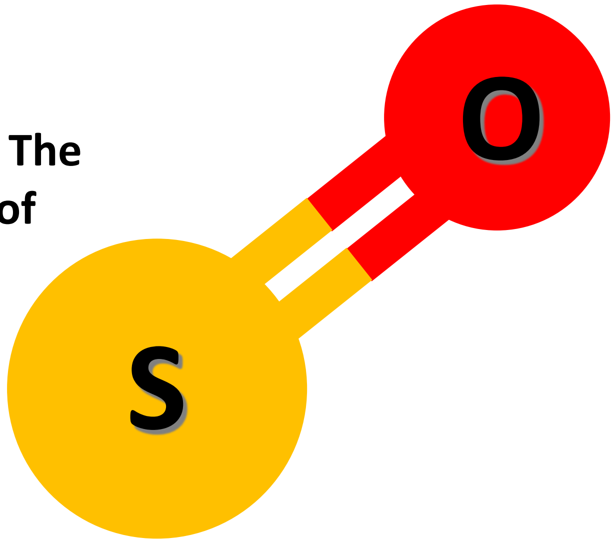
HRMS DIJON 2023: ExoMol Line list – The Semi-Empirical Rovibronic Spectrum of Sulfur Monoxide (32S16O)



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References:

[1] Yurchenko S. N., Lodi L., Tennyson J., Stolyarov A. V., 2016, Comput. Phys. Commun., 202, 262

[2] Furtenbacher T., Császár A. G., Tennyson J., 2007, J. Mol. Spectrosc., 245, 115

[3] Furtenbacher T., Császár A. G., 2012a, J. Quant. Spectrosc. Radiat. Transf., 113, 929

[4] Furtenbacher T., Császár A. G., 2012b, J. Mol. Struct., 1009, 123

[5] Császár A. G., Furtenbacher T., 2011, J. Mol. Spectrosc., 266, 99

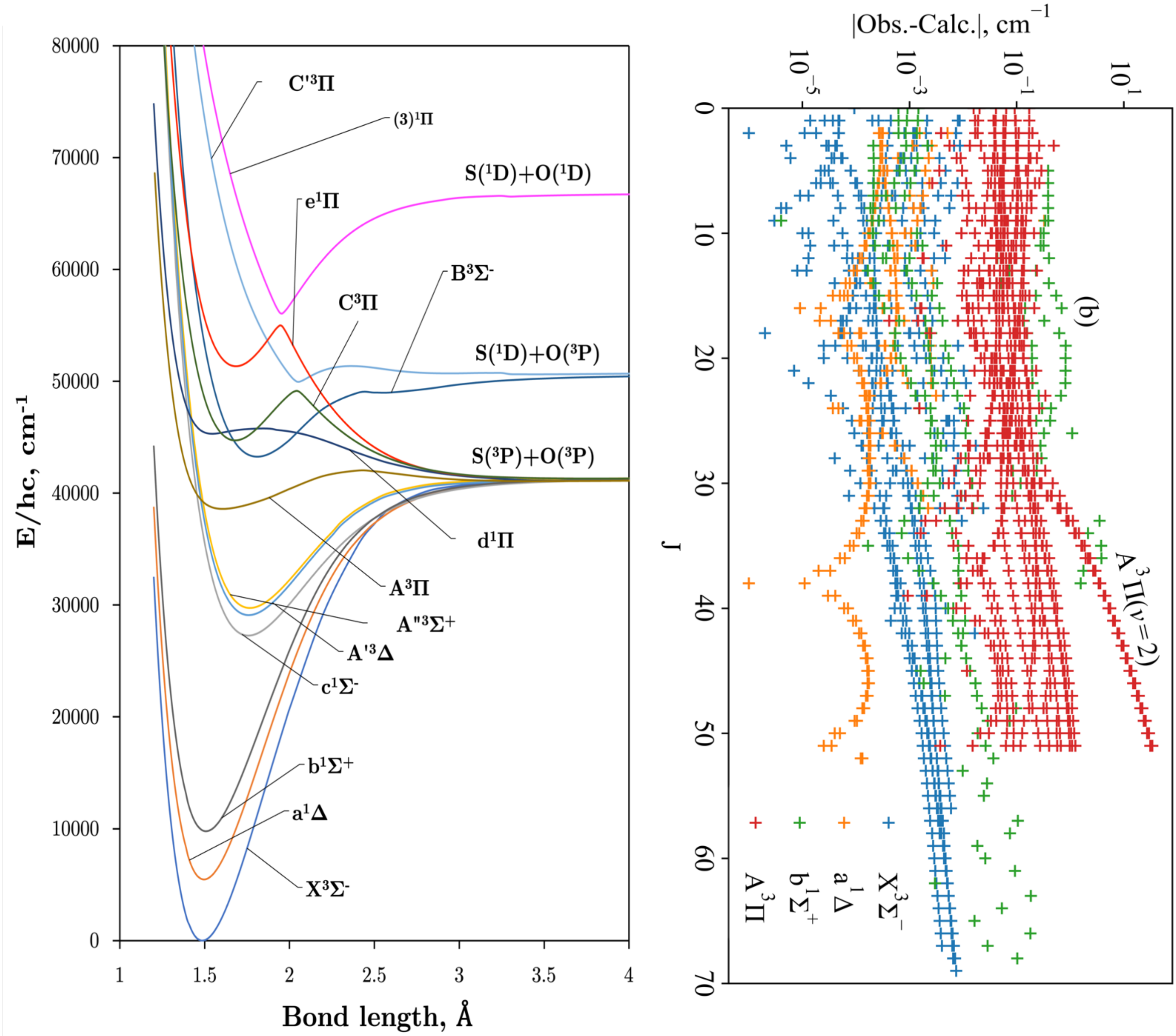
[6] Yurchenko S. N., Al-Refaie A. F., Tennyson J., 2018b, A&A, 614, A131

Data Coverage: (extract from upcoming line list paper on SO)

Table 2. The experimental data sources included in the final MARVEL analysis and their spectroscopic coverage. TAG denotes the identifier used to label the data sources throughout this paper, V/T describes the number of validated (V) data using the MARVEL procedure described in Section 2.1 relative to the total number of provided transitions (T), and the final columns cross-references source specific comments in Section 3.3.

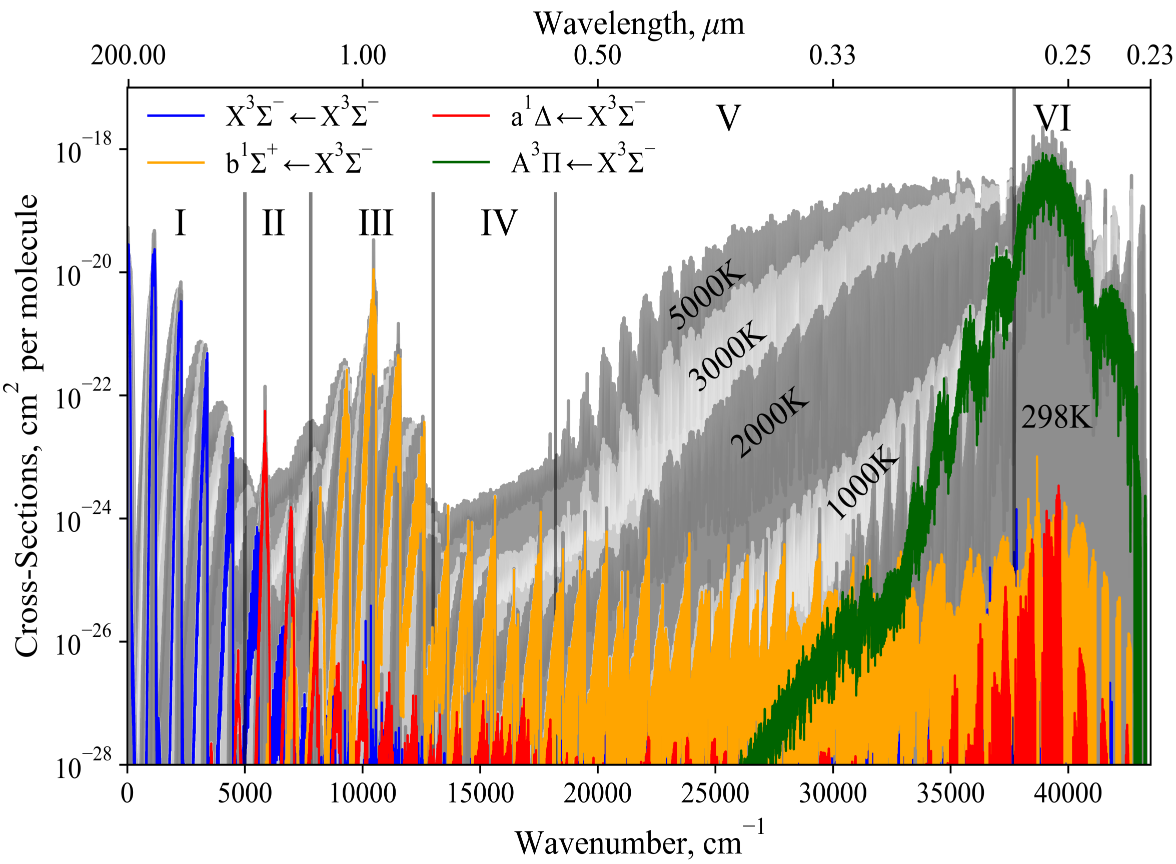
TAG	Source	Range (cm^{-1})	El. states	J	v	$\bar{\sigma}$ (cm^{-1})	V/T	Comment
64PoLi	Powell & Lide (1964)	0.435-2.2	X-X	0-3	0-0	1.07×10^{-5}	5/5	
64WiGoSa	Winnewisser et al. (1964)	2.87-5.74	X-X	1-4	0-0	1.67×10^{-5}	6/6	
69Colin	Colin (1969)	38672.94-39086.99	A-X	0-34	0-2	0.06	446/514	(a),(b)
71BoMa	Bouchoux et al. (1971a)	11354.43-11606.78	b-X	5-96	0-2	0.40	226/227	(a)
72BoMa	Bouchoux & Marchand (1972)	12265.5-12625.29	b-X	8-32	0-4	0.40	164/165	(a)
74Tiemann	Tiemann (1974)	1.21-4.31	X-X	1-4	0-0	8.64×10^{-8}	6/6	
76ClDe	Clark & Delucia (1976)	4.26-11.6	X-X, a-a	0-9	0-0	4.50×10^{-5}	28/28	
82Colin	Colin (1982)	38255.26-39499.71	A-X	1-34	0-1	0.21	254/275	(a),(b)
82WoAmBe	Wong et al. (1982)	3368.19-3386.30	X-X	1-9	0-3	2.00×10^{-3}	28/28	
82WuMoYe	Wu et al. (1982)	23696.68-40816.33	B-X	0-0	1-19	2.00×10^{-4}	0/9	(c)
82Tiemann	Tiemann (1982)	1.21-9.89	X-X	1-9	0-0	3.53×10^{-5}	5/5	
85KaBuKa	Kanamori et al. (1985)	1041.95-1116.20	X-X	1-44	0-6	2.14×10^{-3}	50/94	(c)
86ClTe	Clyne & Tennyson (1986)	38051.24-38108.07	A-X	1-24	0-0	0.15	74/87	(b)
87BuLoHa	Burkholder et al. (1987)	1051.89-2296.98	X-X, a-a	0-47	0-2	1.64×10^{-3}	560/562	(b),(e)
87EnKaHi	Endo et al. (1987)	10.9-12.8	a-a	7-9	0-5	9.00×10^{-7}	12/24	(c)
88KaTiHi	Kanamori et al. (1988)	1022.14-1121.26	a-a	2-41	0-5	2.01×10^{-3}	82/144	(b),(c),(f)
92LoSuOg	Lovas et al. (1992)	0.435-0.435	X-X	1-1	0-0	6.67×10^{-7}	0/1	
93Yamamoto	Yamamoto (1993)	2.8-15.4	b-b	1-11	0-8	5.89×10^{-7}	42/42	(c)
94CaClCo	Cazzoli et al. (1994)	19-62.8	X-X, a-a	9-45	0-0	1.46×10^{-4}	33/33	
94StCaPo	Stuart et al. (1994)	39619.44-40280.32	A-X, B-X	1-26	0-5.	0.03	85/237	(a),(c)
96KlSaBe	Klaus et al. (1996)	19.7-34.4	X-X	12-25	0-7	3.76×10^{-6}	45/71	(c)
97BoCiDe	Bogey et al. (1997)	11.7-31.2	a-a, b-b	8-22	0-13	1.40×10^{-6}	80/143	(b),(c)
97KlBeWi	Klaus et al. (1997)	9.94-35.4	a-a, b-b	6-25	0-7	4.43×10^{-6}	41/55	(c)
99SeFiRa	Setzer et al. (1999)	5792.97-10566.42	a-X, b-X	0-50	0-2	0.01	887/890	
03KiYa	Kim & Yamamoto (2003)	1.11-2.8	b-b	0-2	0-22	6.67×10^{-8}	30/30	(c)
15MaHiMo	Martin-Drumel et al. (2015)	0.435-83.8	X-X	0-60	0-0	2.08×10^{-6}	110/110	(d)
17CaLaCo	Cazzoli et al. (2017)	2.87-28.1	X-X	0-20	0-0	6.67×10^{-5}	19/19	
CDMS	Endres et al. (2016)	0.43-125.40	X-X, a-a	0-69	0-1	3.97×10^{-2}	860/862	(g)
22HeStLy	Heays et al. (2022)	37856.6214-52350.3967	A-X, B-X, C-X	0-51	0-30	0.05	45434/45434	(h)

Refinement of the spectroscopic model to the experimental data:

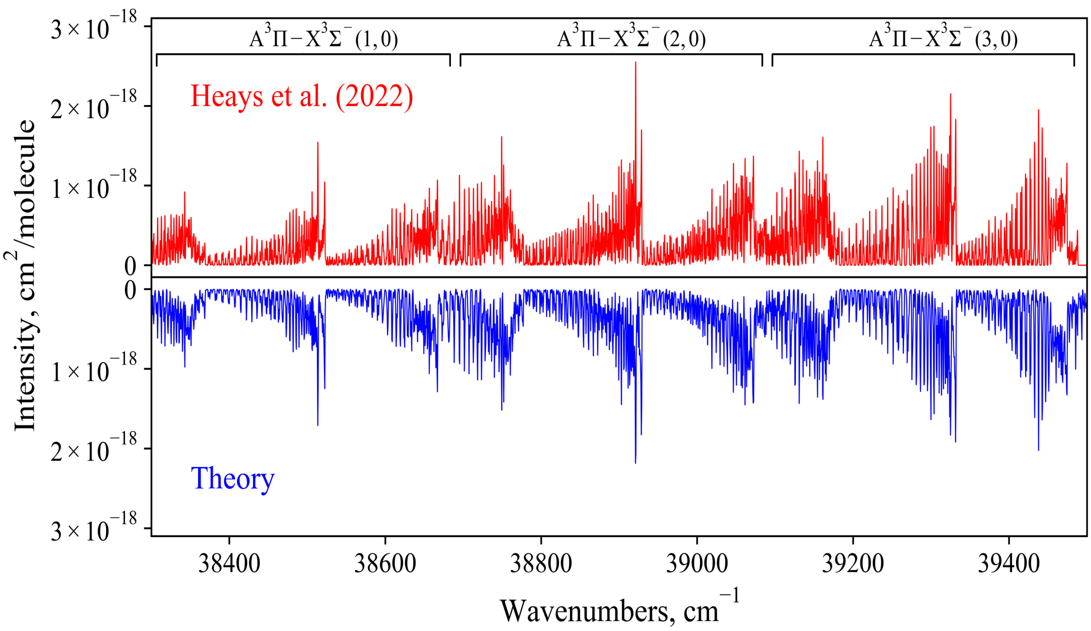


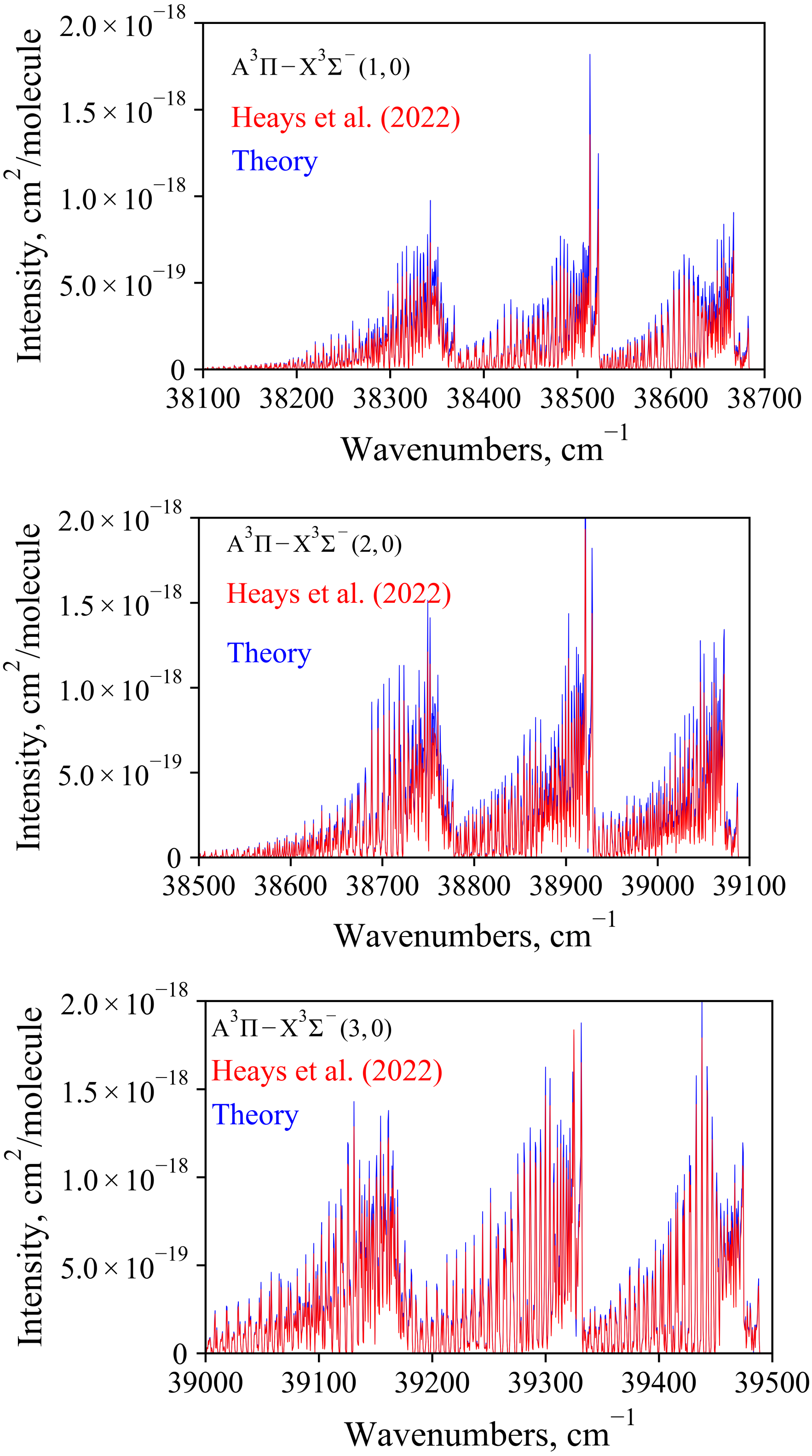
Left shows the ab initio potential energy curves computed for our ab initio spectroscopic model at an ic-MRCI aug-cc-pv5Z level of theory. Right shows the residuals of our computed states relative to the MARVELised data.

Simulated Spectrum: (all extracts from an upcoming line list paper on SO)

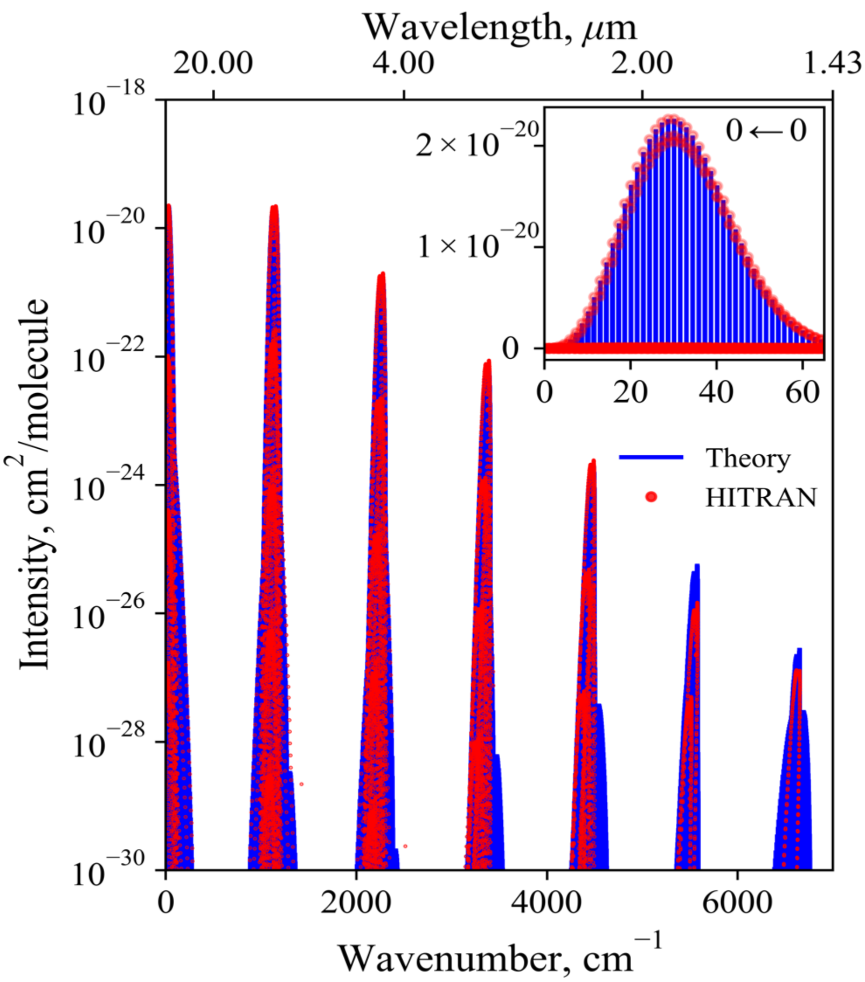


Dipole allowed and forbidden components of the absorption spectrum simulated with our semi-empirical model at 1000 K connecting $X\,^3\Sigma^-$ with $^1\Delta$, $b\,^1\Sigma^+$, and $A\,^3\Pi$. The total SO opacity is also shown for different temperatures as grey shaded regions. We see the intensity deviation is greatest in region V around 18 000-35 000 cm^{-1} where the $B\,^3\Sigma^- \leftarrow X\,^3\Sigma^-$ band begins to dominate opacity. The white shaded region marks the total opacity of SO simulated at 1000 K.





Comparisons between our simulated A-X overtone bands to the semi-empirical spectra produced by Heays et al. (2022). We see fantastic agreement for line positions, intensitites and band structure.



Comparison between our simulated X-X band to HITRAN. We see fantastic agreements up to the 6th vibrational band at about 5500 cm^{-1}.