Species Tag:	18003	Name:		H_2O
Version:	7			Water
Date:	September 2012			ground state
Contributor:	L.H. Coudert			
	S. Yu			
	J.C. Pearson			
Lines Listed:	1376	Q(300.0)=		178.122
Freq. (GHz) <	10 000	Q(225.0)=		116.021
Max. J:	27	Q(150.0)=		63.678
LOGSTR0=	-20	Q(75.00)=		23.170
LOGSTR1=	-20	Q(37.50)=		8.580
Isotope Corr.:	0.0	Q(18.75)=		3.033
Egy. $(cm^{-1}) >$	0.0	Q(9.375)=		1.257
$\mu_a =$		A=		835840.3
$\mu_b =$	1.8546	B=		435351.7
$\mu_c =$		C=		278138.7

This catalog entry represents pure rotation transitions in the ground state only. The frequency analysis includes the ground state and first four excited vibrations and was based on S. Yu, J.C. Pearson, B.J. Drouin, M.-A. Martin-Drumel, O. Pirali, M. Vervloet, L.H. Coudert, H.S.P. Muller and S. Brunken, J. Mol. Spectrosc. 279 (2012) 16-25. The H_2O data set consists of three different types of data: microwave transitions, rotational energy levels, FIR and IR lines recorded using high-resolution techniques. The fit results in a reduced RMS of 1.06 obtained for a combination of the the five states. The following 15 344 data with the maximum J-value of 27 were introduced in a weighted least-squares fit procedure in which each data point was given a weight equal to the inverse of its experimental uncertainty squared:

(a) 642 microwave transitions from

(1) S. Golden, T. Wentink, R. Hillger, M. W. P. Strandberg, Phys. Rev. 73 (1948) 92-93.
(2) W. C. King, W. Gordy, Phys. Rev. 93 (1954) 407-412.
(3) M. Lichtenstein, V. E. Derr, J. J. Gallagher, J. Mol. Spectrosc. 20 (1966) 391-401.
(4) L. Frenkel, T. Sullivan, M. A. Pollack, T. J. Bridges, Appl. Phys. Lett. 11 (1967) 344-345.
(5) M. A. Pollack, L. Frenkel, T. Sullivan, Phys. Lett. A 26 (1968) 381-382.
(6) W. Benedict, M. Pollack, W. Tomlinson, III, IEEE J. Quant. Electronics 5 (1969) 108-124.
(7) S. G. Kukolich, J. Chem. Phys. 50 (1969) 3751-3755.
(8) K. M. Evenson, J. S. Wells, L. M. Matarrese, L. B. Elwell, Appl. Phys. Lett. 16 (1970) 159-162.
(9) G. Steenbeckeliers, J. Bellet, C. R. Acad. Sci. B 273 (1971) 471-474.
(10) C. Huiszoon, Rev. Sci. Instrum. 42 (1971) 477-481.
(11) R. S. Winton, Ph. D. Thesis, Duke University (1972).

(12) F. C. De Lucia, P. Helminger, R. L. Cook, W. Gordy, Phys. Rev. A 5 (1972) 487-490.

(13) T. G. Blaney, C. C. Bradley, G. J. Edwards, D. J. E. Knight, Phys. Lett. A 43 (1973) 471-472.

(14) M. Herman, J. W. C. Johns, A. R. W. McKellar, Can. J. Phys. 57 (1979) 397-401.

(15) H. Kuze, Astrophys. J. 239 (1980) 1131-1133.

(16) A. V. Burenin, T. M. Fevral'skikh, E. N. Karyakin, O. L. Polyansky, S. M. Shapin,J. Mol. Spectrosc. 100 (1983) 182-192.

(17) P. Helminger, J. K. Messer, F. C. De Lucia, Appl. Phys. Lett. 42 (1983) 309-310.

(18) O. I. Baskakov, V. A. Alekseev, E. A. Alekseev, B. I. Pelevoi, Opt. Spectrosk, 63 (1987) 1016-1018.

(19) S. P. Belov, I. N. Kozin, O. L. Polyansky, M. Yu. Tret'yakov, N. F. Zobov, J. Mol. Spectrosc. 126 (1987) 113-117.

(20) J. C. Pearson, T. Anderson, E. Herbst, F. C. De Lucia, P. Helminger, Astrophys. J. 379 (1991) L41-L43.

(21) T. Amano, Flavio Scappini, Chem. Phys. Lett. 182 (1991) 93-95.

(22) J. C. Pearson, Ph. D. Thesis, Duke University (1995).

(23) F. Matsushima, H. Odashima, T. Iwasaki, S. Tsunekawa, K. Takagi, J. Mol. Struct. 352/353 (1995) 371-378.

(24) P. De Natale, L. Lorini, M. Inguscio, I. G. Nolt, J. H. Park, G. Di Lonardo, L. Fusina, P. A. R. Ade, A. G. Murray, Appl. Opt. 33 (1997) 8526-8532.

(25) K. V. Chance, K. Park, K. M. Evenson, J. Quant. Spectrosc. Radiat. Tansfer 59 (1998) 687-688.

(26) G. Yu. Golubiatnikov, J. Mol. Spectrosc. 230 (2005) 196-198.

(27) F. Matsushima, N. Tomatsu, T. Nagai, Y. Moriwaki, K. Takagi, J. Mol. Spectrosc. 235 (2006) 191-199.

(28) G. Yu. Golubiatnikov, V. N. Markov, A. Guarnieri, R. Knöchel, J. Mol. Spectrosc. 240 (2006) 251-254.

(29) G. Cazzoli, C. Puzzarini, M. E. Harding, Jürgen Gauss, Chem. Phys. Lett. 473 (2009) 21-25.

(30) G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini, J. Quant. Spectrosc. Radiat. Tansfer 110 (2009) 609-618.

(31) Yu et al., J. Mol. Spectrosc. 279 (2012) 16-25.

    (b) 2169 rotational energy levels from

(1) R. Lanquetin, L. H. Coudert, C. Camy-Peyret, J. Mol. Spectrosc. 206 (2001) 83-103.

    (c) 12 728 FIR and IR transitions from

(1) J. Kauppinen, K. Jolma, V.-M. Horneman, Appl. Opt. 21 (1982) 3332-3336.

(2) J. W. C. Johns, J. Opt. Soc. Am. B 8 (1985)1340-1354.

(3) V. Dana, J.-Y. Mandin, C. Camy-Peyret, J.-M. Flaud, J.-P. Chevillard, R. L. Hawkins, J.-L. Delfau, Appl. Opt. 31 (1992) 1928-1936.

(4) R. A. Toth, J. Opt. Soc. Am. B 10 (1993) 1526-1544.

(5) R. A. Toth, J. Opt. Soc. Am. B 10 (1993) 2006-2029.

(6) R. Paso, V.-M. Horneman, J. Opt. Soc. Am. B 12 (1995) 1813-1838.

(7) S. N. Mikhailenko, Vl. G. Tyuterev, K. A. Kepler, B. P. Winnewisser, M. Winnewisser, G. Mellau, S. Klee, K. Narahari Rao, J. Mol. Spectrosc. 184 (1997) 330-349.

(8) R. A. Toth, J. Mol. Spectrosc. 190 (1998) 379-396.

(9) R. A. Toth, J. Mol. Spectrosc. 194 (1999) 28-42.

(10) S. N. Mikhailenko, Vl. G. Tyuterev, V. I. Starikov, K. K. Albert, B. P. Winnewisser, M. Winnewisser, G. Mellau, C. Camy-Peyret, R. Lanquetin, J.-M. Flaud, J. W. Brault, J. Mol. Spectrosc. 213 (2002) 91-121.

(11) V.-M. Horneman, R. Anttila,J. Pietilä, S. Alanko, M. Koivusaari, J. Mol. Spectrosc. 229 (2005) 89-107.

(12) L. H. Coudert, O. Pirali, M. Vervloet, R. Lanquetin, C. Camy-Peyret, J. Mol. Spectrosc. 228 (2004) 471-498.

(13) O. L. Polyansky, J. R. Busler, B. Guo, K. Zhang, P. F. Bernath, J. Mol. Spectrosc. 176 (1996) 305-315.

(14) O. L. Polyansky, J. Tennyson, P. F. Bernath, J. Mol. Spectrosc. 186 (1997) 213-221.

(15) O. L. Polyansky, N. F. Zobov, S. Viti, J. Tennyson, P. F. Bernath, L. Wallace, J. Mol. Spectrosc. 186 (1997) 422-427.

(16) O. L. Polyansky, personal communication (1997).

(17) M. P. Esplin, R. B. Watson, M. L. Hokes, L. S. Rothman, J. Quant. Spectrosc. Radiat. Transfer 60 (1998) 711-739.

(18) N. F. Zobov, O. L. Polyansky, J. Tennyson, J. A. Lotoski, P. Colarusso, K.-Q. Zhang, P. F. Bernath, J. Mol. Spectrosc. 193 (1999) 118-136.

(19) N. F. Zobov, O. L. Polyansky, J. Tennyson, S. V. Shirin, R. Nassar, T. Hirao, T. Imajo, P. F. Bernath, L. Wallace, Astrophys. J. 530 (2000) 994-998.

(20) P.-F. Coheur, P. F. Bernath, M. C. Carleer, R. Colin, O. L. Polyansky, N. F. Zobov, S. V. Shirin, R. J. Barber, J. Tennyson, J. Chem. Phys. 122 (2005) 074307.

(21) Yu et al., J. Mol. Spectrosc. (2012), http://dx.doi.org/10.1016/j.jms.2012.07.011.

In this version, the line intensity calculation is slightly more complicated than in the case of a rigid molecule because the current approach treats the bending ν_2 mode as a large amplitude motion parameterized by the large amplitude coordinate $t = \cos(\theta)$, where θ is the bending angle. For this reason, a dipole moment value corresponding to the equilibrium configuration was not used. Instead, the dipole moment function was written as an expansion in terms of the large amplitude corrdinate t. The reader is referred to the following two papers for details:

(1) L. H. Coudert, J. Molec. Spectrosc. 181 (1997) 246-273.

(2) L. H. Coudert, G. Wagner, M. Birk, Yu. I. Baranov, W. J. Lafferty, and J.-M. Flaud, J. Molec. Spectrosc. 251 (2008) 339-357.

Details on the intensities validation can be found in Yu et al. J. Mol. Spectrosc. 279 (2012) 16-25.