

VI.F.5. Crystal-Lattice Model File

The crystal-lattice model of Doppler broadening, discussed in Section III.B.4, requires additional input beyond that needed by other Doppler models:

- (1) In the INPut file, include one of these alphanumeric commands:

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USE CRYSTAL LATTICE model of doppler broadening or CLM
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- (2) Provide the location/name of the CLM file in the input stream, directly after the name of the DATA file.

The format for the CLM file is given in Table VI F5.1, where we have again used the convention that “C:L” implies “card set number: line number” and the notation “f-f ” refers to “free format.”

Table VI F5.1. Format of the SAMMY CLM file (crystal-lattice model)

Note: “f-f” indicates “free-format”

C:L	Variable Name	Format	Possible Values	Default Value	Meaning
1:1	Title	A80			Alphanumeric title
2:1	Mode_ S_Norm	f-f integer	0 or 1	0	Mode of normalization 0 → do not correct the S function 1 → correct the S function
	Nphon	f-f integer	> 0		Phonon-expansion order
	Sub	f-f real	> 0.0	1.0	Number of subdivisions between the spectrum points for beta mesh
	Xdop	f-f real	> 0.0	1.0	Initial Doppler cut of beta mesh
	Eps	f-f real	> 0.0, small	0.08	Precision over normalization and sum rule check of scattering law
	Epsc	f-f real	> 0.0, small	0.001	Precision of convolution integral calculation
2:2	(blank)				
3:1	What	A5	CONTI		Continuous distribution parameters follow
3:2	Del_Phonon	f-f real	> 0.0		Interval (in eV) between points of the phonon distribution

Table VI F5.1 (continued)

C:L	Variable Name	Format	Possible Values	Default Value	Meaning
3:2, cont.	N_Cont	f-f integer	0 or > 0		If greater than zero, line 3 in card set 3 is in free-form real; N_Cont is the number of points to be read. If equal to zero, line 3 is in fixed format (8F10.1); SAMMY will count the number of points.
3:3	Phonon(i)	f-f real, or 8F10.1			Phonon distribution, uniformly spaced in energy
3:4	(blank)				
4:1	What	A5	DISCR		Discrete mode parameters follow. (This card set may be omitted.)
4:2	N_Osc	f-f integer	0 or > 0		If > 0, lines 3 and 4 are free-form real and there are N_Osc values to be read. If = 0, or if this card is absent, Lines 3 and 4 are fixed format (8F10.1) and SAMMY will count how many values there are.
4:3	Osc_Eng(i)	f-f real or 8F10.1			Energies (eV) for discrete mode oscillators
4:4	Osc_Wts(i)	f-f real or 8F10.1			Weights for discrete mode oscillators
4:5	(blank)				
5:1	What	A5	TRANS		Translational parameters follow (This card set may be omitted.)
5:2	Twt	f-f real			Translational weight
	C_Trans	f-f real			Diffusion constant
	Tbeta	f-f real		1.0	Normalization for continuous part