Hot Jupiters & Cool Stars Beware:

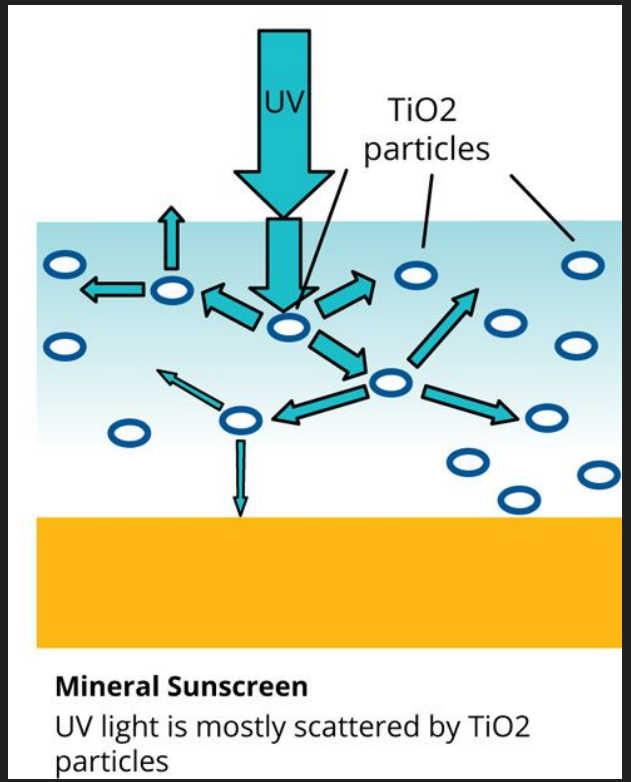
A new TiO line list is here.

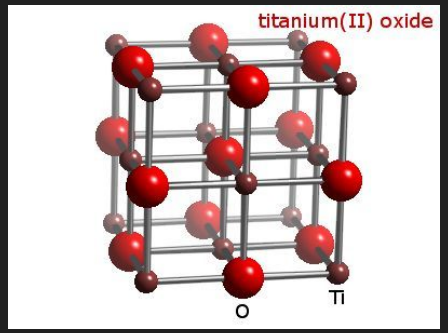
Laura K. McKemmish
University of New South Wales

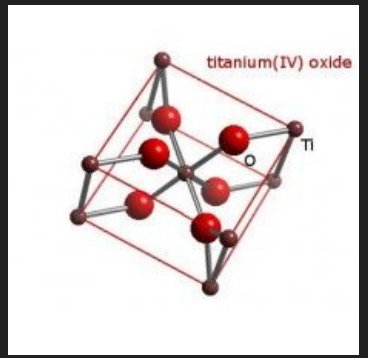
Thomas Masseron
Instituto de Astrofísica de Canarias

Sergey N. Yurchenko, Jonathan Tennyson
University College London

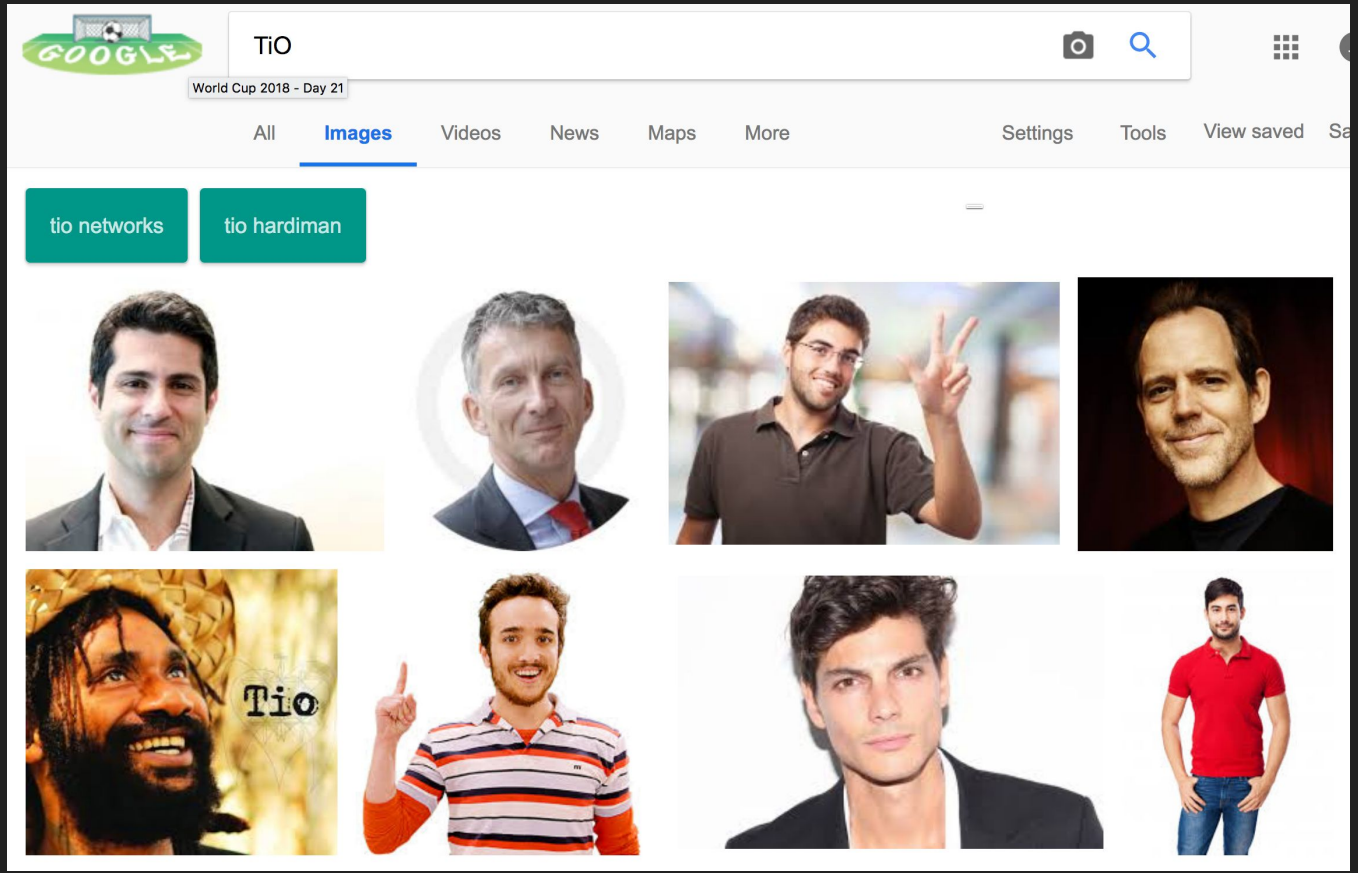
Titanium oxide to chemists



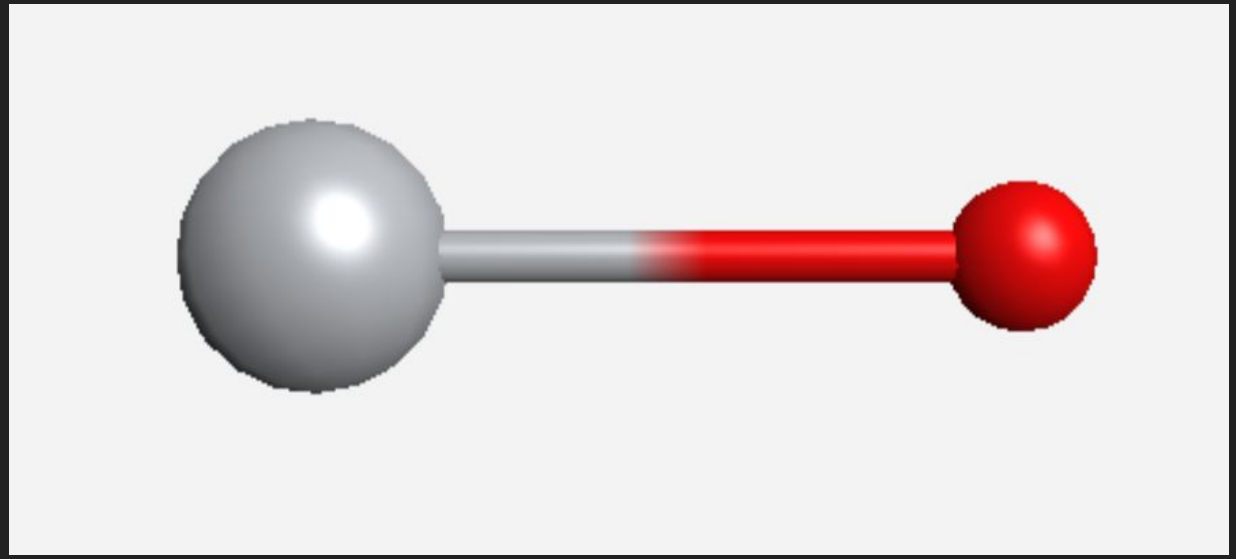




TiO to Google

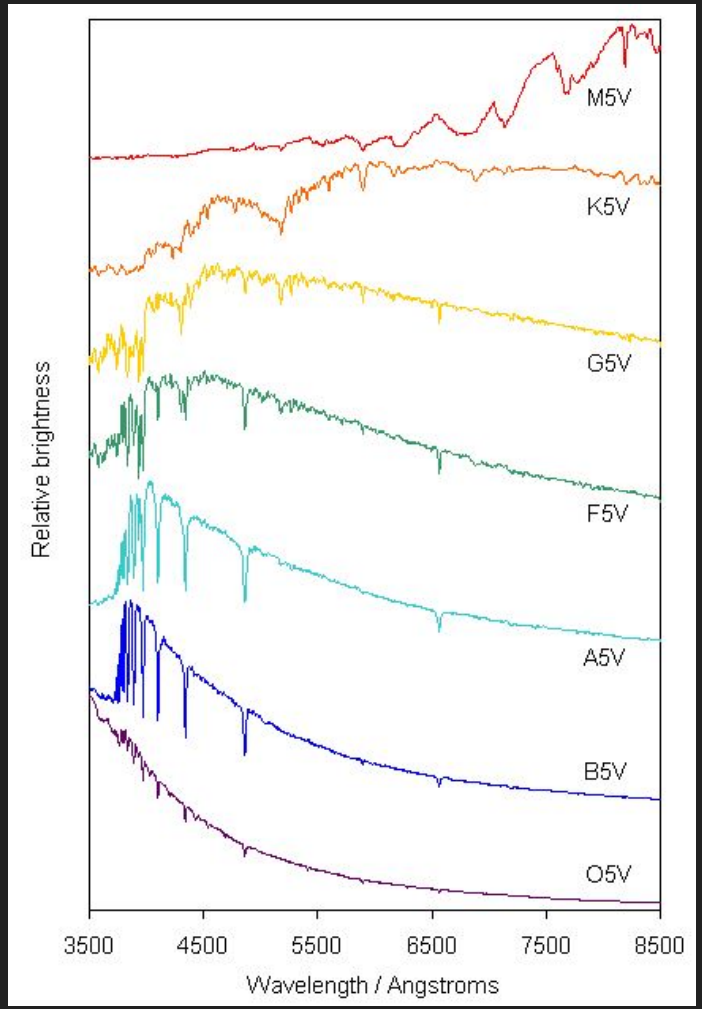


Titanium oxide to astronomers

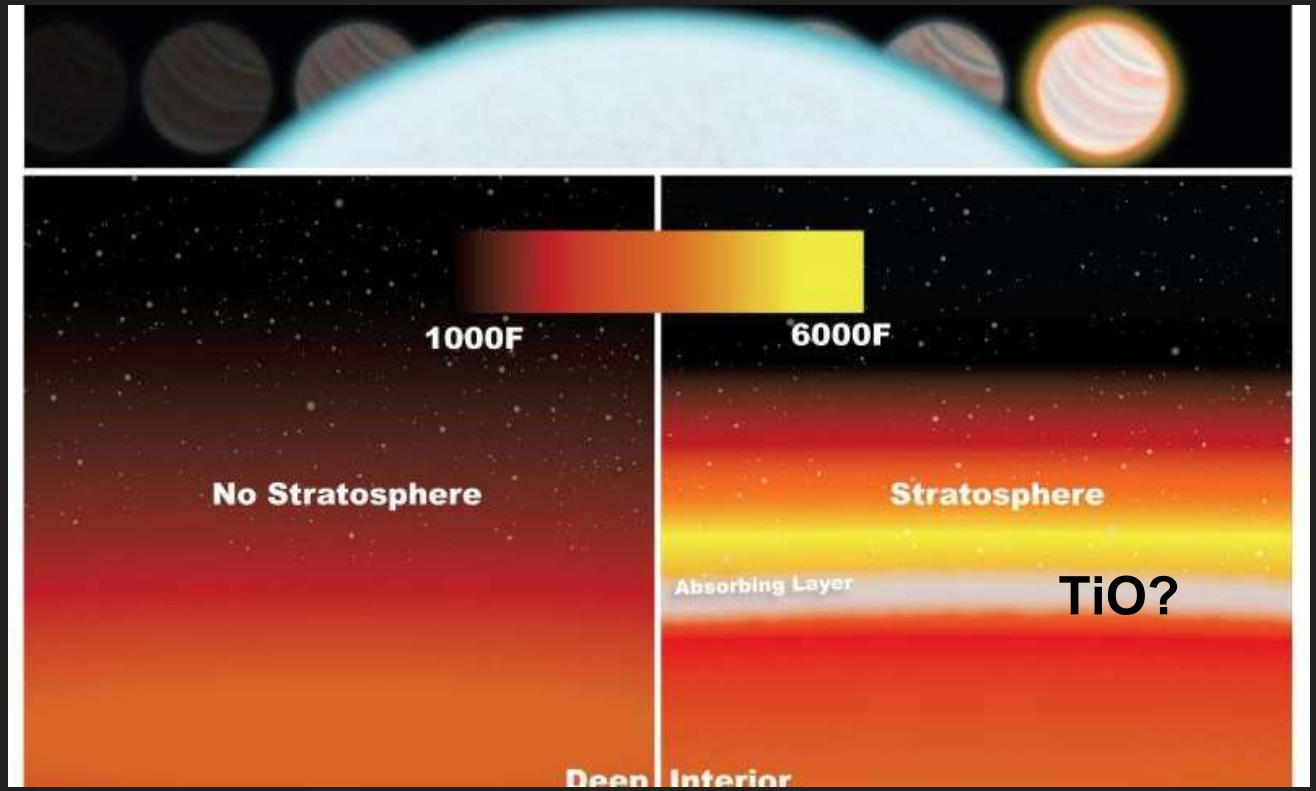


One of top 10 most important molecules

TiO in stars


M5V
K5V
G5V
F5V
A5V
B5V
O5V
Relative brightness
3500
4500
5500
6500
7500
8500
Wavelength / Angstroms

TiO, hot Jupiters and temperature inversion



Hot Jupiter: Recent Results

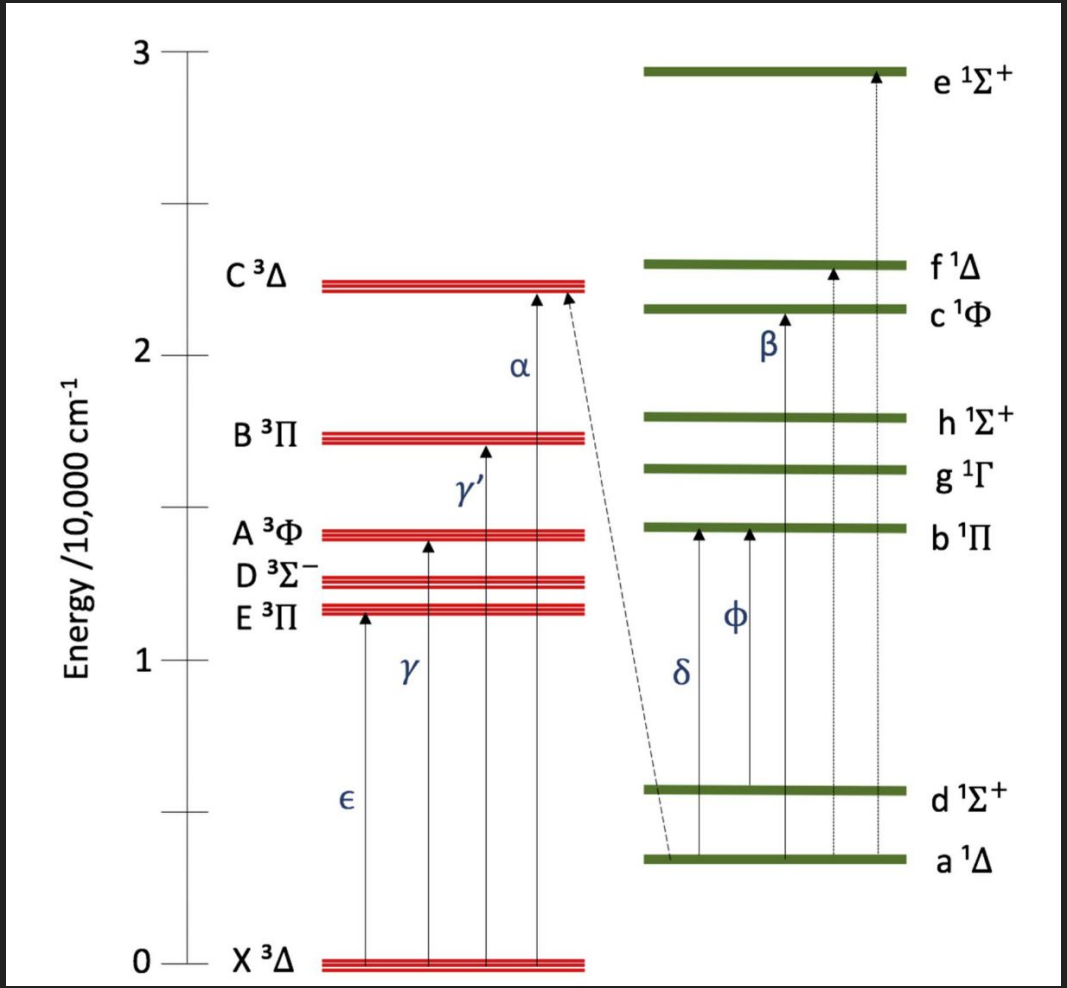
Letter | Published: 13 September 2017

Detection of titanium oxide in the atmosphere of a hot Jupiter

Elyar Sedaghati ✉, Henri M. J. Boffin, Ryan J. MacDonald, Siddharth Gandhi, Nikku Madhusudhan, Neale P. Gibson, Mahmoudreza Oshagh, Antonio Claret & Heike Rauer

Nature **549**, 238–241 (14 September 2017) | Download Citation ↓

Electronic structure of TiO



Schwenke 1998

Faraday Discuss., 1998, **109**, 321–334

Opacity of TiO from a coupled electronic state calculation parametrized by *ab initio* and experimental data

David W. Schwenke
M.S. 230-3, NASA Ames Research Center, Moffett Field, CA 94035-1000, USA

- 13 coupled electronic states considered

Plez 1998

Astron. Astrophys. 337, 495–500 (1998)

ASTRONOMY AND ASTROPHYSICS

A new TiO line list

B. Plez[1,2]

[1] Astronomiska Observatoriet, Box 515, S-751 20 Uppsala, Sweden
[2] Atomspektroskopi, Fysiska Institution, Box 118, S-221 00 Lund, Sweden (plez@fysik.lu.se)

- 9 uncoupled electronic states considered

Plez 1998 … improved in VALD (2012

Astron. Astrophys. 337, 495–500 (1998)

ASTRONOMY AND ASTROPHYSICS

A new TiO line list

B. Plez[1,2]

[1] Astronomiska Observatoriet, Box 515, S-751 20 Uppsala, Sweden
[2] Atomspektroskopi, Fysiska Institution, Box 118, S-221 00 Lund, Sweden (plez@fysik.lu.se)

- 9 uncoupled electronic states considered
- **Incorporates experimental frequencies where available**
  - Shifted isotopologue frequencies by error in ^{48}TiO

High Resolution Ground-based Exoplanet Spectroscopy

Call to action

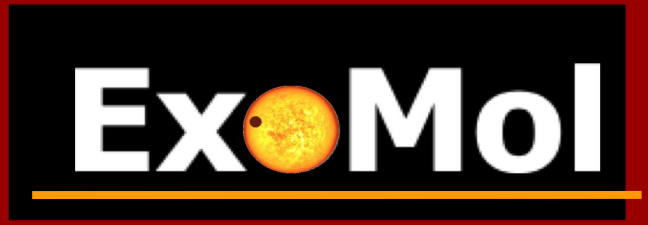
A&A 575, A20 (2015)

A search for TiO in the optical high-resolution transmission spectrum of HD 209458b: Hindrance due to inaccuracies in the line database

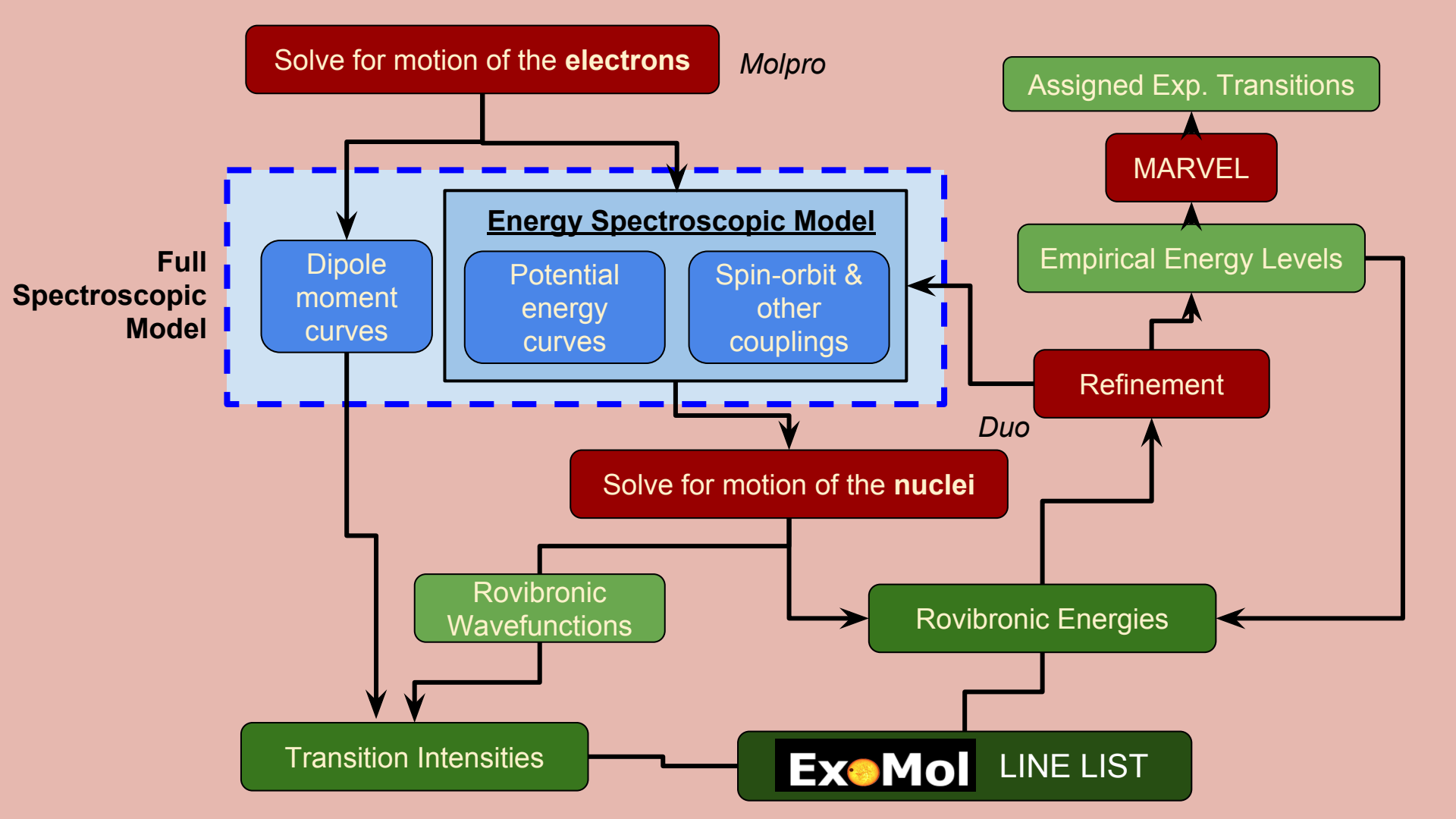
H. J. Hoeijmakers[1], R. J. de Kok[1,2], I. A. G. Snellen[1], M. Brogi[1,⋆], J. L. Birkby[1,3,⋆⋆] and H. Schwarz[1]

Resolutions of 100,000

At 1 um = 1000 A = 10,000 cm^{-1}, this is equivalent to 0.01 A = 0.1 cm^{-1}



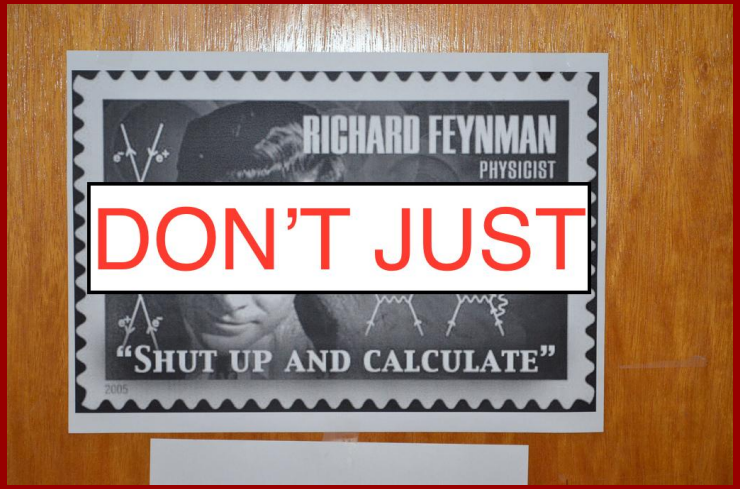
Creating a New TiO Linelist
Methods and Tools


Solve for motion of the **electrons**
Molpro
Assigned Exp. Transitions
MARVEL
Empirical Energy Levels
Full Spectroscopic Model
Dipole moment curves
Energy Spectroscopic Model
Potential energy curves
Spin-orbit & other couplings
Refinement
Duo
Solve for motion of the **nuclei**
Rovibronic Wavefunctions
Rovibronic Energies
Transition Intensities
ExoMol LINE LIST

Ab-initio (Molpro)

Solve for motion of the **electrons**

- Dipole moment curves
- Potential energy curves
- Spin-orbit & other couplings



TOPICAL REVIEW

The *ab initio* calculation of spectra of open shell diatomic molecules

Jonathan Tennyson, Lorenzo Lodi, Laura K McKemmish and Sergei N Yurchenko

Published 5 May 2016 • © 2016 IOP Publishing Ltd
Journal of Physics B: Atomic, Molecular and Optical Physics, Volume 49, Number 10

It's hard and accuracy is low

MARVEL

Assigned Exp. Transitions

MARVEL

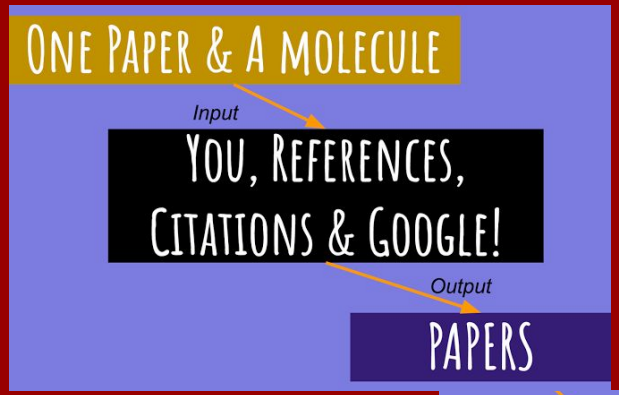
Empirical Energy Levels

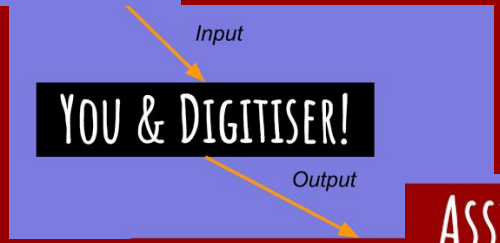
Available online at www.sciencedirect.com
ScienceDirect
Journal of Molecular Spectroscopy 245 (2007) 115–125
ELSEVIER
Journal of MOLECULAR SPECTROSCOPY
www.elsevier.com/locate/jms

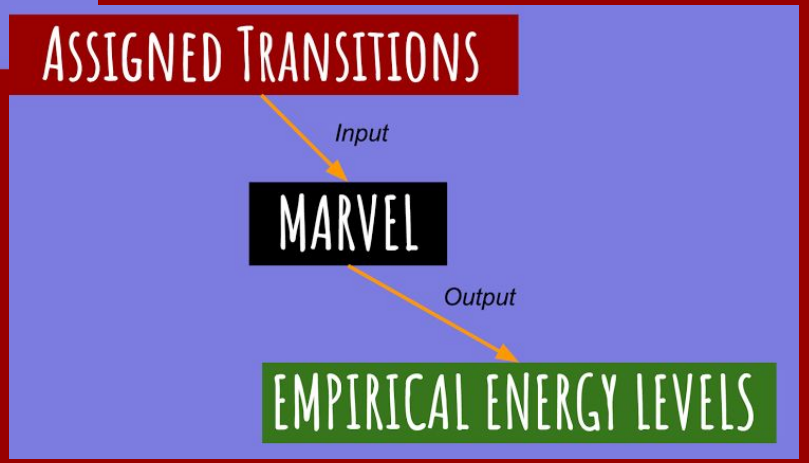
MARVEL: measured active rotational–vibrational energy levels

Tibor Furtenbacher [a], Attila G. Császár [a,*], Jonathan Tennyson [b]

MARVEL Project







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Papers

Input

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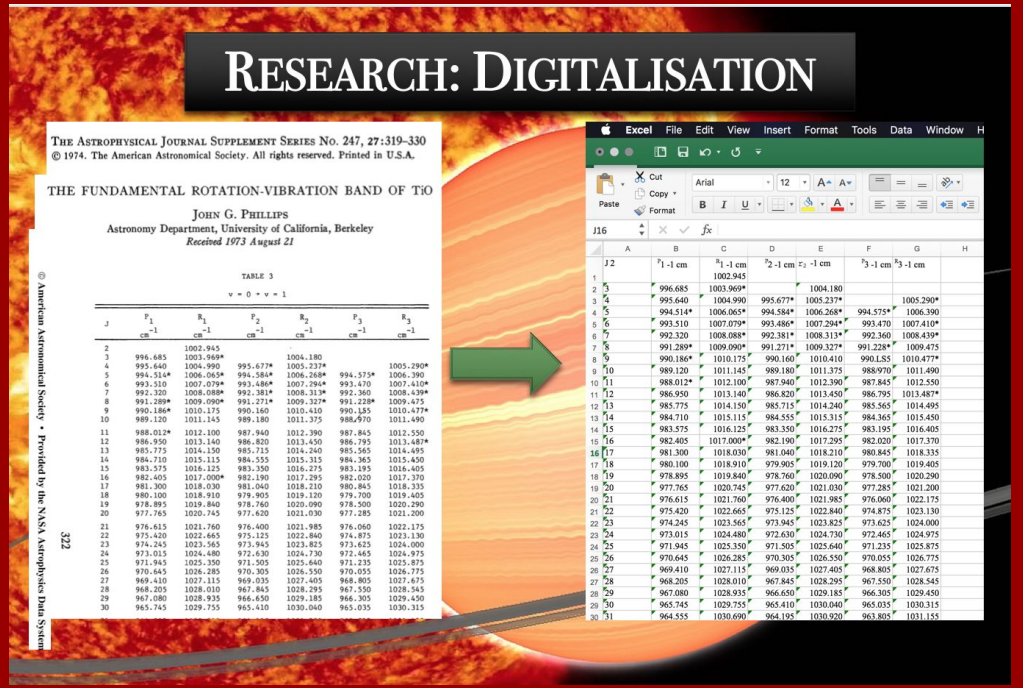
Output

Assigned Transitions

Research: Digitalisation



THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES No. 247, 27:319–330
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THE FUNDAMENTAL ROTATION-VIBRATION BAND OF TiO

JOHN G. PHILLIPS
Astronomy Department, University of California, Berkeley
Received 1973 August 21

TABLE 3

$v = 0 \rightarrow v = 1$

J	P_1 cm^{-1}	R_1 cm^{-1}	P_2 cm^{-1}	R_2 cm^{-1}	P_3 cm^{-1}	R_3 cm^{-1}
2		1002.945				
3	996.685	1003.969*		1004.180		
4	995.640	1004.990	995.677*	1005.237*		1005.290*
5	994.514*	1006.065*	994.584*	1006.268*	994.575*	1006.390
6	993.510	1007.079*	993.486*	1007.294*	993.470	1007.410*
7	992.320	1008.088*	992.381*	1008.313*	992.360	1008.439*
8	991.289*	1009.090*	991.271*	1009.327*	991.228*	1009.475
9	990.186*	1010.175	990.160	1010.410	990.135	1010.477*
10	989.120	1011.145	989.180	1011.375	988.970	1011.490
11	988.012*	1012.100	987.940	1012.390	987.845	1012.550
12	986.950	1013.140	986.820	1013.450	986.795	1013.487*
13	985.775	1014.150	985.715	1014.260	985.565	1014.495
14	984.710	1015.115	984.555	1015.315	984.365	1015.450
15	983.575	1016.125	983.350	1016.275	983.195	1016.405
16	982.405	1017.000*	982.190	1017.295	982.020	1017.370
17	981.300	1018.030	981.040	1018.210	980.845	1018.335
18	980.100	1018.910	979.905	1019.120	979.700	1019.405
19	978.895	1019.840	978.760	1020.090	978.500	1020.290
20	977.765	1020.745	977.620	1021.030	977.285	1021.200
21	976.615	1021.760	976.400	1021.985	976.060	1022.175
22	975.420	1022.665	975.125	1022.840	974.875	1023.130
23	974.245	1023.565	973.945	1023.825	973.625	1024.000
24	973.015	1024.480	972.630	1024.730	972.465	1024.975
25	971.945	1025.350	971.505	1025.640	971.235	1025.875
26	970.645	1026.285	970.305	1026.550	970.055	1026.775
27	969.410	1027.115	969.035	1027.405	968.805	1027.675
28	968.205	1028.010	967.845	1028.295	967.550	1028.545
29	967.080	1028.935	966.650	1029.185	966.305	1029.450
30	965.745	1029.755	965.410	1030.040	965.035	1030.315

322

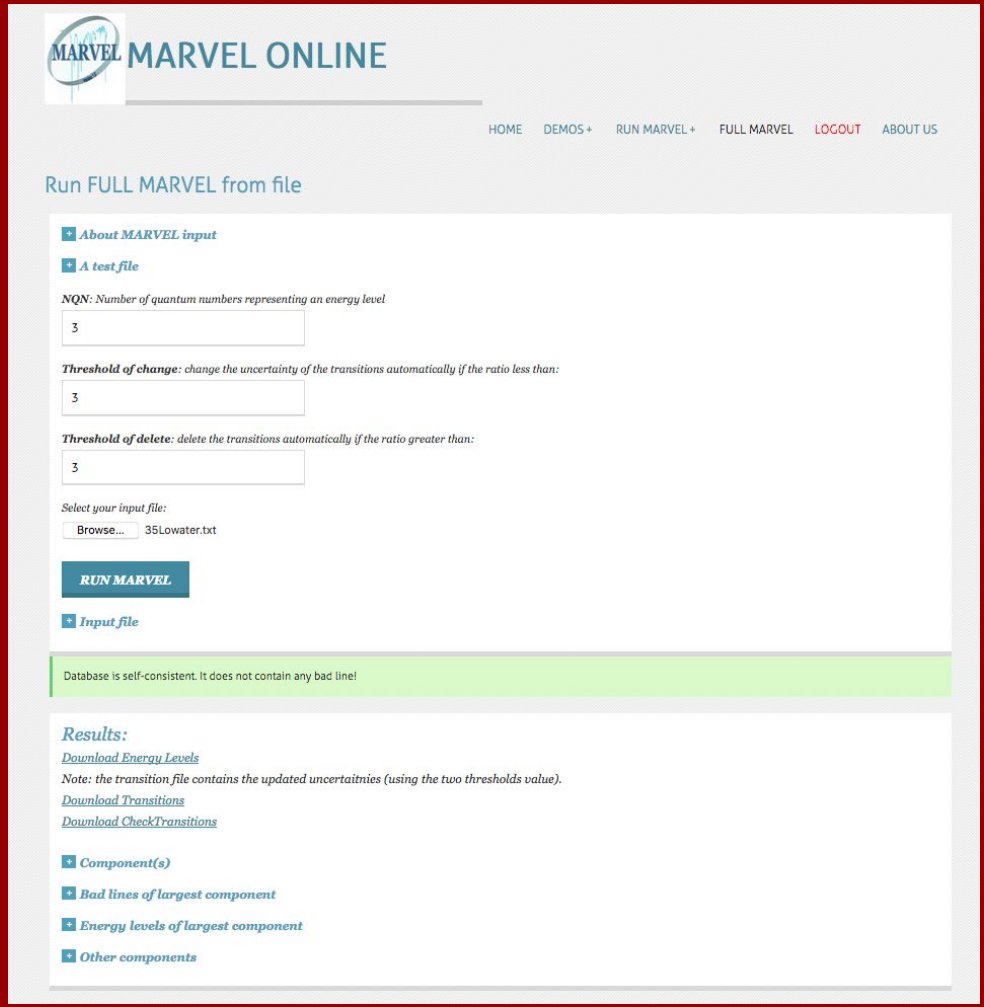
	J 2	P_1 -1 cm	R_1 -1 cm	P_2 -1 cm	r_2 -1 cm	R_3 -1 cm	R_3 -1 cm
1			1002.945				
2	3	996.685	1003.969*		1004.180		
3	4	995.640	1004.990	995.677*	1005.237*		1005.290*
4	5	994.514*	1006.065*	994.584*	1006.268*	994.575*	1006.390
5	6	993.510	1007.079*	993.486*	1007.294*	993.470	1007.410*
6	7	992.320	1008.088*	992.381*	1008.313*	992.360	1008.439*
7	8	991.289*	1009.090*	991.271*	1009.327*	991.228*	1009.475
8	9	990.186*	1010.175	990.160	1010.410	990.LS5	1010.477*
9	10	989.120	1011.145	989.180	1011.375	988.970	1011.490
10	11	988.012*	1012.100	987.940	1012.390	987.845	1012.550
11	12	986.950	1013.140	986.820	1013.450	986.795	1013.487*
12	13	985.775	1014.150	985.715	1014.240	985.565	1014.495
13	14	984.710	1015.115	984.555	1015.315	984.365	1015.450
14	15	983.575	1016.125	983.350	1016.275	983.195	1016.405
15	16	982.405	1017.000*	982.190	1017.295	982.020	1017.370
16	17	981.300	1018.030	981.040	1018.210	980.845	1018.335
17	18	980.100	1018.910	979.905	1019.120	979.700	1019.405
18	19	978.895	1019.840	978.760	1020.090	978.500	1020.290
19	20	977.765	1020.745	977.620	1021.030	977.285	1021.200
20	21	976.615	1021.760	976.400	1021.985	976.060	1022.175
21	22	975.420	1022.665	975.125	1022.840	974.875	1023.130
22	23	974.245	1023.565	973.945	1023.825	973.625	1024.000
23	24	973.015	1024.480	972.630	1024.730	972.465	1024.975
24	25	971.945	1025.350	971.505	1025.640	971.235	1025.875
25	26	970.645	1026.285	970.305	1026.550	970.055	1026.775
26	27	969.410	1027.115	969.035	1027.405	968.805	1027.675
27	28	968.205	1028.010	967.845	1028.295	967.550	1028.545
28	29	967.080	1028.935	966.650	1029.185	966.305	1029.450
29	30	965.745	1029.755	965.410	1030.040	965.035	1030.315
30	31	964.555	1030.690	964.195	1030.920	963.805	1031.155

MARVEL

Assigned Exp. Transitions

MARVEL

Empirical Energy Levels



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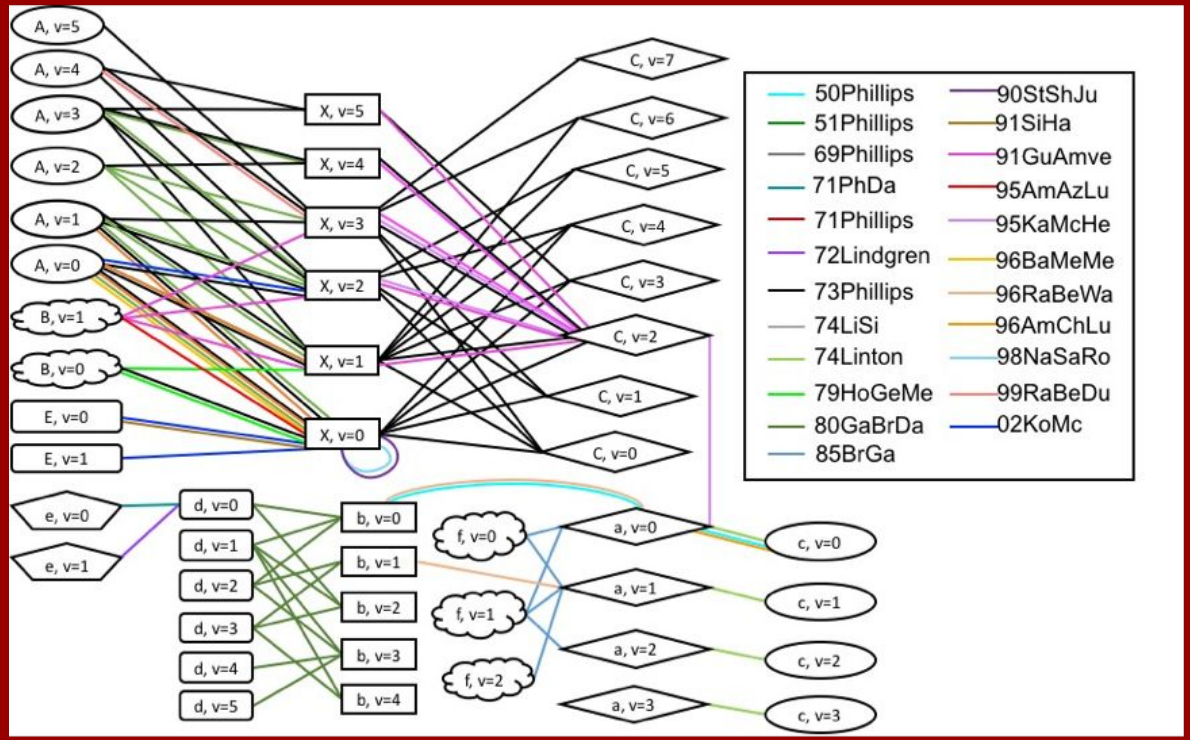
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B, v=1
B, v=0
E, v=0
E, v=1
e, v=0
e, v=1
X, v=5
X, v=4
X, v=3
X, v=2
X, v=1
X, v=0
d, v=0
d, v=1
d, v=2
d, v=3
d, v=4
d, v=5
b, v=0
b, v=1
b, v=2
b, v=3
b, v=4
f, v=0
f, v=1
f, v=2
C, v=7
C, v=6
C, v=5
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C, v=1
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a, v=2
a, v=3
c, v=0
c, v=1
c, v=2
c, v=3
50Phillips
51Phillips
69Phillips
71PhDa
71Phillips
72Lindgren
73Phillips
74LiSi
74Linton
79HoGeMe
80GaBrDa
85BrGa
90StShJu
91SiHa
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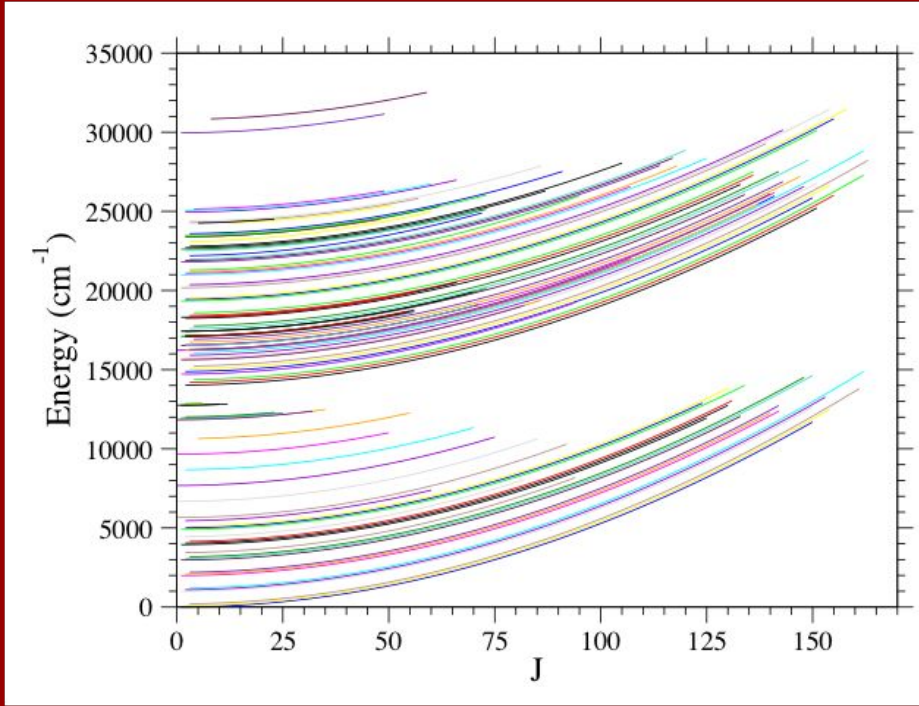
96RaBeWa
96AmChLu
98NaSaRo
99RaBeDu
02KoMc

MARVEL


35000
30000
25000
20000
15000
10000
5000
0
Energy (cm-1)
0
25
50
75
100
125
150
J

MARVEL

Twinkle
ORBYTS

The Astrophysical Journal Supplement Series, 228:15 (22pp), 2017 February https://doi.org/10.3847/1538-4365/228/2/15

OPEN ACCESS

MARVEL Analysis of the Measured High-resolution Rovibronic Spectra of $^{48}Ti^{16}O$

Laura K. McKemmish[1], Thomas Masseron[2], Samuel Sheppard[3], Elizabeth Sandeman[3], Zak Schofield[3], Tibor Furtenbacher[4], Attila G. Császár[4], Jonathan Tennyson[1], and Clara Sousa-Silva[1]

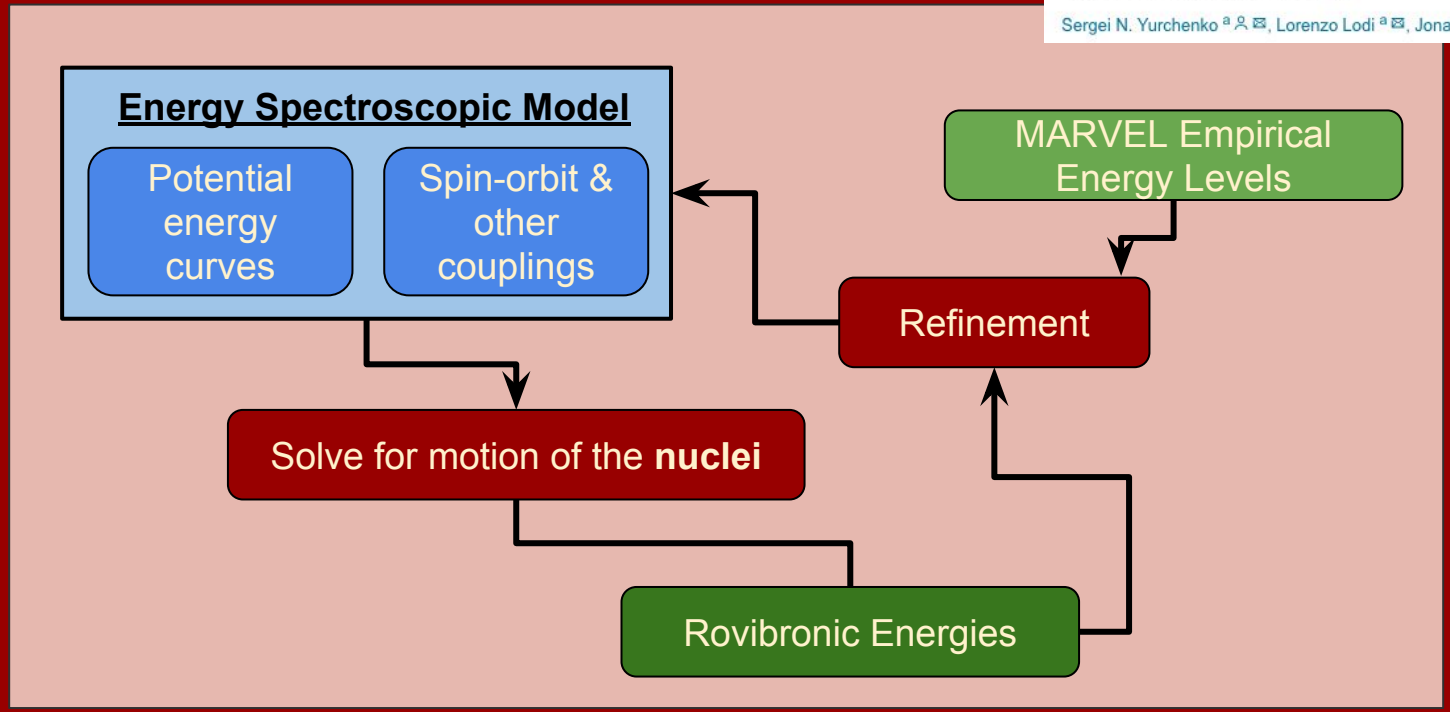
[1] Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK; laura.mckemmish@gmail.com
[2] Institute of Astronomy, University of Cambridge, Madingley Road, Cambridge, CB3 0HA, UK
[3] Highams Park School, Handsworth Avenue, Highams Park, London, E4 9PJ, UK
[4] Institute of Chemistry, Eötvös Loránd University and MTA-ELTE Complex Chemical Systems Research Group, H-1518 Budapest 112, Hungary
Received 2016 September 30; revised 2016 December 22; accepted 2016 December 22; published 2017 February 8

Duo: Role 1

Computer Physics Communications
Volume 202, May 2016, Pages 262-275

DUO: A general program for calculating spectra of diatomic molecules ☆

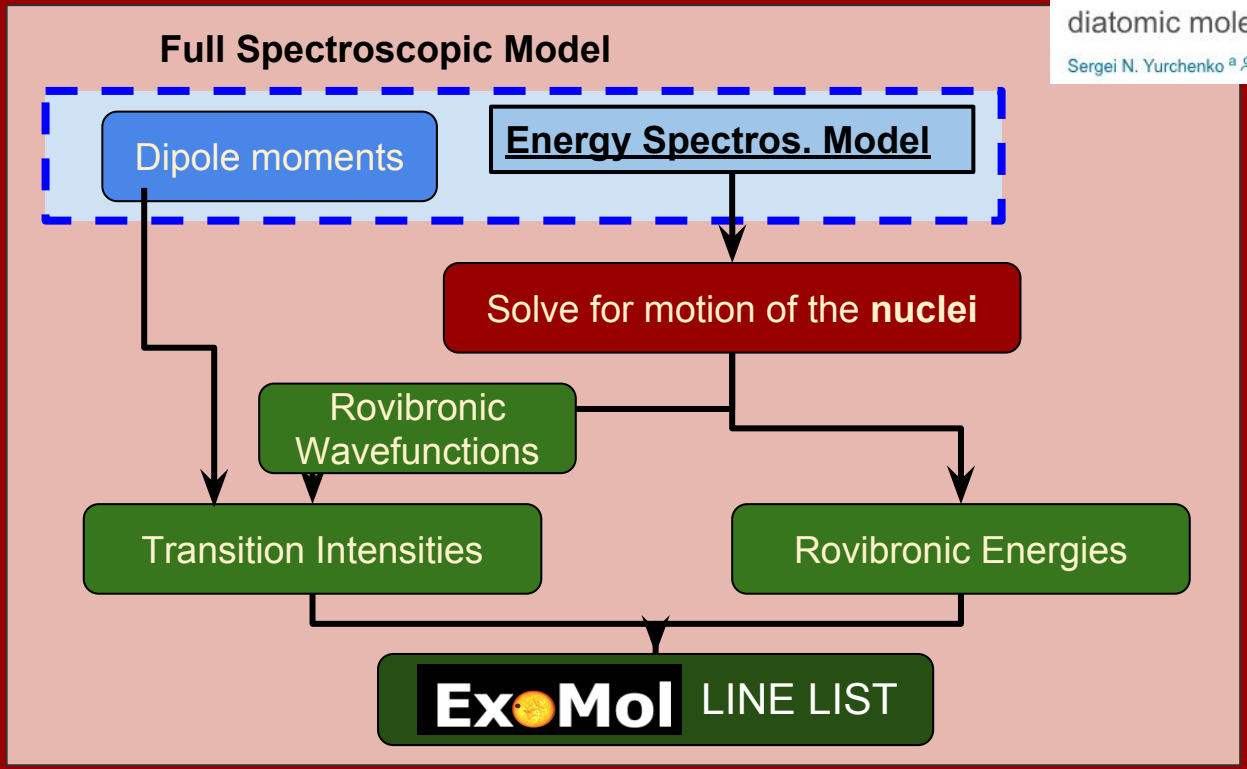
Sergei N. Yurchenko [a], Lorenzo Lodi [a], Jonathan Tennyson [a], Andrey V. Stolyarov [b]



State	v	ExoMol		Plez 1998		Schwenke 1998	
		rmsd	max	rmsd	max	rmsd	max
X $^3\Delta$	0	0.032	0.117	0.624	3.442	0.572	1.126
	1	0.017	0.057	0.599	3.309	0.611	1.282
	2	0.020	0.047	0.317	2.344	0.607	1.579
	3	0.021	0.048	0.497	2.741	0.744	2.416
	4	0.040	0.230	1.101	5.612	1.173	5.457
	5	0.066	0.140	0.741	4.764	0.820	4.017
E $^3\Pi$	0	0.023	0.073	0.720	1.698	1.657	2.998
A $^3\Phi$	0	0.454	0.586	0.628	3.632	0.746	2.113
	1	0.207	0.379	0.602	3.702	0.790	2.257
	2	0.051	0.160	0.594	3.997	0.806	2.239
	3	0.304	0.506	0.300	2.182	0.717	1.955
	4	0.499	0.641	0.412	4.175	0.747	3.584
	5	0.743	1.057	0.492	3.078	0.733	2.228
B $^3\Pi$	0	0.132	0.372	5.901	14.999	18.602	49.894
	1	0.269	1.023	0.988	3.854	27.948	49.896
C $^3\Delta$	0	0.104	0.175	3.693	10.452	0.998	3.521
	1	0.236	0.428	1.944	4.868	1.027	3.865
	2	0.144	0.216	2.074	6.221	1.119	3.370
	3	0.148	0.339	2.148	11.849	2.475	8.545
	4	0.774	4.559	1.401	3.741	2.845	9.800
	5	2.276	8.010	3.030	9.874	3.318	11.107
	6	4.386	10.349	2.424	8.545	7.523	19.053
	7	0.709	3.815	1.381	5.869	10.036	16.303

State	v	ExoMol		Plez 1998		Schwenke 1998	
		rmsd	max	rmsd	max	rmsd	max
a $^1\Delta$	0	0.006	0.015	0.156	0.276	0.19	0.385
	1	0.017	0.059	8.660	19.956	2.219	11.846
	2	0.236	1.39	14.223	14.328	0.195	0.517
	3	0.038	0.089				
d $^1\Sigma^+$	0	0.021	0.104	0.414	1.064	0.121	0.288
	1	0.018	0.034	8.279	8.454	0.116	0.291
	2	0.014	0.048	15.810	15.932	0.103	0.316
	3	0.025	0.049	22.841	22.933	0.080	0.201
	4	0.027	0.091	29.444	29.497	0.059	0.215
	5	0.101	0.195	35.565	35.610	0.051	0.087
b $^1\Pi$	0	0.09	0.336	1.425	4.080	2.984	3.550
	1	0.084	0.345	6.519	6.902	3.227	3.839
	2	0.084	0.352	12.848	13.251	3.189	3.740
	3	0.093	0.492	17.632	18.093	2.943	3.280
	4	0.065	0.265	21.108	21.527	2.603	2.999
c $^1\Phi$	0	0.164	0.939	1.245	5.402	0.205	0.383
	1	0.031	0.136	9.394	19.004	2.201	10.538
	2	0.16	0.904	15.244	15.410	0.783	1.947
	3	0.085	0.268				
f $^1\Delta$	0	0.031	0.14	4.594	4.645	0.155	0.458
	1	0.025	0.089	4.540	4.612	0.345	0.771
	2	0.309	0.606	4.211	4.565	0.301	0.432
e $^1\Sigma^+$	0	0.714	1.281				
	1	1.094	2.306				

Duo: Role 2

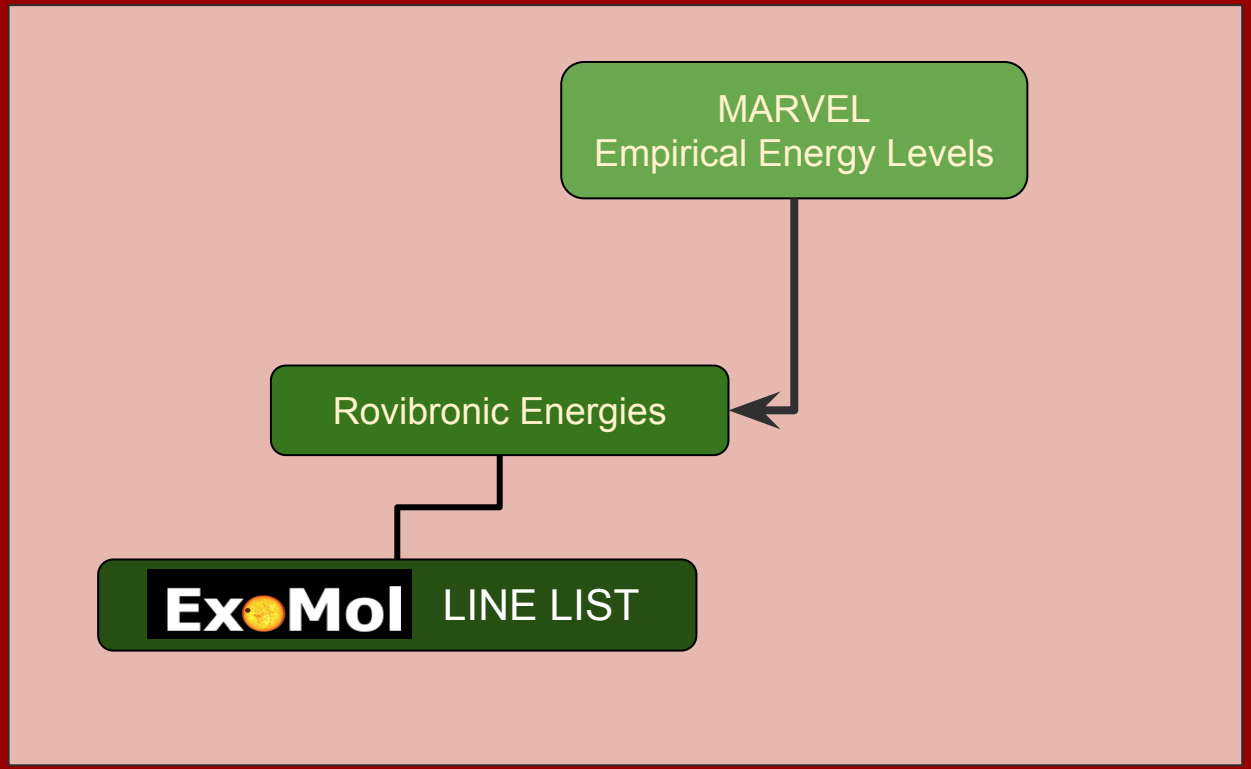


Computer Physics Communications
Volume 202, May 2016, Pages 262-275

DUO: A general program for calculating spectra of diatomic molecules ☆

Sergei N. Yurchenko [a], Lorenzo Lodi [a], Jonathan Tennyson [a], Andrey V. Stolyarov [b]

Final Stage


MARVEL
Empirical Energy Levels
Rovibronic Energies
ExoMol
LINE LIST

Ongoing Science...

Dr Laura McKemmish @laura_mckemmish · Jun 20

Replying to @TroveMaster

It would be great to have their data to improve the upcoming TiO line list!

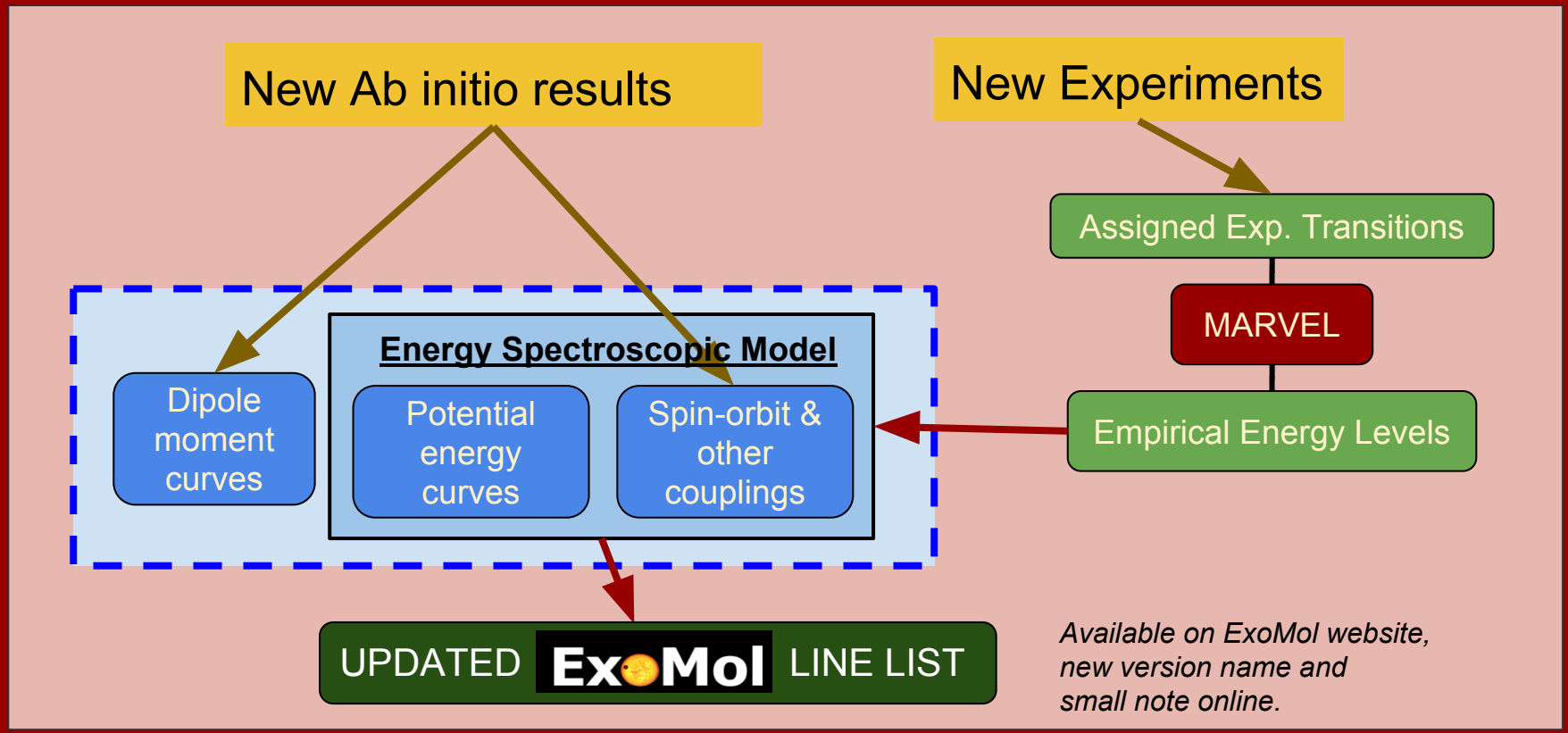
1 2

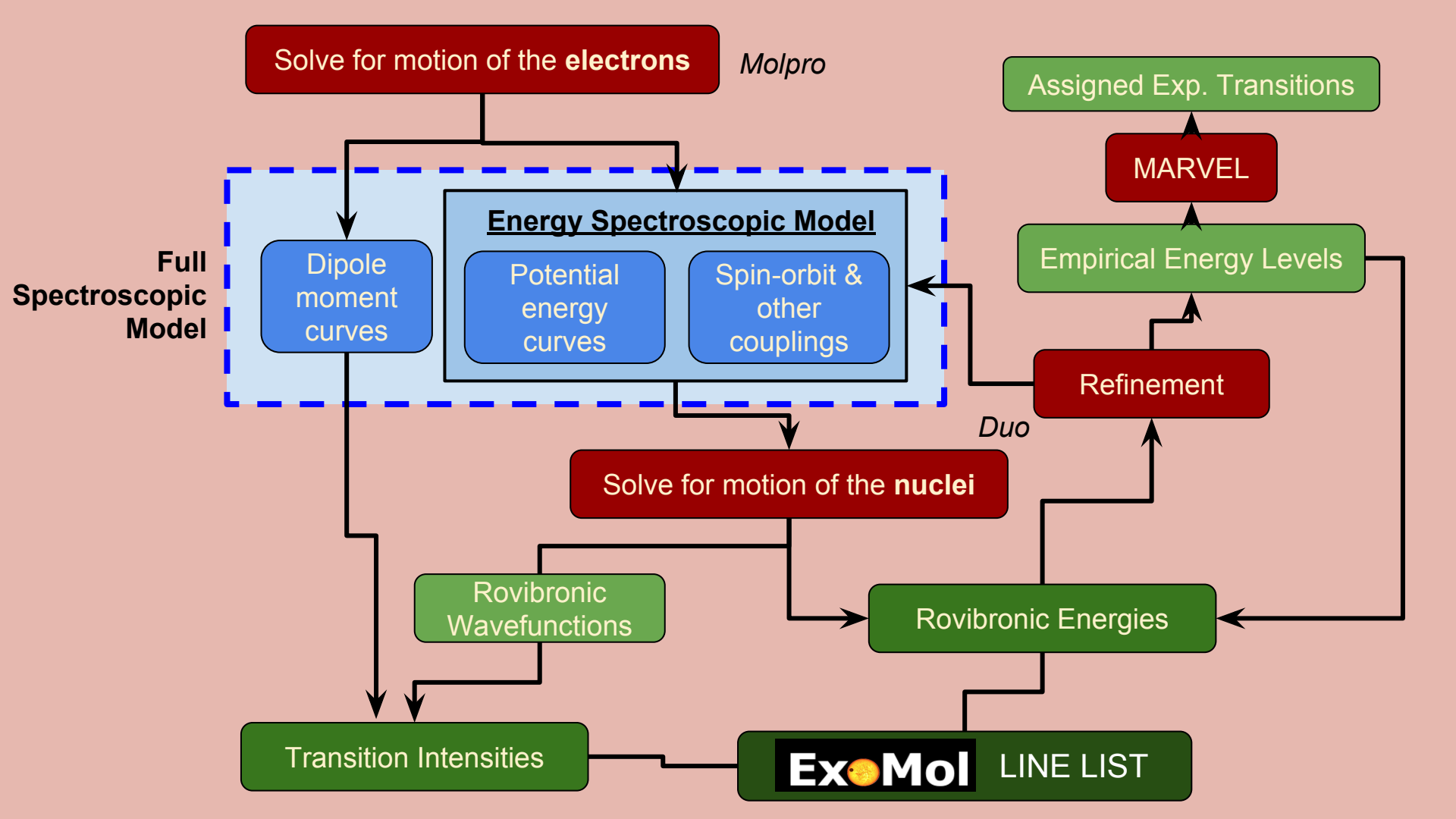
Sergey Yurchenko @TroveMaster · Jun 21

Daniel and Thomas Giessen (head of the group) kindly promised their line position of TiO before publication 😀

1

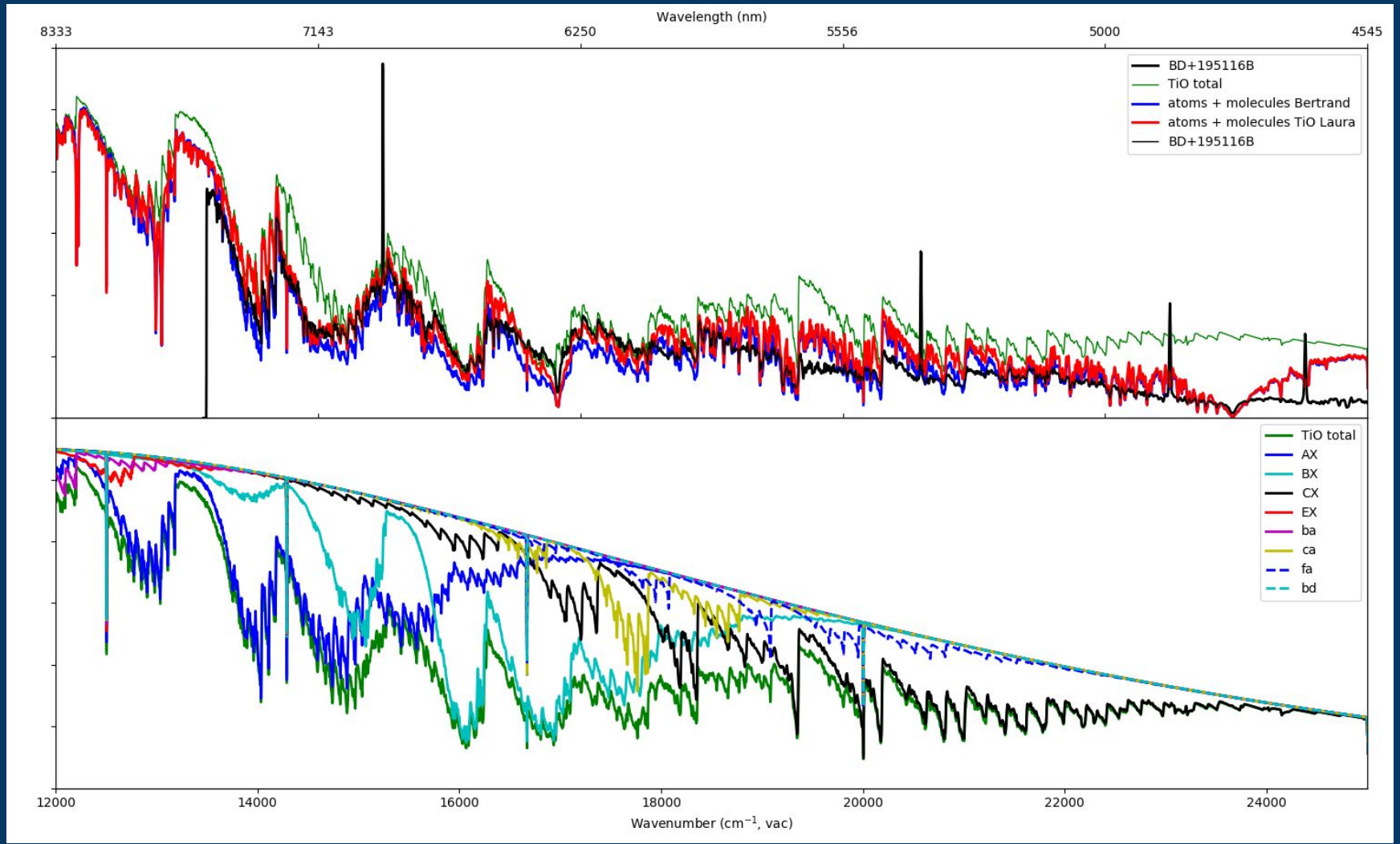
Adding New Information

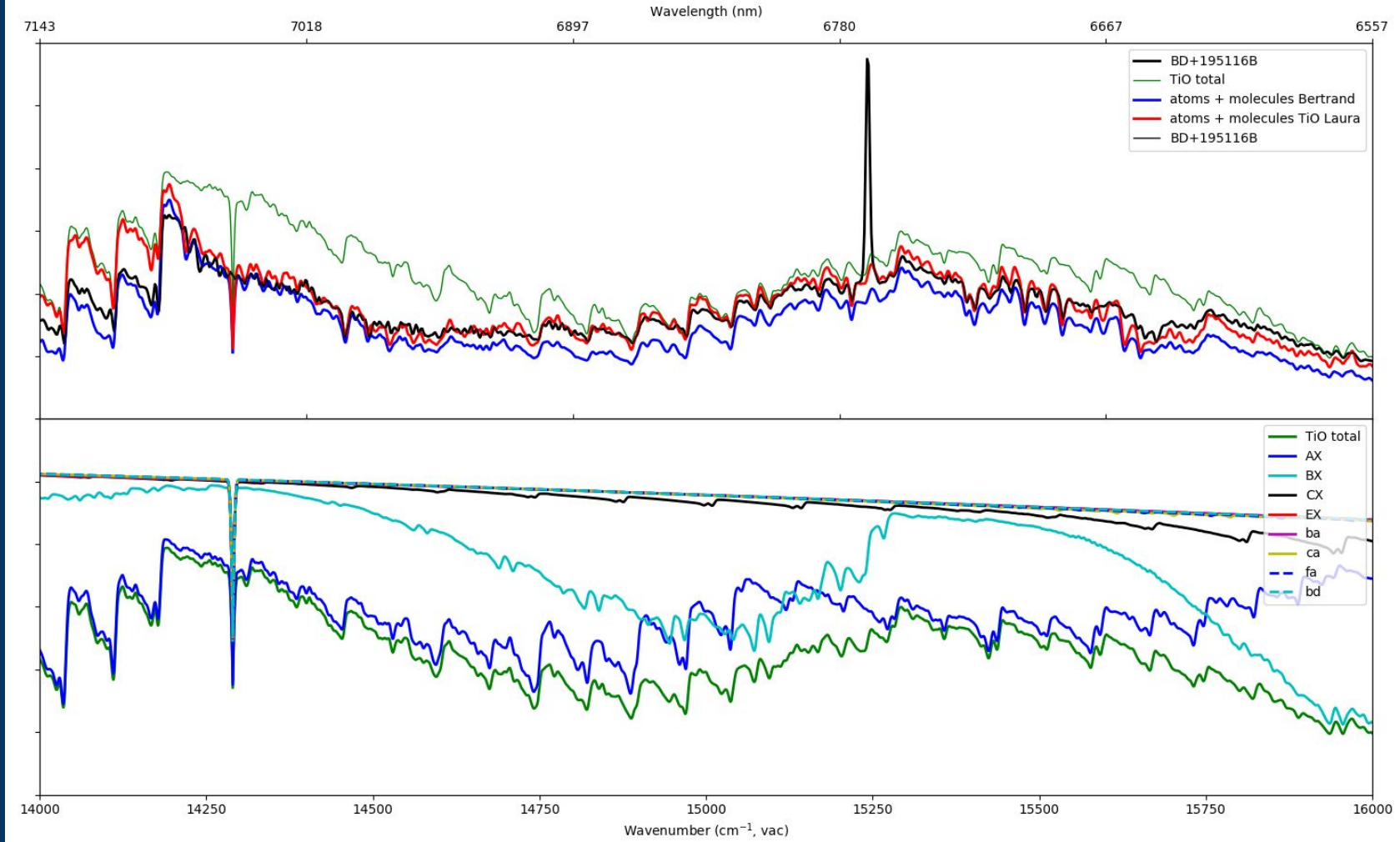


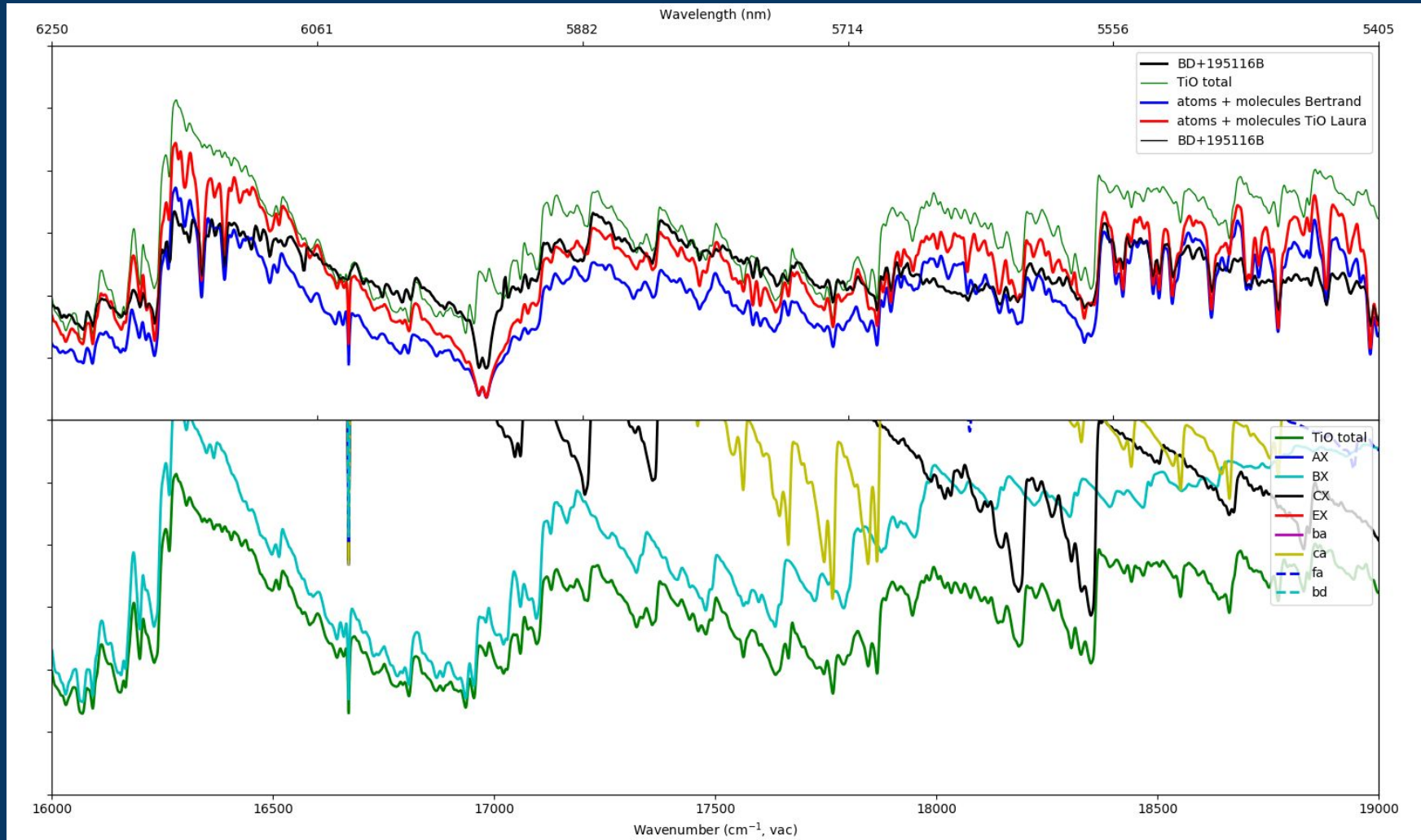

Solve for motion of the **electrons**
Molpro
Assigned Exp. Transitions
MARVEL
Empirical Energy Levels
Full Spectroscopic Model
Dipole moment curves
Energy Spectroscopic Model
Potential energy curves
Spin-orbit & other couplings
Refinement
Duo
Solve for motion of the **nuclei**
Rovibronic Wavefunctions
Rovibronic Energies
Transition Intensities
ExoMol LINE LIST

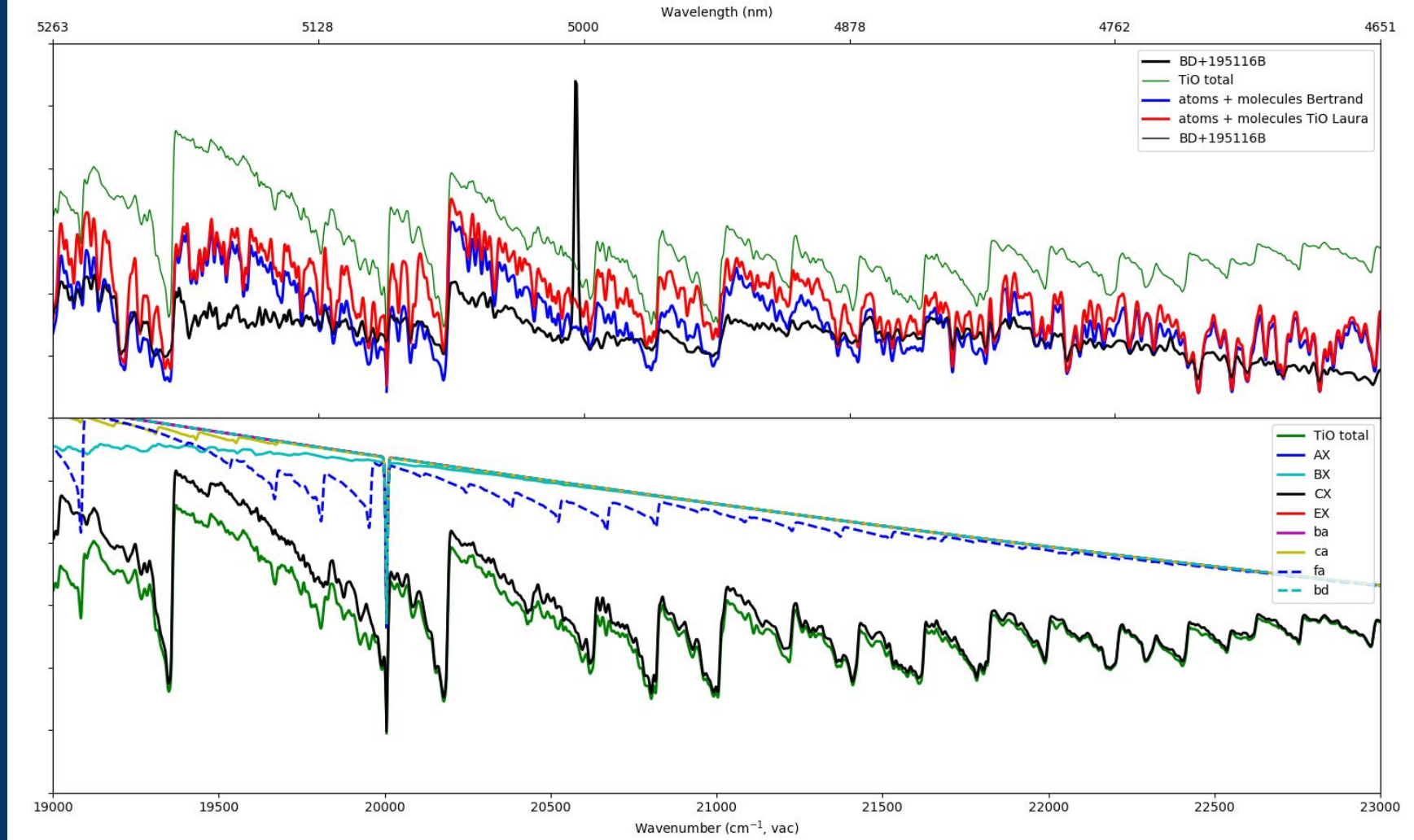
Current TiO line list …
TiO_iota (ExoMol)

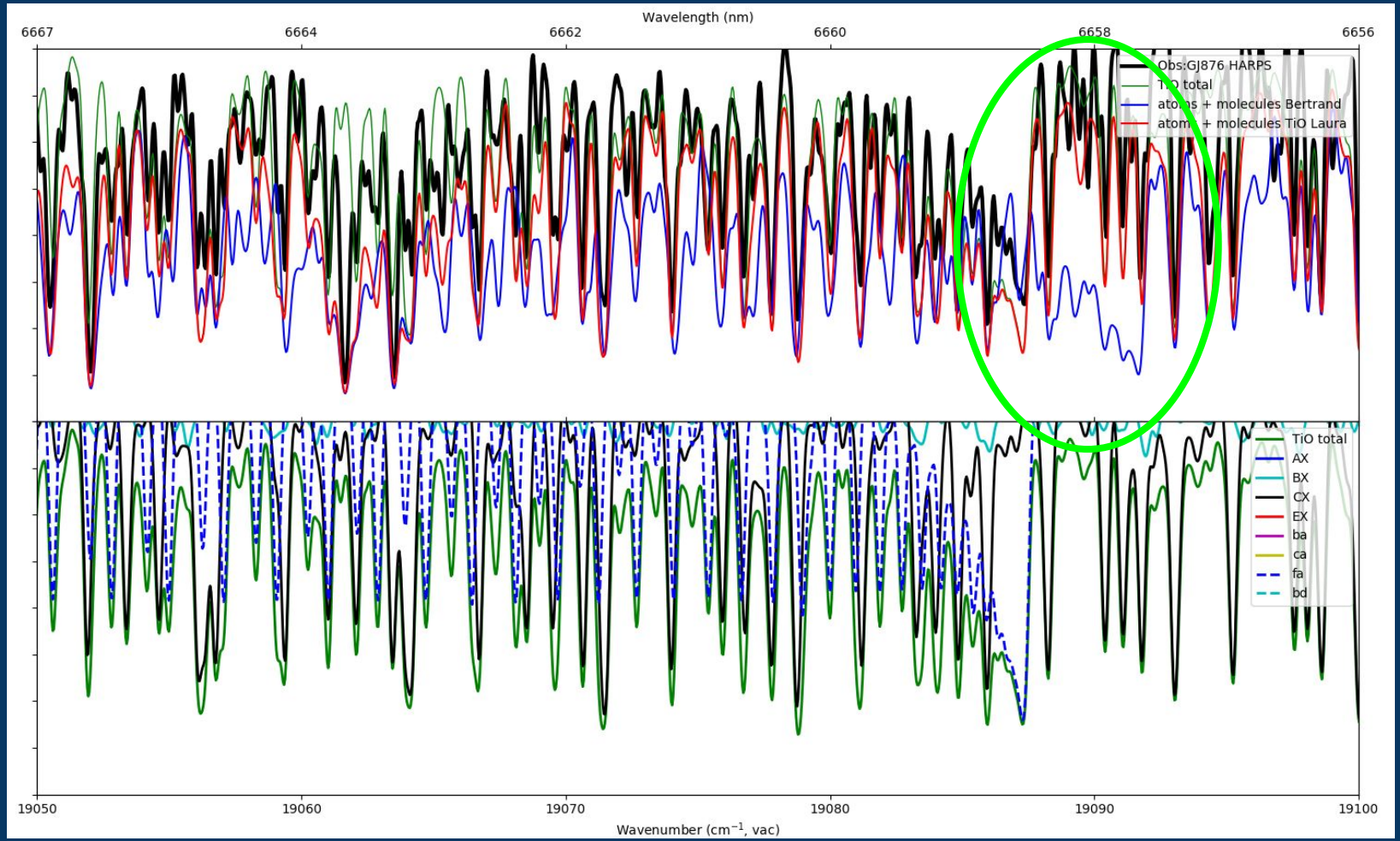
Thanks to Victor Perez for plotting scripts

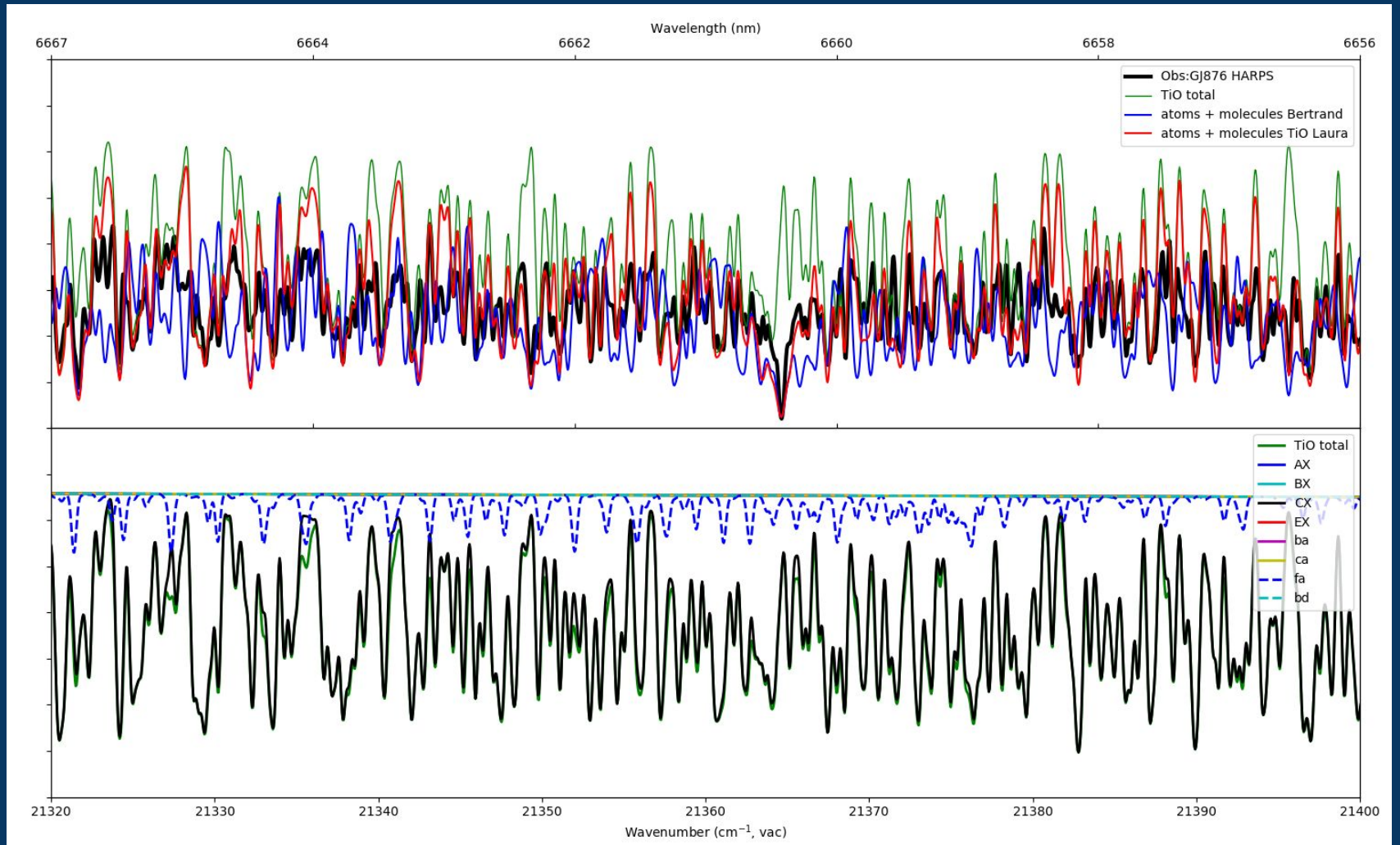

Wavelength (nm)
8333
7143
6250
5556
5000
4545
BD+195116B
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
BD+195116B
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
12000
14000
16000
18000
20000
22000
24000
Wavenumber (cm^{-1}, vac)


Wavelength (nm)
7143
7018
6897
6780
6667
6557
BD+195116B
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
BD+195116B
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
14000
14250
14500
14750
15000
15250
15500
15750
16000
Wavenumber (cm^{-1}, vac)


Wavelength (nm)
6250
6061
5882
5714
5556
5405
BD+195116B
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
BD+195116B
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
16000
16500
17000
17500
18000
18500
19000
Wavenumber (cm^{-1}, vac)

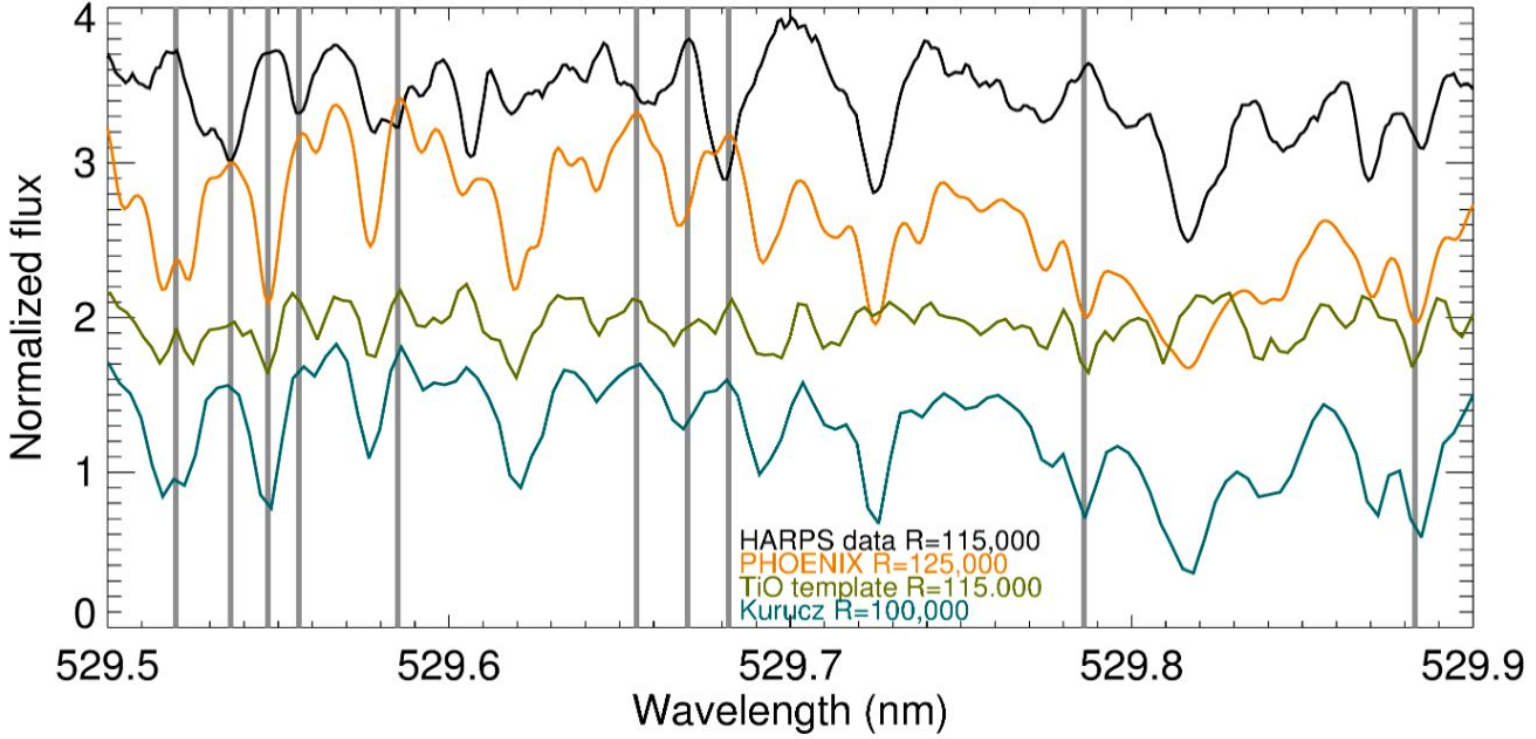

Wavelength (nm)
5263
5128
5000
4878
4762
4651
BD+195116B
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
BD+195116B
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
19000
19500
20000
20500
21000
21500
22000
22500
23000
Wavenumber (cm^{-1}, vac)


Wavelength (nm)
6667
6664
6662
6660
6658
6656
Obs:GJ876 HARPS
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
19050
19060
19070
19080
19090
19100
Wavenumber (cm^{-1}, vac)


Wavelength (nm)
6667
6664
6662
6660
6658
6656
Obs:GJ876 HARPS
TiO total
atoms + molecules Bertrand
atoms + molecules TiO Laura
TiO total
AX
BX
CX
EX
ba
ca
fa
bd
21320
21330
21340
21350
21360
21370
21380
21390
21400
Wavenumber (cm^{-1}, vac)

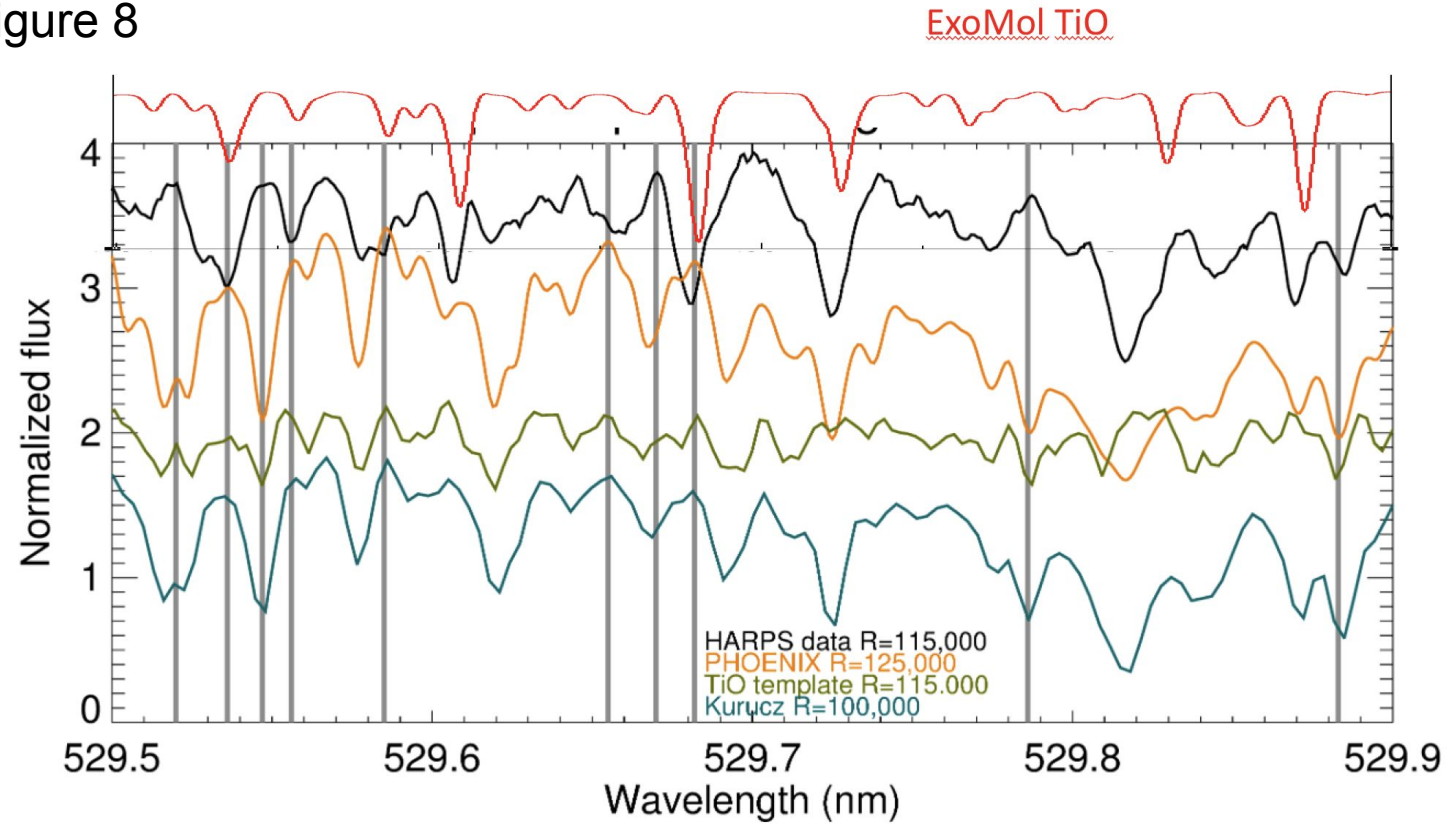
A search for TiO in the optical high-resolution transmission spectrum of HD 209458b: Hindrance due to inaccuracies in the line database

Figure 8



A search for TiO in the optical high-resolution transmission spectrum of HD 209458b: Hindrance due to inaccuracies in the line database

Figure 8



Sending me problem cases for TiO

I'd love to get some to test the new ExoMol line list compared to Plez & Schwenke's lists:

Please

- Use cm^{-1} (I never know whether a wavelength is in air or vacuum …)
- If you have Plez, Schwenke line lists against your data, please send.
- Let me know a specific frequency range of concern; my first question (which I can help you with) is what TiO band is of issue (e.g. B-X 0-0, C-X 1-2 etc)

Upcoming

ZrO

4 year AU$40,000/yr PhD scholarship available at UNSW Chemistry Sydney Australia to work on hot O_2 linelist.