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A COMMENT ON MOLECULAR PARTITION FUNCTIONS

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ABSTRACT

Molecular partition functions computed from recently published approximate expressions can be significantly in error. In particular, H_2 number densities computed from these expressions can be too small by as much as 10%. As a consequence, H, H^-, and hydride number densities and the opacity for H^- all can be overestimated by as much as 20%.

Subject heading: molecular processes

There have been two recent papers on molecular partition functions, Bohn and Wolf (1984) who treat H_2 and CO, and Sauval and Tatum (1984) who treat 300 different species. Both papers used approximate expressions for the molecular partition function instead of summing over the levels explicitly. These expressions are not rigorous because they do not go to sufficiently high order and because they do not keep proper track of the number of bound levels. Approximate expressions should not be used now that computers are readily available to determine the energy levels and to sum the exponentials. Chase et al. (1982) computed the JANAF thermodynamic properties table for H_2 using explicit summation.

In Table 1 we list partition functions and equilibrium constants for H_2 and CO computed by straightforwardly summing over the three lowest states of each molecule using energy levels derived from the work of Dabrowsky (1977; 1984; 1985) for H_2, and of Mantz et al. (1975), Field (1971), and Field et al. (1972) for CO. We also tabulate the errors in the partition functions for the fits listed by Bohn and Wolf (labelled BW), the fits to the partition functions and equilibrium constants listed by Sauval and Tatum (ST), the fits to approximate equilibrium constants by Tsuji (1973; T), the fits to McBride et al. (1963) by Kurucz (1970; K70), the fits to JANAF (Chase et al. 1982) by

Dragon (1983; D), and fits to the present work (K). All these fitting expressions are listed in Table 2. Sauval and Tatum list many other fits as well. The approximate partition functions are about 10% too small for H_2 and about 2% too small for CO. H_2 number densities computed from approximate expressions can be too small by as much as 10%, and, consequently, H, H^-, and hydride number densities, and the H^- opacity can be too large by twice this amount.

The errors for H_2 are probably the largest that one would expect from approximations because the Dunham expansions for H_2 go to very high order. The expansions for hydrides are also high order, but for many other molecules simple expansions are an excellent approximation. Also, for many molecules it is impossible to determine the energy levels exactly because laboratory analyses are very incomplete and do not go to high v or high J. Then any method of computing the partition function is uncertain.

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TABLE 1
Partition Functions and Equilibrium Constants

		% ERROR				% ERROR						% ERROR				% ERROR				
T	$Q(H_2)$	K	BW	ST	$E(H_2)$	K	K70	D	T	ST	Q(CO)	K	BW	ST	E(CO)	K	K70	D	T	ST
1000	6.150	0.7	-4.6	-1.9	2.679E-02	0.7	-3.7	-2.8	-5.6	-1.7	380.2	0.4	-0.8	-0.8	4.025E+30	0.6	20.4	2.0	-3.0	1.2
1100	6.773	0.1	-4.5	-2.1	2.270E-04	0.1	-3.3	-2.5	-5.3	-1.9	425.0	0.1	-0.5	-0.6	3.191E+25	0.2	18.4	1.2	-2.9	0.8
1200	7.406	-0.2	-4.4	-2.2	4.250E-06	-0.2	-2.8	-2.0	-4.8	-2.1	471.9	-0.1	-0.3	-0.4	1.792E+21	0.0	16.9	0.5	-2.2	0.5
1300	8.050	-0.4	-4.4	-2.4	1.465E-07	-0.4	-2.2	-1.4	-4.4	-2.2	520.9	-0.2	-0.2	-0.2	4.539E+17	-0.2	15.7	0.0	-1.2	0.3
1400	8.708	-0.4	-4.4	-2.5	8.158E-09	-0.4	-1.6	-0.8	-4.0	-2.4	572.1	-0.2	-0.1	-0.1	3.756E+14	-0.2	14.8	-0.3	-0.1	0.3
1500	9.381	-0.3	-4.4	-2.6	6.672E-10	-0.3	-1.0	-0.3	-3.7	-2.5	625.6	-0.2	-0.1	0.0	8.014E+11	-0.3	13.9	-0.5	0.8	0.2
1600	10.070	-0.2	-4.4	-2.8	7.458E-11	-0.2	-0.5	0.2	-3.5	-2.6	681.4	-0.1	-0.2	0.1	3.692E+09	-0.3	13.2	-0.7	1.5	0.2
1700	10.777	-0.1	-4.5	-2.9	1.079E-11	-0.1	0.0	0.6	-3.5	-2.8	739.5	-0.1	-0.3	0.1	3.205E+07	-0.2	12.6	-0.8	2.0	0.2
1800	11.503	0.0	-4.5	-3.1	1.934E-12	0.0	0.4	1.0	-3.6	-2.9	800.0	0.0	-0.3	0.1	4.720E+05	-0.2	12.0	-0.8	2.4	0.2
1900	12.248	0.0	-4.6	-3.2	4.155E-13	0.0	0.7	1.2	-3.7	-3.1	862.9	0.0	-0.4	0.1	1.085E+04	-0.1	11.5	-0.8	2.5	0.2
2000	13.014	0.1	-4.8	-3.4	1.041E-13	0.1	0.8	1.4	-4.0	-3.3	928.3	0.1	-0.5	0.1	3.638E+02	-0.1	11.0	-0.7	2.5	0.2
2100	13.802	0.2	-4.9	-3.5	2.978E-14	0.2	1.0	1.5	-4.3	-3.4	996.0	0.1	-0.6	0.0	1.687E+01	0.0	10.5	-0.7	2.4	0.2
2200	14.611	0.2	-5.0	-3.7	9.548E-15	0.2	1.0	1.5	-4.6	-3.6	1066.2	0.1	-0.7	0.0	1.035E+00	0.0	10.0	-0.6	2.1	0.2
2300	15.444	0.2	-5.2	-3.9	3.381E-15	0.2	1.0	1.4	-5.0	-3.8	1138.9	0.1	-0.7	-0.1	8.104E-02	0.1	9.6	-0.5	1.7	0.1
2400	16.300	0.2	-5.3	-4.1	1.306E-15	0.2	0.9	1.3	-5.4	-4.0	1214.0	0.1	-0.8	-0.2	7.848E-03	0.1	9.2	-0.4	1.3	0.1
2500	17.180	0.2	-5.5	-4.3	5.444E-16	0.2	0.7	1.1	-5.8	-4.2	1291.6	0.1	-0.8	-0.2	9.166E-04	0.1	8.7	-0.3	0.8	0.1
2600	18.085	0.2	-5.6	-4.5	2.429E-16	0.2	0.6	0.9	-6.3	-4.4	1371.7	0.1	-0.9	-0.3	1.264E-04	0.1	8.3	-0.2	0.3	0.0
2700	19.016	0.2	-5.8	-4.7	1.151E-16	0.2	0.4	0.7	-6.8	-4.6	1454.3	0.1	-0.9	-0.4	2.019E-05	0.2	7.9	-0.1	-0.3	0.0
2800	19.972	0.1	-5.9	-4.9	5.758E-17	0.1	0.2	0.5	-7.2	-4.8	1539.4	0.1	-0.9	-0.5	3.678E-06	0.2	7.5	0.0	-0.8	-0.1
2900	20.954	0.1	-6.1	-5.1	3.022E-17	0.1	-0.1	0.2	-7.7	-5.0	1627.0	0.1	-0.9	-0.6	7.539E-07	0.2	7.2	0.1	-1.4	-0.1
3000	21.963	0.0	-6.2	-5.3	1.657E-17	0.0	-0.3	0.0	-8.2	-5.2	1717.2	0.0	-0.9	-0.6	1.718E-07	0.2	6.8	0.2	-2.0	-0.2
3100	23.000	0.0	-6.4	-5.5	9.446E-18	0.0	-0.5	-0.3	-8.6	-5.4	1809.9	0.0	-0.8	-0.7	4.310E-08	0.2	6.5	0.3	-2.6	-0.2
3200	24.064	0.0	-6.6	-5.7	5.581E-18	0.0	-0.7	-0.5	-9.1	-5.6	1905.1	0.0	-0.8	-0.8	1.179E-08	0.1	6.1	0.4	-3.1	-0.3
3300	25.156	-0.1	-6.7	-5.9	3.406E-18	-0.1	-0.9	-0.7	-9.5	-5.8	2003.0	0.0	-0.8	-0.9	3.490E-09	0.1	5.9	0.4	-3.7	-0.3
3400	26.277	-0.1	-6.9	-6.1	2.141E-18	-0.1	-1.1	-0.8	-10.0	-6.0	2103.3	-0.1	-0.8	-0.9	1.110E-09	0.1	5.6	0.5	-4.2	-0.4
3500	27.427	-0.1	-7.0	-6.3	1.382E-18	-0.1	-1.2	-1.0	-10.4	-6.2	2206.3	-0.1	-0.8	-1.0	3.772E-10	0.1	5.3	0.5	-4.8	-0.5
3600	28.607	-0.1	-7.2	-6.5	9.151E-19	-0.1	-1.3	-1.1	-10.9	-6.4	2311.9	-0.1	-0.8	-1.1	1.361E-10	0.0	5.1	0.5	-5.3	-0.5
3700	29.817	-0.2	-7.3	-6.7	6.197E-19	-0.2	-1.3	-1.1	-11.3	-6.6	2420.0	-0.1	-0.7	-1.2	5.189E-11	0.0	4.9	0.6	-5.7	-0.6
3800	31.057	-0.2	-7.5	-6.9	4.285E-19	-0.2	-1.4	-1.2	-11.7	-6.8	2530.8	-0.1	-0.7	-1.2	2.082E-11	0.0	4.8	0.6	-6.2	-0.6
3900	32.329	-0.2	-7.6	-7.1	3.021E-19	-0.2	-1.3	-1.1	-12.1	-7.0	2644.1	-0.1	-0.8	-1.3	8.758E-12	0.0	4.6	0.6	-6.6	-0.7
4000	33.632	-0.2	-7.8	-7.3	2.169E-19	-0.2	-1.3	-1.1	-12.6	-7.2	2760.1	-0.1	-0.8	-1.3	3.847E-12	-0.1	4.5	0.6	-7.1	-0.7
4100	34.967	-0.1	-8.0	-7.5	1.583E-19	-0.1	-1.2	-1.0	-13.0	-7.4	2878.7	-0.1	-0.8	-1.4	1.760E-12	-0.1	4.4	0.6	-7.4	-0.8
4200	36.334	-0.1	-8.1	-7.7	1.173E-19	-0.1	-1.0	-0.8	-13.4	-7.6	3000.0	-0.1	-0.8	-1.4	8.354E-13	-0.1	4.4	0.5	-7.8	-0.8
4300	37.735	-0.1	-8.3	-7.9	8.819E-20	-0.1	-0.9	-0.7	-13.7	-7.8	3123.9	-0.1	-0.9	-1.5	4.107E-13	-0.1	4.3	0.5	-8.2	-0.9
4400	39.168	-0.1	-8.5	-8.1	6.720E-20	-0.1	-0.7	-0.5	-14.1	-8.0	3250.4	-0.1	-0.9	-1.5	2.085E-13	-0.1	4.3	0.5	-8.5	-0.9
4500	40.636	-0.1	-8.6	-8.2	5.184E-20	-0.1	-0.5	-0.3	-14.5	-8.2	3379.6	0.0	-1.0	-1.6	1.091E-13	-0.1	4.3	0.4	-8.8	-1.0
4600	42.138	0.0	-8.8	-8.4	4.047E-20	0.0	-0.2	0.0	-14.9	-8.4	3511.5	0.0	-1.0	-1.6	5.876E-14	-0.1	4.3	0.4	-9.1	-1.0
4700	43.676	0.0	-9.0	-8.6	3.194E-20	0.0	0.0	0.2	-15.2	-8.6	3646.1	0.0	-1.1	-1.7	3.249E-14	-0.1	4.2	0.3	-9.3	-1.0
4800	45.248	0.0	-9.2	-8.8	2.546E-20	0.0	0.2	0.5	-15.6	-8.7	3783.4	0.0	-1.2	-1.7	1.841E-14	-0.1	4.3	0.3	-9.6	-1.1
4900	46.857	0.0	-9.4	-9.0	2.050E-20	0.0	0.5	0.7	-15.9	-8.9	3923.3	0.0	-1.3	-1.7	1.068E-14	-0.1	4.3	0.2	-9.8	-1.1
5000	48.501	0.1	-9.5	-9.1	1.665E-20	0.1	0.7	0.9	-16.3	-9.1	4066.0	0.0	-1.4	-1.7	6.331E-15	-0.1	4.2	0.2	-10.0	-1.1
5100	50.183	0.1	-9.7	-9.3	1.364E-20	0.1	0.8	1.1	-16.6	-9.2	4211.4	0.0	-1.4	-1.8	3.831E-15	-0.1	4.2	0.1	-10.2	-1.2
5200	51.902	0.1	-9.9	-9.5	1.126E-20	0.1	0.9	1.2	-16.9	-9.4	4359.5	0.1	-1.5	-1.8	2.364E-15	-0.1	4.2	0.1	-10.3	-1.2
5300	53.659	0.1	-10.1	-9.6	9.372E-21	0.1	1.0	1.2	-17.3	-9.6	4510.4	0.1	-1.5	-1.8	1.486E-15	-0.1	4.1	0.0	-10.5	-1.2
5400	55.453	0.1	-10.3	-9.8	7.854E-21	0.1	1.0	1.2	-17.6	-9.7	4664.0	0.1	-1.6	-1.8	9.500E-16	-0.1	4.0	0.0	-10.6	-1.2
5500	57.287	0.1	-10.4	-9.9	6.626E-21	0.1	0.8	1.0	-17.9	-9.9	4820.4	0.1	-1.6	-1.8	6.174E-16	0.0	3.9	-0.1	-10.8	-1.3
5600	59.159	0.1	-10.6	-10.1	5.626E-21	0.1	0.6	0.8	-18.2	-10.0	4979.5	0.1	-1.5	-1.9	4.075E-16	0.0	3.7	-0.1	-10.9	-1.3
5700	61.071	0.1	-10.8	-10.2	4.806E-21	0.1	0.2	0.4	-18.5	-10.2	5141.4	0.1	-1.5	-1.9	2.729E-16	0.0	3.5	-0.2	-10.9	-1.3
5800	63.023	0.1	-10.9	-10.4	4.129E-21	0.1	-0.3	-0.2	-18.9	-10.3	5306.1	0.1	-1.4	-1.9	1.853E-16	0.0	3.1	-0.2	-11.0	-1.3
5900	65.015	0.1	-11.0	-10.5	3.567E-21	0.1	-1.0	-0.9	-19.2	-10.5	5473.7	0.1	-1.2	-1.9	1.275E-16	0.0	2.7	-0.3	-11.1	-1.3
6000	67.047	0.1	-11.1	-10.7	3.097E-21	0.1	-1.9	-1.9	-19.4	-10.6	5644.1	0.1	-1.0	-1.9	8.886E-17	0.0	2.3	-0.3	-11.1	-1.3
6100	69.121	0.1		-10.8	2.702E-21	0.1			-19.7	-10.8	5817.3	0.1		-1.9	6.266E-17	0.1			-11.2	-1.3
6200	71.235	0.1		-10.9	2.369E-21	0.1			-20.0	-10.9	5993.3	0.0		-1.9	4.468E-17	0.1			-11.2	-1.4
6300	73.391	0.0		-11.1	2.086E-21	0.0			-20.3	-11.0	6172.2	0.0		-1.9	3.221E-17	0.1			-11.2	-1.4
6400	75.589	0.0		-11.2	1.845E-21	0.0				-11.1	6354.0	0.0		-1.9	2.346E-17	0.1				-1.4
6500	77.828	0.0		-11.3	1.638E-21	0.0				-11.3	6538.6	0.0		-1.9	1.725E-17	0.1				-1.4
6600	80.110	0.0		-11.4	1.460E-21	0.0				-11.4	6726.3	0.0		-1.9	1.281E-17	0.1				-1.4
6700	82.434	-0.1		-11.5	1.306E-21	0.0				-11.5	6916.8	0.0		-1.9	9.593E-18	0.1				-1.4
6800	84.800	-0.1		-11.6	1.172E-21	-0.1				-11.6	7110.4	-0.1		-1.9	7.247E-18	0.1				-1.4
6900	87.210	-0.1		-11.7	1.056E-21	-0.1				-11.7	7306.8	-0.1		-1.9	5.520E-18	0.1				-1.4
7000	89.662	-0.1		-11.8	9.537E-22	-0.1				-11.8	7506.3	-0.1		-1.9	4.237E-18	0.1				-1.5
7100	92.157	-0.1		-11.9	8.643E-22	-0.1				-11.9	7708.8	-0.1		-1.8	3.277E-18	0.1				-1.5
7200	94.695	-0.1		-12.0	7.856E-22	-0.1				-12.0	7914.3	-0.1		-1.8	2.553E-18	0.1				-1.5
7300	97.276	-0.1		-12.1	7.161E-22	-0.1				-12.1	8122.9	-0.1		-1.8	2.002E-18	0.1				-1.5
7400	99.900	-0.1		-12.2	6.545E-22	-0.1				-12.1	8333.7	-0.1		-1.8	1.580E-18	0.0				-1.5
7500	102.567	-0.1		-12.2	5.997E-22	-0.1				-12.2	8548.4	-0.1		-1.8	1.256E-18	0.0				-1.5
7600	105.277	-0.1		-12.3	5.508E-22	-0.1				-12.3	8766.3	-0.1		-1.8	1.004E-18	0.0				-1.5
7700	108.030	-0.1		-12.4	5.072E-22	0.0				-12.3	8987.4	-0.1		-1.8	8.070E-19	0.0				-1.5
7800	110.826	0.0		-12.4	4.680E-22	0.0				-12.4	9211.5	0.0		-1.8	6.526E-19	-0.1				-1.6
7900	113.665	0.0		-12.5	4.328E-22	0.0				-12.4	9439.0	0.0		-1.8	5.306E-19	-0.1				-1.6
8000	116.546	0.0		-12.5	4.011E-22	0.1				-12.5	9669.6	0.0		-1.8	4.336E-19	-0.1				-1.6
8100	119.470	0.1		-12.5	3.725E-22	0.1				-12.5	9903.8	0.0		-1.8	3.562E-19	-0.1				-1.7
8200	122.437	0.1		-12.6	3.466E-22	0.1				-12.5	10141.0	0.0		-1.7	2.940E-19	-0.1				-1.7
8300	125.446	0.1		-12.6	3.231E-22	0.1				-12.5	10381.8	0.1		-1.7	2.437E-19	-0.1				-1.7
8400	128.496	0.1		-12.6	3.017E-22	0.2				-12.6	10625.9	0.1		-1.7	2.030E-19	-0.1				-1.7
8500	131.589	0.1		-12.6	2.822E-22	0.4				-12.6	10873.2	0.1		-1.7	1.698E-19	-0.1				-1.8
8600	134.723	0.1		-12.6	2.644E-22	0.2				-12.6	11124.6	0.1		-1.7	1.427E-19	-0.1				-1.8
8700	137.899	0.1		-12.6	2.482E-22	0.1				-12.6	11379.3	0.0		-1.7	1.203E-19	0.0				-1.9
8800	141.115	0.0		-12.6	2.332E-22	0.1				-12.5	11637.4	0.0		-1.7	1.019E-19	0.0				-1.9
8900	144.372	-0.1		-12.6	2.196E-22	-0.1				-12.5	11899.2	-0.1		-1.7	8.662E-20	0.1				-2.0
9000	147.670	-0.2		-12.5	2.070E-22	-0.2				-12.5	12164.8	-0.2		-1.7	7.390E-20	0.2				-2.0

TABLE 2

Polynomial Fits for Partition Functions and Equilibrium Constants

K: This paper for 1000 < T < 9000K,

$\ln Q(H_2) = 0.582145 + 16.3760t - 49.4684t^2 + 112.049t^3 - 149.953t^4 + 106.531t^5 - 30.9791t^6$

$\ln Q(CO) = 4.51349 + 18.4221t - 50.0599t^2 + 102.208t^3 - 128.504t^4 + 87.8414t^5 - 24.8533t^6$

$\ln E(H_2) = 4.478/T_{eV} - 46.4584 + 16.3660t - 49.3992t^2 + 111.822t^3 - 149.567t^4 + 106.206t^5 - 30.8720t^6 - 1.5 \ln T$

$\ln E(CO) = 11.091/T_{eV} - 49.0414 + 14.0306t - 26.6341t^2 + 35.3827t^3 - 26.5424t^4 + 8.32385t^5 - 1.5 \ln T$

K70: Kurucz (1970, fit to McBride et al. (1963)) for 1000 < T < 6000K,

$\ln E(H_2) = 4.477/T_{eV} - 46.628 + 18.031t - 50.239t^2 + 81.424t^3 - 50.501t^4 - 1.5 \ln T$

$\ln E(CO) = 11.108/T_{eV} - 49.170 + 15.802t - 34.347t^2 + 46.870t^3 - 26.563t^4 - 1.5 \ln T$

D: Dragon (1983, fit to JANAF (Chase et al. 1982)) for 1000 < T < 6000K,

$\ln E(H_2) = 4.478/T_{eV} - 46.641 + 18.212t - 51.150t^2 + 83.297t^3 - 51.844t^4 - 1.5 \ln T$

$\ln E(CO) = 11.091/T_{eV} - 48.914 + 12.133t - 16.990t^2 + 13.763t^3 - 4.5299t^4 - 1.5 \ln T$

T: Tsuji (1973) for 1008 < T < 6300K,

$\log E(H_2) = \log kT - 12.739 + 5.1172x - 0.12572x^2 + 0.014149x^3 - 0.00063021x^4$

$\log E(CO) = \log kT - 13.820 + 11.795x - 0.17217x^2 + 0.022888x^3 - 0.0011349x^4$

BW: Bohn and Wolf (1984) for 1000 < T < 6000K,

$Q(H_2) = (57.971t + 4.6761t^2 + 10.886t^3) / (0.95547 + 1.0395t - 7.1985t^2 + 11.544t^3 - 6.4035t^4)$

$Q(CO) = (3598.7t + 238.72t^2 + 51.280t^3) / (1.1377 - 1.7072t - 1.2576t^2 + 6.5767t^3 - 5.2274t^4)$

ST: Sauval and Tatum (1984) for 1000 < T < 9000K,

$\log Q(H_2) = 1.6498 - 1.6265y + 0.7472y^2 - 0.2751y^3$

$\log Q(CO) = 3.6076 - 1.7608y + 0.4172y^2$

$\log E(H_2) = \log kT - 1 - 11.1759 + 0.8735y + 0.7470y^2 - 0.2748y^3 + 4.4781x$

$\log E(CO) = \log kT - 1 - 12.2263 + 0.8829y + 0.1230y^2 + 0.3226y^3 + 11.0920x$

Here and in Table 1, $Q(H_2)$ and $Q(CO)$ are the partition functions, $E(H_2)$ and $E(CO)$ are the equilibrium constants, and where $t = T/10000$, $T_{eV} = 0.000086171\ T = T$ in eV , $x = 5040/T$, and $y = \log x$.
$E(H_2)$ is the number density in cm^{-3} of H_2 divided by the square of the number density of neutral H .
$E(CO)$ is the number density in cm^{-3} of CO divided by the number densities of neutral C and neutral O .