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Erratum

Erratum to ''Relativistic correction to the potential energy surface and vibration–rotation levels of water'' [Chem. Phys. Lett. 293 (1998) 317] [1]

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Due to a programming error, results reported in Tables 2 and 3 for Born–Oppenheimer (BO) potential with both adiabatic and electronic relativistic corrections ($BO + \Delta V^{ad} + \Delta V_{rel}$) are not correct. Corrected results are given here. The new results lead to a slight (about 10%) improvement of the bending band origins but are qualitatively similar to those published.

There is a typographical mistake in Table 1 where the entry '1 1 2 −35.63530' should be replaced by '1 1 4 −35.63530'.

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Table 1
Band origins (in cm^{-1}) for the $H_2{}^{16}O$. Results calculated using BO, BO diagonal correction (ΔV^{ad}) and with the relativistic correction (ΔV_{rel}), are given as observed–calculated

	Obs[a]	b	c	d
(010)	1594.75	−2.65	−2.15	−3.44
(020)	3151.63	−5.12	−4.13	−6.86
(100)	3657.05	−3.49	−3.42	−0.62
(030)	4666.80	−7.53	−6.05	−10.43
(110)	5235.00	−6.20	−5.70	−4.13
(040)	6134.03	−9.90	−7.88	−14.26
(120)	6775.10	−8.64	−7.70	−7.50
(200)	7201.54	−6.38	−6.30	−0.70
(002)	7445.07	−4.89	−5.08	0.70
(050)	7542.39	−12.39	−9.74	−18.70
(130)	8273.98	−11.06	−9.69	−11.07
(210)	8761.59	−9.07	−8.59	−4.18
(060)	8870.5	−14.9	−11.3	−24.0
(012)	9000.14	−7.50	−7.30	−2.57
(220)	10284.37	−11.39	−10.57	−7.41
(022)	10524.3	−7.5	−7.0	−3.4
(300)	10599.69	−8.20	−8.19	0.19
(102)	10868.88	−8.81	−8.82	−0.33
(310)	12139.2	−10.9	−10.6	−3.3
(112)	12407.64	−11.53	−11.18	−4.38
(240)	13205.1	−16.0	−14.3	−14.5
(042)	13453.7	−14.8	−13.5	−13.0
(320)	13640.8	−13.0	−12.3	−6.4
(170)	13661.3	−19.7	−16.0	−27.6
(202)	13828.28	−9.43	−9.48	1.58
(122)	13910.90	−13.82	−13.20	−6.99
(400)	14221.16	−12.00	−11.89	−0.71
(004)	14537.5	−9.2	−9.6	2.0
(330)	15108.1	−15.3	−14.4	−9.4
(212)	15344.50	−12.02	−11.80	−1.89
(410)	15742.80	−14.60	−14.23	−4.11
(222)	16825.23	−12.25	−11.78	−3.36
(302)	16898.4	−10.6	−10.7	2.3
(420)	17227.70	−16.36	−15.78	−6.86
(104)	17458.30	−13.38	−13.32	0.56
(500)	17748.07	−13.06	−13.19	0.96
(312)	18392.98	−12.28	−12.25	−.14
(001)	3755.93	−2.25	−2.38	0.53
(011)	5331.27	−4.83	−4.51	−2.77
(021)	6871.51	−7.39	−6.65	−6.20
(101)	7249.81	−5.32	−5.39	0.29
(031)	8373.8	−9.9	−8.8	−9.8
(111)	8807.00	−7.95	−7.63	−3.06
(041)	9833.58	−12.24	−10.68	−13.47
(121)	10328.73	−10.29	−9.63	−6.25
(201)	10613.36	−7.72	−7.77	0.66
(003)	11032.41	−7.01	−7.32	1.39
(131)	11813.19	−12.73	−11.73	−9.71
(211)	12151.26	−10.30	−10.03	−2.67
(013)	12565.00	−9.63	−9.60	−1.83

Table 1 (continued)

	Obs[a]	b	c	d
(141)	13256.2	−15.0	−13.6	−13.3
(221)	13652.66	−12.33	−11.79	−5.43
(301)	13830.94	−9.36	−9.42	1.63
(071)	13835.37	−20.23	−16.65	−29.10
(023)	14066.19	−12.12	−11.82	−5.06
(103)	14318.81	−10.09	−10.27	1.11
(231)	15119.03	−14.77	−13.96	−8.86
(311)	15347.96	−11.77	−11.60	−1.54
(033)	15534.71	−14.60	−14.05	−8.44
(113)	15832.77	−12.66	−12.57	−2.14
(321)	16821.64	−12.94	−12.61	−2.68
(203)	16898.84	−10.53	−10.63	2.35
(123)	17312.54	−14.76	−14.47	−4.98
(401)	17495.53	−12.30	−12.42	1.57
(331)	18265.82	−15.60	−15.02	−6.35
(213)	18393.31	−12.49	−12.48	−.45
(411)	18989.96	−14.72	−14.68	−1.64
(303)	19781.11	−10.60	−10.68	5.12
(501)	20543.14	−13.65	−13.76	4.29
(511)	21221.8	−14.0	−13.9	0.4
(403)	22529.4	−9.4	−9.6	9.0

[a] Observed fundamentals.
[b] BO potential only.
[c] BO + ΔV^{ad}.
[d] BO + ΔV^{ad} + ΔV_{rel}.

Table 2
Rotational term values (in cm^{-1}) for the vibrational ground state and (010) state of $H_2{}^{16}O$. Results calculated using BO, BO diagonal correction (ΔV^{ad}) and with the relativistic correction (ΔV_{rel}), are given as observed–calculated

	Ground state				(010) state			
	Obs[a]	b	c	d	Obs[a]	b	c	d
20_{020}	4048.252	−0.532	−0.155	0.300	4016.581	−0.428	−0.115	0.556
20_{120}	4048.252	−0.535	−0.155	0.300	4016.581	−0.432	−0.116	0.556
20_{119}	4412.317	−0.568	−0.152	0.329	4428.049	−0.379	−0.037	0.741
20_{219}	4412.317	−0.571	−0.152	0.329	4428.051	−0.377	−0.039	0.739
20_{218}	4738.624	−0.664	−0.195	0.231	4784.599	−0.472	−0.075	0.632
20_{318}	4738.636	−0.667	−0.194	0.232	4784.645	−0.476	−0.075	0.634
20_{317}	5031.796	−0.800	−0.260	0.037	5100.008	−0.605	−0.124	0.406
20_{417}	5031.977	−0.795	−0.261	0.044	5100.554	−0.600	−0.130	0.427
20_{416}	5292.096	−0.985	−0.356	−0.311	5374.660	−0.822	−0.218	−0.0812
20_{516}	5294.035	−0.951	−0.337	−0.212	5379.620	−0.752	−0.193	0.152
20_{515}	5513.266	−1.250	−0.454	−0.980	5598.487	−1.190	−0.344	−1.083
20_{615}	5527.046	−1.081	−0.402	−0.447	5627.511	−0.855	−0.243	−0.019
20_{614}	5680.787	−1.675	−0.656	−2.056	5762.306	−1.508	−0.456	−2.000
20_{714}	5739.232	−1.127	−0.429	−0.429	5857.784	−0.842	−0.253	0.195
20_{713}	5812.074	−1.702	−0.666	−2.063	5909.823	−1.325	−0.408	−1.306
20_{813}	5947.327	−0.999	−0.381	0.045	6090.365	−0.678	−0.227	0.882
20_{812}	5966.827	−1.265	−0.496	−0.702	6101.535	−0.890	−0.333	0.339

Table 2 (continued)

	Ground state				(010) state			
	Obs[a]	b	c	d	Obs[a]	b	c	d
20_{912}	6167.909	−0.621	−0.143	1.011	6339.423	−0.461	−0.194	1.822
20_{911}	6170.964	−0.736	−0.227	0.796	6341.018	−0.489	−0.204	1.738
20_{1011}	6407.084	−0.587	−0.281	1.705	6608.002	−0.249	−0.189	2.782
20_{1010}	6407.446	−0.596	−0.285	1.683	6608.180	−0.252	−0.190	2.773
20_{1110}	6664.138	−0.409	−0.261	2.561	6893.156	−0.079	−0.207	3.699
20_{119}	6664.172	−0.407	−0.259	2.561	6893.153	−0.101	−0.229	3.677
20_{129}	6935.425	−0.241	−0.260	3.386	7191.043	0.064	−0.261	4.558
20_{128}	6935.428	−0.240	−0.259	3.387	7191.041	0.059	−0.267	4.552
20_{138}	7217.560	−0.132	−0.302	4.161	7498.245	0.154	−0.349	5.364
20_{137}	7217.560	−0.133	−0.303	4.160	7498.245	0.151	−0.353	5.360
20_{147}	7507.575	−0.031	−0.365	4.909	7811.766	0.713	−0.445	6.161
20_{146}	7507.575	−0.031	−0.365	4.909	7811.736	0.221	−0.526	6.116
20_{156}	7802.700	0.015	−0.466	5.618	8128.763	0.236	−0.640	6.832
20_{155}	7802.700	0.015	−0.466	5.618	8128.763	0.236	−0.640	6.832
20_{165}	8100.292	0.051	−0.597	6.298	8446.615	0.226	−0.851	7.493
20_{164}	8100.292	0.051	−0.597	6.298	8446.615	0.226	−0.851	7.492
20_{174}	8397.625	−0.008	−0.807	6.905	8762.590	0.157	−1.106	8.110
20_{173}	8397.625	−0.008	−0.807	6.905	8762.590	0.157	−1.106	8.110
20_{183}	8691.916	−0.056	−1.033	7.505	9073.744	0.036	−1.445	8.650
20_{182}	8691.916	−0.056	−1.033	7.505	9073.744	0.036	−1.445	8.650
20_{192}	8979.854	−0.211	−1.355	8.027	9376.758	−0.151	−1.842	9.149
20_{191}	8979.854	−0.211	−1.355	8.027	9376.758	−0.151	−1.842	9.149
20_{201}	9257.408	−0.423	−1.775	8.485	9667.337	−0.396	−2.348	9.574
20_{200}	9257.408	−0.423	−1.775	8.485	9667.337	−0.396	−2.348	9.574

[a] Observed rotational term values.
[b] BO potential only.
[c] BO + ΔV^{ad}.
[d] BO + ΔV^{ad} + ΔV_{rel}.