1 input file `input.dat`

In version 5.0, the input file `input.dat` looks as follows:

Warning: The read-in of the input file is coded in a very low-level fashion, hence it is vital that the structure of the input file remains intact. Don't add or remove lines, don't add or remove any columns! Also, don't add or remove any white space in any of the lines!

The following describes the various input parameters of the input file line by line. notation: $x, y, \ldots$ are placeholders for floating point numbers, 0/1 is a placeholder for a boolean flag, where 0 means FALSE and 1 means TRUE. n is a placeholder for an integer number, *string* is a placeholder for a word like "OCP" or "output.txt".

DO_FIT	0/1		activate(1) chi-squared fitting routines
PHOTON_ENERGY	x		energy of incoming photons in units of eV
SCATTERING_ANGLE	x		scattering angle in degrees ($0 < x < 180$)
ELECTRON_TEMP	x	0/1	x = electron temperature in units of eV ($x > 0.0$) 0/1: fit x to data (no/yes)
ELECTRON_DENSITY	x	0/1	x = electron number density in units of $1/\mathrm{m}^3$ ($x > 0.0$) 0/1: fit x to data (no/yes)
AMPLITUDE	x	0/1	normalize spectrum to peak amplitude x 0/1: fit peak amplitude to data (no/yes)
BASELINE	x	0/1	x: add constant offset x to spectrum 0/1: fit constant offset to data (no/yes)
Z_FREE	x	0/1	x = total average ionization per ion 0/1: fit ionization to data (no/yes)
.....			
only one of the following 8 USE_... parameters can be different from 0			
USE_RPA	0/1		use RPA model for free-free scattering [4]
USE_LINDHARDT	0/1		use Lindhardt model ... []
USE_TSYTOVICH	0/1		use Tsytovich model ... []
USE_STATIC_LFC	0/1		use RPA+static LFC ... []
USE_DYNAMIC_LFC	0/1		use RPA+dynamic LFC ... []
USE_MFF	0/1		use Memory Function Formalism ... []
USE_BMA	0/1		use Born-Mermin Approximation ... [2]
USE_BMA+SLFC	0/1		use BMA+static LFC ... [1]
.....			
USE_CORE	0/1		Add bound-free contribution to total scattering
.....			
ION_TEMP	x	0/1	x=ion temperature in units of eV use this value (no/yes). If "0", $T_{\mathrm{ion}} = T_{\mathrm{electron}}$ is used.
S_ION_FEATURE	x	0/1	x=user-defined ion feature, $x = \lvert f(k) + q(k)\rvert^2 S_{\mathrm{ii}}(k)$ 0/1: use x for ion feature calculation?
DEBYE_TEMP	x	0/1	x = Debye temperature in units of eV 0/1: use Debye temperature in ion feature calculation (Debye-Waller factor) [3]?
band_gap	x	0/1	x = valence-to-conduction band gap in units of eV 0/1: use band-gap in calcuation [3].

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N_DAWSON	n		number of points for Dawson's integral
N_Distribution	n		number of points for integral over el. distribution function integral
N_PVI	n		number of points for principal value integration
N_LANDEN	n		obsolete
N_FFT	n		number of points for fast fourier transform
EPS	n		smallness parameter
STATIC_MODEL...	*string*		ion-feature model. possible are: DH[],OCP[],SOCP[],SOCPN[]
USE_ADV_MIX	0/1		0/1: use advanced mixing model [] (no/yes)
USE_IRS_MODEL	0/1		0/1: use incipient rydberg states [] (no/yes)
HARD_SPHERE_DIAM	x	0/1	x =diameter of hard spheres in SOCPN model in units of m 0/1: use hard sphere diameter in ion-feature calcuation
POLARIZABILITY	x	y	x = real part of polarizability y = imaginary part of polarizability
BOUND-FREE_MODEL...	*string*		bound-free model. possible are: form-factor approximation FFA[6] impulse approximation IA[5] impulse approximation+Compton defect IBA[5]
CONT_LOWR_MODEL	string	x	continuum lowering model possible are: Stewart-Pyatt SP [7], Ecker-Kröll EK [8], and user-defined USR (in which case x is the continuum lowering in units of eV, ($x \geq 0.0$))
GK	x	0/1	x=user defined value for the static local field factor 0/1: use this value in calcuations (no/yes).
RPA	0/1	0/1	0/1: include RPA free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
LINDHARD	0/1	0/1	0/1: include Lindhard free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
SALPETER	0/1	0/1	0/1: include Salpeter free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
RPA_TSYTOVICH	0/1	0/1	0/1: include Tsytovich free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
STATIC_LFC	0/1	0/1	0/1: include static LFC free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
DYNAMIC_LFC	0/1	0/1	0/1: include dynamic LFC free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
MFF	0/1	0/1	0/1: include MFF free-free feature in output (no/yes) 0/1: normalize to AMPLITUDE (no/yes)
BMA(+sLFC)	0/1	0/1	0/1: include BMA free-free feature in output (no/yes)

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			0/1: normalize to `AMPLITUDE` (no/yes)
`CORE`	0/1	0/1	0/1: include bound-free feature in output (no/yes)
			0/1: normalize to `AMPLITUDE` (no/yes)
`TOTAL`	0/1	0/1	0/1: include total scatter in output (no/yes)
			0/1: normalize to `AMPLITUDE` (no/yes)
`NUMBER_OF_SPECIES`	n		n = number of ion species
`TARGET_1`	*string*	n m	*string*=chemical element symbol
			n=number of ions per molecule
			m average charge state
			($m = -1$ for single-ion species see note for multi-ion!)
`MASS_DENSITY`	x		x=mass density in units of (g/cm^3).
			write e.g. `3.0E+23` for 3.0×10^{23} g/cm^3.
`NE_ZF_LOCK`	0/1		1: adjust electron density to be
			consistent with mass density
			and average charge state. 0: use given values
`DATA_FILE`	*string*		*string*=name of ascii file
			containing experimental data (e.g. for use in fit routine)
`NUMBER_POINTS`	n		number of points in `DATA_FILE`
`OPACITY_FILE`	*string*	0/1	*string*=name of ascii file containing target's opacity
			as function of photon energy
			0/1: use opacity file (no/yes)
`USE_FILE`	0/1		0/1: use tabulated values for instrumental
			function (to be read in from ascii file)
`FILE_NAME`	*string*		*string*=name of ascii file containing
			instrument response as function of photon energy
`INST_MODEL`	*string*		*string*=name of instrument function
			valid are "GAUSSIAN" or "LORENTZIAN"
`INST_FWHM`	x		x=width of instrumental function in units of eV
x is not actually the full width at half max but the σ-parameter of a normalized			
Gaussian or Lorentzian function. See note below.			
`MAX_ITERATIONS`	n		n=maximum number of iterations
			for optimization routines
`LEVENBERG_MARQUARDT`	0/1		use LM algorithm (no/yes)
`SIGMA_LM`	x		x=tolerance level for LM algorithm
`SAVE_FILE`	*string*		*string*=name of output file

References

1. Fortmann, C., Wierling, A., and Röpke, G. Influence of local-field corrections on Thomson scattering in collision-dominated two-component plasmas. *Physical Review E* **81,** 26405. ISSN: 1539-3755 (2010).

2. Fortmann, C, Bornath, T, Redmer, R, Reinholz, H, Röpke, G, Schwarz, V, and Thiele, R. X-ray Thomson scattering cross-section in strongly correlated plasmas. *Laser Part. Beams* **27,** 311. ISSN: 0263-0346 (2009).

3. Gregori, G, Tommasini, R, Landen, O. L., Lee, R. W., and Glenzer, S. H. Limits on collective X-ray scattering imposed by coherence. *Europhys. Lett.* **74,** 637 (2006).

4. Gregori, G., Glenzer, S. H., Rozmus, W., Lee, R. W., and Landen, O. L. Theoretical model of x-ray scattering as a dense matter probe. *Phys. Rev. E* **67,** 026412 (2003).

5. Holm, P. and Ribberfors, R. First correction to the nonrelativistic Compton cross section in the impulse approximation. *Phys. Rev. A* **40,** 6251–6259. ISSN: 0556-2791 (1989).

6. Schumacher, M, Smend, F, and Borchert, I. Incoherent scattering of gamma rays by inner-shell electrons. *J. Phys. B: Atomic and Molecular Physics* **8,** 1428–1439. ISSN: 0022-3700 (1975).

7. Stewart, J. C. and Pyatt Jr., K. D. Lowering of ionization potentials in plasmas. *Astrophys. J.* **144,** 1203 (1966).

8. Ecker, G. and Kröll, W. Lowering of the Ionization Energy for a Plasma in Thermodynamic Equilibrium. *Physics of Fluids* **6,** 62–69 (1963).

```
--XRTS---input_file-----------------------------------
--
--fit_parameters------------------------------flag----
DO_FIT                          0
PHOTON_ENERGY                   8000.0
SCATTERING_ANGLE                140.0
ELECTRON_TEMP                   10.0            0
ELECTRON_DENSITY                1.00E+29        0
AMPLITUDE                       1.0             0
BASELINE                        0.0             0
Z_FREE                          2.0             0
--model_for_total_spec---------use-flag-------------
USE_RPA                         1
USE_LINDHARD                    0
USE_TSYTOVICH                   0
USE_STATIC_LFC                  0
USE_DYNAMIC_LFC                 0
USE_MFF                         0
USE_BMA                         0
USE_BMA+sLFC                    0
USE_CORE                        1
--ion_parameters-------------------------------useflag-
ION_TEMP                        10.0            1
S_ION_FEATURE                   0.14            0
DEBYE_TEMP                      0.4             0
BAND_GAP                        4.0             0
--integration-----------------------------------------
N_DAWSON                        32
N_DISTRIBUTION                  32
N_PVI                           128
N_LANDEN                        512
N_RELAXATION                    2048
N_FFT                           2048
EPS                             1.0E-3
--See(k,w)-------------------------------------norm/use-
STATIC_MODEL(DH,OCP,SOCP,SOCPN) SOCP
USE_ADV_MIX                     1
USE_IRS_MODEL                   0
HARD_SPHERE_DIAM                1E-10           0
POLARIZABILITY                  0.0             0.0
BOUND-FREE_MODEL(IA,IBA,FFA)    FFA
CONT-LOWR_MODEL(SP,EK,USR)      EK              0.0
GK                              1.5             0
RPA                             0               0
LINDHARD                        0               0
SALPETER                        0               0
LANDEN                          0               0
RPA_TSYTOVICH                   0               0
STATIC_LFC                      0               0
DYNAMIC_LFC                     0               0
MFF                             0               0
BMA(+sLFC)                      0               0
CORE                            1               0
TOTAL                           1               1
E_MIN                           -1000.0
E_MAX                           300.0
E_STEP                          1.3
--target_spec--------------------------chem----Zfree--
NUMBER_OF_SPECIES               1
TARGET_1                        Be      1       -1
MASS_DENSITY                    5.0
NE_ZF_LOCK                      1
DATA_FILE                       35082_s2_h.txt
NUMBER_POINTS                   2048
OPACITY_FILE                    nofile          0
--instrument_function---------------------------------
USE_FILE                        0
FILE_NAME                       HOPG.INST
INST_MODEL                      GAUSSIAN
INST_FWHM                       50.0
BIN_PER_PIXEL                   1.0
INST_INDEX                      2.0
--additional_parameters-------------------------------
MAX_ITERATIONS                  0
LEVENBERG_MARQUARDT             0
SIGMA_LM                        1.0
SAVE_FILE                       xrts.txt
```

Figure 1: Sample `input.dat` in version 5.0