

Supplementary Material for “Comparative Studies of Density Functional Approximations for Light Atoms in Strong Magnetic Fields”

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TABLE I: Total energies of the Helium atom in B fields. (Energies in Hartree, B in a.u.) “HF” is Hartree-Fock. The XC functionals are PW92 for LDA, PBE for GGA, and TPSS MGGA. The HGGA functional combines exact exchange and the TPSS C functionals. See article for details, as well as for state labeling. The column labeled WFM gives published results from correlated wave function methods, as detailed in the footnotes.

State	$B(\text{au})$	HF, present	HF, prior ^a	LDA	GGA	MGGA	HGGA	WFM ^b
1s ²								
0	-2.861679	-2.861679996	-2.83445	-2.89294	-2.90966	-2.90483	-2.903351	
0.01	-2.861660	-2.861660249	-2.83443	-2.89291	-2.90964	-2.90481		
0.02	-2.861600	-2.861601014	-2.83437	-2.89285	-2.90958	-2.90475	-2.903270	
0.04	-2.861364	-2.861364147	-2.83411	-2.89260	-2.90934	-2.90452	-2.903036	
0.08	-2.860417	-2.860417861	-2.83308	-2.89160	-2.90837	-2.90358	-2.902083	
0.1	-2.859709	-2.859709376	-2.83232	-2.89085	-2.90764	-2.90289		
0.16	-2.856651		-2.82900	-2.88762	-2.90450	-2.89987	-2.898290	
0.24	-2.850435	-2.850435823	-2.82229	-2.88107	-2.89814	-2.89373	-2.892035	
0.4	-2.831013	-2.831013483	-2.80144	-2.86072	-2.87833	-2.87454	-2.872501	
0.5	-2.814450	-2.814450946	-2.78378	-2.84347	-2.86151	-2.85816	-2.855859	
0.8	-2.746839	-2.746839677	-2.71240	-2.77363	-2.79320	-2.79116	-2.787556	
1	-2.688884	-2.688884848	-2.65177	-2.71423	-2.73491	-2.73364	-2.729508	
1.6	-2.467388		-2.42242	-2.48900	-2.51310	-2.51335	-2.507952	
2	-2.289144	-2.289144423	-2.23932	-2.30882	-2.33511	-2.33581	-2.329780	
4	-1.176295	-1.176297919	-1.10685	-1.19083	-1.22647	-1.22546		
5	-0.532442	-0.532445132	-0.45536	-0.54618	-0.58565	-0.58245	-0.574877	
8	1.591275	1.591274097	1.68598	1.57640	1.52752	1.53956		
10	3.110634	3.110633781	3.21416	3.09325	3.03926	3.05817	3.064582	
20	11.319611	11.319608967	11.44959	11.28092	11.20842	11.26517	11.267051	
40	29.012108	29.012106576	29.15918	28.91752	28.82238	28.95636		
50	38.143906	38.143903320	38.29203	38.01980	37.91648	38.08790	38.076320	
80	66.092087	66.092085756	66.23035	65.87939	65.75751	66.03580		
100	85.004179	85.004177725	85.13000	84.73367	84.60239	84.94788	84.918313	
160	142.45118		142.5276	142.0151	141.8630	142.3951		
200	181.10639		181.1452	180.5661	180.4036	181.0506		
240	219.94017		219.9398	219.3000	219.1288	219.8846		
400	376.32909		376.1683	375.3226	375.1265	376.2744		
500	474.58300		474.3231	473.3682	473.1613	474.5288		
560	533.65483		533.3365	532.3210	532.1086	533.6009		
800	770.54396		770.0003	768.7686	768.5391	770.4910		
1000	968.44540		967.7239	966.3349	966.0951	968.3932		
2000	1961.1249		1959.617	1957.605	1957.338	1961.075		
1s2s								

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TABLE I (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b
0		-2.174251		-2.12026	-2.17681	-2.18014	-2.17748	-2.175220
0.01		-2.184058		-2.13007	-2.18662	-2.18996	-2.18729	
0.02		-2.193485		-2.13950	-2.19607	-2.19941	-2.19671	-2.194461
0.04		-2.211243		-2.15730	-2.21392	-2.21727	-2.21440	-2.212236
0.08		-2.242906	-2.2425	-2.18914	-2.24593	-2.24931	-2.24639	-2.243958
0.1		-2.257141		-2.20351	-2.26041	-2.26381	-2.26072	
0.16		-2.295123		-2.24211	-2.29941	-2.30283	-2.29895	-2.296318
0.24		-2.338235		-2.28657	-2.34456	-2.34794	-2.34221	-2.339560
0.4		-2.411242	-2.4111	-2.36399	-2.42389	-2.42715	-2.41487	-2.412723
0.5		-2.452831		-2.40904	-2.47045	-2.47383	-2.45602	-2.454347
0.8		-2.572115	-2.5720	-2.53820	-2.60375	-2.60818	-2.57437	-2.573615
1		-2.649181		-2.62036	-2.68823	-2.69328	-2.65114	-2.650655
1.6		-2.866164	-2.8659	-2.84770	-2.92193	-2.92858	-2.86770	-2.867620
2		-2.998242		-2.98462	-3.06295	-3.07058	-2.99964	-2.999708
4		-3.543618	-3.5435	-3.54665	-3.64375	-3.65564	-3.54473	
5		-3.766671		-3.77613	-3.88168	-3.89539	-3.76771	-3.768199
8		-4.320356	-4.3202	-4.34631	-4.47444	-4.49267	-4.32125	
10		-4.625938		-4.66158	-4.80304	-4.82376	-4.62677	-4.627450
20		-5.771020		-5.84800	-6.04412	-6.07395	-5.77166	-5.772448
40		-7.254434	-7.2543	-7.39836	-7.67512	-7.71613	-7.25491	
50		-7.814002		-7.98735	-8.29724	-8.34223	-7.81443	-7.815256
80		-9.138636	-9.1385	-9.39092	-9.78476	-9.83867	-9.13897	
100		-9.841990		-10.14155	-10.58304	-10.64141	-9.84228	-9.843074
160		-11.49473	-11.4945	-11.92017	-12.48199	-12.55018	-11.49493	
200		-12.36634		-12.86667	-13.49668	-13.56981	-12.36651	
240		-13.12269	-13.1223	-13.69284	-14.38470	-14.46163	-13.12288	
400		-15.46711	-15.4668	-16.28260	-17.18174	-17.26680	-15.46725	
500		-16.60183		-17.55199	-18.55979	-18.64498	-16.60196	
560		-17.20526	-17.2046	-18.23126	-19.29903	-19.38219	-17.20538	
800		-19.22890	-19.2286	-20.53068	-21.81084	-21.87227	-19.22900	
1000		-20.59486		-22.10166	-23.53526	-23.58779	-20.59494	
2000		-25.36397		-27.70952	-29.74620	-29.8569	-25.3640	
1s2p _o								
0		-2.131357		-2.08755	-2.14430	-2.14653	-2.13295	-2.132910
0.01		-2.141222		-2.09743	-2.15418	-2.15642	-2.14281	
0.02		-2.150820		-2.10707	-2.16383	-2.16607	-2.15242	-2.152378
0.04		-2.169254		-2.12566	-2.18245	-2.18470	-2.17089	-2.170822
0.08		-2.203497	-2.2031	-2.16043	-2.21731	-2.21962	-2.20526	-2.205130
0.1		-2.219554		-2.17675	-2.23374	-2.23609	-2.22139	
0.16		-2.264677		-2.22296	-2.28013	-2.28260	-2.26675	-2.266575
0.24		-2.319889		-2.27961	-2.33699	-2.33963	-2.32227	-2.322032
0.4		-2.419758	-2.4197	-2.38199	-2.44011	-2.44328	-2.42268	-2.422361
0.5		-2.477330		-2.44083	-2.49949	-2.50302	-2.48054	-2.480172
0.8		-2.634835	-2.6347	-2.60110	-2.66166	-2.66633	-2.63874	-2.638222
1		-2.730167		-2.69769	-2.75972	-2.76512	-2.73444	-2.733813
1.6		-2.983027	-2.9827	-2.95297	-3.01995	-3.02737	-2.98811	-2.987185
2		-3.130765		-3.10182	-3.17230	-3.18092	-3.13622	-3.135142
4		-3.719107	-3.7186	-3.69519	-3.78302	-3.79634	-3.72547	
5		-3.953988		-3.93291	-4.02888	-4.04403	-3.96052	-3.959235
8		-4.528881	-4.5282	-4.51749	-4.63565	-4.65525	-4.53554	
10		-4.842627		-4.83827	-4.96966	-4.99168	-4.84923	-4.848590
20		-6.004818		-6.03698	-6.22340	-6.25419	-6.01082	-6.011488
40		-7.493280	-7.4932	-7.59400	-7.86234	-7.90398	-7.49824	
50		-8.052221		-8.18433	-8.48637	-8.53193	-8.05679	-8.059466
80		-9.372604	-9.3724	-9.59005	-9.97759	-10.03201	-9.37635	
100		-10.072805		-10.34157	-10.77768	-10.83656	-10.07617	-10.079973
160		-11.717161	-11.7170	-12.12230	-12.68101	-12.74964	-11.71977	
200		-12.584195		-13.07001	-13.69809	-13.77148	-12.58649	
240		-13.336615	-13.3364	-13.89730	-14.58822	-14.66551	-13.33867	
400		-15.669483	-15.6691	-16.49098	-17.39231	-17.48033	-15.67096	
500		-16.799065		-17.76251	-18.77421	-18.86663	-16.80032	

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TABLE I (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b
	560	-17.399901	-17.3996	-18.44306	-19.51570	-19.61026	-17.40105	
	800	-19.415400	-19.4150	-20.74737	-22.03592	-22.13630	-19.41625	
	1000	-20.776400		-22.32220	-23.76654	-23.86966	-20.77715	
	2000	-25.530899		-27.94539	-29.99944	-30.1089	-25.5314	
1s2p ₋₁								
	0	-2.131347		-2.08231	-2.13734	-2.13855	-2.13508	-2.133149
	0.01	-2.146083		-2.09705	-2.15208	-2.15329	-2.14983	
	0.02	-2.160300		-2.11128	-2.16631	-2.16750	-2.16406	-2.162112
	0.04	-2.187279		-2.13832	-2.19333	-2.19446	-2.19110	-2.189128
	0.08	-2.236463	-2.2353	-2.18772	-2.24267	-2.24357	-2.24045	-2.238504
	0.1	-2.259234		-2.21064	-2.26552	-2.26631	-2.26330	
	0.16	-2.322599		-2.27444	-2.32908	-2.32956	-2.32690	-2.325189
	0.24	-2.399271		-2.35158	-2.40585	-2.40606	-2.40383	-2.402393
	0.4	-2.536740	-2.5366	-2.48941	-2.54308	-2.54320	-2.54179	-2.540763
	0.5	-2.615549		-2.56811	-2.62156	-2.62180	-2.62091	-2.620021
	0.8	-2.830207	-2.8301	-2.78140	-2.83493	-2.83575	-2.83658	-2.835619
	1	-2.959686		-2.90948	-2.96349	-2.96467	-2.96675	-2.965504
	1.6	-3.302215	-3.3016	-3.24709	-3.30364	-3.30526	-3.31117	-3.308774
	2	-3.502049		-3.44367	-3.50238	-3.50386	-3.51208	-3.508911
	4	-4.298436	-4.2980	-4.22732	-4.29773	-4.29626	-4.31223	
	5	-4.617248		-4.54168	-4.61775	-4.61440	-4.63229	-4.625491
	8	-5.400409	-5.4000	-5.31616	-5.40773	-5.39922	-5.41799	
	10	-5.829510		-5.74199	-5.84283	-5.83143	-5.84823	-5.839475
	20	-7.427702		-7.33773	-7.47698	-7.45563	-7.44960	-7.440556
	40	-9.488271	-9.4882	-9.41836	-9.61487	-9.58172	-9.51283	
	50	-10.264491		-10.20901	-10.42916	-10.39149	-10.28980	-10.28410
	80	-12.101321	-12.1011	-12.09497	-12.37538	-12.32654	-12.12807	
	100	-13.076652		-13.10498	-13.41981	-13.36467	-13.10402	-13.10478
	160	-15.369297	-15.3690	-15.50258	-15.90486	-15.83383	-15.39781	
	200	-16.579068		-16.78099	-17.23307	-17.15303	-16.60807	
	240	-17.629325	-17.6289	-17.89825	-18.39563	-18.30741	-17.65868	
	400	-20.887774	-20.8876	-21.40843	-22.05850	-21.94290	-20.91800	
	500	-22.466647		-23.13313	-23.86382	-23.73388	-22.49719	
	560	-23.306770	-23.3066	-24.05720	-24.83257	-24.69472	-23.33745	
	800	-26.126547	-26.1264	-27.19100	-28.12546	-27.95970	-26.15762	
	1000	-28.032093		-29.33698	-30.38698	-30.20117	-28.06336	
	2000	-34.698652		-37.02465	-38.53109	-38.26795	-34.73029	
1s3d ₋₁								
	0	-2.055571		-2.00353	-2.05924	-2.06359	-2.05837	-2.055629
	0.01	-2.069689		-2.01775	-2.07351	-2.07785	-2.07253	
	0.02	-2.082246		-2.03054	-2.08646	-2.09074	-2.08519	-2.082319
	0.04	-2.104127		-2.05304	-2.10937	-2.11351	-2.10730	-2.104234
	0.08	-2.140836	-2.1403	-2.09098	-2.14815	-2.15201	-2.14441	-2.141017
	0.1	-2.157219		-2.10789	-2.16546	-2.16918	-2.16096	
	0.16	-2.202000		-2.15416	-2.21275	-2.21610	-2.20612	-2.202291
	0.24	-2.255594		-2.20942	-2.26899	-2.27193	-2.26008	-2.256006
	0.4	-2.351540	-2.3512	-2.30831	-2.36946	-2.37178	-2.35655	-2.352208
	0.5	-2.406693		-2.36508	-2.42704	-2.42906	-2.41196	-2.407521
	0.8	-2.557747	-2.5528	-2.52017	-2.58430	-2.58573	-2.56356	-2.559005
	1	-2.649469		-2.61407	-2.67960	-2.68083	-2.65555	-2.650973
	1.6	-2.894105	-2.8938	-2.86363	-2.93346	-2.93473	-2.90077	-2.896192
	2	-3.037923		-3.00991	-3.08271	-3.08426	-3.04488	-3.040304
	4	-3.615797	-3.6156	-3.59629	-3.68391	-3.68749	-3.62363	
	5	-3.848205		-3.83205	-3.92672	-3.93125	-3.85630	-3.851883
	8	-4.419691	-4.4193	-4.41261	-4.52665	-4.53356	-4.42827	
	10	-4.732709		-4.73132	-4.85704	-4.86522	-4.74148	-4.737490
	20	-5.896107		-5.92166	-6.09603	-6.10869	-5.90526	-5.902110
	40	-7.390126	-7.3900	-7.46463	-7.71176	-7.72964	-7.39934	
	50	-7.951520		-8.04867	-8.32578	-8.34547	-7.96070	-7.959094
	80	-9.277732	-9.2773	-9.43755	-9.79083	-9.81450	-9.28673	
	100	-9.980898		-10.17914	-10.57573	-10.60134	-9.98978	-9.989376

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TABLE I (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b
160	-11.631639		-11.6315	-11.93422	-12.44017	-12.46987	-11.64021	
200	-12.501691			-12.86725	-13.43511	-13.46668	-12.51010	
240	-13.256538		-13.2562	-13.68122	-14.30515	-14.33817	-13.26480	
400	-15.595926		-15.5955	-16.23043	-17.04204	-17.07847	-15.60376	
500	-16.728191			-17.47883	-18.38885	-18.42632	-16.73582	
560	-17.330349		-17.3302	-18.14667	-19.11105	-19.14890	-17.33788	
800	-19.349813		-19.3495	-20.40645	-21.56346	-21.60174	-19.35703	
1000	-20.713142			-21.94965	-23.24574	-23.28355	-20.72015	
2000	-25.474170			-27.45278	-29.29239	-29.32401	-25.48059	
1s3d ₋₂								
0	-2.055211			-2.00274	-2.05764	-2.06192	-2.05915	-2.055635
0.01	-2.073992			-2.02155	-2.07651	-2.08077	-2.07795	
0.02	-2.090571			-2.03821	-2.09334	-2.09755	-2.09459	-2.090760
0.04	-2.119045			-2.06698	-2.12254	-2.12657	-2.12331	-2.119167
0.08	-2.166315		-2.1659	-2.11480	-2.17116	-2.17478	-2.17102	-2.166519
0.1	-2.187305			-2.13603	-2.19274	-2.19618	-2.19218	
0.16	-2.244369			-2.19378	-2.25128	-2.25428	-2.24967	-2.244776
0.24	-2.312137			-2.26245	-2.32063	-2.32310	-2.31789	-2.312786
0.4	-2.432302		-2.4320	-2.38449	-2.44328	-2.44487	-2.43868	-2.433466
0.5	-2.500874			-2.45423	-2.51315	-2.51430	-2.50754	-2.502362
0.8	-2.687529		-2.6871	-2.64415	-2.70305	-2.70317	-2.69480	-2.689916
1	-2.800387			-2.75888	-2.81783	-2.81753	-2.80795	-2.803296
1.6	-3.100793		-3.1005	-3.06360	-3.12336	-3.12234	-3.10907	-3.104935
2	-3.277380			-3.24226	-3.30309	-3.30175	-3.28612	-3.282141
4	-3.989093		-3.9890	-3.96026	-4.02882	-4.02578	-3.99985	
5	-4.276634			-4.24997	-4.32273	-4.31868	-4.28822	-4.284050
8	-4.987052		-4.9866	-4.96603	-5.05093	-5.04363	-5.00052	
10	-5.378085			-5.36068	-5.45305	-5.44360	-5.39247	-5.387931
20	-6.841527			-6.84280	-6.96687	-6.94791	-6.85874	-6.854811
40	-8.738642		-8.7385	-8.77923	-8.95123	-8.91789	-8.75837	
50	-9.455332			-9.51569	-9.70756	-9.66842	-9.47577	-9.476057
80	-11.154700		-11.1540	-11.27323	-11.51580	-11.46230	-11.17646	
100	-12.058706			-12.21479	-12.48636	-12.42486	-12.08100	-12.088566
160	-14.187530		-14.1875	-14.45053	-14.79579	-14.71445	-14.21074	
200	-15.312775			-15.64287	-16.03015	-15.93772	-15.33633	
240	-16.290615		-16.2905	-16.68502	-17.11052	-17.00811	-16.31440	
400	-19.329520		-19.3286	-19.95960	-20.51410	-20.37851	-19.35372	
500	-20.804539			-21.56868	-22.19138	-22.03846	-20.82882	
560	-21.590017		-21.5954	-22.43081	-23.09135	-22.92884	-21.61432	
800	-24.229300		-24.2283	-25.35462	-26.15001	-25.95352	-24.25357	
1000	-26.015249			-27.35677	-28.25025	-28.02904	-26.03943	
2000	-32.276759			-34.52868	-35.81092	-35.49155	-32.30030	
1s4f ₋₂								
0	-2.031249			-1.97866	-2.03299	-2.03801	-2.03361	-2.031254
0.01	-2.048544			-1.99632	-2.05083	-2.05580	-2.05103	
0.02	-2.062148			-2.01052	-2.06536	-2.07018	-2.06484	-2.062177
0.04	-2.084307			-2.03369	-2.08925	-2.09383	-2.08729	-2.084414
0.08	-2.120330		-2.1201	-2.07134	-2.12800	-2.13214	-2.12368	-2.120532
0.1	-2.136321			-2.08783	-2.14496	-2.14894	-2.13981	
0.16	-2.180084			-2.13307	-2.19140	-2.19499	-2.18395	-2.180271
0.24	-2.232571			-2.18702	-2.24662	-2.24982	-2.23674	-2.232769
0.4	-2.326857		-2.3268	-2.28364	-2.34538	-2.34800	-2.33143	-2.327166
0.5	-2.381198			-2.33921	-2.40208	-2.40444	-2.38597	-2.381601
0.8	-2.530386		-2.5299	-2.49136	-2.55713	-2.55906	-2.53561	-2.531094
1	-2.621154			-2.58369	-2.65122	-2.65302	-2.62661	-2.622067
1.6	-2.863780		-2.8637	-2.82974	-2.90223	-2.90403	-2.86972	-2.865215
2	-3.006695			-2.97431	-3.05000	-3.05199	-3.01286	-3.008432
4	-3.582552		-3.5823	-3.55572	-3.64645	-3.65011	-3.58933	
5	-3.814702			-3.79002	-3.88772	-3.89228	-3.82164	-3.817900
8	-4.386458		-4.3861	-4.36774	-4.48443	-4.49143	-4.39369	
10	-4.700010			-4.68519	-4.81326	-4.82166	-4.70735	-4.704423

Continued on the next page

TABLE I (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b
20		-5.866633		-5.87138	-6.04687	-6.06053	-5.87418	-5.872256
40		-7.365670	-7.3654	-7.40894	-7.65535	-7.67558	-7.37321	
50		-7.928889		-7.99071	-8.26638	-8.28899	-7.93638	-7.935933
80		-9.259024	-9.2549	-9.37362	-9.72369	-9.75170	-9.26635	
100		-9.964016		-10.11171	-10.50411	-10.53485	-9.97125	-9.971845
160		-11.618368	-11.6182	-11.85770	-12.35706	-12.39383	-11.62534	
200		-12.489979		-12.78547	-13.34542	-13.38513	-12.49681	
240		-13.246015	-13.2459	-13.59465	-14.20948	-14.25158	-13.25273	
400		-15.588290	-15.5879	-16.12776	-16.92628	-16.97485	-15.59466	
500		-16.721612		-17.36773	-18.26256	-18.31369	-16.72780	
560		-17.324260	-17.3240	-18.03092	-18.97887	-19.03128	-17.33028	
800		-19.345077	-19.3448	-20.27435	-21.41087	-21.46647	-19.35094	
1000		-20.709117		-21.80583	-23.07846	-23.13552	-20.71484	
2000		-25.471793		-27.26433	-29.06882	-29.12687	-25.47699	
1s4f ₋₃								
0		-2.031249		-1.97844	-2.03218	-2.03726	-2.03425	-2.031255
0.01		-2.052700		-2.00030	-2.05425	-2.05925	-2.05588	
0.02		-2.069488		-2.01770	-2.07202	-2.07679	-2.07296	-2.069509
0.04		-2.096912		-2.04600	-2.10106	-2.10549	-2.10079	-2.096967
0.08		-2.141490	-2.1406	-2.09140	-2.14748	-2.15148	-2.14580	-2.141582
0.1		-2.161202		-2.11135	-2.16790	-2.17174	-2.16567	
0.16		-2.214843		-2.16560	-2.22328	-2.22663	-2.21966	-2.214999
0.24		-2.278729		-2.23006	-2.28891	-2.29184	-2.28388	-2.278994
0.4		-2.392422	-2.3923	-2.34474	-2.40523	-2.40743	-2.39811	-2.392988
0.5		-2.457457		-2.41035	-2.47156	-2.47344	-2.46345	-2.458243
0.8		-2.634770	-2.6344	-2.58928	-2.65196	-2.65333	-2.64155	-2.636282
1		-2.742096		-2.69757	-2.76106	-2.76220	-2.74933	-2.744109
1.6		-3.028048	-3.0275	-2.98586	-3.05128	-3.05229	-3.03625	-3.031517
2		-3.196346		-3.15537	-3.22220	-3.22323	-3.20499	-3.200682
4		-3.876023	-3.8759	-3.83878	-3.91318	-3.91481	-3.88597	
5		-4.151209		-4.11526	-4.19356	-4.19541	-4.16158	-4.160555
8		-4.832223	-4.8318	-4.79973	-4.88932	-4.89149	-4.84352	
10		-5.207614		-5.17741	-5.27406	-5.27626	-5.21937	-5.222402
20		-6.614859		-6.59733	-6.72422	-6.72542	-6.62805	-6.636961
40		-8.442698	-8.4426	-8.45412	-8.62727	-8.62542	-8.45720	
50		-9.133925		-9.16047	-9.35291	-9.34939	-9.14881	-9.169700
80		-10.774057	-10.7734	-10.84625	-11.08812	-11.07985	-10.78963	
100		-11.647101		-11.74936	-12.01955	-12.00819	-11.66295	-11.697425
160		-13.704227	-13.7044	-13.89361	-14.23598	-14.21602	-13.72054	
200		-14.792170		-15.03701	-15.42071	-15.39546	-14.80864	
240		-15.737890	-15.7378	-16.03628	-16.45755	-16.42720	-15.75447	
400		-18.678514	-18.6784	-19.17550	-19.72375	-19.67498	-18.69525	
500		-20.106581		-20.71769	-21.33321	-21.27400	-20.12333	
560		-20.867238	-20.8674	-21.54389	-22.19674	-22.13159	-20.88397	
800		-23.423985	-23.4342	-24.34529	-25.13136	-25.04431	-23.44064	
1000		-25.154789		-26.26316	-27.14627	-27.04252	-25.17135	
2000		-31.226978		-33.13018	-34.39868	-34.22428	-31.24305	
1s5g ₋₃								
0		-2.019969		-1.96687	-2.02058	-2.02592	-2.02189	
0.01		-2.039226		-1.98698	-2.04090	-2.04615	-2.04138	
0.02		-2.052769		-2.00136	-2.05576	-2.06073	-2.05519	
0.04		-2.074248		-2.02410	-2.07930	-2.08401	-2.07699	
0.08		-2.109116	-2.1089	-2.06087	-2.11738	-2.12174	-2.11218	-2.10950
0.1		-2.124672		-2.07696	-2.13387	-2.13795	-2.12787	
0.16		-2.167486		-2.12147	-2.17959	-2.18335	-2.17103	
0.24		-2.219055		-2.17454	-2.23400	-2.23740	-2.22291	-2.21919
0.4		-2.312085	-2.3120	-2.26980	-2.33158	-2.33444	-2.31631	-2.31133
0.5		-2.365849		-2.32467	-2.38772	-2.39035	-2.37022	
0.8		-2.513803	-2.5133	-2.47513	-2.54149	-2.54369	-2.51851	-2.51328
1		-2.603968		-2.56655	-2.63489	-2.63696	-2.60886	
1.6		-2.845464	-2.8451	-2.81052	-2.88433	-2.88649	-2.85074	-2.84601

Continued on the next page

TABLE I (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b
2		-2.987898		-2.95406	-3.03130	-3.03370	-2.99337	
4		-3.562747	-3.5607	-3.53224	-3.62514	-3.62938	-3.56877	-3.56063
5		-3.794798		-3.76556	-3.86557	-3.87075	-3.80096	
8		-4.366800	-4.3664	-4.34132	-4.46051	-4.46828	-4.37320	-4.36666
10		-4.680701		-4.65787	-4.78849	-4.79776	-4.68718	
20		-5.849342		-5.84131	-6.01925	-6.03431	-5.85596	
40		-7.351537	-7.3514	-7.37557	-7.62403	-7.64664	-7.35812	
50		-7.915924		-7.95603	-8.23353	-8.25893	-7.92247	
80		-9.248602	-9.2476	-9.33556	-9.68687	-9.71864	-9.25500	
100		-9.954794		-10.07168	-10.46496	-10.49999	-9.96111	
160		-11.611545	-11.6106	-11.81255	-12.31181	-12.35413	-11.61760	
200		-12.484202		-12.73736	-13.29668	-13.34255	-12.49019	
240		-13.241036	-13.2408	-13.54383	-14.15749	-14.20632	-13.24693	
400		-15.585251	-15.5847	-16.06781	-16.86324	-16.92029	-15.59085	
500		-16.719277		-17.30298	-18.19366	-18.25411	-16.72473	
560		-17.322250	-17.3216	-17.96353	-18.90677	-18.96890	-17.32760	
800		-19.343951	-19.3436	-20.19761	-21.32714	-21.39404	-19.34914	
1000		-20.708443		-21.72239	-22.98553	-23.05572	-20.71350	
2000		-25.472106		-27.15517	-28.94442	-29.01818	-25.47679	

^a For the $1s^2$ state, HF atomic energies are B-spline basis calculations; L.B. Zhao and P.C. Stancil, Phys. Rev. A **77**, 035401 (2008). For other states, HF energies are anisotropic GTO basis calculations; M.D. Jones, G. Ortiz, and D.M. Ceperley, Phys. Rev. A **59**, 2875 (1999).

^b For the $1s5g_{-3}$ state, data from fixed-phase QMC calculations; M.D. Jones, G. Ortiz, and D.M. Ceperley, Int. J. Quant. Chem. **64**, 523 (1997). Data for other states from CI calculations with anisotropic GTO basis did by Schmelcher and collaborators. For magnetic quantum number $M = 0$ (states $1s^2$, $1s2s$, $1s2p_0$), see W. Becken, P. Schmelcher, and F.K. Diakonov, J. Phys. B **32**, 1557 (1999). For $M = -1$ (states $1s2p_{-1}$, $1s3d_{-1}$), see W. Becken and P. Schmelcher, J. Phys. B **33**, 545 (2000). For $M = -2, -3$ (states $1s3d_{-2}$, $1s4f_{-2}$, $1s4f_{-3}$), see W. Becken and P. Schmelcher, Phys. Rev. A **63**, 053412 (2001).

TABLE II: As in Table I for the Lithium singly positive ion.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c
$1s^2$									
0		-7.23641	-7.23642	-7.14218	-7.25675	-7.28660	-7.28219	-7.277191	-7.2791930452
0.001		-7.23641	-7.23642	-7.14218	-7.25675	-7.28660	-7.28219	-7.277189	
0.002		-7.23641	-7.23642	-7.14218	-7.25675	-7.28659	-7.28219		
0.005		-7.23641	-7.23641	-7.14218	-7.25675	-7.28659	-7.28219		
0.01		-7.23641	-7.23641	-7.14217	-7.25674	-7.28659	-7.28218	-7.277327	
0.02		-7.23639	-7.23639	-7.14215	-7.25672	-7.28657	-7.28216	-7.277376	-7.2790926140
0.05		-7.23623	-7.23623	-7.14198	-7.25656	-7.28641	-7.28200	-7.277336	
0.1		-7.23567	-7.23567	-7.14140	-7.25598	-7.28584	-7.28145	-7.276897	-7.2784566184
0.17633		-7.23411	-7.23411	-7.13975	-7.25437	-7.28426	-7.27989		
0.2		-7.23345	-7.23345	-7.13906	-7.25369	-7.28359	-7.27924	-7.274673	-7.2762423947
0.5		-7.21798	-7.21798	-7.12282	-7.23773	-7.26791	-7.26385	-7.259522	-7.2607612984
1		-7.16401	-7.16401	-7.06634	-7.18223	-7.21331	-7.21012	-7.205547	-7.2066303684
2		-6.96300	-6.96300	-6.85770	-6.97689	-7.01082	-7.00984	-7.004453	-7.0053327494
2.071814		-6.94440	-6.94440	-6.83849	-6.95796	-6.99213	-6.99131		
2.153		-6.92278	-6.92278	-6.81616	-6.93596	-6.97040	-6.96975		
3		-6.66237	-6.66237	-6.54825	-6.67177	-6.70915	-6.71002		
4		-6.28591		-6.16297	-6.29132	-6.33224	-6.33432		
5		-5.85051	-5.85051	-5.71916	-5.85253	-5.89689	-5.89960	-5.891947	
7		-4.84725	-4.84725	-4.70055	-4.84407	-4.89487	-4.89748		
8		-4.29438		-4.14073	-4.28924	-4.34303	-4.34508		
10		-3.11091	-3.11092	-2.94459	-3.10286	-3.16217	-3.16242	-3.153453	-3.1538963265
20		3.74896	3.74896	3.96179	3.75994	3.67910	3.69503		3.7041245990
50		27.96465	27.96465	28.24616	27.94517	27.82552	27.90822		
100		72.09338	72.09337	72.41532	71.99341	71.83633	72.03587		72.0425222760
200		164.66868	164.66867	164.9938	164.3926	164.1912	164.6109		
500		452.00319	452.0032	452.2001	451.2285	450.9590	451.9462		
1000		939.87972	939.87976	939.7880	938.3865	938.0607	939.8241		
2000		1925.2140		1924.548	1922.527	1922.144	1925.160		
$1s2p_{-1}$									
0		-5.02469	-5.02469	-4.93862	-5.03007	-5.03411	-5.02884	-5.026321	

Continued on the next page

TABLE II (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c
0.001		-5.02619	-5.02619	-4.94012	-5.03157	-5.03561	-5.03034	-5.027815	
0.002		-5.02768	-5.02769	-4.94162	-5.03306	-5.03711	-5.03184		
0.005		-5.03217	-5.03218	-4.94611	-5.03755	-5.04160	-5.03633		
0.01		-5.03962	-5.03963	-4.95355	-5.04500	-5.04904	-5.04377	-5.041247	
0.02		-5.05441	-5.05442	-4.96834	-5.05979	-5.06383	-5.05857	-5.056040	
0.05		-5.09796	-5.09797	-5.01188	-5.10332	-5.10736	-5.10213	-5.099595	
0.1		-5.16788	-5.16789	-5.08177	-5.17318	-5.17721	-5.17209	-5.169539	
0.17633		-5.26874	-5.26874	-5.18255	-5.27391	-5.27790	-5.27304		
0.2		-5.29872	-5.29873	-5.21251	-5.30384	-5.30782	-5.30306	-5.300455	
0.5		-5.64006	-5.64006	-5.55341	-5.64442	-5.64835	-5.64488	-5.643726	
1		-6.11462	-6.11462	-6.02636	-6.11712	-6.12149	-6.12023	-6.119216	
2		-6.89408	-6.89408	-6.80007	-6.89221	-6.89775	-6.90127	-6.899768	
2.071814		-6.94440	-6.94440	-6.84991	-6.94222	-6.94783	-6.95171		
2.153		-7.00056	-7.00057	-6.90553	-6.99805	-7.00372	-7.00799		
3		-7.54672	-7.54672	-7.44583	-7.54096	-7.54698	-7.55539		
4		-8.11772		-8.01006	-8.10886	-8.11464	-8.12769		
5		-8.62942	-8.62943	-8.51546	-8.61830	-8.62335	-8.64051	-8.636273	
7		-9.52492	-9.52492	-9.40002	-9.51118	-9.51401	-9.53783		
8		-9.92437		-9.79476	-9.91004	-9.91158	-9.93803		
10		-10.65131	-10.65131	-10.51354	-10.63686	-10.63571	-10.66624	-10.659060	
20		-13.42974	-13.42974	-13.26695	-13.42576	-13.41286	-13.44849		
50		-18.52547	-18.52548	-18.34630	-18.58346	-18.55075	-18.54854		
100		-23.69994	-23.69994	-23.54518	-23.87532	-23.82420	-23.72567		
200		-30.26077	-30.26077	-30.19725	-30.66265	-30.58676	-30.28868		
500		-41.50392	-41.50393	-41.75408	-42.49454	-42.36925	-41.53404		
1000		-52.32301	-52.3230	-53.06271	-54.11904	-53.93751	-52.35433		
2000		-65.47655		-67.05990	-68.56884	-68.30807	-65.50866		

^a Data from two-dimensional mesh HF calculation; M.V. Ivanov and P. Schmelcher, Phys. Rev. A **57**, 3793 (1998).^b Data from CI calculation; O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A **70**, 033411 (2004).^c Data are from full-core plus correlation method; X. Wang and H. Qiao, Phys. Rev. A **75**, 033421 (2007).

TABLE III: As in Table I for the Lithium atom.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c	WFM 3 ^d
$1s^2 2s$										
0		-7.43275	-7.43275	-7.34328	-7.46217	-7.48906	-7.48223	-7.477766	-7.4763360	-7.4777957
0.001		-7.43325	-7.43326	-7.34378	-7.46267	-7.48956	-7.48273	-7.478032		
0.0018		-7.43364	-7.43365	-7.34418	-7.46307	-7.48996	-7.48313		-7.4772303	-7.4786907
0.002		-7.43374	-7.43375	-7.34428	-7.46317	-7.49006	-7.48323			
0.005		-7.43521	-7.43522	-7.34574	-7.46464	-7.49153	-7.48470			
0.009		-7.43712	-7.43713	-7.34766	-7.46655	-7.49344	-7.48661		-7.4806770	-7.4821719
0.01		-7.43759	-7.43760	-7.34813	-7.46702	-7.49391	-7.48708	-7.482888		
0.018		-7.44125	-7.44125	-7.35179	-7.47069	-7.49758	-7.49075			-7.4863018
0.02		-7.44213	-7.44214	-7.35268	-7.47158	-7.49847	-7.49164	-7.490983	-7.4856398	
0.05		-7.45397	-7.45398	-7.36458	-7.48353	-7.51045	-7.50357	-7.502724		
0.054		-7.45536	-7.45537	-7.36598	-7.48495	-7.51187	-7.50497			-7.5004678
0.1		-7.46856	-7.46857	-7.37939	-7.49852	-7.52548	-7.51840	-7.517154	-7.5122102	-7.5137817
0.126		-7.47407	-7.47408	-7.38509	-7.50432	-7.53131	-7.52406			-7.5193718
0.17633		-7.48162	-7.48162	-7.39310	-7.51259	-7.53961	-7.53189			
0.18		-7.48203	-7.48204	-7.39355	-7.51306	-7.54008	-7.53233			-7.5275049
0.2		-7.48400	-7.48400	-7.39574	-7.51536	-7.54240	-7.53439	-7.533495	-7.5278376	
0.5		-7.47740	-7.47741	-7.39479	-7.51699	-7.54402	-7.52833	-7.528055	-7.5216127	-7.5235946
0.54		-7.47350	-7.47351	-7.39190	-7.51459	-7.54163	-7.52438			-7.5197262
0.9		-7.42504	-7.42504	-7.35304	-7.48078	-7.50875	-7.47525			-7.4710527
1		-7.40878	-7.40879	-7.33924	-7.46832	-7.49671	-7.45885	-7.458550	-7.4529046	
1.26		-7.36225	-7.36226	-7.29818	-7.43050	-7.45994	-7.41204			-7.4072733
1.8		-7.24603	-7.24603	-7.18982	-7.32819	-7.35967	-7.29563		-7.2895540	-7.2876730
2		-7.19621	-7.19621	-7.14208	-7.28261	-7.31483	-7.24582	-7.244919	-7.2397460	
2.153		-7.15566		-7.10292	-7.24510	-7.27788	-7.20531			
2.16		-7.15376		-7.10108	-7.24333	-7.27614	-7.20340			

Continued on the next page

TABLE III (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c	WFM 3 ^d
2.5		-7.05618	-7.05619	-7.00608	-7.15196	-7.18602	-7.10593			
3		-6.89559	-6.89559	-6.84846	-6.99958	-7.03549	-6.94557			
3.6		-6.67876	-6.67874	-6.63433	-6.79166	-6.82974	-6.72906		-6.7221991	-6.6884510
3.96		-6.53737		-6.49428	-6.65528	-6.69465	-6.58787			
4		-6.52118		-6.47823	-6.63963	-6.67915	-6.57170			
4.32		-6.38836		-6.34645	-6.51106	-6.55171	-6.43905			
4.68		-6.23230		-6.19145	-6.35965	-6.40154	-6.28319			
5		-6.08810	-6.08811	-6.04813	-6.21946	-6.26245	-6.13916	-6.136918		
5.04		-6.06973		-6.02986	-6.20159	-6.24471	-6.12081			
5.4		-5.90114	-5.90113	-5.86217	-6.03738	-6.08170	-5.95240	-5.949297	-5.9448544	-5.8555577
7		-5.08909	-5.08909	-5.05354	-5.24374	-5.29312	-5.14110			
10		-3.35784	-3.35777	-3.32762	-3.54382	-3.60153	-3.41095	-3.406556	-3.4020661	
20		3.49120	3.49120	3.50491	3.21595	3.13744	3.43600		3.4446412	
50		27.69135	27.6916	27.65114	27.20402	27.08883	27.63403			
100		71.80766	71.807	71.67426	71.03954	70.88976	71.74951		71.7573135	
200		164.37026	164.371	164.0581	163.1503	162.9614	164.3120			
500		451.68807	451.69	450.9038	449.4404	449.2118	451.6307			
1000		939.55235	939.54	938.1123	936.0146	935.8673	939.4964			
2000		1924.8749		1922.367	1919.363	1919.024	1924.821			
1s ² 2p ₋₁										
0		-7.36507	-7.36509	-7.27909	-7.39752	-7.42270	-7.41506	-7.407126	-7.4088037	-7.4097907
0.001		-7.36607	-7.36609	-7.28009	-7.39852	-7.42370	-7.41606	-7.408174		
0.0018		-7.36687	-7.36689	-7.28088	-7.39931	-7.42449	-7.41685		-7.4105946	-7.4115816
0.002		-7.36706	-7.36709	-7.28108	-7.39951	-7.42469	-7.41705			
0.005		-7.37000	-7.37002	-7.28402	-7.40245	-7.42763	-7.41999			
0.009		-7.37384	-7.37387	-7.28787	-7.40630	-7.43147	-7.42384		-7.4175767	-7.4185656
0.01		-7.37479	-7.37481	-7.28882	-7.40725	-7.43242	-7.42479	-7.416994		
0.018		-7.38216	-7.38218	-7.29621	-7.41464	-7.43979	-7.43218			-7.4268977
0.02		-7.38395	-7.38397	-7.29800	-7.41644	-7.44159	-7.43397		-7.4275717	
0.05		-7.40843	-7.40844	-7.32265	-7.44113	-7.46613	-7.45861	-7.451086		
0.054		-7.41139	-7.41141	-7.32565	-7.44414	-7.46911	-7.46160			-7.4562839
0.1		-7.44174	-7.44176	-7.35647	-7.47501	-7.49961	-7.49225	-7.484773	-7.4858382	-7.4869343
0.126		-7.45649	-7.45650	-7.37154	-7.49008	-7.51445	-7.50716			-7.5018829
0.17633		-7.48160	-7.48162	-7.39731	-7.51580	-7.53974	-7.53258			
0.18		-7.48329	-7.48330	-7.39904	-7.51753	-7.54144	-7.53428			-7.5291175
0.2		-7.49218	-7.49220	-7.40820	-7.52665	-7.55039	-7.54329	-7.536032	-7.5366925	
0.5		-7.58787	-7.58790	-7.50718	-7.62468	-7.64670	-7.64052	-7.634547	-7.6341245	-7.6362483
0.54		-7.59707	-7.59709	-7.51670	-7.63408	-7.65598	-7.64992			-7.6457300
0.9		-7.65627	-7.65628	-7.57752	-7.69439	-7.71604	-7.71103			-7.7070540
1		-7.66652	-7.66653	-7.58789	-7.70476	-7.72652	-7.72182	-7.716679	-7.7151944	
1.26		-7.68285	-7.68288	-7.60399	-7.72115	-7.74337	-7.73957			-7.7350130
1.8		-7.67655	-7.67657	-7.59554	-7.71426	-7.73775	-7.73610		-7.7274957	-7.7296270
2		-7.66245	-7.66246	-7.58026	-7.69981	-7.72379	-7.72297	-7.715709	-7.7137805	
2.153		-7.64784	-7.64785	-7.56468	-7.68492	-7.70926	-7.70909			
2.16		-7.64710	-7.64711	-7.56389	-7.68416	-7.70852	-7.70838			
2.5		-7.60350	-7.60351	-7.51793	-7.63989	-7.66501	-7.66630			
3		-7.51515	-7.51516	-7.42582	-7.55056	-7.57666	-7.57997			
3.6		-7.37638	-7.37638	-7.28241	-7.41076	-7.43782	-7.44336		-7.4298482	-7.4258570
3.96		-7.27825	-7.27826	-7.18151	-7.31213	-7.33966	-7.34641			
4		-7.26672		-7.16968	-7.30055	-7.32813	-7.33500			
4.32		-7.17025	-7.17026	-7.07078	-7.20372	-7.23165	-7.23950			
4.68		-7.05325	-7.05326	-6.95111	-7.08639	-7.11466	-7.12351			
5		-6.94229	-6.94230	-6.83784	-6.97522	-7.00375	-7.01341	-7.002346		
5.04		-6.92799	-6.92800	-6.82325	-6.96090	-6.98945	-6.99921			
5.4		-6.79515	-6.79517	-6.68788	-6.82790	-6.85670	-6.86726	-6.855410	-6.8503299	-6.8361629
7		-6.12668	-6.12670	-6.00911	-6.15966	-6.18913	-6.20221			
10		-4.61775	-4.61777	-4.48455	-4.65417	-4.68388	-4.69801	-4.684076	-4.6811073	
20		1.70566	1.70565	1.86892	1.64374	1.61495	1.61654		1.6398139	
50		24.97943	24.97942	25.15756	24.80802	24.77977	24.88024			
100		68.17349	68.1735	68.30834	67.80872	67.78076	68.06848		74.0993214	
200		159.57484	159.5749	159.5676	158.8469	158.8228	159.4657			

Continued on the next page

TABLE III (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c	WFM 3 ^d
	500	444.90318	444.9033	444.4242	443.2486	443.2428	444.7912			
	1000	930.84309	930.84308	929.6385	927.9366	927.9620	930.7310			
	2000	1913.8069		1911.362	1908.903	1908.983	1913.696			
1s2s2p ₋₁	0	-5.35887	-5.35888	-5.27113	-5.36586	-5.37122	-5.37127	-5.366705		
	0.001	-5.36087	-5.36088	-5.27313	-5.36786	-5.37322	-5.37327	-5.368015		
	0.0018	-5.36247	-5.36247	-5.27473	-5.36946	-5.37482	-5.37487			
	0.002	-5.36286	-5.36288	-5.27513	-5.36985	-5.37522	-5.37527			
	0.005	-5.36883	-5.36884	-5.28109	-5.37582	-5.38118	-5.38123			
	0.009	-5.37673	-5.37673	-5.28899	-5.38371	-5.38908	-5.38913			
	0.01	-5.37869	-5.37871	-5.29095	-5.38568	-5.39104	-5.39110	-5.385841		
	0.018	-5.39429	-5.39429	-5.30654	-5.40127	-5.40663	-5.40670			
	0.02	-5.39815	-5.39817	-5.31040	-5.40513	-5.41050	-5.41057			
	0.05	-5.45441	-5.45442	-5.36660	-5.46134	-5.46672	-5.46690			
	0.054	-5.46167	-5.46168	-5.37385	-5.46860	-5.47398	-5.47418			
	0.1	-5.54148	-5.54149	-5.45355	-5.54836	-5.55377	-5.55420	-5.550268		
	0.126	-5.58376	-5.58376	-5.49579	-5.59064	-5.59608	-5.59663			
	0.18	-5.66585	-5.66585	-5.57794	-5.67291	-5.67838	-5.67909			
	0.2	-5.69451	-5.69451	-5.60667	-5.70169	-5.70716	-5.70789	-5.703511		
	0.5	-6.04786	-6.04787	-5.96423	-6.05994	-6.06524	-6.06329	-6.058463		
	0.54	-6.08745	-6.08746	-6.00476	-6.10057	-6.10582	-6.10311			
	0.9	-6.40175	-6.40175	-6.33035	-6.42732	-6.43195	-6.41880			
	1	-6.48028	-6.48029	-6.41255	-6.50997	-6.51445	-6.49751	-6.494196		
	1.26	-6.67493	-6.67494	-6.61663	-6.71555	-6.71973	-6.69222			
	1.8	-7.05428	-7.05430	-7.01126	-7.11450	-7.11856	-7.07076			
	2	-7.18888	-7.18889	-7.14984	-7.25496	-7.25908	-7.20503	-7.206026		
	2.153	-7.28986		-7.25338	-7.35993	-7.36412	-7.30579			
	2.16	-7.29444	-7.29445	-7.25806	-7.36468	-7.36887	-7.31036			
	2.5	-7.51255	-7.51255	-7.48072	-7.59062	-7.59493	-7.52812			
	3	-7.81834	-7.81834	-7.79143	-7.90620	-7.91060	-7.83365			
	3.6	-8.16336	-8.16336	-8.14086	-8.26142	-8.26573	-8.17864			
	4	-8.38133		-8.36128	-8.48565	-8.48979	-8.39670			
	5	-8.88982	-8.88981	-8.87501	-9.00867	-9.01206	-8.90559	-8.905985		
	5.4	-9.08045	-9.08045	-9.06752	-9.20480	-9.20779	-9.09640	-9.096395		
	10	-10.91057	-10.91059	-10.91657	-11.09161	-11.08850	-10.92864	-10.925976		
	20	-13.69419	-13.69420	-13.73816	-13.97853	-13.96288	-13.71516			
	50	-18.80127	-18.8012	-18.95172	-19.32998	-19.29229	-18.82579			
	100	-23.98639	-23.987	-24.29525	-24.83336	-24.77437	-24.01318			
	200	-30.55891	-30.559	-31.14147	-31.90888	-31.82093	-30.58761			
	500	-41.81816	-41.821	-43.05947	-44.28702	-44.14010	-41.84880			
	1000	-52.64936	-52.65	-54.74854	-56.49632	-56.28188	-52.68111			
	2000	-65.81463		-69.25315	-71.74010	-71.40159	-65.84709			
1s2p02p ₋₁	0	-5.23185	-5.23186	-5.18538	-5.27457	-5.27483	-5.24432	-5.243519		
	0.001	-5.23385	-5.23386	-5.18738	-5.27657	-5.27682	-5.24631	-5.245744		
	0.0018	-5.23544	-5.23546	-5.18898	-5.27816	-5.27842	-5.24791			
	0.002	-5.23584	-5.23586	-5.18938	-5.27856	-5.27882	-5.24831			
	0.005	-5.24181	-5.24182	-5.19534	-5.28453	-5.28479	-5.25428			
	0.009	-5.24972	-5.24973	-5.20326	-5.29244	-5.29270	-5.26219			
	0.01	-5.25169	-5.25170	-5.20523	-5.29441	-5.29467	-5.26416	-5.262918		
	0.018	-5.26732	-5.26734	-5.22087	-5.31005	-5.31031	-5.27981			
	0.02	-5.27120	-5.27121	-5.22475	-5.31393	-5.31419	-5.28369			
	0.05	-5.32785	-5.32786	-5.28147	-5.37063	-5.37089	-5.34042	-5.339046		
	0.054	-5.33519	-5.33521	-5.28883	-5.37799	-5.37825	-5.34778			
	0.1	-5.41641	-5.41643	-5.37030	-5.45942	-5.45969	-5.42924	-5.429067		
	0.126	-5.45991	-5.45992	-5.41400	-5.50310	-5.50338	-5.47290			
	0.18	-5.54554	-5.54555	-5.50017	-5.58924	-5.58954	-5.55888			
	0.2	-5.57584	-5.57585	-5.53070	-5.61977	-5.62007	-5.58931	-5.587442		
	0.5	-5.96955	-5.96957	-5.92833	-6.01748	-6.01794	-5.98458	-5.983849		
	0.54	-6.01600	-6.01603	-5.97528	-6.06447	-6.06497	-6.03120			
	0.9	-6.39611	-6.39613	-6.35912	-6.44902	-6.44997	-6.41256			

Continued on the next page

TABLE III (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c	WFM 3 ^d
1		-6.49246	-6.49248	-6.45627	-6.54647	-6.54755	-6.50922	-6.508527		
1.26		-6.72929	-6.72931	-6.69478	-6.78600	-6.78738	-6.74680			
1.8		-7.17323	-7.17326	-7.14090	-7.23500	-7.23680	-7.19214			
2		-7.32492	-7.32494	-7.29311	-7.38849	-7.39035	-7.34431			
2.153		-7.43710		-7.40562	-7.50201	-7.50389	-7.45684			
2.16		-7.44216	-7.44218	-7.41069	-7.50713	-7.50901	-7.46192			
2.5		-7.68056	-7.71826	-7.64966	-7.74850	-7.75033	-7.70105			
3		-8.00835	-8.00837	-7.97808	-8.08067	-8.08226	-8.02983			
3.6		-8.37213	-8.37214	-8.34250	-8.44980	-8.45090	-8.39465			
4		-8.59964		-8.57046	-8.68096	-8.68163	-8.62277			
5		-9.12552	-9.12554	-9.09765	-9.21626	-9.21564	-9.14996	-9.148122		
5.4		-9.32132	-9.32134	-9.29408	-9.41593	-9.41474	-9.34621			
10		-11.17880	-11.17886	-11.16295	-11.32014	-11.3120	-11.206948	-11.204311		
20		-13.96581	-13.96582	-13.98677	-14.20817	-14.1882	-13.996409			
50		-19.04358	-19.0436	-19.18366	-19.54403	-19.5037	-19.075513			
100		-24.19476	-24.1946	-24.51000	-25.03281	-24.9715	-24.226942			
200		-30.73415	-30.7327	-31.34154	-32.09713	-32.0061	-30.766514			
500		-41.95847	-41.959	-43.24763	-44.46848	-44.3173	-41.991266			
1000		-52.77041	-52.771	-54.93563	-56.68252	-56.4629	-52.803500			
2000		-65.92122		-69.44560	-71.93611	-71.6199	-65.953135			
1s2p-13d-2										
0		-5.08377	-5.08379	-5.00614	-5.09830	-5.09921	-5.09177	-5.142319		
0.001		-5.08676	-5.08679	-5.00913	-5.10129	-5.10220	-5.09476	-5.145464		
0.0018		-5.08914	-5.08915	-5.01151	-5.10366	-5.10457	-5.09714			
0.002		-5.08973	-5.08976	-5.01210	-5.10426	-5.10516	-5.09773			
0.005		-5.09849	-5.09852	-5.02088	-5.11303	-5.11393	-5.10650			
0.009		-5.10986	-5.10988	-5.03229	-5.12443	-5.12531	-5.11792			
0.01		-5.11265	-5.11268	-5.03510	-5.12723	-5.12810	-5.12073	-5.169111		
0.018		-5.13432	-5.13433	-5.05690	-5.14898	-5.14976	-5.14253			
0.02		-5.13957	-5.13960	-5.06219	-5.15425	-5.15501	-5.14782			
0.05		-5.21278	-5.21281	-5.13577	-5.22756	-5.22785	-5.22174	-5.248206		
0.054		-5.22196	-5.22199	-5.14497	-5.23672	-5.23696	-5.23103			
0.1		-5.32138	-5.32140	-5.24405	-5.33574	-5.33547	-5.33166	-5.341030		
0.126		-5.37369	-5.37371	-5.29595	-5.38774	-5.38726	-5.38460			
0.18		-5.47565	-5.47568	-5.39695	-5.48908	-5.48823	-5.48767			
0.2		-5.51149	-5.51151	-5.43245	-5.52472	-5.52376	-5.52385	-5.524939		
0.5		-5.97050	-5.97052	-5.88799	-5.98199	-5.97989	-5.98586	-5.982253		
0.54		-6.02412	-6.02414	-5.94131	-6.03545	-6.03324	-6.03972			
0.9		-6.46060	-6.46061	-6.37567	-6.47067	-6.46761	-6.47789			
1		-6.57079	-6.57081	-6.48534	-6.58053	-6.57729	-6.58846	-6.582361		
1.26		-6.84121	-6.84122	-6.75443	-6.85010	-6.84639	-6.85976			
1.8		-7.34721	-7.34723	-7.25756	-7.35450	-7.34973	-7.36736			
2		-7.52002	-7.52003	-7.42928	-7.52682	-7.52159	-7.54072	-7.530125		
2.153		-7.64784	-7.64785	-7.55625	-7.65430	-7.64869	-7.66894			
2.16		-7.65360	-7.65361	-7.56197	-7.66005	-7.65442	-7.67472			
2.5		-7.92531	-7.92532	-7.83181	-7.93113	-7.92459	-7.94728			
3		-8.29920	-8.29920	-8.20298	-8.30440	-8.29636	-8.32233			
3.6		-8.71463	-8.71464	-8.61532	-8.71954	-8.70953	-8.73905			
3.96		-8.94928	-8.94929	-8.84823	-8.95423	-8.94297	-8.97442			
4		-8.97475		-8.87351	-8.97971	-8.96831	-8.99996			
4.32		-9.17442	-9.17442	-9.07171	-9.17954	-9.16700	-9.20023			
4.68		-9.39098	-9.39099	-9.28671	-9.39642	-9.38258	-9.41742			
5		-9.57693	-9.57694	-9.47135	-9.58275	-9.56775	-9.60391	-9.591769		
5.04		-9.59976	-9.59977	-9.49403	-9.60564	-9.59050	-9.62681			
5.4		-9.80146	-9.80147	-9.69434	-9.80787	-9.79143	-9.82907			
7		-10.62576	-10.62578	-10.51355	-10.63571	-10.61355	-10.65558			
10		-11.93900	-11.93902	-11.82087	-11.95879	-11.92698	-11.97189	-11.957294		
20		-15.16261	-15.16260	-15.04379	-15.22743	-15.17279	-15.20114			
50		-21.05051	-21.0505	-20.98431	-21.26811	-21.17963	-21.09529			
100		-27.01926	-27.0192	-27.07687	-27.47894	-27.36026	-27.06791			
200		-34.58498	-34.5850	-34.89906	-35.47253	-35.3153	-34.636926			

Continued on the next page

TABLE III (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c	WFM 3 ^d
500		-47.55828	-47.5583	-48.56385	-49.48447	-49.2571	-47.613748			
1000		-60.05888	-60.0589	-62.02394	-63.34180	-63.0414	-60.116404			
2000		-75.28238		-78.79694	-80.68240	-80.2856	-75.341552			

^a Data from two-dimensional mesh HF; M.V. Ivanov and P. Schmelcher, Phys. Rev. A **57**, 3793 (1998).

^b Data from CI calculation; O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A **70**, 033411 (2004).

^c Data from full core plus correlation calculation; X. Wang and H. Qiao, Phys. Rev. A **75**, 033421 (2007). The energy for the $1s^2 2p_{-1}$ state in $B = 100$ a.u. appears to be in error.

^d Data from full core plus correlation calculation; X. Guan and B. Li, Phys. Rev. A **63**, 043413 (2001).

TABLE IV: As in Table I for the Beryllium singly positive ion.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c
$1s^2 2s$									
0		-14.27746	-14.27747	-14.11468	-14.29931	-14.33851	-14.32972	-14.3247	-14.32126
0.001		-14.27796	-14.27797	-14.11518	-14.29981	-14.33901	-14.33022	-14.3251	-14.32176
0.002		-14.27846	-14.27846	-14.11568	-14.30031	-14.33951	-14.33072		-14.32226
0.004		-14.27945		-14.11667	-14.30130	-14.34050	-14.33171		-14.32326
0.005		-14.27995	-14.27995	-14.11716	-14.30180	-14.34100	-14.33221		
0.01		-14.28241	-14.28241	-14.11962	-14.30426	-14.34346	-14.33467	-14.3296	-14.32621
0.02		-14.28724	-14.28725	-14.12446	-14.30910	-14.34830	-14.33951		-14.33105
0.0412		-14.29714	-14.29714	-14.13436	-14.31900	-14.35821	-14.34941		
0.05		-14.30110	-14.30111	-14.13832	-14.32297	-14.36218	-14.35338	-14.3482	
0.1		-14.32206	-14.32207	-14.15931	-14.34400	-14.38322	-14.37439	-14.3694	-14.36586
0.2		-14.35648	-14.35648	-14.19383	-14.37868	-14.41796	-14.40897	-14.4038	-14.40026
0.3		-14.38211		-14.21966	-14.40476	-14.44399	-14.43483		-14.42588
0.4		-14.40046	-14.40046	-14.23830	-14.42371	-14.46312	-14.45342		-14.44420
0.5		-14.41281	-14.41282	-14.25106	-14.43683	-14.47628	-14.46600	-14.4606	-14.45737
0.6		-14.42021		-14.25897	-14.44516	-14.48473	-14.47361		-14.46390
0.7		-14.42350		-14.26287	-14.44954	-14.48916	-14.47707		-14.46700
0.8		-14.42334		-14.26344	-14.45065	-14.49036	-14.47704		-14.46697
0.957		-14.41741		-14.25890	-14.44707	-14.48690	-14.47126		
1		-14.41477	-14.41478	-14.25668	-14.44514	-14.48501	-14.46864	-14.4630	-14.45832
2		-14.28223	-14.28225	-14.13758	-14.33533	-14.37716	-14.33577	-14.3300	
4.567		-13.67997		-13.55854	-13.77833	-13.82921	-13.73297		
5		-13.55017	-13.55019	-13.43057	-13.65374	-13.70597	-13.60321	-13.5971	
10		-11.57651	-11.57652	-11.46620	-11.72693	-11.79329	-11.63062	-11.6231	
20		-6.03361	-6.03364	-5.93033	-6.25743	-6.34586	-6.08954		
50		15.42605	15.4261	15.50231	15.02236	14.89210	15.36784		
100		56.55157	56.5516	56.56794	55.90212	55.73070	56.49224		
200		145.1651	145.1649	145.0506	144.1119	143.8912	145.1053		
500		425.4682	425.471	424.9751	423.4801	423.1831	425.4088		
1000		906.3822	906.37	905.3321	903.1998	902.8605	906.334		
2000		1883.062	1883.08	1881.070	1878.029	1877.669	1883.005		
$1s^2 2p_{-1}$									
0		-14.13092	-14.13093	-13.97722	-14.15964	-14.19312	-14.18328	-14.1741	-14.17447
0.001		-14.13192	-14.13195	-13.97822	-14.16064	-14.19412	-14.18428	-14.1751	-14.17547
0.002		-14.13292	-14.13294	-13.97922	-14.16164	-14.19512	-14.18528		-14.17647
0.004		-14.13491		-13.98121	-14.16363	-14.19711	-14.18727		-14.17846
0.005		-14.13590	-14.13593	-13.98220	-14.16463	-14.19810	-14.18827		
0.01		-14.14085	-14.14087	-13.98715	-14.16957	-14.20305	-14.19321	-14.1841	-14.18440
0.02		-14.15063	-14.15066	-13.99693	-14.17936	-14.21283	-14.20300		-14.19418
0.0412		-14.17090		-14.01721	-14.19963	-14.23310	-14.22328		
0.05		-14.17913	-14.17916	-14.02544	-14.20786	-14.24132	-14.23152	-14.2216	
0.1		-14.22387	-14.22390	-14.07022	-14.25263	-14.28603	-14.27632	-14.2672	-14.26740
0.2		-14.30404	-14.30406	-14.15056	-14.33292	-14.36614	-14.35672	-14.3476	-14.34751
0.3		-14.37399		-14.22077	-14.40305	-14.43604	-14.42695		-14.41738
0.4		-14.43597	-14.43599	-14.28305	-14.46523	-14.49800	-14.48923		-14.47926
0.5		-14.49161	-14.49163	-14.33900	-14.52106	-14.55363	-14.54519	-14.5358	-14.53478
0.6		-14.54208		-14.38975	-14.57169	-14.60409	-14.59596		-14.58512
0.7		-14.58819		-14.43612	-14.61793	-14.65021	-14.64240		-14.63109

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TABLE IV (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM 1 ^b	WFM 2 ^c
0.8		-14.63057		-14.47871	-14.66041	-14.69260	-14.68510		-14.67332
0.957		-14.69066	-14.69069	-14.53904	-14.72059	-14.75271	-14.74569		
1		-14.70590	-14.70591	-14.55431	-14.73583	-14.76794	-14.76106	-14.7520	-14.74830
2		-14.95180	-14.95181	-14.79885	-14.98072	-15.01378	-15.01016	-15.0000	
4.567		-15.01237		-14.84477	-15.03438	-15.07161	-15.07787		
5		-14.96818	-14.96820	-14.79755	-14.98899	-15.02679	-15.03467	-15.0184	
10		-13.75772	-13.75773	-13.55316	-13.76896	-13.81027	-13.83277	-13.8087	
20		-9.21789	-9.21791	-8.96403	-9.22874	-9.27041	-9.30217		
50		10.42839	10.42836	10.75039	10.36744	10.32747	10.33266		
100		49.70821	49.70820	50.05480	49.52527	49.48470	49.60529		
200		135.9592	135.95916	136.2626	135.5154	135.4745	135.8507		
500		412.1475	412.14745	412.1699	410.9731	410.9407	412.0343		
1000		889.0264	889.0264	888.5207	886.8026	886.7913	888.9118		
2000		1860.710	1860.7100	1859.211	1856.741	1856.772	1860.595		
1s2p-13d-2									
0		-9.41056	-9.41056	-9.29441	-9.42594	-9.42768	-9.42032	-9.4156	
0.001		-9.41355	-9.41358	-9.29741	-9.42894	-9.43068	-9.42332	-9.4185	
0.002		-9.41654	-9.41657	-9.30040	-9.43193	-9.43367	-9.42631		
0.004		-9.42251		-9.30636	-9.43789	-9.43963	-9.43227		
0.005		-9.42548	-9.42551	-9.30934	-9.44086	-9.44261	-9.43525		
0.01		-9.44025	-9.44028	-9.32411	-9.45563	-9.45737	-9.45003	-9.4452	
0.02		-9.46936	-9.46939	-9.35320	-9.48472	-9.48645	-9.47916		
0.0412		-9.52916		-9.41295	-9.54447	-9.54614	-9.53907		
0.05		-9.55327	-9.55332	-9.43704	-9.56854	-9.57019	-9.56324		
0.1		-9.68353	-9.68356	-9.56699	-9.69849	-9.69991	-9.69395	-9.6888	
0.2		-9.91876	-9.91878	-9.80108	-9.93277	-9.93370	-9.93024	-9.9243	
0.3		-10.13141		-10.01226	-10.14435	-10.14488	-10.14389		
0.4		-10.32814	-10.32817	-10.20747	-10.34004	-10.34025	-10.34148		
0.5		-10.51257	-10.51259	-10.39046	-10.52352	-10.52346	-10.52662	-10.5188	
0.6		-10.68703		-10.56361	-10.69714	-10.69684	-10.70169		
0.7		-10.85321		-10.72858	-10.86255	-10.86205	-10.86840		
0.8		-11.01234		-10.88660	-11.02098	-11.02029	-11.02799		
0.957		-11.25020		-11.12289	-11.25782	-11.25689	-11.26647		
1		-11.31311	-11.31312	-11.18539	-11.32047	-11.31947	-11.32953	-11.3203	
2		-12.59205	-12.59206	-12.45669	-12.59423	-12.59186	-12.61102	-12.6002	
4.567		-15.07308	-15.07310	-14.92176	-15.06648	-15.05917	-15.09620		
5		-15.42816	-15.42817	-15.27438	-15.42061	-15.41221	-15.45187	-15.4367	
10		-18.82017	-18.82018	-18.64327	-18.80967	-18.78709	-18.84917	-18.8283	
20		-23.61200	-23.61200	-23.41126	-23.61815	-23.57048	-23.64699		
50		-32.61958	-32.61959	-32.41627	-32.71905	-32.62912	-32.66181		
100		-41.93409	-41.93414	-41.78903	-42.20788	-42.08259	-41.98087		
200		-53.90637	-53.90638	-53.92572	-54.51380	-54.34654	-53.95701		
500		-74.73620	-74.73619	-75.27535	-76.20668	-75.96495	-74.79106		
1000		-95.0751	-95.07513	-96.4007	-97.7251	-97.4062	-95.1326		
2000		-120.1194	-120.11947	-122.7836	-124.6700	-124.2496	-120.1790		

^a Data from two-dimensional mesh HF calculation; M.V. Ivanov and P. Schmelcher, Eur. Phys. J. D **14**, 279 (2001).^b Data from CI calculation; O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A **70**, 023411 (2004).^c Data from frozen core calculation; X. Guan, B. Li, and K.T. Taylor, J. Phys. B **36**, 2465 (2003).

TABLE V: As in Table I for the Beryllium atom.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b	WFM ^c
1s ² 2s ²									
0		-14.57302	-14.57336	-14.44647	-14.62995	-14.67167	-14.66028	-14.6405	-14.66287
0.001		-14.57302	-14.57336	-14.44647	-14.62994	-14.67167	-14.66027	-14.6410	-14.66287
0.002		-14.57302	-14.57335	-14.44647	-14.62994	-14.67166	-14.66027		-14.66292
0.005		-14.57299	-14.57332	-14.44644	-14.62991	-14.67164	-14.66024		
0.01		-14.57288	-14.57322	-14.44633	-14.62981	-14.67153	-14.66014	-14.6408	-14.66279
0.02		-14.57244	-14.57279	-14.44591	-14.62939	-14.67112	-14.65972		-14.66238
0.03		-14.57173		-14.44520	-14.62869	-14.67043	-14.65902		

Continued on the next page

TABLE V (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b	WFM ^c
0.04	-14.57072			-14.44421	-14.62772	-14.66946	-14.65806		
0.05	-14.56944	-14.56944	-14.56986	-14.44295	-14.62647	-14.66823	-14.65682	-14.6393	
0.07	-14.56605	-14.56605	-14.56657	-14.43962	-14.62319	-14.66496	-14.65353		
0.1	-14.55897			-14.43268	-14.61633	-14.65815	-14.64667	-14.6298	-14.64955
0.15	-14.54227	-14.54227	-14.54367	-14.41630	-14.60016	-14.64206	-14.63043		-14.63338
0.2	-14.52012			-14.39459	-14.57869	-14.62069	-14.60880	-14.5907	-14.61160
0.3	-14.46231	-14.46231	-14.46861	-14.33793	-14.52262	-14.56475	-14.55205		-14.55714
0.3185	-14.44994			-14.32580	-14.51061	-14.55277	-14.53986		
0.4	-14.39023			-14.26732	-14.45267	-14.49490	-14.48094		-14.48793
0.5	-14.30723	-14.30723	-14.32860	-14.18607	-14.37215	-14.41442	-14.39878	-14.3882	-14.40818
0.6	-14.21572			-14.09657	-14.28342	-14.32574	-14.30795		-14.32037
0.8	-14.01379			-13.89949	-14.08801	-14.13043	-14.10695		-14.12710
1	-13.79426	-13.79426	-13.89120	-13.68582	-13.87623	-13.91883	-13.88783	-13.9220	-13.91717
2	-12.58628	-12.58628	-12.88908	-12.51633	-12.71931	-12.76490	-12.67854	-12.9275	
3	-11.32762			-11.29436	-11.51043	-11.56120	-11.41953		
4	-10.04479			-10.03949	-10.26701	-10.32160	-10.13698		
4.501	-9.39066			-9.39684	-9.62986	-9.68604	-9.48295		
5	-8.73080	-8.73080	-9.40602	-8.74720	-8.98563	-9.04328	-8.82315	-9.4907	
10	-1.68968	-1.68968	-2.5988	-1.77633	-2.06612	-2.13609	-1.78197	-2.6936	
20	13.91306	13.91306	12.8201	13.74177	13.36365	13.27463	13.82151		
30	30.57377	30.57377		30.34056	29.88777	29.78414	30.48303		
40	47.82165	47.82165	46.5935	47.53644	47.01798	46.90243	47.73170		
50	65.45129	65.45129	64.186	65.11986	64.54213	64.41646	65.36204		
100	156.6367	156.6367	155.286	156.1171	155.2989	155.1368	156.5502		
200	345.3103	345.3103	343.899	344.5008	343.3306	343.1251	345.2272		
500	925.6925	925.6925	924.20	924.2294	922.3451	922.0730	925.6146		
1000	1906.666	1906.666	1905.14	1904.370	1901.670	1901.349	1906.593		
2000	3883.406	3883.406	3881.5	3879.807	3875.945	3875.568	3883.337		
$1s^2 2s 2p_{-1}$									
0	-14.51205	-14.51205	-14.51206	-14.35660	-14.54197	-14.57726	-14.57325	-14.5598	-14.56237
0.001	-14.51355	-14.51355	-14.51357	-14.35810	-14.54346	-14.57876	-14.57475	-14.5612	-14.56388
0.002	-14.51504	-14.51504	-14.51507	-14.35959	-14.54496	-14.58026	-14.57624		-14.56537
0.005	-14.51951	-14.51951	-14.51953	-14.36405	-14.54942	-14.58472	-14.58071		
0.01	-14.52688	-14.52688	-14.52690	-14.37142	-14.55679	-14.59209	-14.58808	-14.5744	-14.57721
0.02	-14.54136	-14.54136	-14.54138	-14.38589	-14.57126	-14.60656	-14.60258		-14.59170
0.03	-14.55551			-14.40001	-14.58539	-14.62069	-14.61674		
0.04	-14.56931			-14.41379	-14.59917	-14.63448	-14.63058		
0.05	-14.58279	-14.58279	-14.58281	-14.42723	-14.61262	-14.64793	-14.64410	-14.6142	
0.07	-14.60878	-14.60878	-14.60879	-14.45314	-14.63856	-14.67387	-14.67018		
0.1	-14.64546			-14.48971	-14.67518	-14.71050	-14.70705	-14.6936	-14.69575
0.15	-14.70106	-14.70106	-14.70108	-14.54521	-14.73080	-14.76612	-14.76305		-14.75127
0.2	-14.75063			-14.59484	-14.78056	-14.81587	-14.81307	-14.7979	-14.80065
0.3	-14.83519	-14.83519	-14.83520	-14.68001	-14.86602	-14.90124	-14.89858		-14.88560
0.3185	-14.84904	-14.84904	-14.84905	-14.69405	-14.88011	-14.91531	-14.91261		
0.4	-14.90463			-14.75065	-14.93694	-14.97201	-14.96897		-14.95507
0.5	-14.96262	-14.96262	-14.96264	-14.81035	-14.99688	-15.03175	-15.02788	-15.0107	-15.01300
0.6	-15.01170			-14.86153	-15.04829	-15.08294	-15.07782		-15.06181
0.8	-15.08987			-14.94495	-15.13218	-15.16635	-15.15753		-15.13834
1	-15.14895	-15.14895	-15.14899	-15.01031	-15.19809	-15.23178	-15.21787	-15.1982	-15.19348
2	-15.30813	-15.30813	-15.30815	-15.20274	-15.39603	-15.42839	-15.37945	-15.3551	
3	-15.36374			-15.27737	-15.47924	-15.51253	-15.43520		
4	-15.34274			-15.26557	-15.47684	-15.51161	-15.41495		
4.501	-15.30538			-15.23116	-15.44719	-15.48266	-15.37815		
5	-15.25182	-15.25182	-15.25183	-15.17990	-15.40069	-15.43678	-15.32521	-15.3002	
10	-14.03040	-14.03040	-14.03046	-13.96954	-14.23613	-14.27544	-14.10996	-14.0792	
20	-9.49116	-9.49116	-9.49118	-9.44386	-9.78955	-9.82845	-9.57859		
30	-3.59322			-3.56201	-3.97441	-4.01165	-3.68535		
40	3.04027	3.04027	3.04026	3.05306	2.58211	2.54620	2.94491		
50	10.14726	10.14726	10.1472	10.14011	9.61641	9.58143	10.04949		
100	49.41799	49.41799	49.4177	49.30168	48.56446	48.53176	49.31354		
200	135.6582	135.6582	135.659	135.3166	134.2676	134.2388	135.5485		

Continued on the next page

TABLE V (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b	WFM ^c
500		411.8308	411.830	410.8636	409.1803	409.1690	411.7167		
1000		888.6976	888.70	886.8344	884.4256	884.4606	888.5821		
2000		1860.370	1860.40	1857.018	1853.571	1853.693	1860.255		
$1s^2 2p_{-1} 3d_{-2}$									
0		-14.19021	-14.19023	-14.04483	-14.22794	-14.25832	-14.24640		
0.001		-14.19270	-14.1928	-14.04732	-14.23043	-14.26080	-14.24889		
0.002		-14.19517	-14.1952	-14.04978	-14.23289	-14.26327	-14.25135		
0.005		-14.20243	-14.2025	-14.05706	-14.24017	-14.27053	-14.25863		
0.01		-14.21410	-14.2142	-14.06878	-14.25187	-14.28221	-14.27036		
0.02		-14.23604	-14.2361	-14.09086	-14.27388	-14.30411	-14.29247		
0.03		-14.25649		-14.11145	-14.29438	-14.32447	-14.31315		
0.04		-14.27584		-14.13089	-14.31373	-14.34367	-14.33274		
0.05		-14.29433	-14.29437	-14.14941	-14.33218	-14.36198	-14.35148		
0.07		-14.32930	-14.32933	-14.18432	-14.36700	-14.39655	-14.38699		
0.1		-14.37794		-14.23260	-14.41531	-14.44456	-14.43643	-14.4082	
0.15		-14.45142	-14.45145	-14.30523	-14.48825	-14.51710	-14.51110		
0.2		-14.51757		-14.37056	-14.55402	-14.58253	-14.57822	-14.5492	
0.3		-14.63366	-14.63369	-14.48539	-14.66976	-14.69768	-14.69578		
0.3185		-14.65325		-14.50480	-14.68933	-14.71715	-14.71559		
0.4		-14.73394		-14.58490	-14.77005	-14.79743	-14.79717		
0.5		-14.82270	-14.82272	-14.67322	-14.85898	-14.88586	-14.88684	-14.8530	
0.6		-14.90260		-14.75288	-14.93914	-14.96555	-14.96753		
0.8		-15.04230		-14.89240	-15.07940	-15.10498	-15.10862		
1		-15.16177	-15.16178	-15.01185	-15.19940	-15.22433	-15.22931	-15.1975	
2		-15.57494	-15.57496	-15.42448	-15.61430	-15.63738	-15.64768	-15.6217	
3		-15.79983		-15.64688	-15.84001	-15.86186	-15.87699		
4		-15.90158		-15.74483	-15.94233	-15.96290	-15.98264		
4.501		-15.91624	-15.91626	-15.75731	-15.95730	-15.97716	-15.99907		
5		-15.91025	-15.91027	-15.74908	-15.95170	-15.97081	-15.99475	-15.9493	
10		-15.04641	-15.04644	-14.86380	-15.09628	-15.10706	-15.14338	-15.0875	
20		-10.97097	-10.97100	-10.76320	-11.05444	-11.05124	-11.08153		
30		-5.40701		-5.19046	-5.53351	-5.52110	-5.52527		
40		0.95679	0.95677	1.17297	0.783679	0.80234	0.83334		
50		7.83396	7.83395	8.04408	7.612745	7.63598	7.70667		
100		46.25964	46.25962	46.39964	45.79601	45.83266	46.12175		
200		131.4188	131.4188	131.3572	130.4990	130.5516	131.2724		
500		405.7029	405.7027	404.9941	403.6131	403.6999	405.5486		
1000		880.7053	880.706	879.0084	877.0237	877.1543	880.5477		
2000		1850.048	1850.052	1846.661	1843.809	1844.006	1849.889		
$1s 2p_{-1} 3d_{-2} 4f_{-3}$									
0		-9.44320	-9.44321	-9.33439	-9.46626	-9.46612	-9.45631		
0.001		-9.44816	-9.4483	-9.33936	-9.47123	-9.47108	-9.46128		
0.002		-9.45306	-9.4532	-9.34427	-9.47614	-9.47598	-9.46619		
0.005		-9.46737	-9.4675	-9.35866	-9.49050	-9.49031	-9.48059		
0.01		-9.49014	-9.4903	-9.38161	-9.51338	-9.51308	-9.50361		
0.02		-9.53295	-9.5331	-9.42463	-9.55628	-9.55573	-9.54712		
0.03		-9.57337		-9.46500	-9.59670	-9.59610	-9.58825		
0.04		-9.61201		-9.50345	-9.63526	-9.63466	-9.62751		
0.05		-9.64916	-9.6493	-9.54037	-9.67229	-9.67169	-9.66520		
0.07		-9.71974	-9.7198	-9.61050	-9.74268	-9.74198	-9.73666		
0.1		-9.81838		-9.70856	-9.84105	-9.84012	-9.83636		
0.15		-9.96915	-9.9692	-9.85853	-9.99136	-9.98995	-9.98857		
0.2		-10.10810		-9.99665	-10.12973	-10.12780	-10.12875		
0.3		-10.36218	-10.36220	-10.24889	-10.38251	-10.37951	-10.38490		
0.3185		-10.40649		-10.29285	-10.42660	-10.42341	-10.42956		
0.4		-10.59382		-10.47863	-10.61298	-10.60902	-10.61823		
0.5		-10.80900	-10.80901	-10.69200	-10.82716	-10.82241	-10.83479		
0.6		-11.01120		-10.89254	-11.02854	-11.02313	-11.03814		
0.8		-11.38541		-11.26391	-11.40151	-11.39494	-11.41417		
1		-11.72877	-11.72880	-11.60495	-11.74403	-11.73656	-11.75891	-11.7358	
2		-13.16959	-13.16961	-13.03841	-13.18310	-13.17229	-13.20407	-13.1762	

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TABLE V (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA	WFM ^b	WFM ^c
3		-14.35015		-14.21421	-14.36351	-14.34971	-14.38744		
4		-15.38049		-15.24074	-15.39460	-15.37757	-15.42000		
4.501		-15.85572		-15.71430	-15.87051	-15.85175	-15.89623		
5		-16.30689	-16.30690	-16.16394	-16.32254	-16.30199	-16.34832	-16.3139	
10		-20.01752	-20.01753	-19.86565	-20.04976	-20.01032	-20.06580	-20.0242	
20		-25.23248	-25.23250	-25.08498	-25.31809	-25.24742	-25.28819		
30		-29.11101		-28.98206	-29.25793	-29.16534	-29.17086		
40		-32.28414	-32.28415	-32.18034	-32.49411	-32.38523	-32.34674		
50		-35.00766	-35.00768	-34.93257	-35.28060	-35.15884	-35.07229		
100		-45.10517	-45.10519	-45.19278	-45.67967	-45.51598	-45.17550		
200		-58.08260	-58.08264	-58.50541	-59.19451	-58.98266	-58.15784		
500		-80.67355	-80.67357	-82.00237	-83.10096	-82.80752	-80.75427		
1000		-102.7547	-102.75480	-105.3480	-106.9144	-106.5396	-102.8389		
2000		-129.9790	-129.9790	-134.6274	-136.8613	-136.3818	-130.0661		

^a Data from two-dimensional mesh HF calculation; by M.V. Ivanov and P. Schmelcher, Eur. Phys. J. D **14**, 279 (2001).^b Data are from CI calculation; O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A **70**, 023411 (2004).^c Data from frozen core calculation; X. Guan, B. Li, and K.T. Taylor, J. Phys. B **36**, 2465 (2003).

TABLE VI: As in Table I for the Boron singly positive ion.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
$1s^2 2s^2$							
0		-24.23757	-24.23758	-24.0373	-24.2934	-24.3470	-24.3314
0.01		-24.23751	-24.23752	-24.0372	-24.2934	-24.3470	-24.3313
0.05		-24.23592	-24.23593	-24.0357	-24.2918	-24.3454	-24.3298
0.07		-24.23434	-24.23435	-24.0341	-24.2903	-24.3439	-24.3282
0.07811		-24.23355	-24.23356	-24.0333	-24.2895	-24.3431	-24.3274
0.1		-24.23099	-24.23100	-24.0308	-24.2870	-24.3406	-24.3249
0.2		-24.21160	-24.21161	-24.0115	-24.2679	-24.3216	-24.3058
0.3		-24.18034	-24.18047	-23.9805	-24.2372	-24.2910	-24.2749
0.4		-24.13837	-24.13926	-23.9389	-24.1959	-24.2498	-24.2335
0.5		-24.08691	-24.08953	-23.8879	-24.1454	-24.1994	-24.1825
0.6		-24.02709	-24.03268	-23.8286	-24.0866	-24.1407	-24.1232
0.8		-23.88621	-23.90222	-23.6892	-23.9482	-24.0025	-23.9833
1		-23.72226	-23.75518	-23.5270	-23.7872	-23.8417	-23.8201
1.5		-23.24085	-23.34366	-23.0520	-23.3155	-23.3704	-23.3400
1.6761		-23.05383		-22.8678	-23.1327	-23.1878	-23.1532
1.8143		-22.90240		-22.7189	-22.9849	-23.0401	-23.0019
2		-22.69355	-22.89729	-22.5137	-22.7812	-22.8367	-22.7930
2.23984		-22.41643		-22.2417	-22.5114	-22.5672	-22.5158
2.4779		-22.13494		-21.9658	-22.2378	-22.2941	-22.2341
2.5		-22.10854		-21.9399	-22.2121	-22.2685	-22.2077
3		-21.50220	-21.94957	-21.3464	-21.6238	-21.6815	-21.6008
4		-20.25867	-20.94565	-20.1296	-20.4183	-20.4802	-20.3564
5		-18.99538	-19.88877	-18.8909	-19.1902	-19.2571	-19.0931
7		-16.42259	-17.62872	-16.3565	-16.6744	-16.7491	-16.5209
7.957		-15.16589		-15.1141	-15.4403	-15.5181	-15.2645
8		-15.10900	-16.43402	-15.0578	-15.3844	-15.4623	-15.2076
10		-12.42177	-13.93583	-12.3950	-12.7386	-12.8222	-12.5207
20		2.05449	0.03393	2.0012	1.5775	1.4724	1.9551
30		17.70457	15.4428	17.5940	17.0991	16.9777	17.6053
40		34.06427	31.6553	33.9048	33.3459	33.2112	33.9653
50		50.90111	48.3912	50.6975	50.0801	49.9340	50.8025
100		138.99222	136.237	138.6045	137.7461	137.5589	138.8954
200		323.48208	320.558	322.8049	321.5906	321.3537	323.3881
500		896.29425	893.23	894.9632	892.9276	892.7088	896.2055
1000		1869.6592		1867.498	1864.730	1864.350	1869.575
2000		3836.8309		3833.377	3829.432	3828.988	3836.752
$1s^2 2s 2p_{-1}$							
0		-24.12077	-24.12078	-23.8856	-24.1420	-24.1886	-24.1854

Continued on the next page

TABLE VI (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
	0.01	-24.13570	-24.13573	-23.9005	-24.1569	-24.2036	-24.2003
	0.05	-24.19396	-24.19399	-23.9588	-24.2152	-24.2618	-24.2586
	0.07	-24.22223	-24.22226	-23.9870	-24.2435	-24.2901	-24.2869
	0.07811	-24.23353	-24.23356	-23.9983	-24.2548	-24.3014	-24.2982
	0.1	-24.26357	-24.26360	-24.0283	-24.2848	-24.3314	-24.3283
	0.2	-24.39242	-24.39245	-24.1571	-24.4136	-24.4603	-24.4574
	0.3	-24.50850	-24.50852	-24.2732	-24.5298	-24.5765	-24.5738
	0.4	-24.61321	-24.61324	-24.3780	-24.6348	-24.6815	-24.6789
	0.5	-24.70796	-24.70798	-24.4730	-24.7300	-24.7767	-24.7742
	0.6	-24.79399	-24.79401	-24.5595	-24.8166	-24.8633	-24.8607
	0.8	-24.94406	-24.94408	-24.7109	-24.9684	-25.0151	-25.0118
	1	-25.07023	-25.07026	-24.8391	-25.0970	-25.1435	-25.1389
	1.5	-25.31062	-25.31064	-25.0867	-25.3456	-25.3916	-25.3815
	1.6761	-25.37642	-25.37644	-25.1556	-25.4149	-25.4608	-25.4480
	1.8143	-25.42280	-25.42283	-25.2046	-25.4643	-25.5100	-25.4949
	2	-25.47886	-25.47889	-25.2643	-25.5246	-25.5702	-25.5516
	2.23984	-25.54226		-25.3327	-25.5938	-25.6392	-25.6157
	2.4779	-25.59682		-25.3924	-25.6544	-25.6996	-25.6708
	2.5	-25.60152		-25.3976	-25.6596	-25.7048	-25.6756
	3	-25.69387	-25.69390	-25.5005	-25.7648	-25.8099	-25.7688
	4	-25.81860	-25.81863	-25.6430	-25.9132	-25.9586	-25.8945
	5	-25.88462	-25.88465	-25.7212	-25.9981	-26.0445	-25.9611
	7	-25.87125	-25.87128	-25.7204	-26.0119	-26.0609	-25.9490
	7.957	-25.80324		-25.6556	-25.9542	-26.0043	-25.8817
	8	-25.79934	-25.79936	-25.6518	-25.9507	-26.0008	-25.8778
	10	-25.54205	-25.54207	-25.3982	-25.7121	-25.7641	-25.6221
	20	-22.65133	-22.65134	-22.5128	-22.8974	-22.9530	-22.7379
	30	-18.14594	-18.14596	-18.0124	-18.4600	-18.5154	-18.2370
	40	-12.71542	-12.71547	-12.5898	-13.0939	-13.1483	-12.8097
	50	-6.67383	-6.67388	-6.5584	-7.1140	-7.1674	-6.7705
	100	28.47187	28.4719	28.5183	27.7513	27.7007	28.3682
	200	109.16434	109.1648	109.0441	107.9652	107.9170	109.0549
	500	375.31463	375.3157	374.6846	372.9697	372.9327	375.1998
	1000	842.10507	842.10	840.7027	838.2588	838.2463	841.9880
	2000	1801.0937	1801.12	1798.363	1794.879	1794.915	1800.976
$1s^2 2p_{-1} 3d_{-2}$							
	0	-23.39318	-23.39320	-23.1759	-23.4275	-23.4645	-23.4524
	0.01	-23.41788	-23.4180	-23.2006	-23.4522	-23.4892	-23.4771
	0.05	-23.51089	-23.51094	-23.2935	-23.5451	-23.5820	-23.5703
	0.07	-23.55426	-23.55431	-23.3368	-23.5884	-23.6252	-23.6139
	0.07811	-23.57134		-23.3538	-23.6054	-23.6422	-23.6310
	0.1	-23.61608	-23.6162	-23.3984	-23.6500	-23.6867	-23.6760
	0.2	-23.80105	-23.8012	-23.5822	-23.8340	-23.8703	-23.8620
	0.3	-23.96324	-23.9633	-23.7430	-23.9953	-24.0311	-24.0253
	0.4	-24.10931	-24.1094	-23.8877	-24.1405	-24.1759	-24.1723
	0.5	-24.24288	-24.2429	-24.0200	-24.2734	-24.3085	-24.3067
	0.6	-24.36633	-24.36639	-24.1423	-24.3963	-24.4310	-24.4308
	0.8	-24.58910	-24.58915	-24.3633	-24.6182	-24.6525	-24.6549
	1	-24.78669	-24.78674	-24.5595	-24.8153	-24.8490	-24.8535
	1.5	-25.20283	-25.20288	-24.9730	-25.2304	-25.2632	-25.2719
	1.6761	-25.32936		-25.0988	-25.3567	-25.3892	-25.3991
	1.8143	-25.42279	-25.42282	-25.1917	-25.4499	-25.4822	-25.4930
	2	-25.54104	-25.54108	-25.3092	-25.5679	-25.5999	-25.6120
	2.23984	-25.68271	-25.68275	-25.4500	-25.7092	-25.7410	-25.7545
	2.4779	-25.81238	-25.81241	-25.5788	-25.8385	-25.8700	-25.8850
	2.5	-25.82391		-25.5902	-25.8500	-25.8815	-25.8966
	3	-26.06393	-26.06397	-25.8283	-26.0893	-26.1203	-26.1382
	4	-26.44417	-26.44420	-26.2043	-26.4680	-26.4980	-26.5215
	5	-26.71996	-26.71999	-26.4754	-26.7424	-26.7713	-26.8000
	7	-27.03668	-27.03671	-26.7819	-27.0568	-27.0832	-27.1216
	7.957	-27.10002		-26.8403	-27.1193	-27.1445	-27.1870

Continued on the next page

TABLE VI (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
8		-27.10172	-27.10174	-26.8418	-27.1210	-27.1461	-27.1888
10		-27.08415	-27.08417	-26.8140	-27.1025	-27.1247	-27.1751
20		-25.06408	-25.06410	-24.7520	-25.0900	-25.0980	-25.1684
30		-21.18536	-21.18539	-20.8461	-21.2313	-21.2280	-21.2978
40		-16.26387	-16.26392	-15.9074	-16.3360	-16.3244	-16.3820
50		-10.65832	-10.65835	-10.2914	-10.7602	-10.7422	-10.7806
100		22.86886	22.86883	23.2350	22.5989	22.6345	22.7345
200		101.46470	101.46468	101.7316	100.8453	100.8975	101.3204
500		363.90713	363.9071	363.7269	362.3240	362.4072	363.7532
1000		827.00204	827.0020	826.0438	824.0431	824.1654	826.8433
2000		1781.3445	1781.3443	1778.963	1776.102	1776.285	1781.183
1s2p ₋₁ 3d ₋₂ 4f ₋₃							
0		-15.23741	-15.23742	-15.0886	-15.2621	-15.2616	-15.2536
0.01		-15.28652	-15.2868	-15.1377	-15.3112	-15.3107	-15.3027
0.05		-15.46746	-15.4677	-15.3183	-15.4920	-15.4914	-15.4845
0.07		-15.55079	-15.5510	-15.4012	-15.5751	-15.5744	-15.5683
0.07811		-15.58353		-15.4338	-15.6077	-15.6071	-15.6013
0.1		-15.66931	-15.6695	-15.5191	-15.6932	-15.6925	-15.6876
0.2		-16.02513	-16.0252	-15.8727	-16.0476	-16.0465	-16.0454
0.3		-16.34114	-16.3412	-16.1867	-16.3621	-16.3603	-16.3630
0.4		-16.63100	-16.6311	-16.4745	-16.6505	-16.6480	-16.6542
0.5		-16.90165	-16.9017	-16.7432	-16.9198	-16.9166	-16.9260
0.6		-17.15721	-17.1573	-16.9968	-17.1740	-17.1702	-17.1826
0.8		-17.63307	-17.63311	-17.4690	-17.6476	-17.6425	-17.6602
1		-18.07239	-18.07243	-17.9050	-18.0849	-18.0789	-18.1009
1.5		-19.05781	-19.05784	-18.8834	-19.0667	-19.0587	-19.0890
1.6761		-19.37591		-19.1995	-19.3838	-19.3752	-19.4078
1.8143		-19.61712		-19.4392	-19.6243	-19.6153	-19.6495
2		-19.93087	-19.93091	-19.7510	-19.9371	-19.9276	-19.9639
2.23984		-20.32051		-20.1384	-20.3258	-20.3156	-20.3543
2.4779		-20.69200		-20.5079	-20.6964	-20.6855	-20.7264
2.5		-20.72579		-20.5415	-20.7301	-20.7192	-20.7603
3		-21.46199	-21.46202	-21.2738	-21.4647	-21.4525	-21.4977
4		-22.80350	-22.80352	-22.6087	-22.8038	-22.7891	-22.8412
5		-24.01517	-24.01520	-23.8148	-24.0139	-23.9966	-24.0545
7		-26.16678	-26.16682	-25.9571	-26.1642	-26.1411	-26.2088
7.957		-27.09989		-26.8864	-27.0975	-27.0714	-27.1431
8		-27.14062	-27.14064	-26.9270	-27.1382	-27.1120	-27.1839
10		-28.93502	-28.93504	-28.7145	-28.9341	-28.9016	-28.9804
20		-36.02019	-36.02020	-35.7813	-36.0432	-35.9801	-36.0728
30		-41.38294	-41.38296	-41.1416	-41.4430	-41.3554	-41.4399
40		-45.81146	-45.81149	-45.5766	-45.9137	-45.8070	-45.8714
50		-49.63541	-49.63544	-49.4122	-49.7823	-49.6599	-49.6976
100		-63.94724	-63.947265	-63.8180	-64.3235	-64.1511	-64.0158
200		-82.55708	-82.55711	-82.6656	-83.3704	-83.1436	-82.6311
500		-115.33673	-115.33672	-116.1674	-117.2770	-116.9623	-115.4169
1000		-147.71740	-147.71743	-149.6244	-151.1967	-150.7964	-147.8015
2000		-187.99218	-187.99221	-191.7209	-193.9538	-193.4446	-188.0797

^a Data from two-dimensional mesh HF calculation; M.V. Ivanov and P. Schmelcher, J. Phys. B **34**, 2031 (2001).

TABLE VII: As in Table I for the Boron atom.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
1s ² 2s ² 2p ₋₁							
0		-24.53025	-24.53029	-24.3533	-24.6076	-24.6587	-24.6479
0.001		-24.53125	-24.53133	-24.3543	-24.6086	-24.6597	-24.6489
0.002		-24.53224	-24.53232	-24.3553	-24.6096	-24.6606	-24.6499
0.005		-24.53521	-24.53529	-24.3583	-24.6126	-24.6636	-24.6529
0.01		-24.54011	-24.54018	-24.3632	-24.6174	-24.6685	-24.6578
0.02		-24.54968	-24.54976	-24.3727	-24.6270	-24.6781	-24.6674

Continued on the next page

TABLE VII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
	0.03	-24.55897	-24.55905	-24.3820	-24.6363	-24.6874	-24.6767
	0.04	-24.56798	-24.56806	-24.3910	-24.6453	-24.6964	-24.6857
	0.05	-24.57671	-24.57679	-24.3997	-24.6540	-24.7051	-24.6945
	0.07	-24.59334	-24.59340	-24.4163	-24.6706	-24.7217	-24.7112
	0.07811	-24.59977		-24.4227	-24.6770	-24.7281	-24.7177
	0.1	-24.61625	-24.61631	-24.4391	-24.6934	-24.7446	-24.7343
	0.12	-24.63022	-24.63027	-24.4530	-24.7074	-24.7586	-24.7484
	0.15	-24.64928	-24.64933	-24.4720	-24.7264	-24.7776	-24.7678
	0.2	-24.67629	-24.67634	-24.4989	-24.7534	-24.8048	-24.7953
	0.3	-24.71433	-24.71439	-24.5370	-24.7919	-24.8434	-24.8344
	0.4	-24.73414	-24.73424	-24.5573	-24.8126	-24.8642	-24.8554
	0.5	-24.73877	-24.73975	-24.5627	-24.8185	-24.8701	-24.8611
	0.6	-24.73068	-24.73386	-24.5557	-24.8121	-24.8636	-24.8540
	0.7	-24.71179	-24.71863	-24.5382	-24.7951	-24.8466	-24.8361
	0.8	-24.68367	-24.69572	-24.5118	-24.7692	-24.8206	-24.8088
	0.9	-24.64760	-24.66641	-24.4776	-24.7356	-24.7869	-24.7735
	1	-24.60461	-24.63172	-24.4367	-24.6953	-24.7465	-24.7311
	1.2	-24.50128	-24.54933	-24.3382	-24.5980	-24.6490	-24.6289
	1.5	-24.31255	-24.40148	-24.1580	-24.4199	-24.4704	-24.4413
	1.6761	-24.18748		-24.0386	-24.3018	-24.3521	-24.3166
	1.8143	-24.08357		-23.9395	-24.2037	-24.2539	-24.2128
	2	-23.93747	-23.57727	-23.8001	-24.0659	-24.1159	-24.0668
	2.23984	-23.73969		-23.6114	-23.8792	-23.9291	-23.8688
	2.4779	-23.53558		-23.4166	-23.6865	-23.7364	-23.6644
	2.5	-23.51631	-23.26402	-23.3982	-23.6683	-23.7182	-23.6451
	3	-23.06875	-23.43666	-22.9703	-23.2450	-23.2953	-23.1964
	4	-22.12927	-22.66608	-22.0663	-22.3509	-22.4025	-22.2545
	5	-21.14914	-21.81614	-21.1144	-21.4092	-21.4621	-21.2726
	7	-19.07693	-19.91839	-19.0823	-19.3984	-19.4532	-19.1984
	7.957	-18.03329		-18.0529	-18.3798	-18.4352	-18.1539
	8	-17.98564	-18.88687	-18.0059	-18.3332	-18.3886	-18.1062
	10	-15.70237	-16.68963	-15.7450	-16.0861	-16.1437	-15.8198
	12	-13.29922	-14.34380	-13.3580	-13.7298	-13.7741	-13.4132
	15	-9.50364	-10.60422	-9.5807	-9.9840	-10.0204	-9.6139
	20	-2.77368	-3.92689	-2.8752	-3.3274	-3.3500	-2.8811
	30	11.73918		11.5945	11.0545	10.9973	11.6329
	40	27.17247		26.9865	26.3687	26.3143	27.0659
	50	43.21540		42.9890	42.3012	42.2499	43.1084
	100	128.3628		127.946	126.978	126.936	128.253
	200	309.055		308.302	306.929	306.913	308.942
	500	875.204		873.621	871.432	871.42	875.094
	1000	1841.994		1839.292	1836.172	1836.19	1841.88
	2000	3800.985		3796.489	3792.058	3792.14	3800.87
$1s^2 2s 2p_0 2p_{-1}$							
	0	-24.45120	-24.45121	-24.2338	-24.4886	-24.5334	-24.5277
	0.001	-24.45320	-24.45324	-24.2358	-24.4906	-24.5354	-24.5297
	0.002	-24.45519	-24.45523	-24.2378	-24.4926	-24.5374	-24.5317
	0.005	-24.46117	-24.46121	-24.2438	-24.4986	-24.5434	-24.5377
	0.01	-24.47108	-24.47112	-24.2537	-24.5085	-24.5533	-24.5476
	0.02	-24.49071	-24.49075	-24.2733	-24.5281	-24.5729	-24.5672
	0.03	-24.51011	-24.51015	-24.2927	-24.5474	-24.5923	-24.5866
	0.04	-24.52927	-24.52931	-24.3118	-24.5666	-24.6114	-24.6058
	0.05	-24.54819	-24.54823	-24.3307	-24.5854	-24.6303	-24.6247
	0.07	-24.58532	-24.58536	-24.3676	-24.6224	-24.6673	-24.6619
	0.07811	-24.60011	-24.60015	-24.3824	-24.6372	-24.6820	-24.6767
	0.1	-24.63928	-24.63932	-24.4213	-24.6761	-24.7210	-24.7160
	0.12	-24.67412	-24.67416	-24.4559	-24.7108	-24.7557	-24.7509
	0.15	-24.72477	-24.72481	-24.5062	-24.7611	-24.8061	-24.8017
	0.2	-24.80507	-24.80511	-24.5857	-24.8408	-24.8859	-24.8824
	0.3	-24.95177	-24.95180	-24.7309	-24.9863	-25.0318	-25.0298
	0.4	-25.08252	-25.08255	-24.8601	-25.1161	-25.1618	-25.1613

Continued on the next page

TABLE VII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
0.5	-25.19992	-25.19992	-25.19996	-24.9761	-25.2326	-25.2787	-25.2795
0.6	-25.30609	-25.30609	-25.30612	-25.0809	-25.3381	-25.3845	-25.3864
0.7	-25.40266	-25.40266	-25.40269	-25.1764	-25.4342	-25.4808	-25.4837
0.8	-25.49100	-25.49100	-25.49103	-25.2637	-25.5222	-25.5691	-25.5727
0.9	-25.57217	-25.57217	-25.57220	-25.3440	-25.6031	-25.6503	-25.6545
1	-25.64708	-25.64708	-25.64711	-25.4181	-25.6779	-25.7253	-25.7300
1.2	-25.78095	-25.78095	-25.78098	-25.5507	-25.8118	-25.8596	-25.8649
1.5	-25.94995	-25.94995	-25.94997	-25.7184	-25.9816	-26.0300	-26.0352
1.6761	-26.03516	-26.03516	-26.03522	-25.8033	-26.0677	-26.1163	-26.1211
1.8143	-26.09614	-26.09614		-25.8642	-26.1295	-26.1783	-26.1825
2	-26.17107	-26.17107	-26.17110	-25.9392	-26.2059	-26.2549	-26.2580
2.23984	-26.25771	-26.25771	-26.25774	-26.0264	-26.2948	-26.3440	-26.3452
2.4779	-26.33424	-26.33424	-26.33428	-26.1039	-26.3742	-26.4235	-26.4222
2.5	-26.34093	-26.34093	-26.34097	-26.1107	-26.3812	-26.4305	-26.4289
3	-26.47588	-26.47588	-26.47592	-26.2492	-26.5236	-26.5732	-26.5647
4	-26.67272	-26.67272	-26.67276	-26.4567	-26.7401	-26.7898	-26.7627
5	-26.79526	-26.79526	-26.79531	-26.5919	-26.8851	-26.9346	-26.8864
7	-26.86263	-26.86263	-26.86269	-26.6826	-26.9964	-27.0456	-26.9562
7.957	-26.82343	-26.82343		-26.6529	-26.9766	-27.0258	-26.9182
8	-26.82072	-26.82072	-26.82077	-26.6506	-26.9748	-27.0239	-26.9155
10	-26.61077	-26.61077	-26.61083	-26.4574	-26.8022	-26.8511	-26.7079
12	-26.25877	-26.25877	-26.25884	-26.1194	-26.4843	-26.5330	-26.3579
15	-25.51639	-25.51639	-25.51648	-25.3949	-25.7890	-25.8373	-25.6180
20	-23.84221	-23.84221	-23.84231	-23.7462	-24.1865	-24.2341	-23.9471
30	-19.38734	-19.38734	-19.3873	-19.3365	-19.8604	-19.9067	-19.4965
40	-13.98208	-13.98208	-13.9821	-13.9738	-14.5724	-14.6177	-14.0939
50	-7.95405	-7.95405	-7.954	-7.9871	-8.6537	-8.6984	-8.0677
100	27.17968	27.17968	27.178	26.9507	26.0050	25.9617	27.0618
200	107.89267	107.89267	107.896	107.3109	105.9539	105.9130	107.7724
500	374.08692	374.08692	374.06	372.6200	370.4241	370.3986	373.9654
1000	840.90621	840.90621	840.97	838.2429	835.0901	835.0966	840.7847
2000	1799.9146	1799.9146		1795.328	1790.812	1790.880	1799.794
1s ² 2s2p ₋₁ 3d ₋₂							
0	-24.17788	-24.17788	-24.17792	-23.9511	-24.2092	-24.2530	-24.2463
0.001	-24.18087	-24.18087	-24.1818	-23.9541	-24.2122	-24.2560	-24.2493
0.002	-24.18383	-24.18383	-24.185	-23.9571	-24.2151	-24.2589	-24.2522
0.005	-24.19256	-24.19256	-24.193	-23.9659	-24.2239	-24.2677	-24.2610
0.01	-24.20663	-24.20663	-24.207	-23.9800	-24.2381	-24.2818	-24.2751
0.02	-24.23321	-24.23321	-24.234	-24.0070	-24.2650	-24.3086	-24.3018
0.03	-24.25817	-24.25817	-24.259	-24.0324	-24.2903	-24.3337	-24.3269
0.04	-24.28195	-24.28195	-24.2821	-24.0567	-24.3144	-24.3575	-24.3508
0.05	-24.30484	-24.30484	-24.3050	-24.0800	-24.3375	-24.3805	-24.3738
0.07	-24.34864	-24.34864	-24.3489	-24.1246	-24.3817	-24.4242	-24.4178
0.07811	-24.36581	-24.36581		-24.1421	-24.3990	-24.4413	-24.4351
0.1	-24.41079	-24.41079	-24.41099	-24.1877	-24.4442	-24.4861	-24.4803
0.12	-24.45045	-24.45045	-24.450624	-24.2278	-24.4839	-24.5255	-24.5202
0.15	-24.50779	-24.50779	-24.50794	-24.2856	-24.5412	-24.5824	-24.5780
0.2	-24.59852	-24.59852	-24.59863	-24.3766	-24.6316	-24.6722	-24.6697
0.3	-24.76472	-24.76472	-24.76481	-24.5424	-24.7972	-24.8369	-24.8379
0.4	-24.91378	-24.91378	-24.913842	-24.6909	-24.9460	-24.9849	-24.9889
0.5	-25.04843	-25.04843	-25.048475	-24.8251	-25.0808	-25.1189	-25.1253
0.6	-25.17084	-25.17084	-25.17089	-24.9474	-25.2038	-25.2413	-25.2492
0.7	-25.28279	-25.28279	-25.28284	-25.0596	-25.3167	-25.3536	-25.3625
0.8	-25.38572	-25.38572	-25.38575	-25.1631	-25.4209	-25.4573	-25.4667
0.9	-25.48078	-25.48078	-25.48082	-25.2590	-25.5175	-25.5535	-25.5629
1	-25.56896	-25.56896	-25.56899	-25.3483	-25.6074	-25.6431	-25.6521
1.2	-25.72778	-25.72778	-25.72782	-25.5101	-25.7704	-25.8055	-25.8128
1.5	-25.93110	-25.93110	-25.93113	-25.7194	-25.9812	-26.0157	-26.0185
1.6761	-26.03517	-26.03517	-26.03522	-25.8276	-26.0903	-26.1244	-26.1238
1.8143	-26.11044	-26.11044	-26.11049	-25.9064	-26.1697	-26.2036	-26.1999
2	-26.20410	-26.20410	-26.20413	-26.0050	-26.2692	-26.3028	-26.2946

Continued on the next page

TABLE VII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
	2.23984	-26.31434	-26.31437	-26.1219	-26.3872	-26.4205	-26.4060
	2.4779	-26.41397	-26.41401	-26.2282	-26.4947	-26.5276	-26.5066
	2.5	-26.42279	-26.42283	-26.2376	-26.5043	-26.5372	-26.5155
	3	-26.60632	-26.60636	-26.4343	-26.7038	-26.7361	-26.7003
	4	-26.90345	-26.90349	-26.7515	-27.0278	-27.0591	-26.9984
	5	-27.12856	-27.12860	-26.9889	-27.2731	-27.3033	-27.2238
	7	-27.39397	-27.39403	-27.2669	-27.5684	-27.5959	-27.4904
	7.957	-27.44399		-27.3206	-27.6306	-27.6566	-27.5413
	8	-27.44521	-27.44526	-27.3220	-27.6323	-27.6582	-27.5425
	10	-27.41029	-27.41033	-27.2927	-27.6206	-27.6432	-27.5097
	12	-27.22047	-27.22053	-27.1073	-27.4525	-27.4717	-27.3221
	15	-26.70217	-26.70228	-26.5949	-26.9651	-26.9792	-26.8070
	20	-25.36277	-25.36280	-25.2647	-25.6743	-25.6808	-25.4721
	30	-21.47780	-21.4778	-21.3996	-21.8805	-21.8744	-21.5941
	40	-16.55435	-16.5544	-16.4984	-17.0427	-17.0272	-16.6756
	50	-10.94838	-10.9486	-10.9165	-11.5184	-11.4957	-11.0735
	100	22.57559	22.575	22.4739	21.6370	21.6808	22.4393
	200	101.16376	101.165	100.7814	99.6002	99.6652	101.0180
	500	363.59226	363.57	362.4191	360.5369	360.6471	363.4370
	1000	826.67529	826.74	824.3568	821.6736	821.8773	826.5153
	2000	1781.0060		1776.769	1772.941	1773.804	1780.843
$1s^2 2p_0 2p_{-1} 3d_{-2}$							
	0	-23.89386	-23.89391	-23.7320	-23.9815	-24.0160	-23.9622
	0.001	-23.89684	-23.8978	-23.7350	-23.9845	-24.0190	-23.9652
	0.002	-23.89981	-23.9008	-23.7380	-23.9874	-24.0220	-23.9681
	0.005	-23.90856	-23.909	-23.7468	-23.9962	-24.0308	-23.9769
	0.01	-23.92268	-23.924	-23.7610	-24.0104	-24.0449	-23.9910
	0.02	-23.94944	-23.9496	-23.7881	-24.0374	-24.0718	-24.0179
	0.03	-23.97466	-23.97487	-23.8137	-24.0629	-24.0971	-24.0433
	0.04	-23.99873	-23.99895	-23.8383	-24.0873	-24.1213	-24.0675
	0.05	-24.02194	-24.02216	-23.8619	-24.1107	-24.1445	-24.0909
	0.07	-24.06643	-24.06663	-23.9071	-24.1555	-24.1888	-24.1357
	0.07811	-24.08388		-23.9248	-24.1730	-24.2062	-24.1533
	0.1	-24.12967	-24.12988	-23.9713	-24.2190	-24.2519	-24.1994
	0.12	-24.17009	-24.17029	-24.0121	-24.2595	-24.2921	-24.2402
	0.15	-24.22861	-24.22877	-24.0712	-24.3180	-24.3504	-24.2992
	0.2	-24.32139	-24.32153	-24.1645	-24.4108	-24.4429	-24.3930
	0.3	-24.49241	-24.49251	-24.3362	-24.5820	-24.6137	-24.5661
	0.4	-24.64760	-24.64767	-24.4919	-24.7378	-24.7693	-24.7231
	0.5	-24.78992	-24.78997	-24.6348	-24.8809	-24.9122	-24.8670
	0.6	-24.92153	-24.92158	-24.7671	-25.0136	-25.0447	-25.0000
	0.7	-25.04409	-25.04414	-24.8905	-25.1373	-25.1682	-25.1238
	0.8	-25.15887	-25.15892	-25.0062	-25.2533	-25.2840	-25.2397
	0.9	-25.26690	-25.26694	-25.1152	-25.3627	-25.3932	-25.3487
	1	-25.36897	-25.36901	-25.2182	-25.4661	-25.4964	-25.4516
	1.2	-25.55777	-25.55781	-25.4091	-25.6576	-25.6876	-25.6421
	1.5	-25.80957	-25.80961	-25.6639	-25.9134	-25.9430	-25.8959
	1.6761	-25.94300	-25.94305	-25.7990	-26.0491	-26.0785	-26.0304
	1.8143	-26.04136		-25.8987	-26.1493	-26.1784	-26.1296
	2	-26.16569	-26.16572	-26.0247	-26.2759	-26.3049	-26.2549
	2.23984	-26.31434	-26.31437	-26.1754	-26.4275	-26.4561	-26.4048
	2.4779	-26.45015	-26.45018	-26.3131	-26.5661	-26.5945	-26.5418
	2.5	-26.46221	-26.46224	-26.3253	-26.5784	-26.6068	-26.5539
	3	-26.71294	-26.71297	-26.5795	-26.8348	-26.8625	-26.8069
	4	-27.10857	-27.10860	-26.9807	-27.2408	-27.2673	-27.2063
	5	-27.39438	-27.39442	-27.2707	-27.5364	-27.5613	-27.4955
	7	-27.72147	-27.72153	-27.6034	-27.8820	-27.9037	-27.8282
	7.957	-27.78682		-27.6708	-27.9560	-27.9761	-27.8959
	8	-27.78858	-27.78864	-27.6726	-27.9582	-27.9782	-27.8977
	10	-27.77133	-27.77139	-27.6590	-27.9591	-27.9758	-27.8846
	12	-27.58877	-27.58885	-27.4799	-27.7950	-27.8084	-27.7054

Continued on the next page

TABLE VII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
15		-27.07169	-27.07181	-26.9683	-27.3058	-27.3147	-27.1924
20		-25.72293	-25.72295	-25.6299	-26.0042	-26.0065	-25.8487
30		-21.80781	-21.80786	-21.7396	-22.1830	-22.1751	-21.9399
40		-16.85455	-16.85467	-16.8142	-17.3206	-17.3053	-16.9905
50		-11.22283	-11.22288	-11.2118	-11.7759	-11.7548	-11.3614
100		22.38046	22.38035	22.2424	21.4403	21.4792	22.2353
200		101.02798	101.0282	100.6004	99.4491	99.5082	100.8770
500		363.50267	363.5021	362.2793	360.4220	360.5213	363.3451
1000		826.60434	826.602	824.2317	821.5692	821.7182	826.444
2000		1780.9461	1780.96	1776.649	1772.842	1773.082	1780.782
$1s^2 2p_{-1} 3d_{-2} 4f_{-3}$							
0		-23.42580	-23.42589	-23.2157	-23.4674	-23.5025	-23.4884
0.001		-23.43026	-23.429	-23.2202	-23.4719	-23.5070	-23.4929
0.002		-23.43466	-23.434	-23.2246	-23.4763	-23.5114	-23.4973
0.005		-23.44747	-23.433	-23.2375	-23.4892	-23.5242	-23.5102
0.01		-23.46773	-23.468	-23.2580	-23.5096	-23.5445	-23.5307
0.02		-23.50553	-23.507	-23.2961	-23.5477	-23.5824	-23.5692
0.03		-23.54093	-23.5422	-23.3315	-23.5832	-23.6178	-23.6053
0.04		-23.57456	-23.576	-23.3650	-23.6167	-23.6514	-23.6396
0.05		-23.60670	-23.6077	-23.3969	-23.6488	-23.6834	-23.6722
0.07		-23.66727	-23.668	-23.4570	-23.7092	-23.7437	-23.7337
0.07811		-23.69064		-23.4802	-23.7325	-23.7670	-23.7574
0.1		-23.75088	-23.7512	-23.5400	-23.7925	-23.8269	-23.8184
0.12		-23.80289	-23.8031	-23.5917	-23.8444	-23.8785	-23.8710
0.15		-23.87656	-23.87678	-23.6649	-23.9177	-23.9516	-23.9455
0.2		-23.99037	-23.99055	-23.7778	-24.0310	-24.0643	-24.0605
0.3		-24.19402	-24.19415	-23.9797	-24.2334	-24.2657	-24.2663
0.4		-24.37503	-24.37515	-24.1588	-24.4134	-24.4446	-24.4490
0.5		-24.53940	-24.53949	-24.3215	-24.5770	-24.6073	-24.6149
0.6		-24.69060	-24.69068	-24.4712	-24.7276	-24.7572	-24.7673
0.7		-24.83099	-24.83107	-24.6103	-24.8676	-24.8966	-24.9088
0.8		-24.96229	-24.96237	-24.7405	-24.9987	-25.0270	-25.0411
0.9		-25.08577	-25.08586	-24.8630	-25.1221	-25.1499	-25.1655
1		-25.20246	-25.20257	-24.9789	-25.2388	-25.2661	-25.2829
1.2		-25.41848	-25.41860	-25.1935	-25.4549	-25.4814	-25.5004
1.5		-25.70728	-25.70750	-25.4808	-25.7442	-25.7695	-25.7910
1.6761		-25.86086	-25.86112	-25.6337	-25.8982	-25.9229	-25.9456
1.8143		-25.97435		-25.7467	-26.0120	-26.0363	-26.0598
2		-26.11855	-26.11859	-25.8904	-26.1567	-26.1804	-26.2050
2.23984		-26.29140	-26.29144	-26.0626	-26.3302	-26.3533	-26.3791
2.4779		-26.45013	-26.45018	-26.2208	-26.4896	-26.5121	-26.5389
2.5		-26.46427	-26.46431	-26.2349	-26.5038	-26.5262	-26.5531
3		-26.76015	-26.76019	-26.5297	-26.8011	-26.8224	-26.8512
4		-27.23762	-27.23765	-27.0051	-27.2814	-27.3006	-27.3326
5		-27.59735	-27.59737	-27.3627	-27.6439	-27.6610	-27.6959
7		-28.05665	-28.05669	-27.8174	-28.1092	-28.1219	-28.1613
7.957		-28.17991	-28.17996	-27.9384	-28.2355	-28.2461	-28.2871
8		-28.18420	-28.18424	-27.9426	-28.2399	-28.2504	-28.2915
10		-28.27942	-28.27946	-28.0333	-28.3422	-28.3481	-28.3915
12		-28.20034	-28.20038	-27.9503	-28.2709	-28.2722	-28.3165
15		-27.82525	-27.82530	-27.5703	-27.9086	-27.9034	-27.9466
20		-26.68601	-26.68603	-26.4259	-26.7933	-26.7781	-26.8142
30		-23.11969	-23.11975	-22.8582	-23.2801	-23.2492	-23.2577
40		-18.45278	-18.45285	-18.1984	-18.6702	-18.6275	-18.5976
50		-13.06551	-13.06555	-12.8236	-13.3414	-13.2897	-13.2154
100		19.65124	19.65114	19.7910	19.0827	19.1603	19.4867
200		97.19703	97.19700	97.0715	96.0789	96.1814	97.0201
500		357.78007	357.78007	356.8299	355.2528	355.3969	357.5907
1000		819.01476	819.01469	816.8168	814.5654	814.7561	818.8188
2000		1771.0044	1771.00420	1766.675	1763.456	1763.714	1770.804
$1s 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$							

Continued on the next page

TABLE VII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
0		-15.25773	-15.25778	-15.1148	-15.2885	-15.2864	-15.2766
0.001		-15.26515	-15.265	-15.1222	-15.2959	-15.2939	-15.2841
0.002		-15.27241	-15.273	-15.1295	-15.3032	-15.3012	-15.2914
0.005		-15.29339	-15.294	-15.1508	-15.3244	-15.3223	-15.3127
0.01		-15.32665	-15.3272	-15.1842	-15.3578	-15.3557	-15.3467
0.02		-15.38892	-15.3893	-15.2464	-15.4201	-15.4181	-15.4100
0.03		-15.44691	-15.4473	-15.3043	-15.4782	-15.4763	-15.4688
0.04		-15.50171	-15.5019	-15.3590	-15.5331	-15.5312	-15.5244
0.05		-15.55407	-15.5542	-15.4113	-15.5856	-15.5835	-15.5774
0.07		-15.65321	-15.6533	-15.5101	-15.6846	-15.6825	-15.6778
0.07811		-15.69172		-15.5485	-15.7231	-15.7208	-15.7168
0.1		-15.79180	-15.79190	-15.6480	-15.8229	-15.8205	-15.8181
0.12		-15.87908	-15.89	-15.7347	-15.9098	-15.9074	-15.9063
0.15		-16.00397	-16.00408	-15.8587	-16.0342	-16.0315	-16.0324
0.2		-16.19928	-16.19938	-16.0525	-16.2287	-16.2257	-16.2294
0.3		-16.55487	-16.55494	-16.4055	-16.5828	-16.5788	-16.5876
0.4		-16.87764	-16.87770	-16.7260	-16.9044	-16.8994	-16.9125
0.5		-17.17696	-17.17701	-17.0232	-17.2025	-17.1967	-17.2136
0.6		-17.45820	-17.45826	-17.3025	-17.4828	-17.4761	-17.4964
0.7		-17.72483	-17.72490	-17.5673	-17.7485	-17.7410	-17.7644
0.8		-17.97920	-17.97931	-17.8199	-18.0021	-17.9938	-18.0199
0.9		-18.22316	-18.22326	-18.0624	-18.2455	-18.2365	-18.2650
1		-18.45800	-18.45809	-18.2958	-18.4798	-18.4702	-18.5008
1.2		-18.90435	-18.90442	-18.7395	-18.9254	-18.9146	-18.9488
1.5		-19.52639	-19.52650	-19.3582	-19.5467	-19.5344	-19.5729
1.6761		-19.86999		-19.7002	-19.8901	-19.8770	-19.9175
1.8143		-20.13019		-19.9592	-20.1503	-20.1366	-20.1785
2		-20.46836	-20.46842	-20.2959	-20.4885	-20.4740	-20.5175
2.23984		-20.88761		-20.7136	-20.9079	-20.8925	-20.9378
2.4779		-21.28678		-21.1113	-21.3073	-21.2911	-21.3379
2.5		-21.32306	-21.32313	-21.1475	-21.3437	-21.3273	-21.3742
3		-22.11261	-22.11269	-21.9346	-22.1341	-22.1161	-22.1654
4		-23.54727	-23.54735	-23.3658	-23.5714	-23.5502	-23.6028
5		-24.83951	-24.83956	-24.6556	-24.8668	-24.8424	-24.8972
7		-27.12780	-27.12785	-26.9411	-27.1632	-27.1322	-27.1890
7.957		-28.11824		-27.9309	-28.1580	-28.1238	-28.1809
8		-28.16147	-28.16150	-27.9741	-28.2015	-28.1671	-28.2242
10		-30.06359	-30.06363	-29.8759	-30.1138	-30.0726	-30.1289
12		-31.79132	-31.791382	-31.6045	-31.8529	-31.8047	-31.8589
15		-34.13427	-34.134398	-33.9505	-34.2145	-34.1562	-34.2046
20		-37.55464	-37.55469	-37.3796	-37.6684	-37.5947	-37.6287
30		-43.21386	-43.213901	-43.0648	-43.3998	-43.3002	-43.2930
40		-47.88388	-47.883924	-47.7676	-48.1443	-48.0243	-47.9666
50		-51.91495	-51.91499	-51.8351	-52.2499	-52.1136	-52.0003
100		-66.99696	-66.99699	-67.1194	-67.6908	-67.5021	-67.0898
200		-86.60730	-86.60738	-87.1424	-87.9436	-87.6993	-86.7066
500		-121.16486	-121.16488	-122.8138	-124.0820	-123.7496	-121.2715
1000		-155.32948	-155.3296	-158.5373	-160.3384	-159.9217	-155.4409
2000		-197.86533	-197.8655	-203.6170	-206.1778	-205.6546	-197.9808

^a Data are from the two-dimensional mesh Hartree-Fock calculation by M. V. Ivanov and P. Schmelcher, J. Phys. B 34, 2031 (2001).

TABLE VIII: As in Table I for the Carbon atom.

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
$1s^2 2s^2 2p_0 2p_{-1}$							
0		-37.6909	-37.69096	-37.4680	-37.7944	-37.8579	-37.8417
0.001		-37.6924	-37.6925	-37.4695	-37.7959	-37.8594	-37.8432
0.002		-37.6939	-37.6940	-37.4710	-37.7974	-37.8609	-37.8447
0.005		-37.6984	-37.6985	-37.4755	-37.8019	-37.8654	-37.8492
0.01		-37.7058	-37.7059	-37.4829	-37.8093	-37.8728	-37.8566

Continued on the next page

TABLE VIII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
0.02		-37.7205	-37.7205	-37.4976	-37.8239	-37.8875	-37.8713
0.05		-37.7632	-37.7633	-37.5402	-37.8666	-37.9302	-37.9141
0.1		-37.8301	-37.8302	-37.6068	-37.9332	-37.9969	-37.9812
0.2		-37.9485	-37.9486	-37.7243	-38.0508	-38.1148	-38.1002
0.3		-38.0478	-38.0479	-37.8225	-38.1492	-38.2135	-38.2004
0.4		-38.1301	-38.1302	-37.9035	-38.2306	-38.2954	-38.2837
0.5		-38.1972	-38.1973	-37.9695	-38.2970	-38.3622	-38.3519
0.6		-38.2509	-38.2510	-38.0222	-38.3502	-38.4158	-38.4066
0.7		-38.2926	-38.2927	-38.0630	-38.3915	-38.4575	-38.4494
0.8		-38.3237	-38.3238	-38.0933	-38.4224	-38.4888	-38.4815
0.9		-38.3452	-38.3453	-38.1142	-38.4438	-38.5106	-38.5039
1		-38.3581	-38.3582	-38.1266	-38.4568	-38.5239	-38.5177
1.5		-38.3191	-38.3192	-38.0864	-38.4199	-38.4885	-38.4823
2		-38.1548	-38.1549	-37.9233	-38.2602	-38.3301	-38.3203
3		-37.6034	-37.6035	-37.3807	-37.7258	-37.7975	-37.7705
4		-36.8900	-36.8901	-36.6830	-37.0384	-37.1115	-37.0555
5		-36.0968	-36.0969	-35.9089	-36.2763	-36.3509	-36.2585
6		-35.2588		-35.0891	-35.4695	-35.5450	-35.4152
7		-34.3883		-34.2333	-34.6272	-34.7028	-34.5382
8		-33.4872		-33.3434	-33.7508	-33.8261	-33.6307
10		-31.5897		-31.4622	-31.8959	-31.9702	-31.7231
11		-30.5931		-30.4727	-30.9191	-30.9940	-30.7232
12		-29.5660		-29.4524	-29.9113	-29.9853	-29.6937
15		-26.3172		-26.2234	-26.7185	-26.792	-26.441
20		-20.4352		-20.3731	-20.9251	-20.996	-20.556
30		-7.4150		-7.4131	-8.0668	-8.134	-7.535
40		6.7308		6.6755	5.9317	5.867	6.609
50		21.6350		21.5247	20.6990	20.636	21.513
100		102.3865		102.0204	100.8574	100.800	102.262
200		277.1830		276.3664	274.7047	274.673	277.056
500		832.653		830.740	828.063	828.03	832.52
1000		1788.624		1785.264	1781.420	1781.42	1788.50
2000		3733.875		3728.234	3722.747	3722.82	3733.75
$1s^2 2s 2p_0 2p_{-1} 2p_{+1}$							
0		-37.5992	-37.59928	-37.3200	-37.6475	-37.7050	-37.6938
0.001		-37.6012	-37.6013	-37.3220	-37.6495	-37.7070	-37.6958
0.002		-37.6032	-37.6034	-37.3240	-37.6515	-37.7090	-37.6978
0.005		-37.6092	-37.6094	-37.3300	-37.6574	-37.7150	-37.7038
0.01		-37.6191	-37.6193	-37.3399	-37.6673	-37.7249	-37.7137
0.02		-37.6388	-37.6389	-37.3595	-37.6870	-37.7446	-37.7334
0.05		-37.6964	-37.6966	-37.4170	-37.7445	-37.8021	-37.7911
0.1		-37.7880	-37.7882	-37.5082	-37.8357	-37.8934	-37.8828
0.2		-37.9552	-37.9552	-37.6738	-38.0015	-38.0595	-38.0504
0.3		-38.1025	-38.1026	-37.8193	-38.1473	-38.2057	-38.1984
0.4		-38.2322	-38.2323	-37.9470	-38.2755	-38.3343	-38.3288
0.5		-38.3463	-38.3464	-38.0593	-38.3883	-38.4475	-38.4437
0.6		-38.4466	-38.4467	-38.1579	-38.4875	-38.5471	-38.5448
0.7		-38.5346	-38.5346	-38.2444	-38.5747	-38.6346	-38.6336
0.8		-38.6116	-38.6116	-38.3202	-38.6512	-38.7115	-38.7115
0.9		-38.6788	-38.6788	-38.3865	-38.7181	-38.7788	-38.7795
1		-38.7372	-38.7373	-38.4441	-38.7764	-38.8374	-38.8387
1.5		-38.9225	-38.9225	-38.6283	-38.9641	-39.0264	-39.0276
2		-38.9769	-38.9770	-38.6853	-39.0247	-39.0877	-39.0851
3		-38.8417	-38.8418	-38.5633	-38.9097	-38.9730	-38.9546
4		-38.5087	-38.5088	-38.2502	-38.6041	-38.6666	-38.6247
5		-38.0550	-38.0551	-37.8193	-38.1816	-38.2426	-38.1733
6		-37.5163		-37.3029	-37.6745	-37.7338	-37.6363
7		-36.9091	-36.9093	-36.7160	-37.0976	-37.1550	-37.0307
8		-36.2425	-36.2426	-36.0674	-36.4592	-36.5149	-36.3656
10		-34.7537	-34.7539	-34.6080	-35.0208	-35.0731	-34.8798
11		-33.9405		-33.8069	-34.2302	-34.2810	-34.0680

Continued on the next page

TABLE VIII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
12		-33.0864		-32.9637	-33.3974	-33.4468	-33.2153
15		-30.3091		-30.2138	-30.6782	-30.7240	-30.4420
20		-25.1035		-25.0444	-25.5579	-25.5990	-25.2418
30		-13.1909		-13.1911	-13.7951	-13.8310	-13.3367
40		0.0424		-0.0123	-0.6982	-0.7320	-0.1085
50		14.1568		14.0493	13.2881	13.2547	14.0022
100		91.9179		91.5591	90.4854	90.4488	91.7545
200		262.7348		261.9195	260.3808	260.3407	262.5652
500		811.0116		809.0424	806.5504	806.5224	810.8361
1000		1759.749		1756.207	1752.625	1752.632	1759.570
2000		3695.909		3689.821	3684.685	3684.767	3695.727
$1s^2 2s 2p_0 2p_{-1} 3d_{-2}$							
0		-37.2187	-37.2188	-36.9240	-37.2559	-37.3108	-37.3034
0.001		-37.2222	-37.2224	-36.9275	-37.2594	-37.3143	-37.3069
0.002		-37.2257	-37.2259	-36.9310	-37.2629	-37.3177	-37.3104
0.005		-37.2359	-37.2360	-36.9412	-37.2732	-37.3280	-37.3206
0.01		-37.2524	-37.2526	-36.9579	-37.2899	-37.3446	-37.3372
0.02		-37.2840	-37.2842	-36.9898	-37.3218	-37.3764	-37.3689
0.05		-37.3704	-37.3705	-37.0777	-37.4095	-37.4635	-37.4557
0.1		-37.5008	-37.5010	-37.2105	-37.5414	-37.5943	-37.5866
0.2		-37.7386	-37.7388	-37.4515	-37.7801	-37.8313	-37.8251
0.3		-37.9578	-37.9579	-37.6720	-37.9990	-38.0491	-38.0454
0.4		-38.1623	-38.1624	-37.8765	-38.2029	-38.2523	-38.2513
0.5		-38.3539	-38.3541	-38.0675	-38.3937	-38.4426	-38.4445
0.6		-38.5338	-38.5339	-38.2464	-38.5728	-38.6214	-38.6261
0.7		-38.7032	-38.7033	-38.4146	-38.7415	-38.7897	-38.7970
0.8		-38.8631	-38.8632	-38.5732	-38.9007	-38.9486	-38.9583
0.9		-39.0143	-39.0145	-38.7232	-39.0514	-39.0990	-39.1109
1		-39.1577	-39.1577	-38.8653	-39.1942	-39.2417	-39.2555
1.5		-39.7775	-39.7776	-39.4803	-39.8132	-39.8599	-39.8805
2		-40.2769	-40.2769	-39.9767	-40.3135	-40.3599	-40.3837
3		-41.0476	-41.0477	-40.7466	-41.0905	-41.1365	-41.1597
4		-41.6318	-41.6319	-41.3355	-41.6861	-41.7312	-41.7470
5		-42.1015	-42.1016	-41.8142	-42.1718	-42.2156	-42.2186
7		-42.8150	-42.8151	-42.5525	-42.9258	-42.9660	-42.9345
8		-43.0839	-43.0841	-42.8346	-43.2166	-43.2545	-43.2043
10		-43.4768	-43.4769	-43.2522	-43.6525	-43.6858	-43.5992
11		-43.6090		-43.3957	-43.8052	-43.8363	-43.7324
12		-43.7031	-43.7032	-43.5002	-43.9190	-43.9479	-43.8274
15		-43.7839	-43.7842	-43.6086	-44.0551	-44.0779	-43.9112
20		-43.3766	-43.3767	-43.2385	-43.7299	-43.7439	-43.5080
30		-41.1418	-41.1418	-41.0637	-41.6386	-41.6389	-41.2795
40		-37.6518	-37.6519	-37.6260	-38.2772	-38.2675	-37.7937
50		-33.3210	-33.3211	-33.3445	-34.0660	-34.0486	-33.4660
100		-4.7811		-5.0317	-6.0472	-6.0076	-4.9338
200		66.9964		66.3404	64.8850	64.9456	66.8384
500		316.8739		315.1883	312.8296	312.9300	316.7110
1000		767.1167		764.0121	760.6218	760.7741	766.9512
2000		1705.077		1699.652	1694.794	1695.034	1704.910
$1s^2 2p_0 2p_{-1} 3d_{-2} 4f_{-3}$							
0		-36.1168	-36.1170	-35.9037	-36.2234	-36.2617	-36.1921
0.001		-36.1218	-36.122	-35.9087	-36.2284	-36.2667	-36.1971
0.002		-36.1267	-36.1270	-35.9136	-36.2333	-36.2716	-36.2020
0.005		-36.1410	-36.1413	-35.9280	-36.2477	-36.2859	-36.2164
0.01		-36.1638	-36.1641	-35.9510	-36.2707	-36.3088	-36.2395
0.02		-36.2067	-36.2085	-35.9941	-36.3138	-36.3517	-36.2831
0.05		-36.3232	-36.3247	-36.1102	-36.4302	-36.4680	-36.4015
0.1		-36.4929	-36.4932	-36.2793	-36.5998	-36.6373	-36.5729
0.2		-36.7834	-36.7835	-36.5700	-36.8902	-36.9269	-36.8659
0.3		-37.0385	-37.0387	-36.8255	-37.1450	-37.1809	-37.1230
0.4		-37.2715	-37.2716	-37.0586	-37.3775	-37.4128	-37.3579

Continued on the next page

TABLE VIII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
0.5		-37.4879	-37.4881	-37.2752	-37.5936	-37.6284	-37.5761
0.6		-37.6910	-37.6912	-37.4783	-37.7966	-37.8308	-37.7808
0.7		-37.8828	-37.8830	-37.6703	-37.9884	-38.0222	-37.9741
0.8		-38.0649	-38.0650	-37.8525	-38.1707	-38.2040	-38.1576
0.9		-38.2383	-38.2385	-38.0262	-38.3445	-38.3774	-38.3324
1		-38.4041	-38.4043	-38.1922	-38.5107	-38.5432	-38.4994
1.5		-39.1402	-39.1406	-38.9304	-39.2504	-39.2813	-39.2405
2		-39.7620	-39.7621	-39.5550	-39.8769	-39.9065	-39.8664
3		-40.7780	-40.7780	-40.5769	-40.9029	-40.9304	-40.8883
4		-41.5885	-41.5886	-41.3931	-41.7233	-41.7490	-41.7035
5		-42.2548	-42.2549	-42.0645	-42.3993	-42.4231	-42.3738
7		-43.2770	-43.2771	-43.0951	-43.4400	-43.4600	-43.4025
8		-43.6684	-43.6685	-43.4901	-43.8406	-43.8585	-43.7966
10		-44.2658	-44.2659	-44.0938	-44.4562	-44.4698	-44.3989
12		-44.6614	-44.6615	-44.4953	-44.8703	-44.8795	-44.7987
15		-44.9570	-44.9571	-44.7993	-45.1939	-45.1968	-45.0993
20		-44.8467	-44.8468	-44.7034	-45.1317	-45.1251	-44.9957
30		-43.0911	-43.0912	-42.9800	-43.4752	-43.4528	-43.2488
40		-39.9995	-39.9996	-39.9239	-40.4829	-40.4485	-40.1626
50		-36.0196	-36.0197	-35.9812	-36.6004	-36.5564	-36.1863
100		-8.8657	-8.865	-9.0134	-9.8891	-9.8143	-9.0411
200		60.9774	60.973	60.4822	59.2231	59.3311	60.7948
500		307.3113	307.31	305.8632	303.8298	303.9931	307.1192
1000		753.9965	754.1	751.1544	748.2435	748.4701	753.7969
2000		1687.461		1682.271	1678.115	1678.480	1687.256
$1s^2 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$							
0		-35.1185	-35.1186	-34.8393	-35.1633	-35.2027	-35.1878
0.001		-35.1254	-35.126	-34.8462	-35.1702	-35.2096	-35.1948
0.002		-35.1321	-35.133	-34.8530	-35.1770	-35.2164	-35.2016
0.005		-35.1516	-35.152	-34.8727	-35.1967	-35.2360	-35.2214
0.01		-35.1824	-35.1827	-34.9037	-35.2276	-35.2669	-35.2528
0.02		-35.2396	-35.2399	-34.9609	-35.2848	-35.3243	-35.3112
0.05		-35.3898	-35.3900	-35.1107	-35.4353	-35.4747	-35.4636
0.1		-35.6025	-35.6027	-35.3225	-35.6476	-35.6867	-35.6792
0.2		-35.9598	-35.9600	-35.6768	-36.0033	-36.0417	-36.0404
0.3		-36.2651	-36.2653	-35.9795	-36.3072	-36.3446	-36.3483
0.4		-36.5374	-36.5376	-36.2496	-36.5783	-36.6148	-36.6228
0.5		-36.7862	-36.7864	-36.4963	-36.8261	-36.8616	-36.8734
0.6		-37.0168	-37.0170	-36.7250	-37.0558	-37.0904	-37.1055
0.7		-37.2326	-37.2329	-36.9392	-37.2709	-37.3046	-37.3228
0.8		-37.4361	-37.4364	-37.1410	-37.4737	-37.5066	-37.5275
0.9		-37.6291	-37.6293	-37.3325	-37.6662	-37.6984	-37.7217
1		-37.8128	-37.8130	-37.5149	-37.8497	-37.8812	-37.9065
1.5		-38.6240	-38.6242	-38.3209	-38.6604	-38.6892	-38.7218
2		-39.3059	-39.3061	-38.9994	-39.3433	-39.3698	-39.4070
3		-40.4220	-40.4222	-40.1117	-40.4631	-40.4862	-40.5280
4		-41.3179	-41.3180	-41.0055	-41.3636	-41.3839	-41.4279
5		-42.0607	-42.0608	-41.7472	-42.1113	-42.1292	-42.1743
7		-43.2195	-43.2195	-42.9043	-43.2802	-43.2936	-43.3392
8		-43.6733	-43.6734	-43.3575	-43.7393	-43.7505	-43.7958
10		-44.3871	-44.3872	-44.0704	-44.4637	-44.4705	-44.5145
12		-44.8904	-44.8905	-44.5730	-44.9780	-44.9802	-45.0221
15		-45.3346	-45.3348	-45.0168	-45.4394	-45.4350	-45.4719
20		-45.4464	-45.4465	-45.1298	-45.5816	-45.5664	-45.5913
30		-44.0660	-44.0660	-43.7583	-44.2660	-44.2323	-44.2220
40		-41.2854	-41.2855	-40.9936	-41.5534	-41.5048	-41.4495
50		-37.5717	-37.5718	-37.3004	-37.9089	-37.8482	-37.7418
100		-11.3693	-11.3693	-11.2368	-12.0509	-11.9541	-11.5572
200		57.3385	57.3384	57.1382	56.0142	56.1430	57.1350
500		301.7770	301.1777	300.5717	298.8072	298.9804	301.5572
1000		746.5892	746.589	743.8774	741.3741	741.5914	746.3601

Continued on the next page

TABLE VIII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
	2000	1677.675		1672.396	1668.833	1669.112	1677.439
$1s2p_02p_{-1}3d_{-2}4f_{-3}5g_{-4}$							
0		-24.3111	-24.3112	-24.2069	-24.4194	-24.4146	-24.3404
0.001		-24.3190	-24.3193	-24.2149	-24.4274	-24.4226	-24.3484
0.002		-24.3268	-24.3272	-24.2227	-24.4352	-24.4304	-24.3562
0.005		-24.3493	-24.3496	-24.2454	-24.4578	-24.4530	-24.3790
0.01		-24.3850	-24.3853	-24.2814	-24.4938	-24.4890	-24.4155
0.02		-24.4523	-24.4525	-24.3486	-24.5611	-24.5564	-24.4839
0.05		-24.6327	-24.6328	-24.5287	-24.7418	-24.7371	-24.6664
0.1		-24.8958	-24.8959	-24.7910	-25.0047	-24.9996	-24.9325
0.2		-25.3545	-25.3546	-25.2474	-25.4621	-25.4564	-25.3950
0.3		-25.7615	-25.7617	-25.6528	-25.8681	-25.8616	-25.8046
0.4		-26.1357	-26.1358	-26.0260	-26.2415	-26.2343	-26.1809
0.5		-26.4863	-26.4865	-26.3758	-26.5914	-26.5836	-26.5333
0.6		-26.8186	-26.8187	-26.7075	-26.9231	-26.9147	-26.8673
0.7		-27.1360	-27.1362	-27.0244	-27.2400	-27.2311	-27.1863
0.8		-27.4409	-27.4411	-27.3288	-27.5444	-27.5350	-27.4926
0.9		-27.7349	-27.7351	-27.6225	-27.8382	-27.8283	-27.7880
1		-28.0193	-28.0195	-27.9066	-28.1224	-28.1121	-28.0737
1.5		-29.3273	-29.3275	-29.2139	-29.4305	-29.4182	-29.3871
2		-30.4937	-30.4938	-30.3804	-30.5984	-30.5845	-30.5577
3		-32.5444	-32.5445	-32.4330	-32.6545	-32.6377	-32.6145
4		-34.3403	-34.3404	-34.2317	-34.4571	-34.4376	-34.4147
5		-35.9601	-35.9601	-35.8547	-36.0840	-36.0619	-36.0377
7		-38.8324	-38.8325	-38.7340	-38.9717	-38.9442	-38.9151
8		-40.1320	-40.1320	-40.0372	-40.2793	-40.2490	-40.2166
10		-42.5277	-42.5277	-42.4405	-42.6918	-42.6556	-42.6156
12		-44.7092	-44.7094	-44.6300	-44.8912	-44.8488	-44.7998
15		-47.6768	-47.6770	-47.6103	-47.8869	-47.8355	-47.7706
20		-52.0281	-52.0282	-51.9852	-52.2884	-52.2226	-52.1259
30		-59.2746	-59.2747	-59.2852	-59.6420	-59.5514	-59.3774
40		-65.2948	-65.2949	-65.3639	-65.7730	-65.6624	-65.4004
50		-70.5186	-70.5187	-70.6485	-71.1076	-70.9808	-70.6259
100		-90.2751	-90.2751	-90.7042	-91.3832	-91.2017	-90.3844
200		-116.4046	-116.4070	-117.3462	-118.3616	-118.1144	-116.5129
500		-163.2065	-163.209	-165.3937	-167.0815	-166.7213	-163.3161
1000		-209.9844	-209.98	-213.8854	-216.3191	-215.8363	-210.0976
2000		-268.6769	-268.711	-275.3603	-278.8362	-278.0891	-268.7939
$1s2p_{-1}3d_{-2}4f_{-3}5g_{-4}6h_{-5}$							
0		-22.5586	-22.5588	-22.3799	-22.5977	-22.5936	-22.5836
0.001		-22.5689	-22.570	-22.3903	-22.6081	-22.6039	-22.5940
0.002		-22.5789	-22.580	-22.4004	-22.6181	-22.6140	-22.6043
0.005		-22.6079	-22.608	-22.4294	-22.6468	-22.6426	-22.6340
0.01		-22.6535	-22.6539	-22.4749	-22.6924	-22.6886	-22.6803
0.02		-22.7371	-22.7376	-22.5588	-22.7766	-22.7728	-22.7653
0.05		-22.9575	-22.9579	-22.7789	-22.9972	-22.9934	-22.9889
0.1		-23.2739	-23.2743	-23.0936	-23.3129	-23.3090	-23.3090
0.2		-23.8122	-23.8125	-23.6286	-23.8496	-23.8450	-23.8521
0.3		-24.2809	-24.2813	-24.0942	-24.3166	-24.3113	-24.3244
0.4		-24.7062	-24.7067	-24.5165	-24.7404	-24.7344	-24.7523
0.5		-25.1003	-25.1007	-24.9080	-25.1332	-25.1264	-25.1486
0.6		-25.4702	-25.4706	-25.2757	-25.5021	-25.4945	-25.5203
0.7		-25.8207	-25.8211	-25.6242	-25.8518	-25.8434	-25.8725
0.8		-26.1550	-26.1554	-25.9566	-26.1854	-26.1762	-26.2082
0.9		-26.4755	-26.4758	-26.2754	-26.5053	-26.4953	-26.5300
1		-26.7841	-26.7843	-26.5823	-26.8134	-26.8027	-26.8398
1.5		-28.1886	-28.1888	-27.9803	-28.2167	-28.2030	-28.2492
2		-29.4280	-29.4282	-29.2146	-29.4561	-29.4398	-29.4921
3		-31.5923	-31.5925	-31.3726	-31.6229	-31.6026	-31.6613
4		-33.4805	-33.4807	-33.2572	-33.5154	-33.4918	-33.5529
5		-35.1814	-35.1815	-34.9562	-35.2214	-35.1947	-35.2564

Continued on the next page

TABLE VIII (*continued*)

State	$B(\text{au})$	HF, present	HF, lit. ^a	LDA	GGA	MGGA	HGGA
	7	-38.1970	-38.1971	-37.9708	-38.2489	-38.2162	-38.2761
	8	-39.5619	-39.5620	-39.3361	-39.6202	-39.5846	-39.6427
	10	-42.0798	-42.0799	-41.8560	-42.1517	-42.1102	-42.1635
	12	-44.3749	-44.3749	-44.1541	-44.4611	-44.4135	-44.4610
	15	-47.5001	-47.5002	-47.2857	-47.6090	-47.5523	-47.5894
	20	-52.0890	-52.0890	-51.8882	-52.2377	-52.1663	-52.1825
	30	-59.7432	-59.7433	-59.5777	-59.9760	-59.8782	-59.8427
	40	-66.1072	-66.1073	-65.9830	-66.4261	-66.3063	-66.2109
	50	-71.6284	-71.6285	-71.5491	-72.0335	-71.8952	-71.7353
	100	-92.4552	-92.4552	-92.6194	-93.2756	-93.0768	-92.5713
	200	-119.8126	-119.8127	-120.4670	-121.3784	-121.1176	-119.9369
	500	-168.5247	-168.5248	-170.4974	-171.9286	-171.5769	-168.6581
	1000	-217.1411	-217.1413	-220.9600	-222.9848	-222.5500	-217.2806
	2000	-278.1608	-278.1612	-285.0003	-287.8705	-287.3331	-278.3055

^a Data are from two-dimensional mesh HF calculation; M.V. Ivanov and P. Schmelcher, Phys. Rev. A **60**, 3558 (1999). The energy of the $1s^2 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$ state at $B = 500$ a.u. appears to be in error.