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## Empirical rovibrational energy levels for carbonyl sulphide

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### ABSTRACT

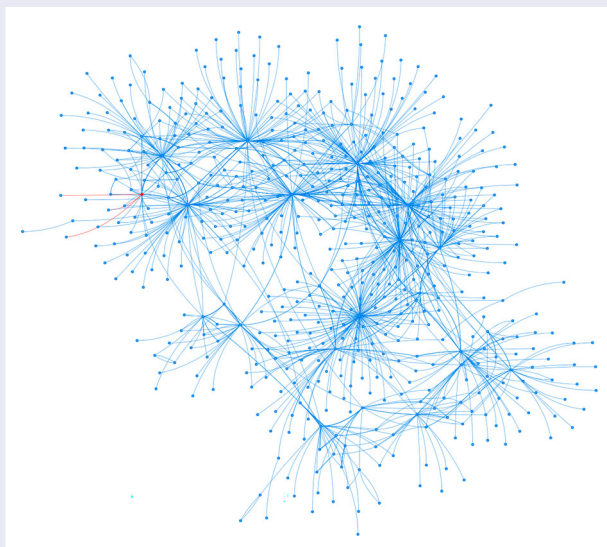
An exhaustive review of the measured rovibrational transitions of the  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  isotopologue of carbonyl sulphide is undertaken. A comprehensive analysis of data from 100 papers is carried out using a consistent set of harmonic oscillator quantum numbers which are recommended for future studies. A corrected compilation of 14,071 OCS transitions is then subjected to a Measured Active Rotational-Vibrational Energy Levels (MARVEL) analysis, resulting in 5729 empirical energy levels. The uncertainties corresponding to these levels are analysed using different procedures; the newly implemented bootstrap method is used to provide final uncertainties.

### ARTICLE HISTORY

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### KEYWORDS

Rotation-vibration energy levels; OCS; uncertainty quantification



## 1. Introduction

Carbonyl sulphide, OCS, is the most abundant sulphur-containing gas in the Earth's atmosphere [1] where it contributes to the formation of stratospheric sulphate aerosols. Atmospheric OCS also affects the radiative properties of the Earth's atmosphere, and hence climate change, and the concentration of stratospheric ozone. Major sources of atmospheric OCS include biomass burning, the oceans and the oxidation of sulphur-bearing molecules such as dimethyl sulphide and  $\text{CS}_2$ ; anthropogenic sources of OCS include coal combustion and aluminium production.

OCS has been detected in Venus [2] and many comets. OCS is commonly found in the interstellar medium and around young stars. Identifying OCS in the atmospheres of exoplanets could provide important clues about the habitability of these distant worlds. Photochemical models of exoplanets [3] suggest the formation of OCS in exoplanet atmosphere where it has also been suggested that it may act as a biomarker [4,5]. The recent detection of  $\text{SO}_2$  alongside  $\text{CO}_2$  in the atmosphere of the hot Jupiter exoplanet WASP-39 b using the James Webb Space Telescope (JWST) [6] raises the prospect of observing OCS in these objects. However, while HITRAN provides

comprehensive data for spectroscopic studies of OCS at terrestrial temperatures [7], we are not aware of a corresponding line list for hot OCS.

There are many high-resolution laboratory studies of the spectrum of OCS [8–163] which are discussed below. In this work, as a first step towards constructing a line list for  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  we have undertaken a comprehensive MARVEL (measured Active rotational-vibrational energy levels) analysis based on these studies. This involves collecting, assessing and validating all available measure high-resolution rotation-vibration transitions of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  and using the results to provide a comprehensive set of empirically determined energy levels.

## 2. Theoretical details

### 2.1. MARVEL

MARVEL provides a means of taking measured and assigned transition frequencies or wavenumbers and inverting them to provide accurate and secure empirical energy levels. The MARVEL methodology was pioneered by Furtenbacher and Császár [164], who have systematically improved the algorithm [165–167]. MARVEL is a generalisation of the X-matrix methodology used by Flaud and co-workers to study the spectrum of water [168]. MARVEL itself was originally developed to facilitate the critical evaluation of water spectra [169–172] giving a database of water transitions [173]. An important point about the MARVEL process is that it is model free: that is MARVEL makes no assumptions about the structure of the energy levels beyond that the bound states of a quantum mechanical system should obey the Rydberg–Ritz combination rules on energy differences between the levels.

The most recent update to the MARVEL procedure introduced a bootstrap method for estimating the uncertainties of the final energy levels which was used to perform a MARVEL study of  $\text{N}_2\text{O}$  [167]. The present work parallels the  $\text{N}_2\text{O}$  MARVEL study in that we also use the bootstrap method to determine energy uncertainties and that  $\text{N}_2\text{O}$  and OCS are both asymmetric linear molecules whose overtone and combination transitions have been extensively studied using high-resolution spectroscopy.

### 2.2. Quantum number labels

Most of states discussed can be well characterised using the standard harmonic oscillator (HO) notation. The standard way to denote these modes for OCS is:  $\nu_1$  corresponds to the carbon–sulphur (C–S) stretch, whose

fundamental lies at about  $859\text{ cm}^{-1}$ ;  $\nu_2$  refers to the bending mode at around  $520\text{ cm}^{-1}$ ; and  $\nu_3$  pertains to the carbon–oxygen (C–O) stretch with a fundamental at about  $2062\text{ cm}^{-1}$ . We note that Mulliken notation for the vibrational modes gives order C–O stretch, C–S stretch and then bend; however, every source we looked at place the bending mode second as  $\nu_2$  and we have retained this universally adopted convention.

Upon excitation of  $\nu_2$ , the bending motions occur in the two, orthogonal planes which can have different phases. Thus, an angular momentum arises as if the bent molecule rotated about the molecular axis. This so-called vibrational angular momentum quantum number,  $\ell$ , takes positive values with  $\ell = \nu_2, \nu_2 - 2, \nu_2 - 4, \dots$ . Therefore, the vibrational states could be labelled as  $(\nu_1 \nu_2^\ell \nu_3)$ ; thus, the vibrational ground state is labelled as  $(\nu_1 \nu_2^\ell \nu_3) = (00^00)$ . While the vibrational quantum numbers are all approximate, the rotational quantum number,  $J$ , and parity are rigorous. States with  $\ell > 0$  can occur with both e and f rotationless parity, while those with  $\ell = 0$  only correspond to e states. The  $\ell$ -splitting in OCS is fairly small and some sources do not specify the parity for transitions between states with  $\ell \geq 1$ , in this case, transitions were assumed to involve both the e and f states, and two transitions with the same wavenumber were included in our transition list. The rotationless parities follow the general dipole selection rule  $\Delta J = 0$  gives e  $\leftrightarrow$  f while  $\Delta J = \pm 1$  gives e – e or f – f [174].

The (harmonic and anharmonic) vibrational fundamentals frequencies obey the approximate relationships  $\nu_3 \approx 2\nu_1 \approx 4\nu_2$ ; this means that some authors prefer to use polyad notation to designate vibrational states. However, our analysis suggests that after checking and reassigning some states by plotting their reduce energy using the formula  $E(\text{cm}^{-1}) = E_{\text{original}} - 0.200123J(J + 1) + 4.3411 \times 10^{-8}J^2(J + 1)^2$ , adopted from 14GoDeHeVa [19], that the standard harmonic notation for the vibrational levels works satisfactorily for the currently observed spectra of OCS. This harmonic notation was therefore adopted for our MARVEL analysis as it is used by a large majority of the sources and, if reliable, contains more information than use of the polyad number with an associated counting number. As discussed in Appendix 1, a number of sources swap quantum numbers  $\nu_1$  and  $\nu_3$ ; this was adjusted on a source-by-source basis.

## 3. Results

A large number of potential sources of transition data were considered as part of this study. Only those sources which gave assigned measured transition wavenumbers

**Table 1.** Experimental sources used to construct the  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  rovibrational spectroscopic network of this study.

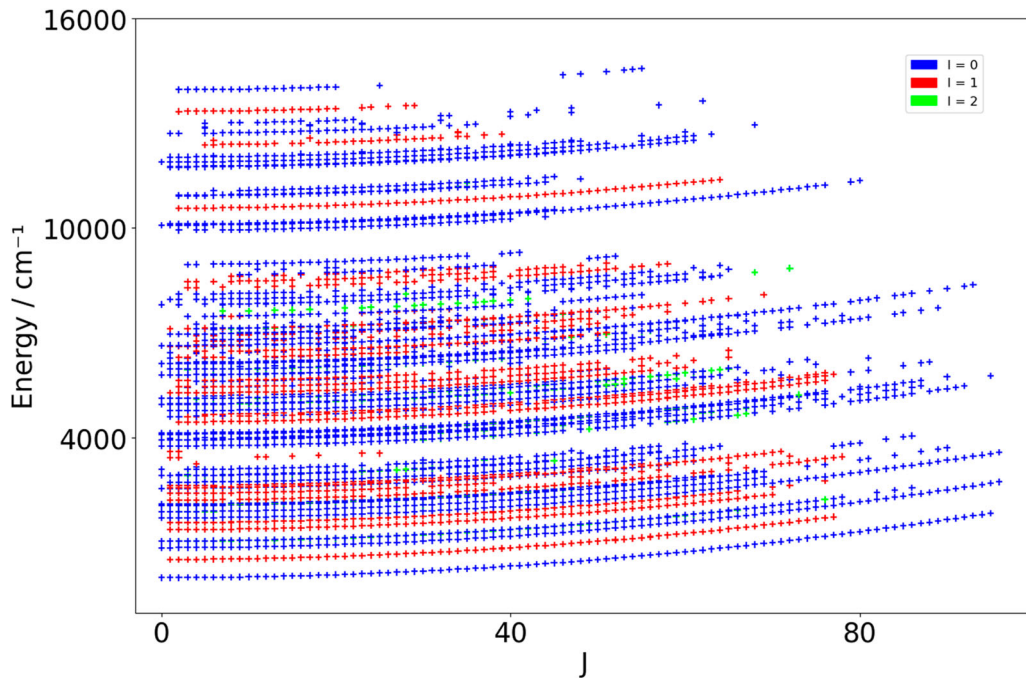
Tag	Range (in $\text{cm}^{-1}$ )	A/V	AIU	AMR	MR
74FaMu [49]	0.00002729–0.001336294	17/17	3.336e–9	3.336e–9	3.336e–9
72ReDyMe [45]	0.00042439–0.03309876	12/12	3.336e–9	6.671e–8	1.195e–8
16GoBeLa [21]	0.40571331–16.21742425	37/37	3.336e–9	6.671e–8	1.529e–8
14GoBeLeAn [20]	1.62284280–17.43187120	24/24	4.003e–9	6.605e–8	1.947e–8
73TaBhSmDa [46]	0.81142545	1/1	3.336e–8	3.336e–8	3.336e–8
95HaBeAnRa [99]	0.80145055–0.80900591	6/6	3.336e–8	3.336e–8	3.336e–8
73WaOaBeKu [47]	0.81142558	1/1	3.347e–8	3.347e–8	3.347e–8
88DeGiDi [78]	1.21350625–1.22135377	7/6	1.334e–8	6.671e–8	3.622e–8
70WiGo [42]	3.65129476–8.51837510	11/11	3.651e–8	8.518e–8	5.827e–8
91GrHeSt [89]	0.3966721–0.4079360	13/13	1.501e–7	1.501e–7	1.501e–7
70ScMuLa [41]	2.0285451	1/1	1.668e–7	1.668e–7	1.668e–7
89EhGrDrHe [80]	0.1378660	1/1	1.668e–7	1.668e–7	1.668e–7
69NaMo [39]	1.2171358	1/1	1.835e–7	1.835e–7	1.835e–7
00MoYaMa [8]	23.2090363–25.9415795	91/91	4.003e–8	3.836e–6	2.128e–7
05GoLaGuKn [14]	1.6228428–36.3875218	40/40	2.335e–8	9.673e–7	2.157e–7
18NeDrTaKi [22]	3.2359385–3.2529659	3/2	3.336e–7	3.336e–7	3.336e–7
72HoRuDi [44]	0.0004263–0.0012732	2/2	3.336e–7	3.336e–7	3.336e–7
74LaWi [51]	0.8114257–10.1401231	48/48	5.003e–7	1.001e–6	6.150e–7
67HiKaHelc [36]	0.4057131	1/1	6.171e–7	6.171e–7	6.171e–7
83ScWi [72]	0.4057133–27.1305593	48/48	6.671e–7	1.001e–6	7.783e–7
20GoKoTsFo [23]	26.3236669	1/1	8.339e–7	8.339e–7	8.339e–7
14GoDeHeVarot [19]	0.4045034–7.7496891	22/22	3.336e–9	1.001e–6	8.712e–7
96SaWaMeUr [103]	2021.2951208–2051.5690121	33/33	7.005e–7	1.868e–6	9.168e–7
98FrMuPaLo [105]	2891.7493048–2909.7971254	10/10	8.006e–7	2.268e–6	9.873e–7
00MuPaUrMa [9]	1870.2452628–2086.6767135	9/9	6.004e–7	1.868e–6	9.896e–7
98FiRuKhLe [104]	1031.814451–1070.736522	239/239	1.000e–6	1.000e–6	1.000e–6
94GeWaSaMu [96]	1885.763454–2064.584096	6/6	5.671e–7	1.601e–6	1.012e–6
48StWeKy [24]	0.811425–2.028539	6/6	3.336e–7	1.668e–6	1.112e–6
Segment tag	Range	A/V	AIU	AMR	MR
75Bogey [52]	1.613122–5.242298	8/8	1.117e–6	1.117e–6	1.117e–6
95MeSaWaGe [100]	2034.762818	1/1	1.151e–6	1.151e–6	1.151e–6
04SuLiLeXu [13]	1033.963099–1061.581466	21/21	1.351e–6	1.351e–6	1.351e–6
80BoBa [62]	1.613122–5.242298	48/48	6.671e–7	2.669e–6	1.452e–6
67Maki [37]	0.267137–0.540174	16/16	1.668e–6	1.668e–6	1.668e–6
74KuOaWa [50]	0.405713–0.811426	2/2	1.668e–6	1.668e–6	1.668e–6
74BoBaMa [48]	2.016394–2.419661	2/2	1.785e–6	1.785e–6	1.785e–6
94DaWeHoMa [95]	2907.921002–2909.412789	2/1	1.668e–6	2.452e–6	2.060e–6
95WeDaHoMa [101]	1688.756026–1885.763455	2/2	1.284e–6	3.452e–6	2.368e–6
84TaltTa [74]	1.618003–4.901654	121/121	1.668e–6	3.336e–6	2.991e–6
76Smith [58]	0.815871–4.079217	9/9	1.668e–6	3.336e–6	3.002e–6
52Tetenbau [27]	1.617994–1.628457	7/7	3.336e–6	3.336e–6	3.336e–6
80DuDeBuBo [63]	0.405713–27.130559	78/78	6.671e–9	1.334e–4	6.496e–6
89VaJeWe [82]	26.323671–37.591558	24/24	6.671e–6	6.671e–6	6.671e–6
09MoHiCuYa [16]	27.130560–42.798593	32/32	6.671e–6	1.334e–5	8.548e–6
67MoMa [38]	0.40793–2.04247	53/53	2.001e–6	1.668e–5	1.020e–5
53KiGo [28]	3.24562–7.30183	6/6	6.671e–6	1.501e–5	1.084e–5
70HeDeGo [40]	23.49749–27.13056	4/4	1.668e–5	1.668e–5	1.668e–5
92HoKoToAl [93]	1022.18546–1077.15949	130/129	2.000e–5	2.000e–5	2.000e–5
83WePeMa [73]	1686.65095–1725.18549	4/4	2.013e–5	3.347e–5	2.513e–5
52KiTo [26]	0.80655–2.02854	17/16	2.669e–5	2.669e–5	2.669e–5
54BuGo [29]	9.73471–12.97701	5/5	2.013e–5	6.683e–5	4.081e–5
92MaWe [94]	1060.05636–1065.98303	54/54	1.300e–5	1.000e–4	5.683e–5
50ShTo [25]	0.81426–0.81586	2/2	6.683e–5	6.683e–5	6.683e–5
56CoGo [32]	16.2174–17.0270	2/2	1.002e–4	1.002e–4	1.002e–4
90FaLaLeHe [84]	1056.5677–1087.6765	23/23	1.000e–4	1.700e–4	1.030e–4
59Dymanus [34]	0.8090–0.8139	5/5	1.184e–4	1.184e–4	1.184e–4
91TaLoLu [91]	830.3675–871.6454	174/174	1.300e–4	1.300e–4	1.300e–4
79WePeMa [61]	1025.0310–1074.2085	122/122	6.671e–5	5.604e–4	1.315e–4
82KiMi [69]	0.4033–10.1630	114/114	1.334e–4	1.334e–4	1.334e–4
92DaMuWeSc [92]	2898.6172–2912.7864	6/6	1.669e–4	3.003e–4	2.114e–4
81WePeMaSu [68]	815.0999–1738.2360	444/444	3.669e–5	2.402e–3	2.268e–4
90WeScMa [87]	2020.9384–2085.3946	23/23	1.001e–4	5.003e–4	2.335e–4
86MaWeHi [77]	1866.8230–1914.8851	10/10	1.335e–4	3.337e–4	2.336e–4
90MaWeJe [85]	2100.8710–2138.0784	4/4	1.001e–4	5.003e–4	2.669e–4
10ToSuBrCr [17]	3880.7740–4174.8571	1509/1506	3.000e–4	3.000e–4	3.000e–4
88MaOlWeVa [79]	1850.7798–1914.6388	57/57	1.669e–4	1.334e–3	4.378e–4
89ScMaVaWe [81]	1363.6303–1397.5967	13/12	1.669e–4	1.334e–3	4.953e–4
95BeFaGu [97]	1885.7634–2912.7864	12/12	8.000e–5	1.000e–3	6.267e–4
98RbBeVaNa [106]	4729.9551–7819.9517	1473/1472	4.000e–4	2.000e–3	6.350e–4

(continued).

**Table 1.** Continued

Segment tag	Range	A/V	AIU	AMR	MR
81SaWoMaLa [66]	834.2665–1086.8752	88/88	1.001e–4	1.001e–3	6.425e–4
90ToHoAl [86]	1020.6628–1082.7131	562/562	8.000e–4	1.600e–3	8.868e–4
18BaSoMaPr [175]	1900.282–1903.957	20/20	1.000e–3	1.000e–3	1.000e–3
54CaTh [30]	2013.750–2130.420	727/0	1.000e–3	1.000e–3	1.000e–3
79HeLyLe [60]	1041.273–1070.463	6/6	1.000e–3	1.000e–3	1.000e–3
06MaRoBoMo [15]	26.725–36.792	10/10	1.001e–3	1.001e–3	1.001e–3
04Horneman [12]	493.260–1079.660	611/469	1.230e–6	3.506e–3	1.900e–3
76MaFr [55]	1037.429–1045.026	2/2	6.672e–4	4.270e–3	2.468e–3
14GoDeHeVa [19]	824.966–13956.648	1277/1262	3.000e–6	5.100e–1	3.021e–3
79Guelachv [59]	2027.980–2083.785	118/118	3.564e–3	3.564e–3	3.564e–3
85HuFoJoMc [75]	2015.435–2017.291	3/3	3.800e–3	3.800e–3	3.800e–3
80MaOlSa [65]	839.985–1733.649	514/514	3.700e–3	6.500e–3	3.977e–3
81SeVa [67]	21.012–42.002	58/58	4.000e–3	4.000e–3	4.000e–3
95ErVaBrFa [98]	2528.183–3116.557	378/378	4.000e–3	4.000e–3	4.000e–3
83KIYaWi [71]	2027.926–2081.737	164/164	4.300e–3	4.300e–3	4.300e–3
13GaArTc [18]	2020.726–2129.436	55/55	4.500e–3	4.500e–3	4.500e–3
91TaLo [90]	1037.789–1069.931	96/96	4.900e–3	4.900e–3	4.900e–3
76MeDuMe [56]	1030.758–2135.202	687/686	2.000e–3	5.000e–3	4.996e–3
85JoHoKaMa [76]	492.522–553.044	379/377	5.000e–3	5.000e–3	5.000e–3
90BIWaBoBo [83]	828.047–868.114	38/38	5.000e–3	5.000e–3	5.000e–3
83JoKaHo [70]	826.174–873.707	226/226	8.000e–3	8.000e–3	8.000e–3
03BeCaDiFa [11]	8944.38–10125.37	465/465	1.000e–2	1.000e–2	1.000e–2
76DoMiSt [54]	1045.02	1/1	1.000e–2	1.000e–2	1.000e–2
02LeBaHuFa [10]	10890.54–13956.85	669/669	3.000e–4	3.930e–2	1.110e–2
76NaNaUeKu [57]	1053.76–1057.38	3/3	2.000e–2	2.000e–2	2.000e–2
75BuDeSm [53]	1876.07–1895.39	102/102	1.050e–2	2.850e–2	2.603e–2
96HoBoStDe [102]	6566.45–12033.56	122/122	1.000e–2	5.000e–2	2.803e–2
55Low [31]	0.81–1.22	16/16	5.003e–2	5.003e–2	5.003e–2
91BICoDeWa [88]	1021.57–1072.27	52/52	5.350e–2	5.350e–2	5.350e–2
65TrCo [35]	3750.3–6969.8	501/499	1.000e–1	1.000e–1	1.000e–1
57AlPIBl [33]	1871.4–6126.9	788/673	1.000e–1	2.000e–1	1.042e–1
80Landsberg [64]	1068.0–1068.9	2/2	3.535e–1	3.535e–1	3.535e–1

Note: The data given include, for each source, the wave number ranges of the validated transitions, the number of actual (A) and validated (V); uncertainties (in  $\text{cm}^{-1}$ ) are AIU = average initial uncertainty, AMR = average MARVEL reproduction of the source's lines, and MR = maximum reproduction in the source.

**Figure 1.** Overview of the energy levels determined in this work labelled by the  $\ell$  and  $J$  angular momentum quantum numbers.

or frequencies were considered. In some cases, mentioned in Appendix 1, where such data were not provided in the original publication, we successfully obtained them either from subsequent papers or directly from the authors.

Table 1 lists the 100 sources used in this study [8–106]; Appendix 1 provides notes on the sources used where appropriate. Appendix 2 lists the other sources considered during this study [107–163], with a brief explanation of why they were not used. The 100 sources we used provide 14,071 independently measured and assigned transition frequencies; of these 13,056, i.e. nearly all of them, are validated by the MARVEL procedure. Of those not transitions not included in the final network, 216 were removed because they did not validate while the remaining transitions formed independent spectroscopic networks. MARVEL provides 5729 empirical energy levels using the transitions in the main network.

Figure 1 provides a visual summary of the energy levels determined. It can be seen that these levels are dominated by ones with low  $\ell$  values; the states largely have  $\ell = 0$  or 1 with some states with  $\ell = 2$ . Our transitions dataset also contains a few transitions involving states with  $\ell = 3$  or 4 but none of these link to the main spectroscopic network.

Table 2 provides a vibrational state by vibrational state summary of the energy levels determined. Also given are vibrational band origins (VBOs), with uncertainties, which are determined by the MARVEL for states with  $J = 0$ . Note that  $J = 0$  levels only exist for states with  $\ell = 0$  and the direct determination of the VBO for states with  $\ell > 0$  is not possible with the MARVEL procedure. An expanded version of this table which considers energy ranges and uncertainties for each vibrational state is given in Appendix 3.

#### 4. Uncertainty analysis

In the present study, we utilised the innovative bootstrap method, as previously described within the context of a MARVEL study on  $N_2O$  [167]. In the bootstrap approach, MARVEL is rerun with transition uncertainties each randomly scaled by between 1 and 10. After a number of such runs, MARVEL checks whether the average of the bootstrapped energies differs from the original MARVEL energy or the standard deviation of the bootstrap energies has increased, if so the uncertainty of the level is increased. The result of this process leaves the energy levels determined by the MARVEL run unchanged but with, hopefully, more robust uncertainties. Our results used 100 iterations in this procedure and proved insensitive to using further iterations.

**Table 2.** Summary of OCS rovibrational states generated in this work by vibrational state.

$(v_1 v_2 v_3 \ell)$	$E(J = \ell)/\text{cm}^{-1}$	$J_{\text{max}}^e$	$N_{\text{lev}}^e$	$J_{\text{max}}^f$	$N_{\text{lev}}^f$
0000	0(0)	95	96		
0101	520.82832405(24)	77	77	76	76
1000	858.966931(10)	96	97		
0200	1047.0420512(10)	86	81		
0202	–	76	66	66	59
1101	1372.864330(13)	70	70	70	69
0301	1573.77360958(32)	72	66	76	69
2000	1710.97631(13)	96	97		
1200	1892.230536(34)	69	70		
1202	1888.1629(16)	47	7	30	6
0010	2062.200896(71)	90	78		
0400	2104.82766(10)	68	63		
0402	2100.7452(14)	53	45	46	44
2101	2218.43266(55)	78	58	77	56
1301	2412.5264(29)	65	39	72	41
0501	–	55	45	43	41
0111	2575.71150(35)	71	67	71	64
3000	2555.9905(57)	86	66		
2200	–	61	59		
1400	–	57	45		
1402	–	32	17	45	18
1010	2918.1051(57)	64	63		
0600	–	47	3		
0210	3095.554411(60)	60	49		
0212	–	51	9	37	5
2301	–	4	1		
1111	–	25	5	25	8
0311	3615.75031(35)	2	2	2	2
2400	–	92	43		
2402	–	68	20		
2010	3768.5(10)	68	61		
1600	–	58	40		
1210	3937.42741(30)	95	83		
1212	3932.5092(16)	78	23	3	1
0020	4101.41(10)	90	87		
0410	4141.22(10)	80	77		
0412	–	75	37		
1311	–	76	66	75	58
0511	–	76	60		
0121	–	76	59	77	46
3010	–	88	51		
2210	–	71	63		
1410	–	62	55		
1412	–	51	28	59	16
1020	4953.87913(30)	81	65		
0610	–	46	30		
0220	5120.98358(40)	74	63		
0222	–	65	50	65	10
2311	5280.943062(40)	59	55	60	49
1121	–	65	46	43	24
0321	–	65	31	65	34
4010	–	51	44		
3210	–	25	21		
2410	–	25	22		
2020	5801.90644(60)	41	30		
11000	–	41	11		
1610	–	32	8		
1220	–	54	54		
1222	–	39	25	32	19
0420	–	64	48		
0030	6117.57641(60)	89	82		
2121	–	26	16	28	14
1321	–	51	36	48	31
0131	6616.252383(60)	8	7	9	5
5010	–	78	30		
4600	–	67	22		
4210	–	62	25		
4212	–	62	8		
3410	–	66	32		

(continued).

**Table 2.** Continued

$(v_1 v_2 v_3 \ell)$	$E(J = \ell)/\text{cm}^{-1}$	$J_{\text{max}}^e$	$N_{\text{lev}}^e$	$J_{\text{max}}^f$	$N_{\text{lev}}^f$
3 0 2 0	6640.1048(10)	93	88		
2 2 2 0	–	22	18		
1 4 2 0	–	31	20		
1 0 3 0	–	43	41		
0 2 3 0	–	55	52		
0 2 3 2	–	46	18	43	17
5 1 1 1	–	50	17	47	13
4 3 1 1	–	51	21	58	20
3 5 1 1	7116.91079(55)	63	25	69	27
3 1 2 1	–	53	20	55	19
1 1 3 1	–	30	8	33	10
6 0 1 0	–	50	16		
5 2 1 0	–	45	13		
4 0 2 0	–	55	45		
3 2 2 2	–	42	15	42	17
2 1 2 0 0	–	17	12		
2 1 2 0 2	–	28	2		
2 4 2 0	–	63	27		
2 4 2 2	–	72	2		
2 0 3 0	7811.9533(10)	64	51		
1 2 3 0	–	65	55		
0 0 4 0	–	64	38		
2 1 3 1	–	49	23	58	26
1 3 3 1	–	51	28	43	16
0 1 4 1	–	38	14	33	11
9 0 0 0	–	47	36		
3 0 3 0	–	52	24		
2 2 3 0	–	20	4		
1 0 4 0	–	41	35		
2 1 6 0 0	–	36	2		
1 2 4 0	–	44	38		
0 4 4 0	–	45	45		
0 0 5 0	10,080.903(10)	80	79		
0 1 5 1	–	64	63	60	7
1 4 4 0	–	48	34		
1 0 5 0	–	44	41		
0 2 5 0	–	45	36		
0 2 5 2	–	35	2		
2 4 4 0	–	48	46		
2 0 5 0	–	61	61		
1 2 5 0	11,886.107(13)	63	60		
0 4 5 0	–	47	6		
0 0 6 0	–	68	49		
1 3 5 1	–	37	26	39	22
0 1 6 1	–	34	4	34	4
3 0 5 0	–	27	1		
2 2 5 0	–	36	32		
1 4 5 0	–	42	5		
1 0 6 0	–	62	8		
0 2 6 0	–	47	19		
1 1 6 1	–	29	24	29	23
0 0 7 0	–	55	26		

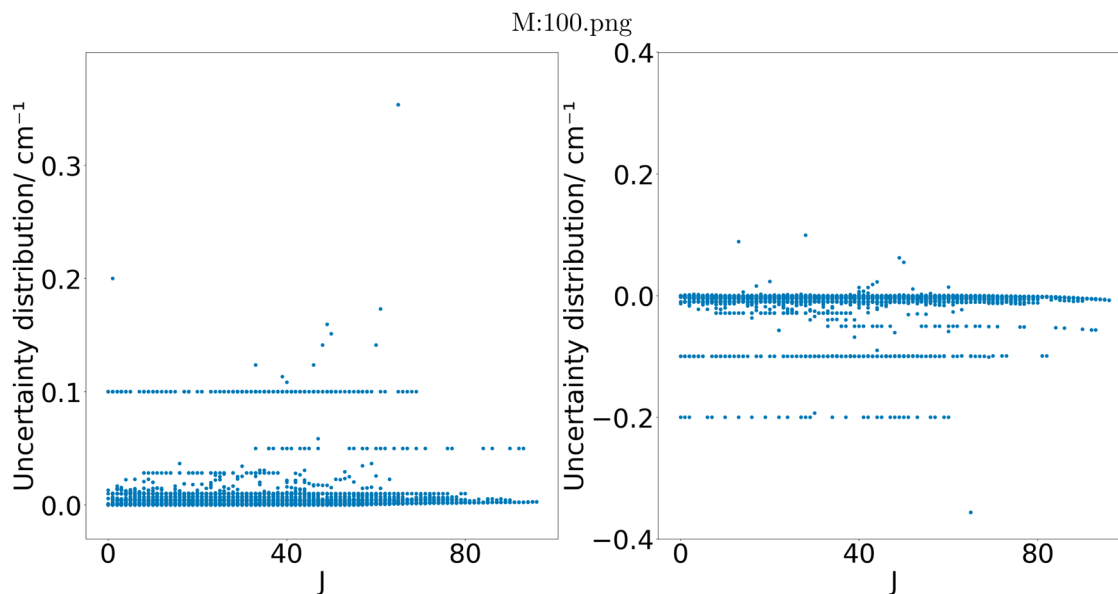
Note: The lowest energy level, the one with  $J = \ell$  and e parity is given where determined by MARVEL; for states with  $\ell = 0$  these correspond to the vibrational band origins (VBOs) (with uncertainties parenthesis in units of the final digit). The number and maximum  $J$  value of MARVEL levels obtained for each vibrational state and rotationless parity are given by  $(N_{\text{lev}}^e, N_{\text{lev}}^f)$  and  $(J_{\text{max}}^e, J_{\text{max}}^f)$ , respectively.

Figure 2 compares uncertainties obtained using the previous MARVEL3 procedure [166], which uses a segmentation procedure to determine uncertainties, with bootstrap procedure. The figure shows the bootstrap approach, which provides a more even-handed approach to the treatment of uncertainties, generally yields reduced uncertainties. This is particularly noticeable for cases

exhibiting a broader uncertainty distribution. Interestingly, even within the same band, we observed considerable variations in uncertainty adjustments; examples showing large changes are given in Tables 3 and 4. It is notable that these energies are determined by several measurements, some of which have comparatively large uncertainties; it is just this situation for which early versions of MARVEL struggled to provide reliable uncertainties and which led to the use of a segmented treatment based on uncertainties in MARVEL3. It would appear that the bootstrap method gives a more robust and consistent treatment of uncertainties.

The most obvious changes occur between the MARVEL3 uncertainties and those for MARVEL4 without bootstrap: the MARVEL4 uncertainties appear to be systematically smaller. A notable instance is for levels determined by a single transition such as  $(2,2^0,1),50,e$ . The uncertainty for this single transition is  $0.1 \text{ cm}^{-1}$  but the MARVEL3 procedure produces a value approximately double this for the level uncertainty. In contrast, MARVEL4 without using the bootstrap method gives a level uncertainty markedly closer to the original transition uncertainty. A similar pattern is evident in the state  $(1,2^0,0),3,e$ . Here four measured transitions are consistent within their measured uncertainties which allows both MARVEL3 and MARVEL4 to assign a smaller uncertainty to the level. However, a difference occurs in the treatment of level  $(2,2^0,1),48,e$ . This level is determined by two lines, with one being significantly more accurate; MARVEL3 and MARVEL4 both use the more accurate line to largely determine the energy level, but MARVEL3 appears to equally weight the less accurate line when calculating the uncertainty. MARVEL4, both without and with bootstrap procedure, largely relies on the accurate line for this which results in an uncertainty closer to the smaller initial line uncertainty. In this case, MARVEL4 suggests an estimated uncertainty less than half than the MARVEL3 value.

A pronounced distinction also emerges when comparing the outcomes with bootstrap = 100 against MARVEL4 calculations with no bootstrap iterations. For transitions determined by a single line, again taking the example of  $(2,2^0,1),50,e$ , this time the uncertainty remains unchanged. But situation gets more complicated when there are multiple lines. For transitions not in agreement because their predicted energies differ significantly such as level  $(2,2^0,1),46$ , there is a noticeable increase in uncertainty with bootstrapping. Conversely, when some of the lines do not agree such as for  $(1,2^0,0),3,e$ ,  $(1,2^0,0),4,e$ , and  $(1,2^0,0),5,e$ , but multiple accurate lines are present, the uncertainties generally stay consistent with and without bootstrapping. However, as in changes from MARVEL3 to MARVEL4, when there is just a single accurate line,



**Figure 2.** Change of uncertainty after applying bootstrap. Left panel: uncertainty distribution provided by MARVEL3; right panel: the change of uncertainty between MARVEL3 and MARVEL4 after 100 bootstrap iterations as a function of the rotational quantum number).

**Table 3.** Energy levels of ( $2\ 2^0\ 1\ e$ ) which show sensitivity to the treatment of uncertainties; all values are in  $\text{cm}^{-1}$ .

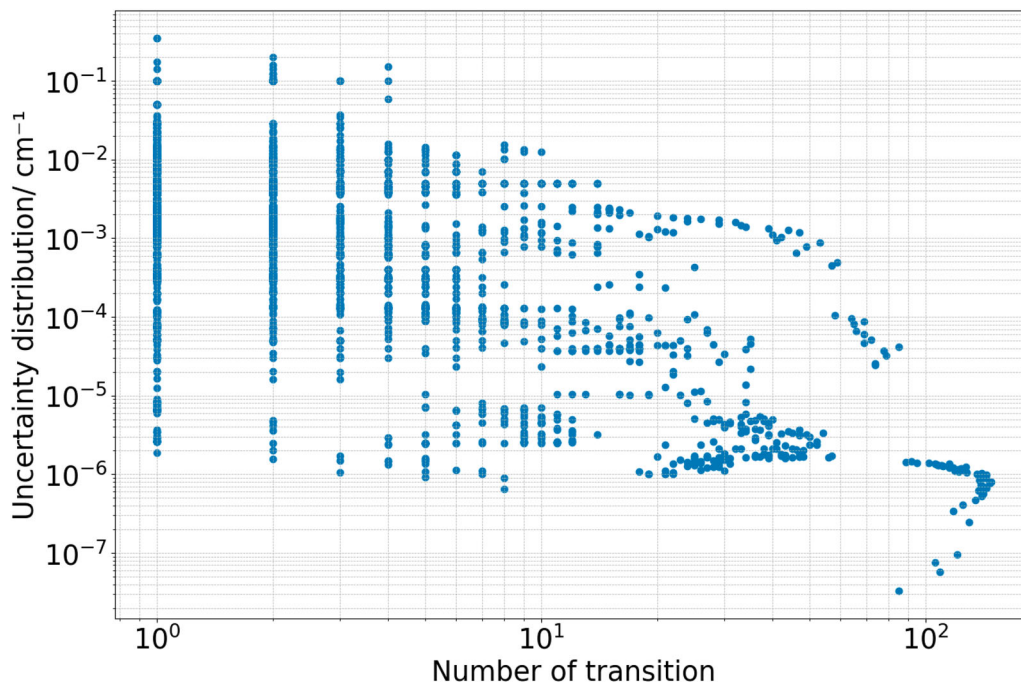
Level	MARVEL energy	MARVEL3 unc	No bootstrap unc	Bootstrap = 100 unc	Tag	Initial unc	Predicted energy
2 2 1 0 46 e	5208.505634	0.200074	0.1000	0.1267	57AIPiBl.535	0.10	5208.667412
					57AIPiBl.581	0.10	5208.343833
2 2 1 0 47 e	5227.406116	0.200117	0.1439	0.1000	57AIPiBl.536	0.10	5227.533331
					57AIPiBl.582	0.10	5227.278873
2 2 1 0 48 e	5246.609403	0.000801	0.000308	0.000307	57AIPiBl.583	0.10	5246.578400
2 2 1 0 49 e	5266.324213	0.000799	0.000305	0.000304	10ToSuBrCr.1030	0.0003	5246.609390
					57AIPiBl.584	0.10	5266.382363
2 2 1 0 50 e	5286.330746	0.200203	0.1	0.1	10ToSuBrCr.1065	0.0003	5266.324198
					57AIPiBl.585	0.10	5286.330720

**Table 4.** Energy levels of ( $1\ 2^0\ 0\ e$ ) which show sensitivity to the treatment of uncertainties; all values are in  $\text{cm}^{-1}$ .

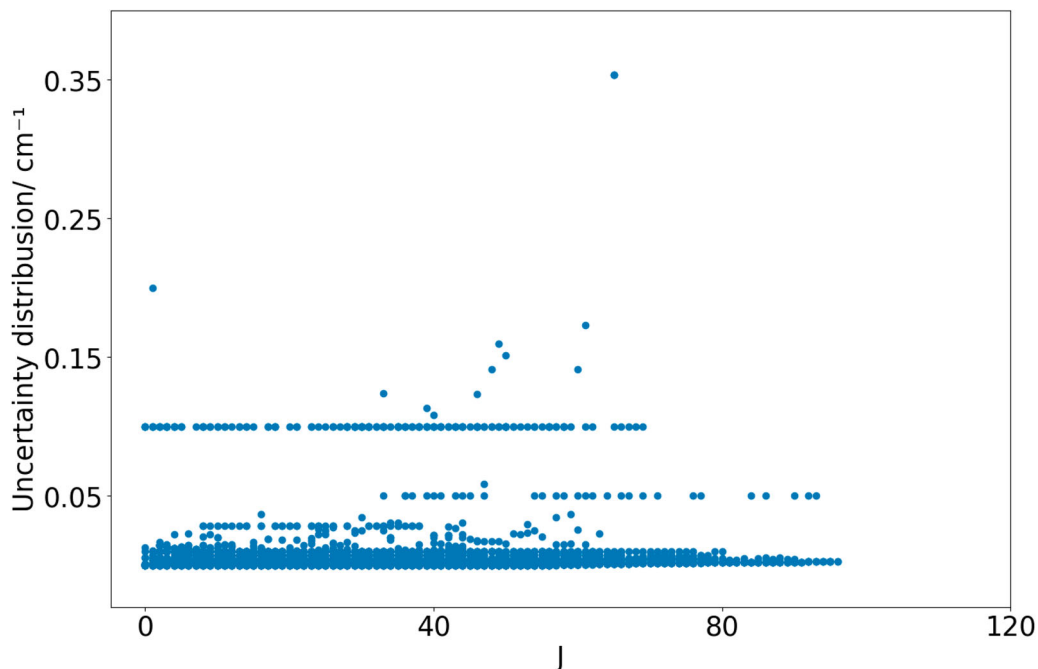
Level	MARVEL energy	MARVEL unc	No bootstrap unc	Bootstrap = 100 unc	Tag	Initial unc	Predicted energy
1 2 0 0 3 e	1894.666079	0.000267	0.000134	0.000134	57AIPiBl.3	0.1	1894.655138
					82KiMi.37	0.000133	1894.666078
					84TaltTa.80	0.000003	1894.666078
					86MaWeHi.6	0.000133	1894.666079
1 2 0 0 4 e	1896.289697	0.000274	0.000134	0.000134	57AIPiBl.4	0.1	1896.244274
					67MoMa.47	0.000005	1896.289694
					84TaltTa.80	0.000003	1896.289697
					84TaltTa.83	0.000003	1896.289699
1 2 0 0 5 e	1898.319214	0.000281	0.000134	0.000134	57AIPiBl.5	0.1	1898.292117
					67MoMa.47	0.000005	1898.319217
					84TaltTa.83	0.000003	1898.319213
					84TaltTa.86	0.000003	1898.319215
1 2 0 0 6 e	1900.754625	0.000287	0.000134	0.000134	57AIPiBl.6	0.1	1900.747663
					84TaltTa.86	0.000003	1900.754625
1 2 0 0 7 e	1903.589460	0.200002	0.1	0.1	57AIPiBl.58	0.1	1903.589459

such as for ( $2,2^0,1$ ),48,e above, the uncertainty may still experience a slight reduction upon bootstrapping compared to MARVEL3. Although more work is required to see if this trend is ubiquitous, the changes in uncertainty between no bootstrap iterations and 100 iterations are always much smaller than the difference between those predicted by MARVEL3 and MARVEL4.

Figure 3 shows the distribution of uncertainties after running the bootstrap procedure. The figure reveals that there are many energy levels with relatively large uncertainties in the  $0.1 - 0.05\ \text{cm}^{-1}$  range; this is caused by the use of several large data sets without stated uncertainties to which we assign with this level of uncertainty and lack of other measurements involving the same energy levels.



**Figure 3.** Distribution of uncertainties after 100 bootstrap iterations.

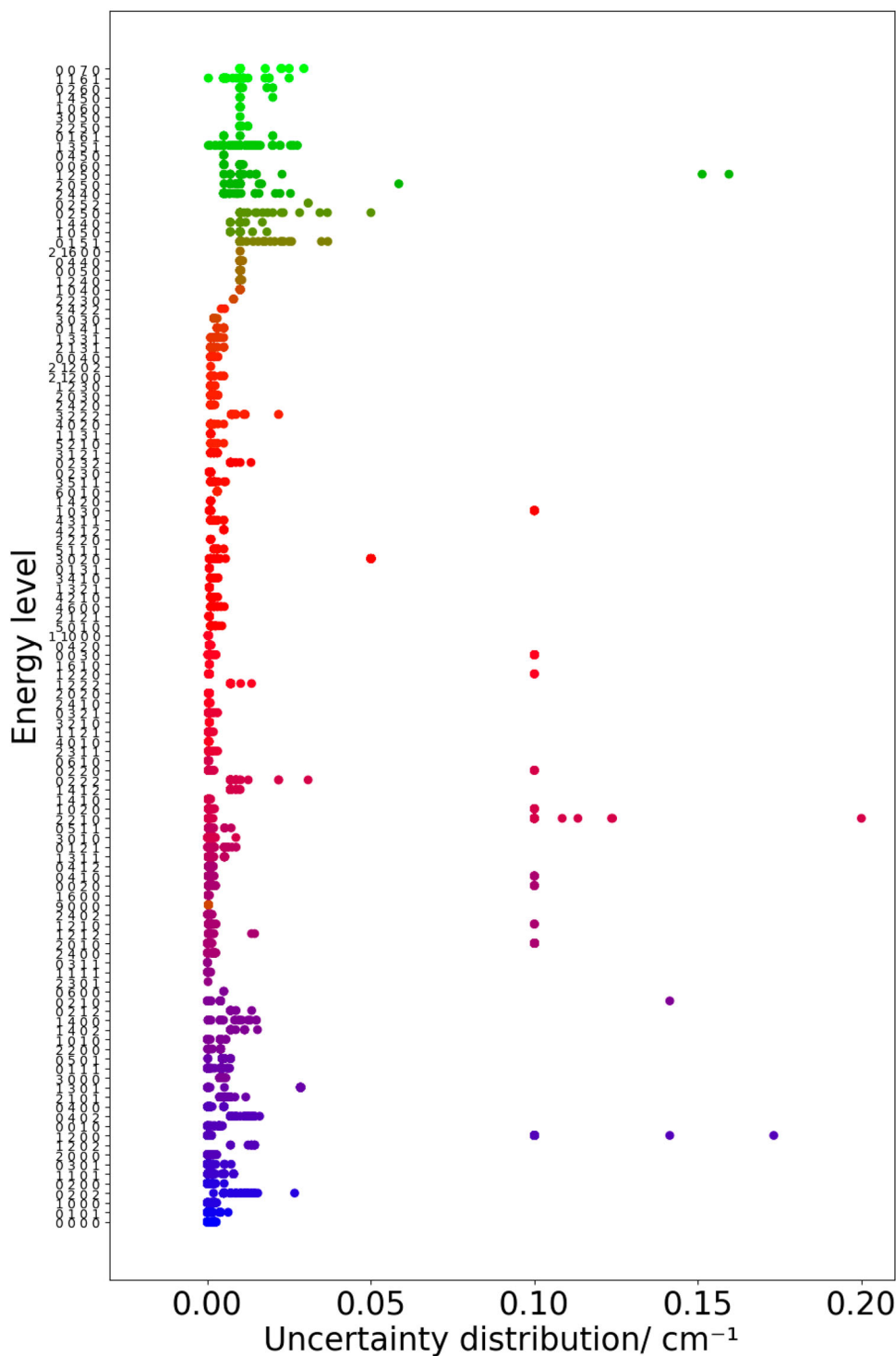


**Figure 4.** Distribution of uncertainty after bootstrap iteration with rotational quantum number  $J$ .

Additional high-resolution investigations would help to improve the accuracy of these levels.

Figures 4 and 5 show the behaviour of the uncertainties as function of rotation and vibrational excitation, respectively. While the difficulty of detecting an energy level generally increases with the level of excitation and hence energy, there is not always a smaller uncertainty for states with lower vibrational or rotational excitation.

What is shown by Figure 3 is that the uncertainty to which a level is determined reduces significantly as with the number of transitions determining that energy. This bears testimony to MARVEL's proficiency in consolidating data from various sources. However, in scenarios with limited data, MARVEL leans heavily on the intrinsic uncertainty of the sources.



**Figure 5.** Distribution of uncertainty after bootstrap iteration depends on vibrational level (given as  $v_1v_2v_3\ell$ ) in order of increasing energy (one extra point outside the range has uncertainty  $0.35 \text{ cm}^{-1}$  in vibrational state  $13^10$ ).

## 5. Conclusions

We present a study of all the published measured and assigned rovibrational lines of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ . By using 100 sources, we compiled a self-consistent network of 13,056 measured transition wavenumbers with

uncertainties and assignments which are based on the use of linear molecule harmonic oscillator quantum numbers. Using the MARVEL procedure this list provided 5729 empirical energy levels. Tests of the treatment of uncertainties, which have changed significantly between

different versions of MARVEL, suggest that the bootstrap method does indeed give an improved treatment and we would recommend its use in future MARVEL studies.

Of course, the results of a MARVEL study can only be as good as the input experimental data. The dataset we produce for OCS is notably smaller than that obtained by the recent MARVEL study on the rather similar linear  $\text{N}_2\text{O}$  molecule [167]. In particular, there is a notable lack of measurements for OCS on states with vibrational angular momentum,  $\ell$ , greater than two. The active nature of the MARVEL procedure is such that should any new high-resolution measurements become available for  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  they can easily be added to the dataset. Indeed, a recent study on formaldehyde,  $\text{H}_2\text{CO}$ , has shown that the addition of relatively few high accuracy measurements to an existing MARVEL network can lead to significant all round improvements in the accuracy of the resulting empirical energy levels [176].

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No potential conflict of interest was reported by the author(s).

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## Data availability statement

The data compiled and generated in this article is given in the supporting information in the form of a MARVEL input transitions file, a MARVEL output energy file and the segment file necessary to run the MARVEL input under MARVEL4; this file gives the units for the transitions by data source.

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## Appendices

### Appendix 1. Notes on data sources

The following sources contained at least some transitions between states with  $\ell \geq 1$  that did not specify the parity: 52Tetenbau [27], 55Low [31], 67MoMa [38], 75BuDeSm [53], 76Smith [58], 80BoBa [62], 81SaWoMaLa [66], 82KiMi [69], 83JoKaHo [70], 83KIYaWi [71], 84TaItTa [74], 88DeGiDi [78], 90FaLaLeHe [84], 90ToHoAl [86], 90WeScMa [87], 95BeFaGu [87]. In these cases we assumed such transitions are actually doublets involving two transitions.

Comments on individual sources are:

**52KiTo** [26] is not a first hand study and uncertainties are not stated, however, it provides novel data. An uncertainty of 0.8 MHz was chosen which is consistent with other data.

**53KiGo** [28]: Transitions are assumed to be within the vibrational ground state although this is not actually stated.

**54CaTh** [30]: This older source provides a very extensive dataset which in many cases do not agree with more modern measurements; because of this, even though the paper provides transitions for which there is no newer measurement, this dataset was excluded from our final compilation.

**54KiGo** [177]: Transition R(11), R(13), R(15), R(17) are a repeat of those from 53KiGo and were excluded

**55Low** [31]: No uncertainty is given so the values given by 78Lovas [137] were adopted.

**57AlPIBl** [33]: Transitions R(28) and R(29) for the  $00^0_2e - 00^0_0e$  do not fit the trend of R branch, transitions; these were corrected to 4111.07 and 4111.35  $\text{cm}^{-1}$ , respectively. No uncertainty is given so a value of 0.1  $\text{cm}^{-1}$  was adopted.

**59Dymanus** [34]: No uncertainty is given so a value of 0.05 MHz was adopted.

**65TrCo** [35]: No uncertainty is given so a value of 0.1  $\text{cm}^{-1}$  was adopted. Some lines do not follow by the trend of data in the source which is presumed to be due to typographical errors. So transition  $20^0_1 - 00^0_0$  R(22) was changed from 3777.795  $\text{cm}^{-1}$  to 3776.795  $\text{cm}^{-1}$ . For  $12^0_2 - 00^0_0$  R(15) was changed from 5964.23  $\text{cm}^{-1}$  to 5965.23  $\text{cm}^{-1}$  and  $12^0_2 - 00^0_0$  P(14) was changed from 5954.25  $\text{cm}^{-1}$  to 5953.25  $\text{cm}^{-1}$ .

**67Maki** [37]: No uncertainty is given so a value of 0.05 MHz was adopted.

**67MoMa** [38]: No uncertainty is given so the values given by 78Lovas [137] were adopted.

**69NaMo** [39]: The transitions frequency were taken from 09Maki [178].

**70HeDeGo** [40]: Lower levels were assigned to the vibrational ground state by comparison with other works although this is not actually stated. No uncertainty is given so a value of 0.05 MHz was adopted.

**72BeKl** [43]: This source provides a single line which proved to be inconsistent with more recent measurements so it was removed.

**74BoBaMa** [48]: No uncertainty is given so a value of 0.05 MHz was adopted.

**74KuOaWa** [50]: No uncertainty is given so a value of 0.05 MHz was adopted.

**74LaWi** [51]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**75BuDeSm** [53]: Some lines do not follow by the trend of data in this source which is presumed to be a typographical error. Both parity of transition  $13^1_0 - 01^1_0$  P(7) has been change from 1889.847 to 1888.847. For transition  $14^0_0 - 02^0_0$  the paper assign the quantum numbering start from P(7) which causes a systematic difference in comparison with other measurements. Lines from P(7) to P(20) were reassigned to P(8) to P(21).

**81SaWoMaLa** [66]: States that the data come from 79WePeMa and 76MeDuMe but some transitions are not given in these references, so the results given in this paper are included.

**82KiMi** [69]: Transition  $10^0_0 - 00^0_0$  R(2)e is given two different values in the source which is probably due to isotopologue misattribution, by comparison with other sources the value 36380.00 MHz was assumed to be the correct one.

**83KIYaWi** [71]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**83ScWi** [72]: Some data given are not first hand, but the papers cited as the source of these could not be found so the data has been included.

**85JoHoKaMa** [76]: For transition  $02^0_0e - 00^0_0e$  the paper assigns transition R(73) to 551.72662  $\text{cm}^{-1}$  and assumes R(71) and R(72) are not observed. This causes a systematic difference with other sources, so lines R(73) to R(76) were reassigned to R(72) to R(75).

**88MaOIWeVa** [79]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**89VaJeWe** [82]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**90BlWaBoBo** [83]: Provides data cited as Maki private communication; an uncertainty of 0.005  $\text{cm}^{-1}$  was assumed.

**90ToHoAl** [86]: The uncertainty claimed is  $8 \times 10^{-5} \text{cm}^{-1}$  but appears to be too small; the uncertainties were increased by a factor of 10.

**90WeScMa** [87]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**91BiCoDeWa** [88]: No uncertainty is given so a value of 0.05  $\text{cm}^{-1}$  was adopted.

**91GrHeSt** [89]: No uncertainty is given so values from 14GoDeHeVa [19] were adopted.

**91TaLoLu** [91]: States that 6 or 7 lines in the R branch were measured using a different method with higher uncertainty; however, it is not specified which lines they are, so all lines in R branch were given the higher uncertainty.

**95BeFaGu** [97]: Some data are presented with an uncertainty of zero, for these the uncertainty was set to  $0.001\text{ cm}^{-1}$ .

**95ErVaBrFa** [98]: The transition data was cited as being from 95BeFaGu [97], but 95BeFaGu only published the corresponding band data, so transitions from 95ErVaBrFa were adopted with uncertainties taken from 95BeFaGu.

**95MeSaWaGe** [100]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**95WeDaHoMa** [101]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**96SaWaMeUr** [103]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**98RbBeVaNa** [106]: This paper does not provide a list of transitions. A set of unassigned transitions were provided by Jean Vander Auwera which we assigned a total of 1473 lines by comparison with the spectroscopic constants given in the paper. This line list can be found as part of the MARVEL input in the supplementary data.

**00MoYaMa** [8]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**00MuPaUrMa** [9]: Vibrational state labels  $\nu_1$  and  $\nu_3$  were swapped to be consistent with other sources.

**02LeBaHuFa** [10] Transitions for this paper were provided by the authors.

**06MaRoBoMo** [15]: The transitions listed are not first hand; all the quoted transitions were included from elsewhere except for the ones with  $J = 65$  to  $73$ , which are cited as A Fayt private communication, which we took from this source.

**10ToSuBrCr** [17] Transitions for this paper were provided by the authors.

**13GaArTc** [18]: We assumed that the quantum number  $\ell = 1$  for all transitions. No uncertainty is given so a value of  $0.001\text{ cm}^{-1}$  was adopted.

**14GoDeHeVa** [19]: This paper presents new measurements in the  $6200\text{--}8200\text{ cm}^{-1}$  region. It also performs a systematic global reanalysis of OCS spectra as a result a significant number of previously measured pure rotational lines are given in supplementary data. Many of these lines are not otherwise available so we have labelled them 14GoDeHeVarot to distinguish them from the newly measured lines.

The 14GoDeHeVarot set contains lines from 74VaDy [179], 87YaKl [180], 87LoSu [145], 91MaLaFa [151] and 99TrBaHuOl [181] which were not provided in the cited references. It also contains lines from the thesis by M-F Grogard-Declerfayt, Université Catholique de Louvain (1972), J.W.C. Johns cited as being reported at the 45th Ohio State University International Symposium on Molecular spectroscopy in 1990, private communication by A. G. Maki (1981), private communication from F. Herleamon (1993), A. Fayt and H. Fichoux unpublished measurements (1997) and private communication by H. Maeder (1999). The parities of some lines correspond to forbidden transitions, these lines are likely reconstructed from band data and have not been included; they comprise 86LaVaFa [144], and two papers by A. Fayt 'Carbonyl sulphide infrared spectra between 2400 and  $7000\text{ cm}^{-1}$ ' from 1970 and 'Molecular constants of carbonyl sulfide' from 1972 which we were unable to obtain copies of.

As discussed in the paper many higher-lying states become heavily mixed which makes the choice of harmonic oscillator assignments somewhat arbitrary and the paper relies heavily on polyads for performing its analysis. We use harmonic oscillator assignments chosen by comparison to other data, calculated band origin data from [182] and the reduced energy method as described in Section IIB which led to some reassignments of the lines. Transition  $20^01\text{--}00^00\text{ e}$  from R(39) to R(91) was reassigned to  $24^00\text{--}00^00\text{ e}$ , transition  $24^00\text{--}00^00\text{ e}$  from R(25) to R(28) and from P(30) to P(40) was reassigned to  $20^01\text{--}00^00$ , transition  $01^12\text{--}01^10$  from R(44) to R(54) was reassigned from e parity to f parity, transition  $00^03\text{--}00^00$  from R(25) to R(31) and from P(35) to P(42) was reassigned to  $10^00\text{--}00^00$ .

**16GoBeLa** [21]: By comparison with other data, the transition with  $J + 1 = 5$  was reassigned to  $J + 1 = 4$  and the original  $J + 1 = 4$  transition deleted.

## Appendix 2. Sources considered but not used

Multiple sources were examined and excluded from further consideration for reasons given below:

**47DaGoCo** [122]: No transitions data given.

**54Anderson** [123]: Data from 54KiGo [177]

**57MaWe** [124]: Electric field method, the zero field data given has been remeasured subsequently more accurately.

**59BaGoPo** [125]: Presents two transitions remeasured more recently.

**59SaWiRa** [183]: Band data only in the paper.

**59Dymanus1** [126]: No transitions data given.

**61DyDi** [127]: No transitions data given.

**62MaPiTi** [128]: Band data only in the paper

**64BuMi** [129]: Constants only; no new line data.

**64KrSrCh** [130]: No transitions data given.

**66BrBo** [131]: Linewidths data only; no new line data.

**66UnFl** [132]: Electric field method; no zero field data given.

**67KrSr** [184]: Presents one transition remeasured more recently.

**69BaCaTa** [185]: Line broadening data only; no new line data.

**70Cattani** [186]: Line broadening data only; no new line data.

**71StMePa** [187]: Two lines taken from 52KiTo [26].

**72NeRoPa** [188]: Presents one transitions remeasured more recently.

**72ReFo** [189]: Presents three transitions remeasured more recently.

**73OlBrPrBo** [190]: Line broadening data only; no new line data.

**73WaLeKuSt** [191]: Presents one transition remeasured more recently.

**74DaMu** [192]: Rotational magnetic moment data; no new line data.

**74ReDy** [193]: Constants only for the main isotopologue.

**75Coy** [133] Pressure relaxation; no new line data

**76KaAmSh** [134]: Presents two transitions remeasured more recently.

**76MaScDr** [135]: Electric field method; the quoted zero field data has been remeasured more recently.

- 76ReLe** [194]: Presents one transition remeasured more recently.
- 77Hewitt** [136]: Line width measurement; no new line data.
- 78DrBeDaVi** [195]: Band data only.
- 78GrCh** [196]: No transition data given.
- 78Lovas** [137]: Useful compilation but not original data.
- 80BoBa1** [197]: Energy transfer process data; no new line data.
- 81BuKaKrSh** [198]: Lines for minor isotopologues only.
- 81BuVaKaKr** [138]: Lines for minor isotopologues only.
- 81ZiBaGu** [139]: Line width measurement; presents one transition remeasured more recently.
- 82KaJoHo** [199]: 83JoKaHo is a later version which contains more data
- 83BoMa** [140]: Electric field method, the zero field data given has been remeasured more recently.
- 84MeBeDrMa** [200] Presents one transition remeasured more recently.
- 84TaItHaTa** [141]: Electric field method, no zero field data given
- 84ZiBaGu** [142]: Lines for minor isotopologues only.
- 86FaVaLa** [143]: No original data.
- 86LaVaFa** [144]: Electric field method, the zero field data given by 14GoDeHeVa [19]
- 87LoSu** [145]: Band data only in the paper, lines positions are given by 14GoDeHeVa [19]
- 87YaKl** [180]: Band data only in the paper, lines positions are given by 14GoDeHeVa [19]
- 88BoBl** [201]: Pressure broadening; no new line data.
- 89CfYYQk** [146]: Band data only in the paper.
- 90BlWaBo** [147]: Line broadening data only; no new line data.
- 90CaDo** [148]: Line width measurement; no new line data.
- 90ZiSe** [149]: Band data of OCS in in liquid Ar and O<sub>2</sub> solution; no new line data.
- 91JoPa** [150]: Line width measurement; no new line data.
- 91MaLaFa** [151]: Electric field method; the zero field data are provided by 14GoDeHeVa [19]
- 91MaWeBu** [202]: Band data only.
- 91MeJaScDr** [152]: Data from 82KiMi[69]
- 92BeLeRe** [153]: Lines for minor isotopologues only.
- 93LeLeRo** [154]: Line broadening data only; no new line data.
- 93StGiGa** [155]: Pressure broadening; no new line data.
- 94DoMaScGu** [156]: Data from 83ScWi[72].
- 94PiOhYa** [157]: Electronic transition; no new line data.
- 95GiGaMi** [158]: Pressure broadening coefficient only; no new line data.
- 96BeBaCo** [159]: Electronic transition band data only.
- 97BeDoSaBo** [160]: Line intensity; no new line data.
- 97RuKhFiLi** [161]: No transitions data given.
- 97YoNa** [162]: Band data only.
- 98NaFaBrBl** [163]: Band data only; the lines are available from 14GoDeHeVa[19] but the quoted transitions violate the parity selection rule so were not used.
- 99TrBaHuOl** [181]: Band data only; the lines are given by 14GoDeHeVa[19].
- 00DoBeBo** [203]: Broadening coefficients only; no new line data.
- 00LuZhXi** [107]: Band data only.
- 00MaSe** [108]: No transitions data given.
- 00ZuBaAlRe** [109]: No original line data
- 02PuDoCa** [110]: Pressure broadening; no new line data.
- 02ReHaThVo** [111]: Line data appears to come from Hitran.
- 03KuFuSa** [112]: Lines for minor isotopologues only.
- 06AuFa** [113]: Line intensity; no new line data.
- 06KoTrLeXu** [114]: Pressure broadening; no new line data
- 08BiMoCuHi** [115]: Removed as line positions differ significantly from other measurements.
- 08BoBuGuKo** [204]: Band data only in the paper
- 09KoTr** [116]: Self-broadening parameters only; no new line data.
- 09SuToBrCr** [117]: Presents two transitions remeasured more recently.
- 11GaBeArTc** [205]: Line data appears to come from Hitran
- 12ScJoMcSc** [118]: Band data only in the paper.
- 13JeGaKwAr** [119]: Line data appears to come from Hitran.
- 13ZhWaLuYa** [120]: Maximum degree of alignment data only.
- 19JeDrMaTc** [121]: Line data appears to come from Hitran.

**Appendix 3. Summary of energy levels and uncertainties by vibrational state****Table A1.** Summary of energy levels for  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  determined in this study by vibrational band.

Energy level ( $\nu_1\nu_2\nu_3 \ell$ parity)	Group Range	Nb. of energy levels	Unc. Range	Avg. of Unc.	Range of energy levels
0000e	0–95	96	0.0000–0.0023	0.0006	0.0000–1846.4411
0010e	0–90	78	0.0000–0.0043	0.0026	2062.2009–3710.7074
0020e	0–90	87	0.0003–0.1000	0.0064	4101.4105–5739.9401
0030e	0–89	82	0.0002–0.1000	0.0225	6117.5764–7710.5031
0040e	2–64	38	0.0010–0.0032	0.0014	8111.9223–8933.8594
0050e	0–80	79	0.0100–0.0101	0.0100	10,080.9027–11,354.7748
0060e	1–68	49	0.0050–0.0105	0.0091	12,028.2901–12,945.6049
0070e	2–55	26	0.0100–0.0295	0.0126	13,953.0053–14,551.4737
0101e	1–77	77	0.0000–0.0063	0.0007	520.8283–1739.1146
0101f	1–76	76	0.0000–0.0038	0.0006	520.8287–1708.7141
0111e	1–71	67	0.0000–0.0061	0.0035	2575.7115–3606.3038
0111f	1–71	64	0.0000–0.0067	0.0035	2575.7119–3607.3925
0121e	3–76	60	0.0001–0.0052	0.0015	4609.5174–5780.6071
0121f	5–77	45	0.0003–0.0087	0.0018	4613.1369–5812.2975
0131e	1–8	7	0.0006–0.0006	0.0006	6616.2524–6630.5193
0131f	1–9	5	0.0006–0.0006	0.0006	6616.2524–6633.8322
0141e	8–38	14	0.0030–0.0050	0.0039	8615.8507–8895.4478
0141f	8–33	11	0.0030–0.0050	0.0037	8615.8698–8824.3483
0151e	2–64	63	0.0100–0.0361	0.0130	10,565.4743–11,383.8637
0151f	9–60	7	0.0100–0.0100	0.0100	10,582.0643–11,286.3524
0161e	6–34	4	0.0050–0.0200	0.0100	12,512.3153–12,737.3640
0161f	6–34	4	0.0050–0.0200	0.0100	12,512.3272–12,737.6851
0200e	0–86	81	0.0000–0.0022	0.0004	1047.0421–2567.4375
0200f	3–4	2	0.0000–0.0000	0.0000	1049.0849–1050.7156
0202e	2–76	66	0.0015–0.0264	0.0064	1042.5109–2230.7237
0202f	2–66	59	0.0050–0.0144	0.0061	1042.5109–1940.5579
0210e	0–60	49	0.0000–0.1414	0.0062	3095.5544–3835.6381
0212e	3–51	9	0.0071–0.0135	0.0082	3091.3335–3625.2612
0212f	19–37	5	0.0071–0.0071	0.0071	3165.8066–3373.3688
0220e	0–74	63	0.0003–0.1000	0.0083	5120.9836–6236.1564
0222e	4–65	50	0.0071–0.0305	0.0084	5117.4123–5975.6390
0222f	22–65	10	0.0071–0.0087	0.0077	5215.1937–5975.7506
0230e	3–55	52	0.0006–0.0010	0.0008	7125.7772–7739.0068
0232e	7–46	18	0.0071–0.0071	0.0071	7125.9843–7547.0494
0232f	9–43	17	0.0071–0.0133	0.0077	7132.7863–7493.1124
0250e	6–45	36	0.0100–0.0500	0.0149	11,067.7193–11,468.6293
0252e	34–35	2	0.0308–0.0308	0.0308	11,283.8285–11,297.6634
0260e	5–47	19	0.0100–0.0200	0.0110	12,999.4105–13,437.1703
0301e	1–72	66	0.0000–0.0072	0.0005	1573.7736–2642.5642
0301f	1–76	69	0.0000–0.0052	0.0005	1573.7744–2765.5644
0311e	1–2	2	0.0000–0.0000	0.0000	3615.7503–3616.5599
0311f	1–2	2	0.0000–0.0000	0.0000	3615.7512–3616.5625
0321e	2–65	31	0.0003–0.0029	0.0006	5635.4527–6496.8908
0321f	8–65	34	0.0003–0.0030	0.0005	5648.7576–6498.7126
0400e	0–68	63	0.0000–0.0051	0.0013	2104.8277–3061.3926
0402e	2–53	45	0.0071–0.0162	0.0083	2100.7452–2682.9781
0402f	2–46	44	0.0071–0.0144	0.0081	2100.7452–2540.4916
0410e	0–80	77	0.0003–0.1000	0.0096	4141.2227–5454.5335
0412e	23–75	37	0.0003–0.0015	0.0005	4246.9006–5289.5530
0420e	2–64	48	0.0006–0.0010	0.0006	6155.9103–6993.2958
0440e	1–45	45	0.0100–0.0109	0.0100	10,114.4241–10,526.8516
0450e	6–47	6	0.0050–0.0050	0.0050	12,070.1700–12,511.8543
0501e	1–55	45	0.0001–0.0071	0.0047	2635.9995–3263.2532
0501f	1–43	41	0.0001–0.0071	0.0048	2635.9997–3022.3757
0511e	5–76	60	0.0003–0.0072	0.0009	4672.1759–5851.9791
0600e	4–47	3	0.0050–0.0050	0.0050	3174.7275–3631.7320
0610e	5–46	30	0.0003–0.0004	0.0003	5202.1117–5635.4925
1000e	0–96	97	0.0000–0.0024	0.0006	858.9669–2738.4925
1010e	0–64	63	0.0000–0.0057	0.0032	2918.1051–3753.8495
1020e	0–81	65	0.0003–0.1000	0.0096	4953.8791–6279.8697
1030e	1–43	41	0.0006–0.1000	0.0396	6966.5713–7342.4061
1040e	3–41	35	0.0100–0.0100	0.0100	8957.2501–9295.7483
1050e	2–44	41	0.0070–0.0182	0.0099	10,921.1777–11,310.2691
1060e	5–62	8	0.0100–0.0100	0.0100	12,867.9362–13,627.4078
1101e	1–70	70	0.0001–0.0080	0.0009	1372.8643–2377.9807

(continued).

**Table A1.** Continued.

Energy level ( $\nu_1\nu_2\nu_3$ $\ell$ parity)	Group Range	Nb. of energy levels	Unc. Range	Avg. of Unc.	Range of energy levels
1101f	1–70	69	0.0001–0.0080	0.0013	1372.8647–2379.1066
1111e	2–25	5	0.0000–0.0010	0.0003	3425.3474–3555.0281
1111f	1–25	8	0.0000–0.0009	0.0002	3424.5428–3555.1822
1121e	2–65	46	0.0003–0.0020	0.0004	5453.6638–6310.7168
1121f	2–43	24	0.0004–0.0004	0.0004	5453.6657–5831.6626
1131e	7–30	8	0.0010–0.0010	0.0010	7468.5873–7642.6095
1131f	11–33	10	0.0010–0.0010	0.0010	7483.7563–7681.1252
1161e	2–29	24	0.0050–0.0250	0.0083	13,333.3959–13,502.8124
1161f	2–29	23	0.0003–0.0189	0.0068	13,333.3981–13,503.1266
1200e	0–69	70	0.0000–0.1732	0.0419	1892.2305–2871.6901
1202e	2–47	7	0.0071–0.0144	0.0118	1888.1629–2344.7413
1202f	2–30	6	0.0071–0.0144	0.0126	1888.1629–2075.7422
1210e	0–95	83	0.0003–0.1000	0.0042	3937.4274–5774.9520
1212e	2–78	23	0.0003–0.0144	0.0012	3932.5093–5173.4306
1212f	3–3	1	0.0135–0.0135	0.0135	3933.7207–3933.7207
1220e	1–54	54	0.0004–0.1000	0.0060	5959.7304–6555.1393
1222e	3–39	25	0.0071–0.0135	0.0075	5954.6753–6265.3949
1222f	8–32	19	0.0071–0.0071	0.0071	5966.7246–6164.2700
1230e	1–65	55	0.0010–0.0023	0.0011	7958.4386–8813.6652
1240e	2–44	38	0.0100–0.0111	0.0100	9934.7273–10326.5485
1250e	0–63	60	0.0050–0.1634	0.0151	11,886.1067–12,681.7382
1301e	1–65	39	0.0000–0.3535	0.0223	2412.5285–3282.2560
1301f	1–72	41	0.0000–0.3535	0.0255	2412.5294–3480.4219
1311e	2–76	66	0.0003–0.0052	0.0009	4451.9713–5631.4583
1311f	7–75	58	0.0003–0.0052	0.0010	4462.0930–5602.9073
1321e	5–51	36	0.0006–0.0006	0.0006	6472.1720–6998.4690
1321f	4–48	31	0.0006–0.0006	0.0006	6470.1722–6939.3675
1331e	3–51	28	0.0020–0.0050	0.0026	8460.7769–8987.8413
1331f	6–43	16	0.0010–0.0020	0.0017	8466.7897–8837.0868
1351e	5–37	26	0.0009–0.0275	0.0124	12,380.0854–12,651.9453
1351f	5–39	22	0.0003–0.0223	0.0110	12,380.0943–12,683.2074
1400e	2–57	45	0.0002–0.0165	0.0047	2938.3675–3609.5680
1402e	3–32	17	0.0071–0.0153	0.0081	2934.6561–3147.1018
1402f	5–45	18	0.0071–0.0114	0.0077	2938.3214–3353.4200
1410e	1–62	55	0.0003–0.0008	0.0003	4970.8345–5760.3006
1412e	8–51	28	0.0071–0.0090	0.0071	4978.8539–5500.7999
1412f	31–59	16	0.0071–0.0100	0.0075	5165.1014–5680.5291
1420e	8–31	20	0.0010–0.0010	0.0010	6995.4322–7180.3386
1440e	2–48	34	0.0070–0.0168	0.0099	10,936.1533–11,401.3648
1450e	5–42	5	0.0100–0.0200	0.0120	12,884.6111–13,234.3665
1600e	1–58	40	0.0003–0.0005	0.0003	3990.5146–4687.8955
1610e	9–32	8	0.0006–0.0006	0.0006	6030.3108–6226.2103
11000e	26–41	11	0.0002–0.0004	0.0003	6256.1784–6460.6996
2000e	0–96	97	0.0000–0.0024	0.0007	1710.9763–3584.6771
2010e	0–68	61	0.0001–0.1000	0.0510	3768.4957–4716.2451
2020e	0–41	30	0.0003–0.0007	0.0004	5801.9064–6145.6920
2030e	0–64	51	0.0010–0.0032	0.0016	7811.9533–8638.0014
2050e	1–61	61	0.0050–0.0607	0.0104	11,762.3841–12,503.2833
2101e	1–78	58	0.0038–0.0131	0.0045	2218.4325–3461.2366
2101f	1–77	56	0.0038–0.0069	0.0044	2218.4340–3430.8257
2121e	3–26	16	0.0004–0.0006	0.0006	6293.3135–6431.2420
2121f	2–28	14	0.0004–0.0006	0.0006	6292.1150–6453.4641
2131e	3–49	23	0.0010–0.0020	0.0013	8294.2201–8778.8647
2131f	4–58	26	0.0010–0.0050	0.0020	8295.8209–8972.8591
2200e	1–61	59	0.0000–0.0041	0.0034	2731.8039–3496.4310
2210e	1–71	63	0.0003–0.2000	0.0410	4773.5636–5801.5521
2220e	5–22	18	0.0010–0.0010	0.0010	6797.5495–6892.9018
2230e	11–20	4	0.0080–0.0080	0.0080	8812.7716–8870.1834
2250e	1–36	32	0.0100–0.0124	0.0102	12,707.3341–12,969.6496
2301e	4–4	1	0.0002–0.0002	0.0002	3249.3111–3249.3111
2311e	1–59	55	0.0004–0.0023	0.0005	5280.9431–5993.1487
2311f	2–60	49	0.0004–0.0029	0.0005	5281.7516–6019.0169
2400e	2–92	43	0.0001–0.0021	0.0009	3764.0412–5479.1957
2402e	30–68	20	0.0001–0.0012	0.0004	3948.4391–4710.9042
2410e	2–25	22	0.0004–0.0008	0.0005	5793.2067–5923.0703
2420e	2–63	27	0.0010–0.0022	0.0011	7799.1646–8605.6742
2422e	68–72	2	0.0042–0.0052	0.0047	8734.7405–8849.7443
2440e	1–48	46	0.0050–0.0254	0.0075	11,741.4442–12,208.2487

(continued).

**Table A1.** Continued.

Energy level ( $\nu_1\nu_2\nu_3 \ell$ parity)	Group Range	Nb. of energy levels	Unc. Range	Avg. of Unc.	Range of energy levels
2 12 0 0 e	4–17	12	0.0010–0.0050	0.0025	7961.3412–8019.7719
2 12 0 2 e	27–28	2	0.0010–0.0010	0.0010	8108.7594–8120.1903
2 16 0 0 e	35–36	2	0.0100–0.0100	0.0100	10,328.6072–10,343.3938
3 0 0 0 e	0–86	66	0.0038–0.0057	0.0041	2555.9906–4057.3208
3 0 1 0 e	1–88	51	0.0001–0.0084	0.0008	4610.2452–6172.7771
3 0 2 0 e	0–93	88	0.0006–0.0500	0.0174	6640.1048–8374.5013
3 0 3 0 e	9–52	24	0.0020–0.0030	0.0020	8664.5067–9191.0371
3 0 5 0 e	27–27	1	0.0100–0.0100	0.0100	12,736.5610–12,736.5610
3 1 2 1 e	5–53	20	0.0010–0.0031	0.0019	7132.8738–7698.2129
3 1 2 1 f	3–55	19	0.0010–0.0030	0.0019	7129.2848–7743.3456
3 2 1 0 e	4–25	21	0.0006–0.0006	0.0006	5606.4886–5733.1259
3 2 2 2 e	7–42	15	0.0073–0.0215	0.0098	7622.5418–7972.5151
3 2 2 2 f	7–42	17	0.0073–0.0115	0.0087	7622.5418–7972.5481
3 4 1 0 e	4–66	32	0.0010–0.0032	0.0014	6615.1292–7501.8536
3 5 1 1 e	1–63	25	0.0020–0.0052	0.0023	7116.9108–7925.2837
3 5 1 1 f	1–69	27	0.0010–0.0055	0.0017	7116.9121–8086.1343
4 0 1 0 e	3–51	44	0.0004–0.0004	0.0004	5447.3513–5973.0145
4 0 2 0 e	3–55	45	0.0010–0.0050	0.0012	7474.5566–8081.7747
4 2 1 0 e	1–62	25	0.0010–0.0031	0.0013	6429.4887–7213.4113
4 2 1 2 e	44–62	8	0.0050–0.0051	0.0050	6821.4210–7208.8358
4 3 1 1 e	4–51	21	0.0010–0.0050	0.0017	6925.9228–7453.8211
4 3 1 1 f	6–58	20	0.0010–0.0030	0.0018	6930.3647–7609.9480
4 6 0 0 e	4–67	22	0.0010–0.0051	0.0020	6422.7098–7337.1497
5 0 1 0 e	1–78	30	0.0010–0.0043	0.0014	6273.5122–7495.0737
5 1 1 1 e	4–50	17	0.0030–0.0030	0.0030	6759.5914–7262.9907
5 1 1 1 f	4–47	13	0.0020–0.0050	0.0027	6759.5978–7205.2014
5 2 1 0 e	4–45	13	0.0010–0.0050	0.0020	7249.7419–7658.9486
6 0 1 0 e	6–50	16	0.0030–0.0030	0.0030	7102.5402–7598.6822
9 0 0 0 e	6–47	36	0.0003–0.0003	0.0003	3977.7307–4421.7407

Note: Provided are the range, in  $\text{cm}^{-1}$ , and energy level count for each band along with the range and average of uncertainties in  $\text{cm}^{-1}$ .