

## Description of the C<sub>2</sub> line list.

Uffe Gråe Jørgensen, September 7, 1999.

The present line list of C<sub>2</sub> data is made available by F.Querci and collaborators. It has been described in detail in F.Querci, M.Querci, V.G.Kunde, A&A, 15, 256–274, 1971 (QQK), and F.Querci, M.Querci, T.Tsuji, A&A, 31, 265–282, 1974 (QQT), and has only been slightly modified by me in the present form, as described below, in order to be consistent with the other line list data available on this ftp site. I kindly ask you to refer to the above mentioned papers if you want to use the data. Also, I kindly ask you not to distribute the lists, but instead refer interested friends and colleagues to the ftp site where you found the data (stella.nbi.dk, anonymous login with your userid as password, cd to pub/scan). The data are occasionally updated if errors are discovered or improved molecular constants etc have become available which can influence the line list data. New lists are added to the old ones when my time permits. So, to optimise the completeness and to minimise the risk of circulating data with errors, each user are asked to look for his data himself at this ftp site when he wants to use them. Therefore, please try to be a bit unfriendly in sharing your data, but friendly in advising the ftp address if somebody asks you for the data. Of course I am also curious about the possible use you have of the data, so I gladly hear about your projects and results. I have described the full data base on the ftp-site you are entering, and compared it to other available data, in U.G.Jørgensen, “Cool Star Models”, In: E.F.vanDishoeck (ed.), *Molecules in Astrophysics: Probes and Processes* (IAU Symp. 178), Kluwer, 1997, p.441–456.

The line strength data,  $s_0$ , on the original list (called the ATLAS tape by the authors) that was distributed through many years by F.Querci, were multiplied with an isotopic factor as described in QQK and QQT in order to fit specific needs (0.5 for <sup>12</sup>C<sup>13</sup>C and 1/16 for <sup>13</sup>C<sup>13</sup>C). This factor has been removed in the present version of the list. Now you therefore multiply directly with the isotopic ratio that applies to your specific purpose. The  $s_0$  values were converted in the present version from units of cm/g first to cm/mol and then further on to the unit-less  $gf$ -values, by multiplying the original  $s_0$  values first with respectively 24, 25, or 26 g/mol and then with  $mc^2/N_A\pi e^2 = 1.875717 \cdot 10^{-12}$ . At some places in QQK the units of  $s_0$  was mentioned as cm/g of stellar material, but we are convinced that the listing was actually in units of cm/g of absorber (i.e., C<sub>2</sub> in this case).

The present C<sub>2</sub> line list contain data for 360,887 spectral lines from <sup>12</sup>C<sub>2</sub>, <sup>12</sup>C<sup>13</sup>C, and <sup>13</sup>C<sub>2</sub>. The data is in the file c2\_querci.dat. Each line in the file contain a listing of wavenumber [cm<sup>-1</sup>],  $gf$ -value [no units], excitation energy [cm<sup>-1</sup>], and isotope identification [1~<sup>12</sup>C<sub>2</sub>, 2~<sup>12</sup>C<sup>13</sup>C, and 3~<sup>13</sup>C<sub>2</sub>], written in the format f9.2, 1pe12.5, 0pf9.2, i2 (but the information can be read in free format from the file). The spectral lines are ordered by increasing wavenumber.

QQK writes that the line data are consistent with the use of the partition functions due to Tatum, described in Tatum 1967, ApJS 124, 21. Tatum’s partition functions are

tabulated in Tatum 1966, Publ.Domin.Astrophys.Obs., vol.13, p.1. For convenience I list below a typing of Tatum's  $C_2$  partition function for each 500 K, which can be used together with the present  $C_2$  line data. The rotational part of the partition function is calculated as  $Q_{rot} = kT/\sigma hc$ , where the symmetry factor,  $\sigma$ , is listed by Tatum to be 2 for homonuclear molecules and 1 for heteronuclear molecules. Since presumably it is the  $^{12}C^{12}C$  partition function which is listed in Tatum (1966), this partition function is also valid for  $^{13}C^{13}C$  according to Tatum's arguments, while it should be multiplied with 2 for  $^{12}C^{13}C$  according to these considerations. However, Tatum's arguments for reaching these factors 1 and 2 for  $\sigma$  seems over-simplified compared to the factors computed for example in Herzberg's text books (e.g., Molecular Spectra and Molecular Structure, vol.I, p.133 *ff*), where the factors not only depends on whether the molecule is homonuclear or heteronuclear, but also (via the nuclear spin statistical weights) on the total nuclear spin of the atoms which are 0 for  $^{12}C$  and 1/2 for  $^{13}C$ . If the rotational partition function is calculated as  $Q_{rot} = \sum g_{J''}(2J''+1)\exp(-E_{rot}/T)$ , the nuclear spin statistical weights,  $g_{J''}$ , enter the rotational partition function and give rise to the statistical weight  $\sigma$ . The nuclear spin statistical weights are  $g_{J''} = 0$  and 1 for  $^{12}C_2$ , 1 and 3 for  $^{13}C_2$ , and 2 and 2 for  $^{12}C^{13}C$  for alternating rotational levels. Consequently, I interpret Herzberg's calculations such that  $1/\sigma$  is 4 times smaller for  $^{12}C_2$  than for any of the two other molecules ( $1/\sigma = 1/2, 2, 2$ , for  $^{12}C_2, ^{13}C_2$ , and  $^{12}C^{13}C$ , respectively).

It is unfortunately not obvious whether the statistical weights are included as above into the  $s_0$  values listed on the original ATLAS tape (which does not list the quantum numbers of the individual lines). Assuming that they are, then the partition function listed by Tatum (1966) (which includes the factor  $1/\sigma = 1/2$  on the rotational part of the partition function) should be adopted directly for  $^{12}C_2$ , and should be multiplied by 4 both for  $^{13}C_2$  and for  $^{12}C^{13}C$ . In order to make it possible to use the same partition function for all the lines (isotopes) on the line list, I have therefore divided the derived  $gf$ -values for all  $^{12}C^{13}C$  and  $^{13}C^{13}C$  lines with 4, while the  $^{12}C^{12}C$  values are unchanged. In this way the partition function from Tatum (1966) (listed below) is in my opinion valid for all lines on the list. Note, however, that this interpretation is in contradiction with the opinion listed in QQK, QQT, and Tatum (1966). You can of course reach the original values by multiplying the  $gf$ -values with 4 for the two rare isotopic combinations.

There exist, to my knowledge, only two other compilations of  $C_2$  line data. One is due to R.F.Kurucz (referred to in several of Kurucz papers and reviews, for example in Kurucz 1994, "Molecules in the Stellar Environment, ed. U.G.Jørgensen, p.282, Springer LNP vol 428). The other is the more recent compilation by D.Goorvitch (1990, ApJS 74, 769; G90). Goorvitch's compilation is only for the Ballik-Ramsay system around  $2\mu m$ . There is quite a large difference between the results of QQK and G90, the integrated band strength of the compilation of Goorvitch being about a factor of 20 smaller than that of QQK in the region covered by G90. The results of Kurucz are in good agreement with the results of QQK in the visual region, but long-ward of  $\approx 1.5\mu m$  the integrated absorption coefficients diverge from one another. In the region of the Ballik-Ramsay transitions, Kurucz' results are in between the results of QQK and those of G90, but

Table 1: Partition functions for C<sub>2</sub> from Tatum (1966).

Temperature	Q <sub>Tatum66</sub>	Temperature	Q <sub>Tatum66</sub>
1000.	799.6	1500.	1721.
2000.	2984.	2500.	4627.
3000.	6693.	3500.	9231.
4000.	12290.	4500.	15910.
5000.	20150.	5500.	25070.
6000.	30700.	6500.	37100.
7000.	44330.	7500.	52440.
8000.	61480.		

closer to the values of G90 than to those of QQK.

It is of course tempting to try to take advantage of the complete wavelength cover of the QQK list (the present list) together with the likely higher accuracy of G90 in the smaller spectral region it covers. One simple compromise (which I have used in some cases) between the 3 data sets, is to adopt the QQK list short-ward of 1.15 $\mu$ m, while long-ward of 1.5 $\mu$ m divide the *gf*-values with 10 (and in between divide with a linearly increasing factor from 1 to 10). The most likely reason for the big discrepancy between the 3 lists in the infrared region, is different adopted values of the rather uncertain electronic *f*-values for the corresponding electronic systems. Unfortunately, the original line lists were constructed in such a way that it is not possible to compare the *f*-values that were used.