Supplementary Material (ESI) for PCCP

SUPPLEMENTAL MATERIAL FOR: Rovibrational levels of HD

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The following tables collect components of the dissociation energy for all rovibrational levels of HD. The abreviations used within the table:

BO – the Born-Oppenheimer component

AD – the adiabatic correction

NA – the nonadiabatic correction

$\boldsymbol{\alpha^2}$ – the relativistic correction of the order α^2

$\boldsymbol{\alpha^3}$ – the QED correction of the order α^3

$\boldsymbol{\alpha^4}$ – the QED correction of the order α^4

Total – the total dissociation energy, D_0

$\boldsymbol{\delta}$ – the uncertainty assigned to D_0

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TABLE I: Components of dissociation energy of HD

$v\backslash J$		0	1	2	3	4	5	6	7	8	9	10	11	12
0	BO	36401.9332	36312.6626	36134.7364	35869.3700	35518.3506	35083.9965	34569.1058	33976.8983	33310.9519	32575.1373	31773.5525	30910.4600	29990.2284
0	AD	4.2509	4.2870	4.3587	4.4653	4.6056	4.7779	4.9805	5.2111	5.4676	5.7473	6.0477	6.3661	6.6998
0	NA	.3267	.3345	.3500	.3731	.4037	.4414	.4862	.5376	.5955	.6594	.7290	.8040	.8840
0	α^2	−.5300	−.5319	−.5358	−.5415	−.5490	−.5581	−.5687	−.5807	−.5938	−.6079	−.6229	−.6384	−.6544
0	α^3	−.1964	−.1956	−.1941	−.1918	−.1888	−.1852	−.1809	−.1760	−.1705	−.1646	−.1582	−.1515	−.1444
0	α^4	−.0016	−.0016	−.0016	−.0016	−.0016	−.0015	−.0015	−.0015	−.0014	−.0014	−.0013	−.0013	−.0012
0	Total	36405.7828	36316.5549	36138.7136	35873.4735	35522.6205	35088.4710	34573.8214	33981.8890	33316.2492	32580.7701	31779.5467	30916.8389	29997.0121
0	δ	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0010	.0011	.0011
1	BO	32768.2136	32682.8029	32512.5786	32258.7206	31922.9637	31507.5569	31015.2138	30449.0553	29812.5476	29109.4390	28343.6959	27519.4427	26640.9053
1	AD	5.1835	5.2164	5.2818	5.3789	5.5065	5.6632	5.8471	6.0562	6.2882	6.5407	6.8112	7.0969	7.3954
1	NA	.9554	.9625	.9764	.9973	1.0249	1.0590	1.0994	1.1458	1.1980	1.2556	1.3185	1.3862	1.4585
1	α^2	−.5509	−.5527	−.5563	−.5616	−.5685	−.5769	−.5867	−.5977	−.6098	−.6227	−.6364	−.6505	−.6651
1	α^3	−.1778	−.1770	−.1756	−.1734	−.1706	−.1671	−.1630	−.1584	−.1533	−.1477	−.1416	−.1353	−.1286
1	α^4	−.0015	−.0015	−.0015	−.0014	−.0014	−.0014	−.0014	−.0013	−.0013	−.0012	−.0012	−.0011	−.0011
1	Total	32773.6224	32688.2505	32518.1034	32264.3604	31928.7546	31513.5337	31021.4092	30455.4998	29819.2695	29116.4637	28351.0463	27527.1389	26648.9644
1	δ	.0012	.0012	.0012	.0012	.0012	.0012	.0012	.0013	.0013	.0013	.0013	.0014	.0014
2	BO	29312.1246	29230.4963	29067.8197	28825.2412	28504.4452	28107.6153	27637.3848	27096.7816	26489.1669	25818.1743	25087.6479	24301.5843	23464.0782
2	AD	5.9800	6.0096	6.0685	6.1560	6.2708	6.4114	6.5763	6.7633	6.9702	7.1947	7.4343	7.6865	7.9487
2	NA	1.5306	1.5369	1.5495	1.5682	1.5930	1.6237	1.6600	1.7018	1.7487	1.8005	1.8571	1.9180	1.9831
2	α^2	−.5677	−.5694	−.5727	−.5775	−.5839	−.5916	−.6006	−.6106	−.6216	−.6334	−.6457	−.6585	−.6716
2	α^3	−.1603	−.1596	−.1582	−.1561	−.1535	−.1502	−.1463	−.1419	−.1371	−.1318	−.1261	−.1201	−.1138
2	α^4	−.0013	−.0013	−.0013	−.0013	−.0013	−.0013	−.0012	−.0012	−.0012	−.0011	−.0011	−.0010	−.0010
2	Total	29318.9058	29237.3125	29074.7056	28832.2304	28511.5704	28114.9074	27644.8730	27104.4929	26497.1260	25826.4033	25096.1664	24310.4092	23473.2237
2	δ	.0015	.0015	.0015	.0015	.0015	.0016	.0016	.0016	.0016	.0017	.0017	.0017	.0018
3	BO	26030.1861	25952.2825	25797.0393	25565.5708	25259.5140	24880.9906	24432.5589	23917.1590	23338.0547	22698.7733	22003.0463	21254.7535	20457.8712
3	AD	6.6368	6.6631	6.7154	6.7928	6.8944	7.0186	7.1637	7.3278	7.5088	7.7044	7.9121	8.1293	8.3537
3	NA	2.0550	2.0607	2.0719	2.0887	2.1109	2.1384	2.1709	2.2082	2.2502	2.2965	2.3471	2.4015	2.4597
3	α^2	−.5804	−.5819	−.5849	−.5893	−.5951	−.6021	−.6102	−.6193	−.6292	−.6397	−.6508	−.6621	−.6737
3	α^3	−.1438	−.1431	−.1418	−.1399	−.1374	−.1343	−.1306	−.1265	−.1219	−.1169	−.1115	−.1058	−.0999
3	α^4	−.0012	−.0012	−.0012	−.0012	−.0012	−.0011	−.0011	−.0011	−.0010	−.0010	−.0010	−.0009	−.0009
3	Total	26038.1525	25960.2800	25805.0987	25573.7219	25267.7856	24889.4100	24441.1515	23925.9482	23347.0616	22708.0166	22012.5422	21264.5155	20467.9102
3	δ	.0019	.0019	.0019	.0019	.0019	.0019	.0019	.0020	.0020	.0020	.0020	.0021	.0021
4	BO	22919.9321	22845.7170	22697.8358	22477.3726	22185.9200	21825.5420	21398.7266	20908.3334	20357.5360	19749.7648	19088.6496	18377.9659	17621.5852
4	AD	7.1493	7.1722	7.2175	7.2846	7.3724	7.4795	7.6042	7.7446	7.8986	8.0640	8.2383	8.4191	8.6038
4	NA	2.5308	2.5358	2.5458	2.5607	2.5804	2.6047	2.6335	2.6666	2.7038	2.7448	2.7895	2.8376	2.8890
4	α^2	−.5887	−.5901	−.5928	−.5968	−.6019	−.6082	−.6155	−.6236	−.6323	−.6416	−.6513	−.6611	−.6710
4	α^3	−.1283	−.1277	−.1265	−.1247	−.1223	−.1193	−.1159	−.1119	−.1076	−.1029	−.0978	−.0925	−.0869
4	α^4	−.0011	−.0011	−.0011	−.0011	−.0010	−.0010	−.0010	−.0010	−.0009	−.0009	−.0009	−.0008	−.0008
4	Total	22928.8940	22854.7061	22706.8788	22486.4954	22195.1476	21834.8977	21408.2320	20918.0081	20367.3975	19759.8282	19098.9275	18388.4681	17632.3192
4	δ	.0022	.0022	.0022	.0022	.0022	.0022	.0023	.0023	.0023	.0023	.0024	.0024	.0025
5	BO	19979.9863	19909.4475	19768.9047	19559.4140	19282.5272	18940.2548	18535.0209	18069.6113	17547.1188	16970.8875	16344.4575	15671.5143	14955.8415
5	AD	7.5122	7.5314	7.5696	7.6259	7.6994	7.7886	7.8919	8.0075	8.1333	8.2670	8.4063	8.5488	8.6918
5	NA	2.9589	2.9633	2.9721	2.9851	3.0023	3.0235	3.0486	3.0774	3.1097	3.1453	3.1840	3.2256	3.2698
5	α^2	−.5925	−.5937	−.5961	−.5996	−.6042	−.6097	−.6161	−.6231	−.6307	−.6387	−.6469	−.6552	−.6634
5	α^3	−.1138	−.1132	−.1121	−.1103	−.1081	−.1053	−.1020	−.0983	−.0943	−.0898	−.0851	−.0800	−.0748
5	α^4	−.0010	−.0010	−.0010	−.0009	−.0009	−.0009	−.0009	−.0009	−.0008	−.0008	−.0008	−.0007	−.0007
5	Total	19989.7501	19919.2343	19778.7372	19569.3140	19292.5156	18950.3510	18545.2424	18079.9739	17557.6361	16981.5705	16355.3151	15682.5527	14967.0643
5	δ	.0025	.0025	.0025	.0025	.0025	.0026	.0026	.0026	.0026	.0027	.0027	.0027	.0027

TABLE II: Components of dissociation energy of HD

$v\backslash J$		0	1	2	3	4	5	6	7	8	9	10	11	12
6	BO	17210.1706	17143.3228	17010.1490	16811.6800	16549.4306	16225.3632	15841.8446	15401.5958	14907.6392	14363.2446	13771.8778	13137.1513	12462.7810
6	AD	7.7196	7.7350	7.7657	7.8107	7.8692	7.9397	8.0207	8.1103	8.2065	8.3070	8.4096	8.5118	8.6110
6	NA	3.3390	3.3428	3.3502	3.3613	3.3759	3.3939	3.4151	3.4394	3.4665	3.4963	3.5284	3.5628	3.5991
6	α^2	−.5915	−.5925	−.5946	−.5977	−.6016	−.6063	−.6117	−.6176	−.6240	−.6305	−.6372	−.6438	−.6501
6	α^3	−.1002	−.0996	−.0985	−.0969	−.0948	−.0922	−.0891	−.0856	−.0818	−.0776	−.0731	−.0684	−.0635
6	α^4	−.0009	−.0009	−.0009	−.0008	−.0008	−.0008	−.0008	−.0008	−.0007	−.0007	−.0007	−.0006	−.0006
6	Total	17220.5367	17153.7075	17020.5709	16822.1567	16559.9785	16235.9975	15852.5788	15412.4415	14918.6057	14374.3390	13783.1048	13148.5131	12474.2769
6	δ	.0028	.0028	.0028	.0028	.0028	.0028	.0029	.0029	.0029	.0029	.0029	.0030	.0030
7	BO	14611.6545	14548.5438	14422.8330	14235.5307	13988.1188	13682.5186	13321.0479	12906.3733	12441.4593	11929.5175	11373.9573	10778.3405	10146.3408
7	AD	7.7660	7.7776	7.8003	7.8336	7.8764	7.9274	7.9850	8.0474	8.1126	8.1784	8.2426	8.3025	8.3557
7	NA	3.6688	3.6718	3.6778	3.6868	3.6985	3.7129	3.7297	3.7489	3.7701	3.7932	3.8178	3.8436	3.8704
7	α^2	−.5853	−.5862	−.5879	−.5904	−.5937	−.5975	−.6019	−.6066	−.6116	−.6166	−.6216	−.6263	−.6306
7	α^3	−.0874	−.0869	−.0858	−.0843	−.0823	−.0798	−.0770	−.0737	−.0701	−.0662	−.0620	−.0576	−.0530
7	α^4	−.0008	−.0008	−.0008	−.0007	−.0007	−.0007	−.0007	−.0007	−.0006	−.0006	−.0006	−.0005	−.0005
7	Total	14622.4158	14559.3194	14433.6367	14246.3756	13999.0170	13693.4808	13332.0831	12917.4886	12452.6597	11940.8057	11385.3335	10789.8022	10157.8828
7	δ	.0031	.0031	.0031	.0031	.0031	.0031	.0031	.0031	.0031	.0032	.0032	.0032	.0032
8	BO	12187.1576	12127.8680	12009.7898	11833.9132	11601.6935	11315.0186	10976.1679	10587.7669	10152.7389	9674.2569	9155.6984	8600.6030	8012.6375
8	AD	7.6472	7.6547	7.6693	7.6903	7.7168	7.7475	7.7808	7.8150	7.8480	7.8777	7.9019	7.9180	7.9234
8	NA	3.9434	3.9456	3.9499	3.9563	3.9646	3.9747	3.9863	3.9993	4.0133	4.0280	4.0431	4.0582	4.0728
8	α^2	−.5734	−.5741	−.5754	−.5774	−.5799	−.5828	−.5860	−.5894	−.5929	−.5962	−.5993	−.6019	−.6039
8	α^3	−.0754	−.0749	−.0740	−.0725	−.0706	−.0683	−.0657	−.0626	−.0592	−.0556	−.0517	−.0476	−.0434
8	α^4	−.0007	−.0007	−.0007	−.0007	−.0006	−.0006	−.0006	−.0006	−.0005	−.0005	−.0005	−.0005	−.0004
8	Total	12198.0988	12138.8186	12020.7590	11844.9092	11612.7237	11326.0890	10987.2827	10598.9285	10163.9474	9685.5103	9166.9919	8611.9292	8023.9861
8	δ	.0033	.0033	.0033	.0033	.0033	.0033	.0033	.0033	.0033	.0033	.0033	.0034	.0034
9	BO	9941.2222	9885.8834	9775.6999	9611.6482	9395.1649	9128.1149	8812.7533	8451.6820	8047.8048	7604.2837	7124.4969	6612.0031	6070.5118
9	AD	7.3614	7.3646	7.3708	7.3792	7.3890	7.3988	7.4072	7.4123	7.4123	7.4051	7.3882	7.3593	7.3158
9	NA	4.1543	4.1555	4.1577	4.1609	4.1649	4.1695	4.1744	4.1794	4.1840	4.1879	4.1904	4.1910	4.1890
9	α^2	−.5551	−.5556	−.5565	−.5579	−.5595	−.5614	−.5634	−.5653	−.5671	−.5686	−.5695	−.5697	−.5690
9	α^3	−.0642	−.0638	−.0629	−.0615	−.0598	−.0576	−.0551	−.0523	−.0492	−.0458	−.0422	−.0384	−.0345
9	α^4	−.0006	−.0006	−.0006	−.0006	−.0005	−.0005	−.0005	−.0005	−.0005	−.0004	−.0004	−.0004	−.0004
9	Total	9952.1180	9896.7836	9786.6084	9622.5684	9406.0989	9139.0636	8823.7159	8462.6556	8058.7844	7615.2618	7135.4634	6622.9449	6081.4127
9	δ	.0034	.0034	.0034	.0034	.0034	.0034	.0035	.0035	.0035	.0035	.0035	.0035	.0035
10	BO	7880.5772	7829.3768	7727.4662	7575.8152	7375.8518	7129.4327	6838.8075	6506.5791	6135.6629	5729.2482	5290.7627	4823.8448	4332.3238
10	AD	6.9108	6.9098	6.9075	6.9031	6.8960	6.8847	6.8678	6.8437	6.8103	6.7657	6.7075	6.6332	6.5401
10	NA	4.2883	4.2880	4.2874	4.2864	4.2846	4.2819	4.2779	4.2721	4.2639	4.2528	4.2378	4.2180	4.1923
10	α^2	−.5297	−.5300	−.5304	−.5311	−.5318	−.5325	−.5331	−.5334	−.5332	−.5325	−.5309	−.5283	−.5244
10	α^3	−.0538	−.0534	−.0525	−.0513	−.0496	−.0477	−.0453	−.0427	−.0398	−.0367	−.0334	−.0300	−.0264
10	α^4	−.0005	−.0005	−.0005	−.0005	−.0005	−.0005	−.0004	−.0004	−.0004	−.0004	−.0003	−.0003	−.0003
10	Total	7891.1923	7839.9908	7738.0776	7586.4219	7386.4504	7140.0186	6849.3743	6517.1183	6146.1638	5739.6971	5301.1434	4834.1375	4342.5051
10	δ	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035	.0035
11	BO	6014.6310	5967.8306	5874.7211	5736.2749	5553.9261	5329.5440	5065.4004	4764.1349	4428.7209	4062.4338	3668.8270	3251.7166	2815.1816
11	AD	6.3035	6.2982	6.2875	6.2705	6.2466	6.2144	6.1725	6.1194	6.0530	5.9713	5.8719	5.7520	5.6087
11	NA	4.3251	4.3230	4.3185	4.3117	4.3020	4.2892	4.2726	4.2517	4.2255	4.1930	4.1530	4.1038	4.0435
11	α^2	−.4962	−.4962	−.4961	−.4960	−.4956	−.4950	−.4939	−.4922	−.4898	−.4864	−.4818	−.4757	−.4679
11	α^3	−.0441	−.0437	−.0429	−.0417	−.0402	−.0384	−.0363	−.0339	−.0312	−.0284	−.0254	−.0223	−.0191
11	α^4	−.0004	−.0004	−.0004	−.0004	−.0004	−.0004	−.0004	−.0003	−.0003	−.0003	−.0003	−.0002	−.0002
11	Total	6024.7189	5977.9115	5884.7877	5746.3189	5563.9384	5339.5138	5075.3150	4773.9795	4438.4781	4072.0831	3678.3444	3261.0743	2824.3466
11	δ	.0036	.0036	.0036	.0036	.0035	.0035	.0035	.0035	.0035	.0035	.0034	.0034	.0033

TABLE III: Components of dissociation energy of HD

$v\backslash J$		0	1	2	3	4	5	6	7	8	9	10	11	12
12	BO	4356.1393	4314.0996	4230.5192	4106.3873	3943.1666	3742.7699	3507.5340	3240.1918	2943.8487	2621.9649	2278.3503	1917.1783	1543.0279
12	AD	5.5540	5.5447	5.5257	5.4965	5.4562	5.4037	5.3374	5.2559	5.1569	5.0382	4.8971	4.7302	4.5334
12	NA	4.2361	4.2313	4.2215	4.2064	4.1857	4.1586	4.1243	4.0819	4.0298	3.9666	3.8899	3.7970	3.6841
12	α^2	−.4532	−.4529	−.4522	−.4511	−.4495	−.4472	−.4441	−.4401	−.4349	−.4282	−.4198	−.4093	−.3962
12	α^3	−.0350	−.0347	−.0340	−.0329	−.0316	−.0299	−.0280	−.0258	−.0234	−.0209	−.0182	−.0154	−.0126
12	α^4	−.0003	−.0003	−.0003	−.0003	−.0003	−.0003	−.0003	−.0003	−.0002	−.0002	−.0002	−.0002	−.0002
12	Total	4365.4408	4323.3876	4239.7798	4115.6059	3952.3271	3751.8548	3516.5234	3249.0634	2952.5769	2630.5204	2286.6991	1925.2806	1550.8364
12	δ	.0035	.0035	.0035	.0035	.0034	.0034	.0034	.0034	.0033	.0033	.0032	.0031	.0030
13	BO	2922.1276	2885.3457	2812.2995	2704.0177	2562.0269	2388.3353	2185.4157	1956.1923	1704.0368	1432.7806	1146.7579	850.8965	550.9027
13	AD	4.6825	4.6692	4.6423	4.6012	4.5449	4.4723	4.3818	4.2714	4.1387	3.9806	3.7929	3.5702	3.3040
13	NA	3.9820	3.9735	3.9561	3.9295	3.8929	3.8454	3.7857	3.7119	3.6219	3.5127	3.3802	3.2189	3.0205
13	α^2	−.3991	−.3984	−.3969	−.3946	−.3914	−.3872	−.3816	−.3746	−.3657	−.3548	−.3412	−.3244	−.3036
13	α^3	−.0267	−.0264	−.0258	−.0248	−.0236	−.0221	−.0204	−.0184	−.0163	−.0141	−.0117	−.0093	−.0069
13	α^4	−.0003	−.0003	−.0003	−.0003	−.0002	−.0002	−.0002	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001
13	Total	2930.3661	2893.5633	2820.4750	2712.1287	2570.0495	2396.2435	2193.1810	1963.7825	1711.4152	1439.9049	1153.5779	857.3517	556.9166
13	δ	.0033	.0033	.0033	.0032	.0032	.0032	.0031	.0030	.0030	.0029	.0028	.0026	.0025
14	BO	1735.1804	1704.3526	1643.2523	1552.9868	1435.2108	1292.1227	1126.4695	941.5659	741.3453	530.4684	314.5506	100.6773	
14	AD	3.7094	3.6920	3.6569	3.6033	3.5302	3.4359	3.3182	3.1743	2.9999	2.7890	2.5319	2.2103	
14	NA	3.5105	3.4965	3.4683	3.4251	3.3658	3.2886	3.1914	3.0710	2.9229	2.7408	2.5144	2.2253	
14	α^2	−.3314	−.3302	−.3278	−.3240	−.3188	−.3119	−.3031	−.2920	−.2781	−.2608	−.2391	−.2112	
14	α^3	−.0191	−.0188	−.0182	−.0174	−.0163	−.0150	−.0135	−.0118	−.0099	−.0080	−.0060	−.0040	
14	α^4	−.0002	−.0002	−.0002	−.0002	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001	−.0001	−.0001	
14	Total	1742.0495	1711.1919	1650.0313	1559.6737	1441.7714	1298.5202	1132.6624	947.5072	746.9799	535.7292	319.3516	104.8977	
14	δ	.0029	.0029	.0028	.0028	.0028	.0027	.0026	.0025	.0024	.0023	.0021	.0018	
15	BO	825.2635	801.4025	754.3116	685.2591	596.1662	489.6422	369.0594	238.7099	104.1687				
15	AD	2.6428	2.6205	2.5752	2.5059	2.4106	2.2863	2.1284	1.9294	1.6753				
15	NA	2.7561	2.7344	2.6904	2.6227	2.5293	2.4067	2.2500	2.0510	1.7947				
15	α^2	−.2471	−.2453	−.2416	−.2358	−.2278	−.2171	−.2033	−.1857	−.1627				
15	α^3	−.0121	−.0118	−.0114	−.0106	−.0097	−.0086	−.0073	−.0058	−.0043				
15	α^4	−.0001	−.0001	−.0001	−.0001	−.0001	−.0001	−.0001	−.0001	−.0001				
15	Total	830.4030	806.5001	759.3242	690.1412	600.8685	494.1095	373.2271	242.4988	107.4717				
15	δ	.0023	.0022	.0022	.0022	.0021	.0020	.0018	.0017	.0015				
16	BO	232.1388	216.8501	187.0898	144.5419	91.8939	33.2087							
16	AD	1.4598	1.4292	1.3665	1.2686	1.1288	.9321							
16	NA	1.6422	1.6083	1.5389	1.4304	1.2756	1.0578							
16	α^2	−.1420	−.1392	−.1334	−.1243	−.1112	−.0926							
16	α^3	−.0058	−.0056	−.0051	−.0045	−.0037	−.0027							
16	α^4	−.0001	−.0001	−.0001	−.0001	.0000	.0000							
16	Total	235.0929	219.7427	189.8566	147.1120	94.1833	35.1032							
16	δ	.0013	.0013	.0013	.0012	.0010	.0009							
17	BO	3.3226	.2368											
17	AD	.1545	.0846											
17	NA	.1822	.1040											
17	α^2	−.0164	−.0096											
17	α^3	−.0004	−.0002											
17	α^4	.0000	.0000											
17	Total	3.6424	.4156											
17	δ	.0001	.0001											

TABLE IV: Components of dissociation energy of HD

$v\backslash J$		13	14	15	16	17	18	19	20	21	22	23	24	25
0	BO	29017.2781	27996.0344	26930.8865	25826.1524	24686.0517	23514.6829	22316.0069	21093.8357	19851.8251	18593.4714	17322.1113	16040.9253	14752.9423
0	AD	7.0460	7.4020	7.7653	8.1332	8.5031	8.8727	9.2397	9.6016	9.9564	10.3017	10.6357	10.9560	11.2608
0	NA	.9688	1.0581	1.1516	1.2489	1.3499	1.4543	1.5620	1.6728	1.7864	1.9029	2.0219	2.1435	2.2676
0	α^2	−.6707	−.6872	−.7035	−.7197	−.7356	−.7511	−.7660	−.7803	−.7938	−.8065	−.8184	−.8292	−.8390
0	α^3	−.1371	−.1296	−.1218	−.1140	−.1060	−.0981	−.0901	−.0821	−.0742	−.0664	−.0586	−.0510	−.0436
0	α^4	−.0012	−.0011	−.0010	−.0010	−.0009	−.0009	−.0008	−.0007	−.0007	−.0006	−.0006	−.0005	−.0004
0	Total	29024.4839	28003.6768	26938.9769	25834.6998	24695.0621	23524.1599	22325.9517	21104.2469	19862.6992	18604.8024	17333.8914	16053.1441	14765.5876
0	δ	.0011	.0012	.0012	.0013	.0013	.0014	.0015	.0016	.0016	.0017	.0018	.0019	.0020
1	BO	25712.3594	24738.0860	23722.3320	22669.2785	21583.0144	20467.5161	19326.6330	18164.0773	16983.4184	15788.0815	14581.3488	13366.3643	12146.1411
1	AD	7.7039	8.0199	8.3406	8.6635	8.9861	9.3061	9.6209	9.9282	10.2259	10.5114	10.7827	11.0375	11.2734
1	NA	1.5352	1.6159	1.7004	1.7886	1.8801	1.9748	2.0726	2.1733	2.2767	2.3827	2.4912	2.6021	2.7153
1	α^2	−.6798	−.6946	−.7093	−.7237	−.7378	−.7513	−.7643	−.7765	−.7879	−.7984	−.8080	−.8164	−.8238
1	α^3	−.1217	−.1146	−.1073	−.0999	−.0924	−.0849	−.0774	−.0699	−.0625	−.0551	−.0479	−.0408	−.0338
1	α^4	−.0010	−.0010	−.0009	−.0009	−.0008	−.0008	−.0007	−.0006	−.0006	−.0005	−.0005	−.0004	−.0004
1	Total	25720.7960	24746.9115	23731.5555	22678.9061	21593.0497	20477.9601	19337.4841	18175.3317	16995.0699	15800.1215	14593.7664	13379.1463	12159.2718
1	δ	.0015	.0015	.0016	.0016	.0017	.0018	.0018	.0019	.0020	.0021	.0022	.0022	.0023
2	BO	22579.2735	21651.3207	20684.3401	19682.3921	18649.4529	17589.3962	16505.9809	15402.8425	14283.4896	13151.3045	12009.5467	10861.3606	9709.7857
2	AD	8.2182	8.4925	8.7689	9.0449	9.3180	9.5857	9.8455	10.0950	10.3319	10.5535	10.7575	10.9414	11.1025
2	NA	2.0521	2.1248	2.2010	2.2804	2.3630	2.4485	2.5367	2.6276	2.7209	2.8165	2.9144	3.0143	3.1161
2	α^2	−.6847	−.6978	−.7108	−.7234	−.7355	−.7470	−.7579	−.7679	−.7771	−.7852	−.7923	−.7982	−.8027
2	α^3	−.1072	−.1005	−.0937	−.0867	−.0797	−.0726	−.0656	−.0586	−.0516	−.0447	−.0380	−.0313	−.0249
2	α^4	−.0009	−.0009	−.0008	−.0008	−.0007	−.0007	−.0006	−.0006	−.0005	−.0005	−.0004	−.0003	−.0003
2	Total	22588.7509	21661.1387	20694.5047	19692.9066	18660.3180	17600.6100	16517.5390	15414.7380	14295.7132	13163.8441	12022.3880	10874.4865	9723.1764
2	δ	.0018	.0019	.0019	.0020	.0021	.0021	.0022	.0023	.0023	.0024	.0025	.0026	.0026
3	BO	19616.4252	18734.4512	17815.9599	16864.9097	15885.1848	14880.5795	13854.7875	12811.3962	11753.8861	10685.6336	9609.9193	8529.9393	7448.8217
3	AD	8.5825	8.8132	9.0432	9.2699	9.4907	9.7031	9.9045	10.0923	10.2640	10.4169	10.5481	10.6549	10.7340
3	NA	2.5214	2.5863	2.6544	2.7253	2.7990	2.8752	2.9539	3.0347	3.1175	3.2022	3.2884	3.3760	3.4646
3	α^2	−.6852	−.6966	−.7076	−.7183	−.7284	−.7378	−.7464	−.7541	−.7608	−.7663	−.7706	−.7735	−.7749
3	α^3	−.0937	−.0874	−.0810	−.0744	−.0678	−.0612	−.0546	−.0480	−.0416	−.0352	−.0289	−.0227	−.0167
3	α^4	−.0008	−.0008	−.0007	−.0007	−.0006	−.0006	−.0005	−.0005	−.0004	−.0004	−.0003	−.0003	−.0002
3	Total	19626.7494	18745.0660	17826.8681	16876.1114	15896.6776	14892.3583	13866.8443	12823.7206	11766.4648	10698.4508	9622.9561	8543.1737	7462.2285
3	δ	.0022	.0022	.0023	.0023	.0024	.0024	.0025	.0026	.0026	.0027	.0028	.0028	.0029
4	BO	16823.4316	15987.4434	15117.5418	14217.6057	13291.4527	12342.8259	11375.3865	10392.7117	9398.2975	8395.5672	7387.8852	6378.5769	5370.9565
4	AD	8.7899	8.9747	9.1557	9.3302	9.4955	9.6491	9.7881	9.9099	10.0115	10.0901	10.1423	10.1649	10.1540
4	NA	2.9433	3.0005	3.0603	3.1225	3.1869	3.2533	3.3215	3.3912	3.4622	3.5341	3.6065	3.6789	3.7507
4	α^2	−.6808	−.6904	−.6995	−.7081	−.7160	−.7231	−.7293	−.7344	−.7383	−.7408	−.7419	−.7413	−.7389
4	α^3	−.0811	−.0752	−.0691	−.0630	−.0568	−.0506	−.0445	−.0384	−.0324	−.0264	−.0206	−.0150	−.0095
4	α^4	−.0007	−.0007	−.0006	−.0006	−.0005	−.0005	−.0004	−.0004	−.0003	−.0003	−.0003	−.0002	−.0002
4	Total	16834.4021	15998.6523	15128.9885	14229.2866	13303.3617	12354.9540	11387.7220	10405.2397	9411.0003	8408.4239	7400.8713	6391.6642	5384.1125
4	δ	.0025	.0025	.0026	.0026	.0027	.0027	.0028	.0028	.0029	.0030	.0030	.0031	.0031
5	BO	14201.2798	13411.6920	12590.9340	11742.8335	10871.1735	9979.6839	9072.0375	8151.8536	7222.7076	6288.1477	5351.7205	4417.0075	3487.6759
5	AD	8.8329	8.9693	9.0985	9.2176	9.3241	9.4149	9.4873	9.5382	9.5644	9.5626	9.5289	9.4591	9.3484
5	NA	3.3165	3.3653	3.4162	3.4688	3.5228	3.5780	3.6340	3.6904	3.7467	3.8023	3.8563	3.9078	3.9555
5	α^2	−.6713	−.6789	−.6859	−.6923	−.6978	−.7023	−.7057	−.7078	−.7085	−.7075	−.7048	−.7000	−.6930
5	α^3	−.0694	−.0638	−.0581	−.0524	−.0467	−.0409	−.0352	−.0295	−.0240	−.0185	−.0132	−.0081	−.0032
5	α^4	−.0006	−.0006	−.0005	−.0005	−.0005	−.0004	−.0004	−.0003	−.0003	−.0002	−.0002	−.0002	−.0001
5	Total	14212.6878	13423.2833	12602.7041	11754.7747	10883.2755	9991.9332	9084.4176	8164.3445	7235.2859	6300.7862	5364.3875	4429.6661	3500.2837
5	δ	.0028	.0028	.0029	.0029	.0029	.0030	.0030	.0031	.0031	.0032	.0032	.0032	.0033

TABLE V: Components of dissociation energy of HD

$v\backslash J$		13	14	15	16	17	18	19	20	21	22	23	24	25
6	BO	11752.5477	11010.2654	10239.7570	9444.8355	8629.2939	7796.9006	6951.4042	6096.5448	5236.0757	4373.7974	3513.6067	2659.5698	1816.0315
6	AD	8.7046	8.7900	8.8644	8.9250	8.9689	8.9931	8.9944	8.9694	8.9146	8.8257	8.6981	8.5261	8.3027
6	NA	3.6371	3.6764	3.7168	3.7579	3.7993	3.8405	3.8808	3.9196	3.9560	3.9887	4.0162	4.0365	4.0466
6	α^2	−.6561	−.6615	−.6661	−.6700	−.6727	−.6743	−.6745	−.6732	−.6700	−.6649	−.6575	−.6473	−.6341
6	α^3	−.0584	−.0532	−.0480	−.0426	−.0373	−.0320	−.0267	−.0215	−.0165	−.0115	−.0067	−.0021	.0022
6	α^4	−.0005	−.0005	−.0005	−.0004	−.0004	−.0003	−.0003	−.0003	−.0002	−.0002	−.0001	−.0001	−.0001
6	Total	11764.1743	11022.0166	10251.6236	9456.8054	8641.3516	7809.0275	6963.5779	6108.7389	5248.2595	4385.9352	3525.6567	2671.4828	1827.7489
6	δ	.0030	.0031	.0031	.0031	.0032	.0032	.0032	.0033	.0033	.0033	.0033	.0033	.0033
7	BO	9481.7095	8788.2487	8069.7908	7330.1868	6573.3025	5803.0243	5023.2747	4238.0424	3451.4272	2667.7112	1891.4663	1127.7257	382.2716
7	AD	8.3996	8.4314	8.4482	8.4472	8.4251	8.3788	8.3047	8.1988	8.0566	7.8727	7.6404	7.3509	6.9911
7	NA	3.8978	3.9253	3.9525	3.9787	4.0034	4.0257	4.0444	4.0582	4.0654	4.0636	4.0496	4.0187	3.9640
7	α^2	−.6343	−.6372	−.6393	−.6402	−.6399	−.6380	−.6344	−.6289	−.6210	−.6105	−.5968	−.5793	−.5569
7	α^3	−.0483	−.0435	−.0386	−.0337	−.0288	−.0239	−.0191	−.0144	−.0098	−.0054	−.0012	.0028	.0065
7	α^4	−.0005	−.0004	−.0004	−.0004	−.0003	−.0003	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001	.0000
7	Total	9493.3238	8799.9242	8081.5132	7341.9385	6585.0622	5814.7666	5034.9701	4249.6560	3462.9182	2679.0314	1902.5582	1138.5187	392.6763
7	δ	.0032	.0033	.0033	.0033	.0033	.0033	.0033	.0034	.0034	.0034	.0033	.0033	.0033
8	BO	7395.5661	6753.2298	6089.5337	5408.4448	4714.0009	4010.3337	3301.7091	2592.5943	1887.7620	1192.4601	512.7007		
8	AD	7.9156	7.8916	7.8485	7.7831	7.6921	7.5715	7.4173	7.2242	6.9858	6.6939	6.3359		
8	NA	4.0864	4.0982	4.1075	4.1133	4.1144	4.1094	4.0961	4.0720	4.0336	3.9756	3.8906		
8	α^2	−.6051	−.6053	−.6042	−.6018	−.5977	−.5917	−.5834	−.5724	−.5583	−.5404	−.5176		
8	α^3	−.0390	−.0346	−.0301	−.0256	−.0211	−.0167	−.0123	−.0081	−.0041	−.0003	.0033		
8	α^4	−.0004	−.0004	−.0003	−.0003	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001	.0000		
8	Total	7406.9236	6764.5794	6100.8550	5419.7136	4725.1884	4021.4061	3312.6267	2603.3098	1898.2188	1202.5889	522.4130		
8	δ	.0034	.0034	.0034	.0034	.0034	.0034	.0034	.0034	.0033	.0033	.0032		
9	BO	5503.8623	4916.0122	4311.0380	3693.1508	3066.7301	2436.3848	1807.0535	1184.1722	573.9630				
9	AD	7.2548	7.1735	7.0686	6.9364	6.7731	6.5736	6.3321	6.0404	5.6867				
9	NA	4.1834	4.1731	4.1569	4.1330	4.0992	4.0526	3.9894	3.9041	3.7882				
9	α^2	−.5672	−.5641	−.5594	−.5528	−.5440	−.5326	−.5181	−.4997	−.4764				
9	α^3	−.0305	−.0264	−.0223	−.0183	−.0142	−.0103	−.0065	−.0029	.0006				
9	α^4	−.0003	−.0003	−.0003	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001				
9	Total	5514.7025	4926.7680	4321.6815	3703.6489	3077.0439	2446.4679	1816.8504	1193.6140	582.9620				
9	δ	.0035	.0034	.0034	.0034	.0034	.0033	.0033	.0032	.0031				
10	BO	3820.2124	3291.7133	2751.2459	2203.5006	1653.5341	1106.9342	570.1135	50.8785					
10	AD	6.4252	6.2852	6.1162	5.9138	5.6721	5.3833	5.0359	4.6103					
10	NA	4.1591	4.1166	4.0624	3.9934	3.9053	3.7920	3.6444	3.4472					
10	α^2	−.5190	−.5118	−.5025	−.4906	−.4755	−.4566	−.4328	−.4022					
10	α^3	−.0228	−.0191	−.0154	−.0118	−.0083	−.0049	−.0017	.0013					
10	α^4	−.0003	−.0002	−.0002	−.0002	−.0001	−.0001	−.0001	.0000					
10	Total	3830.2546	3301.5839	2760.9064	2212.9053	1662.6275	1115.6479	578.3592	58.5350					
10	δ	.0034	.0034	.0033	.0033	.0032	.0031	.0030	.0028					
11	BO	2363.5820	1901.6070	1434.3652	967.5491	507.7385	63.0112							
11	AD	5.4384	5.2367	4.9980	4.7147	4.3751	3.9588							
11	NA	3.9694	3.8781	3.7649	3.6233	3.4431	3.2070							
11	α^2	−.4580	−.4455	−.4299	−.4104	−.3859	−.3545							
11	α^3	−.0158	−.0126	−.0094	−.0063	−.0033	−.0005							
11	α^4	−.0002	−.0002	−.0001	−.0001	−.0001	−.0001							
11	Total	2372.5158	1910.2635	1442.6887	975.4703	515.1674	69.8220							
11	δ	.0033	.0032	.0031	.0030	.0028	.0026							

TABLE VI: Components of dissociation energy of HD

$v\backslash J$		13	14	15	16
12	BO	1160.9721	776.7464	397.0753	30.3683
12	AD	4.3011	4.0256	3.6946	3.2853
12	NA	3.5462	3.3760	3.1621	2.8840
12	α^2	−.3800	−.3599	−.3346	−.3019
12	α^3	−.0098	−.0070	−.0043	−.0017
12	α^4	−.0001	−.0001	−.0001	−.0001
12	Total	1168.4295	783.7811	403.5930	36.2340
12	δ	.0029	.0028	.0026	.0024
13	BO	253.6399			
13	AD	2.9805			
13	NA	2.7712			
13	α^2	−.2772			
13	α^3	−.0045			
13	α^4	−.0001			
13	Total	259.1098			
13	δ	.0023			

TABLE VII: Components of dissociation energy of HD

$v\backslash J$		26	27	28	29	30	31	32	33	34	35	36
0	BO	13461.0478	12167.9931	10876.4064	9588.8060	8307.6152	7035.1791	5773.7842	4525.6820	3293.1165	2078.3596	883.7564
0	AD	11.5479	11.8152	12.0606	12.2817	12.4763	12.6417	12.7751	12.8732	12.9324	12.9484	12.9158
0	NA	2.3940	2.5227	2.6537	2.7869	2.9221	3.0594	3.1987	3.3399	3.4828	3.6272	3.7730
0	α^2	−.8477	−.8553	−.8616	−.8666	−.8703	−.8725	−.8732	−.8723	−.8696	−.8650	−.8582
0	α^3	−.0363	−.0291	−.0222	−.0154	−.0089	−.0025	.0035	.0094	.0150	.0203	.0254
0	α^4	−.0004	−.0003	−.0003	−.0002	−.0002	−.0001	−.0001	.0000	.0000	.0001	.0001
0	Total	13474.1053	12181.4463	10890.2366	9602.9923	8322.1343	7050.0050	5788.8882	4541.0321	3308.6771	2094.0906	899.6125
0	δ	.0021	.0022	.0023	.0024	.0025	.0026	.0027	.0028	.0029	.0030	.0032
1	BO	10923.5711	9701.4378	8482.4306	7269.1634	6064.1955	4870.0580	3689.2869	2524.4643	1378.2761	253.5906	
1	AD	11.4881	11.6790	11.8437	11.9793	12.0827	12.1503	12.1782	12.1617	12.0948	11.9703	
1	NA	2.8307	2.9481	3.0675	3.1887	3.3114	3.4356	3.5609	3.6868	3.8128	3.9381	
1	α^2	−.8299	−.8347	−.8382	−.8401	−.8405	−.8391	−.8359	−.8306	−.8230	−.8128	
1	α^3	−.0270	−.0203	−.0139	−.0077	−.0016	.0042	.0097	.0150	.0200	.0247	
1	α^4	−.0003	−.0003	−.0002	−.0002	−.0001	−.0001	.0000	.0000	.0001	.0001	
1	Total	10937.0326	9715.2096	8496.4896	7283.4834	6078.7473	4884.8089	3704.1998	2539.4972	1393.3807	268.7111	
1	δ	.0024	.0025	.0026	.0027	.0028	.0029	.0030	.0031	.0032	.0033	
2	BO	8557.7710	7408.1924	6263.8753	5127.6224	4002.2492	2890.6318	1795.7709	720.8840			
2	AD	11.2379	11.3448	11.4199	11.4595	11.4593	11.4145	11.3190	11.1649			
2	NA	3.2195	3.3244	3.4305	3.5374	3.6445	3.7514	3.8571	3.9603			
2	α^2	−.8059	−.8076	−.8077	−.8060	−.8023	−.7964	−.7881	−.7770			
2	α^3	−.0185	−.0124	−.0065	−.0008	.0047	.0100	.0149	.0196			
2	α^4	−.0002	−.0002	−.0002	−.0001	−.0001	.0000	.0000	.0001			
2	Total	8571.4037	7422.0415	6277.9114	5141.8124	4016.5555	2905.0113	1810.1737	735.2519			
2	δ	.0027	.0028	.0029	.0030	.0030	.0031	.0032	.0033			
3	BO	6369.6488	5295.4850	4229.4148	3174.5927	2134.3130	1112.1110	111.9184				
3	AD	10.7822	10.7957	10.7702	10.7006	10.5809	10.4032	10.1571				
3	NA	3.5539	3.6432	3.7321	3.8195	3.9043	3.9848	4.0584				
3	α^2	−.7747	−.7726	−.7686	−.7622	−.7534	−.7415	−.7261				
3	α^3	−.0109	−.0053	.0001	.0052	.0101	.0148	.0191				
3	α^4	−.0002	−.0001	−.0001	−.0001	.0000	.0000	.0001				
3	Total	6383.1991	5309.1459	4243.1485	3188.3557	2148.0549	1125.7723	125.4269				
3	δ	.0030	.0030	.0031	.0032	.0032	.0033	.0034				
4	BO	4368.3648	3374.2205	2392.0932	1425.8097	479.6182						
4	AD	10.1053	10.0139	9.8738	9.6772	9.4139						
4	NA	3.8209	3.8886	3.9521	4.0095	4.0576						
4	α^2	−.7345	−.7278	−.7185	−.7061	−.6900						
4	α^3	−.0042	.0008	.0057	.0102	.0145						
4	α^4	−.0001	−.0001	.0000	.0000	.0000						
4	Total	4381.5521	3387.3960	2405.2063	1438.8004	492.4142						
4	δ	.0032	.0032	.0033	.0033	.0034						
5	BO	2567.5532	1660.7354	771.7567								
5	AD	9.1910	8.9793	8.7036								
5	NA	3.9976	4.0315	4.0536								
5	α^2	−.6832	−.6704	−.6537								
5	α^3	.0016	.0060	.0102								
5	α^4	−.0001	.0000	.0000								
5	Total	2580.0600	1673.0818	783.8704								
5	δ	.0033	.0033	.0034								

TABLE VIII: Components of dissociation energy of HD

$v \backslash J$		26	27
6	BO	987.7868	180.3678
6	AD	8.0184	7.6597
6	NA	4.0424	4.0175
6	α^2	$-.6170$	$-.5950$
6	α^3	.0063	.0101
6	α^4	.0000	.0000
6	Total	999.2369	191.4601
6	δ	.0033	.0033