

Supplementary Information to the paper

“Full triples contribution in coupled-cluster and equation-of-motion coupled-cluster methods for atoms and molecules in strong magnetic fields” by Florian Hampe, Niklas Gross, Stella Stopkowicz

angle=60°														
FCI					EOM-EE-CCSDT					EOM-EE-CCSD				
B	Sigma	Pi-1	Pi+1	Delta-2	B	Sigma	Pi-1	Pi+1	Delta-2	B	Sigma	Pi-1	Pi+1	Delta-2
0.00	-38.005861	-37.887716	-37.887716	-37.751762	0.00	-38.005742	-37.887682	-37.887682	-37.750125	0.00	-38.003836	-37.884624	-37.884624	-37.715157
0.05	-38.011128	-37.897652	-37.872131	-37.771497	0.05	-38.011051	-37.897550	-37.871981	-37.770132	0.05	-38.009088	-37.894903	-37.869560	-37.734471
0.10	-38.024263	-37.904170	-37.850934	-37.780438	0.10	-38.024221	-37.904094	-37.850792	-37.779421	0.10	-38.022217	-37.901845	-37.849117	-37.742547
0.15	-38.040606	-37.908786	-37.826338	-37.778770	0.15	-38.040571	-37.908748	-37.826302	-37.777966	0.15	-38.038603	-37.906782	-37.824604	-37.740026
0.20	-38.056860	-37.911411	-37.801319	-37.766488	0.20	-38.056826	-37.911390	-37.801317	-37.765829	0.20	-38.054915	-37.909610	-37.797850	-37.728376
0.25	-38.071184	-37.911405	-37.778394	-37.743461	0.25	-38.071150	-37.911388	-37.778284	-37.742966	0.25	-38.069290	-37.909711	-37.770036	-37.709193
0.30	-38.082599	-37.908269	-37.756495	-37.712530	0.30	-38.082565	-37.908250	-37.756241	-37.712158	0.30	-38.080745	-37.906623	-37.741824	-37.683870
0.35	-38.090607	-37.901768	-37.733644	-37.677413	0.35	-38.090573	-37.901746	-37.733274	-37.677100	0.35	-38.088782	-37.900136	-37.713853	-37.653846
0.40	-38.094985	-37.891874	-37.709766	-37.641291	0.40	-38.094952	-37.891850	-37.709312	-37.640987	0.40	-38.093181	-37.890232	-37.687414	-37.624980
0.45	-38.095677	-37.878686	-37.686366	-37.614011	0.45	-38.095615	-37.878631	-37.685855	-37.613686	0.45	-38.093888	-37.877014	-37.665120	-37.597299
0.50	-38.092731	-37.862388	-37.666054	-37.598565	0.50	-38.092699	-37.862360	-37.665644	-37.598240	0.50	-38.090952	-37.860666	-37.649150	-37.578923
0.55	-38.086254	-37.843219	-37.650009	-37.575917	0.55	-38.086222	-37.843188	-37.649727	-37.575404	0.55	-38.084480	-37.841420	-37.637375	-37.562870
0.60	-38.076388	-37.821460	-37.636113	-37.558557	0.60	-38.076358	-37.821429	-37.635934	-37.558485	0.60	-38.074615	-37.819553	-37.626185	-37.550837
0.65	-38.063293	-37.797434	-37.621897	-37.545685	0.65	-38.063263	-37.797400	-37.621782	-37.545679	0.65	-38.061517	-37.795376	-37.613667	-37.538084
0.70	-38.047130	-37.771495	-37.606116	-37.531365	0.70	-38.047101	-37.771460	-37.606042	-37.531374	0.70	-38.045348	-37.769238	-37.599133	-37.523419
0.75	-38.028058	-37.744032	-37.588313	-37.515064	0.75	-38.028031	-37.743995	-37.588268	-37.515078	0.75	-38.026268	-37.741518	-37.582395	-37.506547
0.80	-38.006231	-37.715461	-37.568358	-37.496570	0.80	-38.006204	-37.715421	-37.568334	-37.496585	0.80	-38.004427	-37.712629	-37.563424	-37.487316
0.85	-37.981789	-37.686198	-37.546249	-37.475687	0.85	-37.981764	-37.686157	-37.546243	-37.475702	0.85	-37.979969	-37.682996	-37.542220	-37.465584
0.90	-37.954868	-37.656628	-37.522033	-37.452223	0.90	-37.954843	-37.656584	-37.522038	-37.452239	0.90	-37.953028	-37.653025	-37.518761	-37.441230
0.95	-37.925593	-37.627042	-37.495792	-37.426047	0.95	-37.925570	-37.626998	-37.495805	-37.426067	0.95	-37.923730	-37.623051	-37.493019	-37.414199
1.00	-37.894084	-37.597583	-37.467667	-37.397136	1.00	-37.894062	-37.597541	-37.467682	-37.397162	1.00	-37.892194	-37.593250	-37.465020	-37.384536
angle=90°														
FCI					EOM-EE-CCSDT					EOM-EE-CCSD				
B	Sigma	Pi-1	Pi+1	Delta-2	B	Sigma	Pi-1	Pi+1	Delta-2	B	Sigma	Pi-1	Pi+1	Delta-2
0.00	-38.005861	-37.887716	-37.887716	-37.751762	0.00	-38.005742	-37.887682	-37.887682	-37.750125	0.00	-38.003836	-37.884624	-37.884624	-37.715157
0.05	-38.013269	-37.889030	-37.880464	-37.745996	0.05	-38.013200	-37.888980	-37.880252	-37.744673	0.05	-38.011225	-37.886101	-37.878270	-37.708763
0.10	-38.030554	-37.892000	-37.863213	-37.730865	0.10	-38.030514	-37.891953	-37.863078	-37.729849	0.10	-38.028513	-37.889439	-37.861910	-37.691635
0.15	-38.050610	-37.894690	-37.841620	-37.711781	0.15	-38.050576	-37.894653	-37.841618	-37.710922	0.15	-38.048620	-37.892459	-37.840569	-37.669959
0.20	-38.069546	-37.895495	-37.817526	-37.692019	0.20	-38.069512	-37.895464	-37.817594	-37.691239	0.20	-38.067611	-37.893494	-37.816305	-37.649085
0.25	-38.085586	-37.893452	-37.791068	-37.670918	0.25	-38.085552	-37.893425	-37.791157	-37.670166	0.25	-38.083696	-37.891604	-37.789450	-37.627960
0.30	-38.097928	-37.888075	-37.762421	-37.647504	0.30	-38.097895	-37.888051	-37.762500	-37.646764	0.30	-38.096072	-37.886332	-37.760278	-37.604949
0.35	-38.106237	-37.879168	-37.732533	-37.622263	0.35	-38.106204	-37.879146	-37.732580	-37.621581	0.35	-38.104411	-37.877506	-37.729814	-37.582498
0.40	-38.110417	-37.866709	-37.703762	-37.600722	0.40	-38.110384	-37.866689	-37.703761	-37.600374	0.40	-38.108614	-37.865106	-37.700550	-37.580002
0.45	-38.110509	-37.850781	-37.680335	-37.585735	0.45	-38.110477	-37.850763	-37.680292	-37.585637	0.45	-38.108724	-37.849219	-37.676900	-37.570930
0.50	-38.106633	-37.831530	-37.665421	-37.563085	0.50	-38.106600	-37.831514	-37.665372	-37.562949	0.50	-38.104862	-37.829996	-37.661955	-37.547823
0.55	-38.098950	-37.809150	-37.656584	-37.531310	0.55	-38.098917	-37.809135	-37.656550	-37.531052	0.55	-38.097191	-37.807625	-37.653085	-37.514278
0.60	-38.087642	-37.783857	-37.649729	-37.494781	0.60	-38.087611	-37.783845	-37.649709	-37.494404	0.60	-38.085893	-37.782319	-37.646186	-37.476531
0.65	-38.072900	-37.755887	-37.642773	-37.456970	0.65	-38.072870	-37.755878	-37.642762	-37.456545	0.65	-38.071157	-37.754306	-37.639193	-37.441564
0.70	-38.054909	-37.725483	-37.635015	-37.423188	0.70	-38.054879	-37.725477	-37.635009	-37.422952	0.70	-38.053168	-37.723820	-37.631405	-37.417067
0.75	-38.033847	-37.692896	-37.626230	-37.399414	0.75	-38.033818	-37.692892	-37.626229	-37.399304	0.75	-38.032107	-37.691101	-37.622599	-37.396140
0.80	-38.009886	-37.658375	-37.616292	-37.377296	0.80	-38.009857	-37.658372	-37.616293	-37.377190	0.80	-38.009242	-37.657484	-37.613741	-37.375339
0.85	-37.983187	-37.622169	-37.605055	-37.353944	0.85	-37.983159	-37.622168	-37.605058	-37.353831	0.85	-37.981442	-37.619908	-37.601388	-37.350771
0.90	-37.953906	-37.584521	-37.592345	-37.329047	0.90	-37.953879	-37.584520	-37.592350	-37.328924	0.90	-37.952155	-37.581891	-37.588651	-37.325666
0.95	-37.922194	-37.545672	-37.577980	-37.302536	0.95	-37.922169	-37.545670	-37.577988	-37.302401	0.95	-37.920436	-37.542559	-37.574246	-37.298906
1.00	-37.888198	-37.505864	-37.561785	-37.274363	1.00	-37.888174	-37.505857	-37.561796	-37.274212	1.00	-37.886430	-37.502128	-37.557988	-37.270448

SI II: Total energies for CH⁺ in a magnetic field at 0° with respect to the bond axis. State labels refer to the field-free case.
Cartesian unc-aug-cc-pCVQZ basis set, R=2.1275 Bohr.

EOM-EE-CCSD

B	Sigma	Pi-1	Pi+1	Delta-2
0.00	-38.080395	-37.966099	-37.966099	-37.783688
0.10	-38.073231	-38.007596	-37.907596	-37.873594
0.20	-38.051956	-38.032437	-37.832437	-37.943812
0.30	-38.017136	-38.041514	-37.741514	-37.995588
0.40	-37.969572	-38.036003	-37.636003	-38.030511
0.50	-37.910170	-38.017160	-37.517160	-38.050219
0.60	-37.839851	-37.986205	-37.386205	-38.056255
0.70	-37.759507	-37.944277	-37.244277	-38.050024
0.80	-37.669971	-37.892420	-37.092420	-38.032781
0.90	-37.572013	-37.831577	-36.931577	-38.005646
1.00	-37.466336	-37.762602	-36.762602	-37.969609

EOM-EE-CCSDT

B	Sigma	Pi-1	Pi+1	Delta-2
0.00	-38.083844	-37.970425	-37.970425	-37.837812
0.10	-38.076671	-38.011912	-37.911912	-37.927804
0.20	-38.055364	-38.036722	-37.836722	-37.998259
0.30	-38.020497	-38.045754	-37.745754	-38.050398
0.40	-37.972875	-38.040189	-37.640189	-38.085785
0.50	-37.913408	-38.021286	-37.521286	-38.106037
0.60	-37.843020	-37.990268	-37.390268	-38.112680
0.70	-37.762606	-37.948280	-37.248280	-38.107107
0.80	-37.673001	-37.896364	-37.096364	-38.090560
0.90	-37.574973	-37.835466	-36.935466	-38.064142
1.00	-37.469228	-37.766441	-36.766441	-38.028830

SI III: Averaged transition wave lengths and total energies for ground and excited states of the sodium atom. The simplified state labels are described in the text.

averaged transitions from NIST						averaged transitions from NIST						averaged transitions from NIST									
s->p	5892.938	p->d	8189.037																		
EOM-CCSD, Cartesian uncontracted aug-cc-pCVQZ basis						EOM-CCSD, Cartesian uncontracted aug-cc-pCVTZ basis						EOM-CCSDT, Cartesian uncontracted aug-cc-pCVTZ basis									
B	Ref	3p-1	3p0	3d-2	3d-1	B	Ref	3p-1	3p0	3d-2	3d-1	B	Ref	3p-1	3p0	3d-2	3d-1				
0.00	-162.221817	-162.145262	-162.145262	-162.086514	-162.086514	0.00	-162.191503	-162.115583	-162.115583	-162.055531	-162.055531	0.00	-162.195133	-162.119040	-162.119040	-162.058903	-162.058903				
0.02	-162.230948	-162.163458	-162.154247	-162.112777	-162.103939	0.02	-162.200627	-162.133762	-162.124558	-162.082180	-162.073221	0.02	-162.204258	-162.137222	-162.128016	-162.085553	-162.076593				
0.04	-162.238377	-162.178329	-162.161298	-162.132214	-162.116509	0.04	-162.208039	-162.148581	-162.131570	-162.102385	-162.086402	0.04	-162.211673	-162.152048	-162.135032	-162.105758	-162.089775				
0.06	-162.244206	-162.190450	-162.166653	-162.146541	-162.125059	0.06	-162.213842	-162.160610	-162.136829	-162.116955	-162.095428	0.06	-162.217481	-162.164087	-162.140297	-162.120332	-162.098803				
0.08	-162.248565	-162.200351	-162.170582	-162.157705	-162.130723	0.08	-162.218165	-162.170378	-162.140581	-162.127291	-162.100917	0.08	-162.221809	-162.173866	-162.144054	-162.130671	-162.104293				
0.10	-162.251580	-162.208415	-162.173310	-162.166977	-162.134524	0.10	-162.221139	-162.178284	-162.143055	-162.135147	-162.103736	0.10	-162.224789	-162.181784	-162.146535	-162.138534	-162.107115				
0.12	-162.253371	-162.214915	-162.175006	-162.174885	-162.137119	0.12	-162.222879	-162.184614	-162.144439	-162.141969	-162.104858	0.12	-162.226535	-162.188126	-162.147927	-162.145364	-162.108241				
0.14	-162.254040	-162.220035	-162.175782	-162.181645	-162.138822	0.14	-162.223492	-162.189580	-162.144887	-162.148351	-162.105092	0.14	-162.227152	-162.193103	-162.148380	-162.151751	-162.108479				
0.16	-162.253678	-162.223912	-162.175711	-162.187411	-162.139790	0.16	-162.223065	-162.193336	-162.144508	-162.154199	-162.104850	0.16	-162.226730	-162.196871	-162.148007	-162.157605	-162.108242				
0.18	-162.252360	-162.226645	-162.174838	-162.192310	-162.140121	0.18	-162.221677	-162.195996	-162.143386	-162.159232	-162.104182	0.18	-162.225347	-162.199543	-162.146892	-162.162645	-162.107578				
0.20	-162.250155	-162.228319	-162.173197	-162.196438	-162.139886	0.20	-162.219391	-162.197640	-162.141575	-162.163250	-162.102950	0.20	-162.223064	-162.201197	-162.145086	-162.166669	-162.106349				
0.22	-162.247118	-162.229003	-162.170811	-162.199850	-162.139125	0.22	-162.216262	-162.198328	-162.139113	-162.166190	-162.101001	0.22	-162.219938	-162.201895	-162.142628	-162.169616	-162.104404				
0.24	-162.243302	-162.228760	-162.167704	-162.202581	-162.137856	0.24	-162.212335	-162.198105	-162.136018	-162.168096	-162.098233	0.24	-162.216013	-162.201682	-162.139538	-162.171530	-162.101640				
0.26	-162.238751	-162.227642	-162.163898	-162.204649	-162.136077	0.26	-162.207648	-162.197009	-162.132304	-162.169075	-162.094605	0.26	-162.211327	-162.200595	-162.135827	-162.172517	-162.098015				
0.28	-162.233506	-162.225698	-162.159417	-162.206064	-162.133769	0.28	-162.202231	-162.195069	-162.127975	-162.169257	-162.090125	0.28	-162.205910	-162.198663	-162.131500	-162.172708	-162.093539				
0.30	-162.227602	-162.222968	-162.154284	-162.206836	-162.130912	0.30	-162.196111	-162.192315	-162.123031	-162.168768	-162.084840	0.30	-162.199790	-162.195918	-162.126560	-162.172227	-162.088259				
0.32	-162.221069	-162.219483	-162.148521	-162.206974	-162.127482	0.32	-162.189306	-162.188768	-162.117471	-162.167697	-162.078812	0.32	-162.192990	-162.192385	-162.121008	-162.171170	-162.082241				
0.34	-162.213936	-162.215274	-162.142149	-162.206491	-162.123463	0.34	-162.181855	-162.184473	-162.111313	-162.166118	-162.072130	0.34	-162.185531	-162.188090	-162.114846	-162.169592	-162.075558				
0.36	-162.206227	-162.210363	-162.135188	-162.205405	-162.118841	0.36	-162.173758	-162.179436	-162.104541	-162.164026	-162.064847	0.36	-162.177432	-162.183060	-162.108077	-162.167507	-162.068279				
0.38	-162.197962	-162.204768	-162.127655	-162.203731	-162.113609	0.38	-162.165039	-162.173689	-162.097167	-162.161406	-162.057024	0.38	-162.168710	-162.177319	-162.100705	-162.164892	-162.060460				
0.40	-162.189161	-162.198505	-162.119566	-162.201492	-162.107767	0.40	-162.155714	-162.167254	-162.089197	-162.158209	-162.048702	0.40	-162.159382	-162.170889	-162.092737	-162.161699	-162.052142				
0.42	-162.179842	-162.191590	-162.110934	-162.198710	-162.101323	0.42	-162.145799	-162.160153	-162.080637	-162.154373	-162.039902	0.42	-162.149464	-162.163795	-162.084180	-162.157866	-162.043346				
0.44	-162.170015	-162.184032	-162.101768	-162.195395	-162.094284	0.44	-162.135312	-162.152412	-162.071499	-162.149829	-162.030629	0.44	-162.138971	-162.156057	-162.075043	-162.153321	-162.0340759				
0.46	-162.159696	-162.175844	-162.092078	-162.191590	-162.086668	0.46	-162.124264	-162.144503	-162.061792	-162.144046	-162.020869	0.46	-162.127919	-162.147696	-162.065338	-162.147996	-162.024316				
0.48	-162.148894	-162.167036	-162.081870	-162.187289	-162.078491	0.48	-162.112670	-162.135073	-162.051526	-162.138330	-162.010600	0.48	-162.116319	-162.138725	-162.055074	-162.141820	-162.014046				
0.50	-162.137620	-162.157619	-162.071150	-162.182517	-162.069775	0.50	-162.100542	-162.125508	-162.040714	-162.131247	-161.999788	0.50	-162.104186	-162.129163	-162.044264	-162.134736	-162.003235				