Supplementary Material

Polarizability tensor invariants of H_2, HD, and D_2

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$\alpha_\perp$: polarizability perpendicular to the internuclear axis
$\alpha_\parallel$: polarizability parallel to the internuclear axis
$\bar{\alpha}$: mean polarizability, $\bar{\alpha} = (2\alpha_\perp + \alpha_\parallel)/3$
γ : polarizability anisotropy, $\gamma = \alpha_\parallel - \alpha_\perp$

S1. Matrix elements of mean polarizability

TABLE T1. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of H_2 for v=0 and v=1.

λ(nm)	$\langle\bar{\alpha}\rangle_{00,00}$	$\langle\bar{\alpha}\rangle_{10,10}$	$\langle\bar{\alpha}\rangle_{10,00}$	$\langle\bar{\alpha}\rangle_{11,01}$	$\langle\bar{\alpha}\rangle_{12,02}$	$\langle\bar{\alpha}\rangle_{13,03}$	$\langle\bar{\alpha}\rangle_{14,04}$	$\langle\bar{\alpha}\rangle_{15,05}$	$\langle\bar{\alpha}\rangle_{16,06}$	$\langle\bar{\alpha}\rangle_{17,07}$	$\langle\bar{\alpha}\rangle_{18,08}$
182.26	7.1074	8.0375	1.2674	1.2706	1.2771	1.2867	1.2996	1.3158	1.3354	1.3583	1.3846
193.00	6.8667	7.7165	1.1819	1.1847	1.1903	1.1987	1.2099	1.2239	1.2408	1.2605	1.2832
213.00	6.5441	7.2947	1.0729	1.0752	1.0798	1.0866	1.0958	1.1073	1.1211	1.1371	1.1555
222.00	6.4350	7.1541	1.0374	1.0395	1.0438	1.0503	1.0588	1.0695	1.0823	1.0973	1.1143
224.30	6.4098	7.1218	1.0293	1.0314	1.0356	1.0420	1.0504	1.0609	1.0735	1.0882	1.1049
235.00	6.3047	6.9876	0.9960	0.9979	1.0019	1.0078	1.0157	1.0255	1.0372	1.0509	1.0664
248.00	6.1991	6.8536	0.9631	0.9649	0.9686	0.9741	0.9814	0.9906	1.0015	1.0142	1.0286
266.00	6.0824	6.7067	0.9276	0.9293	0.9327	0.9377	0.9445	0.9529	0.9630	0.9747	0.9879
275.36	6.0322	6.6438	0.9125	0.9141	0.9174	0.9223	0.9289	0.9370	0.9467	0.9579	0.9707
285.00	5.9864	6.5866	0.8989	0.9005	0.9036	0.9084	0.9147	0.9226	0.9320	0.9429	0.9552
308.00	5.8964	6.4745	0.8724	0.8739	0.8769	0.8814	0.8873	0.8947	0.9035	0.9137	0.9252
325.00	5.8433	6.4087	0.8571	0.8585	0.8614	0.8657	0.8714	0.8785	0.8869	0.8967	0.9078
334.24	5.8181	6.3776	0.8498	0.8512	0.8541	0.8583	0.8639	0.8708	0.8791	0.8887	0.8996
337.10	5.8108	6.3685	0.8477	0.8491	0.8519	0.8561	0.8617	0.8686	0.8769	0.8864	0.8972
347.00	5.7870	6.3391	0.8409	0.8423	0.8451	0.8492	0.8547	0.8615	0.8695	0.8789	0.8895
351.00	5.7780	6.3280	0.8384	0.8397	0.8425	0.8466	0.8520	0.8588	0.8668	0.8761	0.8866
355.00	5.7693	6.3174	0.8359	0.8373	0.8400	0.8441	0.8495	0.8562	0.8641	0.8734	0.8838
385.15	5.7132	6.2483	0.8200	0.8213	0.8240	0.8279	0.8330	0.8395	0.8471	0.8560	0.8659
407.90	5.6794	6.2068	0.8106	0.8119	0.8144	0.8182	0.8232	0.8295	0.8370	0.8456	0.8553
416.10	5.6687	6.1937	0.8076	0.8088	0.8114	0.8151	0.8201	0.8264	0.8337	0.8423	0.8519
435.96	5.6453	6.1651	0.8011	0.8023	0.8048	0.8085	0.8134	0.8195	0.8268	0.8352	0.8446
441.60	5.6392	6.1577	0.7994	0.8006	0.8031	0.8068	0.8117	0.8178	0.8250	0.8333	0.8427
457.90	5.6231	6.1379	0.7949	0.7962	0.7986	0.8023	0.8071	0.8131	0.8202	0.8284	0.8377
488.00	5.5976	6.1069	0.7879	0.7891	0.7915	0.7951	0.7998	0.8057	0.8127	0.8208	0.8299
514.50	5.5790	6.0841	0.7828	0.7840	0.7864	0.7899	0.7946	0.8003	0.8072	0.8152	0.8241
532.00	5.5682	6.0710	0.7799	0.7811	0.7834	0.7869	0.7915	0.7973	0.8041	0.8120	0.8208
546.23	5.5603	6.0613	0.7777	0.7789	0.7812	0.7847	0.7893	0.7950	0.8018	0.8096	0.8184
563.20	5.5516	6.0508	0.7753	0.7765	0.7788	0.7823	0.7868	0.7925	0.7992	0.8070	0.8157
594.10	5.5377	6.0339	0.7716	0.7727	0.7750	0.7784	0.7829	0.7885	0.7952	0.8029	0.8115
611.90	5.5307	6.0253	0.7697	0.7708	0.7731	0.7765	0.7810	0.7865	0.7931	0.8008	0.8094
632.80	5.5232	6.0162	0.7676	0.7688	0.7710	0.7744	0.7789	0.7844	0.7910	0.7986	0.8071
647.10	5.5185	6.0105	0.7664	0.7675	0.7697	0.7731	0.7776	0.7831	0.7896	0.7972	0.8057
670.00	5.5116	6.0022	0.7645	0.7656	0.7679	0.7712	0.7756	0.7811	0.7876	0.7951	0.8036
694.30	5.5051	5.9942	0.7627	0.7639	0.7661	0.7694	0.7738	0.7793	0.7857	0.7932	0.8016
725.00	5.4977	5.9853	0.7608	0.7619	0.7641	0.7674	0.7718	0.7772	0.7836	0.7911	0.7994
754.00	5.4916	5.9779	0.7591	0.7602	0.7624	0.7657	0.7701	0.7755	0.7819	0.7893	0.7976
785.00	5.4858	5.9708	0.7576	0.7587	0.7608	0.7641	0.7685	0.7738	0.7802	0.7876	0.7958
800.00	5.4833	5.9677	0.7569	0.7580	0.7602	0.7634	0.7677	0.7731	0.7795	0.7868	0.7951
836.00	5.4777	5.9610	0.7554	0.7565	0.7586	0.7619	0.7662	0.7715	0.7779	0.7852	0.7934
876.00	5.4723	5.9545	0.7539	0.7550	0.7572	0.7604	0.7647	0.7700	0.7763	0.7836	0.7918
904.00	5.4689	5.9504	0.7530	0.7541	0.7563	0.7595	0.7638	0.7691	0.7754	0.7826	0.7908
911.28	5.4681	5.9494	0.7528	0.7539	0.7561	0.7593	0.7636	0.7688	0.7751	0.7824	0.7905
946.00	5.4645	5.9450	0.7518	0.7529	0.7551	0.7583	0.7625	0.7678	0.7741	0.7813	0.7895
975.00	5.4617	5.9416	0.7511	0.7522	0.7543	0.7575	0.7618	0.7671	0.7733	0.7805	0.7886
1000.00	5.4595	5.9390	0.7505	0.7516	0.7537	0.7569	0.7612	0.7664	0.7727	0.7799	0.7880
1064.00	5.4547	5.9331	0.7492	0.7503	0.7524	0.7556	0.7598	0.7651	0.7713	0.7785	0.7865
1106.00	5.4519	5.9298	0.7485	0.7495	0.7517	0.7549	0.7591	0.7643	0.7705	0.7777	0.7857
1152.00	5.4492	5.9265	0.7478	0.7488	0.7510	0.7541	0.7583	0.7636	0.7697	0.7769	0.7849
1185.00	5.4475	5.9244	0.7473	0.7484	0.7505	0.7537	0.7579	0.7631	0.7693	0.7764	0.7844
1225.00	5.4456	5.9221	0.7468	0.7479	0.7500	0.7531	0.7573	0.7625	0.7687	0.7758	0.7838
1275.00	5.4434	5.9195	0.7462	0.7473	0.7494	0.7526	0.7567	0.7619	0.7681	0.7752	0.7832
1320.00	5.4417	5.9175	0.7458	0.7468	0.7489	0.7521	0.7563	0.7615	0.7676	0.7747	0.7827
Static	5.4179	5.8887	0.7394	0.7405	0.7426	0.7457	0.7498	0.7548	0.7609	0.7678	0.7756

TABLE T2. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of H_2 for v=1 and v=2.

λ(nm)	$\langle\bar{\alpha}\rangle_{20,20}$	$\langle\bar{\alpha}\rangle_{20,10}$	$\langle\bar{\alpha}\rangle_{21,11}$	$\langle\bar{\alpha}\rangle_{22,12}$	$\langle\bar{\alpha}\rangle_{23,13}$	$\langle\bar{\alpha}\rangle_{24,14}$	$\langle\bar{\alpha}\rangle_{25,15}$	$\langle\bar{\alpha}\rangle_{26,16}$	$\langle\bar{\alpha}\rangle_{27,17}$	$\langle\bar{\alpha}\rangle_{28,18}$
182.26	9.0945	1.9519	1.9569	1.9670	1.9821	2.0024	2.0278	2.0584	2.0943	2.1357
193.00	8.6672	1.8026	1.8069	1.8154	1.8283	1.8454	1.8669	1.8927	1.9229	1.9575
213.00	8.1186	1.6165	1.6199	1.6267	1.6369	1.6505	1.6675	1.6879	1.7116	1.7387
222.00	7.9387	1.5569	1.5601	1.5664	1.5758	1.5883	1.6040	1.6227	1.6446	1.6694
224.30	7.8976	1.5434	1.5465	1.5527	1.5619	1.5743	1.5896	1.6080	1.6294	1.6537
235.00	7.7275	1.4879	1.4908	1.4965	1.5051	1.5165	1.5306	1.5476	1.5673	1.5897
248.00	7.5588	1.4336	1.4363	1.4416	1.4495	1.4599	1.4730	1.4886	1.5067	1.5272
266.00	7.3753	1.3754	1.3778	1.3826	1.3898	1.3994	1.4113	1.4255	1.4419	1.4606
275.36	7.2971	1.3508	1.3531	1.3578	1.3647	1.3739	1.3853	1.3990	1.4147	1.4326
285.00	7.2263	1.3287	1.3309	1.3354	1.3421	1.3509	1.3619	1.3751	1.3902	1.4074
308.00	7.0881	1.2859	1.2880	1.2921	1.2984	1.3066	1.3168	1.3290	1.3430	1.3589
325.00	7.0073	1.2611	1.2631	1.2671	1.2730	1.2809	1.2907	1.3023	1.3157	1.3309
334.24	6.9692	1.2495	1.2514	1.2553	1.2612	1.2689	1.2785	1.2898	1.3030	1.3178
337.10	6.9581	1.2461	1.2481	1.2519	1.2577	1.2654	1.2749	1.2862	1.2993	1.3140
347.00	6.9222	1.2352	1.2371	1.2409	1.2466	1.2541	1.2634	1.2745	1.2873	1.3017
351.00	6.9086	1.2311	1.2330	1.2368	1.2424	1.2498	1.2591	1.2701	1.2828	1.2970
355.00	6.8956	1.2271	1.2290	1.2328	1.2384	1.2458	1.2549	1.2659	1.2784	1.2926
385.15	6.8114	1.2018	1.2036	1.2071	1.2125	1.2195	1.2283	1.2387	1.2506	1.2641
407.90	6.7611	1.1867	1.1884	1.1919	1.1971	1.2039	1.2124	1.2225	1.2341	1.2472
416.10	6.7451	1.1819	1.1837	1.1871	1.1922	1.1990	1.2074	1.2174	1.2289	1.2418
435.96	6.7104	1.1716	1.1733	1.1766	1.1817	1.1883	1.1966	1.2063	1.2176	1.2302
441.60	6.7015	1.1689	1.1706	1.1740	1.1790	1.1856	1.1938	1.2035	1.2147	1.2272
457.90	6.6776	1.1618	1.1635	1.1668	1.1717	1.1783	1.1863	1.1959	1.2069	1.2193
488.00	6.6400	1.1507	1.1523	1.1556	1.1604	1.1668	1.1747	1.1840	1.1948	1.2069
514.50	6.6126	1.1426	1.1442	1.1474	1.1521	1.1584	1.1662	1.1754	1.1859	1.1978
532.00	6.5967	1.1380	1.1395	1.1427	1.1474	1.1536	1.1613	1.1704	1.1809	1.1926
546.23	6.5851	1.1345	1.1361	1.1392	1.1439	1.1501	1.1577	1.1667	1.1771	1.1888
563.20	6.5723	1.1308	1.1323	1.1354	1.1401	1.1462	1.1538	1.1627	1.1730	1.1846
594.10	6.5520	1.1248	1.1264	1.1294	1.1340	1.1400	1.1475	1.1564	1.1665	1.1780
611.90	6.5417	1.1218	1.1233	1.1264	1.1309	1.1369	1.1444	1.1532	1.1633	1.1746
632.80	6.5307	1.1186	1.1201	1.1231	1.1277	1.1336	1.1410	1.1497	1.1598	1.1710
647.10	6.5239	1.1166	1.1181	1.1211	1.1256	1.1316	1.1389	1.1476	1.1576	1.1688
670.00	6.5138	1.1137	1.1152	1.1182	1.1226	1.1285	1.1358	1.1445	1.1544	1.1655
694.30	6.5042	1.1109	1.1124	1.1153	1.1198	1.1256	1.1329	1.1415	1.1514	1.1624
725.00	6.4935	1.1077	1.1092	1.1122	1.1166	1.1224	1.1296	1.1382	1.1480	1.1589
754.00	6.4846	1.1052	1.1066	1.1096	1.1140	1.1198	1.1269	1.1354	1.1451	1.1561
785.00	6.4762	1.1027	1.1042	1.1071	1.1115	1.1172	1.1244	1.1328	1.1425	1.1533
800.00	6.4725	1.1016	1.1031	1.1060	1.1104	1.1161	1.1232	1.1316	1.1413	1.1521
836.00	6.4644	1.0993	1.1007	1.1036	1.1080	1.1137	1.1208	1.1291	1.1387	1.1495
876.00	6.4565	1.0970	1.0984	1.1013	1.1056	1.1113	1.1184	1.1267	1.1363	1.1470
904.00	6.4517	1.0956	1.0970	1.0999	1.1042	1.1099	1.1169	1.1252	1.1347	1.1454
911.28	6.4505	1.0952	1.0967	1.0996	1.1038	1.1095	1.1165	1.1248	1.1344	1.1450
946.00	6.4452	1.0937	1.0951	1.0980	1.1023	1.1079	1.1149	1.1232	1.1327	1.1433
975.00	6.4412	1.0925	1.0940	1.0968	1.1011	1.1067	1.1137	1.1220	1.1314	1.1420
1000.00	6.4380	1.0916	1.0930	1.0959	1.1002	1.1058	1.1128	1.1210	1.1304	1.1410
1064.00	6.4309	1.0896	1.0910	1.0938	1.0981	1.1037	1.1106	1.1188	1.1282	1.1387
1106.00	6.4269	1.0884	1.0898	1.0927	1.0969	1.1025	1.1094	1.1176	1.1269	1.1374
1152.00	6.4230	1.0873	1.0887	1.0915	1.0958	1.1013	1.1082	1.1164	1.1257	1.1362
1185.00	6.4205	1.0866	1.0880	1.0908	1.0950	1.1006	1.1075	1.1156	1.1249	1.1354
1225.00	6.4178	1.0858	1.0872	1.0900	1.0942	1.0998	1.1066	1.1147	1.1241	1.1345
1275.00	6.4147	1.0849	1.0863	1.0891	1.0933	1.0988	1.1057	1.1138	1.1231	1.1335
1320.00	6.4122	1.0841	1.0856	1.0884	1.0926	1.0981	1.1049	1.1130	1.1223	1.1327
Static	6.3778	1.0742	1.0756	1.0783	1.0824	1.0879	1.0946	1.1025	1.1115	1.1217

TABLE T3. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of HD for v=0 and v=1.

λ(nm)	$\langle\bar{\alpha}\rangle_{00,00}$	$\langle\bar{\alpha}\rangle_{10,10}$	$\langle\bar{\alpha}\rangle_{10,00}$	$\langle\bar{\alpha}\rangle_{11,01}$	$\langle\bar{\alpha}\rangle_{12,02}$	$\langle\bar{\alpha}\rangle_{13,03}$	$\langle\bar{\alpha}\rangle_{14,04}$	$\langle\bar{\alpha}\rangle_{15,05}$	$\langle\bar{\alpha}\rangle_{16,06}$	$\langle\bar{\alpha}\rangle_{17,07}$	$\langle\bar{\alpha}\rangle_{18,08}$
182.26	7.0472	7.8390	1.1662	1.1684	1.1728	1.1794	1.1883	1.1995	1.2128	1.2285	1.2466
193.00	6.8114	7.5362	1.0888	1.0907	1.0946	1.1004	1.1081	1.1178	1.1295	1.1431	1.1587
213.00	6.4949	7.1368	0.9899	0.9915	0.9947	0.9995	1.0058	1.0138	1.0233	1.0345	1.0472
222.00	6.3877	7.0032	0.9577	0.9591	0.9621	0.9666	0.9725	0.9800	0.9889	0.9993	1.0111
224.30	6.3630	6.9725	0.9503	0.9518	0.9547	0.9591	0.9649	0.9723	0.9810	0.9912	1.0029
235.00	6.2598	6.8448	0.9200	0.9213	0.9241	0.9282	0.9337	0.9405	0.9487	0.9582	0.9691
248.00	6.1559	6.7170	0.8900	0.8913	0.8938	0.8977	0.9028	0.9092	0.9168	0.9257	0.9358
266.00	6.0412	6.5767	0.8576	0.8588	0.8611	0.8647	0.8694	0.8753	0.8824	0.8905	0.8999
275.36	5.9918	6.5166	0.8438	0.8450	0.8473	0.8507	0.8553	0.8610	0.8678	0.8757	0.8847
285.00	5.9467	6.4619	0.8314	0.8325	0.8347	0.8381	0.8425	0.8480	0.8546	0.8622	0.8709
308.00	5.8581	6.3546	0.8073	0.8083	0.8104	0.8135	0.8177	0.8228	0.8290	0.8362	0.8443
325.00	5.8057	6.2915	0.7932	0.7942	0.7962	0.7992	0.8032	0.8082	0.8141	0.8210	0.8289
334.24	5.7810	6.2617	0.7866	0.7876	0.7895	0.7925	0.7964	0.8013	0.8072	0.8139	0.8216
337.10	5.7737	6.2531	0.7847	0.7856	0.7876	0.7906	0.7945	0.7993	0.8051	0.8119	0.8195
347.00	5.7503	6.2249	0.7784	0.7794	0.7813	0.7842	0.7881	0.7928	0.7985	0.8052	0.8127
351.00	5.7414	6.2142	0.7761	0.7771	0.7790	0.7818	0.7857	0.7904	0.7961	0.8026	0.8101
355.00	5.7329	6.2040	0.7738	0.7748	0.7767	0.7796	0.7833	0.7881	0.7937	0.8002	0.8076
385.15	5.6776	6.1377	0.7593	0.7602	0.7621	0.7648	0.7684	0.7730	0.7784	0.7846	0.7917
407.90	5.6443	6.0979	0.7507	0.7516	0.7533	0.7560	0.7596	0.7640	0.7692	0.7753	0.7822
416.10	5.6337	6.0853	0.7479	0.7488	0.7506	0.7532	0.7568	0.7611	0.7663	0.7724	0.7792
435.96	5.6106	6.0578	0.7420	0.7428	0.7446	0.7472	0.7506	0.7549	0.7601	0.7660	0.7727
441.60	5.6047	6.0507	0.7404	0.7413	0.7430	0.7456	0.7491	0.7534	0.7585	0.7644	0.7711
457.90	5.5888	6.0317	0.7364	0.7372	0.7389	0.7415	0.7449	0.7491	0.7541	0.7600	0.7666
488.00	5.5637	6.0019	0.7299	0.7308	0.7325	0.7350	0.7383	0.7424	0.7474	0.7531	0.7596
514.50	5.5453	5.9800	0.7253	0.7261	0.7277	0.7302	0.7335	0.7376	0.7425	0.7481	0.7545
532.00	5.5347	5.9674	0.7226	0.7234	0.7250	0.7275	0.7307	0.7348	0.7396	0.7452	0.7515
546.23	5.5268	5.9581	0.7206	0.7214	0.7230	0.7255	0.7287	0.7327	0.7375	0.7431	0.7494
563.20	5.5183	5.9479	0.7184	0.7192	0.7208	0.7233	0.7265	0.7305	0.7352	0.7408	0.7470
594.10	5.5046	5.9317	0.7149	0.7157	0.7174	0.7197	0.7229	0.7269	0.7316	0.7371	0.7432
611.90	5.4977	5.9235	0.7132	0.7140	0.7156	0.7180	0.7211	0.7251	0.7298	0.7352	0.7413
632.80	5.4903	5.9147	0.7113	0.7121	0.7137	0.7161	0.7192	0.7231	0.7278	0.7332	0.7393
647.10	5.4856	5.9092	0.7102	0.7110	0.7125	0.7149	0.7180	0.7219	0.7266	0.7320	0.7380
670.00	5.4788	5.9012	0.7085	0.7093	0.7108	0.7132	0.7163	0.7202	0.7248	0.7301	0.7362
694.30	5.4724	5.8935	0.7068	0.7076	0.7092	0.7115	0.7146	0.7185	0.7231	0.7284	0.7344
725.00	5.4651	5.8849	0.7050	0.7058	0.7074	0.7097	0.7128	0.7166	0.7212	0.7265	0.7324
754.00	5.4591	5.8778	0.7035	0.7043	0.7058	0.7082	0.7112	0.7150	0.7196	0.7248	0.7308
785.00	5.4534	5.8710	0.7021	0.7029	0.7044	0.7067	0.7098	0.7136	0.7181	0.7233	0.7292
800.00	5.4509	5.8681	0.7015	0.7022	0.7038	0.7061	0.7091	0.7129	0.7174	0.7226	0.7286
836.00	5.4454	5.8616	0.7001	0.7009	0.7024	0.7047	0.7077	0.7115	0.7160	0.7212	0.7271
876.00	5.4401	5.8553	0.6988	0.6995	0.7011	0.7033	0.7064	0.7101	0.7146	0.7198	0.7256
904.00	5.4368	5.8514	0.6979	0.6987	0.7002	0.7025	0.7055	0.7093	0.7137	0.7189	0.7247
911.28	5.4360	5.8504	0.6977	0.6985	0.7000	0.7023	0.7053	0.7091	0.7135	0.7187	0.7245
946.00	5.4324	5.8461	0.6968	0.6976	0.6991	0.7014	0.7044	0.7081	0.7126	0.7177	0.7235
975.00	5.4296	5.8429	0.6962	0.6969	0.6984	0.7007	0.7037	0.7074	0.7119	0.7170	0.7228
1000.00	5.4275	5.8404	0.6956	0.6964	0.6979	0.7002	0.7032	0.7069	0.7113	0.7164	0.7222
1064.00	5.4227	5.8347	0.6944	0.6952	0.6967	0.6989	0.7019	0.7056	0.7100	0.7151	0.7209
1106.00	5.4199	5.8315	0.6938	0.6945	0.6960	0.6983	0.7012	0.7049	0.7093	0.7144	0.7202
1152.00	5.4173	5.8284	0.6931	0.6939	0.6954	0.6976	0.7006	0.7043	0.7086	0.7137	0.7195
1185.00	5.4156	5.8264	0.6927	0.6934	0.6949	0.6972	0.7001	0.7038	0.7082	0.7133	0.7190
1225.00	5.4137	5.8241	0.6922	0.6930	0.6945	0.6967	0.6997	0.7033	0.7077	0.7128	0.7185
1275.00	5.4116	5.8216	0.6917	0.6924	0.6939	0.6962	0.6991	0.7028	0.7072	0.7122	0.7179
1320.00	5.4099	5.8196	0.6913	0.6920	0.6935	0.6957	0.6987	0.7024	0.7067	0.7118	0.7175
Static	5.3864	5.7919	0.6855	0.6862	0.6877	0.6899	0.6928	0.6964	0.7006	0.7056	0.7112

TABLE T4. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of HD for v=1 and v=2.

λ(nm)	$\langle\bar{\alpha}\rangle_{20,20}$	$\langle\bar{\alpha}\rangle_{20,10}$	$\langle\bar{\alpha}\rangle_{21,11}$	$\langle\bar{\alpha}\rangle_{22,12}$	$\langle\bar{\alpha}\rangle_{23,13}$	$\langle\bar{\alpha}\rangle_{24,14}$	$\langle\bar{\alpha}\rangle_{25,15}$	$\langle\bar{\alpha}\rangle_{26,16}$	$\langle\bar{\alpha}\rangle_{27,17}$	$\langle\bar{\alpha}\rangle_{28,18}$
182.26	8.7227	1.7750	1.7784	1.7852	1.7955	1.8092	1.8264	1.8472	1.8714	1.8993
193.00	8.3349	1.6439	1.6468	1.6527	1.6615	1.6732	1.6878	1.7055	1.7261	1.7497
213.00	7.8328	1.4793	1.4817	1.4864	1.4935	1.5029	1.5146	1.5287	1.5451	1.5638
222.00	7.6672	1.4264	1.4286	1.4330	1.4395	1.4482	1.4591	1.4721	1.4872	1.5045
224.30	7.6293	1.4144	1.4166	1.4208	1.4273	1.4358	1.4465	1.4593	1.4741	1.4911
235.00	7.4722	1.3650	1.3670	1.3710	1.3769	1.3849	1.3947	1.4066	1.4203	1.4360
248.00	7.3160	1.3165	1.3184	1.3221	1.3276	1.3349	1.3440	1.3550	1.3677	1.3821
266.00	7.1456	1.2644	1.2661	1.2695	1.2745	1.2812	1.2896	1.2996	1.3112	1.3244
275.36	7.0728	1.2424	1.2440	1.2473	1.2521	1.2586	1.2666	1.2763	1.2874	1.3001
285.00	7.0069	1.2226	1.2241	1.2273	1.2320	1.2382	1.2460	1.2552	1.2660	1.2782
308.00	6.8780	1.1842	1.1856	1.1885	1.1929	1.1987	1.2060	1.2146	1.2246	1.2359
325.00	6.8025	1.1619	1.1633	1.1661	1.1703	1.1758	1.1828	1.1910	1.2006	1.2114
334.24	6.7669	1.1514	1.1528	1.1555	1.1596	1.1651	1.1719	1.1800	1.1894	1.2000
337.10	6.7565	1.1484	1.1497	1.1525	1.1566	1.1620	1.1687	1.1768	1.1861	1.1967
347.00	6.7229	1.1386	1.1399	1.1426	1.1466	1.1519	1.1585	1.1664	1.1755	1.1859
351.00	6.7102	1.1349	1.1362	1.1388	1.1428	1.1481	1.1547	1.1625	1.1716	1.1818
355.00	6.6980	1.1313	1.1326	1.1353	1.1392	1.1445	1.1510	1.1588	1.1678	1.1779
385.15	6.6192	1.1084	1.1097	1.1122	1.1160	1.1210	1.1273	1.1347	1.1433	1.1530
407.90	6.5720	1.0948	1.0961	1.0985	1.1022	1.1071	1.1131	1.1203	1.1287	1.1381
416.10	6.5570	1.0905	1.0918	1.0942	1.0978	1.1027	1.1087	1.1158	1.1241	1.1334
435.96	6.5245	1.0812	1.0824	1.0848	1.0884	1.0931	1.0990	1.1060	1.1141	1.1232
441.60	6.5161	1.0788	1.0800	1.0824	1.0859	1.0907	1.0965	1.1035	1.1115	1.1206
457.90	6.4936	1.0724	1.0736	1.0759	1.0794	1.0841	1.0899	1.0967	1.1047	1.1136
488.00	6.4584	1.0624	1.0635	1.0658	1.0693	1.0738	1.0794	1.0862	1.0939	1.1027
514.50	6.4326	1.0551	1.0562	1.0585	1.0618	1.0663	1.0719	1.0785	1.0861	1.0947
532.00	6.4177	1.0509	1.0520	1.0542	1.0576	1.0620	1.0675	1.0741	1.0816	1.0902
546.23	6.4067	1.0478	1.0489	1.0511	1.0544	1.0588	1.0643	1.0708	1.0783	1.0868
563.20	6.3947	1.0444	1.0455	1.0477	1.0510	1.0554	1.0608	1.0672	1.0747	1.0831
594.10	6.3756	1.0390	1.0401	1.0423	1.0455	1.0498	1.0552	1.0616	1.0689	1.0772
611.90	6.3659	1.0363	1.0373	1.0395	1.0427	1.0470	1.0524	1.0587	1.0660	1.0743
632.80	6.3556	1.0334	1.0344	1.0366	1.0398	1.0441	1.0494	1.0557	1.0629	1.0711
647.10	6.3492	1.0315	1.0326	1.0348	1.0380	1.0422	1.0475	1.0538	1.0610	1.0692
670.00	6.3397	1.0289	1.0300	1.0321	1.0353	1.0395	1.0447	1.0510	1.0582	1.0663
694.30	6.3307	1.0264	1.0274	1.0295	1.0327	1.0369	1.0421	1.0483	1.0555	1.0635
725.00	6.3206	1.0235	1.0246	1.0267	1.0299	1.0340	1.0392	1.0454	1.0525	1.0605
754.00	6.3123	1.0212	1.0222	1.0243	1.0275	1.0316	1.0368	1.0429	1.0500	1.0579
785.00	6.3043	1.0190	1.0200	1.0221	1.0252	1.0294	1.0345	1.0406	1.0476	1.0555
800.00	6.3008	1.0180	1.0190	1.0211	1.0242	1.0284	1.0335	1.0395	1.0465	1.0544
836.00	6.2932	1.0159	1.0169	1.0190	1.0221	1.0262	1.0313	1.0373	1.0443	1.0521
876.00	6.2858	1.0138	1.0148	1.0169	1.0200	1.0241	1.0291	1.0351	1.0421	1.0499
904.00	6.2812	1.0125	1.0136	1.0156	1.0187	1.0228	1.0278	1.0338	1.0407	1.0485
911.28	6.2801	1.0122	1.0132	1.0153	1.0184	1.0224	1.0275	1.0335	1.0404	1.0482
946.00	6.2751	1.0108	1.0119	1.0139	1.0170	1.0210	1.0260	1.0320	1.0389	1.0467
975.00	6.2713	1.0098	1.0108	1.0128	1.0159	1.0199	1.0249	1.0309	1.0378	1.0455
1000.00	6.2684	1.0089	1.0100	1.0120	1.0151	1.0191	1.0241	1.0300	1.0369	1.0446
1064.00	6.2617	1.0071	1.0081	1.0101	1.0132	1.0172	1.0222	1.0281	1.0349	1.0426
1106.00	6.2579	1.0060	1.0071	1.0091	1.0121	1.0161	1.0211	1.0270	1.0338	1.0415
1152.00	6.2543	1.0050	1.0060	1.0081	1.0111	1.0151	1.0200	1.0259	1.0327	1.0404
1185.00	6.2519	1.0044	1.0054	1.0074	1.0104	1.0144	1.0193	1.0252	1.0320	1.0397
1225.00	6.2493	1.0036	1.0047	1.0067	1.0097	1.0137	1.0186	1.0245	1.0312	1.0389
1275.00	6.2464	1.0028	1.0038	1.0058	1.0089	1.0128	1.0178	1.0236	1.0304	1.0380
1320.00	6.2440	1.0022	1.0032	1.0052	1.0082	1.0122	1.0171	1.0229	1.0297	1.0373
Static	6.2116	0.9932	0.9942	0.9961	0.9991	1.0030	1.0078	1.0135	1.0201	1.0275

TABLE T5. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of D_2 for v=0 and v=1.

λ(nm)	$\langle\bar{\alpha}\rangle_{00,00}$	$\langle\bar{\alpha}\rangle_{10,10}$	$\langle\bar{\alpha}\rangle_{10,00}$	$\langle\bar{\alpha}\rangle_{11,01}$	$\langle\bar{\alpha}\rangle_{12,02}$	$\langle\bar{\alpha}\rangle_{13,03}$	$\langle\bar{\alpha}\rangle_{14,04}$	$\langle\bar{\alpha}\rangle_{15,05}$	$\langle\bar{\alpha}\rangle_{16,06}$	$\langle\bar{\alpha}\rangle_{17,07}$	$\langle\bar{\alpha}\rangle_{18,08}$
182.26	6.9768	7.6104	1.0398	1.0411	1.0437	1.0477	1.0529	1.0595	1.0674	1.0767	1.0873
193.00	6.7466	7.3281	0.9722	0.9733	0.9756	0.9791	0.9837	0.9894	0.9964	1.0044	1.0137
213.00	6.4372	6.9536	0.8854	0.8864	0.8883	0.8912	0.8950	0.8997	0.9054	0.9121	0.9197
222.00	6.3323	6.8279	0.8571	0.8580	0.8598	0.8625	0.8660	0.8705	0.8758	0.8820	0.8892
224.30	6.3081	6.7990	0.8506	0.8515	0.8533	0.8559	0.8594	0.8638	0.8691	0.8752	0.8822
235.00	6.2070	6.6785	0.8239	0.8248	0.8264	0.8289	0.8322	0.8363	0.8412	0.8469	0.8535
248.00	6.1052	6.5578	0.7975	0.7983	0.7998	0.8021	0.8052	0.8091	0.8136	0.8190	0.8251
266.00	5.9927	6.4251	0.7689	0.7696	0.7711	0.7732	0.7761	0.7796	0.7839	0.7888	0.7945
275.36	5.9442	6.3681	0.7568	0.7575	0.7589	0.7609	0.7637	0.7671	0.7712	0.7760	0.7815
285.00	5.9000	6.3163	0.7458	0.7465	0.7478	0.7498	0.7525	0.7558	0.7598	0.7644	0.7697
308.00	5.8130	6.2145	0.7245	0.7251	0.7264	0.7282	0.7307	0.7339	0.7376	0.7420	0.7469
325.00	5.7616	6.1545	0.7120	0.7126	0.7138	0.7157	0.7181	0.7211	0.7247	0.7289	0.7337
334.24	5.7372	6.1262	0.7062	0.7068	0.7080	0.7097	0.7121	0.7151	0.7186	0.7228	0.7274
337.10	5.7302	6.1180	0.7045	0.7051	0.7063	0.7080	0.7104	0.7133	0.7169	0.7210	0.7256
347.00	5.7071	6.0911	0.6990	0.6995	0.7007	0.7025	0.7048	0.7077	0.7112	0.7152	0.7198
351.00	5.6984	6.0810	0.6969	0.6975	0.6986	0.7004	0.7027	0.7056	0.7090	0.7130	0.7176
355.00	5.6900	6.0713	0.6949	0.6955	0.6966	0.6983	0.7006	0.7035	0.7069	0.7109	0.7154
385.15	5.6356	6.0082	0.6820	0.6826	0.6837	0.6854	0.6876	0.6903	0.6936	0.6974	0.7018
407.90	5.6029	5.9703	0.6744	0.6749	0.6760	0.6776	0.6798	0.6824	0.6856	0.6894	0.6936
416.10	5.5925	5.9583	0.6719	0.6725	0.6735	0.6752	0.6773	0.6799	0.6831	0.6868	0.6910
435.96	5.5699	5.9321	0.6667	0.6672	0.6682	0.6698	0.6719	0.6745	0.6777	0.6813	0.6854
441.60	5.5640	5.9253	0.6653	0.6658	0.6669	0.6684	0.6705	0.6731	0.6763	0.6799	0.6840
457.90	5.5484	5.9072	0.6617	0.6622	0.6632	0.6648	0.6669	0.6694	0.6725	0.6761	0.6801
488.00	5.5237	5.8787	0.6560	0.6565	0.6575	0.6590	0.6611	0.6636	0.6666	0.6701	0.6741
514.50	5.5056	5.8579	0.6518	0.6523	0.6533	0.6548	0.6568	0.6593	0.6623	0.6658	0.6697
532.00	5.4952	5.8459	0.6494	0.6499	0.6509	0.6524	0.6544	0.6569	0.6598	0.6633	0.6671
546.23	5.4875	5.8370	0.6477	0.6482	0.6492	0.6506	0.6526	0.6551	0.6580	0.6614	0.6653
563.20	5.4790	5.8273	0.6458	0.6462	0.6472	0.6487	0.6507	0.6531	0.6560	0.6594	0.6632
594.10	5.4656	5.8118	0.6427	0.6432	0.6441	0.6456	0.6475	0.6500	0.6528	0.6562	0.6600
611.90	5.4588	5.8039	0.6411	0.6416	0.6426	0.6440	0.6460	0.6484	0.6512	0.6546	0.6583
632.80	5.4515	5.7956	0.6395	0.6400	0.6409	0.6424	0.6443	0.6467	0.6495	0.6528	0.6566
647.10	5.4469	5.7903	0.6385	0.6389	0.6399	0.6413	0.6432	0.6456	0.6485	0.6517	0.6555
670.00	5.4403	5.7826	0.6369	0.6374	0.6384	0.6398	0.6417	0.6441	0.6469	0.6502	0.6539
694.30	5.4339	5.7753	0.6355	0.6360	0.6369	0.6383	0.6402	0.6426	0.6454	0.6487	0.6524
725.00	5.4268	5.7671	0.6339	0.6344	0.6353	0.6367	0.6386	0.6409	0.6437	0.6470	0.6507
754.00	5.4208	5.7603	0.6325	0.6330	0.6340	0.6354	0.6372	0.6396	0.6423	0.6456	0.6492
785.00	5.4152	5.7539	0.6313	0.6317	0.6327	0.6341	0.6359	0.6383	0.6410	0.6442	0.6479
800.00	5.4127	5.7510	0.6307	0.6312	0.6321	0.6335	0.6354	0.6377	0.6405	0.6437	0.6473
836.00	5.4073	5.7448	0.6295	0.6300	0.6309	0.6323	0.6341	0.6364	0.6392	0.6424	0.6460
876.00	5.4021	5.7388	0.6283	0.6288	0.6297	0.6311	0.6329	0.6352	0.6380	0.6412	0.6448
904.00	5.3989	5.7351	0.6276	0.6281	0.6290	0.6304	0.6322	0.6345	0.6372	0.6404	0.6440
911.28	5.3981	5.7342	0.6274	0.6279	0.6288	0.6302	0.6320	0.6343	0.6370	0.6402	0.6438
946.00	5.3945	5.7301	0.6266	0.6271	0.6280	0.6294	0.6312	0.6335	0.6362	0.6394	0.6430
975.00	5.3918	5.7270	0.6260	0.6265	0.6274	0.6288	0.6306	0.6329	0.6356	0.6387	0.6423
1000.00	5.3897	5.7246	0.6255	0.6260	0.6269	0.6283	0.6301	0.6324	0.6351	0.6383	0.6418
1064.00	5.3850	5.7192	0.6245	0.6249	0.6259	0.6272	0.6290	0.6313	0.6340	0.6371	0.6407
1106.00	5.3823	5.7161	0.6239	0.6243	0.6253	0.6266	0.6284	0.6307	0.6334	0.6365	0.6401
1152.00	5.3797	5.7131	0.6233	0.6238	0.6247	0.6260	0.6278	0.6301	0.6328	0.6359	0.6394
1185.00	5.3780	5.7112	0.6229	0.6234	0.6243	0.6257	0.6275	0.6297	0.6324	0.6355	0.6391
1225.00	5.3762	5.7091	0.6225	0.6230	0.6239	0.6252	0.6270	0.6293	0.6320	0.6351	0.6386
1275.00	5.3741	5.7067	0.6220	0.6225	0.6234	0.6248	0.6266	0.6288	0.6315	0.6346	0.6381
1320.00	5.3724	5.7048	0.6217	0.6221	0.6230	0.6244	0.6262	0.6284	0.6311	0.6342	0.6377
Static	5.3493	5.6783	0.6165	0.6170	0.6179	0.6192	0.6210	0.6232	0.6258	0.6288	0.6323

TABLE T6. Mean polarizability matrix elements $\langle\bar{\alpha}\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\bar{\alpha}|\psi_{v',J'}\rangle$ of D_2 for v=1 and v=2.

λ(nm)	$\langle\bar{\alpha}\rangle_{20,20}$	$\langle\bar{\alpha}\rangle_{20,10}$	$\langle\bar{\alpha}\rangle_{21,11}$	$\langle\bar{\alpha}\rangle_{22,12}$	$\langle\bar{\alpha}\rangle_{23,13}$	$\langle\bar{\alpha}\rangle_{24,14}$	$\langle\bar{\alpha}\rangle_{25,15}$	$\langle\bar{\alpha}\rangle_{26,16}$	$\langle\bar{\alpha}\rangle_{27,17}$	$\langle\bar{\alpha}\rangle_{28,18}$
182.26	8.3031	1.5610	1.5629	1.5669	1.5729	1.5809	1.5909	1.6030	1.6170	1.6332
193.00	7.9573	1.4503	1.4520	1.4554	1.4606	1.4675	1.4761	1.4864	1.4985	1.5124
213.00	7.5054	1.3103	1.3117	1.3145	1.3187	1.3243	1.3312	1.3396	1.3494	1.3605
222.00	7.3554	1.2650	1.2663	1.2689	1.2728	1.2780	1.2845	1.2923	1.3013	1.3117
224.30	7.3209	1.2547	1.2560	1.2586	1.2624	1.2675	1.2739	1.2815	1.2904	1.3006
235.00	7.1781	1.2124	1.2135	1.2159	1.2195	1.2242	1.2302	1.2373	1.2455	1.2550
248.00	7.0356	1.1707	1.1718	1.1740	1.1773	1.1817	1.1872	1.1938	1.2015	1.2102
266.00	6.8797	1.1257	1.1268	1.1288	1.1318	1.1359	1.1410	1.1470	1.1541	1.1621
275.36	6.8130	1.1067	1.1077	1.1097	1.1126	1.1165	1.1214	1.1272	1.1340	1.1417
285.00	6.7525	1.0896	1.0905	1.0924	1.0953	1.0990	1.1038	1.1094	1.1159	1.1234
308.00	6.6340	1.0563	1.0572	1.0590	1.0616	1.0652	1.0696	1.0749	1.0810	1.0879
325.00	6.5644	1.0370	1.0379	1.0396	1.0421	1.0455	1.0497	1.0548	1.0607	1.0673
334.24	6.5316	1.0279	1.0288	1.0304	1.0329	1.0363	1.0404	1.0454	1.0511	1.0577
337.10	6.5220	1.0253	1.0261	1.0278	1.0303	1.0336	1.0377	1.0427	1.0484	1.0549
347.00	6.4910	1.0168	1.0176	1.0192	1.0217	1.0249	1.0290	1.0338	1.0394	1.0458
351.00	6.4793	1.0136	1.0144	1.0160	1.0184	1.0216	1.0257	1.0305	1.0361	1.0424
355.00	6.4680	1.0105	1.0113	1.0129	1.0153	1.0185	1.0225	1.0273	1.0328	1.0391
385.15	6.3952	0.9906	0.9914	0.9929	0.9952	0.9983	1.0021	1.0067	1.0120	1.0180
407.90	6.3515	0.9788	0.9795	0.9810	0.9833	0.9863	0.9900	0.9944	0.9996	1.0054
416.10	6.3377	0.9750	0.9758	0.9773	0.9795	0.9825	0.9861	0.9906	0.9957	1.0015
435.96	6.3075	0.9669	0.9676	0.9691	0.9713	0.9742	0.9778	0.9821	0.9872	0.9928
441.60	6.2997	0.9648	0.9656	0.9670	0.9692	0.9721	0.9757	0.9800	0.9850	0.9906
457.90	6.2790	0.9592	0.9600	0.9614	0.9636	0.9664	0.9700	0.9742	0.9791	0.9847
488.00	6.2463	0.9505	0.9512	0.9526	0.9547	0.9575	0.9610	0.9652	0.9700	0.9754
514.50	6.2223	0.9441	0.9448	0.9462	0.9483	0.9510	0.9545	0.9586	0.9633	0.9687
532.00	6.2086	0.9405	0.9411	0.9425	0.9446	0.9473	0.9507	0.9548	0.9595	0.9648
546.23	6.1984	0.9377	0.9384	0.9398	0.9418	0.9446	0.9479	0.9520	0.9566	0.9619
563.20	6.1872	0.9348	0.9355	0.9368	0.9389	0.9416	0.9449	0.9489	0.9535	0.9588
594.10	6.1695	0.9301	0.9308	0.9321	0.9341	0.9368	0.9401	0.9440	0.9486	0.9538
611.90	6.1605	0.9277	0.9284	0.9297	0.9317	0.9344	0.9377	0.9416	0.9461	0.9513
632.80	6.1509	0.9252	0.9259	0.9272	0.9292	0.9318	0.9351	0.9390	0.9435	0.9486
647.10	6.1449	0.9236	0.9243	0.9256	0.9276	0.9302	0.9334	0.9373	0.9418	0.9470
670.00	6.1361	0.9213	0.9219	0.9233	0.9252	0.9278	0.9311	0.9349	0.9394	0.9445
694.30	6.1278	0.9191	0.9197	0.9210	0.9230	0.9256	0.9288	0.9327	0.9371	0.9422
725.00	6.1184	0.9166	0.9173	0.9186	0.9205	0.9231	0.9263	0.9301	0.9345	0.9396
754.00	6.1106	0.9146	0.9152	0.9165	0.9184	0.9210	0.9242	0.9280	0.9324	0.9374
785.00	6.1033	0.9126	0.9133	0.9146	0.9165	0.9190	0.9222	0.9260	0.9304	0.9354
800.00	6.1000	0.9118	0.9124	0.9137	0.9156	0.9182	0.9213	0.9251	0.9295	0.9345
836.00	6.0929	0.9099	0.9106	0.9118	0.9137	0.9163	0.9194	0.9232	0.9275	0.9325
876.00	6.0860	0.9081	0.9088	0.9100	0.9119	0.9144	0.9176	0.9213	0.9257	0.9306
904.00	6.0818	0.9070	0.9076	0.9089	0.9108	0.9133	0.9164	0.9202	0.9245	0.9294
911.28	6.0807	0.9067	0.9074	0.9086	0.9105	0.9130	0.9162	0.9199	0.9242	0.9291
946.00	6.0761	0.9055	0.9061	0.9074	0.9093	0.9118	0.9149	0.9186	0.9229	0.9278
975.00	6.0726	0.9046	0.9052	0.9065	0.9084	0.9109	0.9140	0.9177	0.9220	0.9269
1000.00	6.0698	0.9039	0.9045	0.9058	0.9076	0.9101	0.9132	0.9169	0.9212	0.9261
1064.00	6.0636	0.9022	0.9029	0.9041	0.9060	0.9085	0.9116	0.9153	0.9195	0.9244
1106.00	6.0601	0.9013	0.9020	0.9032	0.9051	0.9076	0.9106	0.9143	0.9186	0.9234
1152.00	6.0567	0.9004	0.9011	0.9023	0.9042	0.9066	0.9097	0.9134	0.9176	0.9225
1185.00	6.0545	0.8999	0.9005	0.9017	0.9036	0.9061	0.9091	0.9128	0.9170	0.9219
1225.00	6.0521	0.8992	0.8999	0.9011	0.9030	0.9054	0.9085	0.9121	0.9164	0.9212
1275.00	6.0494	0.8985	0.8991	0.9004	0.9022	0.9047	0.9078	0.9114	0.9156	0.9204
1320.00	6.0472	0.8980	0.8986	0.8998	0.9017	0.9041	0.9072	0.9108	0.9151	0.9198
Static	6.0170	0.8901	0.8907	0.8919	0.8937	0.8961	0.8991	0.9027	0.9068	0.9115

S2. Matrix elements of polarizability anisotropy

TABLE T7. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of H_2 for v=0.

λ(nm)	$\langle\gamma\rangle_{00,00}$	$\langle\gamma\rangle_{00,02}$	$\langle\gamma\rangle_{01,03}$	$\langle\gamma\rangle_{02,04}$	$\langle\gamma\rangle_{03,05}$	$\langle\gamma\rangle_{04,06}$	$\langle\gamma\rangle_{05,07}$	$\langle\gamma\rangle_{06,08}$	$\langle\gamma\rangle_{07,09}$	$\langle\gamma\rangle_{08,0\,10}$
182.26	3.1512	3.1733	3.2026	3.2469	3.3063	3.3813	3.4724	3.5802	3.7055	3.8491
193.00	2.9784	2.9986	3.0255	3.0660	3.1204	3.1889	3.2721	3.3703	3.4843	3.6147
213.00	2.7537	2.7717	2.7955	2.8314	2.8794	2.9400	3.0133	3.0998	3.1998	3.3139
222.00	2.6795	2.6968	2.7196	2.7540	2.8001	2.8581	2.9282	3.0110	3.1066	3.2156
224.30	2.6626	2.6796	2.7023	2.7363	2.7819	2.8393	2.9088	2.9907	3.0853	3.1931
235.00	2.5922	2.6086	2.6303	2.6630	2.7067	2.7618	2.8283	2.9067	2.9973	3.1004
248.00	2.5223	2.5380	2.5588	2.5901	2.6321	2.6848	2.7485	2.8235	2.9101	3.0086
266.00	2.4461	2.4611	2.4809	2.5108	2.5508	2.6011	2.6618	2.7332	2.8155	2.9091
275.36	2.4136	2.4283	2.4477	2.4770	2.5162	2.5654	2.6248	2.6947	2.7753	2.8668
285.00	2.3841	2.3986	2.4176	2.4464	2.4848	2.5331	2.5914	2.6599	2.7389	2.8286
308.00	2.3266	2.3405	2.3589	2.3866	2.4236	2.4701	2.5262	2.5921	2.6680	2.7541
325.00	2.2930	2.3066	2.3246	2.3516	2.3878	2.4333	2.4881	2.5525	2.6266	2.7107
334.24	2.2771	2.2906	2.3084	2.3352	2.3710	2.4159	2.4702	2.5338	2.6071	2.6903
337.10	2.2725	2.2860	2.3037	2.3304	2.3661	2.4109	2.4650	2.5284	2.6015	2.6843
347.00	2.2576	2.2709	2.2884	2.3149	2.3502	2.3945	2.4480	2.5108	2.5831	2.6651
351.00	2.2519	2.2652	2.2827	2.3090	2.3442	2.3884	2.4417	2.5042	2.5762	2.6578
355.00	2.2465	2.2597	2.2771	2.3034	2.3384	2.3825	2.4355	2.4978	2.5696	2.6509
385.15	2.2115	2.2244	2.2414	2.2670	2.3012	2.3442	2.3960	2.4568	2.5267	2.6059
407.90	2.1905	2.2032	2.2200	2.2453	2.2790	2.3213	2.3723	2.4322	2.5010	2.5790
416.10	2.1839	2.1965	2.2133	2.2384	2.2719	2.3141	2.3648	2.4244	2.4929	2.5705
435.96	2.1694	2.1820	2.1985	2.2234	2.2566	2.2983	2.3486	2.4075	2.4753	2.5520
441.60	2.1657	2.1782	2.1947	2.2195	2.2527	2.2942	2.3444	2.4031	2.4707	2.5473
457.90	2.1558	2.1682	2.1846	2.2092	2.2421	2.2834	2.3332	2.3915	2.4586	2.5346
488.00	2.1402	2.1524	2.1686	2.1930	2.2255	2.2664	2.3156	2.3732	2.4395	2.5146
514.50	2.1288	2.1409	2.1570	2.1812	2.2134	2.2539	2.3027	2.3599	2.4256	2.5001
532.00	2.1222	2.1343	2.1503	2.1743	2.2065	2.2468	2.2953	2.3522	2.4176	2.4917
546.23	2.1173	2.1294	2.1453	2.1693	2.2013	2.2415	2.2898	2.3465	2.4117	2.4855
563.20	2.1120	2.1241	2.1399	2.1638	2.1957	2.2357	2.2839	2.3404	2.4053	2.4787
594.10	2.1036	2.1155	2.1313	2.1550	2.1867	2.2265	2.2744	2.3305	2.3950	2.4680
611.90	2.0993	2.1112	2.1270	2.1506	2.1822	2.2218	2.2696	2.3255	2.3898	2.4625
632.80	2.0947	2.1066	2.1223	2.1459	2.1774	2.2169	2.2644	2.3202	2.3842	2.4567
647.10	2.0919	2.1038	2.1194	2.1429	2.1744	2.2138	2.2612	2.3169	2.3808	2.4531
670.00	2.0877	2.0995	2.1151	2.1386	2.1699	2.2092	2.2565	2.3120	2.3757	2.4478
694.30	2.0837	2.0955	2.1111	2.1345	2.1657	2.2049	2.2521	2.3073	2.3708	2.4427
725.00	2.0793	2.0910	2.1065	2.1298	2.1610	2.2000	2.2471	2.3022	2.3654	2.4371
754.00	2.0756	2.0873	2.1028	2.1260	2.1571	2.1960	2.2429	2.2978	2.3609	2.4324
785.00	2.0721	2.0838	2.0992	2.1224	2.1534	2.1922	2.2390	2.2938	2.3567	2.4279
800.00	2.0705	2.0822	2.0976	2.1208	2.1517	2.1905	2.2372	2.2920	2.3548	2.4259
836.00	2.0672	2.0788	2.0942	2.1173	2.1482	2.1868	2.2334	2.2880	2.3507	2.4217
876.00	2.0639	2.0755	2.0909	2.1139	2.1447	2.1833	2.2298	2.2842	2.3468	2.4175
904.00	2.0619	2.0735	2.0888	2.1118	2.1426	2.1811	2.2275	2.2819	2.3443	2.4150
911.28	2.0614	2.0730	2.0883	2.1113	2.1420	2.1806	2.2269	2.2813	2.3437	2.4143
946.00	2.0592	2.0708	2.0861	2.1090	2.1397	2.1782	2.2245	2.2787	2.3410	2.4115
975.00	2.0575	2.0691	2.0844	2.1073	2.1379	2.1764	2.2226	2.2768	2.3390	2.4094
1000.00	2.0562	2.0678	2.0830	2.1059	2.1366	2.1749	2.2211	2.2753	2.3374	2.4078
1064.00	2.0533	2.0648	2.0800	2.1029	2.1334	2.1717	2.2178	2.2718	2.3339	2.4040
1106.00	2.0516	2.0631	2.0783	2.1012	2.1317	2.1699	2.2160	2.2699	2.3318	2.4019
1152.00	2.0500	2.0615	2.0767	2.0995	2.1300	2.1682	2.2141	2.2680	2.3299	2.3999
1185.00	2.0490	2.0605	2.0756	2.0984	2.1289	2.1670	2.2130	2.2668	2.3286	2.3985
1225.00	2.0478	2.0593	2.0745	2.0972	2.1276	2.1658	2.2117	2.2655	2.3272	2.3971
1275.00	2.0465	2.0580	2.0731	2.0959	2.1263	2.1644	2.2102	2.2640	2.3257	2.3954
1320.00	2.0455	2.0570	2.0721	2.0948	2.1252	2.1633	2.2091	2.2628	2.3244	2.3941
Static	2.0312	2.0426	2.0575	2.0800	2.1101	2.1477	2.1930	2.2461	2.3071	2.3760

TABLE T8. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of H_2 for v=1.

λ(nm)	$\langle\gamma\rangle_{10,10}$	$\langle\gamma\rangle_{10,12}$	$\langle\gamma\rangle_{11,13}$	$\langle\gamma\rangle_{12,14}$	$\langle\gamma\rangle_{13,15}$	$\langle\gamma\rangle_{14,16}$	$\langle\gamma\rangle_{15,17}$	$\langle\gamma\rangle_{16,18}$	$\langle\gamma\rangle_{17,19}$	$\langle\gamma\rangle_{18,1\,10}$
182.26	4.2412	4.2695	4.3064	4.3621	4.4370	4.5316	4.6468	4.7832	4.9421	5.1245
193.00	3.9516	3.9769	4.0097	4.0593	4.1260	4.2100	4.3121	4.4329	4.5731	4.7338
213.00	3.5868	3.6084	3.6365	3.6788	3.7356	3.8072	3.8939	3.9963	4.1147	4.2499
222.00	3.4690	3.4895	3.5162	3.5563	3.6101	3.6778	3.7598	3.8565	3.9683	4.0958
224.30	3.4423	3.4625	3.4888	3.5284	3.5816	3.6484	3.7294	3.8248	3.9351	4.0609
235.00	3.3321	3.3514	3.3763	3.4139	3.4643	3.5276	3.6043	3.6946	3.7989	3.9177
248.00	3.2238	3.2421	3.2657	3.3014	3.3491	3.4091	3.4817	3.5671	3.6657	3.7778
266.00	3.1071	3.1243	3.1466	3.1802	3.2252	3.2817	3.3499	3.4302	3.5227	3.6279
275.36	3.0577	3.0745	3.0963	3.1290	3.1728	3.2278	3.2943	3.3724	3.4625	3.5648
285.00	3.0132	3.0296	3.0508	3.0828	3.1255	3.1793	3.2442	3.3204	3.4082	3.5079
308.00	2.9268	2.9425	2.9628	2.9933	3.0341	3.0853	3.1471	3.2197	3.3033	3.3982
325.00	2.8766	2.8919	2.9116	2.9412	2.9809	3.0307	3.0908	3.1614	3.2425	3.3346
334.24	2.8530	2.8681	2.8876	2.9168	2.9560	3.0051	3.0644	3.1340	3.2140	3.3048
337.10	2.8462	2.8612	2.8806	2.9098	2.9488	2.9977	3.0568	3.1260	3.2058	3.2961
347.00	2.8240	2.8389	2.8580	2.8868	2.9253	2.9736	3.0319	3.1003	3.1790	3.2682
351.00	2.8157	2.8304	2.8495	2.8782	2.9165	2.9646	3.0226	3.0906	3.1689	3.2576
355.00	2.8077	2.8224	2.8413	2.8699	2.9080	2.9559	3.0136	3.0813	3.1593	3.2475
385.15	2.7560	2.7703	2.7887	2.8164	2.8534	2.8999	2.9559	3.0216	3.0971	3.1826
407.90	2.7253	2.7393	2.7574	2.7846	2.8209	2.8666	2.9215	2.9860	3.0601	3.1439
416.10	2.7156	2.7295	2.7475	2.7745	2.8107	2.8560	2.9107	2.9747	3.0484	3.1317
435.96	2.6944	2.7082	2.7260	2.7527	2.7884	2.8331	2.8871	2.9503	3.0230	3.1052
441.60	2.6890	2.7027	2.7204	2.7470	2.7826	2.8272	2.8810	2.9441	3.0165	3.0984
457.90	2.6745	2.6881	2.7057	2.7320	2.7673	2.8115	2.8648	2.9273	2.9991	3.0803
488.00	2.6517	2.6652	2.6825	2.7085	2.7433	2.7869	2.8395	2.9011	2.9718	3.0518
514.50	2.6351	2.6484	2.6656	2.6913	2.7258	2.7690	2.8210	2.8819	2.9519	3.0311
532.00	2.6256	2.6388	2.6559	2.6815	2.7157	2.7586	2.8104	2.8709	2.9405	3.0192
546.23	2.6185	2.6317	2.6487	2.6742	2.7083	2.7510	2.8025	2.8628	2.9321	3.0104
563.20	2.6109	2.6240	2.6409	2.6663	2.7002	2.7427	2.7940	2.8540	2.9229	3.0008
594.10	2.5986	2.6116	2.6284	2.6536	2.6873	2.7295	2.7803	2.8399	2.9082	2.9855
611.90	2.5924	2.6054	2.6221	2.6472	2.6807	2.7228	2.7734	2.8328	2.9009	2.9778
632.80	2.5859	2.5988	2.6154	2.6404	2.6738	2.7157	2.7661	2.8252	2.8930	2.9696
647.10	2.5817	2.5946	2.6112	2.6361	2.6695	2.7112	2.7615	2.8204	2.8881	2.9645
670.00	2.5757	2.5885	2.6051	2.6299	2.6631	2.7047	2.7548	2.8135	2.8809	2.9570
694.30	2.5700	2.5827	2.5992	2.6240	2.6570	2.6985	2.7484	2.8069	2.8740	2.9499
725.00	2.5635	2.5763	2.5927	2.6173	2.6503	2.6916	2.7413	2.7995	2.8663	2.9419
754.00	2.5582	2.5709	2.5873	2.6118	2.6447	2.6858	2.7354	2.7934	2.8600	2.9352
785.00	2.5532	2.5658	2.5821	2.6066	2.6393	2.6804	2.7298	2.7876	2.8540	2.9290
800.00	2.5509	2.5636	2.5799	2.6043	2.6370	2.6780	2.7273	2.7850	2.8513	2.9262
836.00	2.5461	2.5587	2.5749	2.5993	2.6319	2.6727	2.7219	2.7795	2.8455	2.9202
876.00	2.5414	2.5540	2.5702	2.5945	2.6270	2.6677	2.7167	2.7741	2.8399	2.9144
904.00	2.5385	2.5510	2.5672	2.5915	2.6239	2.6645	2.7135	2.7707	2.8365	2.9107
911.28	2.5378	2.5503	2.5665	2.5907	2.6231	2.6638	2.7127	2.7699	2.8356	2.9099
946.00	2.5346	2.5471	2.5632	2.5875	2.6198	2.6603	2.7091	2.7663	2.8318	2.9059
975.00	2.5322	2.5447	2.5608	2.5850	2.6173	2.6578	2.7065	2.7635	2.8290	2.9030
1000.00	2.5303	2.5428	2.5589	2.5830	2.6153	2.6557	2.7044	2.7614	2.8267	2.9006
1064.00	2.5261	2.5386	2.5546	2.5787	2.6108	2.6512	2.6997	2.7565	2.8217	2.8954
1106.00	2.5237	2.5362	2.5522	2.5762	2.6083	2.6486	2.6970	2.7538	2.8189	2.8924
1152.00	2.5214	2.5338	2.5498	2.5738	2.6059	2.6461	2.6945	2.7511	2.8161	2.8895
1185.00	2.5199	2.5323	2.5483	2.5723	2.6043	2.6445	2.6928	2.7494	2.8143	2.8877
1225.00	2.5183	2.5307	2.5466	2.5706	2.6026	2.6427	2.6910	2.7475	2.8124	2.8856
1275.00	2.5164	2.5288	2.5447	2.5687	2.6006	2.6407	2.6889	2.7454	2.8102	2.8833
1320.00	2.5149	2.5273	2.5432	2.5671	2.5991	2.6391	2.6873	2.7437	2.8084	2.8815
Static	2.4945	2.5067	2.5224	2.5460	2.5775	2.6170	2.6645	2.7202	2.7840	2.8561

TABLE T9. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of H_2 for v=2.

λ(nm)	$\langle\gamma\rangle_{20,20}$	$\langle\gamma\rangle_{20,22}$	$\langle\gamma\rangle_{21,23}$	$\langle\gamma\rangle_{22,24}$	$\langle\gamma\rangle_{23,25}$	$\langle\gamma\rangle_{24,26}$	$\langle\gamma\rangle_{25,27}$	$\langle\gamma\rangle_{26,28}$	$\langle\gamma\rangle_{27,29}$	$\langle\gamma\rangle_{28,2\,10}$
182.26	5.6158	5.6518	5.6982	5.7683	5.8626	5.9820	6.1275	6.3001	6.5015	6.7332
193.00	5.1504	5.1816	5.2216	5.2820	5.3632	5.4657	5.5903	5.7379	5.9094	6.1061
213.00	4.5828	4.6085	4.6413	4.6907	4.7570	4.8407	4.9420	5.0616	5.2001	5.3582
222.00	4.4040	4.4280	4.4587	4.5048	4.5668	4.6448	4.7392	4.8506	4.9794	5.1263
224.30	4.3636	4.3873	4.4175	4.4629	4.5239	4.6006	4.6936	4.8031	4.9298	5.0743
235.00	4.1986	4.2208	4.2491	4.2916	4.3487	4.4205	4.5073	4.6096	4.7278	4.8623
248.00	4.0381	4.0589	4.0854	4.1252	4.1785	4.2456	4.3267	4.4222	4.5323	4.6576
266.00	3.8670	3.8864	3.9110	3.9480	3.9975	4.0597	4.1349	4.2233	4.3252	4.4409
275.36	3.7952	3.8140	3.8378	3.8736	3.9216	3.9819	4.0546	4.1402	4.2387	4.3504
285.00	3.7307	3.7490	3.7721	3.8069	3.8535	3.9120	3.9826	4.0656	4.1611	4.2695
308.00	3.6065	3.6238	3.6456	3.6785	3.7224	3.7776	3.8442	3.9223	4.0122	4.1141
325.00	3.5348	3.5515	3.5726	3.6044	3.6468	3.7001	3.7644	3.8398	3.9265	4.0248
334.24	3.5012	3.5177	3.5385	3.5697	3.6115	3.6639	3.7271	3.8013	3.8865	3.9831
337.10	3.4915	3.5079	3.5286	3.5597	3.6012	3.6534	3.7163	3.7901	3.8750	3.9710
347.00	3.4601	3.4762	3.4966	3.5272	3.5681	3.6195	3.6814	3.7540	3.8375	3.9320
351.00	3.4482	3.4643	3.4845	3.5150	3.5556	3.6067	3.6683	3.7405	3.8234	3.9173
355.00	3.4369	3.4528	3.4730	3.5032	3.5437	3.5945	3.6557	3.7274	3.8099	3.9032
385.15	3.3640	3.3794	3.3988	3.4280	3.4670	3.5159	3.5749	3.6440	3.7234	3.8131
407.90	3.3207	3.3358	3.3548	3.3833	3.4215	3.4693	3.5270	3.5945	3.6721	3.7598
416.10	3.3070	3.3220	3.3409	3.3692	3.4071	3.4546	3.5118	3.5789	3.6559	3.7430
435.96	3.2774	3.2922	3.3108	3.3387	3.3760	3.4228	3.4791	3.5451	3.6209	3.7065
441.60	3.2698	3.2845	3.3030	3.3308	3.3680	3.4146	3.4707	3.5364	3.6119	3.6972
457.90	3.2496	3.2641	3.2824	3.3099	3.3467	3.3928	3.4483	3.5133	3.5879	3.6723
488.00	3.2178	3.2321	3.2501	3.2772	3.3133	3.3586	3.4132	3.4771	3.5504	3.6333
514.50	3.1947	3.2088	3.2266	3.2533	3.2890	3.3338	3.3877	3.4508	3.5232	3.6049
532.00	3.1814	3.1955	3.2131	3.2396	3.2751	3.3195	3.3730	3.4357	3.5075	3.5887
546.23	3.1716	3.1856	3.2031	3.2295	3.2648	3.3090	3.3622	3.4245	3.4960	3.5767
563.20	3.1609	3.1748	3.1923	3.2185	3.2536	3.2975	3.3504	3.4124	3.4834	3.5636
594.10	3.1439	3.1577	3.1750	3.2010	3.2358	3.2793	3.3317	3.3931	3.4634	3.5428
611.90	3.1354	3.1491	3.1663	3.1922	3.2268	3.2701	3.3222	3.3833	3.4533	3.5324
632.80	3.1262	3.1399	3.1570	3.1828	3.2172	3.2603	3.3122	3.3729	3.4426	3.5212
647.10	3.1205	3.1342	3.1512	3.1769	3.2112	3.2542	3.3059	3.3665	3.4359	3.5142
670.00	3.1122	3.1257	3.1427	3.1683	3.2024	3.2452	3.2967	3.3570	3.4261	3.5040
694.30	3.1042	3.1177	3.1347	3.1601	3.1941	3.2367	3.2879	3.3479	3.4167	3.4943
725.00	3.0953	3.1088	3.1256	3.1510	3.1848	3.2272	3.2782	3.3379	3.4063	3.4835
754.00	3.0880	3.1014	3.1182	3.1434	3.1770	3.2193	3.2701	3.3295	3.3976	3.4745
785.00	3.0810	3.0944	3.1111	3.1362	3.1697	3.2118	3.2624	3.3216	3.3895	3.4660
800.00	3.0779	3.0913	3.1080	3.1330	3.1665	3.2085	3.2590	3.3181	3.3859	3.4623
836.00	3.0712	3.0845	3.1012	3.1261	3.1595	3.2013	3.2516	3.3105	3.3780	3.4541
876.00	3.0648	3.0780	3.0946	3.1195	3.1527	3.1944	3.2445	3.3032	3.3704	3.4463
904.00	3.0608	3.0740	3.0905	3.1153	3.1485	3.1901	3.2401	3.2986	3.3657	3.4414
911.28	3.0598	3.0730	3.0895	3.1143	3.1475	3.1890	3.2390	3.2975	3.3646	3.4402
946.00	3.0554	3.0686	3.0851	3.1098	3.1429	3.1844	3.2342	3.2926	3.3594	3.4349
975.00	3.0521	3.0653	3.0817	3.1064	3.1395	3.1808	3.2306	3.2888	3.3556	3.4309
1000.00	3.0495	3.0627	3.0791	3.1038	3.1367	3.1780	3.2277	3.2859	3.3525	3.4277
1064.00	3.0437	3.0568	3.0732	3.0977	3.1306	3.1718	3.2213	3.2793	3.3457	3.4206
1106.00	3.0404	3.0535	3.0698	3.0944	3.1272	3.1683	3.2177	3.2755	3.3418	3.4166
1152.00	3.0372	3.0503	3.0666	3.0911	3.1238	3.1649	3.2142	3.2719	3.3381	3.4127
1185.00	3.0352	3.0482	3.0645	3.0890	3.1217	3.1626	3.2119	3.2696	3.3357	3.4102
1225.00	3.0329	3.0459	3.0622	3.0866	3.1193	3.1602	3.2094	3.2670	3.3330	3.4075
1275.00	3.0304	3.0433	3.0596	3.0840	3.1166	3.1575	3.2066	3.2642	3.3300	3.4044
1320.00	3.0283	3.0413	3.0575	3.0819	3.1145	3.1553	3.2044	3.2619	3.3277	3.4019
Static	3.0002	3.0130	3.0289	3.0529	3.0850	3.1252	3.1735	3.2300	3.2947	3.3677

TABLE T10. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of HD for v=0.

λ(nm)	$\langle\gamma\rangle_{00,00}$	$\langle\gamma\rangle_{00,02}$	$\langle\gamma\rangle_{01,03}$	$\langle\gamma\rangle_{02,04}$	$\langle\gamma\rangle_{03,05}$	$\langle\gamma\rangle_{04,06}$	$\langle\gamma\rangle_{05,07}$	$\langle\gamma\rangle_{06,08}$	$\langle\gamma\rangle_{07,09}$	$\langle\gamma\rangle_{08,0\,10}$
182.26	3.0835	3.0998	3.1215	3.1541	3.1977	3.2528	3.3194	3.3979	3.4888	3.5924
193.00	2.9175	2.9325	2.9523	2.9823	3.0223	3.0727	3.1337	3.2056	3.2885	3.3831
213.00	2.7011	2.7144	2.7321	2.7586	2.7942	2.8389	2.8929	2.9563	3.0296	3.1128
222.00	2.6295	2.6423	2.6593	2.6847	2.7189	2.7617	2.8134	2.8743	2.9444	3.0240
224.30	2.6131	2.6258	2.6426	2.6678	2.7016	2.7440	2.7953	2.8555	2.9249	3.0037
235.00	2.5452	2.5573	2.5734	2.5977	2.6301	2.6708	2.7200	2.7777	2.8443	2.9198
248.00	2.4775	2.4892	2.5047	2.5279	2.5591	2.5981	2.6452	2.7006	2.7643	2.8366
266.00	2.4038	2.4149	2.4297	2.4519	2.4816	2.5189	2.5638	2.6166	2.6773	2.7461
275.36	2.3723	2.3833	2.3977	2.4195	2.4486	2.4851	2.5291	2.5808	2.6402	2.7076
285.00	2.3438	2.3545	2.3687	2.3901	2.4186	2.4545	2.4977	2.5484	2.6067	2.6727
308.00	2.2880	2.2984	2.3121	2.3327	2.3602	2.3948	2.4364	2.4852	2.5413	2.6048
325.00	2.2554	2.2655	2.2789	2.2991	2.3260	2.3598	2.4005	2.4482	2.5030	2.5651
334.24	2.2400	2.2501	2.2633	2.2833	2.3099	2.3433	2.3836	2.4308	2.4850	2.5464
337.10	2.2355	2.2456	2.2588	2.2787	2.3052	2.3386	2.3787	2.4257	2.4798	2.5410
347.00	2.2210	2.2309	2.2440	2.2637	2.2900	2.3230	2.3628	2.4093	2.4628	2.5234
351.00	2.2156	2.2254	2.2385	2.2581	2.2843	2.3172	2.3567	2.4031	2.4564	2.5168
355.00	2.2103	2.2201	2.2331	2.2527	2.2788	2.3115	2.3510	2.3972	2.4503	2.5104
385.15	2.1763	2.1859	2.1986	2.2177	2.2432	2.2752	2.3137	2.3588	2.4106	2.4692
407.90	2.1559	2.1654	2.1779	2.1968	2.2219	2.2534	2.2914	2.3358	2.3868	2.4446
416.10	2.1495	2.1589	2.1714	2.1901	2.2151	2.2465	2.2843	2.3285	2.3793	2.4368
435.96	2.1355	2.1448	2.1571	2.1757	2.2005	2.2315	2.2689	2.3127	2.3630	2.4198
441.60	2.1318	2.1412	2.1535	2.1720	2.1967	2.2277	2.2649	2.3086	2.3588	2.4154
457.90	2.1222	2.1314	2.1437	2.1620	2.1866	2.2173	2.2544	2.2977	2.3475	2.4038
488.00	2.1070	2.1162	2.1283	2.1464	2.1707	2.2011	2.2377	2.2806	2.3298	2.3855
514.50	2.0959	2.1050	2.1170	2.1350	2.1591	2.1893	2.2256	2.2681	2.3169	2.3721
532.00	2.0895	2.0986	2.1105	2.1284	2.1524	2.1824	2.2186	2.2609	2.3095	2.3644
546.23	2.0848	2.0938	2.1057	2.1236	2.1475	2.1774	2.2134	2.2556	2.3040	2.3587
563.20	2.0796	2.0886	2.1005	2.1183	2.1421	2.1719	2.2078	2.2498	2.2980	2.3525
594.10	2.0714	2.0803	2.0921	2.1098	2.1335	2.1631	2.1988	2.2405	2.2885	2.3426
611.90	2.0673	2.0762	2.0879	2.1056	2.1291	2.1587	2.1942	2.2359	2.2836	2.3376
632.80	2.0628	2.0717	2.0834	2.1010	2.1245	2.1540	2.1894	2.2309	2.2785	2.3323
647.10	2.0601	2.0689	2.0806	2.0982	2.1216	2.1510	2.1864	2.2278	2.2753	2.3289
670.00	2.0560	2.0648	2.0765	2.0940	2.1174	2.1467	2.1819	2.2232	2.2705	2.3240
694.30	2.0521	2.0609	2.0726	2.0900	2.1133	2.1425	2.1777	2.2188	2.2660	2.3194
725.00	2.0478	2.0566	2.0682	2.0856	2.1088	2.1379	2.1730	2.2140	2.2610	2.3142
754.00	2.0442	2.0530	2.0645	2.0819	2.1050	2.1341	2.1690	2.2099	2.2568	2.3099
785.00	2.0408	2.0495	2.0611	2.0784	2.1015	2.1305	2.1653	2.2061	2.2529	2.3058
800.00	2.0393	2.0480	2.0595	2.0768	2.0999	2.1289	2.1637	2.2044	2.2512	2.3040
836.00	2.0360	2.0447	2.0562	2.0735	2.0965	2.1254	2.1601	2.2007	2.2473	2.3000
876.00	2.0329	2.0415	2.0530	2.0702	2.0932	2.1220	2.1566	2.1972	2.2437	2.2962
904.00	2.0309	2.0395	2.0510	2.0682	2.0911	2.1199	2.1545	2.1950	2.2414	2.2938
911.28	2.0304	2.0391	2.0505	2.0677	2.0906	2.1194	2.1539	2.1944	2.2408	2.2933
946.00	2.0283	2.0369	2.0483	2.0655	2.0884	2.1171	2.1516	2.1920	2.2383	2.2907
975.00	2.0266	2.0353	2.0467	2.0638	2.0867	2.1154	2.1498	2.1902	2.2365	2.2888
1000.00	2.0254	2.0340	2.0454	2.0625	2.0854	2.1140	2.1484	2.1888	2.2350	2.2872
1064.00	2.0225	2.0311	2.0425	2.0596	2.0824	2.1109	2.1453	2.1855	2.2317	2.2838
1106.00	2.0209	2.0295	2.0408	2.0579	2.0807	2.1092	2.1435	2.1837	2.2298	2.2818
1152.00	2.0193	2.0279	2.0393	2.0563	2.0790	2.1075	2.1418	2.1820	2.2280	2.2800
1185.00	2.0183	2.0269	2.0382	2.0553	2.0780	2.1065	2.1407	2.1808	2.2268	2.2787
1225.00	2.0172	2.0258	2.0371	2.0541	2.0768	2.1053	2.1395	2.1796	2.2255	2.2774
1275.00	2.0159	2.0245	2.0358	2.0528	2.0755	2.1039	2.1381	2.1782	2.2241	2.2759
1320.00	2.0149	2.0235	2.0348	2.0518	2.0745	2.1029	2.1370	2.1770	2.2229	2.2747
Static	2.0010	2.0095	2.0207	2.0375	2.0599	2.0880	2.1219	2.1614	2.2068	2.2580

TABLE T11. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of HD for v=1.

λ(nm)	$\langle\gamma\rangle_{10,10}$	$\langle\gamma\rangle_{10,12}$	$\langle\gamma\rangle_{11,13}$	$\langle\gamma\rangle_{12,14}$	$\langle\gamma\rangle_{13,15}$	$\langle\gamma\rangle_{14,16}$	$\langle\gamma\rangle_{15,17}$	$\langle\gamma\rangle_{16,18}$	$\langle\gamma\rangle_{17,19}$	$\langle\gamma\rangle_{18,1\,10}$
182.26	3.9975	4.0177	4.0441	4.0839	4.1372	4.2045	4.2860	4.3822	4.4937	4.6210
193.00	3.7362	3.7544	3.7780	3.8137	3.8615	3.9217	3.9945	4.0804	4.1797	4.2929
213.00	3.4048	3.4204	3.4408	3.4715	3.5126	3.5644	3.6269	3.7004	3.7852	3.8817
222.00	3.2973	3.3121	3.3315	3.3607	3.3998	3.4488	3.5081	3.5779	3.6582	3.7496
224.30	3.2728	3.2875	3.3067	3.3355	3.3741	3.4226	3.4811	3.5500	3.6294	3.7196
235.00	3.1719	3.1859	3.2041	3.2316	3.2683	3.3144	3.3700	3.4354	3.5107	3.5963
248.00	3.0725	3.0858	3.1032	3.1292	3.1641	3.2079	3.2607	3.3227	3.3942	3.4752
266.00	2.9651	2.9777	2.9941	3.0187	3.0517	3.0930	3.1429	3.2014	3.2687	3.3450
275.36	2.9196	2.9319	2.9479	2.9719	3.0041	3.0444	3.0930	3.1501	3.2157	3.2900
285.00	2.8785	2.8906	2.9062	2.9297	2.9611	3.0005	3.0480	3.1037	3.1678	3.2404
308.00	2.7987	2.8103	2.8252	2.8477	2.8777	2.9154	2.9608	3.0140	3.0752	3.1444
325.00	2.7523	2.7635	2.7781	2.8000	2.8292	2.8659	2.9101	2.9618	3.0214	3.0887
334.24	2.7305	2.7416	2.7559	2.7775	2.8064	2.8426	2.8862	2.9374	2.9961	3.0626
337.10	2.7242	2.7352	2.7495	2.7710	2.7998	2.8359	2.8793	2.9303	2.9888	3.0550
347.00	2.7036	2.7145	2.7287	2.7499	2.7784	2.8140	2.8569	2.9072	2.9650	3.0304
351.00	2.6959	2.7067	2.7208	2.7420	2.7703	2.8058	2.8485	2.8986	2.9561	3.0211
355.00	2.6884	2.6993	2.7133	2.7344	2.7625	2.7979	2.8404	2.8902	2.9475	3.0122
385.15	2.6406	2.6511	2.6647	2.6852	2.7126	2.7469	2.7882	2.8366	2.8922	2.9550
407.90	2.6120	2.6224	2.6358	2.6559	2.6828	2.7165	2.7571	2.8047	2.8593	2.9210
416.10	2.6030	2.6133	2.6266	2.6466	2.6734	2.7069	2.7473	2.7946	2.8489	2.9102
435.96	2.5834	2.5935	2.6067	2.6265	2.6529	2.6861	2.7259	2.7726	2.8262	2.8868
441.60	2.5783	2.5884	2.6016	2.6213	2.6477	2.6807	2.7204	2.7670	2.8204	2.8808
457.90	2.5648	2.5749	2.5879	2.6075	2.6336	2.6664	2.7058	2.7520	2.8049	2.8648
488.00	2.5437	2.5536	2.5664	2.5858	2.6116	2.6439	2.6828	2.7283	2.7806	2.8396
514.50	2.5282	2.5381	2.5508	2.5699	2.5955	2.6275	2.6660	2.7111	2.7628	2.8213
532.00	2.5194	2.5291	2.5418	2.5608	2.5862	2.6181	2.6564	2.7012	2.7526	2.8107
546.23	2.5128	2.5225	2.5351	2.5541	2.5794	2.6111	2.6492	2.6939	2.7451	2.8030
563.20	2.5057	2.5153	2.5279	2.5468	2.5719	2.6035	2.6415	2.6859	2.7369	2.7945
594.10	2.4943	2.5039	2.5163	2.5351	2.5601	2.5914	2.6291	2.6732	2.7238	2.7810
611.90	2.4885	2.4981	2.5105	2.5292	2.5541	2.5853	2.6228	2.6668	2.7172	2.7741
632.80	2.4824	2.4919	2.5043	2.5229	2.5477	2.5788	2.6162	2.6600	2.7102	2.7669
647.10	2.4785	2.4881	2.5004	2.5189	2.5437	2.5747	2.6120	2.6557	2.7058	2.7623
670.00	2.4729	2.4824	2.4947	2.5132	2.5378	2.5687	2.6059	2.6494	2.6993	2.7556
694.30	2.4676	2.4770	2.4893	2.5077	2.5323	2.5631	2.6001	2.6435	2.6932	2.7493
725.00	2.4616	2.4710	2.4832	2.5016	2.5260	2.5567	2.5936	2.6368	2.6863	2.7422
754.00	2.4566	2.4660	2.4782	2.4965	2.5209	2.5514	2.5882	2.6313	2.6806	2.7363
785.00	2.4519	2.4613	2.4734	2.4916	2.5160	2.5465	2.5831	2.6260	2.6752	2.7308
800.00	2.4498	2.4592	2.4713	2.4895	2.5138	2.5443	2.5809	2.6237	2.6729	2.7283
836.00	2.4453	2.4547	2.4667	2.4849	2.5091	2.5395	2.5760	2.6187	2.6677	2.7230
876.00	2.4410	2.4503	2.4623	2.4804	2.5046	2.5348	2.5712	2.6138	2.6627	2.7178
904.00	2.4382	2.4475	2.4596	2.4776	2.5017	2.5320	2.5683	2.6108	2.6596	2.7146
911.28	2.4376	2.4469	2.4589	2.4769	2.5011	2.5312	2.5676	2.6101	2.6588	2.7138
946.00	2.4346	2.4439	2.4559	2.4739	2.4980	2.5281	2.5644	2.6068	2.6554	2.7103
975.00	2.4324	2.4417	2.4536	2.4716	2.4957	2.5258	2.5620	2.6043	2.6529	2.7077
1000.00	2.4306	2.4399	2.4519	2.4698	2.4938	2.5239	2.5600	2.6023	2.6508	2.7056
1064.00	2.4267	2.4359	2.4479	2.4658	2.4897	2.5197	2.5558	2.5980	2.6463	2.7009
1106.00	2.4245	2.4337	2.4456	2.4635	2.4874	2.5173	2.5534	2.5955	2.6438	2.6983
1152.00	2.4223	2.4315	2.4434	2.4613	2.4852	2.5151	2.5510	2.5931	2.6413	2.6958
1185.00	2.4209	2.4301	2.4420	2.4599	2.4837	2.5136	2.5495	2.5915	2.6397	2.6941
1225.00	2.4194	2.4286	2.4404	2.4583	2.4821	2.5119	2.5478	2.5898	2.6380	2.6923
1275.00	2.4177	2.4268	2.4387	2.4565	2.4803	2.5101	2.5460	2.5879	2.6360	2.6902
1320.00	2.4163	2.4254	2.4373	2.4551	2.4789	2.5087	2.5445	2.5864	2.6344	2.6886
Static	2.3972	2.4062	2.4179	2.4355	2.4590	2.4884	2.5238	2.5651	2.6125	2.6660

TABLE T12. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of HD for v=2.

λ(nm)	$\langle\gamma\rangle_{20,20}$	$\langle\gamma\rangle_{20,22}$	$\langle\gamma\rangle_{21,23}$	$\langle\gamma\rangle_{22,24}$	$\langle\gamma\rangle_{23,25}$	$\langle\gamma\rangle_{24,26}$	$\langle\gamma\rangle_{25,27}$	$\langle\gamma\rangle_{26,28}$	$\langle\gamma\rangle_{27,29}$	$\langle\gamma\rangle_{28,2\,10}$
182.26	5.1149	5.1398	5.1720	5.2205	5.2857	5.3679	5.4676	5.5854	5.7220	5.8783
193.00	4.7176	4.7394	4.7675	4.8099	4.8667	4.9382	5.0249	5.1271	5.2454	5.3803
213.00	4.2274	4.2456	4.2690	4.3042	4.3514	4.4107	4.4824	4.5668	4.6643	4.7752
222.00	4.0716	4.0887	4.1107	4.1437	4.1880	4.2437	4.3109	4.3900	4.4813	4.5850
224.30	4.0363	4.0532	4.0749	4.1074	4.1511	4.2059	4.2722	4.3501	4.4400	4.5421
235.00	3.8918	3.9078	3.9281	3.9588	3.9998	4.0514	4.1137	4.1868	4.2711	4.3669
248.00	3.7508	3.7658	3.7850	3.8138	3.8524	3.9008	3.9593	4.0279	4.1070	4.1966
266.00	3.5999	3.6139	3.6318	3.6587	3.6947	3.7399	3.7944	3.8584	3.9320	4.0154
275.36	3.5364	3.5500	3.5674	3.5935	3.6284	3.6723	3.7252	3.7872	3.8586	3.9394
285.00	3.4792	3.4925	3.5094	3.5348	3.5688	3.6115	3.6630	3.7233	3.7927	3.8712
308.00	3.3689	3.3815	3.3976	3.4217	3.4539	3.4943	3.5430	3.6001	3.6657	3.7400
325.00	3.3051	3.3173	3.3328	3.3562	3.3874	3.4265	3.4737	3.5289	3.5924	3.6642
334.24	3.2752	3.2872	3.3025	3.3255	3.3563	3.3948	3.4412	3.4956	3.5581	3.6288
337.10	3.2665	3.2785	3.2937	3.3166	3.3472	3.3856	3.4318	3.4860	3.5482	3.6185
347.00	3.2384	3.2503	3.2653	3.2879	3.3180	3.3558	3.4014	3.4547	3.5160	3.5853
351.00	3.2279	3.2396	3.2546	3.2770	3.3070	3.3446	3.3899	3.4430	3.5039	3.5728
355.00	3.2177	3.2294	3.2443	3.2666	3.2965	3.3339	3.3789	3.4317	3.4923	3.5608
385.15	3.1526	3.1639	3.1783	3.1999	3.2287	3.2649	3.3084	3.3593	3.4178	3.4840
407.90	3.1139	3.1250	3.1390	3.1602	3.1884	3.2238	3.2665	3.3164	3.3736	3.4383
416.10	3.1017	3.1127	3.1267	3.1477	3.1757	3.2109	3.2532	3.3028	3.3597	3.4239
435.96	3.0751	3.0860	3.0998	3.1205	3.1481	3.1828	3.2245	3.2734	3.3294	3.3927
441.60	3.0683	3.0791	3.0929	3.1135	3.1411	3.1756	3.2172	3.2658	3.3217	3.3847
457.90	3.0501	3.0609	3.0745	3.0949	3.1222	3.1564	3.1975	3.2457	3.3009	3.3634
488.00	3.0216	3.0322	3.0456	3.0657	3.0925	3.1262	3.1667	3.2141	3.2685	3.3299
514.50	3.0009	3.0113	3.0245	3.0444	3.0710	3.1043	3.1443	3.1912	3.2449	3.3055
532.00	2.9889	2.9993	3.0125	3.0322	3.0586	3.0917	3.1314	3.1780	3.2313	3.2916
546.23	2.9801	2.9905	3.0036	3.0232	3.0495	3.0823	3.1219	3.1682	3.2213	3.2812
563.20	2.9706	2.9808	2.9938	3.0134	3.0395	3.0722	3.1116	3.1576	3.2104	3.2700
594.10	2.9553	2.9655	2.9784	2.9978	3.0236	3.0561	3.0951	3.1407	3.1931	3.2521
611.90	2.9476	2.9577	2.9706	2.9899	3.0156	3.0479	3.0868	3.1322	3.1843	3.2431
632.80	2.9394	2.9495	2.9623	2.9815	3.0071	3.0393	3.0779	3.1231	3.1750	3.2335
647.10	2.9342	2.9443	2.9571	2.9762	3.0018	3.0338	3.0724	3.1175	3.1692	3.2275
670.00	2.9267	2.9367	2.9494	2.9685	2.9940	3.0259	3.0643	3.1092	3.1606	3.2187
694.30	2.9196	2.9295	2.9422	2.9612	2.9866	3.0183	3.0566	3.1013	3.1525	3.2103
725.00	2.9116	2.9215	2.9341	2.9530	2.9783	3.0099	3.0479	3.0924	3.1434	3.2010
754.00	2.9049	2.9148	2.9274	2.9462	2.9714	3.0029	3.0408	3.0851	3.1359	3.1932
785.00	2.8987	2.9085	2.9210	2.9398	2.9649	2.9963	3.0340	3.0782	3.1288	3.1859
800.00	2.8959	2.9058	2.9182	2.9370	2.9620	2.9933	3.0310	3.0751	3.1257	3.1827
836.00	2.8899	2.8997	2.9121	2.9308	2.9557	2.9870	3.0245	3.0685	3.1188	3.1756
876.00	2.8840	2.8938	2.9062	2.9248	2.9497	2.9808	3.0183	3.0621	3.1122	3.1688
904.00	2.8804	2.8902	2.9026	2.9211	2.9460	2.9770	3.0144	3.0581	3.1081	3.1646
911.28	2.8795	2.8893	2.9017	2.9202	2.9450	2.9761	3.0134	3.0571	3.1071	3.1636
946.00	2.8756	2.8854	2.8977	2.9162	2.9410	2.9719	3.0092	3.0527	3.1027	3.1590
975.00	2.8726	2.8824	2.8947	2.9132	2.9379	2.9688	3.0060	3.0495	3.0993	3.1555
1000.00	2.8703	2.8800	2.8923	2.9108	2.9354	2.9663	3.0035	3.0469	3.0967	3.1528
1064.00	2.8650	2.8747	2.8870	2.9054	2.9300	2.9608	2.9978	3.0411	3.0907	3.1467
1106.00	2.8621	2.8718	2.8840	2.9024	2.9269	2.9576	2.9946	3.0378	3.0873	3.1432
1152.00	2.8592	2.8689	2.8811	2.8994	2.9239	2.9546	2.9915	3.0347	3.0841	3.1399
1185.00	2.8574	2.8670	2.8792	2.8975	2.9220	2.9527	2.9895	3.0326	3.0820	3.1377
1225.00	2.8553	2.8650	2.8771	2.8955	2.9199	2.9505	2.9873	3.0304	3.0797	3.1353
1275.00	2.8530	2.8626	2.8748	2.8931	2.9175	2.9481	2.9848	3.0278	3.0771	3.1326
1320.00	2.8512	2.8608	2.8730	2.8912	2.9156	2.9462	2.9829	3.0258	3.0750	3.1305
Static	2.8258	2.8353	2.8473	2.8653	2.8893	2.9194	2.9555	2.9978	3.0463	3.1009

TABLE T13. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of D_2 for v=0.

λ(nm)	$\langle\gamma\rangle_{00,00}$	$\langle\gamma\rangle_{00,02}$	$\langle\gamma\rangle_{01,03}$	$\langle\gamma\rangle_{02,04}$	$\langle\gamma\rangle_{03,05}$	$\langle\gamma\rangle_{04,06}$	$\langle\gamma\rangle_{05,07}$	$\langle\gamma\rangle_{06,08}$	$\langle\gamma\rangle_{07,09}$	$\langle\gamma\rangle_{08,0\,10}$
182.26	3.0053	3.0160	3.0301	3.0514	3.0799	3.1157	3.1589	3.2096	3.2680	3.3344
193.00	2.8470	2.8568	2.8698	2.8894	2.9156	2.9485	2.9882	3.0347	3.0883	3.1491
213.00	2.6400	2.6488	2.6604	2.6778	2.7011	2.7304	2.7656	2.8070	2.8546	2.9084
222.00	2.5714	2.5798	2.5909	2.6077	2.6301	2.6582	2.6920	2.7317	2.7773	2.8290
224.30	2.5556	2.5640	2.5750	2.5916	2.6138	2.6416	2.6752	2.7145	2.7597	2.8108
235.00	2.4904	2.4984	2.5090	2.5250	2.5463	2.5730	2.6053	2.6430	2.6864	2.7355
248.00	2.4254	2.4331	2.4433	2.4586	2.4791	2.5048	2.5357	2.5719	2.6135	2.6606
266.00	2.3545	2.3618	2.3716	2.3862	2.4058	2.4303	2.4599	2.4945	2.5342	2.5791
275.36	2.3241	2.3314	2.3409	2.3553	2.3745	2.3985	2.4275	2.4614	2.5003	2.5443
285.00	2.2966	2.3037	2.3131	2.3272	2.3461	2.3697	2.3981	2.4314	2.4696	2.5128
308.00	2.2429	2.2498	2.2588	2.2725	2.2906	2.3134	2.3408	2.3729	2.4097	2.4513
325.00	2.2115	2.2182	2.2270	2.2404	2.2582	2.2805	2.3073	2.3387	2.3747	2.4154
334.24	2.1966	2.2033	2.2120	2.2252	2.2428	2.2649	2.2915	2.3225	2.3582	2.3984
337.10	2.1923	2.1989	2.2077	2.2208	2.2384	2.2604	2.2869	2.3178	2.3534	2.3935
347.00	2.1783	2.1849	2.1935	2.2066	2.2239	2.2457	2.2719	2.3026	2.3378	2.3775
351.00	2.1730	2.1796	2.1882	2.2012	2.2185	2.2402	2.2663	2.2969	2.3319	2.3715
355.00	2.1679	2.1744	2.1831	2.1960	2.2133	2.2349	2.2609	2.2913	2.3263	2.3657
385.15	2.1351	2.1415	2.1499	2.1625	2.1794	2.2005	2.2259	2.2557	2.2898	2.3283
407.90	2.1155	2.1217	2.1300	2.1425	2.1591	2.1800	2.2050	2.2343	2.2679	2.3059
416.10	2.1092	2.1155	2.1237	2.1361	2.1527	2.1734	2.1984	2.2276	2.2610	2.2988
435.96	2.0957	2.1019	2.1100	2.1223	2.1387	2.1593	2.1840	2.2129	2.2460	2.2834
441.60	2.0922	2.0983	2.1065	2.1188	2.1351	2.1556	2.1802	2.2091	2.2421	2.2794
457.90	2.0828	2.0890	2.0971	2.1092	2.1255	2.1458	2.1703	2.1989	2.2317	2.2688
488.00	2.0682	2.0742	2.0822	2.0943	2.1104	2.1305	2.1547	2.1830	2.2155	2.2521
514.50	2.0574	2.0635	2.0714	2.0834	2.0993	2.1193	2.1433	2.1714	2.2036	2.2399
532.00	2.0513	2.0572	2.0652	2.0771	2.0929	2.1128	2.1367	2.1647	2.1967	2.2329
546.23	2.0467	2.0527	2.0606	2.0724	2.0882	2.1081	2.1319	2.1597	2.1917	2.2277
563.20	2.0417	2.0477	2.0555	2.0673	2.0831	2.1028	2.1266	2.1543	2.1861	2.2220
594.10	2.0338	2.0397	2.0475	2.0592	2.0749	2.0945	2.1181	2.1457	2.1773	2.2130
611.90	2.0297	2.0356	2.0434	2.0551	2.0708	2.0903	2.1139	2.1414	2.1729	2.2084
632.80	2.0255	2.0313	2.0391	2.0508	2.0664	2.0859	2.1093	2.1367	2.1681	2.2036
647.10	2.0228	2.0286	2.0364	2.0480	2.0636	2.0831	2.1065	2.1338	2.1652	2.2005
670.00	2.0188	2.0247	2.0324	2.0440	2.0595	2.0789	2.1023	2.1296	2.1608	2.1961
694.30	2.0151	2.0209	2.0286	2.0402	2.0557	2.0750	2.0983	2.1255	2.1567	2.1918
725.00	2.0109	2.0167	2.0244	2.0360	2.0514	2.0707	2.0938	2.1210	2.1520	2.1871
754.00	2.0074	2.0132	2.0209	2.0324	2.0478	2.0670	2.0901	2.1172	2.1482	2.1831
785.00	2.0041	2.0099	2.0176	2.0291	2.0444	2.0636	2.0867	2.1136	2.1445	2.1794
800.00	2.0027	2.0085	2.0161	2.0276	2.0429	2.0621	2.0851	2.1120	2.1429	2.1777
836.00	1.9995	2.0053	2.0129	2.0243	2.0396	2.0587	2.0817	2.1086	2.1394	2.1741
876.00	1.9964	2.0022	2.0098	2.0212	2.0365	2.0555	2.0785	2.1053	2.1360	2.1707
904.00	1.9945	2.0003	2.0079	2.0193	2.0345	2.0536	2.0765	2.1032	2.1339	2.1685
911.28	1.9941	1.9998	2.0074	2.0188	2.0340	2.0531	2.0760	2.1027	2.1334	2.1680
946.00	1.9920	1.9977	2.0053	2.0167	2.0319	2.0509	2.0738	2.1005	2.1311	2.1656
975.00	1.9904	1.9962	2.0037	2.0151	2.0303	2.0493	2.0721	2.0988	2.1294	2.1639
1000.00	1.9892	1.9949	2.0025	2.0138	2.0290	2.0480	2.0708	2.0974	2.1280	2.1625
1064.00	1.9864	1.9921	1.9997	2.0110	2.0261	2.0451	2.0678	2.0944	2.1249	2.1593
1106.00	1.9849	1.9906	1.9981	2.0094	2.0245	2.0434	2.0662	2.0928	2.1232	2.1575
1152.00	1.9833	1.9890	1.9966	2.0079	2.0230	2.0419	2.0646	2.0911	2.1215	2.1558
1185.00	1.9824	1.9881	1.9956	2.0069	2.0220	2.0408	2.0635	2.0901	2.1204	2.1547
1225.00	1.9813	1.9870	1.9945	2.0058	2.0208	2.0397	2.0624	2.0889	2.1192	2.1535
1275.00	1.9801	1.9858	1.9933	2.0045	2.0196	2.0384	2.0611	2.0876	2.1179	2.1521
1320.00	1.9791	1.9848	1.9923	2.0036	2.0186	2.0374	2.0601	2.0865	2.1168	2.1510
Static	1.9656	1.9713	1.9787	1.9898	2.0047	2.0234	2.0458	2.0719	2.1019	2.1358

TABLE T14. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of D_2 for v=1.

λ(nm)	$\langle\gamma\rangle_{10,10}$	$\langle\gamma\rangle_{10,12}$	$\langle\gamma\rangle_{11,13}$	$\langle\gamma\rangle_{12,14}$	$\langle\gamma\rangle_{13,15}$	$\langle\gamma\rangle_{14,16}$	$\langle\gamma\rangle_{15,17}$	$\langle\gamma\rangle_{16,18}$	$\langle\gamma\rangle_{17,19}$	$\langle\gamma\rangle_{18,1\,10}$
182.26	3.7238	3.7365	3.7531	3.7782	3.8117	3.8538	3.9047	3.9646	4.0335	4.1119
193.00	3.4929	3.5044	3.5195	3.5421	3.5724	3.6104	3.6562	3.7101	3.7722	3.8426
213.00	3.1977	3.2077	3.2208	3.2405	3.2668	3.2998	3.3396	3.3863	3.4399	3.5008
222.00	3.1015	3.1110	3.1235	3.1422	3.1673	3.1987	3.2366	3.2810	3.3321	3.3899
224.30	3.0795	3.0889	3.1013	3.1198	3.1446	3.1756	3.2131	3.2570	3.3075	3.3647
235.00	2.9888	2.9978	3.0096	3.0273	3.0509	3.0805	3.1162	3.1581	3.2062	3.2606
248.00	2.8992	2.9078	2.9190	2.9359	2.9584	2.9866	3.0207	3.0605	3.1063	3.1581
266.00	2.8022	2.8103	2.8209	2.8369	2.8583	2.8850	2.9172	2.9550	2.9983	3.0473
275.36	2.7610	2.7689	2.7793	2.7949	2.8158	2.8419	2.8734	2.9102	2.9525	3.0003
285.00	2.7237	2.7315	2.7417	2.7569	2.7774	2.8029	2.8337	2.8698	2.9112	2.9579
308.00	2.6512	2.6587	2.6685	2.6831	2.7027	2.7272	2.7567	2.7912	2.8309	2.8756
325.00	2.6090	2.6163	2.6258	2.6401	2.6592	2.6831	2.7118	2.7455	2.7841	2.8277
334.24	2.5891	2.5963	2.6057	2.6198	2.6387	2.6623	2.6907	2.7240	2.7621	2.8052
337.10	2.5834	2.5905	2.5999	2.6140	2.6328	2.6563	2.6846	2.7177	2.7557	2.7987
347.00	2.5646	2.5717	2.5810	2.5949	2.6135	2.6368	2.6647	2.6975	2.7351	2.7775
351.00	2.5576	2.5647	2.5739	2.5877	2.6062	2.6294	2.6573	2.6899	2.7273	2.7695
355.00	2.5508	2.5579	2.5670	2.5808	2.5993	2.6223	2.6501	2.6825	2.7198	2.7618
385.15	2.5071	2.5140	2.5229	2.5364	2.5543	2.5767	2.6037	2.6353	2.6715	2.7124
407.90	2.4811	2.4878	2.4966	2.5098	2.5274	2.5495	2.5761	2.6072	2.6428	2.6830
416.10	2.4728	2.4795	2.4883	2.5014	2.5189	2.5409	2.5673	2.5982	2.6337	2.6736
435.96	2.4549	2.4615	2.4701	2.4831	2.5005	2.5222	2.5483	2.5789	2.6139	2.6534
441.60	2.4502	2.4569	2.4655	2.4784	2.4957	2.5174	2.5434	2.5739	2.6088	2.6482
457.90	2.4379	2.4445	2.4530	2.4659	2.4831	2.5045	2.5304	2.5606	2.5952	2.6343
488.00	2.4185	2.4250	2.4335	2.4462	2.4631	2.4843	2.5099	2.5397	2.5739	2.6125
514.50	2.4044	2.4108	2.4192	2.4318	2.4486	2.4696	2.4949	2.5244	2.5583	2.5965
532.00	2.3963	2.4027	2.4110	2.4235	2.4402	2.4611	2.4863	2.5157	2.5494	2.5874
546.23	2.3903	2.3966	2.4050	2.4174	2.4340	2.4549	2.4799	2.5092	2.5428	2.5806
563.20	2.3837	2.3901	2.3983	2.4108	2.4273	2.4481	2.4730	2.5021	2.5355	2.5732
594.10	2.3733	2.3796	2.3878	2.4001	2.4166	2.4372	2.4619	2.4909	2.5241	2.5615
611.90	2.3680	2.3743	2.3825	2.3948	2.4111	2.4317	2.4563	2.4852	2.5182	2.5555
632.80	2.3624	2.3686	2.3768	2.3890	2.4054	2.4258	2.4504	2.4791	2.5121	2.5492
647.10	2.3589	2.3651	2.3732	2.3855	2.4018	2.4222	2.4467	2.4754	2.5082	2.5453
670.00	2.3537	2.3599	2.3680	2.3802	2.3964	2.4168	2.4412	2.4698	2.5025	2.5395
694.30	2.3488	2.3550	2.3631	2.3752	2.3914	2.4117	2.4360	2.4645	2.4971	2.5339
725.00	2.3433	2.3495	2.3576	2.3696	2.3858	2.4060	2.4302	2.4586	2.4911	2.5278
754.00	2.3388	2.3449	2.3530	2.3650	2.3811	2.4012	2.4254	2.4537	2.4861	2.5226
785.00	2.3345	2.3406	2.3486	2.3606	2.3766	2.3967	2.4208	2.4490	2.4814	2.5178
800.00	2.3326	2.3387	2.3467	2.3587	2.3747	2.3947	2.4188	2.4470	2.4793	2.5157
836.00	2.3284	2.3345	2.3425	2.3545	2.3704	2.3904	2.4144	2.4425	2.4747	2.5110
876.00	2.3244	2.3305	2.3384	2.3504	2.3663	2.3862	2.4102	2.4382	2.4703	2.5065
904.00	2.3219	2.3280	2.3359	2.3478	2.3637	2.3837	2.4076	2.4355	2.4676	2.5037
911.28	2.3213	2.3274	2.3353	2.3472	2.3631	2.3830	2.4069	2.4349	2.4669	2.5030
946.00	2.3186	2.3247	2.3326	2.3445	2.3603	2.3802	2.4041	2.4320	2.4639	2.5000
975.00	2.3165	2.3226	2.3305	2.3424	2.3582	2.3781	2.4019	2.4298	2.4617	2.4977
1000.00	2.3149	2.3210	2.3289	2.3407	2.3566	2.3764	2.4002	2.4280	2.4599	2.4958
1064.00	2.3113	2.3174	2.3252	2.3371	2.3528	2.3726	2.3964	2.4241	2.4559	2.4918
1106.00	2.3093	2.3153	2.3232	2.3350	2.3508	2.3705	2.3942	2.4219	2.4537	2.4895
1152.00	2.3073	2.3133	2.3212	2.3330	2.3487	2.3684	2.3921	2.4198	2.4515	2.4873
1185.00	2.3060	2.3120	2.3199	2.3317	2.3474	2.3671	2.3908	2.4184	2.4501	2.4858
1225.00	2.3046	2.3106	2.3185	2.3302	2.3459	2.3656	2.3893	2.4169	2.4485	2.4842
1275.00	2.3030	2.3090	2.3169	2.3286	2.3443	2.3640	2.3876	2.4152	2.4468	2.4825
1320.00	2.3017	2.3078	2.3156	2.3273	2.3430	2.3627	2.3863	2.4138	2.4454	2.4810
Static	2.2842	2.2901	2.2979	2.3095	2.3250	2.3444	2.3677	2.3949	2.4261	2.4613

TABLE T15. Polarizability anisotropy matrix elements $\langle\gamma\rangle_{vJ,v'J'} \equiv \langle\psi_{v,J}|\gamma|\psi_{v',J'}\rangle$ of D_2 for v=2.

λ(nm)	$\langle\gamma\rangle_{20,20}$	$\langle\gamma\rangle_{20,22}$	$\langle\gamma\rangle_{21,23}$	$\langle\gamma\rangle_{22,24}$	$\langle\gamma\rangle_{23,25}$	$\langle\gamma\rangle_{24,26}$	$\langle\gamma\rangle_{25,27}$	$\langle\gamma\rangle_{26,28}$	$\langle\gamma\rangle_{27,29}$	$\langle\gamma\rangle_{28,2\,10}$
182.26	4.5704	4.5855	4.6050	4.6345	4.6740	4.7236	4.7835	4.8541	4.9354	5.0279
193.00	4.2424	4.2558	4.2731	4.2992	4.3341	4.3779	4.4308	4.4929	4.5646	4.6459
213.00	3.8322	3.8436	3.8582	3.8803	3.9098	3.9468	3.9914	4.0438	4.1041	4.1724
222.00	3.7006	3.7113	3.7252	3.7460	3.7738	3.8088	3.8509	3.9003	3.9571	4.0215
224.30	3.6707	3.6813	3.6950	3.7155	3.7430	3.7775	3.8190	3.8678	3.9238	3.9873
235.00	3.5479	3.5580	3.5709	3.5904	3.6163	3.6489	3.6882	3.7343	3.7872	3.8471
248.00	3.4276	3.4370	3.4493	3.4677	3.4922	3.5230	3.5601	3.6036	3.6535	3.7100
266.00	3.2981	3.3071	3.3186	3.3358	3.3589	3.3878	3.4226	3.4634	3.5102	3.5631
275.36	3.2435	3.2522	3.2634	3.2802	3.3026	3.3308	3.3646	3.4043	3.4498	3.5013
285.00	3.1943	3.2027	3.2137	3.2300	3.2519	3.2794	3.3124	3.3511	3.3954	3.4456
308.00	3.0990	3.1070	3.1174	3.1330	3.1539	3.1800	3.2114	3.2482	3.2904	3.3380
325.00	3.0436	3.0515	3.0616	3.0767	3.0970	3.1223	3.1528	3.1885	3.2295	3.2757
334.24	3.0177	3.0255	3.0354	3.0503	3.0703	3.0953	3.1254	3.1606	3.2009	3.2465
337.10	3.0102	3.0179	3.0278	3.0427	3.0626	3.0875	3.1174	3.1525	3.1927	3.2380
347.00	2.9858	2.9934	3.0032	3.0179	3.0375	3.0621	3.0916	3.1262	3.1658	3.2106
351.00	2.9766	2.9842	2.9939	3.0085	3.0281	3.0525	3.0819	3.1163	3.1558	3.2003
355.00	2.9678	2.9753	2.9850	2.9996	3.0190	3.0433	3.0726	3.1068	3.1461	3.1904
385.15	2.9111	2.9184	2.9278	2.9419	2.9607	2.9843	3.0126	3.0458	3.0838	3.1267
407.90	2.8773	2.8845	2.8937	2.9075	2.9260	2.9491	2.9770	3.0095	3.0468	3.0888
416.10	2.8666	2.8738	2.8829	2.8967	2.9150	2.9380	2.9657	2.9980	3.0351	3.0769
435.96	2.8435	2.8505	2.8596	2.8731	2.8913	2.9139	2.9412	2.9731	3.0097	3.0509
441.60	2.8375	2.8445	2.8536	2.8671	2.8851	2.9077	2.9349	2.9667	3.0031	3.0443
457.90	2.8216	2.8286	2.8375	2.8509	2.8688	2.8912	2.9181	2.9496	2.9857	3.0265
488.00	2.7967	2.8036	2.8124	2.8256	2.8432	2.8653	2.8918	2.9229	2.9584	2.9986
514.50	2.7785	2.7853	2.7940	2.8071	2.8245	2.8464	2.8727	2.9034	2.9385	2.9782
532.00	2.7681	2.7748	2.7835	2.7965	2.8138	2.8355	2.8616	2.8922	2.9271	2.9666
546.23	2.7604	2.7671	2.7757	2.7886	2.8059	2.8275	2.8535	2.8839	2.9187	2.9579
563.20	2.7520	2.7587	2.7672	2.7801	2.7973	2.8188	2.8446	2.8749	2.9095	2.9485
594.10	2.7386	2.7452	2.7537	2.7665	2.7835	2.8049	2.8305	2.8605	2.8948	2.9336
611.90	2.7318	2.7384	2.7469	2.7596	2.7766	2.7978	2.8234	2.8532	2.8875	2.9260
632.80	2.7246	2.7312	2.7396	2.7523	2.7692	2.7904	2.8158	2.8455	2.8796	2.9180
647.10	2.7201	2.7267	2.7351	2.7477	2.7646	2.7857	2.8110	2.8407	2.8747	2.9130
670.00	2.7135	2.7201	2.7284	2.7410	2.7578	2.7788	2.8041	2.8336	2.8674	2.9056
694.30	2.7072	2.7138	2.7221	2.7346	2.7514	2.7723	2.7975	2.8269	2.8606	2.8986
725.00	2.7002	2.7067	2.7150	2.7275	2.7442	2.7650	2.7901	2.8194	2.8529	2.8908
754.00	2.6944	2.7009	2.7092	2.7216	2.7382	2.7590	2.7839	2.8131	2.8466	2.8843
785.00	2.6889	2.6953	2.7036	2.7160	2.7325	2.7532	2.7781	2.8072	2.8405	2.8781
800.00	2.6865	2.6929	2.7011	2.7135	2.7300	2.7507	2.7756	2.8046	2.8379	2.8754
836.00	2.6812	2.6876	2.6958	2.7081	2.7246	2.7452	2.7700	2.7989	2.8321	2.8695
876.00	2.6760	2.6824	2.6906	2.7029	2.7194	2.7399	2.7646	2.7935	2.8265	2.8638
904.00	2.6729	2.6793	2.6874	2.6997	2.7161	2.7366	2.7612	2.7901	2.8230	2.8602
911.28	2.6721	2.6785	2.6867	2.6989	2.7153	2.7358	2.7604	2.7892	2.8222	2.8594
946.00	2.6686	2.6750	2.6832	2.6954	2.7117	2.7322	2.7568	2.7855	2.8184	2.8555
975.00	2.6660	2.6724	2.6805	2.6928	2.7091	2.7295	2.7540	2.7827	2.8156	2.8526
1000.00	2.6640	2.6703	2.6785	2.6907	2.7070	2.7274	2.7519	2.7805	2.8133	2.8503
1064.00	2.6593	2.6657	2.6738	2.6860	2.7022	2.7226	2.7470	2.7756	2.8083	2.8452
1106.00	2.6567	2.6631	2.6712	2.6833	2.6995	2.7199	2.7443	2.7728	2.8054	2.8423
1152.00	2.6542	2.6605	2.6686	2.6808	2.6970	2.7172	2.7416	2.7701	2.8027	2.8394
1185.00	2.6526	2.6589	2.6670	2.6791	2.6953	2.7155	2.7399	2.7683	2.8009	2.8376
1225.00	2.6508	2.6571	2.6652	2.6773	2.6934	2.7137	2.7380	2.7664	2.7989	2.8356
1275.00	2.6488	2.6551	2.6631	2.6752	2.6914	2.7116	2.7359	2.7642	2.7967	2.8334
1320.00	2.6472	2.6535	2.6615	2.6736	2.6897	2.7099	2.7342	2.7625	2.7950	2.8316
Static	2.6248	2.6310	2.6390	2.6509	2.6668	2.6867	2.7106	2.7386	2.7706	2.8067

TABLE T16. Conversion factors for polarizability.

Atomic units[a]		Conversion factor	Resulting units
$1\ e^2a_0^2E_h^{-1}$	$\rightarrow$	$1.648\,777\,254 \times 10^{-41}$	$C^2m^2J^{-1}$
$1\ e^2a_0^2E_h^{-1}$	$\rightarrow$	$1.481\,847\,096 \times 10^{-1}$	$Å^3$
$1\ e^2a_0^2E_h^{-1}$	$\rightarrow$	$1.481\,847\,096 \times 10^{-25}$	cm^3

[a] With the factor of $1/4\pi\epsilon_0$ incorporated.

S3. Static polarizability components and invariants for H_2 at selected distances

TABLE T17. Static polarizability components and invariants for H_2, HD and D_2 at selected distances obtained from linear response procedures with CCSD method and a composite basis: aug-mcc-pV6Z+5×BF(8s6p)basis set. These results were obtained using the cutoff for linear dependence of AOs as 1.0 $\times 10^{-6}$, the convergence criteria for SCF energy gradient set to 1.0 $\times 10^{-11}$ a.u., CC energy convergence criteria of 1.0 $\times 10^{-9}$ a.u. and response solutions convergence criteria of 1.0 $\times 10^{-7}$ a.u.

r	$\alpha_\perp$	$\alpha_\parallel$	$\bar{\alpha}$	γ
0.5	2.062 408 7	2.197 581 2	2.107 466 2	0.135 172 5
0.6	2.285 903 8	2.494 674 5	2.355 494 0	0.208 770 7
0.7	2.527 715 7	2.832 014 5	2.629 148 6	0.304 298 8
0.8	2.785 790 1	3.210 424 6	2.927 334 9	0.424 634 5
0.9	3.058 315 2	3.630 936 6	3.249 189 0	0.572 621 4
1.0	3.343 620 7	4.094 559 1	3.593 933 5	0.750 938 4
1.1	3.640 107 1	4.602 054 0	3.960 756 1	0.961 946 9
1.2	3.946 050 6	5.153 830 7	4.348 644 0	1.207 780 1
1.3	4.259 757 2	5.749 774 1	4.756 429 5	1.490 016 9
1.4	4.579 413 2	6.389 121 8	5.182 649 4	1.809 708 6
1.5	4.903 176 6	7.070 300 2	5.625 551 1	2.167 123 6
1.6	5.229 102 7	7.790 806 0	6.083 003 8	2.561 703 3
1.7	5.555 137 9	8.547 074 3	6.552 450 0	2.991 936 4
1.8	5.879 189 0	9.334 315 4	7.030 897 8	3.455 126 4
1.9	6.199 123 3	10.146 415 0	7.514 887 2	3.947 291 7
2.0	6.512 695 8	10.975 978 0	8.000 456 5	4.463 282 2
2.1	6.817 707 4	11.814 141 0	8.483 185 3	4.996 433 6
2.2	7.111 958 7	12.650 714 0	8.958 210 5	5.538 755 3
2.3	7.393 267 5	13.474 246 0	9.420 260 3	6.080 978 5
2.4	7.659 668 9	14.272 359 0	9.863 898 9	6.612 690 1
2.5	7.909 223 8	15.031 928 0	10.283 458 5	7.122 704 2
2.6	8.140 242 8	15.739 587 0	10.673 357 5	7.599 344 2
2.7	8.351 253 9	16.382 154 0	11.028 220 6	8.030 900 1
2.8	8.541 228 7	16.947 542 0	11.343 333 1	8.406 313 3
2.9	8.709 382 2	17.424 939 0	11.614 567 8	8.715 556 8
3.0	8.855 379 0	17.805 679 0	11.838 812 3	8.950 300 0
3.1	8.979 301 5	18.083 846 0	12.014 149 7	9.104 544 5
3.2	9.081 669 6	18.256 526 0	12.139 955 1	9.174 856 4
3.3	9.163 427 5	18.324 121 0	12.216 992 0	9.160 693 5
3.4	9.225 898 3	18.290 329 0	12.247 375 2	9.064 430 7
3.5	9.270 723 2	18.161 902 0	12.234 449 5	8.891 178 8
3.6	9.299 784 2	17.948 203 0	12.182 590 5	8.648 418 8
3.7	9.315 117 4	17.660 585 0	12.096 939 9	8.345 467 6
3.8	9.318 823 6	17.311 690 0	11.983 112 4	7.992 866 4
3.9	9.312 983 0	16.914 721 0	11.846 895 7	7.601 738 0
4.0	9.299 582 0	16.482 757 0	11.693 973 7	7.183 175 0
4.2	9.257 241 6	15.562 186 0	11.358 889 7	6.304 944 4
4.4	9.204 034 2	14.633 575 0	11.013 881 1	5.429 540 8
4.6	9.148 702 8	13.756 300 0	10.684 568 5	4.607 597 2
4.8	9.096 792 3	12.964 991 0	10.386 191 9	3.868 198 7
5.0	9.051 249 1	12.275 188 0	10.125 895 4	3.223 938 9
5.2	9.013 235 3	11.688 681 0	9.905 050 5	2.675 445 7
5.4	8.982 775 3	11.199 031 0	9.721 527 2	2.216 255 7
5.6	8.959 258 2	10.795 648 0	9.571 388 1	1.836 389 8
5.8	8.941 779 0	10.466 495 0	9.450 017 7	1.524 716 0
6.0	8.929 350 2	10.199 707 0	9.352 802 5	1.270 356 8
6.2	8.921 020 5	9.984 434 8	9.275 491 9	1.063 414 3
6.4	8.915 935 3	9.811 200 1	9.214 356 9	0.895 264 8
6.6	8.913 403 1	9.672 014 8	9.166 273 7	0.758 611 7
6.8	8.912 738 8	9.560 112 0	9.128 529 9	0.647 373 2
7.0	8.913 478 5	9.470 076 3	9.099 011 1	0.556 597 8
7.5	8.919 076 1	9.313 750 0	9.050 634 1	0.394 673 9
8.0	8.927 047 2	9.220 486 1	9.024 860 2	0.293 438 9
8.5	8.935 313 0	9.162 867 6	9.011 164 5	0.227 554 6
9.0	8.942 973 4	9.125 582 0	9.003 842 9	0.182 608 6
9.5	8.949 725 8	9.100 174 5	8.999 875 4	0.150 448 7
10.0	8.955 533 7	9.081 982 2	8.997 683 2	0.126 448 5
10.5	8.960 468 5	9.068 372 8	8.996 436 6	0.107 904 3
11.0	8.964 641 2	9.057 797 3	8.995 693 2	0.093 156 1
11.5	8.968 171 6	9.049 318 9	8.995 220 7	0.081 147 3
12.0	8.971 173 0	9.042 370 9	8.994 905 6	0.071 197 9

S4. Development of the bond functions used in this work

The improvement in the energy of H_2 by introduction of bond functions has been studied by Wright and coworkers[2–4] who showed that employing bond functions of type $2s2p$ and $3s3p2d$ gives improved energies for H_2. We tested the bond functions as given in Ref. 2 and 3 namely, $2s2p2d$ and $3s3p3d$, while adding more $s-$ and $p-$ functions, which however, did not result in significant improvement of the polarizability. The bond functions mentioned in Ref. 2–4 were optimized only at r=1.4 a.u. for the energy of the molecule, and hence as expected they did not perform well at larger distances as shown in Fig. F1, where the difference of the invariants of static polarizability to the data given by Rychlewski[5] are plotted against the internuclear distance. In the present work, we are computing integrals up to the v=1,J=10 state and the wavefunction for the highest state diminish to zero at r=3.4 a.u., hence we need accurate polarizability at least up to this distance.

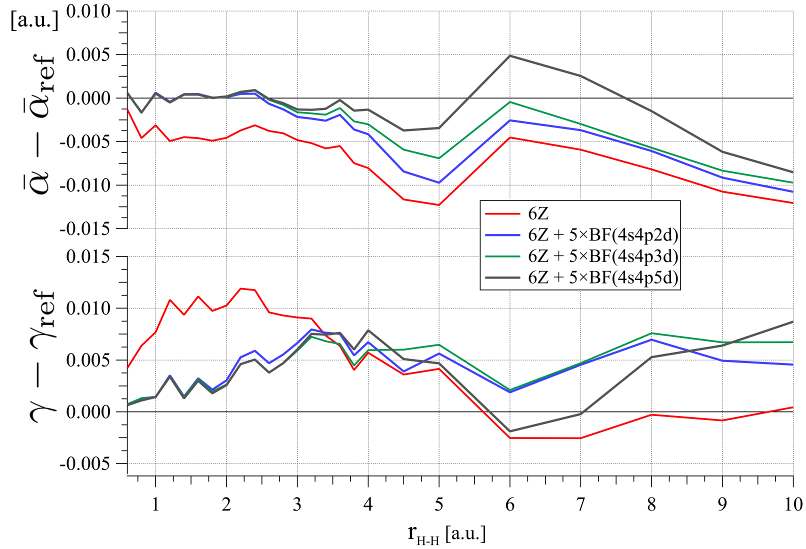


FIG. F1. The values of $\bar{\alpha} - \bar{\alpha}_{\mathrm{ref}}$ and $\gamma - \gamma_{\mathrm{ref}}$ for the static polarizabilities of H_2 as a function of the internuclear distance. The $\bar{\alpha}$ and γ invariants are computed with CCSD methodology using the composite aug-mcc-pV6Z+5×BF basis set. The reference values $\bar{\alpha}_{\mathrm{ref}}$ and γ_{ref} are taken from the work of Rychlewski (Ref. 5). The basis sets is composed of aug-cc-pV6Z basis as the AO basis and the bond functions given in the legend. These bond functions were taken from the work of Wright and coworkers[2, 3] where we have added additional diffuse functions following the same ratio for the exponents as in the original work.

It seems important to investigate which types of functions (namely $s-$, $p-$ or $d-$) are important as bond functions, and what are the appropriate size and the number of functions needed. To answer these questions, different sized $s-$, $p-$ and $d-$ functions were placed on a number of equally spaced points along the H−H bond, and the static polarizability was computed at several internuclear distances. By comparing the results with those given by Rychlewski (Ref. 5) it was found that less than 5 number of equally spaced points with bond functions do not provide all the basis functions needed for larger distances especially r>3 a.u. (see Fig. F2). Hence, we chose to place bond functions on 5 equidistant points along the internuclear distance.

Upon testing many different sized $s-$, $p-$ and $d-$ functions we found that $p-$functions are the most important towards the improvement of polarizability. Differently sized $p-$functions were then checked and optimized to obtain a $6p-$function set as a good candidate (see main text for the exponents). After the $p-$functions, the $s-$functions were found to be the most relevant. It was found that the $d-$functions affect the polarizability values to the least degree, as shown in Fig. F4.

Since we added additional basis functions for our calculations, we checked the consistency of our results by changing the parameters controlling the cut-off for numerical linear dependence of basis functions, the convergence criteria for SCF and CCSD energies and the convergence criteria for response solutions.

- In the DALTON package, the linear dependence of basis functions is controlled within the program by computing the overlap matrix of the basis functions (also known as AO overlap matrix) and removing the eigenvectors whose eigenvalues are less than the cutoff defining the numerical linear dependence (default cutoff=1×10^{-6}). This cutoff governs which basis functions are removed to avoid mathematically incorrect results. AOs with bond functions supply excess basis functions to be used for generating the MOs, and this check for linear dependence removes functions not needed. In our tests, the cut-off

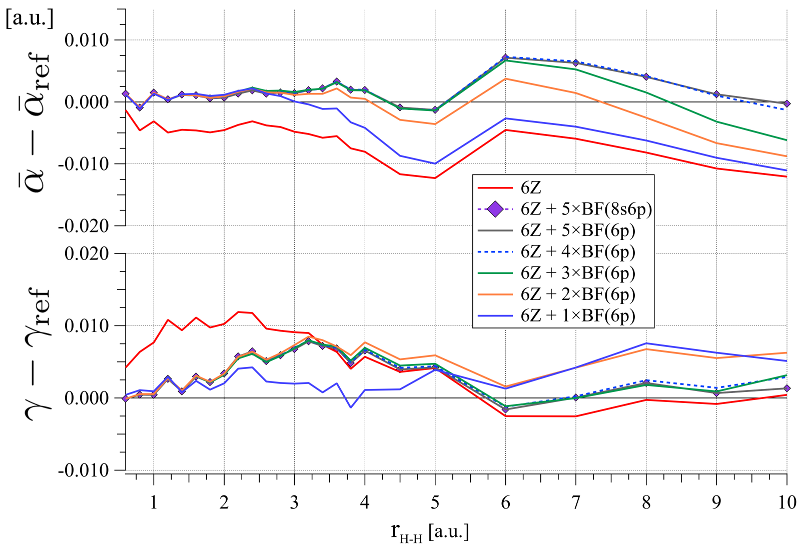


FIG. F2. The values of $\bar{\alpha} - \bar{\alpha}_{\mathrm{ref}}$ and $\gamma - \gamma_{\mathrm{ref}}$ for the static polarizabilities of H_2 as a function of internuclear distance. The $\bar{\alpha}$ and γ invariants are computed with CCSD using the composite aug-mcc-pV6Z+n×BF basis set. The reference values $\bar{\alpha}_{\mathrm{ref}}$ and γ_{ref} are taken from the work of Rychlewski (Ref. 5). The basis sets include the aug-cc-pVDZ as the AO functions and the different number of bond functions placed at n-equidistant points along the H−H are given in the legend.

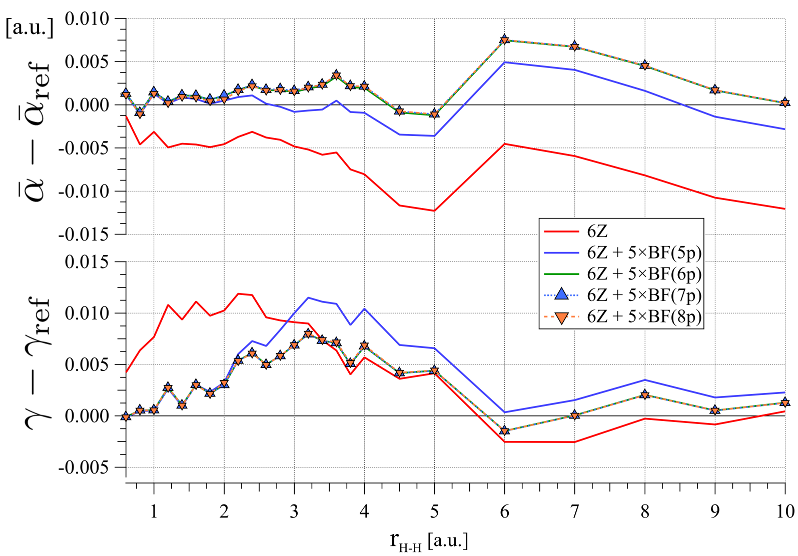


FIG. F3. The values of $\bar{\alpha} - \bar{\alpha}_{\mathrm{ref}}$ and $\gamma - \gamma_{\mathrm{ref}}$ for the static polarizabilities of H_2 as a function of internuclear distance. The $\bar{\alpha}$ and γ invariants are computed with CCSD using the composite aug-mcc-pV6Z+5×BF basis set. The reference values $\bar{\alpha}_{\mathrm{ref}}$ and γ_{ref} are taken from the work of Rychlewski (Ref. 5). Deviation observed for the 6Z+5×BF(5p), shown in violet, from the lines for larger basis at r=1.5 a.u. for $\bar{\alpha}$ and r=1.75 a.u. for γ indicates that this basis does not have enough functions for the larger internuclear distances. 6$p-$ and larger bond functions along with 6Z AO basis show same differences at all distances indicating they give converged results since no significant departure in the differences are observed at any distance for these cases.

for linear dependence was varied within 10^{-6} to 10^{-11} to check the effect on the polarizability (see table T18). The default cutoff for linear dependence(10^{-6}) gave reproducible results up to the fourth decimal digit for both $\alpha_{\perp}$ and $\alpha_{\parallel}$. The cut-off at 10^{-7} – 10^{-11} gave converged results for both the components of polarizability shown in Table T18. In the present work, the default cutoff (of 10^{-6}) been used which, however, causes a change of 1.0×10^{-5} for $\bar{\alpha}$ and 1.0×10^{-4} for γ. This effect of the cutoff for linear dependence is accounted when describing the error in the computed matrix elements.

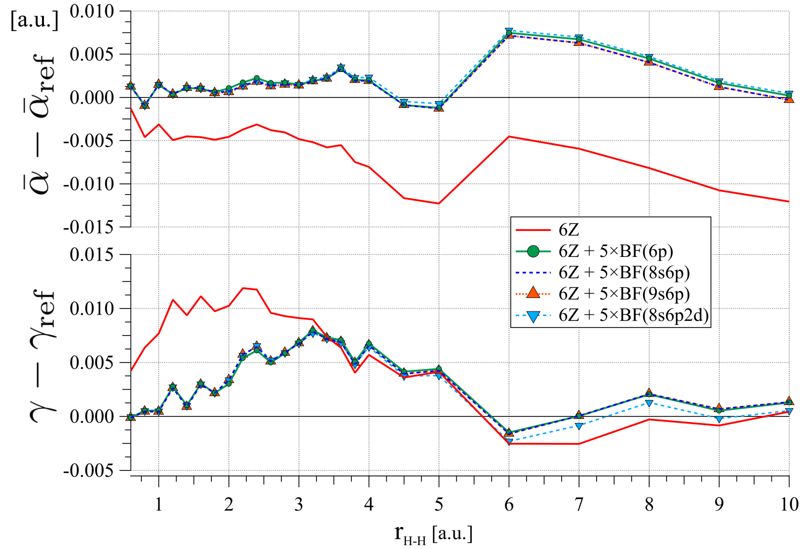


FIG. F4. The values of $\bar{\alpha} - \bar{\alpha}_{\text{ref}}$ and $\gamma - \gamma_{\text{ref}}$ for the static polarizabilities of H_2 as a function of internuclear distance. The $\bar{\alpha}$ and γ invariants are computed with CCSD using the composite aug-mcc-pV6Z+5×BF basis set. The reference values $\bar{\alpha}_{\text{ref}}$ and γ_{ref} are taken from the work of Rychlewski (Ref. 5). This plot shows that $6p-$ bond functions gives similar polarizability as with larger bond-functions indicating that polarizability is nearly converged. Additional $s-$functions affect polarizability only by less than 0.002 a.u. across all distances, and $d-$functions only affect the polarizability at distances larger than 5 a.u. and only by ~0.001 a.u. or less.

TABLE T18. Change of static polarizability r=1.4 a.u. with the cutoff for linear dependence of atomic orbital basis functions when using the composite basis: aug-mcc-pV6Z+5×BF($8s6p$). The following test was performed using the convergence criteria for SCF energy gradient as 1.0×10^{-11} a.u., convergence criteria for CC energy as 1.0×10^{-9} a.u. and the convergence criteria for response solutions as 1.0×10^{-7} a.u.

AO linear dependence cutoff	$\boldsymbol{\alpha_\perp}$	$\boldsymbol{\alpha_\parallel}$	$\boldsymbol{\bar{\alpha}}$	$\boldsymbol{\gamma}$
1.0×10^{-6}	4.579 413 2	6.389 121 8	5.182 649 4	1.809 708 6
1.0×10^{-7}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2
1.0×10^{-8}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2
1.0×10^{-9}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2
1.0×10^{-10}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2
1.0×10^{-11}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2

- Convergence of the wavefunctions and the respective energy was ascertained by tightening the SCF convergence criteria for the energy gradient to 10^{-11} a.u. and the CCSD energy convergence criteria to 10^{-9} a.u. The response results (for example, polarizability) were checked by tightening the convergence criteria for response solutions to 10^{-7} a.u. (see table T19). The change in the values of polarizability was found to be consistent with the set convergence criteria, indicating stable converged results and the final calculations were performed using these tightened parameters.

TABLE T19. Change of static polarizability at r=1.4 a.u. with the convergence criteria for the SCF energy gradient, CC energy and the solutions to the response equations respectively, when using the composite basis: aug-mcc-pV6Z+5×BF(8s6p). Two tests were performed where, (i) AO linear dependence cutoff as 1.0×10^{-6} a.u. and (ii) AO linear dependence cutoff as 1.0×10^{-11} a.u. For both the tests, the convergence criteria for the SCF energy gradient was changed from 1.0×10^{-6} to 1.0×10^{-11} a.u., convergence criteria for CC energy was two orders of magnitude larger than that for the case of SCF energy gradient while the convergence criteria for response solutions was two orders of magnitude larger than that for the case of CC energy. All numbers are in the respective a.u.

	Convergence threshold						
AO linear dependence cutoff	**SCF energy**	**CC energy**	**Linear Response**	$\alpha_\perp$	$\alpha_\parallel$	$\bar{\alpha}$	γ
1.0×10^{-6}	1.0×10^{-6}	1.0×10^{-4}	1.0×10^{-2}	4.580 875 2	6.390 956 0	5.184 235 5	1.810 080 8
	1.0×10^{-7}	1.0×10^{-5}	1.0×10^{-3}	4.579 510 5	6.389 124 3	5.182 715 1	1.809 613 8
	1.0×10^{-8}	1.0×10^{-6}	1.0×10^{-4}	4.579 476 6	6.389 129 5	5.182 694 2	1.809 652 9
	1.0×10^{-9}	1.0×10^{-7}	1.0×10^{-5}	4.579 417 0	6.389 124 5	5.182 652 8	1.809 707 5
	1.0×10^{-10}	1.0×10^{-8}	1.0×10^{-6}	4.579 413 2	6.389 121 8	5.182 649 4	1.809 708 6
	1.0×10^{-11}	1.0×10^{-9}	1.0×10^{-7}	4.579 413 2	6.389 121 8	5.182 649 4	1.809 708 6
1.0×10^{-11}	1.0×10^{-6}	1.0×10^{-4}	1.0×10^{-2}	4.580 917 7	6.390 970 4	5.184 268 6	1.810 052 7
	1.0×10^{-7}	1.0×10^{-5}	1.0×10^{-3}	4.579 535 9	6.389 107 2	5.182 726 3	1.809 571 3
	1.0×10^{-8}	1.0×10^{-6}	1.0×10^{-4}	4.579 502 3	6.389 113 3	5.182 706 0	1.809 611 0
	1.0×10^{-9}	1.0×10^{-7}	1.0×10^{-5}	4.579 494 3	6.389 108 7	5.182 699 1	1.809 614 4
	1.0×10^{-10}	1.0×10^{-8}	1.0×10^{-6}	4.579 438 8	6.389 106 1	5.182 661 2	1.809 667 3
	1.0×10^{-11}	1.0×10^{-9}	1.0×10^{-7}	4.579 438 8	6.389 106 0	5.182 661 2	1.809 667 2

S5. Details of the numerical procedure used for the solution of the 1D Schrödinger equation

A. Introduction

Consider the Schrödinger equation

$$\Omega\psi(x) = E\psi(x) \tag{1}$$

where operator Ω is some form of differential operator representing the Hamiltonian in one dimension(say x). Let the eigenvectors be given as $\psi(x)$ while the eigenvalues as E. The objective is to obtain a solution which comprises of, the eigenvalue E and the eigenvector ψ, for a given operator Ω. Consider a finite region in x where the solution exists and is real valued. For such a region, one can consider a finite number of points in x giving us a grid of points with uniform step h. If the operator Ω can be expressed explicitly for each of these points on x, then one can map the equations onto a square matrix (described as H-matrix) where each diagonal element corresponds to the point in the finite grid on x. Eigendecomposition of this matrix would yield the left and right eigenvectors arranged in the form of square matrices and a square diagonal matrix having eigenvalues. This is the outline of the process for obtaining a solution to the Schrödinger equation. The focus then shifts to the process of mapping the differential operator Ω spanning over some finite region in x on some chosen grid points.

B. Finite difference formulae for approximating the derivative

The finite difference method for obtaining a numerical solution to the differential equations is based on the concept of using appropriate differences over a grid of points (discretization) rather than continuous derivatives (differentiation) of analytic functions. In this method, truncated Taylor series expansion at each grid point can be used to effectively compute numerical derivatives as differences shown in the following description. For a general function $f(x)$, the central difference formula of the order h^4 (i.e. using up to the 4^{th}-order derivative) can be derived using the Taylor series expansion about x for $f(x-2h)$, $f(x-h)$, $f(x)$,

$f(x+h)$ and $f(x+2h)$ which are;

$$
\begin{aligned}
f(x-2h) &= f(x) - 2hf^{(1)}(x) + \frac{4h^2 f^{(2)}(x)}{2!} - \frac{8h^3 f^{(3)}(x)}{3!} + \frac{16h^4 f^{(4)}(x)}{4!} - \frac{32h^5 f^{(5)}(\tau_2)}{5!} \\
f(x-h) &= f(x) - hf^{(1)}(x) + \frac{h^2 f^{(2)}(x)}{2!} - \frac{h^3 f^{(3)}(x)}{3!} + \frac{h^4 f^{(4)}(x)}{4!} - \frac{h^5 f^{(5)}(\tau_1)}{5!} \\
f(x) &= f(x) + 0 + 0 + 0 + 0 \\
f(x+h) &= f(x) + hf^{(1)}(x) + \frac{h^2 f^{(2)}(x)}{2!} + \frac{h^3 f^{(3)}(x)}{3!} + \frac{h^4 f^{(4)}(x)}{4!} + \frac{h^5 f^{(5)}(\tau_1)}{5!} \\
f(x+2h) &= f(x) + 2hf^{(1)}(x) + \frac{4h^2 f^{(2)}(x)}{2!} + \frac{8h^3 f^{(3)}(x)}{3!} + \frac{16h^4 f^{(4)}(x)}{4!} + \frac{32h^5 f^{(5)}(\tau_2)}{5!}
\end{aligned}
\tag{2}
$$

where τ is some point within $(x-2h)$ and $(x+2h)$. Note that the above equations have the 5^{th} derivative term which is included for error estimation in this approximation.

Difference of the last and the first term in Eqn. 2 gives,

$$f(x+2h) - f(x-2h) = 4hf^{(1)}(x) + \frac{16h^3 f^{(3)}(x)}{3!} + \frac{64h^5 f^{(5)}(\tau_2)}{5!} \tag{3}$$

while, the difference between the second last and the second term in Eqn. 2 gives,

$$f(x+h) - f(x-h) = 2hf^{(1)}(x) + \frac{2h^3 f^{(3)}(x)}{3!} + \frac{2h^5 f^{(5)}(\tau_1)}{5!} \tag{4}$$

Subtracting Eqn. 3 from Eqn. 4 and rearranging gives,

$$-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h) = 12hf^{(1)} + \frac{h^5(16f^{(5)}(\tau_1) - 64f^{(5)}(\tau_2))}{120} \tag{5}$$

Assuming that the $f^{(5)}$ is smooth over the $(x-2h)$ .. $(x+2h)$ and preserves its sign over this interval, the second term in Eqn. 5 can be simplified using a common value of τ which is within the interval $(x-2h)$ .. $(x+2h)$, giving ,

$$16f^{(5)}(\tau_1) - 64f^{(5)}(\tau_2) = -48f^{(5)}(\tau) \tag{6}$$

Using Eqn. 6, Eqn. 5 can be rewritten for $f^{(1)}$ as,

$$f^{(1)} = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{h^4 f^{(5)}(\tau)}{30} \tag{7}$$

The first term of the right hand side in the above expression is an approximation for the first derivative, where the coefficients (also known as difference quotients), namely, $(\frac{-1}{12h}, \frac{8}{12h}, \frac{-8}{12h}, \frac{1}{12h})$ are derived algebraically for the present case. The second term of the right hand side is the truncation error. The truncation error is dependent on the step size (h) and for the first derivative it is generalized as,

$$\text{Error}(h^n) = \frac{h^n f^{(n+1)}(x)}{(n+1)(n+2)} \tag{8}$$

Using a similar treatment, other numerical derivative approximations specifically, forward and backward difference, and various versions of asymmetric difference formulations can be obtained. It is to be noted that the expression for the truncation error will be different for each case. The process of obtaining the coefficients for the relevant derivative can also be treated as a problem of set of linear equations (for example, see section S5 C) which can be solved using a matrix equation, allowing for convenient implementation on a computer code. Formulae for numerous other kind of differences for the approximation of derivative can be found in Ref. [6, 7].

C. Matrix mathematics approach to coefficients of the terms in the finite difference method

Consider a general function $f(x)$ whose value at $f(x+h)$ can be written in terms of Taylor series expansion and the series can be truncated up to the 4^{th} derivative term giving,

$$f(x+h) = f(x) + hf^{(1)}(x) + \frac{h^2 f^{(2)}(x)}{2!} + \frac{h^3 f^{(3)}(x)}{3!} + \frac{h^4 f^{(4)}(x)}{4!} \tag{9}$$

Consider a point x_0 around which the numerical values of $f(x_0)$ and $f(x_0+nh)$ are available. For evaluating the derivative at x_0 the 5-point numerical derivative (an example of left handed asymmetric derivative also known as forward difference) can be employed,

$$\begin{aligned}
f(x_0) &= f(x_0) + 0 + 0 + 0 + 0 \\
f(x_0+h) &= f(x_0) + hf^{(1)}(x_0) + \frac{h^2 f^{(2)}(x_0)}{2!} + \frac{h^3 f^{(3)}(x_0)}{3!} + \frac{h^4 f^{(4)}(x_0)}{4!} \\
f(x_0+2h) &= f(x_0) + 2hf^{(1)}(x_0) + \frac{4h^2 f^{(2)}(x_0)}{2!} + \frac{8h^3 f^{(3)}(x_0)}{3!} + \frac{16h^4 f^{(4)}(x_0)}{4!} \\
f(x_0+3h) &= f(x_0) + 3hf^{(1)}(x_0) + \frac{9h^2 f^{(2)}(x_0)}{2!} + \frac{27h^3 f^{(3)}(x_0)}{3!} + \frac{81h^4 f^{(4)}(x_0)}{4!} \\
f(x_0+4h) &= f(x_0) + 4hf^{(1)}(x_0) + \frac{16h^2 f^{(2)}(x_0)}{2!} + \frac{64h^3 f^{(3)}(x_0)}{3!} + \frac{256h^4 f^{(4)}(x_0)}{4!}
\end{aligned} \tag{10}$$

The objective is then to obtain the required derivative in terms of appropriate coefficients (C_0, C_1, C_2, C_3 and C_4). This can be performed by constructing a set of 5-linear equations, one each for one of the derivative and solving them to obtain the required coefficients.

Set of Eqns. 10 can be transformed into a matrix (F) where the elements are the numerical values of the Taylor series coefficients. Transpose of this matrix would arrange the coefficients such that each row corresponds to the coefficients C_0, C_1, C_2, C_3 and C_4 for the derivative of a certain degree.

$$F = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{24} \\ 1 & 2 & 2 & \frac{8}{6} & \frac{16}{24} \\ 1 & 3 & \frac{9}{2} & \frac{27}{6} & \frac{81}{24} \\ 1 & 4 & \frac{16}{2} & \frac{64}{6} & \frac{256}{24} \end{bmatrix} \tag{11}$$

$$A = F^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \\ 0 & \frac{1}{2} & 2 & \frac{9}{2} & \frac{16}{2} \\ 0 & \frac{1}{6} & \frac{8}{6} & \frac{27}{6} & \frac{64}{6} \\ 0 & \frac{1}{24} & \frac{16}{24} & \frac{81}{24} & \frac{256}{24} \end{bmatrix} \tag{12}$$

$$[A]_{5\times5}[C]_{5\times1} = [B]_{5\times1} \tag{13}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \\ 0 & \frac{1}{2} & 2 & \frac{9}{2} & \frac{16}{2} \\ 0 & \frac{1}{6} & \frac{8}{6} & \frac{27}{6} & \frac{64}{6} \\ 0 & \frac{1}{24} & \frac{16}{24} & \frac{81}{24} & \frac{256}{24} \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = \begin{bmatrix} f^{(0)} \\ f^{(1)} \\ f^{(2)} \\ f^{(3)} \\ f^{(4)} \end{bmatrix} \tag{14}$$

Using the matrix eqn. 14 the coefficients (C_0, C_1, C_2, C_3 and C_4) can be obtained for any of the derivative by assigning it as unity in the column matrix B. Such condition(s) are shown below for the first and the second derivative.

$$B = \begin{bmatrix}0\\1\\0\\0\\0\end{bmatrix} \quad \text{for first derivative; and} \quad B = \begin{bmatrix}0\\0\\1\\0\\0\end{bmatrix} \quad \text{for second derivative} \tag{15}$$

Matrix equation $AC = B$ can be solved as $C = A^{-1}B$
Each coefficient has to be divided with the value of (h^n) for the specific n^{th}-order derivative, for example,

$$C : \left(\frac{C_0}{h}, \frac{C_1}{h}, \frac{C_2}{h}, \frac{C_3}{h}, \frac{C_4}{h}\right), \text{ for the first derivative} \quad \text{and} \tag{16}$$

$$C : \left(\frac{C_0}{h^2}, \frac{C_1}{h^2}, \frac{C_2}{h^2}, \frac{C_3}{h^2}, \frac{C_4}{h^2}\right), \text{ for the second derivative.} \tag{17}$$

The explanation given above is for the 5-point forward difference. A similar technique can be used to compute the required coefficients for the backward and central difference methods.

Mapping the operator Ω on a matrix followed by eigendecomposition

As shown in the previous section, numerical derivatives can be computed by appropriately choosing 5 points when using Taylor series expansion up to the 4^{th} degree. For the present case, the region over the one-dimensional space over which the solution of the differential equation is sought can be divided into a finite number of points, say from x_0 to x_n having step of h. For the first point (x_0), the derivative can be described using the forward difference. For the second point (x_1), asymmetric derivative using expansions over $f(x_1 - h)$, $f(x_1)$, $f(x_1 + h)$ $f(x_1 + 2h)$, and $f(x_1 + 3h)$ can be used. From the 3^{rd} point (x_2) up to the $n - 2^{\text{th}}$ point symmetric derivative using expansions over $f(x_2 - 2h)$, $f(x_2 - h)$,$f(x_2)$, $f(x_2 + h)$ and $f(x_2 + 2h)$ can be employed. For the $n - 1^{\text{th}}$ point, asymmetric derivative similar to the x_1 can be used. For the very last point (x_n), backward difference can be used. This is shown using Table T20.

TABLE T20. Taylor expansions required for computing derivative at certain point on a grid spanning from x_0 to x_n with step of h.

Point on grid	Taylor expansions required				
x_0	$f(x_0)$	$f(x_0 + h)$	$f(x_0 + 2h)$	$f(x_0 + 3h)$	$f(x_0 + 4h)$
x_1	$f(x_1 - h)$	$f(x_1)$	$f(x_1 + h)$	$f(x_1 + 2h)$	$f(x_1 + 3h)$
x_2	$f(x_2 - 2h)$	$f(x_2 - h)$	$f(x_2)$	$f(x_2 + h)$	$f(x_2 + 2h)$
x_3	$f(x_3 - 2h)$	$f(x_3 - h)$	$f(x_3)$	$f(x_3 + h)$	$f(x_3 + 2h)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_{n-2}	$f(x_{n-2} - 2h)$	$f(x_{n-2} - h)$	$f(x_{n-2})$	$f(x_{n-2} + h)$	$f(x_{n-2} + 2h)$
x_{n-1}	$f(x_{n-1} - 3h)$	$f(x_{n-1} - 2h)$	$f(x_{n-1} - h)$	$f(x_{n-1})$	$f(x_{n-1} + h)$
x_n	$f(x_n - 4h)$	$f(x_n - 3h)$	$f(x_n - 2h)$	$f(x_n - h)$	$f(x_n)$

As shown in the previous discussion, for each derivative required in the relevant operator, the appropriate coefficients for numerical differentiation can be computed by solving a set of linear equations. This provides us with the coefficients (C_0, C_1, C_2, C_3 and C_4) for each point x_0 to x_n. Using these coefficients the numerical derivative can be explicitly defined, as shown using the following example.

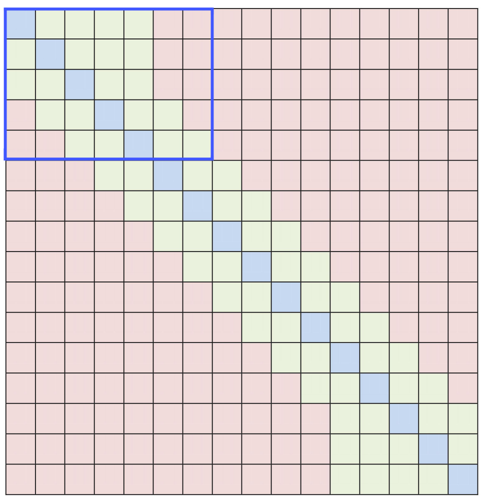
Consider the operator Ω as,

$$\Omega = \frac{\partial^2}{\partial x^2} + k(x) \simeq \frac{d^2}{dx^2} + k(x) \tag{18}$$

In Eqn. 18, the second derivative term $(\frac{d^2}{dx^2})$ can now be expressed using C_0/h^2, C_1/h^2, C_2/h^2, C_3/h^2 and C_4/h^2 and the numerical value of the $k(x)$ term is added to the respective equation. This is shown using Eqns. 19.

$$
\begin{aligned}
\left(\frac{C_0^{x_0}}{h^2} + k(x_0) + \frac{C_1^{x_0+h}}{h^2} + \frac{C_2^{x_0+2h}}{h^2} + \frac{C_3^{x_0+3h}}{h^2} + \frac{C_4^{x_0+4h}}{h^2}\right)\psi(x_0) &= E\psi(x_0) \\
\left(\frac{C_0^{x_1-h}}{h^2} + \frac{C_1^{x_1}}{h^2} + k(x_1) + \frac{C_2^{x_1+h}}{h^2} + \frac{C_3^{x_1+2h}}{h^2} + \frac{C_4^{x_1+3h}}{h^2}\right)\psi(x_1) &= E\psi(x_1) \\
\left(\frac{C_0^{x_2-2h}}{h^2} + \frac{C_1^{x_1-h}}{h^2} + \frac{C_2^{x_2}}{h^2} + k(x_2) + \frac{C_3^{x_2+h}}{h^2} + \frac{C_4^{x_2+2h}}{h^2}\right)\psi(x_2) &= E\psi(x_2) \\
\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad &= \vdots \\
\left(\frac{C_0^{x_n-4h}}{h^2} + \frac{C_1^{x_n-3h}}{h^2} + \frac{C_2^{x_n-2h}}{h^2} + \frac{C_3^{x_n-h}}{h^2} + \frac{C_4^{x_n}}{h^2} + k(x_n)\right)\psi(x_n) &= E\psi(x_n)
\end{aligned}
\tag{19}
$$

Following Eqns. 19, the H-matrix can be formulated where the derivative term takes 5 columns, which are asymmetric (around the diagonal) for the first and last two rows, while symmetric for the other rows. The $k(x)$ term is added to the diagonal term. This is shown using Fig. F5. Eigendecomposition of the resulting H-matrix gives three square matrices (F6), two for the eigenvectors and one for the eigenvalues.

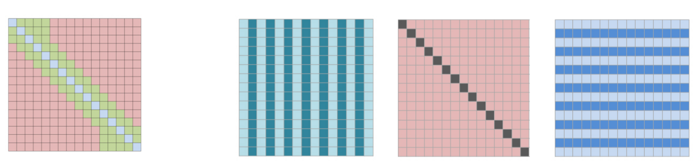


(C_0/h^2) $+k(x_0)$	(C_1/h^2)	(C_2/h^2)	(C_3/h^2)	(C_4/h^2)	0	0
(C_0/h^2)	(C_1/h^2) $+k(x_1)$	(C_2/h^2)	(C_3/h^2)	(C_4/h^2)	0	0
(C_0/h^2)	(C_1/h^2)	(C_2/h^2) $+k(x_2)$	(C_3/h^2)	(C_4/h^2)	0	0
0	(C_0/h^2)	(C_1/h^2)	(C_2/h^2) $+k(x_3)$	(C_3/h^2)	(C_4/h^2)	0
0	0	(C_0/h^2)	(C_1/h^2)	(C_2/h^2) $+k(x_4)$	(C_3/h^2)	(C_4/h^2)

(a) Second derivative = blue and green elements
k(x) = blue elements
Red elements are zero.

(b) Zoom up of the blue enclosed region of the matrix (in left) with the respective elements.

FIG. F5. (a) General structure of the H-matrix shown using small sized representation. The numerical derivative are centered on the blue elements and occupy 5 elements on each row, owing to 5-point numerical derivative approximation. Non-derivative term like $k(x)$ are present in the diagonal elements. Other elements are zero (shown in red). (b) A zoom up of the blue enclosed region showing the detailed composition of the respective elements.



$$\left[\mathbf{H}\right] = \left[\boldsymbol{\psi}\right]\left[\mathbf{E}\right]\left[\boldsymbol{\psi}^\dagger\right]$$

FIG. F6. Eigendecomposition of the H-matrix to obtain the eigenvectors, $\psi(x)$ and $\psi^\dagger(x)$) in the form of two square matrices, and the eigenvalues as diagonals of a square matrix.

Comparison of the present implementation of the finite difference method with other methods for the solution of 1D Schrödinger equation

To verify our implementation of the above described procedure involving the finite difference approximation for numerical derivative, we compare the results obtained using the same potential on LEVEL16 program by Le Roy[8] which is based on the Cooley method[9]. A comparison of dissociation energies from different vibrational levels is presented in Table T21 showing that a non-systematic difference in dissociation energies (in cm^{-1}) appears on the third digit after decimal for any of the J-state. For comparing the accuracy of the wavefunction, a comparison of the matrix elements computed with respective wavefunctions is shown in Table T22 where it is seen that the difference in the numerical value of the matrix element is of the order of 10^{-7}. These comparisons indicate that the present implementation of the procedure based on finite difference approximation is accurate enough for present purpose.

TABLE T21. Comparison of dissociation energies (D_e) for H_2 from different vibrational levels (v=0–4,J=0) obtained from our implementation of procedure described in Section S5 and LEVEL16 program implementing the Cooley method.

v, J	Our program	LEVEL16[a]	Δ
0,0	−36 118.217	−36 118.210	−0.006
1,0	−31 957.282	−31 957.281	−0.001
2,0	−28 031.632	−28 031.627	−0.005
3,0	−24 336.385	−24 336.379	−0.006
4,0	−20 868.501	−20 868.493	−0.008

[a] Ref. 8

TABLE T22. Matrix elements (a.u.) for H_2 obtained by wavefunctions from the present implementation of procedure described in Section S5 and LEVEL16 based on the Cooley method.

	Matrix element	Our program	LEVEL16[a]	Δ
H_2	$\langle\psi_{00}\vert\bar{\alpha}\vert\psi_{00}\rangle$	5.417 943 315	5.417 943 279	0.000 000 037
	$\langle\psi_{00}\vert\gamma\vert\psi_{00}\rangle$	2.031 207 900	2.031 207 449	0.000 000 451

[a] Ref. 8

S6. Error estimation for matrix elements

In the present work, errors can be introduced from many different sources which have to be identified and the magnitude of each error has to be estimated. The present section is devoted to the details of the identified sources and magnitude of each error.
The potential energies and the corrections were interpolated using cubic spline interpolation procedure while solving the radial nuclear Schrödinger equation. The error introduced by the cubic spline interpolation was estimated by removing each data point one by one and generating new interpolated data which was compared to the original value thus giving information about the maximal oscillation of the cubic spline in the absence of a data point. The maximal shift in the numerical value of the potential and the corrections for the potential was found to be $\sim 10^{-7}$ a.u. A similar analysis on the polarizability data points over distance showed a maximal shift of $\sim 10^{-6}$ a.u.
Any effect of random noise in the potential energy surface was investigated by introducing artificial white noise oscillating within $\pm 1\times 10^{-6}$ having random statistical distribution. Wavefunctions obtained by such perturbed potentials were used to calculate the matrix elements. This was done for 31 random noise vectors for statistical analysis and the 3σ standard deviation in the values of the matrix elements is shown in Table T23, where it is observed that the effect on the matrix element is below 10^{-5} a.u.

TABLE T23. Effect of random noise (oscillating within $\pm 10^{-6}$ a.u.) in the potential energy on the matrix elements (static)

Matrix element	3 $\boldsymbol{\sigma}$
$\langle\psi_{0,0}\vert\gamma\vert\psi_{0,0}\rangle$	8.7×10^{-6}
$\langle\psi_{0,0}\vert\bar{\alpha}\vert\psi_{0,0}\rangle$	7.1×10^{-6}
$\langle\psi_{0,0}\vert\gamma\vert\psi_{0,2}\rangle$	8.8×10^{-6}
$\langle\psi_{0,0}\vert\bar{\alpha}\vert\psi_{1,0}\rangle$	2.7×10^{-6}

During generation of the H-matrix, the reduced nuclear mass(μ) of the molecule is required. The masses of proton and deuteron have their respective uncertainties which propagates to the reduced mass and then to the elements of the H-matrix. In order to estimate the maximal error due to uncertainty in nuclear masses, two H-matrices were setup, one with the error added to both the nuclei and second, where the error was subtracted. The resulting wavefunctions were used to calculate the matrix elements, from which the maximal error in respective matrix elements was determined. These are shown in Table T24 where it is seen that the error due to uncertainty of nuclear masses is of the order of 10^{-11} a.u. Among the three isotopologues, due to the smaller nuclear mass of a proton the contribution of error due to nuclear mass is more in H_2, which decreases in HD and is the lowest in D_2.

TABLE T24. Maximal error in the matrix elements (static) due to the uncertainty in nuclear mass

	$\boldsymbol{\Delta\langle\psi_{0,0}\vert\bar{\alpha}\vert\psi_{0,0}\rangle}$	$\boldsymbol{\Delta\langle\psi_{0,0}\vert\gamma\vert\psi_{0,0}\rangle}$
H_2	2.5×10^{-11}	3.6×10^{-11}
HD	1.2×10^{-11}	1.5×10^{-11}
D_2	6.3×10^{-12}	6.3×10^{-12}

In the presently used technique involving finite differences to solve the 1D Schrödinger equation, the H-matrix is setup using an array of inter-nuclear distance of certain step size. The choice of step size (h) is crucial to obtain resulting wavefunctions of sufficient accuracy. With the step (h) of 0.004 a.u., the truncation error when keeping the Taylor series expansion up to the 4$^{\text{th}}$-order derivative was estimated using Eqn. 8 for the first derivative (see Section S5 B) and a similar equation for the second derivative, giving a net maximal error of the order of 10^{-8} a.u. Effect of the step size and numerical rounding off in computation on the matrix element was estimated by calculating matrix elements of $\bar{\alpha}$ and γ using the wavefunctions obtained from using different step sizes. From this analysis it was found that uncertainty of the order of 10^{-8} a.u. exists due to above mentioned numerical errors and approximations, for any matrix element when h=0.004 a.u. was used.

When computing the wavelength dependent matrix elements of the polarizability invariants, the exact wavelength (say λ_i) at which the matrix element is sought might differ by up to a few nanometers with respect to the wavelength at which the invariant over distance is available (say $\lambda_i \pm q_i$). In the present work, q_i is up to $\sim$5 nm. In such case, there are two ways to compute the matrix element. First, the polarizability invariant can be interpolated over wavelength to obtain the required invariant as a function of distance for λ_i followed by computation of the matrix element. Secondly, the matrix elements can be computed at $\lambda_i + q_i$ (or $\lambda_i - q_i$) followed by interpolation (of the matrix elements) to obtain an interpolated value at λ_i. Both of these methods were tested to compute the respective matrix element at a given wavelength and the difference was found to be less than 1.0×10^{-7} a.u. revealing the low error in spline interpolation procedure achievable due to the densely spaced polarizability data points over wavelength.

The combined effect of all the errors discussed above, namely error due to spline interpolation, random noise in the potential, uncertainty in nuclear mass, the step size when generating the H-matrix, the uncertainty due to numerical rounding and interpolation of matrix elements over wavelength is no more than $\pm 1\times10^{-5}$ a.u. for any matrix element, and we regard this as the maximal numerical error.

S7. Tables of dissociation and transitions energies of H_2, D_2 and HD

TABLE T25. Dissociation energy (cm^{-1}) for H_2, HD and D_2.

Molecule	**Theory**					**Expt.**	
	Our	**Ref. 10**	Δ	**Others**	Δ	**Expt.**	Δ
H_2	36118.2167	36118.060	0.156	36118.069 [a]	0.147	36118.06962(37) [b]	0.1471
HD	36405.8720	36705.774	0.098	36405.7828 [c]	0.0892	36405.828(16) [b]	0.044
D_2	36748.4080	36748.355	0.053	36748.363 [a]	0.045	36748.36286(68) [d]	0.0451

[a] Ref. 11
[b] Ref. 12
[c] Ref. 13
[d] Ref. 14

TABLE T26. Transition energies (cm^{-1}) for H_2

	S0				O1			
	Our			Expt.	Our			Expt.
J_i	**Our**	Δ[a]	Δ[b]	Δ[c]	**Our**	Δ[a]	Δ[b]	Δ[d]
0	354.2035	−0.188	−0.1696	−0.1700				
1	586.7532	−0.279	−0.2788	−0.2789				
2	814.0419	−0.383	−0.3825	−0.3829	3806.7324	−0.043		−0.127
3	1034.1920	−0.480	−0.4787	−0.4782	3568.2741	0.070		0.035
4	1245.5336	−0.567	−0.5659	−0.5645	3329.2045	0.180		0.061
5	1446.6380	−0.644	−0.6429	−0.6408	3091.4729	0.288		0.332
6	1636.3370	−0.710			2856.8554	0.388		
7	1813.7288				2626.9195			
8	1978.1708				2403.0013			
	Q1				S1			
	Our			Expt.	Our			Expt.
J_i	**Our**	Δ[a]	Δ[b]	Δ[e]	**Our**	Δ[a]	Δ[b]	Δ[e]
0	4160.9359	−0.231	−0.2302	−0.2271	4497.4500	−0.391	−0.3884	−0.3891
1	4155.0273	−0.209	−0.2265	−0.2274	4712.4182	−0.471	−0.4864	−0.4872
2	4143.2464	−0.203	−0.2189	−0.2196	4916.4310	−0.562	−0.5753	−0.5759
3	4125.6649	−0.192	−0.2077	−0.2090	5107.7495	−0.641	−0.6534	−0.6545
4	4102.3891	−0.179	−0.1929	−0.1929	5284.8720	−0.709		
5	4073.5575	−0.162			5446.5641	−0.764		
6	4039.3383	−0.142			5591.8744	−0.805		
7	3999.9261				5720.1347			
8	3955.5374				5830.9481			

[a] Ref. 10
[b] Ref. 11
[c] Ref. 15
[d] Ref. 16
[e] Ref. 17

TABLE T27. $\Delta G(v+1/2)$ (cm^{-1}) for HD

	Theory				
v	**Our**	Δ[a]	Δ[b]	Δ[c]	Δ[d]
0	3632.0067	−0.147	−0.154	−0.1537	−0.1528
1	3454.5877	−0.129	−0.129		
2	3280.6508	−0.109	−0.103		
3	3109.1838	−0.084	−0.075		
4	2939.0983	−0.054	−0.046		
5	2769.1972	−0.023	−0.017		

[a] Ref. 10
[b] Ref. 18
[c] Ref. 13
[d] Ref. 19

TABLE T28. $P_v(J)$ and $R_v(J)$ line positions (cm^{-1}) for HD

Transition	Theory		Expt.
	Our	Δ^a	Δ^b
P1(3)	3355.3165	−0.052	−0.044
P1(2)	3450.3752	−0.085	−0.088
P1(1)	3542.8109	−0.118	−0.121
R1(0)	3717.3482	−0.181	−0.184
R1(1)	3798.2393	−0.210	−0.216
R1(2)	3874.1158	−0.236	−0.241
R1(3)	3944.4594	−0.260	−0.261
R1(4)	4008.8087	−0.279	−0.279

[a] Ref. 10
[b] Ref. 20

TABLE T29. Transition energies (cm^{-1}) for D_2

	S0				O1			
	Our			**Expt.**	**Our**			**Expt.**
J_i	**Our**	Δ^a	Δ^b	Δ^c	**Our**	Δ^a	Δ^b	Δ^d
0	179.0239	−0.045	−0.043	−0.044				
1	297.4623	−0.072	−0.071	−0.071				
2	414.5495	−0.099	−0.099	−0.099	2814.507	−0.032	−0.043	−0.039
3	529.7747	−0.126	−0.125	−0.125	2693.960	−0.003	−0.013	−0.012
4	642.6558	−0.151	−0.150	−0.150	2572.660	0.025	0.015	0.017
5	752.7452	−0.176	−0.174	−0.178	2451.132	0.053		
6	859.6354	−0.198	−0.197	−0.210	2329.879	0.081		
7	962.9626	−0.217			2209.372	0.109		
8	1062.4090	−0.236			2090.051	0.893		

	Q1				S1			
	Our			**Expt.**	**Our**			**Expt.**
J_i	**Our**	Δ^a	Δ^b	Δ^d	**Our**	Δ^a	Δ^b	Δ^d
0	2993.5309	−0.077	−0.1017	−0.0827	3166.2333	−0.119	−0.1272	−0.1263
1	2991.4216	−0.075	−0.0854	−0.0862	3278.3696	−0.143	−0.1535	−0.1526
2	2987.2093	−0.074	−0.0841	−0.0809	3387.0842	−0.169	−0.1784	−0.1764
3	2980.9073	−0.072	−0.0821	−0.0778	3491.8920	−0.192	−0.2017	−0.1993
4	2972.5350	−0.070	−0.0791		3592.3424	−0.215		
5	2962.1173	−0.067			3688.0251	−0.234		
6	2949.6866	−0.063			3778.5753	−0.252		
7	2935.2800	−0.058			3863.6767	−0.266		
8	2918.9400	−0.054			3943.0637	−0.279		

[a] Ref. 10
[b] Ref. 11
[c] Ref. 21
[d] Ref. 22

S8. Comparison of rotationally averaged mean polarizability and anisotropy with previous results

TABLE T30. Comparison of present rotationally averaged mean polarizability and anisotropy with the theoretical results of Schwartz and Le Roy (Ref. 1) at 488 nm.

Molecule	$\langle\psi_{v,J}\vert\gamma\vert\psi_{v',J'}\rangle$					$\langle\psi_{v,J}\vert\bar{\alpha}\vert\psi_{v',J'}\rangle$				
	$\vert v,J\rangle$	$\vert v',J'\rangle$	**Our**	**Ref. 1**	Δ	$\vert v,J\rangle$	$\vert v',J'\rangle$	**Our**	**Ref. 1**	Δ
H_2	$\vert 0,0\rangle$	$\vert 0,2\rangle$	2.1524	2.1514	0.0010	$\vert 0,0\rangle$	$\vert 1,0\rangle$	0.7879	0.7883	−0.0004
	$\vert 0,1\rangle$	$\vert 0,3\rangle$	2.1686	2.1677	0.0009	$\vert 0,1\rangle$	$\vert 1,1\rangle$	0.7891	0.7895	−0.0004
	$\vert 0,2\rangle$	$\vert 0,4\rangle$	2.1929	2.1920	0.0009	$\vert 0,2\rangle$	$\vert 1,2\rangle$	0.7915	0.7919	−0.0004
	$\vert 0,3\rangle$	$\vert 0,5\rangle$	2.2255	2.2246	0.0009	$\vert 0,3\rangle$	$\vert 1,3\rangle$	0.7951	0.7955	−0.0004
	$\vert 1,0\rangle$	$\vert 1,2\rangle$	2.6651	2.6641	0.0010					
	$\vert 1,1\rangle$	$\vert 1,3\rangle$	2.6824	2.6815	0.0009					
	$\vert 1,2\rangle$	$\vert 1,4\rangle$	2.7085	2.7075	0.0010					
	$\vert 1,3\rangle$	$\vert 1,5\rangle$	2.7432	2.7423	0.0009					
HD	$\vert 0,0\rangle$	$\vert 0,2\rangle$	2.1161	2.1151	0.0010	$\vert 0,0\rangle$	$\vert 1,0\rangle$	0.7299	0.7303	−0.0004
	$\vert 0,1\rangle$	$\vert 0,3\rangle$	2.1282	2.1272	0.0010	$\vert 0,1\rangle$	$\vert 1,1\rangle$	0.7307	0.7311	−0.0004
	$\vert 0,2\rangle$	$\vert 0,4\rangle$	2.1464	2.1454	0.0010	$\vert 0,2\rangle$	$\vert 1,2\rangle$	0.7324	0.7328	−0.0004
	$\vert 0,3\rangle$	$\vert 0,5\rangle$	2.1706	2.1697	0.0009	$\vert 0,3\rangle$	$\vert 1,3\rangle$	0.7349	0.7353	−0.0004
	$\vert 1,0\rangle$	$\vert 1,2\rangle$	2.5535	2.5525	0.0010					
	$\vert 1,1\rangle$	$\vert 1,3\rangle$	2.5664	2.5654	0.0010					
	$\vert 1,2\rangle$	$\vert 1,4\rangle$	2.5857	2.5847	0.0010					
	$\vert 1,3\rangle$	$\vert 1,5\rangle$	2.6115	2.6105	0.0010					
D_2	$\vert 0,0\rangle$	$\vert 0,2\rangle$	2.0742	2.0732	0.0010	$\vert 0,0\rangle$	$\vert 1,0\rangle$	0.6559	0.6563	−0.0004
	$\vert 0,1\rangle$	$\vert 0,3\rangle$	2.0822	2.0812	0.0010	$\vert 0,1\rangle$	$\vert 1,1\rangle$	0.6564	0.6568	−0.0004
	$\vert 0,2\rangle$	$\vert 0,4\rangle$	2.0942	2.0933	0.0009	$\vert 0,2\rangle$	$\vert 1,2\rangle$	0.6575	0.6578	−0.0003
	$\vert 0,3\rangle$	$\vert 0,5\rangle$	2.1103	2.1094	0.0009	$\vert 0,3\rangle$	$\vert 1,3\rangle$	0.6590	0.6593	−0.0003
	$\vert 1,0\rangle$	$\vert 1,2\rangle$	2.4250	2.4239	0.0011					
	$\vert 1,1\rangle$	$\vert 1,3\rangle$	2.4334	2.4324	0.0010					
	$\vert 1,2\rangle$	$\vert 1,4\rangle$	2.4461	2.4451	0.0010					
	$\vert 1,3\rangle$	$\vert 1,5\rangle$	2.4631	2.4620	0.0011					

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