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The VoTe room temperature $H_2{}^{16}O$ line list up to 25000 cm^{-1}

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ABSTRACT

A preliminary version of the line list of dipole-allowed transition of the water molecule is presented. The line lists is created on the basis of VoTe calculations (Voronin, Tennyson et al. in preparation). The cut-of values used for this line list are:25000 cm^{-1} in wavenmumber and 10^{-30} cm/molecule at T=296 K in intensity. Calculated line-lists are available on the site ftp://ftp.iao.ru/pub/VTT/VoTe/.

Keywords: $H_2{}^{16}O$, VoTe, line list, water vapour

1. INTRODUCTION

The role of water vapor on Earth and in the Universe is unique. In particular, $H_2{}^{16}O$ is the dominant absorber of both incoming and outgoing radiation in the Earth's atmosphere As a result water is molecule number in both the HITRAN[1] and GEISA[2] atmospheric databases. On Earth, water contains a number of isotopologues, but $H_2{}^{16}O$ has the major abundance of about 99.7317%. For these reasons water vapor is the object of thousand experimental and theoretical studies. Theoretical work of note here is the study of temperature-dependent partition function by Vidler and Tennyson[3], and various previous line lists namely SP[4] and PS[5], BT2[6] and calculations by S.Tashkun with using PS technology[7]. Very recently a new $H_2{}^{16}O$ line list called POKAZATEL[8], which treats energy levels and associated transitions up to dissociated dissociation, has been completed.

2. CALCULATIONS

The first version of VoTe (Voronin, Tennyson et al.[9]) line list was produced using the DVR3D package which employees a discrete variable representation (DVR) for the vibrational degrees of freedom [10] and a two-step approach for solving the full rotation-vibration nuclear motion problem. Calculations uses the high accuracy, empirical potential energy surface (PES) of Bubukina *et al.* [11] and the CVR water dipole moment surface (DMS) [12]. Vibration - rotation energy levels up to $J = 27$ are obtained and a novel method of labeling is used which allows more thorough labelling of the energy levels with approximate vibrational and rotational quantum numbers than previous water line lists computed using DVR3D.

Figure 1 presents and overview comparison of VoTe and the 2016 version of the HITRAN database (as sampled 30 May 2018). The 8000-11000 cm^{-1} region displays a possible technical problem with HITRAN 2016 for lines with intensity about 10^{-28} cm/molecule. Figure 2 shows this region more clearly. In addition, above 20000 cm^{-1} HITRAN is also missing a large number of transtions.

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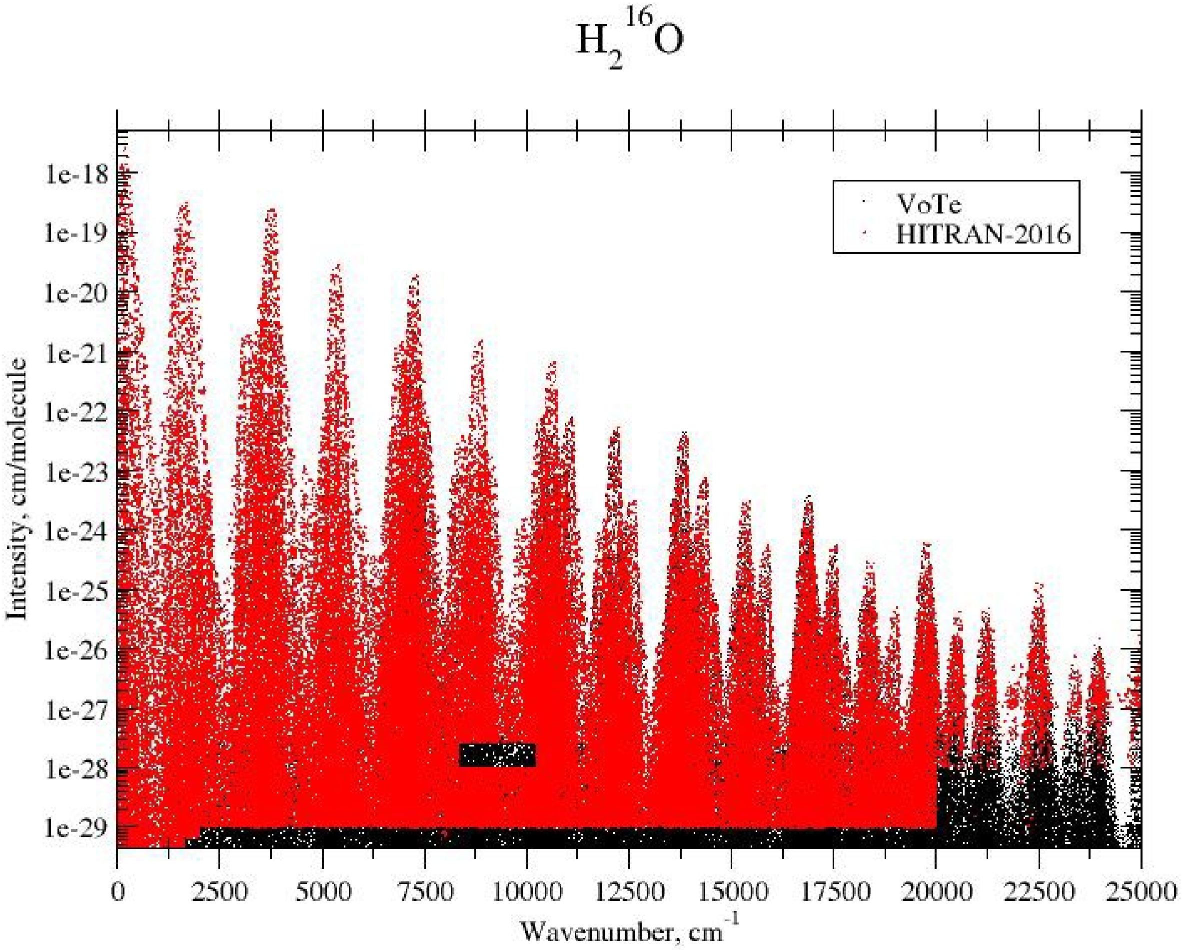

Figure 1. Overview of VoTe and HITRAN 2016[1].

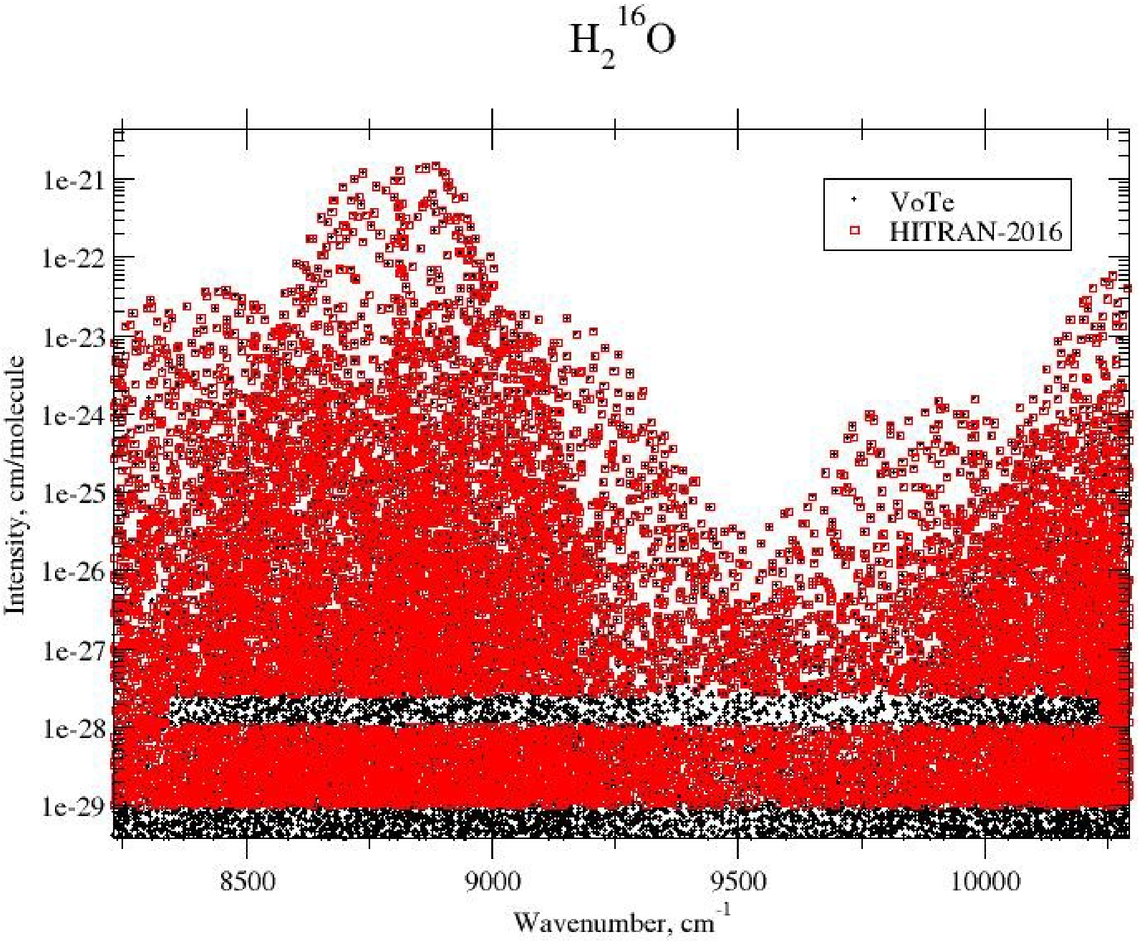

Figure 2. Overview of VoTe and HITRAN 2016 (30 May 2018) [1] for the region 8000-11000 cm^{-1}.

Table 1 presents a sample part line list for 100 first lines in the 0-25.8 cm^{-1} region. Table 2 and Figure 3 show energy levels for J=0 states with A_1 symmetry. Table 2 also gives energy levels from BT2[6], VoTe and our assignment.

Figure 3 gives a comparison between VoTe energy levels from Table 2, BT2 [6] and POKAZATEL[8] with the comprehensive empirical energy levels compiled as part of a IUPAC study [13]. We take IUPAC's J=0 levels (36 levels) comparison with calculations, sorted it by value and result on figure 3 is presented.

From figure 3 it is possible to see that for J=0 POKAZATEL [8] performs slightly better than our calculation especially for one point - the vibrational level (060) up to 0.2 cm^{-1} for VoTe and 0.4 cm^{-1} for BT2 and less than 0.1 cm^{-1} for POKAZATEL. It mean that in general, high bending levels are better predicted by POKAZATEL [8].

Table 1. Example of line list VoTe (first 100 lines).

J	sym	*J*	sym	frequencies	Intensity	*J*	sym	*J*	sym	frequencies	Intensit
top		low		cm^{-1}	cm/molecule	top		low		cm^{-1}	cm/molecul
4	1	5	2	0.068992	0.189E-29	9	1	8	2	14.666146	0.193E-27
4	3	3	4	0.414104	0.253E-27	9	3	8	4	14.750115	0.586E-27
5	4	4	3	0.916209	0.380E-27	4	1	3	2	15.466273	0.133E-24
6	4	5	3	0.747725	0.447E-24	4	3	3	4	15.977325	0.191E-28
4	4	3	3	2.267379	0.124E-25	5	2	4	1	15.501423	0.175E-29
2	1	3	2	3.995253	0.143E-25	5	2	4	1	15.837750	0.109E-21
4	1	5	2	3.191462	0.153E-26	6	1	5	2	15.712037	0.274E-22
14	3	15	4	4.642175	0.118E-27	6	1	7	2	16.286489	0.222E-22
3	2	4	1	4.560971	0.486E-29	7	1	6	2	16.652829	0.113E-25
5	3	6	4	4.008329	0.360E-29	8	1	7	2	16.835713	0.106E-23
6	2	5	1	4.935305	0.185E-29	8	3	7	4	16.805220	0.318E-23
8	1	9	2	4.298485	0.204E-29	1	1	1	2	17.487548	0.188E-27
8	3	9	4	4.295883	0.610E-29	14	4	13	3	17.705425	0.228E-25
15	1	16	2	5.898335	0.121E-28	18	1	17	2	17.837466	0.126E-29
3	2	2	1	6.117072	0.776E-22	2	1	3	2	17.214729	0.135E-27
3	2	2	1	6.575057	0.171E-29	7	2	6	1	17.573301	0.176E-28
5	2	6	1	6.950630	0.166E-26	8	1	7	2	17.780870	0.202E-29
5	4	6	3	7.737247	0.619E-26	10	2	9	1	18.342780	0.324E-28
13	1	14	2	8.657644	0.601E-27	10	4	9	3	18.329616	0.971E-28
14	1	15	2	8.236511	0.272E-27	1	4	1	3	18.036654	0.951E-27
3	3	2	4	8.478762	0.526E-29	1	4	1	3	18.576797	0.525E-19
6	4	7	3	8.927750	0.337E-29	3	4	2	3	18.487603	0.959E-27
7	2	8	1	8.737750	0.705E-28	3	4	4	3	18.565166	0.223E-27
7	4	8	3	8.756231	0.212E-27	5	1	4	2	18.248005	0.202E-24
6	1	7	2	9.893196	0.616E-27	5	4	4	3	18.944529	0.395E-29
6	3	7	4	9.767186	0.180E-26	8	1	7	2	18.832846	0.130E-29
10	3	9	4	10.725326	0.256E-23	8	3	7	4	18.897355	0.396E-28
14	4	13	3	10.778491	0.416E-29	12	3	13	4	19.064682	0.308E-25
5	2	4	1	10.850457	0.910E-22	14	4	15	3	19.722947	0.560E-27
5	2	4	1	10.897322	0.160E-29	17	1	18	2	19.768381	0.330E-29
5	3	4	4	10.780963	0.258E-29	4	2	3	1	19.750675	0.632E-29
6	2	7	1	10.775629	0.163E-29	5	3	4	4	19.466338	0.459E-29
16	3	17	4	11.291329	0.220E-28	6	4	5	3	19.868877	0.225E-24
17	3	16	4	11.850900	0.102E-28	7	3	6	4	19.307971	0.456E-25
3	3	4	4	11.041507	0.165E-27	9	1	8	2	19.800074	0.656E-26
5	3	6	4	11.215263	0.545E-25	5	4	4	3	20.707899	0.569E-21
4	4	3	3	12.685355	0.828E-21	7	1	6	2	20.378075	0.419E-28
4	4	3	3	12.815371	0.158E-28	1	4	1	3	21.946340	0.302E-22
10	2	11	1	13.000993	0.288E-24	9	2	8	1	21.550447	0.236E-24
4	1	5	2	13.457346	0.443E-28	9	4	8	3	21.555101	0.708E-24
6	3	5	4	13.446287	0.109E-27	6	4	5	3	22.698246	0.220E-29
8	3	7	4	13.113786	0.517E-29	5	1	4	2	23.338532	0.144E-29
4	1	3	2	14.346881	0.407E-29	2	2	2	1	24.521926	0.635E-27
4	3	3	4	14.946689	0.866E-21	2	3	2	4	24.171489	0.115E-26
6	3	5	4	14.653440	0.715E-22	4	3	5	4	24.017938	0.102E-27
7	2	6	1	14.594634	0.482E-23	10	2	11	1	25.856272	0.599E-27
7	3	8	4	14.926346	0.130E-29	11	1	10	2	25.068656	0.532E-29
7	4	6	3	14.783806	0.149E-22	11	2	12	1	25.565051	0.165E-24
8	2	7	1	14.730459	0.147E-26	11	3	10	4	25.070659	0.160E-28
8	4	7	3	14.228153	0.411E-26	2	1	1	2	25.869729	0.288E-26

Table.2. Energy levels for *J*=0 symmetry A_1.

N	BT2	v_1	v_2	v_3	VoTe	N	BT2	v_1	v_2	v_3	VoTe
	cm^{-1}	BT2			cm^{-1}		cm^{-1}	BT2			cm^{-1}
1	0	0	0	0	0	81	19864.081197	5	2	0	19864.791751
2	1594.873096	0	1	0	1594.762713	82	20030.241581	0	14	0	20029.974810
3	3151.677108	0	2	0	3151.635009	83	20080.346141	2	4	2	20079.477238
4	3657.155752	1	0	0	3657.014674	84	20312.476876	1	12	0	20310.675376
5	4666.724999	0	3	0	4666.788344	85	20386.324038	0	4	4	20386.366229
6	5235.220005	1	1	0	5234.964853	86	20419.087331	3	2	2	20419.386357
7	6133.839271	0	4	0	6134.021227	87	20493.277195	3	7	0	20491.476460
8	6775.244828	1	2	0	6775.080936	88	20533.474474	4	0	2	20533.377490
9	7201.52985	2	0	0	7201.537462	89	20700.213077	1	2	4	20699.925626
10	7445.096222	0	0	2	7445.022256	90	20722.413727	1	7	2	20720.529259
11	7542.213797	0	5	0	7542.411014	91	20836.233018	2	10	0	20832.929838
12	8274.095037	1	3	0	8273.976792	92	20906.792176	2	0	4	20905.977904
13	8761.699748	2	1	0	8761.586243	93	21005.467403	0	10	2	21002.767295
14	8870.269363	0	6	0	8870.161865	94	21052.026793	4	5	0	21052.000615
15	9000.159482	0	1	2	9000.118412	95	21221.997007	6	1	0	21221.448877
16	9724.331337	1	4	0	9724.195642	96	21274.538307	0	0	6	21275.132676
17	10086.96294	0	7	0	10086.06147	97	21312.543562	5	3	0	21313.606899
18	10284.35665	2	2	0	10284.36642	98	21431.632424	2	5	2	21430.268374
19	10521.80515	0	2	2	10521.72936	99	21629.389078	1	13	0	21628.468945
20	10599.59969	3	0	0	10599.68999	100	21705.631963	3	8	0	21703.187819
21	10868.84851	1	0	2	10868.87014	101	21764.320866	0	5	4	21764.338901
22	11098.88228	1	5	0	11098.35868	102	21845.069230	3	3	2	21844.710317
23	11254.83175	0	8	0	11253.46174	103	21917.043288	0	15	0	21915.885001
24	11767.4744	2	3	0	11767.38536	104	21974.410286	1	8	2	21971.944533
25	12007.91128	0	3	2	12007.76303	105	22007.097573	4	1	2	22006.982079
26	12139.32932	3	1	0	12139.31173	106	22128.390074	1	3	4	22127.796095
27	12381.60462	1	6	0	12380.49598	107	22168.184163	2	11	0	22165.032444
28	12407.66462	1	1	2	12407.65182	108	22328.592440	0	11	2	22325.606361
29	12534.623	0	9	0	12533.30908	109	22376.948406	4	6	0	22376.758263
30	13205.05407	2	4	0	13204.78697	110	22386.942954	2	1	4	22386.019184
31	13453.68258	0	4	2	13453.50663	111	22529.232550	7	0	0	22529.300289
32	13640.4711	3	2	0	13640.66577	112	22626.934319	6	2	0	22627.266860
33	13661.89937	1	7	0	13660.04778	113	22701.353972	2	6	2	22699.628341
34	13828.2889	4	0	0	13828.2637	114	22732.912543	0	1	6	22733.449559
35	13858.59367	0	10	0	13857.05781	115	22743.306226	5	4	0	22744.105409
36	13910.81599	1	2	2	13910.88254	116	22875.932292	3	9	0	22872.349403
37	14221.06219	2	0	2	14221.15668	117	23058.977254	1	9	2	23056.949540
38	14537.42249	0	0	4	14537.49042	118	23148.520733	0	6	4	23146.854760
39	14579.34228	2	5	0	14578.6148	119	23232.952449	3	4	2	23232.325384
40	14820.55066	1	8	0	14818.46413	120	23253.504262	1	14	0	23252.580040
41	14882.52045	0	5	2	14881.33868	121	23401.123958	4	2	2	23400.966039
42	15108.06541	3	3	0	15108.08547	122	23466.649633	5	0	2	23466.677845

43	15296.15521	0	11	0	15295.06895	123	23521.146374	1	4	4	23520.352132
44	15344.59249	4	1	0	15344.49749	124	23550.936962	2	12	0	23549.418666
45	15377.83046	1	3	2	15377.7183	125	23644.771196	4	7	0	23644.022002
46	15742.80346	2	1	2	15742.81751	126	23656.963056	0	12	2	23655.939656
47	15871.21273	2	6	0	15869.62695	127	23778.298806	0	16	0	23776.250790
48	16046.88912	0	1	4	16046.96132	128	23824.410661	2	2	4	23823.364291
49	16074.48393	1	9	0	16071.81358	129	23942.486983	7	1	0	23941.561032
50	16215.46345	0	6	2	16215.09824	130	23955.631972	2	7	2	23953.849944
51	16534.44512	3	4	0	16534.26879	131	23978.552183	3	0	4	23977.311326
52	16796.16168	1	4	2	16795.77869	132	24012.495323	5	5	0	24013.112644
53	16823.12188	4	2	0	16823.29461	133	24082.944360	3	10	0	24079.350125
54	16825.15624	0	12	0	16824.60122	134	24141.606886	6	3	0	24143.056820
55	16898.53561	5	0	0	16898.417	135	24161.511835	0	2	6	24162.335236
56	17139.83846	2	7	0	17137.584	136	24293.453833	1	0	6	24292.429191
57	17227.23543	2	2	2	17227.32832	137	24304.664082	1	10	2	24300.657403
58	17385.344	1	10	0	17382.69052	138	24426.144170	0	7	4	24424.882249
59	17458.13092	3	0	2	17458.20029	139	24578.096242	3	5	2	24577.112151
60	17491.97719	0	7	2	17490.96744	140	24796.722825	4	3	2	24795.787074
61	17526.26312	0	2	4	17526.42449	141	24818.333776	2	13	0	24817.100889
62	17748.3223	1	0	4	17748.09703	142	24866.027368	1	5	4	24864.851396
63	17911.61849	3	5	0	17911.18885	143	24875.945270	4	8	0	24874.663073
64	18162.54655	1	5	2	18161.49556	144	24913.852749	5	1	2	24914.134242
65	18267.09667	4	3	0	18267.15116	145	25086.840752	1	15	0	25085.974866
66	18334.74269	2	8	0	18331.64195	146	25119.746242	8	0	0	25120.249681
67	18392.69512	5	1	0	18392.78566	147	25148.258541	2	8	2	25145.615836
68	18425.6882	0	13	0	18424.7627	148	25225.920709	2	3	4	25224.100322
69	18644.80067	0	8	2	18643.52699	149	25258.540044	3	11	0	25255.467643
70	18675.18903	2	3	2	18674.67392	150	25312.650630	5	6	0	25313.453611
71	18806.9233	1	11	0	18804.2388	151	25353.240425	0	13	2	25349.644217
72	18955.83525	3	1	2	18955.77619	152	25369.410000	7	2	0	25370.995277
73	18977.12853	0	3	4	18977.33246	153	25436.983726	3	1	4	25435.722974
74	19223.69024	3	6	0	19222.66125	154	25468.227079	0	17	0	25468.553012
75	19242.41006	1	1	4	19242.10541	155	25517.128496	6	4	0	25518.777624
76	19442.38645	1	6	2	19440.14127	156	25563.710199	0	3	6	25564.739849
77	19576.44127	2	9	0	19573.60471	157	25597.931896	0	8	4	25595.898005
78	19677.79336	4	4	0	19677.86671	158	25681.197330	1	11	2	25676.952012
79	19779.7995	0	9	2	19778.12365	159	25738.065010	1	1	6	25736.799543
80	19782.01609	6	0	0	19781.30931	160	25855.201400	3	6	2	25853.416485

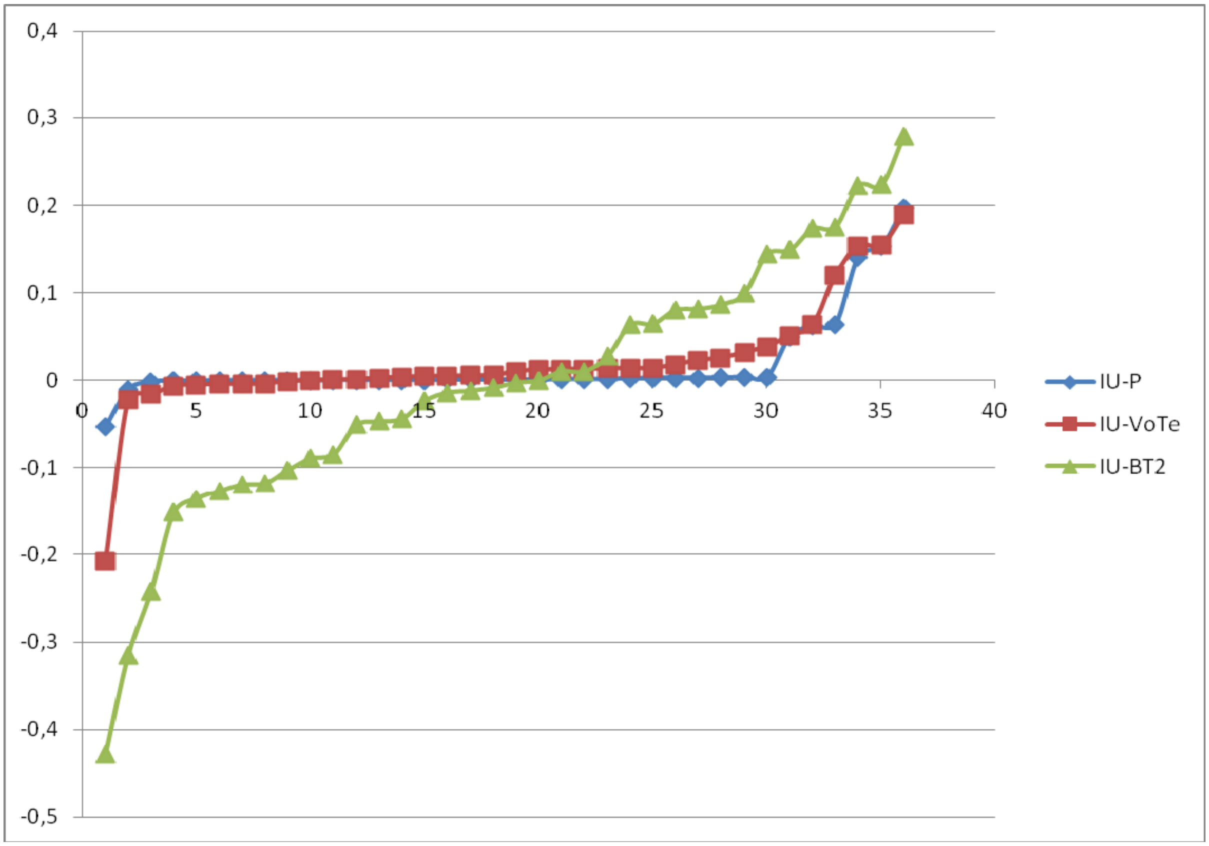

Figure 3. Comparison of energy levels from IUPAC compilation (IU) [13] IU and calculations P (POKAZATEL) [8], BT2 [6] and this work, VoTe.

The VoTe line list is available from the site ftp://ftp.iao.ru/pub/VTT/VoTe where one the files readmeVoTe-H216O.txt and VoTe-linelist.296K.25000.dat which gives the VoTe line list with a cut off intensity of 10^{-30} at T=296 K and assuming $H_2{}^{16}O$ in 100% abundance. The line list covers the region 0-25000 cm^{-1} for J up to 27 and contains 252 252 transitions.

At file readmeVoTe-H216O.txt you can see description of VoTe-linelist.296K.25000.dat , like at table 1.

The format of file VoTe-linelist.296K.25000.dat is, in Fortran notation, format(2(i2,i2,1x),f13.6,1x,1(e9.3))

```
JUp,SymUp,Jlow,SymLow, rFr,  rInt
 4 1  5 2      0.068992 0.189E-29
 4 3  3 4      0.414104 0.253E-27
 5 4  4 3      0.916209 0.380E-27
 6 4  5 3      0.747725 0.447E-24
 4 4  3 3      2.267379 0.124E-25
 JUp, SymUp          top rotational quantum numbers (J', Sym')
 Jlow,SymLo          low rotational quantum numbers (J , Sym)
 rFr                 Frequency of transition, cm-1
 rInt                Intensity, cm/molecule
Sym = 1,2,3,4 (by BT2 linelist)
```

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