ASCII MS Spectrum File format (*.spectrum)

The ASCII MS Spectrum File format (*.spectrum) is fully compatible to the NIST mass spectra file format and has the following specifications:

Each row of the file is introduced by a special case-insensitive keyword, which is immediately followed by a colon, separating the key from the corresponding value(s). Spaces or other characters between the keyword and the colon are not allowed. Some keywords can be abbreviated; the optional part is listed in parentheses in the table below.

The order of the keywords is irrelevant, but the first one must be the *Name* keyword and the last one must be the *Num Peaks* keyword. Other keywords are optional, but may appear only once (except for the *Synonym* keyword).

Note: Some keywords accept only predefined arguments, which are listed in braces.

Keyword	***Description***
Name	This entry is required, only ASCII characters between ' ' (ASCII no. 32) and '~' (ASCII no. 126) are allowed, see table II a below. For Greek characters see table II b below.
CAS	The chemical abstracts registry number (with or without '-').
NIST	The database entry number of NIST libraries.
UN	The four-digit *United Nations* number of the compound.
MW	The molecular weight in the sense of a nominal mass (an integer number).
Form(ula)	The chemical formula.
Syn(onym)	A synonym for the compound. This entry can appear multiply.
Com(ment)	Any comment.
Struc(*ture*)	The hex decimally coded structure information of an MDL® MOL file, continuously written in the same line. Each single byte value is a two-digit number, where each digit must be a hexadecimal number (0..9,A..F,a..f). *Example: The first five bytes of some arbitrary MDL MOL file with the molecule name H2O in the first line should start with Structure: 48324F0D0A...*
Cont(ributor)	Contributor, recommended as "Name, Organization".
InstType	Type of instrument. Recognized symbols are: {**IT**, **TQ**, **Q**, **TOF**, **ICR**, **FTMS**, **ESI-TOF**}.
InstName	Any description for the instrument.
IoniMethod	Method of ionization. Recognized symbols are: {**EI**, **CI**, **APCI**, **ESI**, **nano-ESI**, **TS**, **MALDI**, **CAESIUM**, **APMALDI**, **APPI**}.
IonPol(arity)	Ion polarity. The following symbols are recognized: {**neg** or **0** for negative, **pos** or **1** for positive, **-1** for undefined polarity, **both** or **2** for both polarities}.
MSMS(Stage)	An integer number *n* describing the MS^n stage.
PreIon	A comma-separated list of precursor ions in *m/z* (floating-point numbers). Although not obligatory, it is recommended to provide a list of *n-1* precursor ions, if the MSMS stage was specified to be of order *n*.
ProdIon	A floating-point number describing the product ion in *m/z.*
TrapDrive	A floating-point number describing the trap drive value of the *esquire* instruments.
Skim1	A floating-point number describing the skim 1 value of the *esquire* instruments.
FragAmpl	A floating-point number describing the fragmentation amplitude value in *V.*
IsolWidth	A floating-point number describing the isolation width value in *m/z.*
TargetGas	Any identifier for the target gas.
TargetGasPres(sure)	A floating-point number describing the target gas pressure in *hPa.*
ReagentIon	Any identifier for the reagent ion.
ReagentGasPres(sure)	A floating-point number describing the reagent gas pressure in *hPa.*
ColEnergy	A floating-point number describing the collision energy in *eV.*
PeakWidth	A floating-point number describing the original mass spectral peak width of the raw spectrum in *m/z.*
Refl(ector)	Integer number describing the reflector mode as linear {**0**} or reflector {**1**}.
PSD	Integer number describing whether the spectrum is a post source decay spectrum

	{**0**, **1**}.
ChargeDecon (volved)	Integer number denoting whether the spectrum has been charge deconvoluted into the singly charged state {**0**, **1**}.
Date	Date and time of the analysis given as a local time in the ISO 8601 format: `YYYY-MM-DD[T| ]HH:MM:SS[+|-]hh:mm` *Each item is presented as an integer value, hh:mm corresponds to the time offset between local time and the Coordinated Universal Time (UTC), such that UTC = local time - hh:mm*
Column	Any description of the chromatographic column.
RetTime	A floating-point number describing the retention time of the spectrum in analysis in seconds.
SSID	Unique software system ID of the analysis (Bruker-specific).
AnalID	Unique ID of the analysis (Bruker-specific).
AnalName	Any descriptive identifier of the analysis.
Mass(Range)	Two comma-separated floating-point numbers describing the lowest and the highest mass values of the MS measurement range.
Num(Peaks)	This item is obligatory and must be the last one of the list. The format is as follows: An integer number of peaks followed by pairs of mass (floating-point) and intensity (floating-point) values delimited by characters of the set " \n,;:')([]{}".

List of ASCII symbols allowed in the *Name* field:

SPACE	!	"	#	$	%	&	'	(	)
*	+	,	-	.	/	0-9	:	;	<
=	>	?	@	A-Z	[	\	]	^	_
`	a-z	{	|	}	~				

Greek characters in the *Name* and *Synonym* fields can be embedded by placing their English transcription between dots:

.alpha.	.beta.	.gamma.	.delta.	.epsilon.	.zeta.
.eta.	.theta.	.iota.	.kappa.	.lambda.	.mu.
.nu.	.xi.	.omicron.	.pi.	.rho.	.sigma.
.tau.	.upsilon.	.phi.	.chi.	.psi.	.omega.