BT2 water line list reveals new lines in post-impact spectra of Comet 9P/Tempel 1

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Presentation to EPSC , Berlin, 22.09.2006

Reference

Barber R. J., Miller S., Stallard T., Tennyson J., Hirst P., Carroll T., Adamson A., 2006, ICARUS (in press)

'*UKIRT Deep Impact observations: light curve, ejecta expansion rates and water spectral features*'

The BT2 H_2O Line List

Barber R. J., Tennyson J., Harris G. J., Tolchenov R., 2006, MNRAS, 368, 1087

Data downloadable from:
http://www.tampa.phys.ucl.ac.uk/ftp/astrodata/water/BT2
or *ftp://cdsarc.u-strasbg.fr/cats/VI/119*

Produced using the DVR3D suite of programs

Tennyson J., Kostin M., Barletta P., Harris G.J., Polyansky O.L., Ramanial J., Zobov N.F., 2004, Comput. Phys. Commun., 163, 85

Ro-vibration **energy levels** are solutions to Schrödinger Equation for nuclei moving in potential well due to electrons - requires **potential energy surface**.

We used that of:

Shirin S.V. et al., 2003, J. Chem Phys., 118

Intensities are dipole transition moments between pairs of wavefunctions - requires **dipole moment surface**.

We used that of:

Schwenke D.W., Partridge H., 2000, J. Chem Phys. 113

Synthetic spectra are generated by:

‘spectra-BT2.f90’

The BT2 line list

- 50,000 processor hrs.
- Wavefunctions > 0.8 terabites
- 221,100 E levels ~ 7% known experimentally
- 506 million transitions (PS list has 308m). Only ~ 0.02% known experimentally
- Good agreement with experiment

Extract from the BT2 Energy Levels File (221,100 entries)

43432	11	1	50	**8730.136998**	0	2	1	**11**	3	8
43433	11	1	51	**8819.773962**	0	4	0	**11**	6	6
43434	11	1	52	**8918.536215**	0	0	2	**11**	2	10
43435	11	1	53	**8965.496130**	0	2	1	**11**	5	6
43436	11	1	54	**8975.145175**	2	0	0	**11**	4	8
43437	11	1	55	**9007.868894**	1	0	1	**11**	3	8
43438	11	1	56	**9082.413891**	1	2	0	**11**	6	6
43439	11	1	57	**9170.343871**	1	0	1	**11**	5	6
43440	11	1	58	**9223.444158**	0	0	2	**11**	4	8
43441	11	1	59	**9264.489815**	2	0	0	**11**	6	6
43442	11	1	60	**9267.088316**	0	5	0	**11**	2	10
43443	11	1	61	**9369.887722**	0	2	1	**11**	7	4
43444	11	1	62	**9434.002547**	0	4	0	**11**	8	4

Extract from Transitions File (506 million entries)

Upper #	Lower #	A_{if}
115309	108520	7.42E-04
196018	198413	1.95E-04
7031	7703	1.13E-02
149176	150123	1.69E-04
81528	78734	2.30E-01
80829	78237	8.83E-04
209672	210876	2.51E-01
207026	203241	2.72E-04
188972	184971	1.25E-01
152471	153399	1.12E-02
39749	37479	1.46E-07

BT2 is **spectroscopically accurate** at the temperatures of early M type stars (**3,500 K**). Comets are not an obvious application.

However……………….

The **fundamental transitions** of H_2O that dominate the spectra of comets are **absorbed** by Earth's atmosphere.

Solar pumped fluorescent (SPF) transitions are **not absorbed** and **can be observed** from earth.

These exist because they are produced in non-LTE regions. In LTE they would be characteristic of temperatures of **several thousand K**

The Mechanism for producing SPF lines

Molecules sublime from the cometary nucleus with ro-vibrational temperatures equal to the surface temperature (~170 K at 1AU)

The molecules are collisionally ‘thermalised’ within the first ~500 metres of the inner coma, adopting a rotational ground state Boltzmann distribution that is characteristic of the temperature of this region.

Energy transfer from incident solar photons and electron collisions raises the H_2O molecules into higher vibrational states.

These excited levels decay radiatively either to the ground vibrational state (fundamental) or to higher vibrational states. The latter, which we term ‘SPF’ lines, are not absorbed telluricly.

(Intensities of SPF lines can be used to determine T)

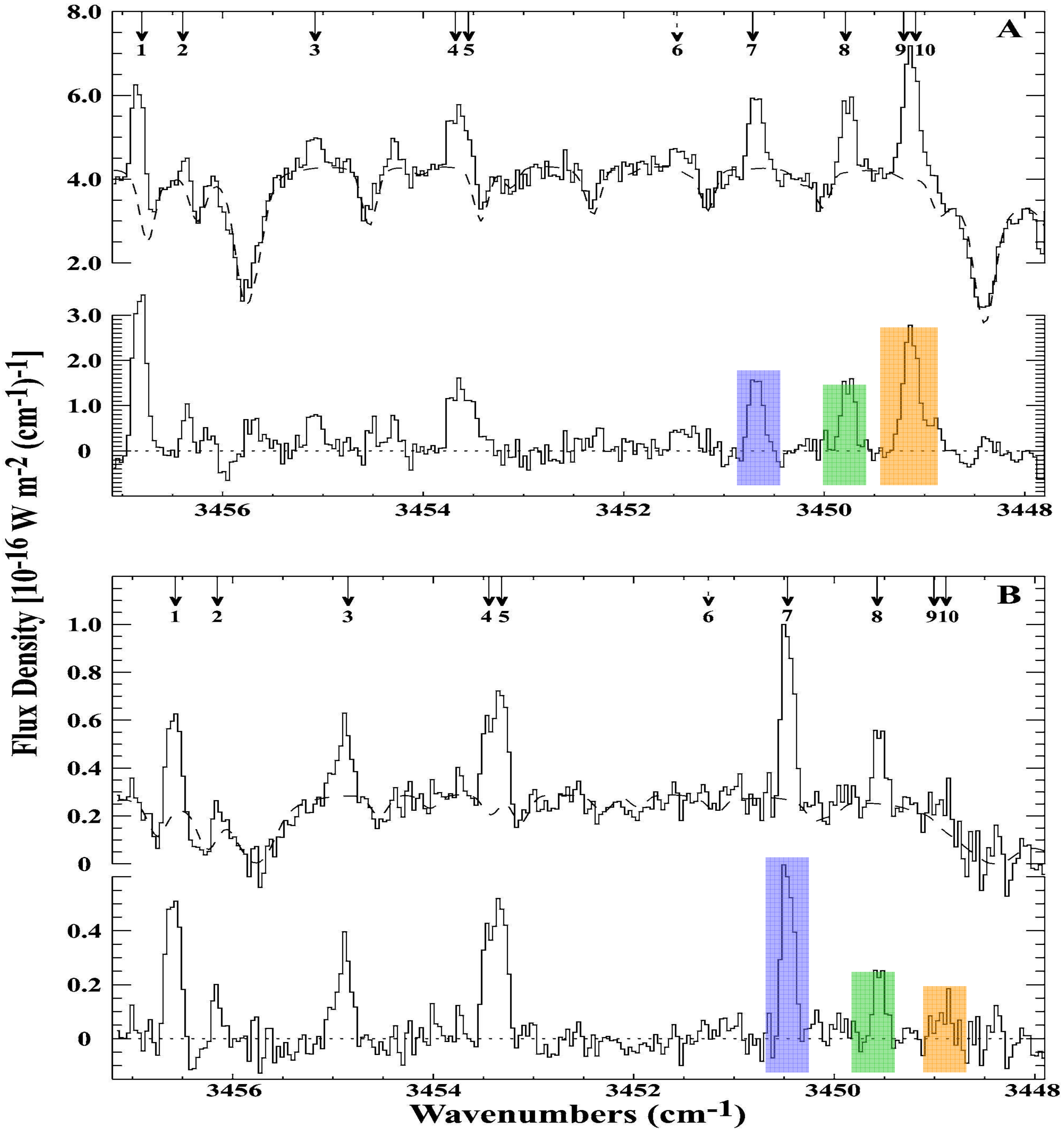


Fig. 2. Detection of 2.9-μm hot-band lines in Comet Ikeya–Zhang. (A) UT 2002 March 22, 00:31. (B) UT 2002 April 13, 18:45. Top: Flux-calibrated

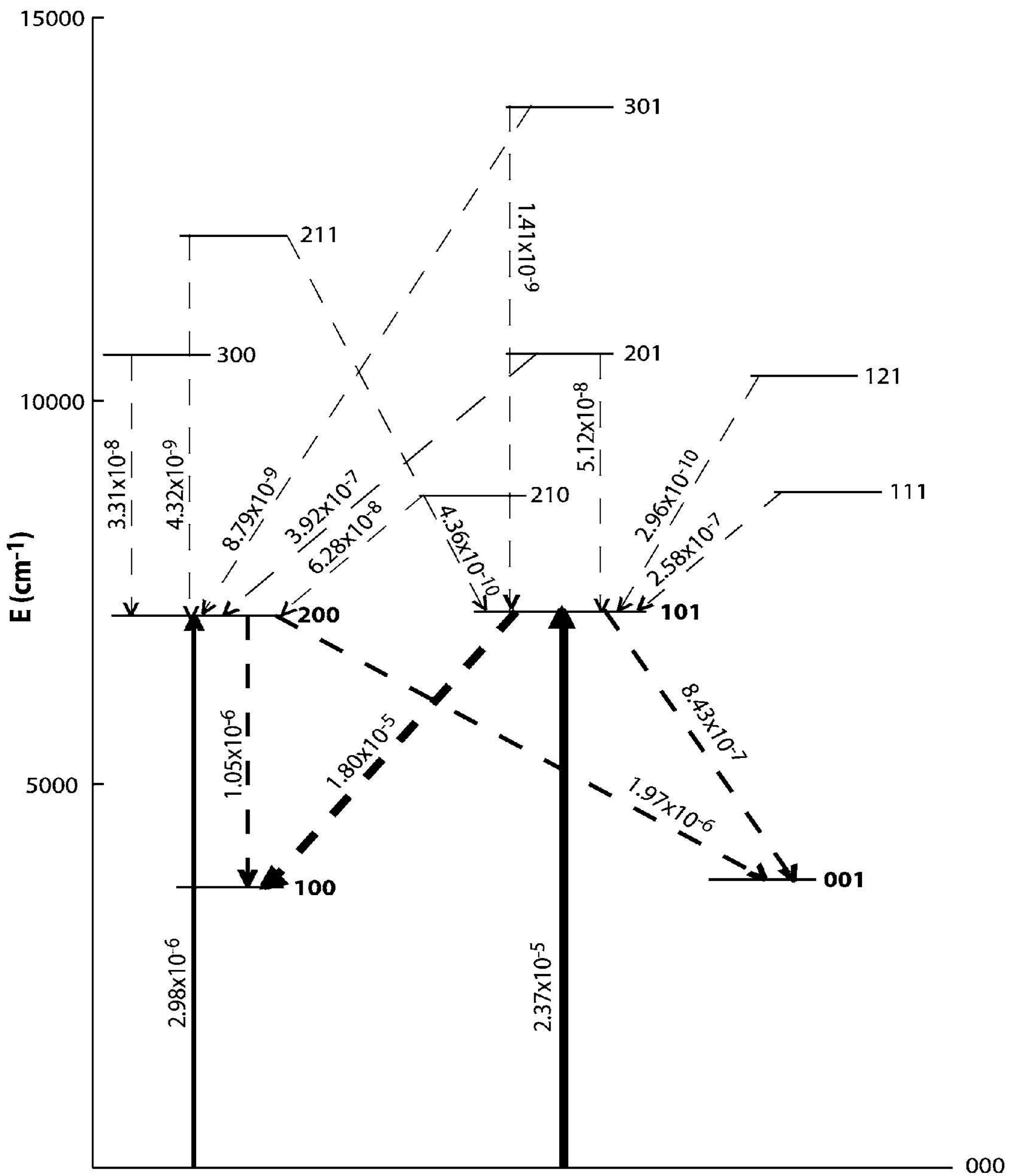
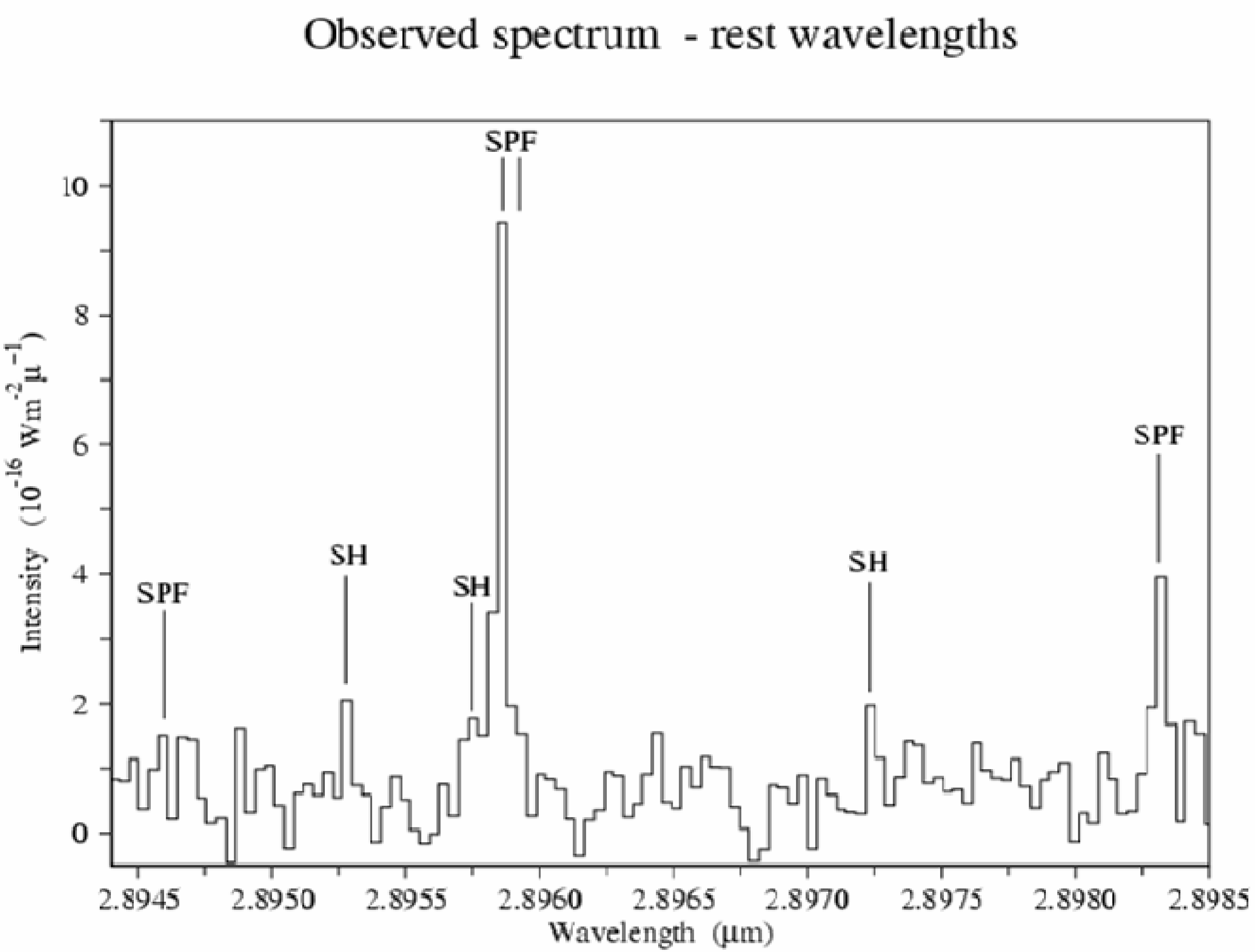
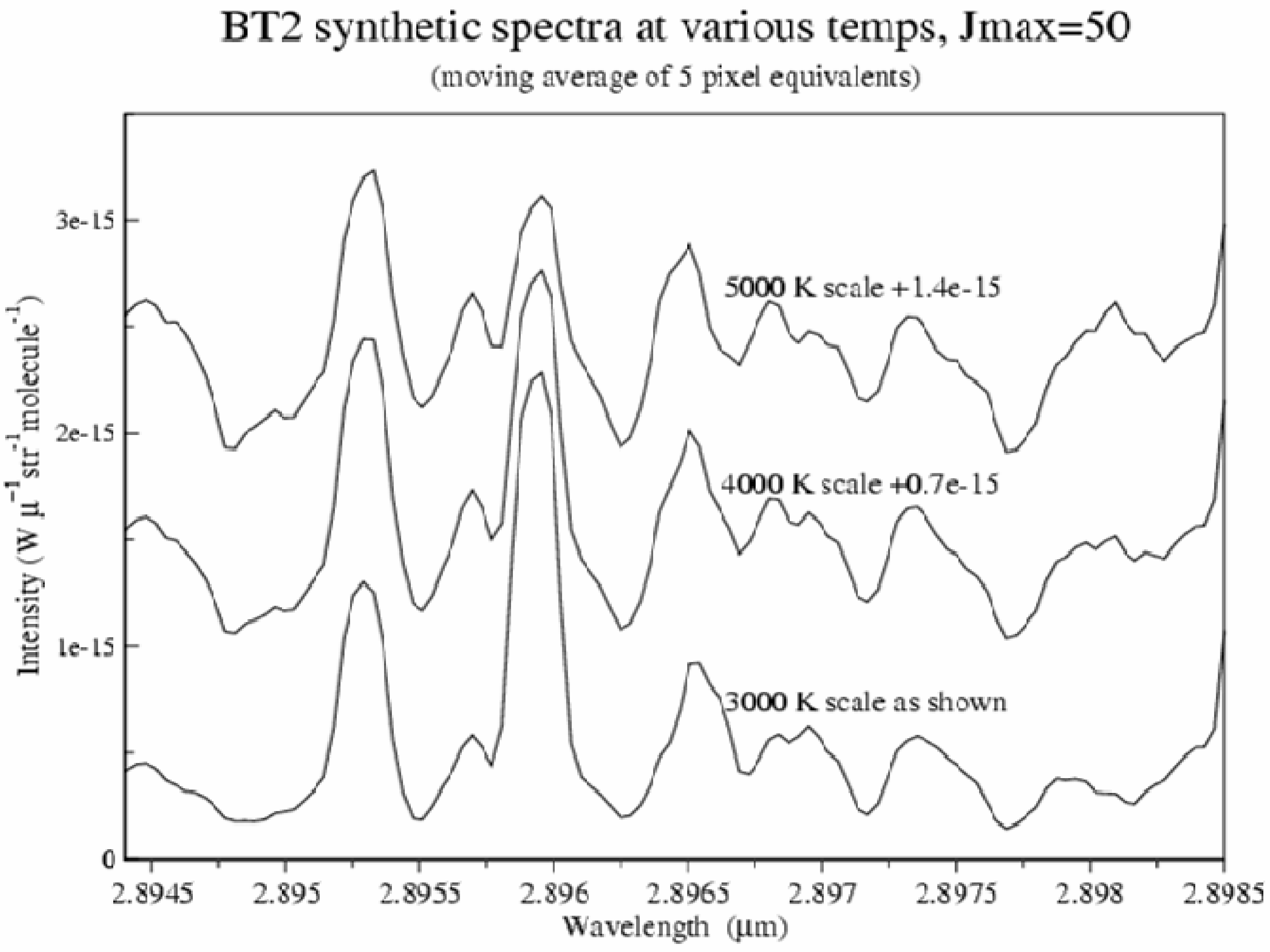


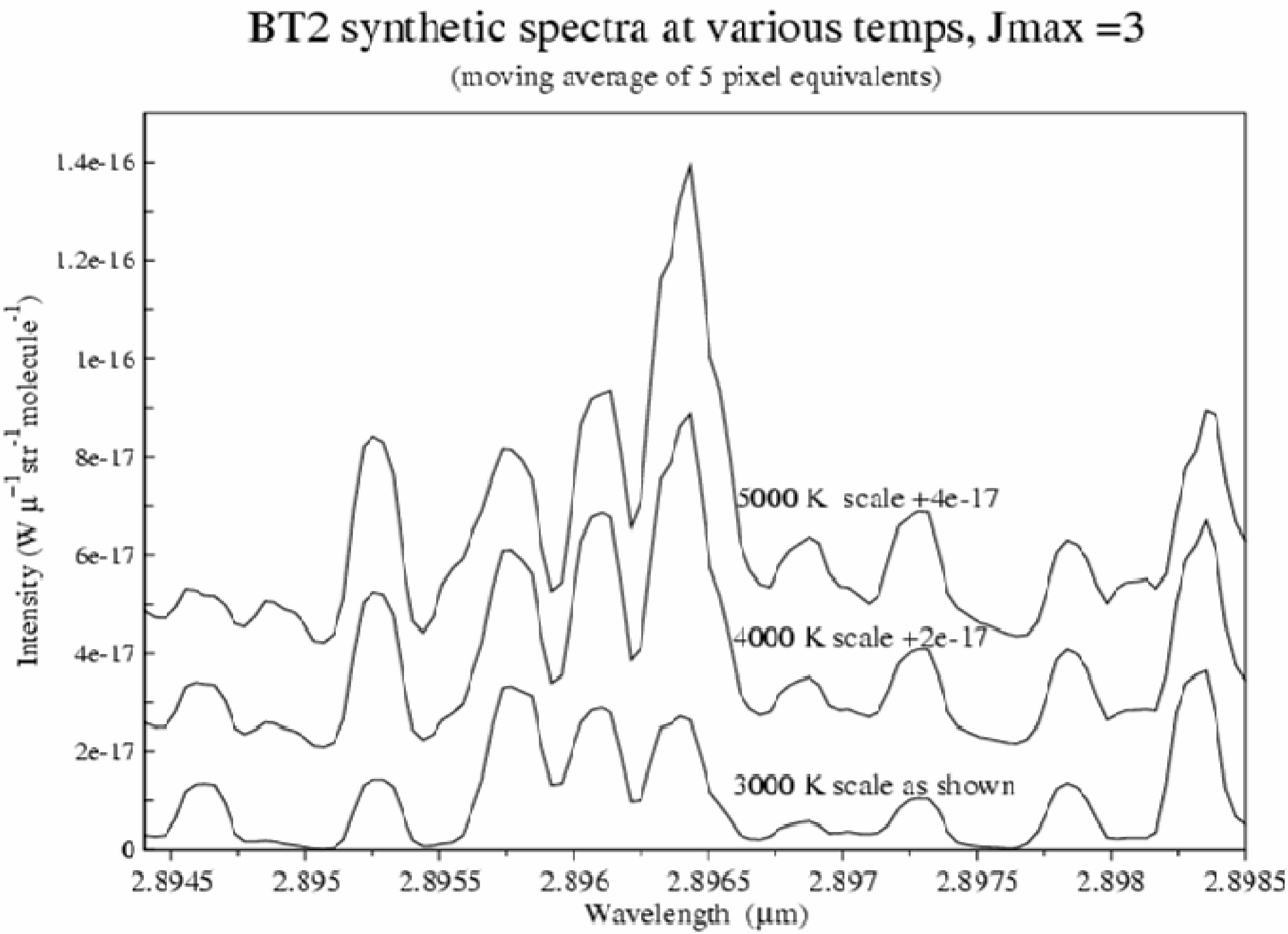
Fig. 4. Schematic showing pump and cascade rates (s^{-1}) for bands of interest near 2.9-μm (200–001, 200–100, 101–100, 101–001). The solid arrows indicate pump rates into the upper vibrational states, dashed arrows indicate cascade rates.

Spectra of Tempel 1 post-impact

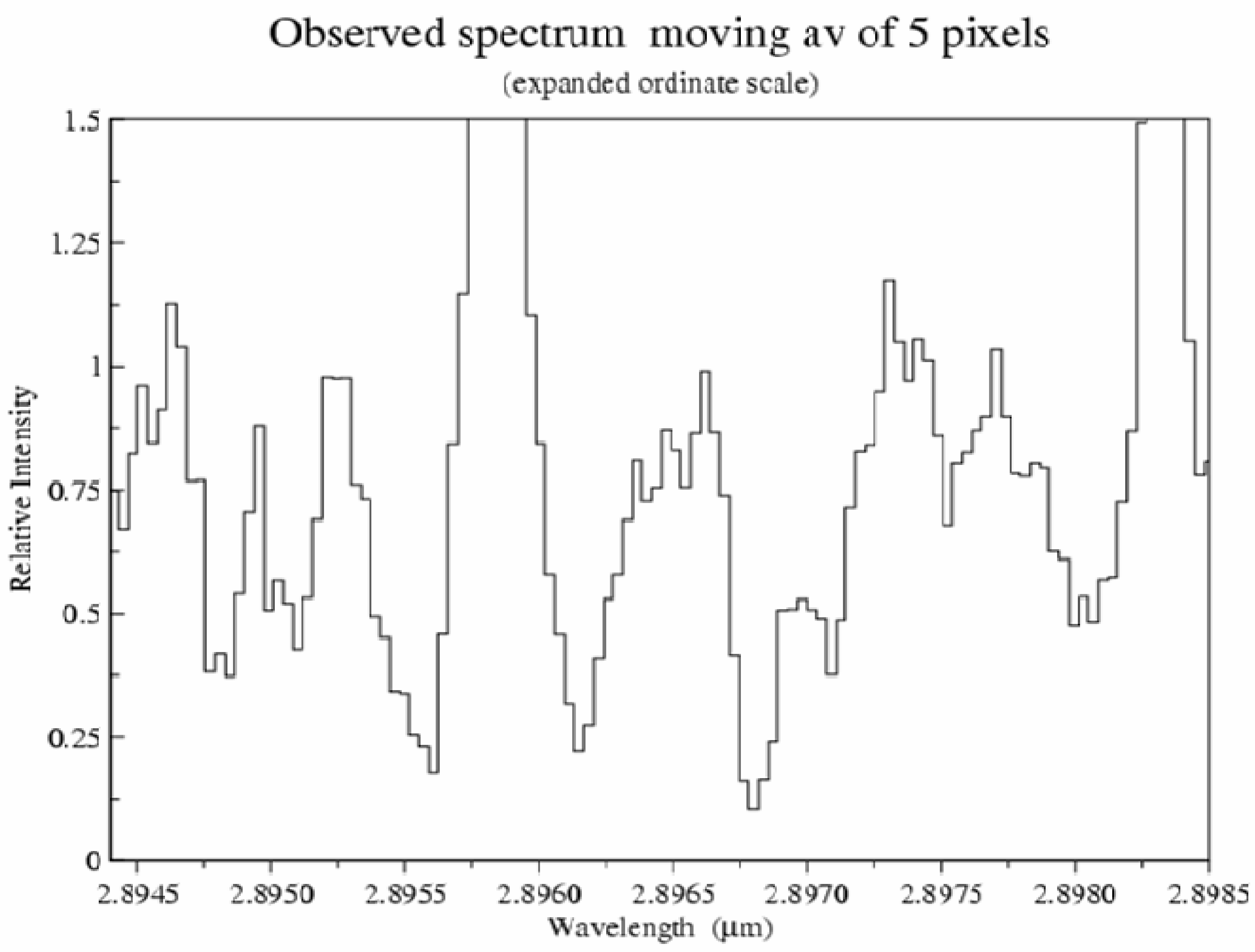

Observed spectrum - rest wavelengths
Intensity (10^-16 Wm^-2 μ^-1)
Wavelength (μm)
SPF
SH
SH
SPF
SH
SPF
10
8
6
4
2
0
2.8945
2.8950
2.8955
2.8960
2.8965
2.8970
2.8975
2.8980
2.8985



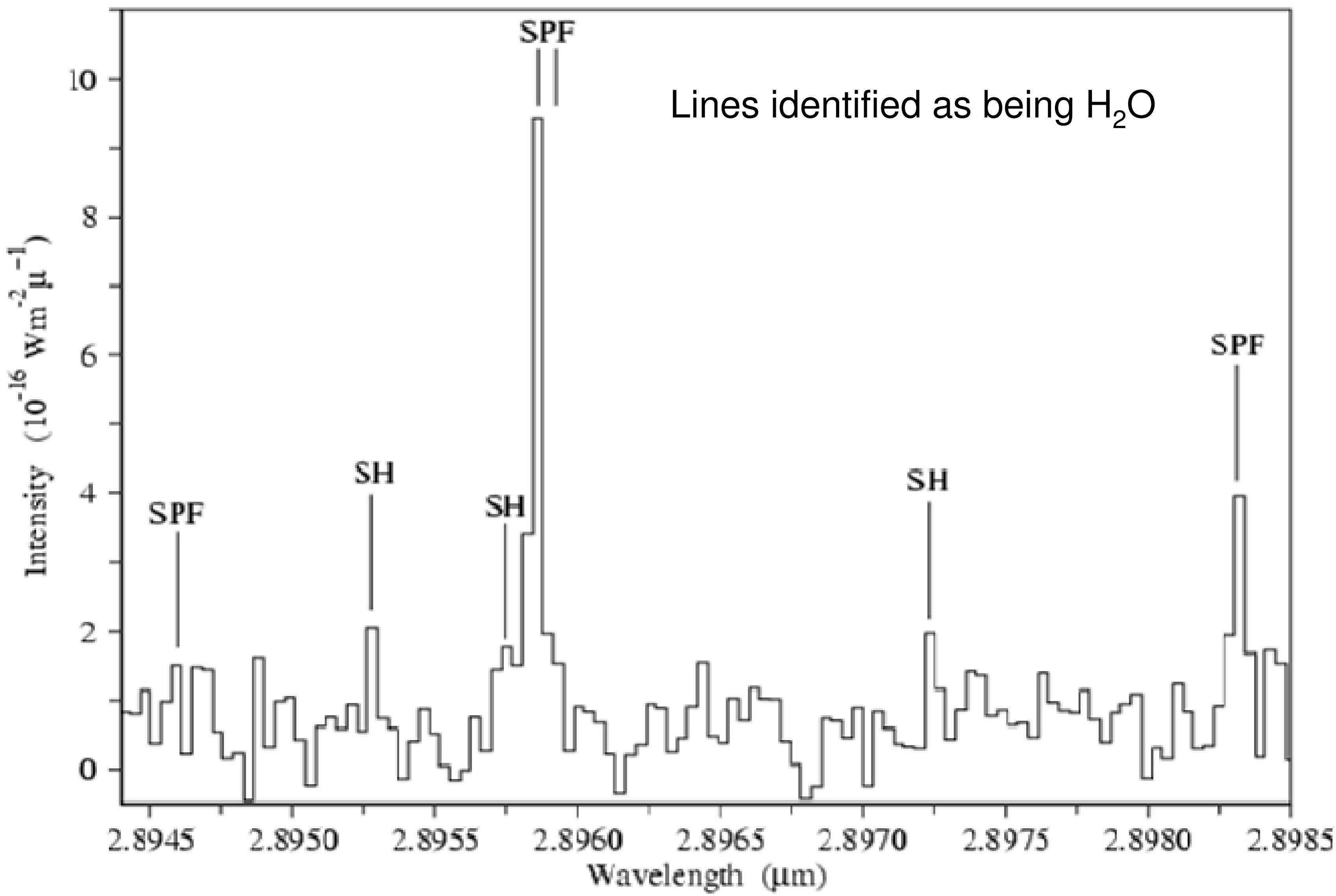
BT2 synthetic spectra at various temps, Jmax=50
(moving average of 5 pixel equivalents)
5000 K scale +1.4e-15
4000 K scale +0.7e-15
3000 K scale as shown
Intensity (W μ-1 str-1 molecule-1)
3e-15
2e-15
1e-15
0
2.8945
2.895
2.8955
2.896
2.8965
2.897
2.8975
2.898
2.8985
Wavelength (μm)



BT2 synthetic spectra at various temps, Jmax =3
(moving average of 5 pixel equivalents)
Intensity (W μ^-1 str^-1 molecule^-1)
1.4e-16
1.2e-16
1e-16
8e-17
6e-17
4e-17
2e-17
0
5000 K scale +4e-17
4000 K scale +2e-17
3000 K scale as shown
2.8945
2.895
2.8955
2.896
2.8965
2.897
2.8975
2.898
2.8985
Wavelength (μm)


Observed spectrum moving av of 5 pixels
(expanded ordinate scale)
Relative Intensity
1.5
1.25
1
0.75
0.5
0.25
0
2.8945
2.8950
2.8955
2.8960
2.8965
2.8970
2.8975
2.8980
2.8985
Wavelength (µm)

Observed spectrum - rest wavelengths



In addition to the SPF lines, we observed a second, weak component, that we call ‘SH’. This does not imply a knowledge of the production route, except to indicate the origin as being some form of solar heating

$\lambda_{observed}$	Idendification		$\lambda_{laboratory}$	Type
μm ± 0.00005	Upper	Lower	μm	
2.89458	(101)[211] -	(001)[220]	2.89462	SPF
2.89527	(103)[110] -	(102)[110]	2.89526	SH
2.89527	(211)[322] -	(210)[211]	2.89528	SH
2.89573	(210)[101] -	(011)[000]	2.89570	SH
2.89580	(200)[110] -	(100)[221]	2.89578	SPF
2.89591	(101)[202] -	(100)[321]	2.89590	SPF
2.89723	(220)[212} -	(021)[111]	2.89728	SH
2.89831	(200)[110] -	(001)[111]	2.89830	SPF

Low S/N greatly restricted our temporal resolution. However, by aggregating the SU data, we determined that the combined intensities of the ‘SU’ transitions peaked ~30 mins. after impact and declined during the next ~20 mins.

Keck spectrum of Tempel 1 (UT 2006 July 4 6:43-7:25)
Reproduced from Mumma et al., Science 272, 1310