Supplementary Material

Effects of spin–orbit coupling on the coupled $3\,^3\Pi$ and $4\,^3\Pi$ excited states of NaK

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Table 1. Calculated values of the spin–orbit coupling constants for the adiabatic states that correlate with the $3s3d$ limit, in cm^{-1}.

$R\,(a_0)$	A_1^{sd}	A_2^{sd}	A_3^{sd}	A_4^{sd}	A_5^{sd}	A_6^{sd}	A_7^{sd}	A_8^{sd}	A_9^{sd}	A_{10}^{sd}
6.0	0.7305	0.5632	0.3024	7.2787	0.4077	0.6086	7.8060	3.1971	2.2660	2.6774
6.5	0.6242	0.3453	0.1642	6.5584	0.3231	0.3815	7.1713	2.6711	1.9564	2.1962
7.0	0.5499	0.2222	0.0667	6.0528	0.2544	0.1819	6.6714	2.2064	1.6733	1.6304
7.5	0.4988	0.1365	0.0054	5.7391	0.1927	0.0037	6.2173	1.7584	1.3581	0.9231
8.0	0.4656	0.0406	0.0633	5.6297	0.1289	0.1770	5.7199	1.1619	0.7790	0.1648
8.5	0.4474	0.2584	0.1139	5.9934	0.0151	0.3222	5.4743	1.4748	1.2640	0.2159
9.0	0.4425	2.3424	0.1613	14.4177	0.5074	0.4116	6.9046	2.2542	1.7723	1.7403
9.5	0.4482	2.0328	0.2065	12.7688	0.3497	0.4430	5.6645	1.3756	0.6860	1.6368
10.0	0.4630	1.7311	0.2497	11.1536	0.1840	0.4419	4.6839	1.1480	0.2571	1.5975
10.5	0.4833	1.4739	0.2894	9.8148	0.0326	0.4326	3.8307	1.5154	0.7860	1.5961
11.0	0.5044	1.2546	0.3236	8.7539	0.0978	0.4300	3.0890	1.7477	0.7822	1.5691
11.5	0.5219	1.0697	0.3507	7.9093	0.2027	0.4389	2.4416	1.7496	0.6900	1.4984
12.0	0.5329	0.9175	0.3704	7.1893	0.2812	0.4561	1.8863	1.6733	0.4544	1.3944
12.5	0.5365	0.7955	0.3834	6.5131	0.3350	0.4750	1.4308	1.5795	0.8103	1.2727
13.0	0.5337	0.6994	0.3914	5.8393	0.3675	0.4902	1.0797	1.4706	0.9921	1.1453
13.5	0.5262	0.6244	0.3958	5.1690	0.3827	0.4991	0.8265	1.3421	0.9231	1.0184
14.0	0.5157	0.5657	0.3979	4.5273	0.3852	0.5016	0.6546	1.1976	0.8180	0.8973
14.5	0.5041	0.5211	0.3990	3.9279	0.3808	0.4990	0.5443	1.0389	0.6985	0.7856
15.0	0.4917	0.4865	0.3986	3.3870	0.3723	0.4927	0.4754	0.8832	0.5814	0.6858
15.5	0.4800	0.4616	0.3981	2.8919	0.3646	0.4843	0.4344	0.7272	0.4620	0.5982
16.0	0.4695	0.4446	0.3979	2.4400	0.3594	0.4754	0.4114	0.5762	0.3435	0.5214
16.5	0.4596	0.4326	0.3972	2.0385	0.3561	0.4660	0.3992	0.4419	0.2343	0.4537
17.0	0.4509	0.4247	0.3965	1.6872	0.3552	0.4570	0.3934	0.3261	0.1336	0.3937
18.0	0.4364	0.4159	0.3951	1.1485	0.3583	0.4410	0.3917	0.1803	0.0354	0.2939
19.0	0.4254	0.4111	0.3940	0.8151	0.3640	0.4282	0.3939	0.1861	0.1580	0.2190
20.0	0.4171	0.4073	0.3930	0.6300	0.3694	0.4183	0.3958	0.2461	0.2405	0.1658
22.0	0.4062	0.4009	0.3917	0.4783	0.3766	0.4052	0.3968	0.3279	0.3277	0.1073
24.0	0.3998	0.3960	0.3907	0.4304	0.3803	0.3977	0.3955	0.3619	0.3619	0.0924
26.0	0.3959	0.3927	0.3901	0.4113	0.3824	0.3934	0.3937	0.3751	0.3751	0.1155
28.0	0.3934	0.3906	0.3896	0.4022	0.3837	0.3909	0.3923	0.3805	0.3805	0.1706
30.0	0.3917	0.3894	0.3892	0.3973	0.3846	0.3895	0.3913	0.3830	0.3829	0.3107
32.0	0.3906	0.3886	0.3888	0.3944	0.3852	0.3886	0.3906	0.3843	0.3843	0.3778
34.0	0.3898	0.3881	0.3886	0.3925	0.3857	0.3881	0.3900	0.3851	0.3851	0.3862
36.0	0.3893	0.3877	0.3884	0.3912	0.3860	0.3877	0.3895	0.3858	0.3858	0.3876
38.0	0.3888	0.3875	0.3882	0.3903	0.3862	0.3875	0.3891	0.3862	0.3862	0.3878
40.0	0.3885	0.3873	0.3880	0.3896	0.3864	0.3873	0.3888	0.3865	0.3865	0.3877
50.0	0.3877	0.3870	0.3876	0.3880	0.3868	0.3870	0.3878	0.3868	0.3868	0.3872
75.0	0.3873	0.3870	0.3872	0.3873	0.3870	0.3870	0.3873	0.3870	0.3870	0.3870
100.0	0.3872	0.3871	0.3872	0.3872	0.3871	0.3871	0.3872	0.3871	0.3871	0.3871

Table 2. Calculated values of the spin–orbit coupling constants for the adiabatic states that correlate with the $3s5p$ limit, in cm^{-1}.

$R\,(a_0)$	A_1^{sp}	A_2^{sp}	A_3^{sp}	A_4^{sp}	A_5^{sp}
6.0000	15.2021	6.4519	1.4553	0.0596	2.2655
6.5000	13.6783	5.4846	1.2895	0.3680	2.3694
7.0000	11.9670	4.5984	0.1801	0.6925	2.3424
7.5000	10.5279	3.6922	0.8101	1.0416	2.0550
8.0000	9.3296	2.8008	1.8514	1.4597	1.7084
8.5000	8.0789	2.1541	2.7306	1.3386	1.5885
9.0000	2.9684	3.1489	2.1004	1.9274	1.7182
9.5000	3.0715	3.4707	1.7738	1.6508	1.4007
10.0000	3.3850	3.8220	1.4394	1.2649	1.1091
10.5000	3.7874	4.1380	1.0501	0.8463	0.7492
11.0000	4.1830	4.3684	0.6892	0.4696	0.3242
11.5000	4.4426	4.4725	0.3949	0.1710	0.1377
12.0000	4.5135	4.4689	0.1537	0.0610	0.6836
12.5000	4.4430	4.4060	0.0629	0.2560	1.4729
13.0000	4.3078	4.3220	4.0506	3.6617	4.5760
13.5000	4.1696	4.2381	4.3684	3.7155	4.2692
14.0000	4.0528	4.1626	4.6036	3.7455	3.9720
14.5000	3.9753	4.1071	4.7803	3.7618	3.6961
15.0000	3.9271	4.0618	4.8864	3.7601	3.4287
15.5000	3.9206	4.0457	4.9533	3.7690	3.1507
16.0000	3.9543	4.0632	4.9974	3.8012	2.9477
16.5000	4.0060	4.0945	5.0055	3.8397	2.7390
17.0000	4.0762	4.1456	4.9970	3.8963	2.5374
18.0000	4.2386	4.2837	4.9501	4.0492	2.1550
19.0000	4.3923	4.4292	4.8873	4.2156	1.8011
20.0000	4.5151	4.5481	4.8247	4.3545	1.4833
22.0000	4.6655	4.6867	4.7302	4.5170	0.9845
24.0000	4.7349	4.7446	4.6889	4.5940	0.6674
25.0000	4.7534	4.7593	4.6853	4.6218	0.5693
26.0000	4.7656	4.7688	4.6896	4.6470	0.5078
28.0000	4.7788	4.7793	4.7107	4.6912	0.5072
30.0000	4.7845	4.7840	4.7347	4.7255	0.7215
32.0000	4.7871	4.7864	4.7535	4.7489	0.8236
34.0000	4.7885	4.7879	4.7658	4.7633	0.8790
36.0000	4.7893	4.7889	4.7737	4.7723	1.0320
38.0000	4.7899	4.7790	4.7782	4.7896	1.5439
40.0000	4.7903	4.7829	4.7824	4.7901	3.8305
42.0000	4.7905	4.7858	4.7854	4.7903	4.7316
44.0000	4.7906	4.7877	4.7874	4.7905	4.7799
46.0000	4.7907	4.7889	4.7887	4.7906	4.7873
48.0000	4.7907	4.7896	4.7894	4.7906	4.7892
50.0000	4.7907	4.7900	4.7899	4.7907	4.7899
75.0000	4.7907	4.7906	4.7905	4.7907	4.7906
100.0000	4.7907	4.7906	4.7906	4.7906	4.7906

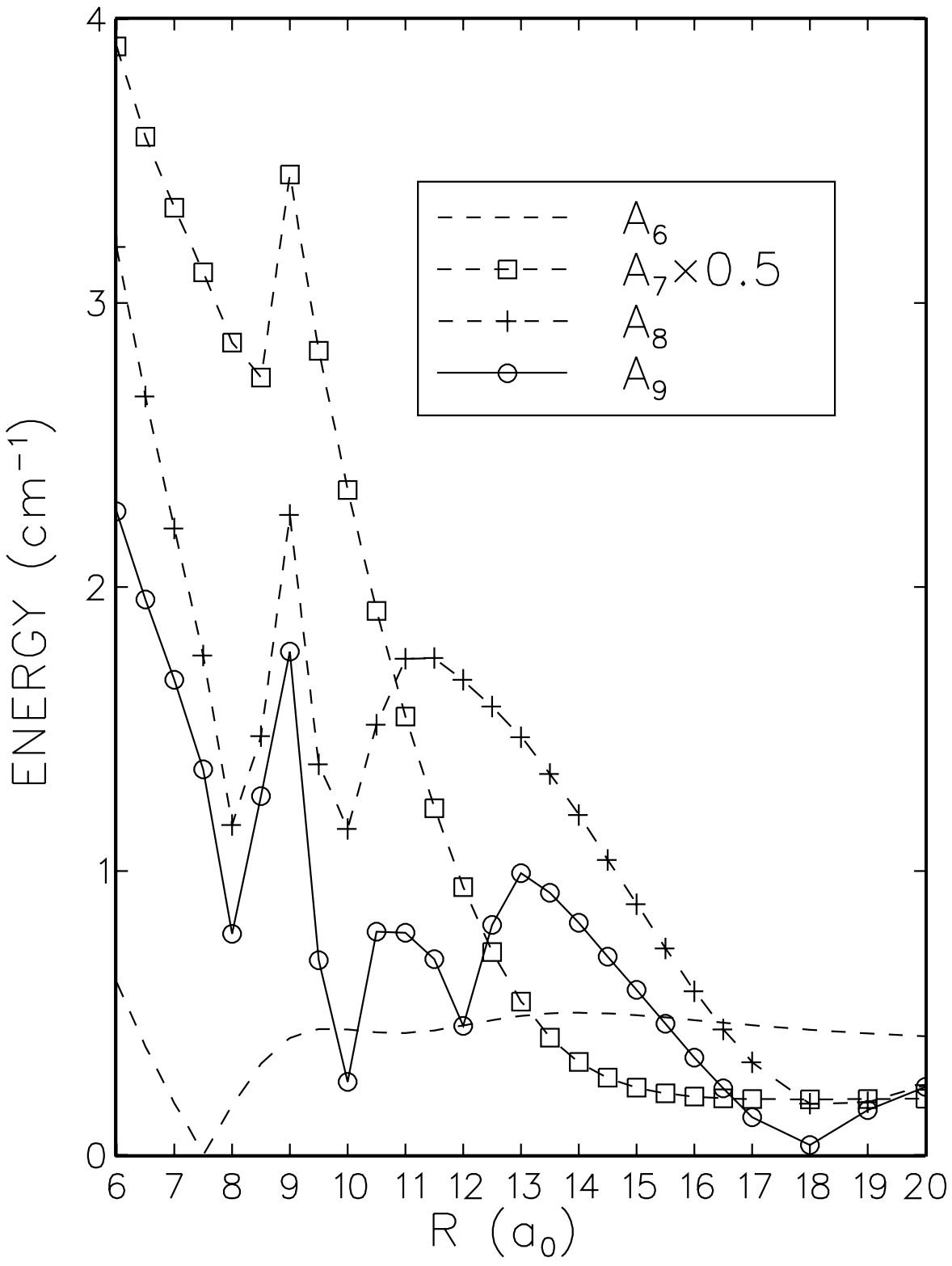

Figure 1. Calculated values of the spin–orbit coupling matrix elements A_6^{sd}, A_7^{sd}, A_8^{sd}, and A_9^{sd} for the adiabatic states that correlate with the $3s3d$ limit, in cm^{-1}. The curve marked by the square boxes (□) corresponds to 50% of the calulated value of A_7^{sd}.

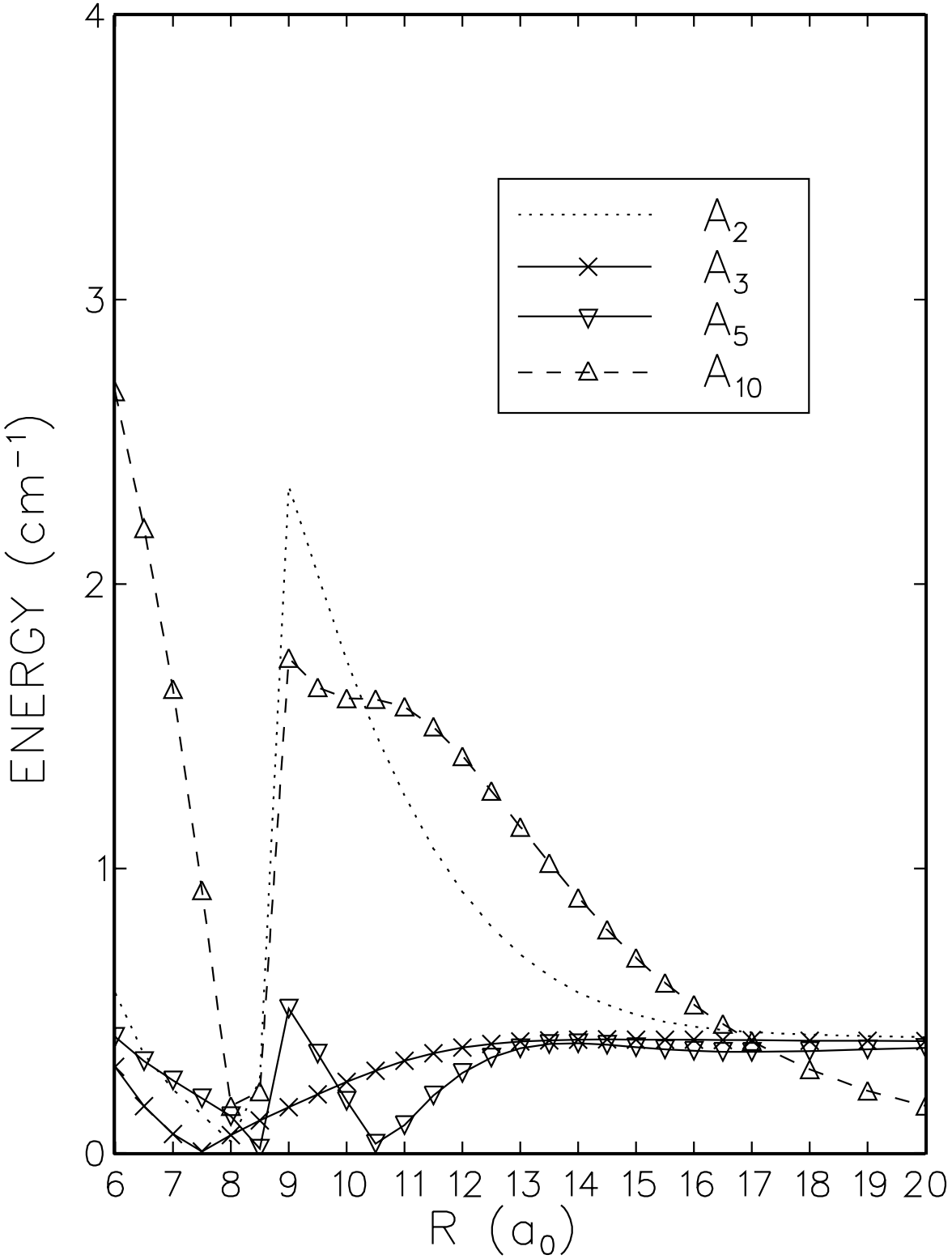

Figure 2. Calculated values of the spin–orbit coupling matrix elements A_2^{sd}, A_3^{sd}, A_5^{sd}, and A_{10}^{sd} for the adiabatic states that correlate with the $3s3d$ limit, in cm^{-1}.

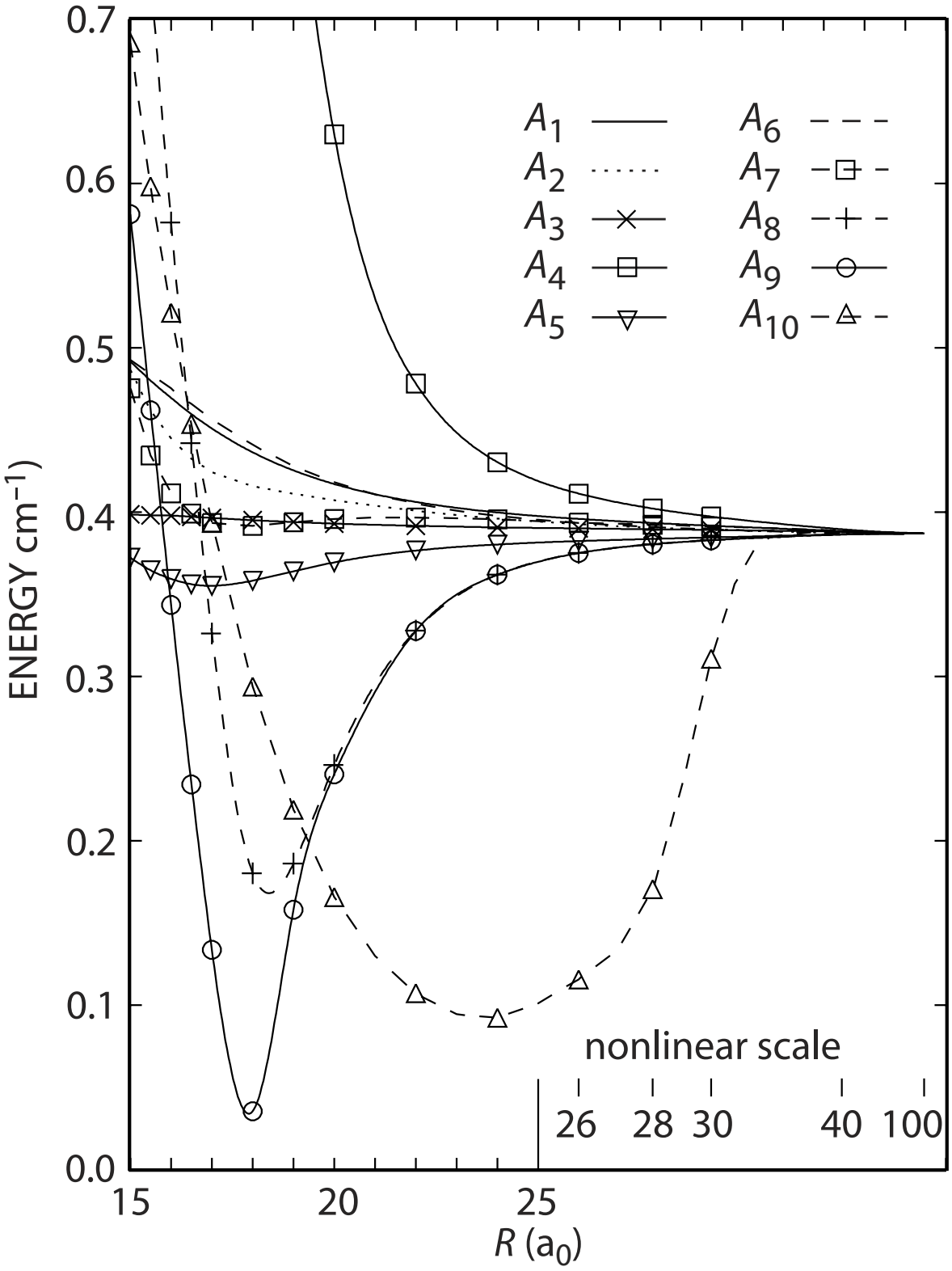

Figure 3. Calculated spin–orbit coupling constants A_1^{sd}–A_{10}^{sd} for the electronic states $5^1\Sigma^+$, $5^3\Sigma^+$, $3^1\Pi$, $3^3\Pi$, $1^1\Delta$, and $1^3\Delta$ that correlate with the $3s3d$ limit. This figure is a larger version of Fig. 3 in the original publication.

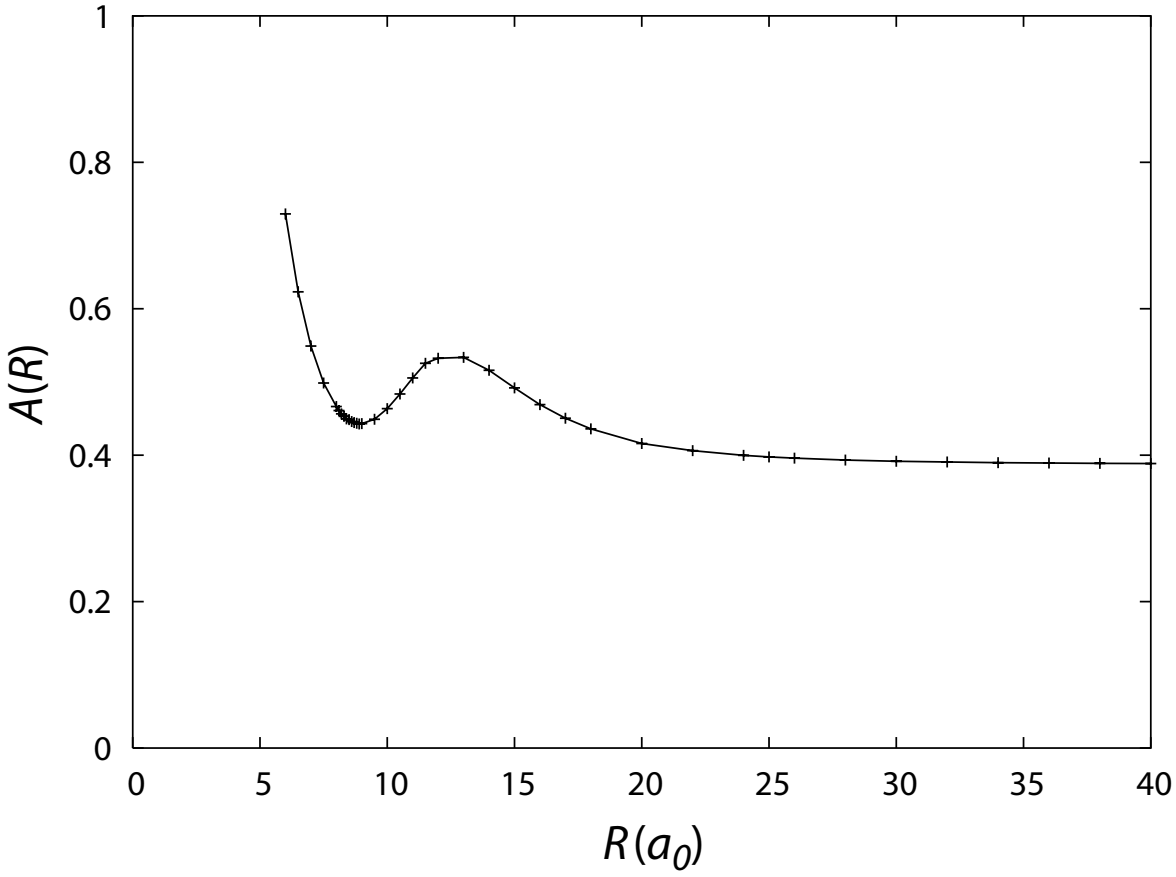

Figure 4. Calculated spin–orbit coupling constant A_1^{sd} for the $1\,^3\Delta$ state.

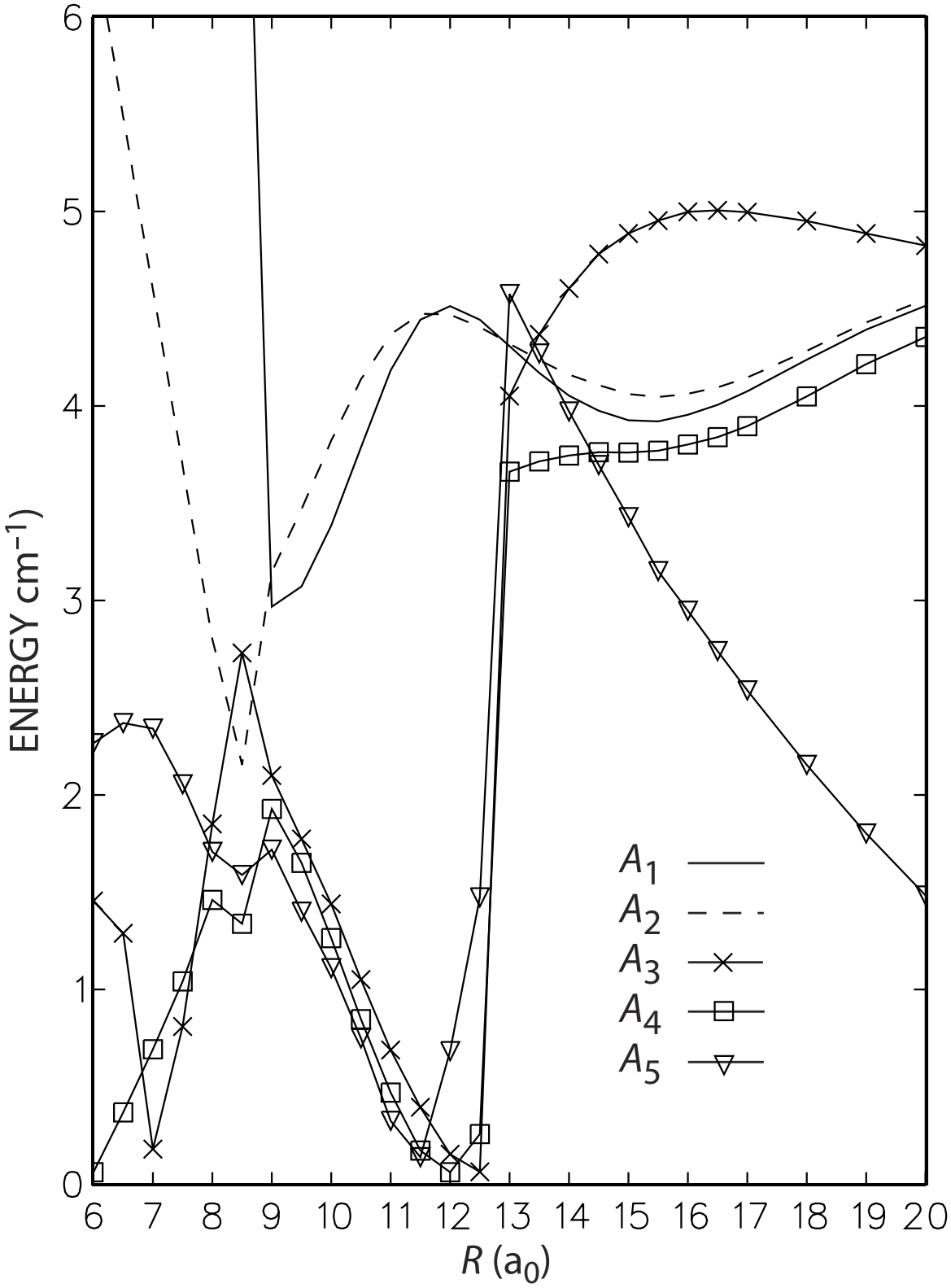

Figure 5. Calculated spin–orbit coupling constants A_1^{sp}–A_5^{sp} for the electronic states $6^1\Sigma^+$, $6^3\Sigma^+$, $4^1\Pi$, and $4^3\Pi$ that correlate with the $3s5p$ limit.

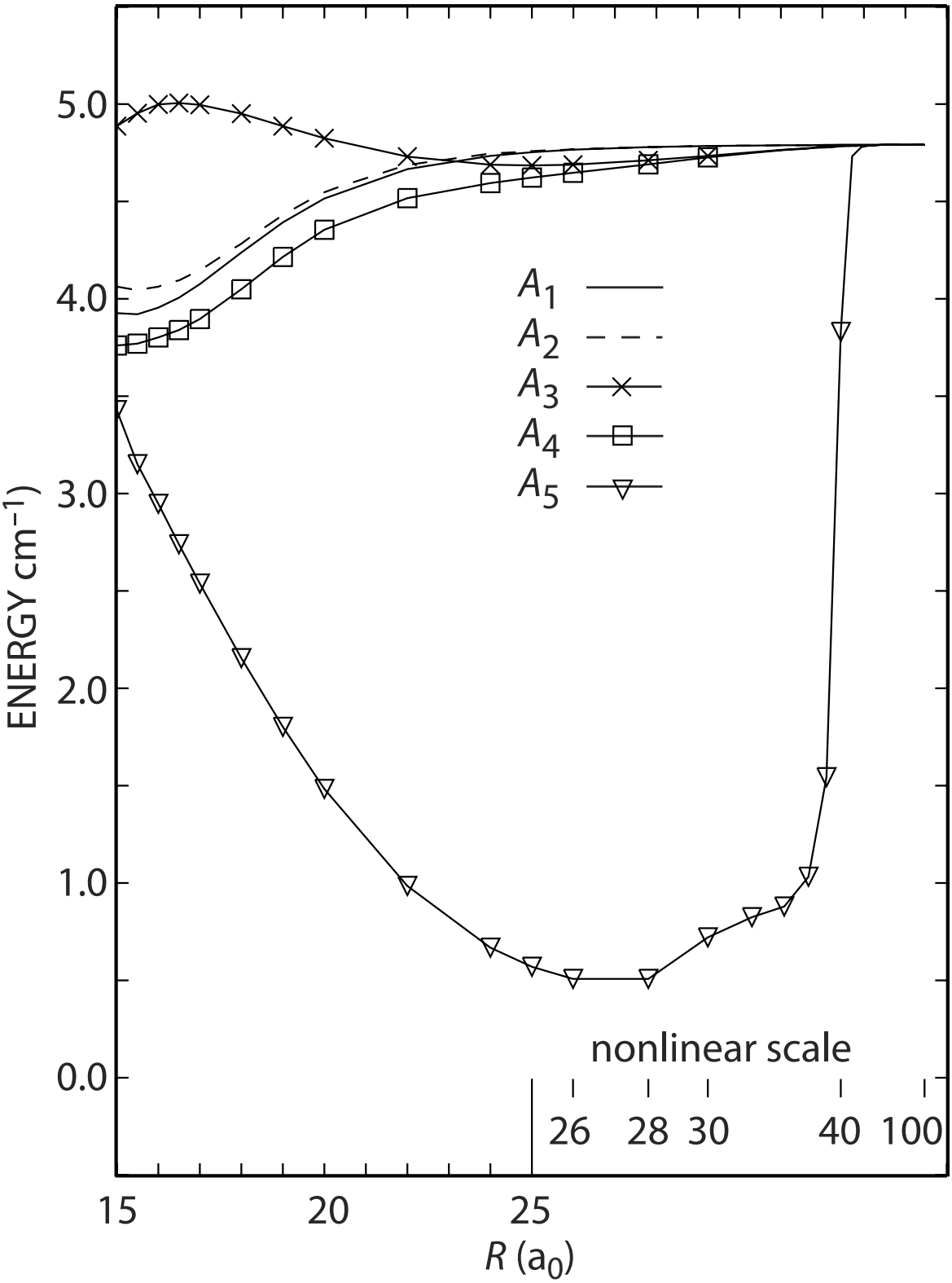

Figure 6. Calculated spin–orbit coupling constants A_1^{sp}–A_5^{sp} for the electronic states $6^1\Sigma^+$, $6^3\Sigma^+$, $4^1\Pi$, and $4^3\Pi$ that correlate with the $3s5p$ limit. This figure is a larger version of Fig. 4 in the original publication.