The Jülich Photolysis Frequency Browser

Version 2016 zu VDI-Richtlinie 3783 Blatt 18 1.5.2016

Manual

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After opening the link to the Jülich Photolysis Frequency Browser a short introduction appears, stating what is to be expected. This page also contains buttons for the contact to the scientist in charge of the catalog. and the others show the imprint.

To reach the catalog of the photolysis frequencies press one of the buttons [continue to data]. Due to the fact that the Technical Guideline VDI-3783 part 18 refers to this browser, [version 2016] represents the reference state of the guideline. The button [current version] represents the actual datasets which may be corrected and/or extended.

Photolysis Frequency Browser	JÜLICH FORSCHUNGSZENTRUM
Photolysis Frequencies	
The rate constants of tropospheric photolysis reactions, i.e. the photolysis frequencies, are listed for a variety of meteorological conditions. The photolysis frequencies are given for a ground-level altitude o 200m to represent mean European conditions and for 1000m above ground. The data are based on the actinic photon flux densities calculated by a state-of-the-art model.	
continue to version 2016	
continue to current version	
Contact Impressum Imprint	

Photolysis Frequency	Brows	ser												J,	
1) Select the general format															
dependence on global irrad	iance	depend	lence on	solar ze	nith angle	value	es at fixed	l solar	zenith an	igles	photonfl	ux densit	ies	global in	radiances
2) Choose condition:															
clear sky at ground level	overca	i <mark>st sky</mark> a	t ground	llevel	clear sky	1 km al	oove grou	nd	overcast	sky 1 ki	n above	ground			
3) Choose appropriate ozone	column	density	[Dobsor	units]:	4) Selec	t the bou	ndary I	ayer aero	osol type					
240 270 300 330	360	390	420	450		clean	averag	e p	olluted						
5) Select optical depth of the	cloud:				6	5) For v	which cos	(SZA)?	10.						
10 20 30 40						0.95	0.85	0.75	0.65	0.55	0.45	0.35	0.25	0.15	0.05

After pressing one of the two buttons for the respective version, the next page allows the choice of the requested simulation conditions:

Bar 1 : Select the general format

There are three possibilities for the depiction of the photolysis frequencies. To reach the calculated values for 10 fixed solar zenith angles (cos(SZA)= from 0.95 to 0.05, step width 0.10), press the button [values at fixed solar zenith angles].

The button [dependence on solar zenith angle] brings you to the parameters of the solar-zenith-angle-dependent functions of the photolysis frequencies. Both of these formats require the correct meteorological conditions (see below).

If the meteorological conditions are not known, there is the possibility of coupling the photolysis frequencies to the measured or estimated global irradiance. This button [dependence on global irradiance] opens a list of photolysis frequency functions, depending on the global irradiance and, if necessary, on the ozone column density.

The other two buttons [photoflux densities] and [global irradiances] open tables of the input data used for the determination of the photolysis frequencies and their functions. Besides the photolysis frequencies, the original actinic photon flux densities are made available. These data were calculated with the program libRadtran (Mayer and Kylling, 2005) by P. Köpke and B. Mayer of the LMU. After pressing the respective button, the

appropriate simulation conditions must be selected, e.g. the solar zenith angle (SZA). The respective buttons of Bar 6 indicate the cosine of the SZA, the related angles are assigned to their cosine in the following table:

cos(SZA)	0.95	0.85	0.75	0.65	0.55	0.45	0.35	0.25	0.15	0.05
SZA/dgr	18.2	31.8	41.45	49.5	56.6	63.3	69.5	75.5	81.4	87.1

Accordingly, for the global irradiances, the conditions have to be selected, too (see below).

Bar 2 : Choose conditions

The spectral actinic photon flux densities were calculated for two general conditions: [clear sky] and [overcast sky]. For both conditions, the photolysis frequencies are displayed for two altitudes: [ground level] (200 m above sea level) and [1 km above ground]. These conditions can be chosen by the relevant button.

Bar 3 : Choose appropriate ozone column density, Bar 4 : Select the boundary layer aerosol type, and Bar 5 : Select optical depth of the cloud

There are three essential meteorological data to be specified:

- 1) The ozone column density, which is important for the decay of the sun's irradiation towards shorter wavelengths : The range of the ozone column density considered reaches from 240 Dobson Units to 450 Dobson Units with a step width of 30 Dobson Units. An annual mean value for Central Europe is 330 Dobson Units.
- The aerosol type which governs the scattered light in the planetary boundary layer : The menu items for the aerosol type are [continental clean], [continental average], and [continental polluted].
- 3) And the optical depth of the cloud (COD) in case of an overcast sky : There are four COD to choose from: 10, 20, 30, and 40 with a mean value of 20.

In the following examples are given for the different possibilities to depict the photolysis frequencies. If the relevant buttons are activated, the name of the respective file appears on the display, together with the requested values and a legend. But the tables only appear if all necessary buttons are activated. With a click on the file's name, the file itself is displayed and can be printed or stored for further use.

	ct the general forma	t:													
depen	dence on global irra	diance d	ependenc	e on <mark>solar</mark> ze	nith angle	value	es at fixe	d solar	zenith a	ngles	photonf	lux densit	ies	global irr	adiances
) Choo	se condition:														
clear	sky at ground level	overcast	sky at gr	ound level	clear sky	1 km at	ove gro	und	overcast	sky 1 k	m above	ground			
) Choo	se appropriate ozon	e column de	ensity [Do	bson units]:	4	1) Selec	t the bou	Indary	ayer aer	osol typ	e:				
240	270 300 33	0 360	390 4	20 450		dean	averag	ge p	olluted						
) Selec	ct optical depth of th	e cloud:			6	5) For w	hich cos	(SZA)?	1						
10	20 30 40					0.95	0.85	0.75	0.65	0.55	0.45	0.35	0.25	0.15	0.05
ile (FG2	A36.TXT):														
Photoly	sis Frequencies as	Function of	the Sola	ar Zenith An	gle										
102 103 103 103 1205 10N0 1N03	-hv-> NO + 0 -hv-> products -hv-> NO2 + 0 -hv-> NO + 02 -hv-> NO3 + NO2 -hv-> OH + NO2 -hv-> OH + NO2	5.003E-03 1.313E-01 1.197E-01 1.089E-02 2.723E-05 8.200E-04 2.987E-07	3.18886 2.97391 2.83956 2.92423 3.87379 3.17369 5.20829	0.69537 0.72078 0.73082 0.72824 0.68163 0.69643 0.69643	j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b	(1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co)	s(cX))] s(cX))] s(cX))] s(cX))] s(cX))] s(cX))] s(cX))]								
INO3 INO4 INO4 INO4 INO4 INO4 INO4 INO2 INO3	-hv-> HONO +0 -hv-> HO2 + NO2 -hv-> OH + NO3 -hv-> CHO + H -hv-> products	3.493E-10 3.461E-06 9.430E-08 1.771E-05 4.590E-05	5.82887 4.59820 4.85200 3.76024 3.56819	0.66806 0.66887 0.66526 0.70600 0.69789	j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b	(1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co)	s(cX))] s(cX))] s(cX))] s(cX))] s(cX))]								
CH20 CH302 CH300H CH300H C2H502	-hv-> C0 + H2 -hv-> CH30 + 0 -hv-> CH30 + 0H -hv-> C2H50 + 0 -hv-> CH4 + C0	2.831E-05 4.957E-05 2.899E-06 1.777E-04 4.545E-09	3.37793 4.98610 3.80286 4.31735 6.19712	0.69897 0.67319 0.68588 0.67337 0.66582	j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b j=a*exp[b	(1-1/co) (1-1/co) (1-1/co) (1-1/co) (1-1/co)	s(cX))] s(cX))] s(cX))] s(cX))] s(cX))]								

If the general formats [dependence on solar zenith angle] or [values at fixed solar zenith angles] are chosen, a selection of the solar zenith angle is not required. The display then shows the photolysis reactions and the parameters of the related frequency function, resp. a table with all 10 SZA values for every listed photolysis reaction. If the overcast sky version is selected, the button for the optical depth of the cloud must be pressed.

L) Sele	ct the general forma	t:										
depen	idence on global irra	diance	dependen	ce on <mark>solar</mark>	zenith ang	jle valu	es at fixed	solar zenit	th angles	photonflu	x densities	global irradiance
2) Choo	se condition:				1.044							
clear	sky at ground level	overca	st sky at g	round level	clear s	sky 1 km a	bove grou	nd over	cast sky 1	km above g	round	
3) Choo	se appropriate ozon	e column	density [D	obson units	i]:	4) Selec	ct the boun	dary layer	aerosol ty	pe:		
240	270 300 330	0 360	390	420 450)	dean	average	pollute	ed			
5) Sele	ct optical depth of th	e cloud:				6) For v	which cos(s	SZA)?				
10	20 30 40					0.95	0.85	0.75 0.0	55 0.55	0.45	0.35 0.25	0.15 0.05
ile (WG	0P30.TXT):											
Photoly	sis Frequencies at	Fixed Sol	ar Zenith	Angles								
NO3 NO3 NO3 NO3 NO3 N205 HONO	-nv-> 0(10) + 02 -hv-> 0(3P) + 02 -hv-> 0H + 0H -hv-> NO + 0 -hv-> products -hv-> NO + 02 -hv-> NO + 02 -hv-> NO + NO2 -hv-> NO + NO2 -hv-> NO + NO2	2.942-05 3.45E-04 6.69E-06 7.59E-03 2.09E-01 1.92E-01 1.75E-02 4.14E-05 1.23E-03	2.25E-05 3.27E-04 5.86E-06 7.02E-03 2.00E-01 1.84E-01 1.69E-02 3.65E-05 1.13E-03 4.00E-07	1.64E-05 3.07E-04 4.98E-06 6.35E-03 1.90E-01 1.74E-01 1.61E-02 3.12E-05 1.02E-03 2.16E-02	1.12E-05 2.81E-04 4.07E-06 5.55E-03 1.76E-01 1.61E-01 1.50E-02 2.57E-05 8.81E-04 2.37E-07	7.01E-06 2.50E-04 3.15E-06 4.62E-03 1.58E-01 1.45E-01 1.36E-02 2.00E-05 7.27E-04	3.95E-06 2.12E-04 2.26E-06 3.59E-03 1.35E-01 1.23E-01 1.18E-02 1.45E-05 5.59E-04	1.95E-06 1.65E-04 1.47E-06 2.53E-03 1.06E-01 9.65E-02 9.41E-03 9.55E-06 3.89E-04 4.65E-02	6.25E-07 1.10E-04 8.41E-07 1.53E-03 7.04E-02 6.40E-02 6.40E-03 5.50E-06 2.36E-04 2.06E-02	2.85E-07 5.10E-05 3.96E-07 7.57E-04 3.23E-02 2.93E-02 2.99E-03 2.62E-06 1.19E-04	0.322-08 1.07E-05 1.18E-07 2.53E-04 7.12E-03 6.54E-03 5.78E-04 7.94E-07 3.98E-05 2.99E-05	
HNO3 HNO4 HNO4 CH20 CH20	-hv-> HONO +0 -hv-> HO2 + NO2 -hv-> HO2 + NO2 -hv-> OH + NO3 -hv-> CHO + H -hv-> products	5.94E-10 5.42E-06 1.50E-07 2.71E-05 6.90E-05	4.74E-10 4.61E-06 1.26E-07 2.35E-05 6.10E-05	3.62E-10 3.79E-06 1.02E-07 1.97E-05 5.23E-05	2.62E-10 2.99E-06 7.94E-08 1.58E-05 4.30E-05	1.77E-10 2.22E-06 5.81E-08 1.20E-05 3.36E-05	1.09E-10 1.53E-06 3.93E-08 8.37E-06 2.43E-05	5.94E-11 9.49E-07 2.39E-08 5.28E-06 1.60E-05	2.78E-11 5.17E-07 1.28E-08 2.90E-06 9.20E-06	1.04E-11 2.30E-07 5.55E-09 1.29E-06 4.37E-06	2.39E-03 6.32E-08 1.49E-09 3.44E-07 1.29E-06	
CH20 CH302 CH300H C2H502	-hv-> C0 + H2 -hv-> CH30 + 0 -hv-> CH30 + 0H -hv-> C2H50 + 0	4.21E-05 7.96E-05 4.41E-06 2.74E-04 7.90E-09	3.77E-05 6.62E-05 3.89E-06 2.35E-04 6.19E-09	3.27E-05 5.29E-05 3.33E-06 1.96E-04 4.65E-09	2.74E-05 4.03E-05 2.73E-06 1.56E-04 3.29E-09	2.17E-05 2.88E-05 2.13E-06 1.17E-04 2.17E-09	1.60E-05 1.89E-05 1.54E-06 8.21E-05 1.30E-09	1.07E-05 1.12E-05 1.01E-06 5.20E-05 6.86E-10	6.32E-06 5.72E-06 5.84E-07 2.89E-05 3.10E-10	3.10E-06 2.36E-06 2.78E-07 1.32E-05 1.10E-10	9.50E-07 5.93E-07 8.41E-08 3.54E-06 2.44E-11	

Likewise, the tables of the 'Dependence on the global irradiance' are displayed. They consist of the reactions, the values of the parameters and the type of the function:

	Charles and the second second second	A MARKA PARAMETER							FURSCHI	JNGSZEI
1) Select the g	general format:	_							1	
dependence	on global irradian	ice deper	ndence on so	lar zenith and	jle value	s at fixed solar zenith and	gles p	photonflux densities	global irradiand	es
2) Choose con	dition:	1			-			19		
no cloud in fr	ont of sun at grou	ind sun c	overed by clo	ouds at <mark>groun</mark>	d no clou	id in front of sun 1 km abo	ove grou	ind sun covered b	y clouds 1 km abov	e groun
3) Choose app	ropriate ozone co	lumn densit	y [Dobson u	nits]:	4) Select	the boundary layer aero	sol type	:		
240 270	300 330	360 390	420	450	clean	average polluted				
5) Select optio	al depth of the cl	oud:			6) For w	hich cos(SZA)?				
10 20	30 40				0.95	0.85 0.75 0.65	0.55	0.45 0.35 0.2	5 0.15 0.05	
File (GG1XXX.T)	(T):									
Photolysis Fr	equencies as Fund	ction of the	Global Irr	adiance						
03 -hv-> H202 -hv-> N02 -hv-> N03 -hv-> N03 -hv-> N03 -hv-> N03 -hv-> N03 -hv-> H003 -hv-> H003 -hv->	O(3P) + 02 OH + OH NO + 0 products NO2 + 0 NO3 + NO2 OH + NO OH + NO2 HONO +0	3.69E-07 8.68E-09 1.02E-05 2.41E-04 2.22E-04 1.90E-05 5.42E-08 1.69E-06 4.89E-10 5.04E-13	2.22E-10 -5.80E-12 -2.03E-09 6.01E-08 5.08E-08 9.58E-09 -3.22E-11 -3.56E-10 -6.72E-13 -7.87E-16	-2.58E-13 3.83E-12 -7.76E-11 -6.67E-11 -1.13E-11 1.96E-11 1.06E-12 1.70E-15	-2.62E-15 -1.41E-14 -1.36E-15 -2.55E-18)=G(a+bG+cG*G)]=G(a+bC)+(c+dC)G}]=G(a+bG+CG*G)]=G(a+bG+cG*G)]=G(a+bG+cG*G)]=G(a+bG+cG*G)]=G(a+bC)+(c+dC)G}]=G(a+bC)+(c+dC)G}]=G((a+bC)+(c+dC)G)]=G((a+bC)+(c+dC)G)				
HN04 -hV-> HN04 -hV-> CH20 -hV-> CH20 -hV->	OH + NO2 OH + NO3 CHO + H products	6.41E-09 1.68E-10 3.55E-08 7.45E-08	-6.29E-12 -1.83E-13 -3.34E-11 2.17E-11	6.82E-12 2.34E-13 1.91E-11	-7.10E-15 -2.73E-16 -2.14E-15]=G{(a+bC)+(c+dC)G}]=G{(a+bC)+(c+dC)G}]=G{(a+bC)+(c+dC)G}]=G{a+bG}				
CH20 -hv-> CH302 -hv-> CH300H -hv-> CH300H -hv-> CH502 -hv-> CH3CH0 -hv->	C0 + H2 CH30 + 0 CH30 + 0H C2H50 + 0 CH4 + C0	5.08E-08 8.49E-08 5.78E-09 3.43E-07 6.04E-12	3.20E-12 -1.07E-10 -3.46E-12 -2.99E-10 -1.00E-14	1.49E-10 2.09E-12 2.53E-10 2.56E-14	-1.77E-13 -1.45E-15 -2.13E-13 -4.08E-17]=G{a+bG}]=G{(a+bC)+(c+dC)G}]=G{(a+bC)+(c+dC)G}]=G{(a+bC)+(c+dC)G}]=G{(a+bC)+(c+dC)G}				

In this case the buttons of Bar 2 change their inscription: Here we distinguish between [no clouds in front of sun] and [sun covered by clouds], which better describe the situation than 'clear sky' and 'overcast sky'.

To reach the files with the photon flux spectra, it is necessary to declare all four conditions: ozone column density, aerosol type, solar zenith angle, and, for overcast sky conditions, the optical cloud depth.

) Select the		1	Selan Ala											UKSCHUN	GSZE
The second second	e general to	ormat:	and a second second	and the second second second		The second	a marine and a second second	and the state of the state of the	Concernant of the	Providence of	and the state	and the second se	10 all all the and	Same and Party And In-	
dependent	ce on global	irradiance	dependenc	e on solar :	zenith angle	values	at fixed	solar zenith a	ngles	photonf	lux dens	ities	global in	radiances	5
) Choose c	ondition:														
clear sky a	at around le	vel overc	ast sky at or	ound level	clear sky	1 km abo	ove group	d overcast	tskv 1 k	m above	around				
) Choose a	opropriato	ozono colum	a doncity [Do	hean unite		I) Select	the bound	any layor aor	encol tra	0.	Call Start in				
Choose a	ppropriate		I density [Do			J Select	the bound	ary layer der	USUI LYP	e.					
240 27	0 300	330 360	390 4	20 450		ciean	average	polluted							
) Select op	tical depth	of the cloud:			6	5) For wh	ich cos(S	ZA)?							
10 20	30 40					0.95	0.85 0	.75 0.65	0.55	0.45	0.35	0.25	0.15	0.05	
	TVTL				6	ACCORDENCE				INCOME.	and the second second	1	- Streeten.		
le (<u>0H2P39</u>	. <u>1,11</u>):	diffune des		1											_
wavelength	direct	photon flux	vn dilluse u	1p											
[nm]	Ini	otons/(cm^2	nm s)]												
280.05	4.1988-21	2.864F-11	4 566F-12	altitu	de: 1km abov	e ground									
290.15	1 2358-23	6 206F-11	1.0108-11	overce	at COD-20	e ground									
200.13	1.233E-22	1 6405 14	2 5505 11	Overca	200 00-20										
280.25	4.200E-22	1.6402-10	2.050E-11	ozone:	390 D0	linted									
200.35	1 5028 21	2.002E-10	7 175F 11	deroso	Al- 0 65	utuced									
200.45	2 2105 24	4.4042-10 0 170F 1/	1 1 2205 10	CO3 (52	A/- 0.03										
280.55	3.316E-21	1 2005 0	1.3356-10												
260.65	5./00E-23	1.2000-05	2.1122-10	1											
280.75	9.185E-21	1.884E-09	3.095E-10	<u>.</u>											
280.85	1.104E-20	2.262E-09	3.722E-10	1											
280.95	1.417E-20	2.790E-05	4.594E-10	1											
281.05	1.834E-20) 3.401E-09	5.615E-10)											
281.15	3.236E-20	5.223E-09	8.651E-10	2											
281.25	8.508E-20) 1.077E-08	1.793E-09	9											
281.35	3.183E-19	3.054E-08	5.118E-09	1											
281.45	1.064E-18	8.002E-08	1.350E-08	1											
281.55	2.667E-18	1.610E-07	2.731E-08												
281.65	4.915E-18	2.530E-01	4.313E-08												
281.75	9.135E-18	4.044E-01	6.927E-08												
281.85	1.441E-17	5.837E-01	1.004E-07	1.											
	2.028E-17	7.680E-01	1.322E-07	50 C											
281.95	2 2725 15	8.706E-07	7 1.502E-07	1											
281.95 282.05	2.3/20-1														
281.95 282.05 282.15	2.312E-17	8.521E-07	7 1.470E-07												
281.95 282.05 282.15 282.25	2.312E-17 2.792E-17	8.521E-07 9.740E-07	1.470E-07 1.682E-07												
281.95 282.05 282.15 282.25 282.35	2.372E-1 2.312E-1 2.792E-1 4.189E-1	8.521E-07 9.740E-07 1.367E-06	7 1.470E-07 7 1.682E-07 5 2.367E-07												
281.95 282.05 282.15 282.25 282.35 282.45	2.312E-1 2.312E-1 2.792E-1 4.189E-1 7.646E-1	7 8.521E-07 7 9.740E-07 7 1.367E-06 7 2.170E-06	7 1.470E-07 7 1.682E-07 5 2.367E-07 5 3.769E-07												

For the table with the dependence of the photolysis frequencies on the global irradiance, it is only necessary to press the relevant button for the general format and then click on the respective general condition:

L) Selec	t the gener	ral format:											_
depend	dence on gl	lobal irradia	nce	depende	nce on solar :	zenith angle	values	at fixed sola	r zenith a	ngles ph	otonflux densities	global irradi	ances
2) Choos	se condition	n:									_		
no clou	ud in front o	of sun at gro	und	sun cove	ered by clouds	at ground	no cloud	l in front of s	un 1 km al	bove groun	d sun covered by	clouds 1 km a	bove grou
3) Choos	se appropri	iate ozone c	olumn	density [Dobson units	1:	4) Select t	the boundary	layer aer	osol type:			
240	270 30	00 330	360	390	420 450		dean	average	polluted				
5) Selec	t optical de	epth of the c	loud:				6) For whi	ich cos(SZA)	?				
10	20 30	40					0.95	0.85 0.75	0.65	0.55 0	0.45 0.35 0.2	5 0.15 0	05
ile (<u>IHO</u>	PXX.TXT):												
IHOPXX.1	IXT ove ground	i clear	skv		contir	ental pollu	ited						
		0.05				0.45	0.25	0.25	0.15	0.05			
240 DU	1246.60	1108.30	970.6	9 834.	.08 698.40	563.51	429.22	295.66	164.53	47.37			
270 DU	1245.30	1107.00	969.4	8 832.	.91 697.28	562.44	428.23	294.77	163.85	47.03			
300 DU 330 DU	1244.10	1105.80	968.2	9 831. 1 830.	.62 695.06	561.40	427.20	293.91	162.19	46.82			
360 DU	1241.60	1103.40	965.9	8 829.	.52 694.02	559.33	425.31	292.13	161.70	46.02			
390 DU	1240.40	1102.20	964.8	4 828.	.42 692.95	558.30	424.34	291.24	160.97	45.70			
420 DU 450 DU	1239.30	1101.10	963.7	3 827.	.34 691.92	557.32	423.43	290.42	160.31	45.33			
cosX : ozone o global	cos(solar column dens irradiance	zenith angl sity in Dobs s in W/m^2	le) son Uni	ts				57636A-					
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For users of the VDI-Guideline 3783 part 19, the following table of the photolysis reaction numbers in this catalog and in the guideline may be useful:

VDI-Guideline	3783 sheet 19	this	catalog
reaction	number	number	reaction
$NO_2 \rightarrow O(^{3}P) + NO$	1	4	NO2-hv->NO+O
$O_3 \rightarrow O(^1D) + O_2$	6	1	03-hv->0(D)+02
HCHO \rightarrow 2 HO ₂ + CO	10	14	CH2O-hv->CHO+H
$O_3 \rightarrow O(^{3}P) + O2$	16	2	O3-hv->O(P)+O2
$NO_3 \rightarrow NO + O_2$	19	7	NO3-hv->NO+O2
$NO_3 \rightarrow NO_2 + O(^3P)$	20	6	NO3-hv->NO2+O
HCHO \rightarrow H ₂ + CO	21	16	CH2O-hv->CO+H2

References are listed in the download file 'list of spectra'.