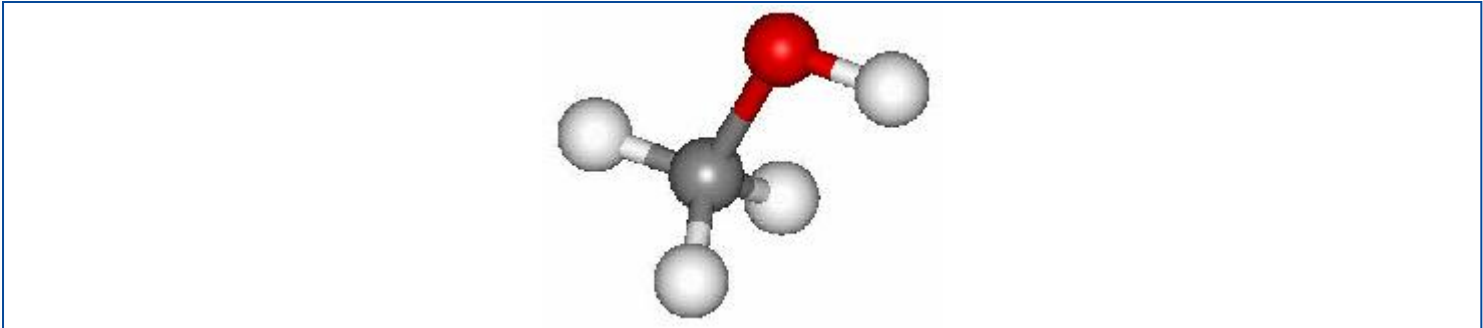


CH₃OH, $v_t = 0 - 2$

Methanol, $v_t = 0 - 2$



Species tag	032504
Version	3*
Date of Entry	May 2016
Contributors	L.-H. Xu C. P. Endres H. S. P. Müller

Please read this documentation carefully. This entry is a new calculation, trying to avoid various intensity issues. Caveats and suggestions for dealing with maser or low energy lines will be given toward the end. The third version of the methanol entry has been extended considerably in J , K , v_t , and in frequency. The entry is based on

(1) L.-H. Xu, J. Fisher, R. M. Lees, H. Y. Shi, J. T. Hougen, J. C. Pearson, B. J. Drouin, G. A. Blake, R. Braakman, 2008, *J. Mol. Spectrosc.* **251**, 305.

Details on the RAM (RHO axis method) and fitting program employed to reduce the data is available in

(2) L.-H. Xu and J. T. Hougen, 1995, *J. Mol. Spectrosc.* **169**, 396 and

(3) L.-H. Xu and J. T. Hougen, 1995, *J. Mol. Spectrosc.* **173**, 540 and references therein.

These three papers also give details on the extensive data sets considered in the fits. Because of the internal rotation (torsion), torsion-rotation interaction, and large effects of centrifugal distortion, global modeling of the methanol spectrum is a challenging task. The input data are original data from (1) to a large extent. Important additional sources are

(4) R. M. Lees and J. G. Baker, 1968, *J. Chem. Phys.* **48**, 5299;

(5) H. M. Pickett, E. A. Cohen, D. E. Brinza, M. M. Schaefer, 1981, *J. Mol. Spectrosc.* **89**, 542;

(6) K. V. L. N. Sastry, R. M. Lees, F. C. De Lucia, 1984, *J. Mol. Spectrosc.* **103**, 486;

(7) E. Herbst, J. K. Messer, F. C. De Lucia, P. Helminger, 1984, *J. Mol. Spectrosc.* **108**, 42;

(8) T. Anderson, F. C. De Lucia, E. Herbst, 1990, *Astrophys. J. Suppl. Ser.* **72**, 797;

(9) F. Matsushima, K. M. Evenson, L. R. Zink, 1994, *J. Mol. Spectrosc.* **164**, 517;

(10) H. Odashima, F. Matsushima, K. Nagai, S. Tsunekawa, K. Takagi, 1995, *J. Mol. Spectrosc.* **173**, 404;

(11) S. P. Belov, G. Winnewisser, E. Herbst, 1995, *J. Mol. Spectrosc.* **174**, 253;

(12) S. Tsunekawa, T. Ukai, A. Toyama, K. Takagi, 1995, *University of Toyama Methanol Atlas*, online available;

(13) H. S. P. Müller, K. Menten, and H. Mäder, 2004, *Astron. Astrophys.* **428**, 1019.

Full line by line references are available via the VAMDC version of the CDMS.

In order to achieve a balanced fit, small experimental uncertainties have been set to 50 kHz for most of the microwave lines in the fit.

Certain prediction, in particular those of higher J , may be found outside three times the uncertainties. However, because of the large body of transitions observed by FTFIR spectroscopy, it is expected that these deviations are within 6 MHz, an uncertainty value assigned to the FTFIR data).

Please note: No experimental lines have been merged in the present entry. On average, the entry is expected to be much better than the previous one. However, the reproduction of some low energy transitions, important for studies of dark clouds or methanol maser sources, may be better in the previous version. We recommend to inspect both entries for studies of dark clouds or methanol masers. In addition we recommend to inspect the experimental microwave and millimeter-wave transition frequencies, which have not been merged, but are available in a [line file](#). The coding of the [references](#) is also given.

It contains data with uncertainties small enough for these purposes. This refers especially to data from (13), including cited data. In addition, we list very recent data from

(14) L. H. Coudert, C. Gutlé, T. R. Huet, J.-U. Grabow, and S. A. Levshakov, 2015, *J. Chem. Phys.* **143**, Art. No. 044304.

Also listed are transition frequencies from astronomical observations. As space and time variability of these frequencies turned out to be negligible with respect to the reported uncertainties, we do recommend using these as well. They were published by

(15) M. A. Voronkov, K. J. Brooks, A. M. Sobolev, S. P. Ellingsen, A. B. Ostrovskii, J. L. Caswell, 2006, *Mon. Not. R. Astron. Soc.* **373**, 411;

(16) M. A. Voronkov, A. J. Walsh, J. L. Caswell, S. P. Ellingsen, S. L. Breen, S. N. Longmore, C. R. Purcell, J. S. Urquhart, 2011, *Mon. Not. R. Astron. Soc.* **413**, 2339;

(17) M. A. Voronkov, J. L. Caswell, S. P. Ellingsen, J. A. Green, S. L. Breen, 2014, *Mon. Not. R. Astron. Soc.* **439**, 2584.

State numbers 0, 3, and 6 refer to lines with A symmetry with $v_t = 0, 1$, and 2; state numbers 1, 4, and 7 refer to lines with E symmetry with $K_a \geq 0$ and with $v_t = 0, 1$, and 2; state numbers 2, 5, and 8 refer to lines with E symmetry with $K_a < 0$ and with $v_t = 0, 1$, and 2. Please note that parities of the A state lines can be extracted from a [catalog file with 5 quantum numbers](#). The 5th quantum number is the parity for A states only, i.e., having state numbers 0, 3, and 6.

Lower state energies are given referenced to the $J = K = 0$, A , $v_t = 0$ level, which is about 127 cm⁻¹ above the bottom of the torsional potential well. The energies given in the documentation refer to the 0₀₀ rotational levels of the $v_t = 0$, A and E states, the $v_t = 1$, E and A states, and the $v_t = 2$, A and E states, respectively.

The partition function considers states with $v_t \leq 3$, $J \leq 44$, and $K \leq 20$. The K levels are sufficient well beyond 300 K, the vibrational and J levels are about sufficient at 300 K.

The dipole moment values were taken from

(18) E. V. Ivash, PhD thesis, University of Michigan, 1952.

Note: The current entry takes into account contributions of the permanent dipole moment **only** ! Torsional or rotational dependences as well as changes in the dipole moment with torsional state have not yet been determined – or only to an insufficient amount. The effects of these contributions may be non-negligible in certain instances, but should be usually rather small.

Lines Listed	38643
Frequency / GHz	< 3000
Max. J	40
log STR0	
log STR1	
Isotope Corr.	-0.000
Egy / cm ⁻¹	0.000 / 9.122 / 208.912 / 294.451 / 353.518 / 510.320
μ_a / D	0.899
μ_b / D	-1.44
μ_c / D	
A / MHz	127523.4
B / MHz	24692.5
C / MHz	23760.3
Q(1000.)	347799.0417
Q(500.0)	102146.4089
Q(300.0)	37027.3292
Q(225.0)	20991.8100
Q(150.0)	9750.0398
Q(75.00)	2924.3023
Q(37.50)	920.9637
Q(18.75)	274.9880
Q(9.375)	78.1736
Q(5.000)	26.7190
Q(2.725)	11.8899
detected in ISM/CSM	yes

