C.
- The repulsive potential seems to have an additional factor $(1 + const/r)$, presumably to strongly prohibit atoms penetrating to the center of another atom. The const is small, about 0.3.
- $N_i^{(C)}$, $N_i^{(H)}$, $N_i^{(t)}$ are really N_{ij} values since j is excluded in the sums.
- G_i for carbon has been made dependent on $N_i^{(t)}$: the program switches smoothly to a different representation for G_i between 4.2 and 4.7 neighbors to the i-atom (including j), i.e. it switches in the range $3.2 < N_i^{(t)} < 3.7$
- δ_{ij} has been hardcoded in pibond to be 0.5 for CC, CH, HC, HH
- The program seems to square the sums in N_{ij}^{conj}
- The program includes a "torsional interaction" for CC bonds. The added torsional potential is:
    $V^{tor} = V_A(|r_{ij}|) A_{ij}(N_i^{(t)}, N_j^{(t)}, N_{ij}^{conj}) \Sigma_{kl} \sin^2(\varphi_{ijkl}) f_{ik} f_{jl}$
  where φ_{ijkl} is the angle between the ijk and the ijl planes, and the sum extends over $k \neq ij$, $l \neq ij$, $|\sin(\theta_{ijk})| > 0.1$, and $|\sin(\theta_{jil})| > 0.1$. The f-values are hardcoded to special values for H.
- The conditions on the sines in V^{tor} imply that energy is NOT conserved when three atoms become almost along the same line. So, if there is a problem with energy conservation, try turning of the torsional potential by setting ndihed to 10 in Subroutines/Bond$_{Order}$/param.f.
- Alternatively, the subroutine has been modified to allow the restrictions to be smoothed. Setting SINHI to 0.2 and SINLO to 0.0 smooths the cut-off at 0.1 over that range and energy should again be conserved:
    $V^{tor} = V_A(|r_{ij}|) A_{ij}(N_i^{(t)}, N_j^{(t)}, N_{ij}^{conj}) \Sigma_{kl} \sin^2(\varphi_{ijkl}) f_{ik} f_{jl} Z_{ijk} Z_{jil}$
  where in the smoothing range
    $Z_{ijk} = 1 + \cos(\pi (\sin(\theta_{ijk}) - SINHI)/(SINHI - SINLO))$

$$Z_{jil} = 1 + \cos(\pi \,(\sin(\theta_{jil})\text{-SINHI})/(\text{SINHI-SINLO}))$$

- The program includes a Lennard-Jones potential: $V_{LJ}= 4\, \varepsilon_{ij}\, [(\sigma_{ij}/r_{ij})^{12} - (\sigma_{ij}/r_{ij})^{6}]$

  where ε is read in in K (corresponding to energy k K).
  Interactions between two different type atoms use a geometrically average of the ε values of each atom and a straigth average σ.

  The Lennard-Jones potential is set to zero for $r_{ij} > 2.5\, \sigma_{ij}$ and in the range $r_{ij} < R_{ij}^{(2)}$ in which the bond order potential is nonzero. In the range $R_{ij}^{(2)} < r_{ij} < 0.95\, \sigma_{ij}$;, the potential is furthermore replaced by a cubic which vanishes quadratically at $R_{ij}^{(2)}$ and which meets the Lennard-Jones expression with continuous first derivative at $0.95\, \sigma_{ij}$.

  The discontinuity at $2.5\, \sigma_{ij}$ means that energy is *not* preserved. I put in a variable ISMTH which can be changed to a nonzero value to substract the potential value at the cut-off, thus making the potential continuous. Note however that this changes the forces in the range described by the cubic.

Common blocks

The program uses common blocks for most variables which are loaded into each subroutine through common_files.inc:

- common_ch.inc: hydrocarbon potential common blocks
- common_lj_new.inc: Lennard-Jones common blocks
- common_tb.inc: tight binding
- common_md.inc: general
- common_leon.inc: added by me

I/O units

The following Fortran I/O units are in use by the code:

- 1: xmol.d (to be post converted to xmol.xyz)
- 9: output.d
- 11: coord.d
- 13: input.d
- 14-18: REBO potential splines
- 23: for bombard.f
- 41: (used in the periodic box straining modification)
- 50: overwrite.d
- 51: load.d
- 53: fort.53 debug file
- 55: max_ke.d
- 85: pair_energy.d eigenvectors.d
- 86: eigen_energies.d
- 87: dos.d
- 88: ldos.d

I moved pair_energy.d to I/O unit 84.

Files are opened in open.inc, closed in close.inc.

Subroutines

Here is a list of subroutines and what they do:

Bcuint
>   Bicubic interpolation of CLM; also returns derivatives.

Bere
>   Berendsen thermostat: KFLAG=1 damping; KFLAG=other(=5): rescale velocity.

Bombard
>   Adds a single atom from file bombard.d.

Caguts
>   Finds forces on atoms from pair potentials.

Ccorr
>   Call the corrector.

Cpred
>   Calls Pred (if there are nonrigid molecules) and increments time.

Damage
>   Checks whether the number of carbons less than 1.8 apart changes, indicating damage..

Gleq
>   Langevin (friction and random force).

Hoov
>   Evans-Hoover thermostat.

Ljcont
>   Seems to give net Lennard-Jones potential exerted by e semi-infinite continuum with a normal in the 'ndir' direction, at a location 'surf'.

Model
>   Calls Caguts (if not tight binding).

Mtable
>   Creates tables of the potentials V_A and V_R from the Brenner paper..

Param
>   C and H potentials.

Pibond
>   Finds bonding forces involving C and H atoms.

Pred
>   Nordsieck scheme prediction of z_{n+1} from z_n only.

Radic
>   Tricubic interpolation of CLMN.

Rannum
>   Random number generator. Its argument is unused..

Read_data
>   Reads input.d and coord.d.

Set_md
>   Initialize time and such, also sets ENPR.

Setgle
>   Set langevin parameters..

Setin
>   Initialize kt, xmass, noa, sig, eps, pi, bolz, avo, epsi, econv.

Setpc

Set Nordsieck parameters (except F22=1).

Setpp

Calls param and mtable.

Setran

Initializes RNG, called once at the start..

Setrn

Random number initialization. Only called once, inside setran.

Thermos

Chooses thermostat routine.

Tor

Torsional interaction TLMN tricubic interpolation.

Write_data1

Writes to output.d.

Write_data2

Writes to unit 9, output.d, the step number, average energy per atom, some kinetic energy; writes to unit 6 (the screen) total potential energy. Modified by me to write more output to the screen less frequently.

Write_data3

Overwrites 11, coord.d, .

Xmol

Writes to 1, xmol.d data to be converted later to .xyz files..

Zero

Zero velocities.

vscale

Seems to be some attempt to select the scalings that give minimum potential energy.

Variable Names (General)

The meaning of variable names, as well as I can make out follows. See Phys. Rev. B, Vol 42, pp 9458-9471 for formulae and their symbols. Also, I define the additional variables:

- $e_{ijk} = \exp(\alpha_{ijk}[(r_{ij} - R_{ij}^e) - (r_{ik}-R_{ik}^e)])$
- $f_{ij} = f_{ij}(|r_{ij}|)$
- $V_{ijkl}^{tor} = V_A(|r_{ij}|)\, A_{ij}(N_i^{(t)},N_j^{(t)},N_{ij}^{conj})\, \sin^2(\varphi_{ijkl})\, f_{ik}\, f_{jl}$ (a term in the torsional potential)
- b_{ij} is defined by the relation $B_{ij} = b_{ij}^{-\delta}$

- AD(KT1,KT2): $D_{ij}^e\, S_{ij}\, \exp(AXL\, R_{ij}^e)/(1 - S_{ij})$ value 1
- ATABLE(KT1,KT2,$1 + r_{ij}/DDtab$): attractive potential $V_A/2$ function table
- ATT: = 3.2; the value of $N_i^{(t)}$ at which the evaluation of G_i for $0<\theta<109$ starts to smoothly switch to a different polynomial
- AXL(KT1,KT2): $\sqrt{2/S_{ij}}\,\beta_{ij}$ value 1
- BD(KT1,KT2): $D_{ij}^e\, S_{ij}\, \exp(AXL\, R_{ij}^e)/(1 - S_{ij})$ value 2
- BXL(KT1,KT2): $\sqrt{2/S_{ij}}\,\beta_{ij}$ value 2
- CD(KT1,KT2): $D_{ij}^e\, S_{ij}\, \exp(AXL\, R_{ij}^e)/(1 - S_{ij})$ value 3
- CLM(KT2,$1+N_i^{(H)}$,$1+N_i^{(C)}$,term): bicubic splines H_{CC} and H_{CH} in inter2d$_{iv}$.d

- CLMN(1,1+$N_i^{(t)}$,1+$N_j^{(t)}$,N_{ij}^{conj},term): tricubic splines 2 F_{CC} from inter3d$_{iv}$.d
- CLMN(2,1+$N_i^{(t)}$,1+$N_j^{(t)}$,N_{ij}^{conj},term): tricubic splines 2 F_{CH} from inter3d$_{ch}$.d
- CLMN(3,1+$N_i^{(t)}$,1+$N_j^{(t)}$,N_{ij}^{conj},term): tricubic splines 2 F_{HH} from inter3d$_h$.d
- COM: (in Corr) velocity of center of gravity
- COR(K,.): R0(I,.) - R0(j,.) by interacting atom pair index K
- CUBE(3): cube dimensions, set to 1e20 if not periodic
- CUBE2(3): cube dimensions/2, set to .5e20 if not periodic (never used)
- CXL(KT1,KT2): sqrt(2/S_{ij}) β_{ij} value 3
- DATABLE(KT1,KT2,1 + r_{ij}/DDtab): attractive potential's derivative * 2 table
- DD(KT1,KT2): D_{ij}^e exp(DXL R_{ij}^e) /(1 - S_{ij})
- DDTAB(KT1,KT2): r_{ij}-spacing of the potential tables
- DELLJ: table spacing for Lennard-Jones potential, 0.001 A
- DELTA: time step
- DELTSQ: DELTA^2/2
- DEXX1(K): derivative of the attractive potential V_A / 2 of a pair K
- DRTABLE(KT1,KT2,1 + r_{ij}/DDtab): repulsive potential's derivative table
- DWW(K): derivative of $f_{ij}(r_{ij})$ for a pair of neighbors
- DXL(KT1,KT2): sqrt(2 S_{ij}) β_{ij}
- EATOM(I): potential energy of an atom
- ECONV: Conversion factor: 103.6434 eV per (amu A^2/fs^2)
- EN(NSMAX): never used, intended to store an energy?
- EPS(KT1,KT2): Initially depth ε of Lennard-Jones potential in K (i.e. energy kK), converted internally to 4 eV units
- EPSS: strength constant in the LJ potential induced by a semi-infinite solid
- ETOT(NSMAX): never used, probably intended to store the time history of the total energy
- EXX1(K): attractive potential V_A / 2 of a pair of neighbors K
- I2D: potential version number in inter2d$_{iv}$.d
- I3D: potential version number in inter3d$_{iv}$.d, inter3d$_h$.d, inter3d$_{ch}$.d
- IDUM: set to 0 by make_tube, set to 3 by xmol, maybe to indicate that only one parameter, position, exists in the .d file.
- IGC: Interpolation index, 4 for 1>=c>-1/3, 3 for -1/3>=c>-1/2, 2 for -1/2>=c>-2/3, 1 for -2/3>=c, with c=cos(θ), used for the G_i function of carbon
- IGH: Interpolation index, 3 for 1>=c>-1/2, 2 for -1/2>=c>-5/6, 1 for -5/6>=c>-2/3, with c=cos(θ), used for the G_i function of hydrogen
- IN2(term,variable): powers of the terms of the 2D spline
- IN2(term,variable): powers of the terms of the 3D spline
- IPIB: number of times pibond has been called
- IPOT: 1=REBO, 2=Tight binding
- IT: in Caguts, the interpolation interval
- ITD: potential version number in inter3dtors.d
- ITR: 2 is nonmoving, 1=moving and thermostated, other=moving only
- IVCT2B: first atom of the pair in the list of interacting atom pairs
- JVCT2B: second atom of the pair in the list of interacting atom pairs ($\neq$I)
- KEND: number of interacting atom pairs
- KFLAG: thermostat flag: -1 Langevin; 1 Berendsen; 2 zero velocity; 3 Evans-Hoover; 5 Berendsen after corrector; 6 minimize energy; 8 rescale to minimize energy

- KT2: inverse array to KT
- KT: atom code indexed by atom number (C=1, H=2, ...)
- KTYPE: atom code kt, but by atom index
- KVC: number of steps to take
- LCHECK: 1=both C|H; 2=both Si|Ge; 0=one C|H, one Si|Ge, or distance > RMAX
- LCHK: 1=update neighbors list; 2=still OK
- LIST: Same as JVCT2B
- LSTEP: step number
- MAXKB: steps between data writing using write$_{data2}$
- MLIST: atoms that get advanced in time (all atoms with itr$\neq$2)
- NABORS: start in (IVCT2B,JVCT2B,LIST) of the list of neigbors of an atom
- NATX: number of atoms used in tight-binding matrices. MUST be set equal to np before compiling.
- NDIR: direction of the surface normal of a neighboring semi-infinite continuum
- NLA: never used or assigned a value. Probably number of Langevin atoms, to be ignored in adaptive time step modifications
- NLIST: atoms that get damping and random forces added in Gleq, damping in Bere
- NLMAX: maximum number elements in neighbor list
- NMA: number of atoms in MLIST
- NOA: number of atoms of each type
- NP: number of atoms
- NPMAX: maximum number of atoms
- NRA: never used or assigned a value. Probably number of rigid atoms, to be ignored in adaptive time step modifications
- NSMAX: (or NSMAS) maximum number of steps. Derived arrays never used.
- NTA: number of atoms in NLIST
- NTAB: array size for potential table look-up
- NTYPES: maximum number of different types of atoms allowed for Len-Jon potential
- NXMOL: number of steps between xmol writes
- PSEED: random number seed
- R0: position / Nordsieck component 0
- R0L: position when the neighborhood list was updated
- R1: velocity when read from 11, internally converted into Nordsieck component 1
- R2: Nordsieck component 2
- R3: Nordsieck component 3
- R4: Read from coord.d and written to it but never used anywhere, all zeros
- RB1: distance $R_{ij}^{(1)}$ at the start of the bond order potential decay
- RB2: distance $R_{ij}^{(2)}$ at which the bond order potential is gone
- RCOR: distance between a pair of interacting atoms
- REG: $\exp(\alpha_{ijk} [R_{ik}^{e} - R_{ij}^{e}])$
- RLIST: square interaction distance between two atom types, used to create neighbor list = $(R_{ij}^{(2)})^2$
- RLL: .5*RLL is the distance over which molecules can move without changing the neighbor list; RLL must be less than min(RB2)
- RMAX: largest square distance at which interaction is computed = $(R_{ij}^{(2)})^2$
- RMAXLJ: largest square distance at which LJ interaction is computed; $(2.5 \, \sigma_{ij})^2$ or 0 if ε=0
- RNP: force on the atoms
- RPP: gradient of potential energy for a pair

- RSLJ: square distance within which atoms might interact through LJ; (sqrt(RMAXLJ)+RLL)^2 or 0 if ε=0
- RSPL: start of the cubic LJ potential range; 0, or for C-H or Si-G pairs with nonzero ε set to 0.95 σ_{ij}
- RSPLS: RSPL^2 or undefined if ε=0
- RTABLE(KT1,KT2,1 + r_{ij}/DDtab): repulsive potential V_R function table
- SIG(KT1,KT2): equilibrium distance σ of Lennard-Jones potential, converted internally to its square
- SIGS: scale constant in the LJ potential induced by a semi-infinite solid
- SPGC: $G_C(\theta) = \Sigma_{p=0}^{5}$ SPGC(p+1,IGC) cos$^p(\theta)$ where IGC depends on the interval in which cos(θ) is, with IGC=5 an alternate version for the last interval switched to for large enough $N_i^{(t)}$
- SPGH: $G_H(\theta) = \Sigma_{p=0}^{5}$ SPGC(p+1,IGH) cos$^p(\theta)$ where IGH depends on the interval in which cos(θ) is
- RSPL(KT1,KT2): set to 0.95 σ
- SURF: NDIR-location of the surface of a neighboring continuum
- TABDFC(KT1,KT2,1 + r_{ij}/DDtab): cut-off function's derivative table
- TABFC(KT1,KT2,1 + r_{ij}/DDtab): cut-off function table
- TEM: temperature
- TLMN(1+N_i^t,1+N_j^t,N_{ij}^{conj},term): tricubic splines for 2 A_{ij} from inter3dtors.d
- TOTE: total potential energy
- TTCONV: 2/(3 NP)
- TTIME: total time
- VOL: box volume (never used)
- WW(K): $f_{ij}(r_{ij})$ for a pair of neighbors
- XDB: α_{ijk}
- XH(KT2,1+N$^{(H)}$,1+N$^{(C)}$): values of H_{CC} and H_{CH} at the spline collocation points
- XH1: derivative of XH wrt N^C
- XH2: derivative of XH wrt N^H
- XHC(I,1): 1 + sum of atom i's C neighbors' f_{ij} values
- XHC(I,2): 1 + sum of atom i's H neighbors' f_{ij} values
- XMASS: atomic mass, ordered by KT
- XM(KT1,KT2): sqrt(XMM) or undefined if ε=0
- XMM(KT1,KT2): minimum square distance for LJ interaction; 0, or ($R_{ij}^{(2)})^2$ for C-H or Si-G pairs with nonzero ε
- XMMS(KT1,KT2): square radius of the inner range in which we will definitely not compute a LJ potential; corrected to max(0,sqrt(XMM)-RLL)^2 or undefined if ε=0
- XMT: total mass
- XQM: = 3.7; the value of $N_i^{(t)}$ at which the evaluation of G_i for 0<θ<109 ends switching to a different polynomial

Variable Names (pibond.f)

Since subroutine pibond is probably the most impenetrable one, I include a separate list of local variables in pibond:

- AA: $d(V_{ijkl}^{tor})/d(T2)$ keeping V_A, A_{ij}, $T1$, f_{ik}, f_{jl}, Z_{ijk}, Z_{jil} fixed
- AAA1: $V_{ijkl}^{tor}/f_{ik} \, f_{jl} \, Z_{ijk} \, Z_{jil}$
- AT2: $- T1 \, d(V_{ijkl}^{tor})/d(T1)$ keeping V_A, A_{ij}, $T2$, f_{ik}, f_{jl}, Z_{ijk}, Z_{jil} fixed
- ATOR: $A_{ij}(N_i^{(t)}, N_j^{(t)}, N_{ij}^{conj}) * 2$ in the torsional potential
- BIJ: B_{ij}
- BJI: B_{ji}
- BTOR: $\Sigma_{kl} \sin^2(\varphi_{ijkl}) \, f_{ik} \, f_{jl}$ in the torsional potential
- BTOT: bar $B_{ij} * 2$
- CFUNI(NK): $F(x_{ik})$
- CFUNJ(NL): $F(x_{jl})$
- CJ: $r_i - r_j = r_{ij}$
- CK: $r_i - r_k = r_{ik}$
- CL: $r_j - r_l = r_{jl}$
- CONJUG: N_{ij}^{conj}
- CONK: $\Sigma_k \, f_{ik} \, F(x_{ik})$
- CONL: $\Sigma_l \, f_{jl} \, F(x_{jl})$
- COSK(NK): $\cos(\theta_{ijk})$
- COSL(NK): $\cos(\theta_{jil})$
- CRKX: x-component of $r_{ik} \times r_{ij}$
- CRKY: y-component of $r_{ik} \times r_{ij}$
- CRKZ: z-component of $r_{ik} \times r_{ij}$
- CRLX: x-component of $r_{ij} \times r_{jl}$
- CRLY: y-component of $r_{ij} \times r_{jl}$
- CRLZ: z-component of $r_{ij} \times r_{jl}$
- DALDIK: $d(G_i)/d(N_i^{(t)})$
- DALDJL: $d(G_j)/d(N_j^{(t)})$
- DATORC: $d(A_{ij})/d(N_{ij}^{conj})$
- DATORI: $d(A_{ij})/d(N_i^{(t)})$
- DATORJ: $d(A_{ij})/d(N_j^{(t)})$
- DBDZI: $d(B_{ij})/d(b_{ij})$
- DBDZJ: $d(B_{ji})/d(b_{ji})$
- DBTOR*: never used
- DCFUNI: $f_{ik} \, d(F(x_{ik}))/d(x_{ik})$
- DCFUNJ: $f_{jl} \, d(F(x_{jl}))/d(x_{jl})$
- DCTIJ(NK): $d(\cos(\theta_{ijk}))/d(|r_{ij}|^2/2)$
- DCTIK(NK): $d(\cos(\theta_{ijk}))/d(|r_{ik}|^2/2)$
- DCTIL(NL): $d(\cos(\theta_{jil}))/d(|r_{il}|^2/2)$
- DCTJI(NL): $d(\cos(\theta_{jil}))/d(|r_{ij}|^2/2)$

- DCTJK(NK): $d(\cos(\theta_{ijk}))/d(|r_{jk}|^2/2)$
- DCTJL(NL): $d(\cos(\theta_{jil}))/d(|r_{jl}|^2/2)$
- DEXNI(1): $d(H_{ij})/d(N_i^{(C)})$
- DEXNI(2): $d(H_{ij})/d(N_i^{(H)})$
- DEXNJ(1): $d(H_{ji})/d(N_j^{(C)})$
- DEXNJ(2): $d(H_{ji})/d(N_j^{(H)})$
- DFCK: $d(FCK)/d(|r_{ik}|)$
- DFCL: $d(FCL)/d(|r_{jl}|)$
- DGDTHET: $d(G_i)/d(\cos\theta_{ijk})$ respectively $d(G_j)/d(\cos\theta_{jil})$
- DRADI: $d(\text{bar }B_{ij})/d(N_i^{(t)}) * 2$
- DRADJ: $d(\text{bar }B_{ij})/d(N_j^{(t)}) * 2$
- DRDC: $d(\text{bar }B_{ij})/d(N_{ij}^{\text{conj}}) * 2$
- DT1DIJ: $d(T1)/d(|r_{ij}|^2/2)/T1$
- DT1DIK: $d(T1)/d(|r_{ik}|^2/2)/T1$
- DT1DIL: $d(T1)/d(|r_{il}|^2/2)/T1$
- DT1DJK: $d(T1)/d(|r_{jk}|^2/2)/T1$
- DT1DJL: $d(T1)/d(|r_{jl}|^2/2)/T1$
- DT2DIJ(.): $d(T2)/d(r_{ij}(.))$
- DT2DIK(.): $d(T2)/d(r_{ik}(.))$
- DT2DJL(.): $d(T2)/d(r_{jl}(.))$
- EXNIJ: H_{ij}
- EXNJI: H_{ji}
- EXX: $e_{ijk} = \exp(\alpha_{ijk}[(r_{ij} - R_{ij}^e) - (r_{ik} - R_{ik}^e)])$ respectively e_{jil}
- FCK: f_{ik} (modified for H to $R_{ij}^1 = 1.3$, $R_{ij}^2 = 1.6$)
- FCL: f_{jl} (modified for H to $R_{ij}^1 = 1.3$, $R_{ij}^2 = 1.6$)
- GANGLE1: alternate value of GANGLE used for high $N_i^{(t)}$ or $N_j^{(t)}$
- GANGLE: $G_i(\theta_{ijk})$ respectively $G_j(\theta_{jil})$
- IG: G_i-interpolation interval index
- J: pair list index of pairs with i the first atom
- JN: j value, with iKI: KTYPE(i)
- KIKJ: KI+KJ
- KJ: KTYPE(j)
- KK: KTYPE(k)
- KN: second neighbor k≠j to i
- L: pair list index of pairs with j the first atom
- NK: counts number of secondary neighbors k of i
- NL: counts number of secondary neighbors l of j
- QI: $N_i^{(t)} = N_i^{(C)} + N_i^{(H)}$ (does not include j)
- QJ: $N_j^{(t)} = N_j^{(C)} + N_j^{(H)}$ (does not include i)

- RCK: $|r_{ik}|$
- RCL: $|r_{jl}|$
- RSQ2: $|r_{jk}|^2$ respectively $|r_{il}|^2$
- RSQ3: $|r_{ik}|^2$ respectively $|r_{jl}|^2$
- RSQIJ: $|r_{ij}|^2$
- S3: $|r_{ik}|$ respectively $|r_{jl}|$
- SDALIK: $d(\Sigma_k\, G_i\, f_{ij}\, e_{ijk})/d(N_i^{(t)})$
- SDALJL: $d(\Sigma_l\, G_j\, f_{ji}\, e_{jil})/d(N_j^{(t)})$
- SIJ: $|r_{ij}|$
- SINK(NK): $\sin(\theta_{ijk})$
- SINL(NK): $\sin(\theta_{jil})$
- SSUMK: $\Sigma_k\, G_i\, f_{ij}\, e_{ijk}$
- SSUML: $\Sigma_l\, G_j\, f_{ji}\, e_{jil}$
- T1: $|r_{ik} \times r_{ij}|\, |r_{jl} \times r_{ji}|$
- T2: $(r_{ik} \times r_{ij}) \cdot (r_{jl} \times r_{ji})$; negative if k and l point to the same side of i-j
- VATT: $V_A / 2$
- VDBDI: $d(V)/d(b_{ij})$
- VDBDJ: $d(V)/d(b_{ji})$
- VDRDC: $d(V)/d(N_{ij}^{conj})$
- VDRDI: $d(V)/d(N_i^{(t)})$
- VDRDJ: $d(V)/d(N_j^{(t)})$
- XK: $r_j - r_k = r_{jk}$
- XL: $r_i - r_l = r_{il}$
- XNI(1): $= 1 + N_i^{(C)} = 1 +$ atom i's C neighbors f_{ik} values excluding j
- XNI(2): $= 1 + N_i^{(H)} = 1 +$ atom i's C neighbors f_{ik} values excluding j
- XNJ(1): $= 1 + N_j^{(C)} = 1 +$ atom j's C neighbors f_{jl} values excluding i
- XNJ(2): $= 1 + N_j^{(H)} = 1 +$ atom j's C neighbors f_{jl} values excluding i
- XNT1: $N_i^{(t)}+1$
- XNT2: $N_j^{(t)}+1$
- XSIJ: $d(\Sigma_k\, G_i\, f_{ij}\, e_{ijk})/d(|r_{ij}|^2/2)$
- XSIK(NK): $d(G_i\, f_{ij}\, e_{ijk})/d(|r_{ik}|^2/2)$
- XSIL(NL): $d(G_j\, f_{ji}\, e_{jil})/d(|r_{il}|^2/2)$
- XSJI: $d(\Sigma_l\, G_j\, f_{ji}\, e_{jil})/d(|r_{ij}|^2/2)$
- XSJK(NK): $d(G_i\, f_{ij}\, e_{ijk})/d(|r_{jk}|^2/2)$
- XSJL(NL): $d(G_j\, f_{ji}\, e_{jil})/d(|r_{jl}|^2/2)$
- XX: x_{ik} respectively
- ZF1: Z_{ijk}
- ZF1DCT: $d(Z_{ijk})/d(\cos(\theta_{ijk}))$

- ZF2: Z_{jil}
- ZF2DCT: $d(Z_{jil})/d(\cos(\theta_{jil}))$

[Return](#)