

Incremental evaluation of coupled cluster dipole polarizabilities

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Table 1: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.54942	0.10274	-15.8
2	-0.65653	-0.00437	0.7
3	-0.65208	0.00008	-0.0
full	-0.65216		

Table 2: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.46865	0.12061	-20.5
2	-0.58786	0.00139	-0.2
3	-0.58923	0.00002	-0.0
full	-0.58925		

Table 3: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.36591	0.22335	-37.9
2	-0.59223	-0.00298	0.5
3	-0.58914	0.00011	-0.0
full	-0.58925		

Table 4: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	140.8	-5.0	-3.4
2	147.4	1.6	1.1
3	145.9	0.2	0.1
full	145.7		

Table 5: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	138.6	-4.5	-3.1
2	144.7	1.6	1.1
3	143.2	0.1	0.1
full	143.1		

Table 6: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	136.7	-4.1	-2.9
2	142.4	1.5	1.1
3	141.0	0.1	0.1
full	140.8		

Table 7: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	136.4	-4.0	-2.9
2	142.0	1.5	1.1
3	140.6	0.1	0.1
full	140.5		

Table 8: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.58072	0.09560	-14.1
2	-0.68044	-0.00412	0.6
3	-0.67630	0.00002	-0.0
full	-0.67632		

Table 9: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.51367	0.11194	-17.9
2	-0.62505	0.00056	-0.1
3	-0.62564	-0.00003	0.0
full	-0.62561		

Table 10: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.41808	0.20753	-33.2
2	-0.62917	-0.00356	0.6
3	-0.62562	-0.00001	0.0
full	-0.62561		

Table 11: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	114.7	-5.5	-4.5
2	122.7	2.5	2.1
3	120.0	-0.2	-0.2
full	120.2		

Table 12: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	113.0	-5.0	-4.3
2	120.4	2.4	2.0
3	117.9	-0.2	-0.2
full	118.0		

Table 13: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	111.6	-4.7	-4.0
2	118.6	2.3	2.0
3	116.1	-0.2	-0.2
full	116.2		

Table 14: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	111.4	-4.6	-4.0
2	118.3	2.3	2.0
3	115.8	-0.2	-0.2
full	116.0		

Table 15: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.62704	0.11079	-15.0
2	-0.73932	-0.00150	0.2
3	-0.73784	-0.00002	0.0
full	-0.73782		

Table 16: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.54460	0.13477	-19.8
2	-0.67887	0.00050	-0.1
3	-0.67940	-0.00002	0.0
full	-0.67938		

Table 17: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.43382	0.24556	-36.1
2	-0.68038	-0.00100	0.1
3	-0.67942	-0.00004	0.0
full	-0.67938		

Table 18: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	169.0	-26.6	-13.6
2	191.3	-4.3	-2.2
3	195.7	0.1	0.1
full	195.6		

Table 19: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	164.7	-21.7	-11.7
2	183.4	-3.0	-1.6
3	186.6	0.1	0.1
full	186.5		

Table 20: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	161.2	-18.4	-10.2
2	177.4	-2.2	-1.2
3	179.7	0.1	0.1
full	179.6		

Table 21: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.7	-17.9	-10.0
2	176.5	-2.1	-1.2
3	178.7	0.1	0.1
full	178.6		

Table 22: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.62138	0.11691	-15.8
2	-0.74183	-0.00354	0.5
3	-0.73835	-0.00006	0.0
full	-0.73829		

Table 23: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.53388	0.14538	-21.4
2	-0.67900	0.00026	-0.0
3	-0.67925	0.00001	-0.0
full	-0.67926		

Table 24: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.41697	0.26229	-38.6
2	-0.68254	-0.00328	0.5
3	-0.67932	-0.00005	0.0
full	-0.67926		

Table 25: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.9	-24.4	-13.2
2	181.4	-4.0	-2.2
3	185.2	-0.2	-0.1
full	185.4		

Table 26: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	157.8	-21.7	-12.1
2	176.2	-3.2	-1.8
3	179.4	-0.1	-0.1
full	179.5		

Table 27: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	155.1	-19.6	-11.2
2	172.0	-2.6	-1.5
3	174.6	-0.0	-0.0
full	174.7		

Table 28: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	154.7	-19.2	-11.1
2	171.4	-2.6	-1.5
3	173.9	-0.0	-0.0
full	174.0		

Table 29: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.65349	0.11924	-15.4
2	-0.77617	-0.00345	0.4
3	-0.77283	-0.00010	0.0
full	-0.77273		

Table 30: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.56136	0.14407	-20.4
2	-0.70484	0.00059	-0.1
3	-0.70550	-0.00007	0.0
full	-0.70543		

Table 31: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.44212	0.26331	-37.3
2	-0.70829	-0.00286	0.4
3	-0.70561	-0.00017	0.0
full	-0.70543		

Table 32: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	168.6	-11.9	-6.6
2	177.1	-3.4	-1.9
3	180.6	0.1	0.1
full	180.5		

Table 33: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	165.5	-10.5	-6.0
2	173.0	-3.0	-1.7
3	176.2	0.1	0.1
full	176.0		

Table 34: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	162.9	-9.4	-5.5
2	169.7	-2.7	-1.6
3	172.5	0.1	0.1
full	172.4		

Table 35: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	162.5	-9.2	-5.4
2	169.1	-2.7	-1.5
3	171.9	0.1	0.1
full	171.8		

Table 36: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.67205	0.10111	-13.1
2	-0.77620	-0.00305	0.4
3	-0.77312	0.00004	-0.0
full	-0.77315		

Table 37: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.58347	0.12180	-17.3
2	-0.70401	0.00126	-0.2
3	-0.70523	0.00004	-0.0
full	-0.70527		

Table 38: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.48236	0.22291	-31.6
2	-0.70705	-0.00178	0.3
3	-0.70519	0.00008	-0.0
full	-0.70527		

Table 39: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	166.6	-10.0	-5.6
2	176.9	0.3	0.2
3	176.6	0.1	0.0
full	176.6		

Table 40: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	163.6	-8.9	-5.2
2	172.9	0.4	0.2
3	172.6	0.0	0.0
full	172.5		

Table 41: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	161.0	-8.1	-4.8
2	169.5	0.4	0.2
3	169.2	0.0	0.0
full	169.1		

Table 42: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.6	-8.0	-4.7
2	169.0	0.4	0.3
3	168.6	0.0	0.0
full	168.6		

Table 43: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.66005	0.11323	-14.6
2	-0.77577	-0.00250	0.3
3	-0.77334	-0.00007	0.0
full	-0.77327		

Table 44: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.56828	0.13778	-19.5
2	-0.70571	0.00036	-0.1
3	-0.70610	-0.00004	0.0
full	-0.70606		

Table 45: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.45506	0.25100	-35.5
2	-0.70820	-0.00214	0.3
3	-0.70617	-0.00010	0.0
full	-0.70606		

Table 46: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	166.0	-12.3	-6.9
2	179.1	0.8	0.4
3	178.2	-0.1	-0.1
full	178.3		

Table 47: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	163.0	-11.0	-6.3
2	174.9	0.9	0.5
3	173.9	-0.1	-0.1
full	174.0		

Table 48: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.5	-9.9	-5.8
2	171.4	1.0	0.6
3	170.3	-0.1	-0.0
full	170.4		

Table 49: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.1	-9.7	-5.7
2	170.9	1.0	0.6
3	169.8	-0.1	-0.0
full	169.8		

Table 50: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.70440	0.09832	-12.2
2	-0.80656	-0.00384	0.5
3	-0.80262	0.00011	-0.0
full	-0.80273		

Table 51: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.63262	0.11810	-15.7
2	-0.74978	0.00094	-0.1
3	-0.75066	0.00005	-0.0
full	-0.75072		

Table 52: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.53429	0.21642	-28.8
2	-0.75361	-0.00290	0.4
3	-0.75056	0.00016	-0.0
full	-0.75072		

Table 53: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	136.6	-8.1	-5.6
2	145.7	0.9	0.7
3	144.8	0.0	0.0
full	144.8		

Table 54: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	134.6	-7.5	-5.3
2	143.1	1.0	0.7
3	142.1	-0.0	-0.0
full	142.1		

Table 55: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	132.9	-7.0	-5.0
2	140.9	1.0	0.7
3	139.9	-0.0	-0.0
full	139.9		

Table 56: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	132.6	-6.9	-5.0
2	140.5	1.0	0.7
3	139.5	-0.0	-0.0
full	139.6		

Table 57: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.72698	0.16548	-18.5
2	-0.90186	-0.00940	1.1
3	-0.89275	-0.00029	0.0
full	-0.89246		

Table 58: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.64961	0.20321	-23.8
2	-0.84878	0.00404	-0.5
3	-0.85371	-0.00089	0.1
full	-0.85282		

Table 59: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.48413	0.36869	-43.2
2	-0.85818	-0.00536	0.6
3	-0.85400	-0.00118	0.1
full	-0.85282		

Table 60: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	158.8	-5.4	-3.3
2	171.5	7.3	4.4
3	164.7	0.5	0.3
full	164.2		

Table 61: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	155.6	-4.0	-2.5
2	166.5	6.8	4.3
3	159.9	0.3	0.2
full	159.7		

Table 62: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	153.0	-3.0	-1.9
2	162.4	6.4	4.1
3	156.1	0.1	0.1
full	156.0		

Table 63: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	152.6	-2.9	-1.9
2	161.8	6.3	4.1
3	155.6	0.1	0.0
full	155.5		

Table 64: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.76892	0.14000	-15.4
2	-0.91569	-0.00677	0.7
3	-0.90881	0.00012	-0.0
full	-0.90892		

Table 65: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.66608	0.17267	-20.6
2	-0.83744	0.00130	-0.2
3	-0.83880	-0.00006	0.0
full	-0.83875		

Table 66: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.52608	0.31267	-37.3
2	-0.84421	-0.00547	0.7
3	-0.83869	0.00006	-0.0
full	-0.83875		

Table 67: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	189.2	-18.5	-8.9
2	210.9	3.2	1.5
3	207.5	-0.2	-0.1
full	207.7		

Table 68: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	186.1	-16.5	-8.1
2	205.9	3.3	1.6
3	202.4	-0.1	-0.1
full	202.6		

Table 69: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	183.5	-14.9	-7.5
2	201.8	3.4	1.7
3	198.3	-0.1	-0.1
full	198.4		

Table 70: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	183.1	-14.7	-7.4
2	201.1	3.4	1.7
3	197.6	-0.1	-0.1
full	197.7		

Table 71: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **11**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.77693	0.15207	-16.4
2	-0.93175	-0.00276	0.3
3	-0.92906	-0.00007	0.0
full	-0.92899		

Table 72: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **11**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.66627	0.18287	-21.5
2	-0.84820	0.00094	-0.1
3	-0.84919	-0.00005	0.0
full	-0.84914		

Table 73: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **11**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.51421	0.33493	-39.4
2	-0.85096	-0.00182	0.2
3	-0.84926	-0.00012	0.0
full	-0.84914		

Table 74: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **11**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.5	-16.6	-7.6
2	213.6	-4.6	-2.1
3	218.0	-0.2	-0.1
full	218.2		

Table 75: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **11**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	198.0	-14.8	-6.9
2	208.8	-3.9	-1.9
3	212.6	-0.1	-0.1
full	212.7		

Table 76: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **11**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	194.9	-13.3	-6.4
2	204.8	-3.5	-1.7
3	208.2	-0.1	-0.0
full	208.3		

Table 77: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **11**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	194.5	-13.1	-6.3
2	204.2	-3.4	-1.6
3	207.5	-0.1	-0.0
full	207.6		

Table 78: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79755	0.13601	-14.6
2	-0.94313	-0.00957	1.0
3	-0.93281	0.00074	-0.1
full	-0.93356		

Table 79: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.68953	0.16645	-19.4
2	-0.85369	0.00228	-0.3
3	-0.85561	0.00037	-0.0
full	-0.85597		

Table 80: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.55352	0.30245	-35.3
2	-0.86327	-0.00729	0.9
3	-0.85486	0.00111	-0.1
full	-0.85597		

Table 81: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.4	-16.2	-7.5
2	220.9	3.3	1.5
3	218.6	1.1	0.5
full	217.6		

Table 82: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	197.8	-14.1	-6.6
2	215.5	3.6	1.7
3	212.9	0.9	0.4
full	211.9		

Table 83: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	194.9	-12.4	-6.0
2	211.1	3.8	1.8
3	208.2	0.8	0.4
full	207.3		

Table 84: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	194.4	-12.2	-5.9
2	210.4	3.8	1.8
3	207.4	0.8	0.4
full	206.6		

Table 85: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **13**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.83224	0.12015	-12.6
2	-0.95631	-0.00393	0.4
3	-0.95241	-0.00002	0.0
full	-0.95239		

Table 86: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **13**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.73553	0.14934	-16.9
2	-0.88480	0.00008	-0.0
3	-0.88482	0.00006	-0.0
full	-0.88488		

Table 87: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **13**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.61538	0.26949	-30.5
2	-0.88872	-0.00385	0.4
3	-0.88483	0.00004	-0.0
full	-0.88488		

Table 88: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **13**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	180.8	-24.3	-11.9
2	202.0	-3.2	-1.6
3	204.9	-0.2	-0.1
full	205.1		

Table 89: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **13**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	177.3	-21.6	-10.9
2	196.5	-2.5	-1.2
3	198.8	-0.1	-0.1
full	198.9		

Table 90: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **13**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.3	-19.5	-10.1
2	192.0	-1.9	-1.0
3	193.8	-0.1	-0.0
full	193.9		

Table 91: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **13**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	173.9	-19.2	-10.0
2	191.3	-1.8	-1.0
3	193.0	-0.1	-0.0
full	193.1		

Table 92: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **14**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.83218	0.12021	-12.6
2	-0.95631	-0.00392	0.4
3	-0.95241	-0.00002	0.0
full	-0.95239		

Table 93: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **14**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.73546	0.14943	-16.9
2	-0.88479	0.00010	-0.0
3	-0.88483	0.00006	-0.0
full	-0.88489		

Table 94: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **14**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.61525	0.26964	-30.5
2	-0.88871	-0.00382	0.4
3	-0.88485	0.00004	-0.0
full	-0.88489		

Table 95: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **14**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	180.9	-24.5	-11.9
2	202.2	-3.2	-1.6
3	205.2	-0.2	-0.1
full	205.4		

Table 96: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **14**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	177.4	-21.8	-10.9
2	196.7	-2.5	-1.2
3	199.0	-0.1	-0.1
full	199.1		

Table 97: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **14**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.4	-19.7	-10.2
2	192.2	-1.9	-1.0
3	194.0	-0.1	-0.0
full	194.1		

Table 98: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **14**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	173.9	-19.4	-10.0
2	191.5	-1.9	-1.0
3	193.3	-0.0	-0.0
full	193.3		

Table 99: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.83261	0.12076	-12.7
2	-0.95713	-0.00376	0.4
3	-0.95343	-0.00005	0.0
full	-0.95337		

Table 100: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.73608	0.14999	-16.9
2	-0.88578	0.00029	-0.0
3	-0.88606	0.00001	-0.0
full	-0.88607		

Table 101: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.61532	0.27074	-30.6
2	-0.88954	-0.00347	0.4
3	-0.88611	-0.00005	0.0
full	-0.88607		

Table 102: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	181.6	-24.2	-11.8
2	203.3	-2.6	-1.2
3	205.7	-0.1	-0.1
full	205.8		

Table 103: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	178.1	-21.5	-10.8
2	197.7	-1.9	-0.9
3	199.5	-0.0	-0.0
full	199.6		

Table 104: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	175.1	-19.4	-10.0
2	193.1	-1.4	-0.7
3	194.5	0.0	0.0
full	194.5		

Table 105: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.6	-19.1	-9.9
2	192.4	-1.3	-0.7
3	193.7	0.0	0.0
full	193.7		

Table 106: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.78345	0.17577	-18.3
2	-0.96652	-0.00730	0.8
3	-0.95928	-0.00006	0.0
full	-0.95922		

Table 107: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.68651	0.20744	-23.2
2	-0.89220	0.00174	-0.2
3	-0.89409	-0.00015	0.0
full	-0.89394		

Table 108: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.51073	0.38321	-42.9
2	-0.89950	-0.00556	0.6
3	-0.89415	-0.00021	0.0
full	-0.89394		

Table 109: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	171.8	-7.4	-4.1
2	180.1	0.9	0.5
3	179.1	-0.1	-0.1
full	179.2		

Table 110: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	169.3	-6.6	-3.7
2	176.8	0.9	0.5
3	175.8	-0.1	-0.0
full	175.9		

Table 111: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	167.2	-5.9	-3.4
2	174.0	1.0	0.6
3	173.0	-0.1	-0.0
full	173.1		

Table 112: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	166.8	-5.8	-3.4
2	173.6	1.0	0.6
3	172.6	-0.1	-0.0
full	172.6		

Table 113: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.78082	0.18388	-19.1
2	-0.96892	-0.00423	0.4
3	-0.96496	-0.00027	0.0
full	-0.96469		

Table 114: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.65932	0.21678	-24.7
2	-0.87470	0.00140	-0.2
3	-0.87632	-0.00023	0.0
full	-0.87610		

Table 115: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.47544	0.40065	-45.7
2	-0.87893	-0.00283	0.3
3	-0.87659	-0.00049	0.1
full	-0.87610		

Table 116: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	208.9	-7.4	-3.4
2	214.0	-2.2	-1.0
3	216.4	0.1	0.0
full	216.3		

Table 117: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.7	-6.6	-3.1
2	210.2	-2.1	-1.0
3	212.4	0.1	0.1
full	212.3		

Table 118: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.9	-6.0	-2.9
2	206.9	-2.0	-0.9
3	209.0	0.1	0.1
full	208.9		

Table 119: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.4	-5.9	-2.8
2	206.4	-2.0	-0.9
3	208.5	0.1	0.1
full	208.4		

Table 120: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.84505	0.12431	-12.8
2	-0.97558	-0.00622	0.6
3	-0.96924	0.00012	-0.0
full	-0.96936		

Table 121: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.76473	0.14750	-16.2
2	-0.91069	0.00154	-0.2
3	-0.91205	0.00018	-0.0
full	-0.91223		

Table 122: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.64042	0.27181	-29.8
2	-0.91690	-0.00467	0.5
3	-0.91193	0.00030	-0.0
full	-0.91223		

Table 123: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	158.0	-10.3	-6.1
2	171.5	3.2	1.9
3	168.6	0.3	0.2
full	168.3		

Table 124: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	155.6	-9.3	-5.6
2	168.0	3.1	1.9
3	165.1	0.3	0.2
full	164.9		

Table 125: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	153.5	-8.5	-5.3
2	165.0	3.0	1.9
3	162.2	0.2	0.2
full	162.0		

Table 126: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	153.1	-8.4	-5.2
2	164.5	3.0	1.8
3	161.8	0.2	0.1
full	161.5		

Table 127: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.83716	0.13390	-13.8
2	-0.97951	-0.00845	0.9
3	-0.97048	0.00058	-0.1
full	-0.97106		

Table 128: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.72398	0.16112	-18.2
2	-0.88183	0.00327	-0.4
3	-0.88514	-0.00004	0.0
full	-0.88510		

Table 129: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.59008	0.29502	-33.3
2	-0.89028	-0.00518	0.6
3	-0.88457	0.00053	-0.1
full	-0.88510		

Table 130: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	208.5	-4.6	-2.1
2	221.6	8.5	4.0
3	211.2	-1.9	-0.9
full	213.1		

Table 131: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.3	-3.9	-1.9
2	217.4	8.1	3.9
3	207.5	-1.8	-0.9
full	209.3		

Table 132: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.6	-3.4	-1.7
2	213.8	7.8	3.8
3	204.3	-1.7	-0.8
full	206.0		

Table 133: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.2	-3.4	-1.6
2	213.3	7.8	3.8
3	203.8	-1.7	-0.8
full	205.5		

Table 134: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.85317	0.12373	-12.7
2	-0.98093	-0.00403	0.4
3	-0.97706	-0.00016	0.0
full	-0.97690		

Table 135: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.77627	0.14769	-16.0
2	-0.92312	0.00084	-0.1
3	-0.92414	-0.00018	0.0
full	-0.92396		

Table 136: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.65254	0.27142	-29.4
2	-0.92714	-0.00318	0.3
3	-0.92430	-0.00033	0.0
full	-0.92396		

Table 137: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	145.1	-9.8	-6.3
2	154.2	-0.7	-0.5
3	155.4	0.4	0.3
full	154.9		

Table 138: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	143.0	-9.1	-6.0
2	151.5	-0.6	-0.4
3	152.4	0.4	0.2
full	152.1		

Table 139: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	141.2	-8.5	-5.7
2	149.1	-0.5	-0.4
3	150.0	0.4	0.2
full	149.7		

Table 140: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	140.9	-8.4	-5.6
2	148.7	-0.5	-0.4
3	149.6	0.3	0.2
full	149.3		

Table 141: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **21**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81184	0.17659	-17.9
2	-0.99247	-0.00405	0.4
3	-0.98867	-0.00025	0.0
full	-0.98842		

Table 142: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **21**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.70406	0.20780	-22.8
2	-0.91067	0.00119	-0.1
3	-0.91207	-0.00021	0.0
full	-0.91186		

Table 143: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **21**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.52747	0.38439	-42.2
2	-0.91472	-0.00286	0.3
3	-0.91232	-0.00046	0.1
full	-0.91186		

Table 144: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **21**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	182.8	-7.6	-4.0
2	189.5	-1.0	-0.5
3	190.6	0.1	0.1
full	190.5		

Table 145: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **21**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	180.1	-6.9	-3.7
2	186.1	-0.9	-0.5
3	187.2	0.1	0.1
full	187.0		

Table 146: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **21**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	177.8	-6.4	-3.5
2	183.3	-0.9	-0.5
3	184.3	0.1	0.1
full	184.1		

Table 147: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **21**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	177.4	-6.3	-3.4
2	182.8	-0.9	-0.5
3	183.8	0.1	0.1
full	183.7		

Table 148: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.84852	0.16415	-16.2
2	-1.01899	-0.00632	0.6
3	-1.01303	-0.00036	0.0
full	-1.01267		

Table 149: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.75572	0.19260	-20.3
2	-0.94709	0.00123	-0.1
3	-0.94870	-0.00038	0.0
full	-0.94832		

Table 150: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.59158	0.35674	-37.6
2	-0.95341	-0.00509	0.5
3	-0.94906	-0.00074	0.1
full	-0.94832		

Table 151: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	155.1	-9.8	-6.0
2	166.6	1.8	1.1
3	165.4	0.5	0.3
full	164.9		

Table 152: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	152.9	-9.1	-5.6
2	163.7	1.7	1.1
3	162.5	0.5	0.3
full	162.0		

Table 153: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	151.1	-8.5	-5.3
2	161.2	1.7	1.1
3	160.0	0.5	0.3
full	159.5		

Table 154: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	150.8	-8.4	-5.3
2	160.8	1.7	1.1
3	159.6	0.5	0.3
full	159.1		

Table 155: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.82946	0.19027	-18.7
2	-1.02286	-0.00313	0.3
3	-1.01975	-0.00002	0.0
full	-1.01973		

Table 156: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.71270	0.23474	-24.8
2	-0.94573	0.00171	-0.2
3	-0.94750	-0.00006	0.0
full	-0.94744		

Table 157: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.52243	0.42501	-44.9
2	-0.94887	-0.00143	0.2
3	-0.94752	-0.00008	0.0
full	-0.94744		

Table 158: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	212.9	-12.9	-5.7
2	231.8	6.0	2.6
3	227.1	1.3	0.6
full	225.8		

Table 159: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	209.0	-11.4	-5.2
2	226.0	5.7	2.6
3	221.4	1.1	0.5
full	220.3		

Table 160: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.6	-10.2	-4.7
2	221.2	5.4	2.5
3	216.8	1.0	0.5
full	215.8		

Table 161: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.1	-10.0	-4.6
2	220.5	5.4	2.5
3	216.0	1.0	0.4
full	215.1		

Table 162: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **24**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.88284	0.15444	-14.9
2	-1.04103	-0.00375	0.4
3	-1.03744	-0.00016	0.0
full	-1.03728		

Table 163: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **24**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.78719	0.18895	-19.4
2	-0.97481	0.00133	-0.1
3	-0.97633	-0.00019	0.0
full	-0.97614		

Table 164: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **24**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.63275	0.34339	-35.2
2	-0.97856	-0.00242	0.2
3	-0.97649	-0.00035	0.0
full	-0.97614		

Table 165: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **24**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.2	-17.4	-7.9
2	218.7	0.2	0.1
3	218.5	-0.0	-0.0
full	218.5		

Table 166: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **24**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	197.4	-15.0	-7.1
2	213.0	0.6	0.3
3	212.4	-0.0	-0.0
full	212.4		

Table 167: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **24**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	194.2	-13.3	-6.4
2	208.4	0.9	0.4
3	207.5	0.0	0.0
full	207.5		

Table 168: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **24**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.7	-13.0	-6.3
2	207.7	0.9	0.4
3	206.8	0.0	0.0
full	206.8		

Table 169: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **25**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.90426	0.15158	-14.4
2	-1.05953	-0.00368	0.3
3	-1.05595	-0.00010	0.0
full	-1.05585		

Table 170: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **25**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.77993	0.18749	-19.4
2	-0.96704	0.00038	-0.0
3	-0.96743	-0.00002	0.0
full	-0.96742		

Table 171: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **25**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.62834	0.33907	-35.0
2	-0.97072	-0.00330	0.3
3	-0.96754	-0.00012	0.0
full	-0.96742		

Table 172: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **25**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	223.7	-28.0	-11.1
2	250.6	-1.1	-0.4
3	251.9	0.2	0.1
full	251.7		

Table 173: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **25**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	219.7	-25.1	-10.2
2	244.2	-0.5	-0.2
3	245.0	0.3	0.1
full	244.8		

Table 174: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **25**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	216.3	-22.8	-9.6
2	239.0	-0.1	-0.1
3	239.4	0.3	0.1
full	239.1		

Table 175: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **25**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	215.8	-22.5	-9.4
2	238.2	-0.1	-0.0
3	238.5	0.3	0.1
full	238.3		

Table 176: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **26**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.90440	0.15153	-14.4
2	-1.05949	-0.00355	0.3
3	-1.05600	-0.00006	0.0
full	-1.05594		

Table 177: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **26**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.78005	0.18740	-19.4
2	-0.96699	0.00047	-0.0
3	-0.96745	0.00001	-0.0
full	-0.96746		

Table 178: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **26**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.62852	0.33894	-35.0
2	-0.97054	-0.00308	0.3
3	-0.96751	-0.00006	0.0
full	-0.96746		

Table 179: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **26**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	223.7	-27.8	-11.0
2	250.4	-1.1	-0.4
3	251.6	0.1	0.1
full	251.5		

Table 180: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **26**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	219.7	-24.8	-10.2
2	244.0	-0.5	-0.2
3	244.7	0.2	0.1
full	244.5		

Table 181: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **26**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	216.3	-22.6	-9.4
2	238.7	-0.1	-0.1
3	239.0	0.2	0.1
full	238.8		

Table 182: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **26**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	215.7	-22.2	-9.3
2	237.9	-0.1	-0.0
3	238.1	0.2	0.1
full	237.9		

Table 183: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.92130	0.16441	-15.1
2	-1.08848	-0.00277	0.3
3	-1.08578	-0.00007	0.0
full	-1.08570		

Table 184: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79472	0.19743	-19.9
2	-0.99107	0.00109	-0.1
3	-0.99220	-0.00005	0.0
full	-0.99215		

Table 185: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.63032	0.36184	-36.5
2	-0.99384	-0.00168	0.2
3	-0.99227	-0.00012	0.0
full	-0.99215		

Table 186: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	235.8	-12.6	-5.1
2	242.4	-6.0	-2.4
3	248.1	-0.3	-0.1
full	248.4		

Table 187: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	231.5	-11.3	-4.7
2	237.3	-5.5	-2.3
3	242.7	-0.2	-0.1
full	242.9		

Table 188: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	228.0	-10.3	-4.3
2	233.1	-5.1	-2.2
3	238.1	-0.1	-0.1
full	238.3		

Table 189: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	227.4	-10.1	-4.3
2	232.5	-5.1	-2.1
3	237.4	-0.1	-0.1
full	237.5		

Table 190: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **28**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.92164	0.19391	-17.4
2	-1.12675	-0.01120	1.0
3	-1.11525	0.00030	-0.0
full	-1.11555		

Table 191: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **28**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.80921	0.22887	-22.0
2	-1.03596	0.00212	-0.2
3	-1.03789	0.00019	-0.0
full	-1.03808		

Table 192: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **28**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.61530	0.42279	-40.7
2	-1.04715	-0.00907	0.9
3	-1.03759	0.00049	-0.0
full	-1.03808		

Table 193: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **28**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	204.4	-11.2	-5.2
2	215.4	-0.2	-0.1
3	215.1	-0.4	-0.2
full	215.6		

Table 194: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **28**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.4	-10.1	-4.8
2	211.5	-0.0	-0.0
3	211.2	-0.4	-0.2
full	211.5		

Table 195: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **28**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	198.9	-9.3	-4.5
2	208.2	0.1	0.0
3	207.8	-0.3	-0.1
full	208.1		

Table 196: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **28**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	198.5	-9.1	-4.4
2	207.7	0.1	0.0
3	207.3	-0.3	-0.1
full	207.6		

Table 197: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **29**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.92384	0.20605	-18.2
2	-1.13932	-0.00943	0.8
3	-1.13064	-0.00076	0.1
full	-1.12989		

Table 198: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **29**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81323	0.24737	-23.3
2	-1.05575	0.00485	-0.5
3	-1.06169	-0.00109	0.1
full	-1.06060		

Table 199: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **29**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.60718	0.45341	-42.8
2	-1.06518	-0.00459	0.4
3	-1.06245	-0.00185	0.2
full	-1.06060		

Table 200: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **29**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.6	-16.0	-7.6
2	213.8	4.2	2.0
3	208.7	-0.9	-0.4
full	209.5		

Table 201: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **29**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	190.6	-14.1	-6.9
2	209.2	4.6	2.2
3	203.9	-0.7	-0.4
full	204.6		

Table 202: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **29**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	188.0	-12.6	-6.3
2	205.4	4.8	2.4
3	199.9	-0.7	-0.3
full	200.6		

Table 203: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **29**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	187.6	-12.4	-6.2
2	204.8	4.8	2.4
3	199.3	-0.7	-0.3
full	200.0		

Table 204: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.96849	0.16718	-14.7
2	-1.14082	-0.00515	0.5
3	-1.13591	-0.00024	0.0
full	-1.13567		

Table 205: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.87243	0.19933	-18.6
2	-1.07047	0.00129	-0.1
3	-1.07196	-0.00019	0.0
full	-1.07176		

Table 206: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.70526	0.36651	-34.2
2	-1.07562	-0.00386	0.4
3	-1.07220	-0.00044	0.0
full	-1.07176		

Table 207: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	179.7	-11.0	-5.8
2	189.7	-1.0	-0.5
3	190.9	0.1	0.1
full	190.7		

Table 208: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	177.1	-10.1	-5.4
2	186.3	-0.8	-0.4
3	187.3	0.2	0.1
full	187.1		

Table 209: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.8	-9.3	-5.0
2	183.4	-0.7	-0.4
3	184.3	0.2	0.1
full	184.1		

Table 210: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.5	-9.2	-5.0
2	182.9	-0.7	-0.4
3	183.8	0.2	0.1
full	183.6		

Table 211: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.95689	0.20583	-17.7
2	-1.16944	-0.00673	0.6
3	-1.16372	-0.00101	0.1
full	-1.16271		

Table 212: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.85318	0.24291	-22.2
2	-1.09325	0.00284	-0.3
3	-1.09699	-0.00089	0.1
full	-1.09610		

Table 213: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.64736	0.44874	-40.9
2	-1.09999	-0.00389	0.4
3	-1.09800	-0.00190	0.2
full	-1.09610		

Table 214: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.5	-16.1	-7.3
2	220.7	-1.0	-0.4
3	220.6	-1.1	-0.5
full	221.6		

Table 215: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.3	-14.1	-6.5
2	216.0	-0.4	-0.2
3	215.5	-0.9	-0.4
full	216.4		

Table 216: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.6	-12.7	-6.0
2	212.2	-0.0	-0.0
3	211.4	-0.9	-0.4
full	212.2		

Table 217: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.1	-12.4	-5.9
2	211.6	0.0	0.0
3	210.7	-0.8	-0.4
full	211.6		

Table 218: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **32**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.04334	0.12356	-10.6
2	-1.17097	-0.00407	0.3
3	-1.16692	-0.00002	0.0
full	-1.16690		

Table 219: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **32**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.93745	0.15343	-14.1
2	-1.09069	0.00019	-0.0
3	-1.09084	0.00004	-0.0
full	-1.09088		

Table 220: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **32**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81389	0.27699	-25.4
2	-1.09476	-0.00388	0.4
3	-1.09086	0.00002	-0.0
full	-1.09088		

Table 221: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **32**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	200.3	-25.1	-11.2
2	223.9	-1.6	-0.7
3	225.3	-0.1	-0.0
full	225.4		

Table 222: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **32**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	196.4	-22.4	-10.3
2	217.9	-0.9	-0.4
3	218.8	-0.0	-0.0
full	218.8		

Table 223: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **32**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.1	-20.3	-9.5
2	213.0	-0.5	-0.2
3	213.5	0.0	0.0
full	213.5		

Table 224: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **32**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.6	-20.0	-9.4
2	212.2	-0.4	-0.2
3	212.7	0.0	0.0
full	212.6		

Table 225: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **33**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.04349	0.12464	-10.7
2	-1.17192	-0.00379	0.3
3	-1.16818	-0.00005	0.0
full	-1.16813		

Table 226: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **33**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.93822	0.15425	-14.1
2	-1.09217	0.00030	-0.0
3	-1.09246	0.00000	-0.0
full	-1.09247		

Table 227: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **33**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81358	0.27889	-25.5
2	-1.09596	-0.00349	0.3
3	-1.09251	-0.00005	0.0
full	-1.09247		

Table 228: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **33**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.8	-26.0	-11.5
2	223.5	-2.4	-1.0
3	226.0	0.1	0.1
full	225.9		

Table 229: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **33**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	196.0	-23.2	-10.6
2	217.5	-1.7	-0.8
3	219.4	0.2	0.1
full	219.2		

Table 230: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **33**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.8	-21.0	-9.8
2	212.7	-1.2	-0.6
3	214.1	0.2	0.1
full	213.9		

Table 231: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **33**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.3	-20.7	-9.7
2	211.9	-1.1	-0.5
3	213.2	0.2	0.1
full	213.0		

Table 232: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **34**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.04261	0.12578	-10.8
2	-1.17065	-0.00225	0.2
3	-1.16844	-0.00004	0.0
full	-1.16840		

Table 233: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **34**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.93798	0.15503	-14.2
2	-1.09226	0.00074	-0.1
3	-1.09303	-0.00003	0.0
full	-1.09300		

Table 234: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **34**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81219	0.28081	-25.7
2	-1.09451	-0.00151	0.1
3	-1.09307	-0.00007	0.0
full	-1.09300		

Table 235: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **34**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.5	-26.7	-11.8
2	222.8	-3.4	-1.5
3	226.2	-0.0	-0.0
full	226.2		

Table 236: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **34**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	195.8	-23.9	-10.9
2	217.0	-2.7	-1.2
3	219.6	0.0	0.0
full	219.6		

Table 237: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **34**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.6	-21.7	-10.1
2	212.1	-2.1	-1.0
3	214.3	0.1	0.0
full	214.3		

Table 238: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **34**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.1	-21.3	-10.0
2	211.4	-2.1	-1.0
3	213.5	0.1	0.0
full	213.4		

Table 239: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **35**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.01228	0.16039	-13.7
2	-1.18230	-0.00962	0.8
3	-1.17251	0.00017	-0.0
full	-1.17268		

Table 240: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **35**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.90855	0.18824	-17.2
2	-1.09509	0.00170	-0.2
3	-1.09679	-0.00000	0.0
full	-1.09679		

Table 241: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **35**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.74816	0.34863	-31.8
2	-1.10471	-0.00792	0.7
3	-1.09663	0.00016	-0.0
full	-1.09679		

Table 242: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **35**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	189.7	-9.3	-4.7
2	202.6	3.6	1.8
3	198.8	-0.2	-0.1
full	199.0		

Table 243: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **35**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	186.9	-8.6	-4.4
2	199.1	3.5	1.8
3	195.4	-0.2	-0.1
full	195.5		

Table 244: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **35**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	184.6	-8.0	-4.2
2	196.0	3.5	1.8
3	192.4	-0.2	-0.1
full	192.6		

Table 245: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **35**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	184.2	-7.9	-4.1
2	195.6	3.5	1.8
3	191.9	-0.2	-0.1
full	192.1		

Table 246: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **36**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.10481	0.15098	-12.0
2	-1.26105	-0.00527	0.4
3	-1.25581	-0.00003	0.0
full	-1.25578		

Table 247: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **36**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.00379	0.18170	-15.3
2	-1.18391	0.00158	-0.1
3	-1.18538	0.00012	-0.0
full	-1.18549		

Table 248: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **36**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.85282	0.33267	-28.1
2	-1.18918	-0.00369	0.3
3	-1.18541	0.00008	-0.0
full	-1.18549		

Table 249: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **36**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.3	-25.3	-11.0
2	224.9	-5.7	-2.5
3	231.9	1.4	0.6
full	230.6		

Table 250: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **36**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.8	-22.6	-10.1
2	219.6	-4.8	-2.2
3	225.7	1.3	0.6
full	224.4		

Table 251: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **36**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	198.8	-20.6	-9.4
2	215.3	-4.2	-1.9
3	220.6	1.2	0.5
full	219.5		

Table 252: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **36**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	198.4	-20.3	-9.3
2	214.6	-4.1	-1.9
3	219.9	1.2	0.5
full	218.7		

Table 253: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **37**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.10003	0.15768	-12.5
2	-1.26503	-0.00733	0.6
3	-1.25766	0.00005	-0.0
full	-1.25771		

Table 254: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **37**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.99988	0.18931	-15.9
2	-1.18747	0.00172	-0.1
3	-1.18915	0.00004	-0.0
full	-1.18919		

Table 255: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **37**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.84220	0.34699	-29.2
2	-1.19480	-0.00560	0.5
3	-1.18910	0.00009	-0.0
full	-1.18919		

Table 256: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **37**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.8	-12.7	-5.9
2	217.1	1.6	0.8
3	214.6	-0.9	-0.4
full	215.4		

Table 257: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **37**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.6	-11.2	-5.3
2	212.9	2.1	1.0
3	210.2	-0.6	-0.3
full	210.8		

Table 258: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **37**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	197.0	-10.1	-4.9
2	209.3	2.2	1.1
3	206.6	-0.5	-0.2
full	207.1		

Table 259: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **37**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	196.6	-10.0	-4.8
2	208.8	2.3	1.1
3	206.0	-0.5	-0.2
full	206.5		

Table 260: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **38**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.13123	0.16126	-12.5
2	-1.29595	-0.00346	0.3
3	-1.29260	-0.00012	0.0
full	-1.29249		

Table 261: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **38**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.02185	0.19238	-15.8
2	-1.21257	0.00166	-0.1
3	-1.21427	-0.00004	0.0
full	-1.21423		

Table 262: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **38**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.86059	0.35364	-29.1
2	-1.21603	-0.00180	0.1
3	-1.21439	-0.00016	0.0
full	-1.21423		

Table 263: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **38**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	216.8	-15.8	-6.8
2	227.1	-5.5	-2.4
3	232.4	-0.1	-0.1
full	232.6		

Table 264: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **38**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	213.5	-14.5	-6.4
2	222.9	-5.1	-2.2
3	227.9	-0.1	-0.0
full	227.9		

Table 265: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **38**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	210.6	-13.5	-6.0
2	219.4	-4.7	-2.1
3	224.0	-0.1	-0.0
full	224.1		

Table 266: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **38**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	210.1	-13.3	-6.0
2	218.8	-4.7	-2.1
3	223.4	-0.1	-0.0
full	223.4		

Table 267: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **39**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.10130	0.19503	-15.0
2	-1.30434	-0.00801	0.6
3	-1.29670	-0.00037	0.0
full	-1.29633		

Table 268: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **39**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.98894	0.23194	-19.0
2	-1.21819	0.00269	-0.2
3	-1.22125	-0.00036	0.0
full	-1.22088		

Table 269: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **39**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79391	0.42697	-35.0
2	-1.22620	-0.00532	0.4
3	-1.22161	-0.00073	0.1
full	-1.22088		

Table 270: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **39**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	210.4	-17.4	-7.7
2	229.3	1.4	0.6
3	228.8	0.9	0.4
full	227.9		

Table 271: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **39**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	207.3	-15.8	-7.1
2	224.6	1.5	0.7
3	223.9	0.8	0.4
full	223.1		

Table 272: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **39**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	204.6	-14.6	-6.6
2	220.6	1.5	0.7
3	219.9	0.8	0.3
full	219.1		

Table 273: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **39**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	204.1	-14.4	-6.6
2	220.0	1.5	0.7
3	219.2	0.8	0.3
full	218.5		

Table 274: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.15621	0.18435	-13.8
2	-1.34726	-0.00670	0.5
3	-1.34124	-0.00068	0.1
full	-1.34056		

Table 275: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.06045	0.21985	-17.2
2	-1.27895	0.00135	-0.1
3	-1.28098	-0.00069	0.1
full	-1.28030		

Table 276: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.87610	0.40420	-31.6
2	-1.28565	-0.00535	0.4
3	-1.28166	-0.00137	0.1
full	-1.28030		

Table 277: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	205.6	-12.4	-5.7
2	220.7	2.6	1.2
3	215.9	-2.1	-1.0
full	218.0		

Table 278: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	202.8	-11.4	-5.3
2	216.8	2.6	1.2
3	212.2	-2.0	-0.9
full	214.1		

Table 279: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	200.3	-10.5	-5.0
2	213.5	2.6	1.3
3	209.0	-1.9	-0.9
full	210.8		

Table 280: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.9	-10.4	-4.9
2	212.9	2.6	1.3
3	208.5	-1.9	-0.9
full	210.3		

Table 281: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **41**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.18743	0.18534	-13.5
2	-1.37636	-0.00359	0.3
3	-1.37290	-0.00013	0.0
full	-1.37277		

Table 282: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **41**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.02633	0.22819	-18.2
2	-1.25399	0.00054	-0.0
3	-1.25458	-0.00005	0.0
full	-1.25453		

Table 283: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **41**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.84099	0.41354	-33.0
2	-1.25757	-0.00305	0.2
3	-1.25470	-0.00018	0.0
full	-1.25453		

Table 284: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **41**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	286.7	-32.5	-10.2
2	319.9	0.7	0.2
3	319.8	0.6	0.2
full	319.2		

Table 285: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **41**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	281.8	-29.4	-9.5
2	312.3	1.1	0.3
3	311.8	0.6	0.2
full	311.2		

Table 286: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **41**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	277.7	-27.0	-8.8
2	305.9	1.3	0.4
3	305.1	0.5	0.2
full	304.6		

Table 287: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **41**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	277.0	-26.6	-8.8
2	304.9	1.4	0.5
3	304.1	0.5	0.2
full	303.6		

Table 288: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **42**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.18718	0.18661	-13.6
2	-1.37758	-0.00379	0.3
3	-1.37385	-0.00007	0.0
full	-1.37379		

Table 289: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **42**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.02612	0.22992	-18.3
2	-1.25549	0.00056	-0.0
3	-1.25604	0.00000	-0.0
full	-1.25604		

Table 290: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **42**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.83951	0.41653	-33.2
2	-1.25928	-0.00323	0.3
3	-1.25611	-0.00007	0.0
full	-1.25604		

Table 291: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **42**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	286.9	-29.7	-9.4
2	318.9	2.3	0.7
3	317.0	0.4	0.1
full	316.6		

Table 292: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **42**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	282.0	-26.8	-8.7
2	311.4	2.6	0.8
3	309.2	0.3	0.1
full	308.8		

Table 293: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **42**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	277.9	-24.5	-8.1
2	305.1	2.7	0.9
3	302.7	0.3	0.1
full	302.4		

Table 294: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **42**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	277.2	-24.2	-8.0
2	304.1	2.8	0.9
3	301.7	0.3	0.1
full	301.4		

Table 295: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **43**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.25469	0.12600	-9.1
2	-1.38471	-0.00402	0.3
3	-1.38072	-0.00003	0.0
full	-1.38069		

Table 296: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **43**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.13977	0.15613	-12.0
2	-1.29568	0.00021	-0.0
3	-1.29586	0.00003	-0.0
full	-1.29590		

Table 297: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **43**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.01376	0.28213	-21.8
2	-1.29970	-0.00381	0.3
3	-1.29589	0.00000	-0.0
full	-1.29590		

Table 298: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **43**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	217.6	-27.4	-11.2
2	243.1	-1.9	-0.8
3	245.0	0.0	0.0
full	244.9		

Table 299: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **43**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	213.4	-24.5	-10.3
2	236.8	-1.2	-0.5
3	238.1	0.1	0.0
full	238.0		

Table 300: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **43**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	210.0	-22.3	-9.6
2	231.5	-0.8	-0.3
3	232.4	0.1	0.0
full	232.3		

Table 301: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **43**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	209.4	-22.0	-9.5
2	230.7	-0.7	-0.3
3	231.5	0.1	0.0
full	231.4		

Table 302: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **44**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.25458	0.12775	-9.2
2	-1.38640	-0.00406	0.3
3	-1.38238	-0.00005	0.0
full	-1.38233		

Table 303: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **44**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.14006	0.15811	-12.2
2	-1.29793	0.00025	-0.0
3	-1.29817	0.00001	-0.0
full	-1.29818		

Table 304: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **44**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.01231	0.28587	-22.0
2	-1.30199	-0.00381	0.3
3	-1.29822	-0.00005	0.0
full	-1.29818		

Table 305: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **44**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	218.9	-27.0	-11.0
2	244.3	-1.5	-0.6
3	246.0	0.1	0.0
full	245.9		

Table 306: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **44**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	214.7	-24.2	-10.1
2	238.0	-0.9	-0.4
3	239.1	0.1	0.1
full	238.9		

Table 307: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **44**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	211.2	-22.0	-9.4
2	232.8	-0.5	-0.2
3	233.4	0.2	0.1
full	233.2		

Table 308: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **44**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	210.7	-21.7	-9.3
2	232.0	-0.4	-0.2
3	232.5	0.2	0.1
full	232.4		

Table 309: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **45**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.25490	0.13012	-9.4
2	-1.38882	-0.00380	0.3
3	-1.38509	-0.00007	0.0
full	-1.38502		

Table 310: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **45**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.14138	0.16026	-12.3
2	-1.30138	0.00027	-0.0
3	-1.30164	-0.00000	0.0
full	-1.30164		

Table 311: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **45**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.01126	0.29038	-22.3
2	-1.30517	-0.00353	0.3
3	-1.30171	-0.00007	0.0
full	-1.30164		

Table 312: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **45**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	219.3	-26.6	-10.8
2	244.4	-1.6	-0.6
3	246.1	0.1	0.0
full	246.0		

Table 313: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **45**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	215.2	-23.8	-10.0
2	238.1	-1.0	-0.4
3	239.2	0.2	0.1
full	239.0		

Table 314: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **45**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	211.8	-21.6	-9.3
2	232.9	-0.6	-0.2
3	233.6	0.2	0.1
full	233.4		

Table 315: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **45**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	211.2	-21.3	-9.2
2	232.1	-0.5	-0.2
3	232.7	0.2	0.1
full	232.6		

Table 316: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **46**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.22290	0.22927	-15.8
2	-1.47058	-0.01841	1.3
3	-1.45093	0.00124	-0.1
full	-1.45217		

Table 317: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **46**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.05659	0.27517	-20.7
2	-1.32450	0.00726	-0.5
3	-1.33164	0.00012	-0.0
full	-1.33176		

Table 318: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **46**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.82732	0.50444	-37.9
2	-1.34291	-0.01115	0.8
3	-1.33041	0.00136	-0.1
full	-1.33176		

Table 319: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **46**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	307.3	-5.0	-1.6
2	329.6	17.3	5.5
3	308.4	-3.9	-1.3
full	312.3		

Table 320: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **46**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	302.7	-4.2	-1.4
2	323.5	16.6	5.4
3	303.0	-3.9	-1.3
full	306.9		

Table 321: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **46**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	298.7	-3.5	-1.2
2	318.2	16.0	5.3
3	298.4	-3.8	-1.3
full	302.2		

Table 322: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **46**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	298.1	-3.4	-1.1
2	317.4	15.9	5.3
3	297.7	-3.8	-1.3
full	301.5		

Table 323: Errors of the incremental CCSD/cc-pVDZ expansion of the energy for **47**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.35169	0.25543	-15.9
2	-1.61790	-0.01078	0.7
3	-1.60715	-0.00003	0.0
full	-1.60712		

Table 324: Errors of the incremental MP2/cc-pVDZ expansion of the energy for **47**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.20224	0.30277	-20.1
2	-1.50256	0.00244	-0.2
3	-1.50484	0.00017	-0.0
full	-1.50501		

Table 325: Errors of the incremental CCSD|MP2/cc-pVDZ expansion of the energy for **47**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.94681	0.55820	-37.1
2	-1.51334	-0.00834	0.6
3	-1.50487	0.00014	-0.0
full	-1.50501		

Table 326: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 355.00 nm for **47**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	275.3	-31.2	-10.2
2	301.9	-4.6	-1.5
3	307.0	0.5	0.2
full	306.4		

Table 327: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 436.00 nm for **47**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	271.2	-28.5	-9.5
2	295.8	-3.9	-1.3
3	300.2	0.5	0.2
full	299.7		

Table 328: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 589.00 nm for **47**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	267.7	-26.4	-9.0
2	290.7	-3.4	-1.2
3	294.6	0.6	0.2
full	294.0		

Table 329: Errors of the incremental CCSD/cc-pVDZ expansion for the polarizability at 633.00 nm for **47**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	267.1	-26.0	-8.9
2	289.8	-3.3	-1.1
3	293.7	0.6	0.2
full	293.2		

Table 330: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.56302	0.11066	-16.4
2	-0.67848	-0.00479	0.7
3	-0.67351	0.00018	-0.0
full	-0.67369		

Table 331: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.48246	0.12920	-21.1
2	-0.61051	0.00115	-0.2
3	-0.61151	0.00015	-0.0
full	-0.61166		

Table 332: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **1**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.37180	0.23987	-39.2
2	-0.61530	-0.00364	0.6
3	-0.61134	0.00032	-0.1
full	-0.61166		

Table 333: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	163.0	-6.4	-3.8
2	170.7	1.3	0.8
3	169.7	0.3	0.2
full	169.4		

Table 334: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	160.2	-5.6	-3.4
2	167.1	1.3	0.8
3	166.1	0.3	0.2
full	165.8		

Table 335: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	157.9	-5.0	-3.1
2	164.1	1.3	0.8
3	163.1	0.2	0.2
full	162.8		

Table 336: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **1**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	157.5	-4.9	-3.0
2	163.6	1.3	0.8
3	162.6	0.2	0.1
full	162.3		

Table 337: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.60227	0.10445	-14.8
2	-0.71142	-0.00470	0.7
3	-0.70669	0.00003	-0.0
full	-0.70672		

Table 338: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.53631	0.12175	-18.5
2	-0.65789	0.00017	-0.0
3	-0.65808	-0.00001	0.0
full	-0.65806		

Table 339: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **2**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.43186	0.22620	-34.4
2	-0.66259	-0.00453	0.7
3	-0.65805	0.00002	-0.0
full	-0.65806		

Table 340: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	138.2	-6.6	-4.6
2	148.4	3.6	2.5
3	144.5	-0.3	-0.2
full	144.8		

Table 341: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	135.9	-6.0	-4.2
2	145.3	3.5	2.4
3	141.5	-0.3	-0.2
full	141.9		

Table 342: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	133.9	-5.4	-3.9
2	142.7	3.3	2.4
3	139.0	-0.3	-0.2
full	139.4		

Table 343: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **2**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	133.6	-5.3	-3.8
2	142.3	3.3	2.4
3	138.7	-0.3	-0.2
full	139.0		

Table 344: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.64209	0.11860	-15.6
2	-0.76269	-0.00200	0.3
3	-0.76076	-0.00007	0.0
full	-0.76069		

Table 345: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.56052	0.14426	-20.5
2	-0.70472	0.00006	-0.0
3	-0.70486	-0.00007	0.0
full	-0.70478		

Table 346: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **3**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.44193	0.26286	-37.3
2	-0.70673	-0.00194	0.3
3	-0.70493	-0.00014	0.0
full	-0.70478		

Table 347: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	207.1	-32.0	-13.4
2	233.3	-5.9	-2.5
3	239.1	-0.0	-0.0
full	239.1		

Table 348: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	201.1	-25.2	-11.1
2	222.4	-3.8	-1.7
3	226.2	0.0	0.0
full	226.2		

Table 349: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	196.1	-20.6	-9.5
2	214.2	-2.6	-1.2
3	216.7	0.0	0.0
full	216.7		

Table 350: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **3**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	195.3	-20.0	-9.3
2	212.9	-2.4	-1.1
3	215.3	0.0	0.0
full	215.3		

Table 351: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.63597	0.12520	-16.4
2	-0.76516	-0.00398	0.5
3	-0.76147	-0.00029	0.0
full	-0.76117		

Table 352: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.54887	0.15556	-22.1
2	-0.70440	0.00002	-0.0
3	-0.70465	-0.00022	0.0
full	-0.70442		

Table 353: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **4**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.42366	0.28076	-39.9
2	-0.70838	-0.00396	0.6
3	-0.70494	-0.00051	0.1
full	-0.70442		

Table 354: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	197.0	-26.0	-11.6
2	218.1	-5.0	-2.2
3	222.7	-0.3	-0.1
full	223.0		

Table 355: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.5	-22.3	-10.4
2	211.0	-3.8	-1.8
3	214.6	-0.2	-0.1
full	214.8		

Table 356: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	188.6	-19.6	-9.4
2	205.3	-3.0	-1.4
3	208.2	-0.1	-0.0
full	208.3		

Table 357: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **4**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	188.0	-19.2	-9.3
2	204.4	-2.9	-1.4
3	207.2	-0.1	-0.0
full	207.3		

Table 358: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.66964	0.12803	-16.1
2	-0.80235	-0.00468	0.6
3	-0.79781	-0.00015	0.0
full	-0.79766		

Table 359: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.57795	0.15423	-21.1
2	-0.73262	-0.00044	0.1
3	-0.73233	-0.00014	0.0
full	-0.73218		

Table 360: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **5**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.44992	0.28226	-38.6
2	-0.73730	-0.00512	0.7
3	-0.73248	-0.00029	0.0
full	-0.73218		

Table 361: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	200.7	-12.6	-5.9
2	209.7	-3.5	-1.7
3	213.1	-0.2	-0.1
full	213.3		

Table 362: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	196.4	-10.7	-5.2
2	204.1	-3.0	-1.5
3	206.9	-0.1	-0.1
full	207.1		

Table 363: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.7	-9.3	-4.6
2	199.4	-2.6	-1.3
3	202.0	-0.1	-0.0
full	202.1		

Table 364: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **5**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.2	-9.1	-4.5
2	198.7	-2.6	-1.3
3	201.2	-0.1	-0.0
full	201.3		

Table 365: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.68900	0.10904	-13.7
2	-0.80144	-0.00340	0.4
3	-0.79790	0.00014	-0.0
full	-0.79804		

Table 366: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.60114	0.13086	-17.9
2	-0.73094	0.00106	-0.1
3	-0.73184	0.00016	-0.0
full	-0.73200		

Table 367: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **6**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.49210	0.23990	-32.8
2	-0.73434	-0.00234	0.3
3	-0.73170	0.00030	-0.0
full	-0.73200		

Table 368: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	200.0	-11.4	-5.4
2	211.6	0.2	0.1
3	211.5	0.0	0.0
full	211.4		

Table 369: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	195.6	-9.8	-4.8
2	205.7	0.3	0.1
3	205.4	0.0	0.0
full	205.4		

Table 370: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	191.9	-8.7	-4.3
2	200.9	0.3	0.2
3	200.6	0.0	0.0
full	200.5		

Table 371: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **6**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	191.3	-8.5	-4.2
2	200.1	0.3	0.2
3	199.8	0.0	0.0
full	199.8		

Table 372: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.67623	0.12208	-15.3
2	-0.80180	-0.00348	0.4
3	-0.79836	-0.00005	0.0
full	-0.79831		

Table 373: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.58498	0.14797	-20.2
2	-0.73349	-0.00053	0.1
3	-0.73295	0.00000	-0.0
full	-0.73295		

Table 374: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **7**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.46290	0.27006	-36.8
2	-0.73697	-0.00402	0.5
3	-0.73300	-0.00005	0.0
full	-0.73295		

Table 375: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	197.5	-14.0	-6.6
2	212.9	1.4	0.7
3	211.1	-0.4	-0.2
full	211.5		

Table 376: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.3	-12.0	-5.9
2	207.0	1.6	0.8
3	205.0	-0.3	-0.2
full	205.4		

Table 377: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	189.9	-10.6	-5.3
2	202.2	1.7	0.9
3	200.1	-0.3	-0.2
full	200.4		

Table 378: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **7**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	189.3	-10.4	-5.2
2	201.4	1.7	0.9
3	199.4	-0.3	-0.2
full	199.7		

Table 379: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.72791	0.10685	-12.8
2	-0.83884	-0.00408	0.5
3	-0.83452	0.00024	-0.0
full	-0.83476		

Table 380: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.65747	0.12764	-16.3
2	-0.78427	0.00084	-0.1
3	-0.78489	0.00021	-0.0
full	-0.78511		

Table 381: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **8**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.55062	0.23448	-29.9
2	-0.78834	-0.00324	0.4
3	-0.78465	0.00045	-0.1
full	-0.78511		

Table 382: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	162.2	-9.4	-5.5
2	172.8	1.2	0.7
3	171.5	-0.0	-0.0
full	171.6		

Table 383: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	159.4	-8.5	-5.0
2	169.1	1.2	0.7
3	167.8	-0.0	-0.0
full	167.8		

Table 384: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	157.0	-7.7	-4.7
2	166.0	1.3	0.8
3	164.7	-0.0	-0.0
full	164.7		

Table 385: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **8**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	156.6	-7.6	-4.6
2	165.5	1.3	0.8
3	164.2	-0.0	-0.0
full	164.3		

Table 386: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.74704	0.17745	-19.2
2	-0.93414	-0.00965	1.0
3	-0.92448	0.00001	-0.0
full	-0.92449		

Table 387: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.67029	0.21778	-24.5
2	-0.88394	0.00412	-0.5
3	-0.88861	-0.00055	0.1
full	-0.88807		

Table 388: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **9**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.49285	0.39522	-44.5
2	-0.89359	-0.00553	0.6
3	-0.88861	-0.00054	0.1
full	-0.88807		

Table 389: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.6	-11.4	-5.6
2	216.3	11.3	5.5
3	203.9	-1.1	-0.5
full	205.0		

Table 390: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	189.0	-8.8	-4.5
2	208.7	10.8	5.5
3	196.4	-1.4	-0.7
full	197.8		

Table 391: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	185.2	-7.1	-3.7
2	202.6	10.4	5.4
3	190.7	-1.5	-0.8
full	192.2		

Table 392: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **9**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	184.6	-6.8	-3.6
2	201.7	10.3	5.4
3	189.8	-1.6	-0.8
full	191.4		

Table 393: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79349	0.15341	-16.2
2	-0.95546	-0.00857	0.9
3	-0.94675	0.00015	-0.0
full	-0.94689		

Table 394: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.69051	0.18814	-21.4
2	-0.87868	-0.00002	0.0
3	-0.87868	-0.00002	0.0
full	-0.87865		

Table 395: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **10**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.53711	0.34154	-38.9
2	-0.88724	-0.00859	1.0
3	-0.87853	0.00012	-0.0
full	-0.87865		

Table 396: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	232.8	-20.3	-8.0
2	258.3	5.2	2.1
3	252.4	-0.7	-0.3
full	253.1		

Table 397: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	228.3	-17.6	-7.2
2	251.3	5.4	2.2
3	245.3	-0.6	-0.3
full	245.9		

Table 398: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	224.5	-15.6	-6.5
2	245.5	5.4	2.3
3	239.5	-0.6	-0.2
full	240.1		

Table 399: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **10**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	223.9	-15.3	-6.4
2	244.6	5.4	2.3
3	238.6	-0.6	-0.2
full	239.2		

Table 400: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81711	0.14808	-15.3
2	-0.97542	-0.01023	1.1
3	-0.96439	0.00079	-0.1
full	-0.96518		

Table 401: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.70938	0.18063	-20.3
2	-0.88794	0.00207	-0.2
3	-0.88960	0.00041	-0.0
full	-0.89001		

Table 402: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **12**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.56130	0.32870	-36.9
2	-0.89817	-0.00817	0.9
3	-0.88880	0.00120	-0.1
full	-0.89001		

Table 403: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	234.9	-18.0	-7.1
2	255.2	2.3	0.9
3	253.7	0.9	0.3
full	252.9		

Table 404: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	230.3	-15.1	-6.2
2	248.4	3.0	1.2
3	246.1	0.7	0.3
full	245.4		

Table 405: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	226.4	-13.0	-5.4
2	242.9	3.5	1.5
3	240.0	0.6	0.3
full	239.4		

Table 406: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **12**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	225.7	-12.7	-5.3
2	242.0	3.6	1.5
3	239.1	0.6	0.3
full	238.4		

Table 407: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.86267	0.13075	-13.2
2	-0.99771	-0.00429	0.4
3	-0.99371	-0.00028	0.0
full	-0.99342		

Table 408: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.76814	0.16188	-17.4
2	-0.92995	0.00007	-0.0
3	-0.93025	-0.00023	0.0
full	-0.93002		

Table 409: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **15**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.63739	0.29264	-31.5
2	-0.93424	-0.00422	0.5
3	-0.93054	-0.00051	0.1
full	-0.93002		

Table 410: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	225.8	-25.9	-10.3
2	250.2	-1.5	-0.6
3	251.0	-0.7	-0.3
full	251.6		

Table 411: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	220.7	-22.4	-9.2
2	242.4	-0.6	-0.3
3	242.5	-0.5	-0.2
full	243.1		

Table 412: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	216.4	-19.8	-8.4
2	236.2	-0.0	-0.0
3	235.8	-0.5	-0.2
full	236.2		

Table 413: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **15**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	215.8	-19.4	-8.3
2	235.2	0.0	0.0
3	234.7	-0.5	-0.2
full	235.2		

Table 414: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.80788	0.18870	-18.9
2	-1.00579	-0.00921	0.9
3	-0.99692	-0.00034	0.0
full	-0.99659		

Table 415: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.71203	0.22198	-23.8
2	-0.93372	0.00029	-0.0
3	-0.93446	-0.00044	0.0
full	-0.93402		

Table 416: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **16**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.52333	0.41069	-44.0
2	-0.94293	-0.00892	1.0
3	-0.93480	-0.00078	0.1
full	-0.93402		

Table 417: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	199.1	-10.9	-5.2
2	212.4	2.4	1.1
3	209.5	-0.5	-0.3
full	210.0		

Table 418: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	195.9	-9.6	-4.7
2	207.9	2.4	1.2
3	205.0	-0.5	-0.2
full	205.5		

Table 419: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	193.2	-8.6	-4.2
2	204.1	2.4	1.2
3	201.3	-0.5	-0.2
full	201.7		

Table 420: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **16**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	192.7	-8.4	-4.2
2	203.5	2.4	1.2
3	200.7	-0.5	-0.2
full	201.1		

Table 421: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79923	0.19783	-19.8
2	-1.00262	-0.00557	0.6
3	-0.99787	-0.00081	0.1
full	-0.99706		

Table 422: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.67812	0.23185	-25.5
2	-0.90957	0.00041	-0.0
3	-0.91081	-0.00084	0.1
full	-0.90997		

Table 423: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **17**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.48029	0.42968	-47.2
2	-0.91514	-0.00516	0.6
3	-0.91163	-0.00165	0.2
full	-0.90997		

Table 424: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	239.2	-9.7	-3.9
2	246.0	-2.8	-1.1
3	248.7	-0.2	-0.1
full	248.9		

Table 425: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	235.0	-8.5	-3.5
2	240.9	-2.6	-1.1
3	243.4	-0.1	-0.0
full	243.5		

Table 426: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	231.5	-7.6	-3.2
2	236.6	-2.5	-1.0
3	239.0	-0.1	-0.0
full	239.0		

Table 427: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **17**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	230.9	-7.4	-3.1
2	235.9	-2.4	-1.0
3	238.3	-0.0	-0.0
full	238.3		

Table 428: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.87401	0.13676	-13.5
2	-1.01691	-0.00614	0.6
3	-1.01049	0.00028	-0.0
full	-1.01077		

Table 429: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79521	0.16135	-16.9
2	-0.95459	0.00197	-0.2
3	-0.95620	0.00036	-0.0
full	-0.95656		

Table 430: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **18**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.65845	0.29811	-31.2
2	-0.96072	-0.00416	0.4
3	-0.95591	0.00065	-0.1
full	-0.95656		

Table 431: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	191.8	-16.4	-7.9
2	212.7	4.4	2.1
3	208.3	0.0	0.0
full	208.3		

Table 432: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	188.3	-14.5	-7.1
2	207.1	4.3	2.1
3	202.8	0.0	0.0
full	202.8		

Table 433: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	185.4	-13.0	-6.6
2	202.5	4.1	2.1
3	198.4	-0.0	-0.0
full	198.4		

Table 434: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **18**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	184.9	-12.8	-6.5
2	201.8	4.1	2.1
3	197.7	-0.0	-0.0
full	197.7		

Table 435: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.85754	0.14746	-14.7
2	-1.01332	-0.00832	0.8
3	-1.00476	0.00024	-0.0
full	-1.00500		

Table 436: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.74478	0.17619	-19.1
2	-0.91732	0.00366	-0.4
3	-0.92130	-0.00032	0.0
full	-0.92098		

Table 437: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **19**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.59733	0.32365	-35.1
2	-0.92563	-0.00466	0.5
3	-0.92106	-0.00008	0.0
full	-0.92098		

Table 438: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	237.6	-7.8	-3.2
2	254.6	9.3	3.8
3	243.1	-2.2	-0.9
full	245.3		

Table 439: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	233.5	-6.5	-2.7
2	249.0	9.0	3.7
3	237.9	-2.1	-0.9
full	240.0		

Table 440: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	230.0	-5.5	-2.4
2	244.2	8.6	3.7
3	233.6	-2.0	-0.9
full	235.6		

Table 441: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **19**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	229.5	-5.4	-2.3
2	243.4	8.6	3.6
3	232.9	-2.0	-0.8
full	234.9		

Table 442: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.88365	0.13729	-13.4
2	-1.02570	-0.00476	0.5
3	-1.02090	0.00004	-0.0
full	-1.02094		

Table 443: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.80794	0.16292	-16.8
2	-0.97051	0.00035	-0.0
3	-0.97078	0.00008	-0.0
full	-0.97086		

Table 444: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **20**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.67064	0.30021	-30.9
2	-0.97527	-0.00441	0.5
3	-0.97074	0.00012	-0.0
full	-0.97086		

Table 445: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	174.2	-12.7	-6.8
2	187.9	0.9	0.5
3	187.1	0.1	0.1
full	187.0		

Table 446: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	171.4	-11.6	-6.4
2	184.0	1.0	0.5
3	183.1	0.1	0.1
full	183.0		

Table 447: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	169.0	-10.8	-6.0
2	180.8	1.0	0.6
3	179.8	0.1	0.0
full	179.7		

Table 448: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **20**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	168.6	-10.6	-5.9
2	180.2	1.0	0.6
3	179.3	0.1	0.0
full	179.2		

Table 449: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.88275	0.17980	-16.9
2	-1.07031	-0.00775	0.7
3	-1.06326	-0.00071	0.1
full	-1.06255		

Table 450: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.79200	0.20999	-21.0
2	-1.00174	0.00025	-0.0
3	-1.00275	-0.00076	0.1
full	-1.00199		

Table 451: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **22**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.61220	0.38979	-38.9
2	-1.00950	-0.00751	0.7
3	-1.00346	-0.00147	0.1
full	-1.00199		

Table 452: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	187.6	-12.2	-6.1
2	202.6	2.9	1.4
3	200.1	0.3	0.1
full	199.8		

Table 453: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	184.6	-11.1	-5.7
2	198.5	2.8	1.4
3	195.9	0.3	0.1
full	195.7		

Table 454: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	182.0	-10.2	-5.3
2	195.0	2.8	1.4
3	192.5	0.3	0.1
full	192.2		

Table 455: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **22**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	181.6	-10.1	-5.3
2	194.4	2.7	1.4
3	191.9	0.3	0.1
full	191.7		

Table 456: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.84771	0.20383	-19.4
2	-1.05668	-0.00515	0.5
3	-1.05176	-0.00022	0.0
full	-1.05154		

Table 457: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.73167	0.25083	-25.5
2	-0.98253	-0.00003	0.0
3	-0.98275	-0.00026	0.0
full	-0.98250		

Table 458: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **23**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.52784	0.45466	-46.3
2	-0.98767	-0.00518	0.5
3	-0.98298	-0.00048	0.0
full	-0.98250		

Table 459: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	252.7	-14.8	-5.5
2	276.3	8.8	3.3
3	267.6	0.1	0.0
full	267.5		

Table 460: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	247.0	-12.5	-4.8
2	267.9	8.4	3.2
3	259.5	-0.0	-0.0
full	259.5		

Table 461: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	242.3	-10.7	-4.2
2	261.0	8.0	3.2
3	252.9	-0.1	-0.1
full	253.0		

Table 462: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **23**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	241.6	-10.5	-4.1
2	260.0	7.9	3.1
3	251.9	-0.2	-0.1
full	252.0		

Table 463: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.94359	0.17788	-15.9
2	-1.12544	-0.00397	0.4
3	-1.12176	-0.00029	0.0
full	-1.12147		

Table 464: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.81794	0.21245	-20.6
2	-1.03035	0.00005	-0.0
3	-1.03069	-0.00029	0.0
full	-1.03040		

Table 465: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **27**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.64006	0.39034	-37.9
2	-1.03431	-0.00391	0.4
3	-1.03098	-0.00058	0.1
full	-1.03040		

Table 466: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	276.9	-15.4	-5.3
2	285.4	-6.9	-2.3
3	291.9	-0.4	-0.1
full	292.3		

Table 467: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	271.0	-13.4	-4.7
2	278.1	-6.2	-2.2
3	284.1	-0.3	-0.1
full	284.3		

Table 468: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	266.0	-11.9	-4.3
2	272.2	-5.7	-2.1
3	277.7	-0.2	-0.1
full	277.9		

Table 469: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **27**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	265.3	-11.6	-4.2
2	271.2	-5.7	-2.0
3	276.7	-0.2	-0.1
full	276.9		

Table 470: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.00164	0.18312	-15.5
2	-1.19113	-0.00637	0.5
3	-1.18528	-0.00052	0.0
full	-1.18476		

Table 471: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.90719	0.21676	-19.3
2	-1.12358	0.00037	-0.0
3	-1.12441	-0.00046	0.0
full	-1.12395		

Table 472: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **30**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.72407	0.39988	-35.6
2	-1.12995	-0.00600	0.5
3	-1.12493	-0.00098	0.1
full	-1.12395		

Table 473: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	212.9	-15.6	-6.8
2	228.0	-0.6	-0.3
3	228.6	0.1	0.0
full	228.6		

Table 474: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	209.4	-14.0	-6.3
2	223.1	-0.4	-0.2
3	223.6	0.1	0.0
full	223.5		

Table 475: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	206.5	-12.8	-5.8
2	219.0	-0.2	-0.1
3	219.4	0.1	0.1
full	219.2		

Table 476: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **30**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	206.0	-12.6	-5.8
2	218.4	-0.2	-0.1
3	218.7	0.1	0.1
full	218.6		

Table 477: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.99724	0.22714	-18.6
2	-1.23322	-0.00884	0.7
3	-1.22636	-0.00198	0.2
full	-1.22438		

Table 478: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.89554	0.26621	-22.9
2	-1.16015	0.00160	-0.1
3	-1.16361	-0.00186	0.2
full	-1.16175		

Table 479: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **31**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.66839	0.49336	-42.5
2	-1.16899	-0.00724	0.6
3	-1.16559	-0.00384	0.3
full	-1.16175		

Table 480: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	246.8	-23.4	-8.7
2	269.3	-0.9	-0.3
3	268.9	-1.3	-0.5
full	270.1		

Table 481: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	242.5	-20.1	-7.7
2	262.5	-0.1	-0.0
3	261.5	-1.1	-0.4
full	262.6		

Table 482: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	238.9	-17.7	-6.9
2	257.0	0.4	0.2
3	255.6	-1.0	-0.4
full	256.6		

Table 483: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **31**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	238.3	-17.4	-6.8
2	256.1	0.5	0.2
3	254.7	-1.0	-0.4
full	255.7		

Table 484: Errors of the incremental CCSD/aug-cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.20631	0.20801	-14.7
2	-1.42206	-0.00774	0.5
3	-1.41526	-0.00094	0.1
full	-1.41432		

Table 485: Errors of the incremental MP2/aug-cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-1.11216	0.24559	-18.1
2	-1.35673	0.00102	-0.1
3	-1.35866	-0.00091	0.1
full	-1.35775		

Table 486: Errors of the incremental CCSD|MP2/aug-cc-pVDZ expansion of the energy for **40**.

order	Value	error	rel. error
	a.u.	a.u.	%
1	-0.90414	0.45361	-33.4
2	-1.36447	-0.00672	0.5
3	-1.35960	-0.00185	0.1
full	-1.35775		

Table 487: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 355.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	246.2	-18.9	-7.1
2	269.8	4.6	1.7
3	262.3	-2.9	-1.1
full	265.2		

Table 488: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 436.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	242.5	-17.2	-6.6
2	264.2	4.6	1.8
3	256.9	-2.7	-1.0
full	259.6		

Table 489: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 589.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	239.3	-15.7	-6.2
2	259.5	4.5	1.8
3	252.4	-2.6	-1.0
full	255.0		

Table 490: Errors of the incremental CCSD/aug-cc-pVDZ expansion for the polarizability at 633.00 nm for **40**.

order	pol.	error	rel. error
	a.u.	a.u.	%
1	238.8	-15.5	-6.1
2	258.8	4.5	1.8
3	251.7	-2.5	-1.0
full	254.3		

Table 491: BP86/def2-TZVP optimized structure of **1**.

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C	-4.1422675	-1.1039702	2.2038240
H	-3.7926509	-0.5467807	3.0863140
H	-3.7838416	-0.5721240	1.3107747
H	-5.2420633	-1.0586105	2.1996848
C	-3.6481185	-2.5522508	2.2327874
H	-3.9828962	-3.0753855	1.3204362
H	-2.5451333	-2.5672969	2.2011472
C	-4.1252261	-3.3332403	3.4621887
H	-3.7908105	-2.8098816	4.3745442
H	-5.2282228	-3.3185503	3.4935958
C	-3.6306153	-4.7813575	3.4914351
H	-3.9890890	-5.3132205	4.3844552
H	-3.9798306	-5.3387599	2.6089207
H	-2.5308058	-4.8263579	3.4958528

Table 492: BP86/def2-TZVP optimized structure of **2**.

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C	-3.9821401	-0.4768005	-0.0222555
H	-3.5777072	-1.5004354	-0.0811282
H	-3.5780855	0.0712108	-0.8893864
C	-3.4386292	0.1797989	1.2389724
H	-2.3362918	0.2516345	1.1782698
H	-3.8402906	1.2083217	1.3282270
O	-3.8302509	-0.6150713	2.3692303
H	-3.5340508	-0.1601669	3.1745820
C	-5.5110653	-0.5105974	-0.0845680
H	-5.8602014	-1.0061396	-1.0014915
H	-5.9253093	-1.0530894	0.7752338
H	-5.9305974	0.5073228	-0.0745103

Table 493: BP86/def2-TZVP optimized structure of **3**.

13

C	-4.6025430	-0.4144223	-0.0076923
H	-4.0580319	-1.3490922	-0.1995187
H	-4.8092239	0.0679687	-0.9774539
H	-5.5844774	-0.6708881	0.4232618
C	-3.8354730	0.4960996	0.8963467
H	-4.3089518	1.4541735	1.1422793
C	-2.6233989	0.2314382	1.4222669
H	-2.1371300	-0.7225619	1.1846825
C	-1.8961169	1.1326667	2.2953820
H	-2.3905216	2.0818982	2.5309265
C	-0.6823123	0.8811049	2.8179518
H	-0.1801229	1.5964907	3.4686033
H	-0.1550045	-0.0521422	2.6079301

Table 494: B3LYP/aug-cc-pVDZ optimized structure of **4**.

13

C	0.00000000	0.00000000	0.00000000
C	-0.87382800	0.87178900	0.87038800
C	-0.87382800	2.18536200	0.87080500
C	-0.87382800	3.49893500	0.87038800
H	-0.19165900	4.01714100	1.55371200
C	-1.74765600	4.37072400	0.00000000
H	-2.39264800	3.76601200	-0.64911100
H	-2.38616500	5.02111900	0.61760600
H	-1.13340200	5.02895100	-0.63367100
H	-1.55599700	0.35358300	1.55371200
H	0.64499200	0.60471200	-0.64911100
H	0.63850900	-0.65039500	0.61760600
H	-0.61425400	-0.65822700	-0.63367100

Table 495: BP86/def2-TZVP optimized structure of **5**.

15

C	-5.7674510	-0.2385587	0.0009820
H	-5.4369928	-1.2786257	-0.1396223
H	-5.2649376	0.3756375	-0.7597296
H	-6.8496771	-0.2028289	-0.1900752
C	-5.4368666	0.2619653	1.4168770
H	-5.7855580	1.3000403	1.5390345
H	-6.0027886	-0.3448749	2.1460200
C	-3.9719071	0.1846221	1.7381648
H	-3.5208959	-0.8155103	1.6898230
C	-3.1903290	1.2235134	2.0565524
H	-3.6434811	2.2217757	2.1003411
C	-1.7260195	1.1453058	2.3679845
H	-1.1353928	1.7649808	1.6736542
H	-1.5111084	1.5228973	3.3810182
H	-1.3545836	0.1129248	2.3038521

Table 496: BP86/def2-TZVP optimized structure of **6**.

15

C	-3.6830792	0.9445218	-0.0165601
H	-3.6858988	-0.1554502	0.0193263
H	-3.1554585	1.2441023	-0.9347236
H	-4.7264921	1.2781747	-0.1083071
C	-3.0140417	1.5376931	1.2253463
H	-3.0484794	2.6383076	1.1814464
H	-3.5817351	1.2502747	2.1261089
C	-1.5495823	1.0901697	1.3885046
H	-1.5258908	-0.0149524	1.4190707
H	-0.9672134	1.3910492	0.5020431
C	-0.8999958	1.6318871	2.6279932
H	-1.3818599	1.3627375	3.5757339
C	0.1864114	2.4091353	2.6569899
H	0.6054035	2.7752388	3.5952483
H	0.7001268	2.7059223	1.7389309

Table 497: BP86/def2-TZVP optimized structure of **7**.

15

C	-0.5097383	-4.5740903	4.8207808
H	0.1239067	-4.8152462	5.6871676
H	0.1552673	-4.3816644	3.9669119
H	-1.1146728	-5.4628237	4.5898863
C	-1.4019915	-3.3553816	5.1104822
H	-2.0401407	-3.1472324	4.2394996
H	-2.0876770	-3.6103493	5.9382800
C	-0.6090166	-2.1386912	5.4960304
H	0.0614894	-2.2807633	6.3515534
C	-0.6195630	-0.9270736	4.9194752
H	0.0386535	-0.1635064	5.3478164
C	-1.4381657	-0.4748263	3.7466682
H	-2.1167366	0.3447489	4.0347479
H	-0.7918499	-0.0751695	2.9487171
H	-2.0490299	-1.2781889	3.3160268

Table 498: BP86/def2-TZVP optimized structure of **8**.

13

C	-0.9254826	0.2645932	0.0251623
C	0.5471115	0.2620089	-0.0247424
O	-0.1868799	1.5095659	0.0018759
H	-1.4487690	0.0584803	-0.9183270
H	1.0696106	0.0514038	0.9182016
C	1.3264270	-0.0376901	-1.2773368
H	2.2439260	0.5673981	-1.3180675
H	1.6207792	-1.0979570	-1.3047612
H	0.7281820	0.1836770	-2.1714199
C	-1.7058801	-0.0355846	1.2769502
H	-2.6211537	0.5727560	1.3193438
H	-2.0041197	-1.0948304	1.3015463
H	-1.1067744	0.1812216	2.1715747

Table 499: BP86/def2-TZVP optimized structure of **9**.

12

C	-1.0473788	-0.3248815	-0.0000894
C	0.3157443	-0.3189623	0.0000682
C	0.7092986	1.0605147	0.0000459
C	-0.4403337	1.8029541	-0.0001518
O	-1.5291810	0.9602151	-0.0002045
H	-1.7963627	-1.1080016	-0.0001391
H	0.9636730	-1.1892879	0.0001911
H	1.7212499	1.4529576	0.0001905
C	-0.7259856	3.2608304	-0.0001897
H	-1.3052692	3.5593137	-0.8876110
H	-1.3052590	3.5594236	0.8872050
H	0.2156838	3.8228104	-0.0002252

Table 500: BP86/def2-TZVP optimized structure of **10**.

15

C	-5.8057801	-0.4654868	-0.0058792
H	-5.4903521	-1.4946208	-0.2225655
H	-5.3110745	0.2013812	-0.7258871
H	-6.8908970	-0.4013951	-0.1676456
C	-5.4544772	-0.0721045	1.4370308
H	-5.7877616	0.9584979	1.6362734
H	-6.0015228	-0.7253227	2.1369387
C	-3.9878127	-0.1388270	1.7546861
C	-3.2018896	0.9053662	2.0479760
H	-3.7068255	1.8772608	2.0513132
C	-1.7423340	0.9056505	2.3674480
H	-1.1824309	1.5128026	1.6379818
H	-1.5587673	1.3554670	3.3563188
H	-1.3249286	-0.1080900	2.3648447
Cl	-3.3261184	-1.7771979	1.7126182

Table 501: BP86/def2-TZVP optimized structure of **11**.

18

C	-5.2409926	-0.0151442	0.1206020
H	-4.9109554	-1.0592119	0.0122771
H	-4.7504134	0.5721065	-0.6686787
H	-6.3258640	0.0125824	-0.0562641
C	-4.8912179	0.5350048	1.5131531
H	-5.2378136	1.5769464	1.6035220
H	-5.4471986	-0.0456850	2.2707320
C	-3.4219861	0.4672926	1.8175019
H	-2.9713094	-0.5338661	1.7905296
C	-2.6351762	1.5139459	2.0959439
H	-3.0857639	2.5151992	2.1228175
C	-1.1659023	1.4461512	2.3996746
H	-0.6100718	2.0242332	1.6399087
H	-0.8201437	0.4036909	2.3120519
C	-0.8149263	2.0002663	3.7902383
H	-1.3071376	1.4171637	4.5816029
H	0.2698493	1.9702747	3.9672709
H	-1.1421712	3.0456175	3.8947604

Table 502: BP86/def2-TZVP optimized structure of **12**.

18

C	-5.1606767	-0.7204353	-0.0257976
H	-4.6870339	-1.6895917	-0.2111033
H	-5.2709870	-0.2111580	-0.9981155
H	-6.1849242	-0.9115397	0.3369446
C	-4.4115949	0.1596713	0.9464154
C	-3.2653599	-0.2002619	1.5695385
C	-2.5810270	-1.5333741	1.3821345
H	-1.5570452	-1.3908700	0.9969864
H	-2.4740698	-2.0496577	2.3511005
H	-3.1009679	-2.2137456	0.7000659
C	-2.5135306	0.6818276	2.5377830
H	-1.4770300	0.8347949	2.1924117
H	-2.9623573	1.6688013	2.6875151
H	-2.4378186	0.1945675	3.5246956
C	-5.0991300	1.4904561	1.1384403
H	-4.6008573	2.1552010	1.8514169
H	-5.1762247	2.0270855	0.1776951
H	-6.1343305	1.3409046	1.4891035

Table 503: B3LYP/aug-cc-pVDZ optimized structure of **13**.

16

C	0.00000000	0.00000000	0.00000000
C	0.77513300	-0.86446300	0.96685700
C	1.75138800	-1.68483600	0.64157900
C	2.72878900	-2.50275900	0.32460700
H	2.47586700	-3.54207000	0.08906100
C	4.19053000	-2.12927600	0.26664100
H	4.34353700	-1.07279000	0.51791400
H	4.77372800	-2.74399900	0.96909700
H	4.59807600	-2.31265700	-0.73922600
H	0.49821400	-0.78365500	2.02403300
H	0.34099500	-0.15021800	-1.03152600
H	-1.07603900	-0.22511700	0.05201500
H	0.11887700	1.06403000	0.25463200
O	-0.81170100	-3.90343600	0.41632100
H	-1.05678100	-3.87980500	-0.51599800
H	-0.24943400	-3.12399100	0.54334700

Table 504: B3LYP/aug-cc-pVDZ optimized structure of **14**.

16

C	0.00000000	0.00000000	0.00000000
C	-1.46444400	-0.36643000	0.02694600
C	-2.44105800	0.44524100	0.36174100
C	-3.41923100	1.26314500	0.68806000
H	-3.71780300	1.32103000	1.74107500
C	-4.16801100	2.15536700	-0.27447800
H	-3.80129000	2.02991300	-1.30007100
H	-5.24434000	1.92768500	-0.25838400
H	-4.05435400	3.21167600	0.01259000
H	-1.72145400	-1.39204600	-0.25890200
H	0.15629600	1.04448300	0.29557800
H	0.57342800	-0.64609200	0.68212100
H	0.41596400	-0.14458000	-1.00872300
O	-5.05428200	-1.67323100	-0.06746500
H	-4.46520000	-0.94134100	0.17201000
H	-5.19373900	-2.15473700	0.75630300

Table 505: B3LYP/aug-cc-pVDZ optimized structure of **15**.

16

C	0.00000000	0.00000000	0.00000000
C	-1.08720600	0.07487600	-1.04749400
C	-2.36957500	-0.12569500	-0.82712600
C	-3.64403900	-0.34763600	-0.60044200
H	-4.00374300	-1.37869000	-0.69309100
C	-4.66981700	0.69348400	-0.22085700
H	-4.22230900	1.69065000	-0.13536600
H	-5.47501200	0.73116600	-0.97051900
H	-5.13770400	0.43668700	0.74165000
H	-0.76399100	0.28996800	-2.07271100
H	-0.41778100	-0.21467400	0.99069100
H	0.72331700	-0.78966200	-0.25403200
H	0.55725100	0.94707400	0.05408100
O	-1.94239400	3.30347000	-0.44922800
H	-1.84543000	2.36401900	-0.66909100
H	-1.95035800	3.75595100	-1.30090400

Table 506: BP86/def2-TZVP optimized structure of **16**.

16

C	-0.3615266	-0.1980464	0.0641078
C	1.1074466	-0.1984814	-0.0130496
O	0.3714008	1.0406521	0.1238659
H	-0.9579886	-0.3449232	-0.8423803
H	-0.8468851	-0.4968848	0.9995724
H	1.5566282	-0.3217108	-1.0079048
C	1.9835274	-0.5984281	1.1474438
H	2.1992635	-1.6791268	1.0689901
H	1.4198988	-0.4537416	2.0837092
C	3.3007313	0.1879918	1.2039729
H	3.0689768	1.2633644	1.2576641
H	3.8528376	0.0379060	0.2608481
C	4.1848631	-0.2135980	2.3868435
H	4.4503075	-1.2811032	2.3441759
H	5.1207927	0.3623073	2.4011450
H	3.6711294	-0.0385659	3.3442636

Table 507: BP86/def2-TZVP optimized structure of **17**.

20

C	-4.6823563	0.2169856	-0.0251357
H	-4.3431254	-0.8293569	-0.0634004
H	-4.3428002	0.7076904	-0.9499921
H	-5.7817254	0.2110534	-0.0354489
C	-4.1348017	0.9311616	1.2132125
H	-4.5195645	1.9650473	1.2427263
H	-4.5198060	0.4394608	2.1228515
C	-2.6035404	0.9625046	1.2685090
H	-2.2174212	1.4538791	0.3577117
H	-2.2176299	-0.0722457	1.2391591
C	-2.0447193	1.6759764	2.5037276
H	-2.4304365	1.1847080	3.4147444
H	-2.4310281	2.7105930	2.5328804
C	-0.5134493	1.7081009	2.5585761
H	-0.1289374	2.1959041	1.6466233
H	-0.1281827	0.6742972	2.5335980
C	0.0340797	2.4283235	3.7934312
H	-0.3053807	1.9422851	4.7207885
H	1.1334493	2.4344319	3.8036728
H	-0.3052728	3.4747975	3.8263925

Table 508: BP86/def2-TZVP optimized structure of **18**.

15

C	0.5983713	-3.2397468	4.8706794
O	1.3807422	-3.1400687	5.8106107
C	-0.3529309	-4.4246947	4.7109653
H	-1.1247819	-4.2132929	3.9531352
H	0.2511765	-5.2616882	4.3190680
C	-0.9972906	-4.8414489	6.0381019
H	-1.6390535	-4.0219053	6.4002439
H	-0.1981150	-4.9579421	6.7841374
C	-1.8147425	-6.1286936	5.9206566
H	-2.2681096	-6.3999323	6.8844828
H	-2.6301781	-6.0266869	5.1879200
H	-1.1847291	-6.9724377	5.6001447
N	0.5327886	-2.2961897	3.8788715
H	1.1829977	-1.5180805	3.9083267
H	-0.0922937	-2.3852754	3.0882930

Table 509: BP86/def2-TZVP optimized structure of **19**.

20

C	-4.5584682	0.2282043	-0.0089355
H	-4.1695922	-0.8014746	-0.0159524
H	-4.1708984	0.7396842	-0.9035018
H	-5.6539790	0.1751386	-0.1002105
C	-4.1449100	0.9680190	1.2765079
C	-2.5950677	0.9980432	1.3327014
H	-2.2317253	1.4799706	0.4085385
H	-2.2339061	-0.0443211	1.2909336
C	-1.9604245	1.6958637	2.5395585
H	-2.2455404	1.2191050	3.4882377
H	-2.2445098	2.7563280	2.5987420
C	-4.7171740	2.3965403	1.2349194
H	-4.4892523	2.9566559	2.1532126
H	-4.3090109	2.9625082	0.3831185
H	-5.8121213	2.3731331	1.1271592
C	-4.7204419	0.2167489	2.4905944
H	-5.8158395	0.1415332	2.4174475
H	-4.3180177	-0.8062714	2.5506858
H	-4.4881575	0.7276531	3.4360146
H	-0.8636580	1.6566022	2.4723026

Table 510: BP86/def2-TZVP optimized structure of **20**.

14

C	0.0572829	0.4618038	0.5737342
H	0.6427834	-0.4667797	0.5390639
H	0.6761872	1.2454355	1.0292216
H	-0.1575757	0.7721850	-0.4573499
C	-1.2299348	0.2491465	1.3649281
H	-1.0157906	-0.0955862	2.3900957
H	-1.8568603	-0.5389354	0.9193922
C	-2.0719649	1.5043234	1.4822023
O	-1.7516106	2.6157481	1.1105254
O	-3.2644720	1.2291366	2.0819021
C	-4.1350112	2.3684285	2.2586734
H	-5.0336848	1.9762861	2.7450381
H	-3.6536077	3.1279802	2.8885980
H	-4.3842587	2.8172975	1.2882616

Table 511: BP86/def2-TZVP optimized structure of **21**.

18

C	-5.3804589	-0.2595548	-0.0044228
H	-5.0459063	-1.3072580	-0.0464861
H	-5.0483772	0.2305270	-0.9323143
H	-6.4797885	-0.2611855	-0.0038154
C	-4.8194386	0.4518208	1.2291639
H	-5.1984983	1.4873571	1.2629314
H	-5.1969734	-0.0385788	2.1422661
C	-3.2873343	0.4759770	1.2692699
H	-2.9099967	0.9664574	0.3544841
H	-2.9088393	-0.5612575	1.2353704
C	-2.7234036	1.1878632	2.5029511
H	-3.0881714	0.6984541	3.4209438
H	-3.0859269	2.2284847	2.5367879
C	-1.2030144	1.2044639	2.5353122
H	-0.8135249	1.7099817	1.6303099
H	-0.8155232	0.1669814	2.5304609
O	-0.7867804	1.8961787	3.7220810
H	0.1846164	1.9057242	3.7384942

Table 512: BP86/def2-TZVP optimized structure of **22**.

16

C	-5.3093910	-0.2003364	0.0166488
H	-4.9070849	0.2534237	-0.9096586
H	-6.4111117	-0.1023540	-0.0092855
C	-4.7596660	0.5345812	1.2311104
H	-5.1696779	1.5589875	1.2220112
H	-5.1535001	0.0450525	2.1377669
C	-3.2290022	0.5796182	1.2781957
H	-2.8419074	1.1037048	0.3885294
H	-2.8255305	-0.4429046	1.2484271
C	-2.7056844	1.2828900	2.5204941
H	-3.0543520	0.7506289	3.4266894
H	-3.1040696	2.3158297	2.5669088
O	-4.9286647	-1.5811826	0.1113941
H	-5.2126319	-2.0286218	-0.7025538
O	-1.2721366	1.2962481	2.4584155
H	-0.9413088	1.7186445	3.2683766

Table 513: BP86/def2-TZVP optimized structure of **23**.

17

C	-2.5392138	-1.3138540	0.0116742
C	-1.1524361	-0.9924259	-0.4682039
C	-0.3772200	-0.0557466	0.0898238
C	-0.7931418	0.8067934	1.2537111
C	-2.1836224	0.4710433	1.7291439
C	-2.9638545	-0.4636855	1.1749437
H	-0.7746098	-1.5687330	-1.3174424
H	-3.2616902	-1.2037200	-0.8203961
H	-2.6054871	-2.3855792	0.2832985
H	-0.0890974	0.6171356	2.0900734
H	-2.5606162	1.0523424	2.5764234
H	-3.9658380	-0.6372643	1.5773706
H	0.6244122	0.1230732	-0.3136302
C	-0.6639825	2.3090383	0.9140815
H	-0.9244358	2.9314391	1.7829738
H	0.3653072	2.5573349	0.6159571
H	-1.3356841	2.5769969	0.0860829

Table 514: BP86/def2-TZVP optimized structure of **24**.

16

C	-5.7611943	-0.1122497	-0.1592148
H	-5.4417661	-1.1389096	-0.3860821
H	-5.2798154	0.5599418	-0.8832965
H	-6.8482163	-0.0563909	-0.3096396
C	-5.3966924	0.2771378	1.2808873
H	-5.7262018	1.3049704	1.4937923
H	-5.9341398	-0.3818161	1.9824936
C	-3.9110015	0.1935581	1.5712940
C	-3.1485750	1.2596039	1.8993763
H	-3.6575582	2.2272976	1.9584485
C	-1.6857233	1.2517145	2.1928762
H	-1.1480650	1.9175107	1.4986204
H	-1.4920013	1.6404555	3.2056341
H	-1.2524801	0.2462756	2.1170456
C	-3.3218742	-1.1090273	1.4735683
N	-2.8807231	-2.1859334	1.3863565

Table 515: B3LYP/aug-cc-pVDZ optimized structure of **25**.

18

C	0.00000000	0.00000000	0.00000000
C	0.74302000	-1.31403500	0.04799100
C	0.18899700	-2.48679900	0.25475700
C	-0.37176300	-3.65842400	0.45657100
H	-0.47162000	-4.01591700	1.48773800
C	-0.90619300	-4.56656800	-0.62607800
H	-0.76072600	-4.12810800	-1.62075600
H	-0.40297800	-5.54548300	-0.59923000
H	-1.98128100	-4.75359900	-0.48116400
H	1.82684400	-1.26867700	-0.10359000
H	-1.07587800	-0.14304300	0.15734500
H	0.37836200	0.68734600	0.77209900
H	0.14945400	0.49355400	-0.97247900
C	3.92703700	-3.72601500	0.61002600
Cl	4.68297000	-2.40289800	-0.37186100
H	4.35665500	-4.67541800	0.27946800
H	4.16016700	-3.53704800	1.66138500
H	2.84731100	-3.70138700	0.438339000

Table 516: B3LYP/aug-cc-pVDZ optimized structure of **26**.

18

C	0.00000000	0.00000000	0.00000000
C	1.24256100	-0.79025100	0.33472100
C	1.30267600	-2.09405100	0.48213900
C	1.37420100	-3.39894200	0.62254900
H	1.22171200	-3.82323700	1.62158600
C	1.66992500	-4.37951200	-0.48798200
H	1.80940200	-3.86438600	-1.44593100
H	2.58140000	-4.95502600	-0.26489400
H	0.84931600	-5.10492100	-0.59901500
H	2.16710300	-0.21621300	0.46400400
H	-0.87231500	-0.65123700	-0.13031700
H	-0.22183400	0.72849000	0.79495100
H	0.14578600	0.57233500	-0.92876200
Cl	-3.50416800	-2.45442800	-0.29073600
C	-2.69867600	-3.17112000	1.16544500
H	-3.09350900	-4.18101200	1.30456500
H	-2.93600700	-2.53870300	2.02527300
H	-1.62093300	-3.19077900	0.97997700

Table 517: BP86/def2-TZVP optimized structure of **27**.

21

C	-5.9062970	0.6476486	0.1159437
H	-5.5230491	-0.3815987	0.0444482
H	-5.6802616	1.1506975	-0.8365939
H	-7.0000372	0.5898708	0.2105467
C	-5.2780112	1.3908945	1.2973871
H	-5.7093513	2.4041215	1.3675340
H	-5.5469693	0.8817864	2.2385829
C	-3.7521945	1.4991054	1.2022326
H	-3.4818616	2.0166892	0.2645772
H	-3.3201451	0.4856338	1.1228693
C	-3.1132887	2.2300617	2.3869658
H	-3.3692252	1.7100757	3.3254544
H	-3.5470510	3.2418847	2.4709697
C	-1.5814857	2.3426590	2.2775848
H	-1.3375238	2.8599781	1.3313377
H	-1.1369418	1.3360602	2.2079070
C	-0.9614037	3.0896152	3.4219965
H	-1.3115683	4.1190233	3.5656383
C	-0.0483950	2.5976781	4.2644089
H	0.3579239	3.1937115	5.0827298
H	0.3296620	1.5772569	4.1633392

Table 518: BP86/def2-TZVP optimized structure of **28**.

19

C	-0.9294495	0.1584081	-0.0056092
C	0.5424674	0.1757344	-0.0009524
O	-0.2081335	1.4158937	-0.0178856
H	-1.4194749	-0.0625152	-0.9648160
H	1.0373471	-0.0110834	0.9630169
C	1.3785786	-0.1266524	-1.2205379
H	1.6245567	-1.2025778	-1.2149022
H	0.7706674	0.0576336	-2.1199844
C	2.6654065	0.7050654	-1.2737552
H	3.2546319	0.4687917	-2.1708129
H	2.4332043	1.7788577	-1.2924036
H	3.3005171	0.5125693	-0.3962664
C	-1.7586604	-0.1348562	1.2208671
H	-1.9780078	-1.2163041	1.2414287
H	-1.1560313	0.0861934	2.1156333
C	-3.0657403	0.6658459	1.2535807
H	-3.6493320	0.4375201	2.1563600
H	-2.8601289	1.7451362	1.2453745
H	-3.6956511	0.4358932	0.3812839

Table 519: BP86/def2-TZVP optimized structure of **29**.

18

N	0.2460360	-0.0019614	-0.0963981
C	-0.0389802	-1.3859284	0.2703448
H	-0.1091597	-1.9574030	-0.6675877
H	0.8240691	-1.7936227	0.8260154
C	-1.3174916	-1.5755874	1.0902339
H	-2.1955289	-1.2051584	0.5433939
H	-1.4689580	-2.6433161	1.3053839
H	-1.2641220	-1.0479921	2.0522568
C	0.6212858	0.9698918	0.9378470
H	0.9665979	0.4009905	1.8142945
H	1.4744027	1.5455466	0.5490415
C	-0.5039883	1.9341493	1.3224521
H	-1.3759744	1.4029166	1.7275429
H	-0.1480959	2.6398463	2.0871414
H	-0.8216742	2.5123043	0.4457923
C	0.2951958	0.3867458	-1.4052108
H	0.0347145	-0.4459510	-2.1004943
O	0.5903314	1.5105568	-1.7965985

Table 520: BP86/def2-TZVP optimized structure of **30**.

17

C	-5.1881509	-0.6174908	0.0461318
H	-4.8384688	-1.6593292	0.0997731
H	-4.8533307	-0.2044928	-0.9171762
H	-6.2870439	-0.6350530	0.0376274
C	-4.6528831	0.2079511	1.2186773
H	-5.0448738	1.2373260	1.1562386
H	-5.0329574	-0.2062770	2.1675004
C	-3.1218665	0.2547095	1.2652606
H	-2.7244563	-0.7705728	1.3473105
H	-2.7336090	0.6685117	0.3214728
C	-2.5951572	1.0975784	2.4439326
H	-2.9586974	0.6922981	3.3971002
H	-2.9584442	2.1322275	2.3433756
O	-0.3994187	0.5188180	3.3171376
O	-0.5433734	1.8832797	1.5172929
H	0.4278928	1.8093643	1.6267062
C	-1.0864484	1.1142270	2.5113937

Table 521: BP86/def2-TZVP optimized structure of **31**.

17

C	-5.7909350	-0.0326302	-0.0038164
H	-5.4444805	-1.0740577	-0.0807765
H	-5.4797721	0.4894589	-0.9211119
H	-6.8896466	-0.0471555	0.0153433
C	-5.2215707	0.6496908	1.2421972
H	-5.6128019	1.6786072	1.3129229
H	-5.5751364	0.1259378	2.1458164
C	-3.6866562	0.6885600	1.2506770
H	-3.3326914	1.2180454	0.3494277
H	-3.2890133	-0.3360778	1.1888228
C	-3.1299648	1.3696817	2.4977470
H	-3.3504016	0.8223309	3.4269189
H	-3.4995031	2.4011784	2.6055941
S	-1.3103233	1.5741603	2.4885592
O	-0.9647909	2.2625814	3.7531478
O	-1.0788665	-0.0968149	2.6781490
H	-0.1380781	-0.2642264	2.4756617

Table 522: B3LYP/aug-cc-pVDZ optimized structure of **32**.

19

C	0.00000000	0.00000000	0.00000000
C	0.26477900	1.03884700	-1.06696700
C	0.56015700	2.30375500	-0.83875300
C	0.83496600	3.56412300	-0.59452500
H	-0.00959500	4.25611400	-0.50356100
C	2.21476600	4.15233000	-0.42384100
H	2.99872800	3.39492300	-0.53440400
H	2.38454300	4.94546300	-1.16749500
H	2.30884200	4.61568400	0.56986200
H	0.18570200	0.70228600	-2.10743600
H	0.12621900	0.42155100	1.00389900
H	-1.02488300	-0.38960500	-0.08956600
H	0.68272600	-0.85590700	-0.10944200
O	-2.87464200	2.41510700	-0.95783500
H	-1.92973100	2.22146300	-1.04758200
H	-3.13904700	2.75649700	-1.82011600
O	3.74237700	0.99978500	-1.12117400
H	2.77423800	0.99876200	-1.14959700
H	4.00489100	0.11189900	-1.38963100

Table 523: B3LYP/aug-cc-pVDZ optimized structure of **33**.

19

C	0.00000000	0.00000000	0.00000000
C	-1.44827100	-0.19878300	-0.37414100
C	-2.04293800	-1.34109300	-0.63119900
C	-2.68127000	-2.46113000	-0.90325200
H	-2.70581400	-2.80500100	-1.94367500
C	-3.43835000	-3.30180600	0.10062400
H	-3.33195300	-2.90198400	1.11643300
H	-4.50941200	-3.32458000	-0.15155100
H	-3.08607700	-4.34443800	0.09053700
H	-2.06263300	0.70676300	-0.44062800
H	0.57245600	-0.93371400	-0.01848400
H	0.47734100	0.70448400	-0.69712200
H	0.07879600	0.44089000	1.00548800
O	0.15967200	-4.02968900	-0.29487100
H	0.01948200	-4.32455700	0.61314400
H	-0.55841300	-3.39689800	-0.46706900
O	2.62937400	-2.59048900	-0.37227000
H	1.83843900	-3.15933300	-0.41732900
H	3.29832400	-3.04389800	-0.89678700

Table 524: B3LYP/aug-cc-pVDZ optimized structure of **34**.

19

C	0.00000000	0.00000000	0.00000000
C	-0.68993100	0.77192600	-1.10217500
C	-1.45636700	1.82937600	-0.92486600
C	-2.21599400	2.88398500	-0.73882600
H	-3.29196000	2.73537300	-0.59301700
C	-1.71400400	4.30789300	-0.70633000
H	-0.62848200	4.35809500	-0.85427200
H	-2.20409300	4.90441000	-1.49058700
H	-1.96035800	4.77879100	0.25736000
H	-0.50274400	0.42985300	-2.12701700
H	-0.24966800	0.40872400	0.98636800
H	-0.28947700	-1.06153400	-0.02166600
H	1.09239800	0.03953500	-0.12845300
O	-3.81044900	-0.49812700	-0.97321900
H	-3.97267500	-0.80889100	-1.87218800
H	-2.94915000	-0.04659600	-1.01545900
O	-5.48231700	1.72505300	-0.32587800
H	-6.07453600	1.54082000	0.41142100
H	-5.00805100	0.88779600	-0.49047700

Table 525: BP86/def2-TZVP optimized structure of **35**.

19

C	-5.8098344	-0.3051512	-0.1638047
H	-5.4696274	-1.3520664	-0.1435670
H	-5.4993083	0.1343960	-1.1255539
H	-6.9085278	-0.3149452	-0.1669585
C	-5.2702270	0.4797216	1.0353978
H	-5.6092938	1.5280295	0.9848614
H	-5.6687297	0.0569685	1.9687760
C	-3.7422051	0.4724858	1.1304943
H	-3.3891120	-0.5777649	1.1978837
C	-3.2242579	1.2128470	2.3709371
H	-3.5764323	2.2616747	2.3020226
C	-1.7030776	1.1948687	2.4717243
H	-1.2505659	1.6628969	1.5883477
H	-1.3675622	1.7500774	3.3620270
H	-1.3372651	0.1602713	2.5501135
O	-3.8336173	0.5651313	3.5036192
H	-3.4251616	0.9370019	4.3032609
O	-3.1287505	1.1229108	0.0028909
H	-3.4569138	0.6832130	-0.7992760

Table 526: BP86/def2-TZVP optimized structure of **36**.

18

C	-6.1059266	0.1856256	-0.0814315
H	-5.8417510	-0.8811467	-0.0219748
H	-5.6487553	0.5892421	-0.9977804
H	-7.1965441	0.2516267	-0.1978092
C	-5.6371066	0.9469419	1.1604162
H	-5.9472675	2.0009623	1.0983977
H	-6.1250657	0.5436455	2.0602793
C	-4.1209910	0.8805465	1.3396996
H	-3.5950991	1.3012518	0.4662465
H	-3.7738644	-0.1649429	1.4063473
C	-3.6212286	1.6019304	2.5693293
O	-2.2381582	1.5270606	2.6222869
O	-4.2937212	2.1657604	3.4022098
C	-1.6014934	2.1300982	3.6957509
H	-2.2727169	2.6193047	4.4014162
C	-0.2745351	2.0808142	3.8001278
H	0.3429923	1.5744510	3.0591226
H	0.2139173	2.5571591	4.6473549

Table 527: BP86/def2-TZVP optimized structure of **37**.

18

C	-6.4381742	0.0215126	0.5315285
H	-6.5399858	-0.0866928	-0.5600375
H	-6.4444171	1.1024182	0.7413467
H	-7.2768895	-0.4767752	1.0293242
C	-5.1271582	-0.5799233	0.9765780
C	-3.8593715	0.1657557	0.5284721
H	-3.0477192	-0.5670866	0.4400633
H	-4.0286682	0.6842190	-0.4236888
C	-3.5271522	1.2258219	1.5928091
C	-2.5800120	0.7801852	2.6889826
H	-1.6143295	0.5475510	2.2036924
H	-2.9461019	-0.1963262	3.0535911
C	-2.4055015	1.7885677	3.8188390
H	-3.3627059	1.9914253	4.3171806
H	-1.7002663	1.4081170	4.5699798
H	-2.0256142	2.7455614	3.4389379
O	-5.0512669	-1.5713600	1.6817123
O	-4.0403215	2.3310875	1.5554570

Table 528: BP86/def2-TZVP optimized structure of **38**.

20

C	-5.3885354	-0.0844422	0.0101512
H	-5.1822207	-1.1641002	-0.0445496
H	-4.9996164	0.3740843	-0.9115263
H	-6.4798622	0.0459531	0.0119444
C	-4.7491329	0.5399460	1.2525535
H	-5.0008044	1.6127486	1.2990928
H	-5.1823331	0.0866584	2.1597811
C	-3.2250466	0.3791747	1.2899134
H	-2.7909599	0.8317551	0.3809837
H	-2.9731962	-0.6949601	1.2448079
C	-2.5811383	1.0033610	2.5336624
H	-2.9995784	0.5476144	3.4450858
H	-2.8187875	2.0788943	2.5819936
C	-1.0695332	0.8264817	2.5481651
H	-0.6006664	1.3330383	1.6862986
H	-0.7928460	-0.2371543	2.5089959
O	-0.5010844	1.3421533	3.7780113
C	0.2571613	2.4626383	3.6965135
H	0.3669830	2.8330366	2.6496639
O	0.7566476	2.9845392	4.6588284

Table 529: BP86/def2-TZVP optimized structure of **39**.

20

C	-4.5944442	-0.6646077	-0.1491908
H	-4.3466277	-0.5335488	-1.2179280
H	-5.6950776	-0.6445585	-0.0926740
C	-4.0616960	0.5368019	0.6348076
H	-4.5929824	1.4529790	0.3172928
H	-4.2899147	0.3838566	1.7056219
N	-2.6201725	0.6815885	0.4633789
H	-2.2106742	0.2958197	-0.3824227
C	-1.8265974	1.6687644	1.0166461
O	-0.6825559	1.8890809	0.6223670
N	-2.4220203	2.4125955	2.0288001
H	-3.1861189	2.0091731	2.5612803
H	-1.7568476	2.9581968	2.5666024
C	-4.0834319	-2.0248189	0.3416676
H	-2.9826830	-2.0435748	0.3077556
H	-4.3534933	-2.1453461	1.4045693
C	-4.6440365	-3.1959362	-0.4685224
H	-4.2660919	-4.1582209	-0.0959884
H	-5.7430926	-3.2272796	-0.4185996
H	-4.3634771	-3.1170163	-1.5296932

Table 530: BP86/def2-TZVP optimized structure of **40**.

18

C	-5.7387190	-0.0618156	0.0050331
H	-5.4151186	-1.1132610	-0.0031963
H	-5.3856795	0.4027416	-0.9275210
H	-6.8373211	-0.0511403	-0.0111970
C	-5.1960259	0.6752543	1.2315649
H	-5.5652023	1.7144220	1.2322413
H	-5.5916075	0.2083885	2.1489040
C	-3.6615916	0.6841373	1.2854027
H	-3.2597982	1.1730669	0.3847725
H	-3.2889846	-0.3526525	1.2829910
C	-3.1416652	1.4067805	2.5257689
H	-3.4355963	0.9109613	3.4618183
H	-3.4888085	2.4506384	2.5699339
O	-1.0101547	2.1809188	3.8676826
O	-0.8976320	-0.0113478	2.7228731
H	-0.4652626	-0.2351449	1.8745028
S	-1.3508978	1.5594808	2.6108494
O	-0.8365583	2.0605814	1.3485140

Table 531: B3LYP/aug-cc-pVDZ optimized structure of **41**.

23

C	0.00000000	0.00000000	0.00000000
C	1.19160100	0.86227500	0.34292900
C	1.22405700	2.17260800	0.25877400
C	1.25214800	3.48378200	0.17130800
H	1.57118900	3.93342600	-0.77565700
C	0.87332400	4.44043400	1.27742400
H	0.57195600	3.90190700	2.18419100
H	1.71663700	5.10259700	1.52761600
H	0.03968700	5.08714800	0.96364700
H	2.09241600	0.33933600	0.68164900
H	-0.85220100	0.60790900	-0.32699100
H	0.25355900	-0.70813500	-0.80375300
H	-0.30984300	-0.59775600	0.87087000
Cl	8.44077800	2.95538800	0.43334400
C	8.63278300	1.23955100	-0.12506100
H	9.55626100	0.84921300	0.31087100
H	8.68857100	1.24931400	-1.21690800
H	7.76262200	0.67541800	0.22104600
H	5.72104900	2.42660900	1.60115300
C	4.81604200	1.87298700	1.86360800
Cl	5.10325300	0.12400000	1.46022000
H	3.95706700	2.21349600	1.27932900
H	4.61188600	1.93380900	2.93571900

Table 532: B3LYP/aug-cc-pVDZ optimized structure of **42**.

23

C	0.00000000	0.00000000	0.00000000
C	-0.69924200	0.11906200	-1.33363500
C	-0.69015200	1.18501400	-2.10211400
C	-0.67576300	2.25116400	-2.87020700
H	-1.46190100	3.00181700	-2.73371200
C	0.34984700	2.53550600	-3.94199000
H	1.08936500	1.72879000	-4.01157700
H	-0.13573200	2.65139800	-4.92303700
H	0.87836200	3.47779300	-3.73143300
H	-1.25513000	-0.76228200	-1.67195900
H	0.52637000	0.92684600	0.25858800
H	-0.72190100	-0.22843700	0.79911500
H	0.73108300	-0.82257800	-0.01732200
Cl	-4.12870500	4.08005900	-1.63501000
C	-3.90801500	2.83638800	-0.33019400
H	-4.55033000	1.98441300	-0.56694700
H	-4.19385700	3.29740700	0.61843300
H	-2.85568400	2.54060800	-0.32528400
Cl	-5.26051700	-0.40888100	-2.26681700
C	-4.41886600	0.53442900	-3.56980700
H	-3.35913000	0.59751600	-3.30883400
H	-4.56324600	0.00032500	-4.51227100
H	-4.86916500	1.52954300	-3.60635100

Table 533: B3LYP/aug-cc-pVDZ optimized structure of **43**.

22

C	0.00000000	0.00000000	0.00000000
C	-0.20326800	0.97693100	-1.13625800
C	-0.57645500	2.23394000	-1.00054100
C	-0.95846700	3.48148900	-0.85280000
H	-2.03513200	3.68459700	-0.85211200
C	-0.04246900	4.66947200	-0.68078500
H	1.01305100	4.37586700	-0.69539300
H	-0.21619300	5.40241900	-1.48321300
H	-0.25567800	5.17764400	0.27191000
H	-0.02682900	0.59284900	-2.14768900
H	-0.17823800	0.47800200	0.97028200
H	-0.68461700	-0.85536400	-0.09999400
H	1.02460900	-0.40081500	-0.01112100
O	2.89034700	2.68916100	-0.97204700
H	2.07351400	2.17985000	-1.05554300
H	3.61100800	2.04384600	-1.06439500
O	-3.61030900	0.67205900	-1.30742200
H	-3.90304200	0.81063500	-2.21571100
H	-2.68039600	0.94516900	-1.30434800
O	5.22081600	0.93999300	-1.20746900
H	5.77191300	1.23456700	-1.94337800
H	5.77100200	1.04999700	-0.42178600

Table 534: B3LYP/aug-cc-pVDZ optimized structure of **44**.

22

C	0.00000000	0.00000000	0.00000000
C	-0.59626500	0.82620200	-1.11738900
C	-1.40240700	1.85998500	-0.96750300
C	-2.24513900	2.85717400	-0.82448500
H	-3.31233700	2.61278600	-0.79383500
C	-1.88196200	4.31699000	-0.70408700
H	-0.79995400	4.47775100	-0.78468500
H	-2.37597300	4.90002000	-1.49565700
H	-2.22751200	4.72262100	0.25889000
H	-0.32836800	0.52442500	-2.13663000
H	-0.27541200	0.40056200	0.98294100
H	-0.35874800	-1.03867800	-0.06370100
H	1.09507000	-0.03400000	-0.08853900
O	1.85698700	3.07257600	-0.95683000
H	0.97519100	2.66718900	-1.00838700
H	1.90369500	3.45525700	-0.07205400
O	-4.10978500	-0.03813900	-1.08307200
H	-4.25107400	-0.97011000	-1.28452200
H	-3.15319300	0.09206200	-1.15331400
O	3.33315900	0.62293600	-1.08100400
H	4.16715900	0.66545300	-1.56126200
H	2.97304400	1.52898900	-1.10427500

Table 535: B3LYP/aug-cc-pVDZ optimized structure of **45**.

22

C	0.00000000	0.00000000	0.00000000
C	0.06712100	1.23305200	-0.87185000
C	0.24182600	2.46360900	-0.43773200
C	0.38579200	3.69457400	-0.00307400
H	-0.52373200	4.25039500	0.25188900
C	1.69361500	4.42675200	0.17707600
H	2.55227700	3.80972200	-0.11149800
H	1.70646000	5.34388800	-0.43079300
H	1.82164600	4.73431500	1.22599600
H	-0.06524400	1.07718500	-1.94855400
H	0.16016100	0.24943000	1.05579000
H	-0.98310700	-0.48474900	-0.09824700
H	0.75560500	-0.73888100	-0.30624600
O	3.40128600	1.17915800	-1.30558500
H	3.76693800	0.79406200	-0.48640800
H	2.47009300	1.37237500	-1.11935100
O	5.24211800	0.77584700	0.80939500
H	5.22145400	0.95666000	1.75559300
H	5.57411900	1.59409300	0.38643300
O	5.47324400	2.96143500	-0.92533000
H	6.11124600	3.02361400	-1.64503400
H	4.69583100	2.48845200	-1.29465500

Table 536: BP86/def2-TZVP optimized structure of **46**.

29

C	-6.1428565	-0.6536743	-0.0450249
H	-5.7493391	-1.6532989	-0.2794150
H	-5.9552542	-0.0028345	-0.9095328
H	-7.2336510	-0.7505765	0.0615203
C	-5.5451498	-0.0755965	1.2562831
C	-3.9503315	-0.0775818	1.2110817
C	-3.3841257	0.7826779	2.3794277
H	-3.9087592	0.5156448	3.3109985
H	-3.6295037	1.8382693	2.1848970
C	-1.8760539	0.6794036	2.6400620
H	-1.2794091	0.9267646	1.7497791
H	-1.5794942	-0.3249822	2.9723715
H	-1.5817247	1.3843484	3.4311036
C	-6.1066187	1.3530474	1.4254495
H	-5.7246951	2.0450469	0.6606253
H	-7.2026121	1.3329156	1.3273509
H	-5.8757048	1.7760747	2.4126384
C	-6.0761309	-0.9291416	2.4281323
H	-7.1689892	-0.8210781	2.4995118
H	-5.8616136	-1.9977583	2.2894150
H	-5.6552945	-0.6213895	3.3961093
C	-3.4089407	-1.5184168	1.3236848
H	-2.3303815	-1.5427617	1.1137646
H	-3.5583831	-1.9413549	2.3272673
H	-3.8903641	-2.1906399	0.5993631
C	-3.4455253	0.5125545	-0.1227553
H	-3.8687578	1.5077902	-0.3229474
H	-2.3518360	0.6200990	-0.1046876
H	-3.6889800	-0.1373647	-0.9739058

Table 537: BP86/def2-TZVP optimized structure of **47**.

26

C	2.6484069	-2.8401340	-1.2154493
O	1.4202120	-2.9097428	-1.1828892
N	3.3805128	-2.8769457	-2.3947989
H	4.3690066	-3.0984007	-2.3185830
N	3.4326207	-2.7181110	-0.0755330
H	4.3827409	-2.3813831	-0.2034572
C	2.7408986	-3.1902157	-3.6658519
H	2.8540852	-4.2637860	-3.9099595
H	1.6674418	-3.0101459	-3.5188872
C	2.8273235	-2.4655173	1.2256600
H	2.8078295	-1.3815377	1.4486657
H	1.7813838	-2.7904257	1.1439038
C	3.5460916	-3.2118289	2.3522559
H	4.6095375	-2.9160509	2.3700196
H	3.5282106	-4.2903262	2.1294059
C	3.2861287	-2.3384340	-4.8152115
H	4.3765738	-2.4886208	-4.8997105
H	3.1380053	-1.2753344	-4.5681276
C	2.6189945	-2.6716307	-6.1515202
H	3.0282116	-2.0578838	-6.9659320
H	2.7695491	-3.7275168	-6.4223353
H	1.5345965	-2.4914730	-6.1099516
C	2.9176515	-2.9408897	3.7208915
H	3.4510175	-3.4770197	4.5179904
H	2.9407927	-1.8686846	3.9674798
H	1.8664482	-3.2639221	3.7464009