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Einstein A-coefficients for pure rotational transitions in D_2O

SURESH CHANDRA, D A VARSHALOVICH* and
W H KEGEL**

Department of Physics, University of Gorakhpur, Gorakhpur 273 001, India
*Ioffe Physical-Technical Institute of the Academy of Sciences of the USSR, Leningrad, USSR
**Institut für Theoretische Physik der Universität Frankfurt/Main Robert-Mayer-Str. 10, D 6000 Frankfurt/Main, FRG

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Abstract. Einstein A-coefficients for the electric-dipole transitions between the rotational levels up to 785 cm^{-1} in the ground vibrational state of D_2O are calculated. The A-values are used to compute the mean-radiative life-times of the levels.

Keywords. Heavy water; Einstein A-coefficients; rotational spectra.

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1. Introduction

Heavy water has been a subject of extensive investigation. For example, Benedict *et al* (1970) and Steenbeckliers and Bellet (1973) calculated the rotational constants for ground vibrational state, while Clough *et al* (1973) computed the electric dipole moment from Stark measurements. Gupta (1981a, b) analyzed the high-resolution rotation-vibration spectra of D_2O. Recently, it has been utilized in laboratory laser (Behn *et al* 1983). It is quite likely that it may be used in laboratory masers also. Further, since the universe is much more stranger than one can think, D_2O might be found in the interstellar molecular clouds as, besides H_2O, HDO has already been observed in astronomical objects (Chandra *et al* 1984a). Therefore, it would be worthwhile to understand the Einstein A-coefficients, and the mean-radiative life-times of energy levels.

By using the molecular data reported by Gupta (1981a, b), we have calculated the Einstein A-coefficients for electric-dipole transitions between the rotational levels up to 785 cm^{-1} in the ground vibrational (000) state. The A-values are used to compute the mean-radiative life-times of levels.

2. Molecular details

D_2O is a *b*-type asymmetric rotor with dipole moment $\mu = 1{\cdot}8558$ Debye (Clough *et al* 1973) and rotational constants A, B and C equal to 15·41970 cm^{-1}, 7·27265 cm^{-1} and 4·84538 cm^{-1} respectively (Gupta 1981a, b). Theoretical details for *b*-type rotors have

Table 1. Einstein A-coefficients for the transitions even, odd ↔ odd, even.

J'	τ'	J	τ	A (sec^{-1})	J'	τ'	J	τ	A (sec^{-1})	J'	τ'	J	τ	A (sec^{-1})
1	1	1	−1	6·3720D−4	2	−1	1	−1	8·7071D−3	2	1	1	1	4·2961D−2
2	1	2	−1	5·6836D−3	3	−3	2	−1	5·6939D−3	3	−1	2	1	1·4719D−4
3	1	2	−1	5·6101D−2	3	3	2	1	2·1163D−1	3	−1	3	−3	2·3651D−3
3	1	3	−1	4·6159D−3	3	3	3	−3	1·1691D−3	3	3	3	1	1·4033D−2
4	−3	3	−3	3·6138D−2	4	−3	3	1	2·5088D−6	4	−1	3	−1	7·7250D−2
4	−1	3	3	4·8245D−8	4	1	3	−3	1·0622D−2	4	1	3	1	2·3427D−1
4	3	3	−1	1·7495D−3	4	3	3	3	5·8728D−1	4	−1	4	−3	1·3392D−2
4	1	4	−1	2·3720D−2	4	3	4	−3	3·8635D−4	4	3	4	1	3·2037D−2
4	1	5	−5	6·4869D−5	4	3	5	−3	3·6031D−5	4	3	5	1	6·8472D−10
5	−5	4	−3	5·1052D−2	5	−3	4	−1	1·3911D−2	5	−1	4	−3	7·1486D−2
5	−1	4	1	5·2844D−4	5	1	4	−1	2·7894D−1	5	3	4	−3	3·4527D−3
5	3	4	1	6·4334D−1	5	5	4	−1	1·5961D−3	5	5	4	3	1·2472
5	−3	5	−5	9·9505D−3	5	−1	5	−3	6·8319D−3	5	1	5	−5	6·7065D−3
5	1	5	−1	1·8100D−2	5	3	5	−3	3·5927D−3	5	3	5	1	4·6288D−2
5	5	5	−5	3·6708D−5	5	5	5	−1	5·7577D−4	5	5	5	3	5·4113D−2
5	3	6	−5	5·6680D−5	5	5	6	−3	2·7876D−5	5	5	6	1	2·2937D−6
6	−5	5	−5	1·0617D−1	6	−5	5	−1	2·3687D−7	6	−3	5	−3	1·4064D−1
6	−3	5	1	2·1908D−4	6	−1	5	−5	4·8224D−2	6	−1	5	−1	2·8475D−1
6	−1	5	3	2·4767D−5	6	1	5	−3	2·7195D−2	6	1	5	1	6·9058D−1
6	3	5	−5	3·4167D−4	6	3	5	−1	6·7202D−3	6	3	5	3	1·3289
6	5	5	−3	3·2899D−5	6	5	5	1	1·9304D−3	6	5	5	5	2·2473
6	−3	6	−5	2·6759D−2	6	−1	6	−3	3·8118D−2	6	1	6	−5	2·3887D−3
6	1	6	−1	6·0348D−2	6	3	6	−3	1·9518D−3	6	3	6	1	8·6103D−2
6	5	6	−5	3·5894D−6	6	5	6	−1	5·3859D−4	6	5	6	3	8·0696D−2
6	−1	7	−7	8·5928D−5	6	1	7	−5	1·0715D−4	6	3	7	−7	1·2311D−5
6	3	7	−3	8·4450D−5	6	5	7	−5	2·8681D−6	6	5	7	−1	2·4428D−5
6	5	7	3	7·2977D−6	7	−7	6	−5	1·5999D−1	7	−5	6	−3	1·0559D−1
7	−3	6	−5	8·1288D−2	7	−3	6	−1	1·8593D−2	7	−1	6	−3	3·1498D−1
7	−1	6	1	1·0456D−3	7	1	6	−5	1·0987D−2	7	1	6	−1	7·7280D−1

7	1	6	3	6·7886D−6	7	3	6	−3	1·3659D−2	7	3	6	1	1·4294
7	5	6	−5	3·5887D−5	7	5	6	−1	6·9557D−3	7	5	6	3	2·3641
7	7	6	−3	7·8986D−6	7	7	6	1	2·2133D−3	7	7	6	5	3·6302
7	−5	7	−7	2·9560D−2	7	−3	7	−5	1·7260D−2	7	−1	7	−7	8·8577D−3
7	−1	7	−3	1·7438D−2	7	1	7	−5	1·7909D−2	7	1	7	−1	5·0905D−2
7	3	7	−7	3·8206D−4	7	3	7	−3	6·7258D−3	7	3	7	1	1·0385D−1
7	5	7	−5	1·6320D−4	7	5	7	−1	2·0570D−3	7	5	7	3	1·3239D−1
7	7	7	−7	2·3967D−7	7	7	7	−3	8·1570D−6	7	7	7	1	5·1821D−4
7	7	7	5	1·0997D−1	7	−3	8	−7	6·6005D−6	7	1	8	−7	1·1971D−4
7	3	8	−5	1·6426D−4	7	5	8	−7	1·5942D−6	7	5	8	−3	9·1867D−5
7	7	8	−5	4·3199D−7	7	7	8	−1	2·3311D−5	7	7	8	3	1·2482D−5
8	−7	7	−7	2·4692D−1	8	−5	7	−5	2·6726D−1	8	−5	7	−1	3·0131D−4
8	−3	7	−7	8·9974D−2	8	−3	7	−3	3·6484D−1	8	−3	7	1	1·1953D−3
8	−1	7	−5	1·2658D−1	8	−1	7	−1	7·5273D−1	8	−1	7	3	1·8418D−4
8	1	7	−7	1·7219D−3	8	1	7	−3	4·6077D−2	8	1	7	1	1·5146
8	1	7	5	1·7636D−7	8	3	7	−5	1·0772D−3	8	3	7	−1	1·6894D−2
8	3	7	3	2·5033	8	−5	8	−7	4·9128D−2	8	−3	8	−5	6·1168D−2
8	−1	8	−7	4·6496D−3	8	−1	8	−3	7·9947D−2	8	1	8	−5	7·8355D−3
8	1	8	−1	1·2155D−1	8	3	8	−7	4·5336D−5	8	3	8	−3	5·0596D−3
8	3	8	1	1·6797D−1	8	−3	9	−9	1·2558D−4	8	−1	9	−7	8·9724D−5
8	1	9	−9	4·0643D−5	8	1	9	−5	1·6092D−4	8	3	9	−7	4·2195D−5
8	3	9	−3	1·5760D−4	9	−9	8	−7	3·4919D−1	9	−7	8	−5	3·1737D−1
9	−5	8	−7	1·0285D−1	9	−5	8	−3	1·3681D−1	9	−3	8	−5	3·1090D−1
9	−3	8	−1	2·0168D−2	9	−1	8	−7	1·3702D−2	9	−1	8	−3	8·4567D−1
9	−1	8	1	1·7967D−3	9	1	8	−5	3·9024D−2	9	1	8	−1	1·6337
9	1	8	3	8·1086D−5	9	−7	9	−9	6·0773D−2	9	−5	9	−7	4·8338D−2
9	−3	9	−9	7·0887D−3	9	−3	9	−5	2·5688D−2	9	−1	9	−7	3·1279D−2
9	−1	9	−3	4·2547D−2	9	1	9	−9	9·0813D−4	9	1	9	−5	2·8885D−2
9	1	9	−1	1·1303D−1	9	−5	10	−9	7·0792D−5	9	−1	10	−9	1·3253D−4
9	1	10	−7	3·0910D−4	10	−9	9	−9	4·8196D−1	10	−7	9	−7	4·9579D−1
10	−7	9	−3	2·3166D−5	10	−5	9	−9	1·2521D−1	10	−5	9	−5	5·3216D−1
10	−5	9	−1	2·8223D−3	10	−7	10	−9	8·1397D−2	10	−5	10	−7	9·9918D−2
10	−5	11	−11	2·0206D−4	11	−11	10	−9	6·4092D−1					

Table 2. Einstein A-coefficients for the transitions odd, odd ↔ even, even.

J'	τ'	J	τ	A (sec^{-1})	J'	τ'	J	τ	A (sec^{-1})	J'	τ'	J	τ	A (sec^{-1})
1	0	0	0	2·9935D−3	2	−2	1	0	5·7769D−4	2	2	1	0	4·3866D−2
2	0	2	−2	1·1398D−3	2	2	2	0	3·8559D−3	3	−2	2	−2	1·8911D−2
3	−2	2	2	8·6517D−10	3	0	2	0	5·7499D−2	3	2	2	−2	2·2692D−3
3	2	2	2	2·0915D−1	3	0	3	−2	9·1880D−3	3	2	3	0	1·5668D−2
3	2	4	−4	3·8218D−5	4	−4	3	−2	2·1258D−2	4	−2	3	0	2·5716D−3
4	0	3	−2	6·5692D−2	4	0	3	2	7·7816D−6	4	2	3	0	2·4437D−1
4	4	3	−2	1·0155D−3	4	4	3	2	5·8805D−1	4	−2	4	−4	5·0037D−3
4	0	4	−2	5·2634D−3	4	2	4	−4	3·7577D−3	4	2	4	0	1·7925D−2
4	4	4	−2	8·1849D−4	4	4	4	2	3·1532D−2	4	4	5	−4	2·1598D−5
4	4	5	0	8·6318D−8	5	−4	4	−4	6·3975D−2	5	−4	4	0	3·0063D−6
5	−2	4	−2	1·0374D−1	5	−2	4	2	4·0117D−5	5	0	4	−4	2·6978D−2
5	0	4	0	2·5898D−1	5	2	4	−2	8·5864D−3	5	2	4	2	6·3834D−1
5	4	4	−4	6·5123D−5	5	4	4	0	1·6673D−3	5	4	4	4	1·2471
5	−2	5	−4	1·9091D−2	5	0	5	−2	3·0448D−2	5	2	5	−4	1·2312D−3
5	2	5	0	4·9084D−2	5	4	5	−2	5·2842D−4	5	4	5	2	5·4207D−2
5	0	6	−6	7·6342D−5	5	2	6	−4	8·5063D−5	5	4	6	−6	3·3331D−6
5	4	6	−2	2·7721D−5	5	4	6	2	2·0331D−6	6	−6	5	−4	9·6730D−2
6	−4	5	−2	4·5043D−2	6	−2	5	−4	7·5761D−2	6	--2	5	0	4·3455D−3
6	0	5	−2	3·0465D−1	6	0	5	2	7·0584D−5	6	2	5	−4	7·1192D−3
6	2	5	0	7·0840D−1	6	4	5	−2	5·8296D−3	6	4	5	2	1·3302
6	6	5	−4	7·0559D−6	6	6	5	0	1·9369D−3	6	6	5	4	2·2473
6	−4	6	−6	1·8043D−2	6	−2	6	−4	1·0353D−2	6	0	6	−6	8·5855D−3
6	0	6	−2	1·7363D−2	6	2	6	−4	9·4233D−3	6	2	6	0	5·1723D−2
6	4	6	−6	1·6090D−4	6	4	6	−2	2·4279D−3	6	4	6	2	8·5397D−2
6	6	6	−4	2·4066D−5	6	6	6	0	5·3045D−4	6	6	6	4	8·0682D−2
6	−2	7	−6	2·1407D−7	6	2	7	−6	9·2300D−5	6	4	7	−4	8·7165D−5
6	6	7	−6	3·6275D−7	6	6	7	−2	2·6387D−5	6	6	7	2	7·3704D−6
7	−6	6	−6	1·6614D−1	7	−4	6	−4	1·9330D−1	7	−4	6	0	3·7391D−4
7	−2	6	−6	6·9931D−2	7	−2	6	−2	3·1775D−1	7	−2	6	2	3·2786D−4

7	0	6	−4	6·5901D−2	7	0	6	0	7·3002D−1	7	0	6	4	4·6318D−6
7	2	6	−6	9·1798D−4	7	2	6	−2	1·8954D−2	7	2	6	2	1·4236
7	4	6	−4	2·6326D−4	7	4	6	0	6·9440D−3	7	4	6	4	2·3639
7	6	6	−6	4·2663D−7	7	6	6	−2	1·2105D−5	7	6	6	2	2·2110D−3
7	6	6	6	3·6302	7	−4	7	−6	3·6714D−2	7	−2	7	−4	4·8035D−2
7	0	7	−6	3·6036D−3	7	0	7	−2	6·9847D−2	7	2	7	−4	4·4344D−3
7	2	7	0	1·0679D−1	7	4	7	−6	1·7160D−5	7	4	7	−2	2·0837D−3
7	4	7	2	1·3252D−1	7	6	7	−4	4·0903D−6	7	6	7	0	5·2100D−4
7	6	7	4	1·0998D−1	7	−2	8	−8	1·0139D−4	7	0	8	−6	1·0091D−4
7	2	8	−8	2·5791D−5	7	2	8	−4	1·4195D−4	7	4	8	−6	1·5288D−5
7	4	8	−2	8·0844D−5	7	6	8	−8	2·7679D−8	7	6	8	−4	1·0914D−6
7	6	8	0	2·2708D−5	7	6	8	4	1·2471D−5	8	−8	7	−6	2·4321D−1
8	−6	7	−4	1·9745D−1	8	−4	7	−6	9·0055D−2	8	−4	7	−2	5·6693D−2
8	−2	7	−4	3·1362D−1	8	−2	7	0	5·6530D−3	8	0	7	−6	1·3541D−2
8	0	7	−2	8·2354D−1	8	0	7	2	2·6610D−4	8	2	7	−4	2·5220D−2
8	2	7	0	1·5339	8	2	7	4	2·1010D−7	8	4	7	−6	1·0039D−4
8	4	7	−2	1·6556D−2	8	4	7	2	2·5045	8	−6	8	−8	4·4024D−2
8	−4	8	−6	2·9356D−2	8	−2	8	−8	8·0838D−3	8	−2	8	−4	1·9707D−2
8	0	8	−6	2·6295D−2	8	0	8	−2	4·6854D−2	8	2	8	−8	6·5602D−4
8	2	8	−4	1·5138D−2	8	2	8	0	1·1275D−1	8	4	8	−6	5·5672D−4
8	4	8	−2	5·1784D−3	8	4	8	2	1·6731D−1	8	−4	9	−8	2·8773D−5
8	0	9	−8	1·3386D−4	8	2	9	−6	2·4227D−4	8	4	9	−8	3·9110D−6
8	4	9	−4	1·9170D−4	9	−8	8	−8	3·5130D−1	9	−6	8	−6	3·6697D−1
9	−6	8	−2	1·2603D−4	9	−4	8	−8	1·0821D−1	9	−4	8	−4	4·3364D−1
9	−4	8	0	2·3241D−3	9	−2	8	−6	1·9924D−1	9	−2	8	−2	7·6986D−1
9	−2	8	2	1·0590D−3	9	0	8	−8	2·5663D−3	9	0	8	−4	1·0086D−1
9	0	8	0	1·5838	9	0	8	4	7·3962D−5	9	−6	9	−8	6·4040D−2
9	−4	9	−6	7·8280D−2	9	−2	9	−8	5·4128D−3	9	−2	9	−4	9·2372D−2
9	0	9	−6	1·1710D−2	9	0	9	−2	1·3358D−1	9	−4	10	−10	1·5926D−4
9	−2	10	−8	8·8213D−5	9	0	10	−10	5·3756D−5	9	0	10	−6	1·3293D−4
10	−10	9	−8	4·8080D−1	10	−8	9	−6	4·6339D−1	10	−6	9	−8	1·1893D−1
10	−6	9	−4	2·7237D−1	10	−8	10	−10	7·9459D−2	10	−6	10	−8	7·4801D−2
10	−6	11	−10	1·3082D−4	11	−10	10	−10	6·4154D−1					

Table 3. Energies and mean-radiative life-times of levels.

J'	τ'	E (cm^{-1})	T (sec)	J'	τ'	E (cm^{-1})	T (sec)
1	−1	12·116	—	0	0	0·0	—
1	1	22·684	1·569D+3	1	0	20·259	3·341D+2
2	−1	42·069	1·148D+2	2	−2	35·878	1·731D+3
3	−3	70·447	1·756D+2	2	0	49·338	8·774D+2
2	1	73·675	2·056D+1	2	2	74·141	2·095D+1
3	−1	88·969	3·980D+2	3	−2	74·506	5·288D+1
3	1	112·249	1·647D+1	3	0	110·033	1·500D+1
4	−3	117·312	2·767D+1	4	−4	114·986	4·704D+1
3	3	156.661	4.409	4	−2	141·083	1·320D+2
4	−1	158·105	1·103D+1	3	2	156·604	4·403
5	−5	169·039	1·959D+1	4	0	164·174	1·409D+1
5	−3	204·934	4·191D+1	5	−4	170·244	1·563D+1
4	1	205·881	3·722	4	2	206·274	3·759
5	−1	229·987	1·268D+1	5	−2	217·584	8·139
6	−5	233·107	9·419	6	−6	232·523	1·034D+1
5	1	269·007	3·292	5	0	267·528	3·160
4	3	269·374	1·609	4	4	269·380	1·609
6	−3	288·092	5·966	6	−4	279·561	1·584D+1
7	−7	305·496	6·250	7	−6	305·768	6·019
5	3	331·122	1·435	6	−2	309·258	1·105D+1
6	−1	341·386	2·694	5	2	331·070	1·434
7	−5	364·043	7·399	6	0	345·442	3·024
8	−7	388·143	4·050	7	−4	369·265	4·341
7	−3	401·254	8·536	8	−8	388·020	4·112
6	1	405·281	1·281	6	2	405·529	1·287
5	5	411.543	7·671D−1	5	4	411·543	7·671D−1
7	−1	436·053	2·921	7	−2	427·196	2·293
8	−5	460·764	3·158	8	−6	457·820	4·141
9	−9	480·125	2·864	9	−8	480·181	2·847
6	3	485·593	7·022D−1	6	4	485·599	7·022D−1
7	1	492·877	1·173	7	0	492·019	1·150
8	−3	524·607	1·933	8	−4	505·040	5·678
9	−7	560·751	2·644	8	−2	540·873	2·881
7	3	572·162	6·434D−1	9	−6	562·315	2·319
10	−9	581·847	2·075	7	2	572·128	6·431D−1
6	5	582·412	4·291D−1	10	−10	581·823	2·080
8	−1	591·217	1·037	6	6	582·412	4·291D−1
9	−5	619·552	3·471	8	0	593·583	1·098
9	−3	659·406	2·748	9	−4	633·214	1·606
7	5	668·849	3·991D−1	7	4	668·848	3·991D−1
8	1	671·193	5·910D−1	8	2	671·334	5·925D−1
10	−7	673·714	1·732	10	−8	672·915	1·842
11	−11	693·108	1·560	11	−10	693·120	1·559
9	−1	708·166	1·069	9	−2	702·702	9·363D−1
10	−5	752·607	1·315	10	−6	743·793	2·145
8	3	767·710	3·711D−1	8	4	767·714	3·711D−1
7	7	781·170	2·672D−1	7	6	781·170	2·672D−1
9	1	783·269	5·507D−1	9	0	782·810	5·456D−1

Table 4. $A/\mu^2\nu^3$ values for some H_2O and D_2O lines.

	$A/\mu^2\nu^3$ (sec^{-1} $Debye^{-2}$ GHz^{-3})	
Transition	H_2O	D_2O
$6_{-5} \rightarrow 5_{-1}$	$4.908\ 10^{-14}$	$8.405\ 10^{-14}$
$4_{-3} \rightarrow 3_1$	$1.583\ 10^{-13}$	$2.083\ 10^{-13}$
$4_{-1} \rightarrow 3_3$	$1.702\ 10^{-13}$	$1.727\ 10^{-13}$
$3_{-2} \rightarrow 2_2$	$1.688\ 10^{-13}$	$1.917\ 10^{-13}$
$5_{-4} \rightarrow 4_0$	$9.416\ 10^{-14}$	$1.449\ 10^{-13}$

been discussed earlier (Allen and Cross 1963; Gordy and Cook 1970; Chandra *et al* 1984b). The formulae for line-strength, Einstein A-coefficient and mean-radiative life-time are same as those used by Chandra *et al* (1984b).

3. Results and discussion

The Einstein A-values are calculated and reported in tables 1 and 2. The A-values are used to calculate the mean-radiative life-times of levels, which are given in table 3.

The results reported here may be used in spectroscopic/astronomical studies and for laboratory masers. The spectral resolution of Fourier transform spectrometer (Kitt Peak National Observatory, Tucson) used by Gupta (1981a, b) was better than $0.02\ cm^{-1}$, which is superior to previous measurements. Hence, the present data are reliable. In table 4, we have given the values of parameter $A/\mu^2\nu^3$ for some lines of H_2O and D_2O. A comparison shows that the lines from D_2O are more intense than those from H_2O.

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