

Optical Rotation calculated with Time-Dependent Density Functional Theory: A new benchmark – Supporting Information

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The optimized B3LYP/6-311G(d,p) geometries of molecules **1-42** studied in the paper (the atomic symbol followed by three cartesian coordinates, in Å). The structures labels correspond to those of Figure 1.

1			
C	−1.0434290	0.6153280	−0.0615190
C	0.1515990	−0.0360920	0.4888630
H	0.1531120	−0.2526560	1.5570100
O	−0.8257760	−0.7892730	−0.2415100
H	−0.9522010	1.2186250	−0.9624750
H	−1.8701630	0.8793260	0.5941530
C	1.5090730	0.0997910	−0.1483000
H	2.0832840	0.9000390	0.3286960
H	1.4131530	0.3248980	−1.2127570
H	2.0755690	−0.8302050	−0.0468100
2			
C	−0.5972470	−0.0937810	−0.4278450
C	0.5972490	−0.0937800	0.4277950
O	−0.0000170	1.1417930	0.0000170
C	−1.9791090	−0.3871020	0.0939390

H	-0.4434820	-0.3018460	-1.4872730
H	0.4434500	-0.3019120	1.4872090
C	1.9791270	-0.3870870	-0.0939200
H	-2.2393330	-1.4382610	-0.0649790
H	-2.7225440	0.2268110	-0.4227770
H	-2.0426510	-0.1686000	1.1621540
H	2.2391470	-1.4383500	0.0646400
H	2.7226020	0.2265060	0.4231170
H	2.0428320	-0.1681980	-1.1620470
3			
C	-0.5215310	0.1664740	0.5013290
C	0.3608860	1.1560240	-0.1530790
S	1.1010510	-0.5251380	-0.0542020
C	-1.7827430	-0.3109090	-0.1772290
H	-0.5809580	0.2343720	1.5835450
H	0.8477830	1.9076320	0.4578760
H	-2.6043330	0.3855110	0.0259730
H	-2.0778570	-1.2969080	0.1881590
H	-1.6438530	-0.3769100	-1.2583410
H	0.1027320	1.4789830	-1.1561080
4			
C	0.6009830	-0.3748390	0.4305560
C	-0.6009830	-0.3748360	-0.4305330
S	0.0000110	1.3232590	-0.0000030
C	1.9454160	-0.8191970	-0.0941400
H	0.4192650	-0.6096550	1.4763780
C	-1.9454370	-0.8191770	0.0941330
H	2.0395690	-1.9083680	-0.0141890
H	2.7591460	-0.3677950	0.4779230
H	2.0700040	-0.5361380	-1.1412780
H	-2.0395890	-1.9083540	0.0142600
H	-2.7591220	-0.3678220	-0.4780360
H	-2.0700860	-0.5360360	1.1412370
H	-0.4192400	-0.6096780	-1.4763470
5			
C	0.6078350	-0.0642750	0.4464900
C	-0.6077900	-0.0643850	-0.4463590
C	0.0000160	1.2458920	-0.0000680
C	1.9597670	-0.5015520	-0.0733600
H	0.4166430	-0.3331290	1.4824750
C	-1.9598140	-0.5015160	0.0733290
H	2.0771640	-1.5885870	-0.0161000
H	2.7734400	-0.0467280	0.5008680
H	2.0909470	-0.2089470	-1.1194750

H	-0.4164290	-0.3334530	-1.4822640
H	0.5461950	1.8349430	-0.7290170
H	-0.5462260	1.8349690	0.7288210
H	-2.7733830	-0.0461460	-0.5006150
H	-2.0908830	-0.2094290	1.1196120
H	-2.0775570	-1.5884800	0.0155010
6			
C	0.6345300	-0.4331080	0.4389180
C	-0.6338330	-0.4340930	-0.4388710
C	-0.0003830	0.8187310	-0.0003910
C	1.9720970	-0.8794870	-0.1201420
H	0.4634280	-0.7107570	1.4786300
C	-1.9710330	-0.8814570	0.1202950
H	2.0811250	-1.9669900	-0.0626060
H	2.8004570	-0.4284000	0.4344660
H	2.0754260	-0.5815670	-1.1668470
H	-0.4623230	-0.7124660	-1.4783270
C	-0.0015060	2.1381590	0.0000130
H	-2.7997770	-0.4315330	-0.4346800
H	-2.0747930	-0.5830290	1.1668140
H	-2.0789450	-1.9691040	0.0633870
H	0.7554420	2.7061360	0.5325030
H	-0.7592710	2.7052410	-0.5322700
7			
C	0.6057450	-0.0506600	0.4223180
C	-0.5962640	-0.1026890	-0.4477090
N	0.0326000	1.1949710	-0.1302810
C	1.9840860	-0.4286420	-0.0612360
H	0.4224200	-0.2428420	1.4787860
C	-1.9561310	-0.4519120	0.1087680
H	2.1726280	-1.4973090	0.0818240
H	2.7537770	0.1283460	0.4817890
H	2.0910910	-0.1957720	-1.1229160
H	-0.4434510	-0.3956820	-1.4844730
H	-0.5161100	1.6712300	0.5823320
H	-2.7499790	0.0709400	-0.4341970
H	-2.0322140	-0.1742120	1.1650970
H	-2.1509780	-1.5260800	0.0308830
8			
C	1.0140930	-0.1462930	-0.3759200
C	0.4111600	0.9596080	0.4186900
N	-0.0298440	-0.4472020	0.6274270
C	2.3727030	-0.7432520	-0.1079350
H	0.6830490	-0.1787960	-1.4107250

C	-0.4500300	2.0257680	-0.2106240
H	3.1441750	-0.1934090	-0.6556540
H	2.4061230	-1.7887790	-0.4259230
H	2.6101490	-0.7037150	0.9567460
H	0.9496810	1.2912910	1.3047010
Cl	-1.6282860	-0.8702980	-0.0827490
H	-1.2368220	2.3454500	0.4778960
H	-0.9215190	1.6813790	-1.1309940
H	0.1673760	2.8970660	-0.4465680
9			
C	1.4314650	-0.3373060	-0.3738050
C	1.1943330	0.9031340	0.4159820
N	0.3680610	-0.3106320	0.6525450
C	2.5612030	-1.3044620	-0.1198730
H	1.0942080	-0.2769290	-1.4055910
C	0.6804340	2.1713940	-0.2186220
H	3.4505180	-1.0076710	-0.6845890
H	2.2822600	-2.3158650	-0.4279760
H	2.8172700	-1.3306600	0.9409630
H	1.8249460	1.0720960	1.2878730
Br	-1.4549230	-0.2877230	-0.0391740
H	0.0426280	2.7229860	0.4774910
H	0.1046140	1.9704280	-1.1223090
H	1.5248290	2.8137790	-0.4846790
10			
C	0.6433180	1.2720450	0.4948820
C	1.1638870	0.1889470	-0.3812890
N	-0.2139940	0.7131120	-0.5696700
H	0.9063030	2.3134230	0.3415010
H	0.4107920	0.9998510	1.5188190
C	1.4785160	-1.1860180	0.1520780
H	1.7682230	0.4808710	-1.2369320
Cl	-1.5303220	-0.3426070	0.0540760
H	1.2734200	-1.9501300	-0.6022190
H	0.9000380	-1.4224680	1.0450480
H	2.5403200	-1.2388610	0.4081660
11			
C	-2.2369360	-0.6283850	-0.0763210
C	-0.9372490	-0.0562280	0.4298430
N	0.1263840	0.0992870	-0.5842760
Cl	1.7615650	-0.3171320	0.0357410
C	-0.4414280	1.2982050	0.0663850
H	0.1734600	1.8201630	0.7898700
H	-0.9960550	1.9319550	-0.6185720

H	-0.6070680	-0.4152760	1.3997390
H	-2.1872410	-1.7192590	-0.1244180
H	-2.4632100	-0.2521960	-1.0757240
H	-3.0574990	-0.3507060	0.5919940
12			
C	-1.8159600	-0.6194240	-0.0685170
N	-0.6850230	-0.0462640	-0.7204380
O	-1.7216530	0.7815160	-0.0280960
H	-1.7002500	-1.1272370	0.8867460
H	-2.5771040	-1.0337980	-0.7276560
C	0.6231730	-0.0146140	0.0068140
C	1.4073980	-1.1948630	-0.5863770
C	0.5376130	-0.1255890	1.5370410
C	1.2717620	1.3192920	-0.3893960
H	1.4648570	-1.1124200	-1.6737000
H	0.9327640	-2.1488220	-0.3384450
H	2.4237000	-1.2097230	-0.1844460
H	0.2616860	-1.1306120	1.8663340
H	-0.1846910	0.5894060	1.9353840
H	1.5137750	0.1006330	1.9721960
H	2.2932880	1.3803830	-0.0052060
H	0.6979150	2.1557390	0.0156780
H	1.2985320	1.4193590	-1.4764370
13			
C	1.4808660	-0.0045580	0.3432200
N	0.3709650	0.0027110	-0.5549020
O	1.0469630	-1.2627650	-0.1222000
H	1.2884370	0.1627730	1.4024890
C	2.7985050	0.5077930	-0.1666250
C	-1.0181850	0.1037480	-0.0096980
C	-1.3943100	1.5794780	-0.2140540
C	-1.1900650	-0.3056670	1.4614730
C	-1.8730330	-0.8006500	-0.9092670
H	-1.2672320	1.8692260	-1.2592360
H	-0.7720930	2.2346460	0.4027340
H	-2.4376620	1.7424230	0.0677890
H	-0.7493950	0.4213960	2.1483670
H	-0.7414910	-1.2838950	1.6444590
H	-2.2546200	-0.3710070	1.6986070
H	-2.9332030	-0.6970210	-0.6636410
H	-1.5862820	-1.8462940	-0.7773700
H	-1.7279990	-0.5373910	-1.9590670
H	2.8793320	0.3125220	-1.2360440
H	3.6227620	0.0107170	0.3527220

H	2.8843090	1.5841870	0.0098090
14			
C	-1.4980150	-0.1264960	-0.2732690
C	-0.5937580	-1.0419050	0.0886350
C	0.4640210	-0.0182310	0.4821740
C	-0.6035010	1.0577260	0.0452660
H	-2.5131260	-0.1891460	-0.6492770
C	1.7852590	-0.0327470	-0.2800710
H	0.6564980	0.0088610	1.5611730
H	-0.3004130	1.6681140	-0.8113480
H	-0.9495250	1.7224920	0.8433080
H	-0.5947450	-2.1266710	0.1075340
H	2.3906340	0.8459330	-0.0361420
H	1.6129140	-0.0382630	-1.3607140
H	2.3737220	-0.9213990	-0.0309530
15			
O	-0.3936350	-1.0635510	-0.0803610
C	0.4786460	0.0357160	-0.4669500
C	-0.5759330	1.0727420	-0.0179550
C	-1.4732890	-0.1526110	0.2338930
H	0.6337700	0.0249200	-1.5535530
H	-0.9163820	1.7730920	-0.7808340
H	-0.2976160	1.6231760	0.8823090
H	-2.3117140	-0.2620540	-0.4630920
H	-1.8369920	-0.2918150	1.2561370
C	1.8097520	-0.0059900	0.2520390
H	2.3500310	-0.9215860	-0.0033930
H	2.4296020	0.8493870	-0.0360640
H	1.6633250	0.0141430	1.3352190
16			
C	-0.9859730	1.4050640	-0.0728460
C	0.2407960	1.4874100	-0.5879070
S	0.7215490	-0.1529840	-0.0056170
C	-1.0529730	0.0424620	0.5960890
H	-1.7844280	2.1364270	-0.1078410
O	1.7071180	-0.1276920	1.0743440
O	0.8470830	-1.1323130	-1.0858030
H	-1.0526840	0.0964660	1.6876520
C	-2.0430740	-0.9748420	0.0582540
H	0.7942520	2.2330350	-1.1400290
H	-1.8896500	-1.9475700	0.5295110
H	-1.9313570	-1.0972930	-1.0201550
H	-3.0671940	-0.6538500	0.2708790
17			

C	-0.0000020	-0.4140180	-0.0000820
C	1.2460740	-0.4124290	-0.3898150
C	-1.2459090	-0.4119140	0.3901890
H	-1.5373900	-1.0897580	1.1922810
C	2.3353570	0.4600290	0.1851310
H	1.5379560	-1.0912810	-1.1909070
C	-2.3355030	0.4597100	-0.1854250
H	1.9512980	1.1010180	0.9798820
H	2.7742720	1.0968600	-0.5903120
H	3.1462750	-0.1507210	0.5961800
H	-3.1466880	-0.1516020	-0.5951030
H	-1.9518880	1.0995170	-0.9813430
H	-2.7739380	1.0977020	0.5893370
18			
C	-0.5782070	0.4665130	0.4119930
H	-0.6188970	0.5932940	1.4884070
F	-0.7841510	1.6451220	-0.2030040
Br	1.2185660	-0.1872310	-0.0282360
Cl	-1.8531960	-0.6850230	-0.0673570
19			
C	0.5215240	1.3008300	-0.3962120
C	-0.9262670	1.0353730	0.0662890
C	0.1708380	-0.8694010	0.6679370
C	1.2293270	-0.0172300	-0.0299220
H	0.6353970	1.5247270	-1.4596940
H	0.9865290	2.1179160	0.1660120
C	-0.6823980	0.2177310	1.3579190
C	-1.5493300	-0.0319330	-0.8647640
H	-2.6220670	-0.1280970	-0.6809550
H	-1.4215030	0.2210550	-1.9199350
C	-0.7907210	-1.3392160	-0.4658530
H	-1.4759290	-2.0935160	-0.0721510
H	-0.2509740	-1.7923350	-1.2996440
O	2.3735080	-0.3110000	-0.2651880
H	0.5923140	-1.6700720	1.2727030
H	-1.6013620	-0.1792740	1.7966030
H	-0.1378660	0.7750280	2.1252370
H	-1.5304480	1.9356370	0.1809690
20			
C	1.1757860	-0.0069620	-0.0484540
C	-0.8100310	-1.2831360	-0.5280540
C	0.1167890	-0.9119490	0.6298460
C	0.4248100	1.2892770	-0.4231390
C	-1.0266460	0.9550630	0.0290500

C	-1.4930270	-0.1871510	-0.8725130
H	-0.8056540	-2.2442270	-1.0246230
H	0.5436000	-1.7256560	1.2107680
H	0.5260180	1.5173680	-1.4847770
H	0.8578210	2.1195540	0.1439830
H	-1.6922410	1.8132420	0.1087690
H	-2.1795940	-0.0787570	-1.7023480
O	2.3380230	-0.2538320	-0.2305820
C	-0.7412690	0.1667950	1.3346370
H	-1.6420920	-0.2528140	1.7856890
H	-0.1905180	0.7503100	2.0789600
21			
C	1.4455650	0.0723020	0.2888210
C	0.0669460	0.6077220	-1.6352840
C	0.2960290	-0.5001730	-0.5527250
C	0.8592070	1.2522370	1.0802830
C	-0.6066740	1.2603410	0.6022500
C	-0.5928630	1.7834510	-0.8531180
H	1.0053660	0.8910340	-2.1178060
C	0.5602740	-1.8889410	-1.1008300
H	1.4043380	2.1730660	0.8575750
H	0.9704790	1.0643780	2.1509140
H	-1.2921690	1.7915500	1.2656350
H	-0.0241690	2.7123280	-0.9381220
O	2.5862900	-0.3165790	0.3147850
C	-0.9170710	-0.2631140	0.4179260
C	-2.2919220	-0.5401550	-0.2083170
C	-0.8283420	-1.0837680	1.7172940
H	-0.5870540	0.2207830	-2.4199440
H	-1.6004390	1.9921300	-1.2168430
H	-0.2523420	-2.2204510	-1.7531770
H	0.6776760	-2.6206010	-0.2974000
H	1.4881030	-1.8962350	-1.6781180
H	-3.0847340	-0.2160770	0.4736210
H	-2.4278380	-1.6119990	-0.3780850
H	-2.4515640	-0.0340910	-1.1605640
H	-1.5828660	-0.7445770	2.4338530
H	0.1447530	-1.0279120	2.2084150
H	-1.0247520	-2.1401080	1.5139670
22			
C	0.0175750	-0.9227620	-0.3281650
C	-1.3709520	1.0135170	-0.8869310
C	-1.2622060	-0.1969650	0.1012970
C	1.2187540	-0.0405500	0.0934790

C	0.4667810	1.1889500	0.6930760
C	-0.2468580	1.9886630	-0.4217540
H	-1.2641290	0.6984580	-1.9278710
C	-2.4907070	-1.0818000	0.1842860
C	2.1332080	0.2375890	-1.1093210
C	2.0455480	-0.7805180	1.1667210
H	1.0989210	1.8000550	1.3406000
H	0.4173490	2.2933350	-1.2306470
O	0.0893520	-1.9835840	-0.8991190
C	-0.7529780	0.5227820	1.3741180
H	-1.4742280	1.2518480	1.7540890
H	-0.5000060	-0.1641410	2.1839650
H	-2.3623150	1.4636800	-0.7866380
H	-0.6760760	2.9018640	-0.0017750
H	-3.3750000	-0.5008370	0.4621120
H	-2.3561320	-1.8756700	0.9239450
H	-2.6820840	-1.5635030	-0.7777920
H	2.9458410	0.9147920	-0.8287090
H	1.5998830	0.6773940	-1.9536710
H	2.5729030	-0.7000740	-1.4563850
H	2.9178870	-0.1809430	1.4442480
H	2.3969150	-1.7360690	0.7709670
H	1.4764710	-0.9849510	2.0756890
23			
C	-1.1865460	-1.1637010	0.0488260
C	0.3076810	-1.1493080	0.3778710
C	0.5425230	1.0579860	0.4472220
C	-0.9208630	1.3732590	0.1164640
H	-1.4111420	-1.9956340	-0.6245770
H	-0.9858760	2.2732090	-0.5045580
O	0.5842220	-0.1047910	1.2945220
O	1.0778450	-0.8496940	-0.7920860
C	1.3547980	0.5584290	-0.7585110
H	2.4278110	0.7147680	-0.6103380
H	1.0496580	1.0155230	-1.7040410
H	0.6654740	-2.0870680	0.8059290
H	1.0281490	1.8747010	0.9821130
H	-1.7319260	-1.3346690	0.9830760
C	-1.5889300	0.1774800	-0.5940100
H	-1.2823180	0.1644820	-1.6440410
H	-2.6759990	0.2933040	-0.5893920
H	-1.4323360	1.5923960	1.0591650
24			
C	-1.7672240	-0.1218590	-0.7459030

C	-0.8392880	-1.1694780	-0.1316510
C	0.3666930	0.2039840	1.1312870
C	-0.3431890	1.4797420	0.6567090
H	-1.9982560	-0.3836550	-1.7824850
H	0.3685630	2.3066600	0.5641900
O	-0.6103970	-0.8491990	1.2318970
O	0.4455300	-1.1300320	-0.7661580
C	1.3427410	-0.4447670	0.1339530
H	1.9193220	-1.2028290	0.6804060
H	-1.2383330	-2.1845230	-0.1823780
H	0.8110240	0.3362750	2.1189520
H	-2.7049780	-0.1405700	-0.1810660
C	-1.0969870	1.2636320	-0.6749260
H	-0.3969950	1.3479980	-1.5087590
H	-1.8410320	2.0529790	-0.8129970
H	-1.0495160	1.7565990	1.4457360
C	2.3012610	0.4470030	-0.6337830
H	3.0145430	0.9126640	0.0530460
H	2.8673320	-0.1510870	-1.3510350
H	1.7832250	1.2337950	-1.1836400
25			
C	-1.7760650	-0.8866630	-0.1246260
C	-0.3678660	-1.2120930	0.3772910
C	0.3312340	0.8836260	0.5842990
C	-0.9753610	1.5230750	0.1000810
H	-2.0901600	-1.6336780	-0.8590960
H	-0.7645590	2.4303540	-0.4764410
O	0.0128830	-0.2773470	1.3726650
O	0.5921180	-1.0649620	-0.6724250
C	1.1724350	0.2518270	-0.5456970
H	1.0278270	0.7786660	-1.4948590
H	-0.2823660	-2.2159160	0.7964110
H	0.9093430	1.5604380	1.2145160
H	-2.4575830	-0.9526580	0.7301780
C	-1.7939540	0.5238380	-0.7435180
H	-1.3684420	0.4664460	-1.7495180
H	-2.8214970	0.8783700	-0.8604930
H	-1.5413260	1.8265750	0.9866450
C	2.6548860	0.1331780	-0.2235900
H	2.7909460	-0.3203290	0.7609760
H	3.1502570	-0.4971480	-0.9651650
H	3.1356840	1.1166150	-0.2305100
26			
C	-1.1463780	1.1556290	-0.7146310

C	-1.1249810	-0.2319710	-0.0548390
C	0.7562780	0.0776050	1.1204990
C	1.0343310	1.4867120	0.5816040
H	-1.5382390	1.0810260	-1.7330700
H	2.1089000	1.6429690	0.4405000
O	-0.6635010	-0.0759110	1.2862620
O	-0.1266070	-1.0483540	-0.7034690
C	1.0318380	-1.0861320	0.1529000
H	0.9960300	-2.0165200	0.7354650
H	1.2205080	-0.0774410	2.0960220
H	-1.8340280	1.7829600	-0.1385860
C	0.2701750	1.7586250	-0.7311160
H	0.8175390	1.3244730	-1.5703250
H	0.2199830	2.8354190	-0.9162680
H	0.7106310	2.1889320	1.3564920
C	2.3107470	-1.0667860	-0.6653170
H	3.1806760	-1.1577020	-0.0077760
H	2.3206720	-1.9138640	-1.3545290
H	2.4115600	-0.1524420	-1.2515100
C	-2.4564670	-0.9517250	-0.0506660
H	-2.3544530	-1.8991460	0.4802370
H	-3.2170260	-0.3452300	0.4459520
H	-2.7751480	-1.1510700	-1.0755520
27			
C	1.8191250	0.1400410	-0.3790980
C	0.5444030	0.8929250	0.0400260
C	-0.5535310	-0.9205510	0.7551730
C	0.5622660	-1.9201040	0.4322050
H	2.2448810	0.6023380	-1.2740890
H	0.1356510	-2.8725280	0.0993440
O	0.0381820	0.2980690	1.2318880
O	-0.4874040	0.6776270	-0.9404820
C	-1.3112240	-0.4170080	-0.4921790
H	-1.3286730	-1.1755130	-1.2823620
H	-1.2211120	-1.2891150	1.5353440
H	2.5488020	0.2473660	0.4302730
C	1.5065510	-1.3442320	-0.6402650
H	1.0353130	-1.4329700	-1.6233530
H	2.4310680	-1.9264610	-0.6852270
H	1.1102110	-2.1152770	1.3596580
C	-2.7222480	0.0768560	-0.2048340
H	-2.7182840	0.7618420	0.6462990
H	-3.1168120	0.6081710	-1.0736180
H	-3.3901650	-0.7610350	0.0192710

C	0.7394030	2.3781920	0.2552290
H	-0.1963920	2.8215250	0.5971070
H	1.5142160	2.5557390	1.0039520
H	1.0366020	2.8536320	-0.6813950
28			
C	1.2853760	1.2543460	-0.3070330
C	1.1164640	-0.2616090	-0.1166150
C	-1.1403850	-0.2516720	-0.0901230
C	-1.2589970	1.2738430	-0.2594220
H	2.1686960	1.6003410	0.2368730
H	-2.1197680	1.6508370	0.3032300
O	-0.0083160	-0.6932690	-0.8715170
O	0.7647340	-0.5300590	1.2571290
C	-0.6595420	-0.6419810	1.3229040
H	-0.9349890	-1.6754380	1.5592160
H	-1.0470200	0.0191000	2.1041540
H	1.4550860	1.4410590	-1.3724690
C	0.0288830	1.9902590	0.1875410
H	0.0598540	2.0356170	1.2799860
H	0.0270010	3.0248170	-0.1669630
H	-1.4529690	1.4679750	-1.3195240
C	2.3289750	-1.0843990	-0.4955330
H	2.0952960	-2.1435750	-0.3816410
H	2.6137710	-0.8903580	-1.5317070
H	3.1676670	-0.8325840	0.1561160
C	-2.3733430	-1.0018690	-0.5603070
H	-2.1932500	-2.0784550	-0.5302310
H	-3.2321910	-0.7711780	0.0761390
H	-2.6230970	-0.7230480	-1.5865490
29			
O	-1.0774230	-1.1752590	0.0877250
C	-1.5450620	0.0097520	-0.5774280
C	-0.9988550	1.2875490	0.0824530
C	0.4818060	1.0861260	0.4304420
O	0.5609080	-0.0687260	1.2913600
C	0.2866740	-1.1069600	0.3832640
H	-1.1386520	2.1433940	-0.5859570
H	-1.2479390	-0.0368650	-1.6309230
H	-2.6328670	-0.0301610	-0.5264860
H	0.9121920	1.9367620	0.9572960
H	0.5764440	-2.0645440	0.8061960
H	-1.5353040	1.4910860	1.0125830
O	1.0547530	-0.8151340	-0.7738930
C	1.3288630	0.5965400	-0.7506890

H	1.0438710	1.0369830	-1.7094010
H	2.3957880	0.7582460	-0.5731070
30			
O	-0.3807630	1.3901860	-0.1988180
C	1.0161670	1.3876810	-0.5238450
C	1.8187490	0.4721380	0.4144740
C	1.0381990	-0.8289720	0.6352010
O	-0.2481440	-0.4698120	1.1701060
C	-0.8881000	0.1004300	0.0450890
H	2.8088230	0.2756640	-0.0097010
H	1.1370570	1.0708940	-1.5659950
H	1.3418280	2.4246980	-0.4418630
H	1.5277520	-1.5000570	1.3403580
H	1.9538940	0.9511940	1.3874920
O	-0.5648200	-0.7710930	-1.0409260
C	0.6063710	-1.5117530	-0.6680780
H	1.3492300	-1.4455850	-1.4673740
H	0.3406730	-2.5599050	-0.5009170
C	-2.3763010	0.1993480	0.2505500
H	-2.7733220	-0.7846700	0.4975720
H	-2.5852540	0.8961630	1.0622670
H	-2.8413770	0.5641290	-0.6650750
31			
C	1.0877520	-0.3264330	0.2062970
C	-0.1259630	-0.6396790	-0.7579530
C	-1.4445470	-0.2871570	-0.0840530
C	-1.5126110	0.9074270	0.5129860
C	-0.2984550	1.8110140	0.5339150
C	0.8640030	1.1656770	-0.2428510
C	0.3119380	0.6080160	-1.5853000
C	-2.5734940	-1.2744180	-0.1397750
H	0.0003810	2.0216050	1.5696510
H	-0.5412870	2.7859920	0.0907040
H	-2.4227460	1.2436240	1.0025450
H	-0.1484180	-1.6172230	-1.2464720
H	1.7421750	1.8174940	-0.2718180
H	-2.8391510	-1.5125330	-1.1767490
H	-3.4660270	-0.8955660	0.3633120
H	-2.2892770	-2.2216080	0.3343970
H	-0.4866210	1.1718990	-2.0705830
H	1.0951020	0.3933760	-2.3107070
C	2.4104670	-0.8986010	-0.3253170
C	0.9787290	-0.6805390	1.6894060
H	1.8084220	-0.2319000	2.2466690

H	0.0459020	-0.3448350	2.1410770
H	1.0445350	-1.7652220	1.8275600
H	3.2552160	-0.4808000	0.2325060
H	2.4350350	-1.9852610	-0.1935070
H	2.5798470	-0.6908850	-1.3827150
32			
C	-1.0765220	-0.2835340	0.1959240
C	-0.7359440	1.2327740	-0.0281470
C	0.5025910	1.6488230	0.7809710
C	1.7474220	0.8034850	0.3838420
C	1.3930670	-0.5310990	-0.2632700
C	0.0294050	-0.5549880	-0.9031190
C	-0.2985700	0.8600630	-1.4727610
C	2.2198510	-1.5762850	-0.2703180
C	-2.4821180	-0.6405730	-0.3078410
C	-0.8869840	-0.8948300	1.5837660
H	0.7137880	2.7080540	0.6039680
H	0.5221230	1.4266450	-1.9176140
H	-1.1274850	0.8410600	-2.1783090
H	-1.5554650	1.9464780	0.0983040
H	2.4065690	0.6475090	1.2413240
H	2.3346560	1.3737350	-0.3441290
H	0.1077140	-0.7265960	1.9961020
H	-1.6203250	-0.4848090	2.2867480
H	0.2937110	1.5515200	1.8501550
H	-0.1081920	-1.4286340	-1.5449590
H	-2.6064710	-1.7272160	-0.3569990
H	-2.6993320	-0.2374910	-1.2985370
H	-3.2404840	-0.2519480	0.3800210
H	-1.0392650	-1.9781860	1.5427650
H	1.9588160	-2.5001820	-0.7756160
H	3.1864510	-1.5429480	0.2224840
33			
C	-1.1583760	-0.3462450	0.2745630
C	-0.7728670	0.9310700	-0.5716510
C	0.4993580	1.5641070	-0.0089850
C	1.5938950	0.5885190	0.2043210
C	1.3448440	-0.7115950	-0.0408210
C	-0.0296620	-1.0596760	-0.5794240
C	-0.3487480	-0.0391860	-1.7159090
O	0.5950310	2.7496790	0.2442100
C	2.3318610	-1.8143750	0.1842360
H	-0.1416050	-2.1278900	-0.7798990
C	-1.0374870	-0.2892910	1.7980910

H	0.4887300	0.2656490	-2.3444630
H	-1.1844370	-0.3368060	-2.3472390
H	-1.5281370	1.6976640	-0.7509370
H	2.5405320	0.9564920	0.5846480
H	2.5116730	-2.3683550	-0.7442810
H	1.9384370	-2.5392810	0.9065740
H	3.2861570	-1.4374600	0.5555590
C	-2.5595160	-0.8674560	-0.0734990
H	-2.7094150	-1.8623750	0.3582040
H	-3.3214620	-0.2066720	0.3509590
H	-2.7448560	-0.9401710	-1.1457120
H	-1.2199830	-1.2785640	2.2307790
H	-0.0628570	0.0551140	2.1413980
H	-1.7928320	0.3899950	2.2052010

34

C	0.6217300	1.5931600	0.8058610
C	-0.2294250	0.8939530	-1.4560830
C	-0.6400010	1.2593820	-0.0032620
C	1.7915290	0.6341830	0.4542540
C	1.3605420	-0.6397710	-0.2853990
C	-0.0048180	-0.5562790	-0.9337820
H	0.9159930	2.6265500	0.6003210
H	0.6292000	1.4155400	-1.8851230
H	-1.0546830	0.9475890	-2.1639400
C	-1.0715990	-0.2379990	0.1897840
H	-1.4163940	2.0161360	0.1391000
H	2.3700560	0.3339240	1.3298530
H	2.5029220	1.1321260	-0.2141530
H	0.0947150	-0.7847810	1.9840940
H	-1.6186890	-0.4790750	2.2750640
H	0.3988660	1.5432900	1.8752300
H	-0.1730510	-1.4138100	-1.5867800
C	-2.5008400	-0.4969290	-0.3053280
C	-0.9039120	-0.8990390	1.5597300
H	-2.6896780	-1.5718080	-0.3844560
H	-2.7042500	-0.0513010	-1.2806200
H	-3.2243960	-0.0834510	0.4048360
H	-1.1023040	-1.9726080	1.4864940
O	2.0665570	-1.6202860	-0.3418230

35

C	0.4077940	-0.5273520	-1.3772270
C	-0.4077940	0.5273520	-1.3772270
H	-1.4839640	0.3534370	-1.3578100
C	0.0484950	1.8726060	-0.9134840

H	1.4839640	-0.3534370	-1.3578100
H	0.4984840	-2.7073330	-1.3636340
C	-0.1657200	1.8854480	0.6317600
H	-0.4984840	2.7073330	-1.3636340
H	1.1123760	2.0138760	-1.1319840
C	0.4077940	0.6687560	1.4037570
H	-1.2403670	1.9583870	0.8382470
H	0.2819450	2.8007450	1.0361740
H	1.4313510	0.4748990	1.0639220
C	-0.4077940	-0.6687560	1.4037570
H	0.5074630	0.9889180	2.4462460
C	0.1657200	-1.8854480	0.6317600
H	-1.4313510	-0.4748990	1.0639220
H	-0.5074630	-0.9889180	2.4462460
H	-0.2819450	-2.8007450	1.0361740
H	1.2403670	-1.9583870	0.8382470
C	-0.0484950	-1.8726060	-0.9134840
H	-1.1123760	-2.0138760	-1.1319840
36			
C	-1.6509570	0.3338290	-0.6879520
C	-0.6929360	0.9059900	-1.7245510
C	0.6929080	0.9065850	1.7244610
N	0.4765800	1.5630100	-1.1113950
C	1.6510120	0.3344610	0.6879640
C	1.4918670	0.6499430	-0.6695150
H	-1.2104600	1.6435110	-2.3500030
H	0.3444330	0.1144360	2.3900370
H	-0.3443930	0.1138550	-2.3901080
H	1.2102310	1.6442280	2.3499420
C	-1.4920190	0.6500090	0.6696290
N	-0.4767250	1.5632690	1.1111390
C	-0.0001630	2.3873580	-0.0002560
H	-0.8112910	3.0242920	-0.3580700
H	0.8108530	3.0245470	0.3573580
C	-3.5608740	-1.0909990	-0.1457200
C	-2.6905970	-0.5188630	-1.0710600
C	-2.3581530	0.0773270	1.6083880
C	-3.3686330	-0.7839740	1.2086610
H	-2.8087250	-0.7578910	-2.1253830
H	-2.2373540	0.3377770	2.6543390
H	-4.0298130	-1.2138100	1.9546940
C	2.3585450	0.0774950	-1.6082240
C	3.3693860	-0.7829540	-1.2082750
C	3.5616200	-1.0896900	0.1464180

C	2.6914450	-0.5174470	1.0714480
H	2.2379780	0.3382090	-2.6541370
H	4.0312640	-1.2121670	-1.9540830
H	2.8101760	-0.7553500	2.1259360
C	4.6848320	-2.0007420	0.5809150
H	4.7001980	-2.9232450	-0.0067380
H	5.6597850	-1.5186350	0.4515040
H	4.5897260	-2.2754410	1.6335440
C	-4.6863620	-1.9986460	-0.5814500
H	-4.7475170	-2.8897080	0.0496270
H	-5.6541790	-1.4894120	-0.5172580
H	-4.5554180	-2.3272300	-1.6146960
37			
O	5.3803250	0.3993440	-0.9308480
C	4.2672880	0.1364180	-0.5123880
H	3.6706050	2.2033340	-0.2610000
C	3.2932560	1.1880030	-0.1778290
C	2.0429670	0.9573760	0.2652860
C	3.8140090	-1.2867160	-0.2426560
H	4.3810060	-1.9581860	-0.8909420
H	4.1016900	-1.5291580	0.7881060
C	2.3051610	-1.4495170	-0.4407510
H	2.0143020	-2.4727070	-0.1909350
H	2.0805600	-1.3104310	-1.5047290
C	1.4442270	-0.4485750	0.3733040
C	-0.0096010	-0.4262440	-0.2349820
H	0.1314900	-0.1831880	-1.2988290
C	-0.9040070	0.7213660	0.3217330
H	-1.0461960	0.5899980	1.4017580
C	1.4433660	-0.8584590	1.8693430
H	2.4544510	-0.8158280	2.2806730
H	1.0774960	-1.8795690	1.9970460
H	0.8184090	-0.2011810	2.4764870
C	-0.2224360	2.0736000	0.0925310
H	-0.1438440	2.2619790	-0.9856780
H	-0.8292390	2.8824240	0.5110480
C	1.1779790	2.1065460	0.7187970
H	1.0724290	2.0533370	1.8109950
H	1.6813280	3.0521650	0.5028450
C	-0.7058720	-1.8110900	-0.1901730
H	-0.7315710	-2.1772400	0.8394360
H	-0.1084360	-2.5343570	-0.7503770
C	-2.1430980	-1.8265520	-0.7594770
H	-2.1131710	-1.6751010	-1.8447180

H	-2.5858180	-2.8150300	-0.5904420
C	-2.9921020	-0.7172170	-0.1232430
C	-2.2584280	0.6266300	-0.3819010
H	-2.0397150	0.6189390	-1.4597630
C	-3.2406400	-1.0194880	1.3769990
H	-3.7492380	-0.1878600	1.8698410
H	-2.3221690	-1.2257660	1.9298980
H	-3.8854210	-1.8986440	1.4722710
C	-4.3457660	-0.3933910	-0.7402480
H	-5.4845880	1.4047390	-1.0574990
C	-4.5635700	0.9236210	-0.7482780
C	-3.3611770	1.6946500	-0.2297000
H	-3.1565700	2.6033230	-0.8030670
H	-3.5134500	2.0057460	0.8134700
H	-5.0662830	-1.1522520	-1.0273140
38			
C	0.0263200	3.8009350	-1.4246110
C	-0.2089270	0.6482000	3.2399550
C	0.6715620	3.3381190	-2.5477230
C	1.1485290	2.0144760	-2.5720970
C	0.9123220	1.1656060	-1.5127350
C	0.1888230	1.5849670	-0.3683600
C	-0.0551680	0.7224800	0.7820760
C	-0.1888230	2.9611030	-0.3059500
C	-0.3320020	1.3651980	2.0178480
C	-0.6923380	3.5018600	0.9161550
C	-0.6955940	2.7478870	2.0455450
H	1.7159810	1.6597490	-3.4250840
H	0.8436440	3.9954290	-3.3924540
H	-0.3952690	1.1724180	4.1710340
H	-0.9945080	4.5433460	0.9416990
H	-0.9784230	3.1817730	2.9987900
H	1.3054730	0.1602070	-1.5505810
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C	1.8668870	1.1965310	-2.4334080
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C	1.3579080	0.8365560	-1.2044030
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C	-0.7858090	2.3316150	1.4929860
C	-0.8297590	3.7730780	-0.4630830
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H	2.6233580	0.5762830	-2.9006510
H	1.8105240	2.6300880	-4.0545880
H	-0.5607480	1.0644180	4.6445710
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41			
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C	0.8689090	0.9710080	3.0299930
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H	2.0214750	3.9461270	1.8796130
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H	-0.6891730	-0.1806240	2.1654520
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H	-2.7554670	-4.2828670	1.0259650
H	0.6267860	0.1403690	-1.0376860
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C	1.8513200	-3.2815580	-0.2926120
C	1.8603190	-2.0633200	-1.0369010
C	0.6986740	-1.2324890	-1.0498630
C	-0.4409010	-1.5871760	-0.2166140
C	-1.5833370	-0.7274970	0.0323130
C	-0.4677950	-2.8993640	0.3217150
C	-2.8192930	-1.3615880	0.3477600
C	-1.6778430	-3.4335250	0.8495750
C	-2.8346660	-2.7200810	0.7733960
H	2.7490380	-3.8903230	-0.2769270
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C	0.6986930	1.2324790	1.0498630
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C	-2.8346250	2.7201220	-0.7733960
H	2.7490960	3.8902820	0.2769260
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H	-1.6724860	4.4454090	-1.2402770
H	-3.7820920	3.1608320	-1.0641290
H	0.6699290	4.6790090	-0.7911990
C	0.6806910	-0.1628280	-1.9779220
C	1.7723440	0.1306060	-2.7662730
C	2.9503280	-0.6314940	-2.6695370
C	2.9819470	-1.7178930	-1.8266290

H	-0.2183520	0.4225170	-2.0965990
H	1.7156200	0.9506440	-3.4730850
H	3.8119250	-0.3836070	-3.2790910
H	3.8625030	-2.3499570	-1.7773040
C	0.6806940	0.1628180	1.9779220
C	1.7723420	-0.1306310	2.7662740
C	2.9503370	0.6314520	2.6695380
C	2.9819730	1.7178500	1.8266300
H	-0.2183580	-0.4225140	2.0965990
H	1.7156060	-0.9506680	3.4730860
H	3.8119310	0.3835530	3.2790920
H	3.8625370	2.3499010	1.7773040

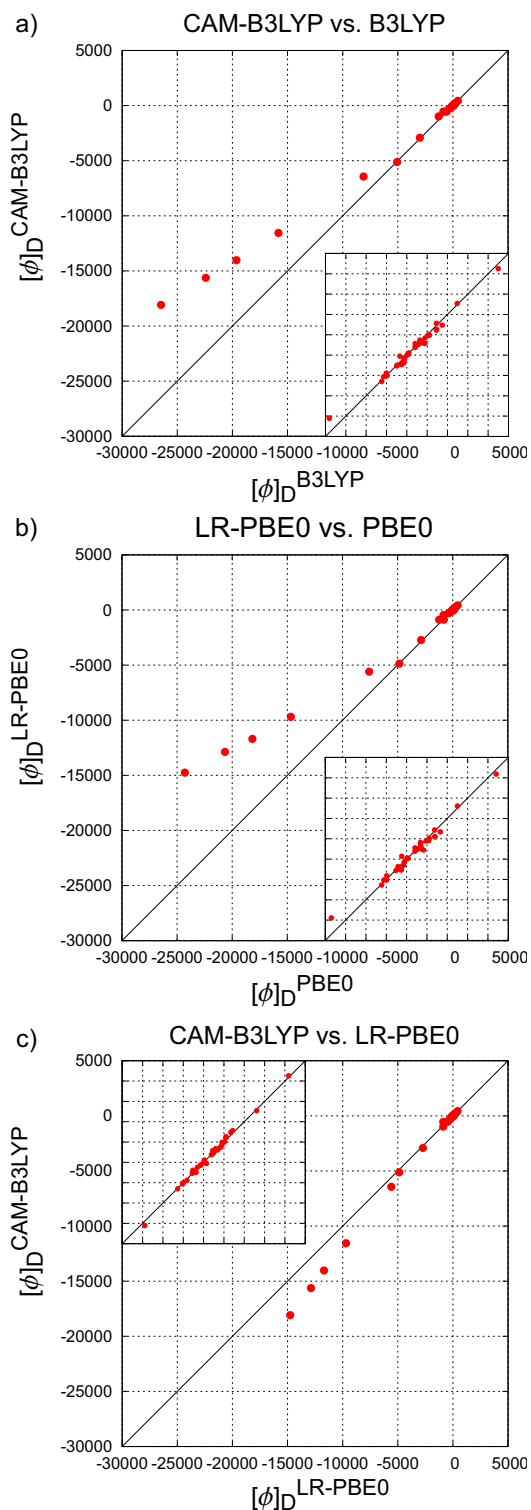


Figure S1: Comparison of calculated molar rotations: CAM-B3LYP/augD vs. B3LYP/augD (panel **a**), LR-PBE0/augD vs. PBE0/augD (panel **b**) and CAM-B3LYP/augD vs. LR-PBE0/augD (panel **c**). The insets show the optical rotations in the range of -400 to 500 $\text{deg cm}^2 \text{dmol}^{-1}$, i.e. excluding molecules **20**, **36**, **38-45**. The line is of slope +1.

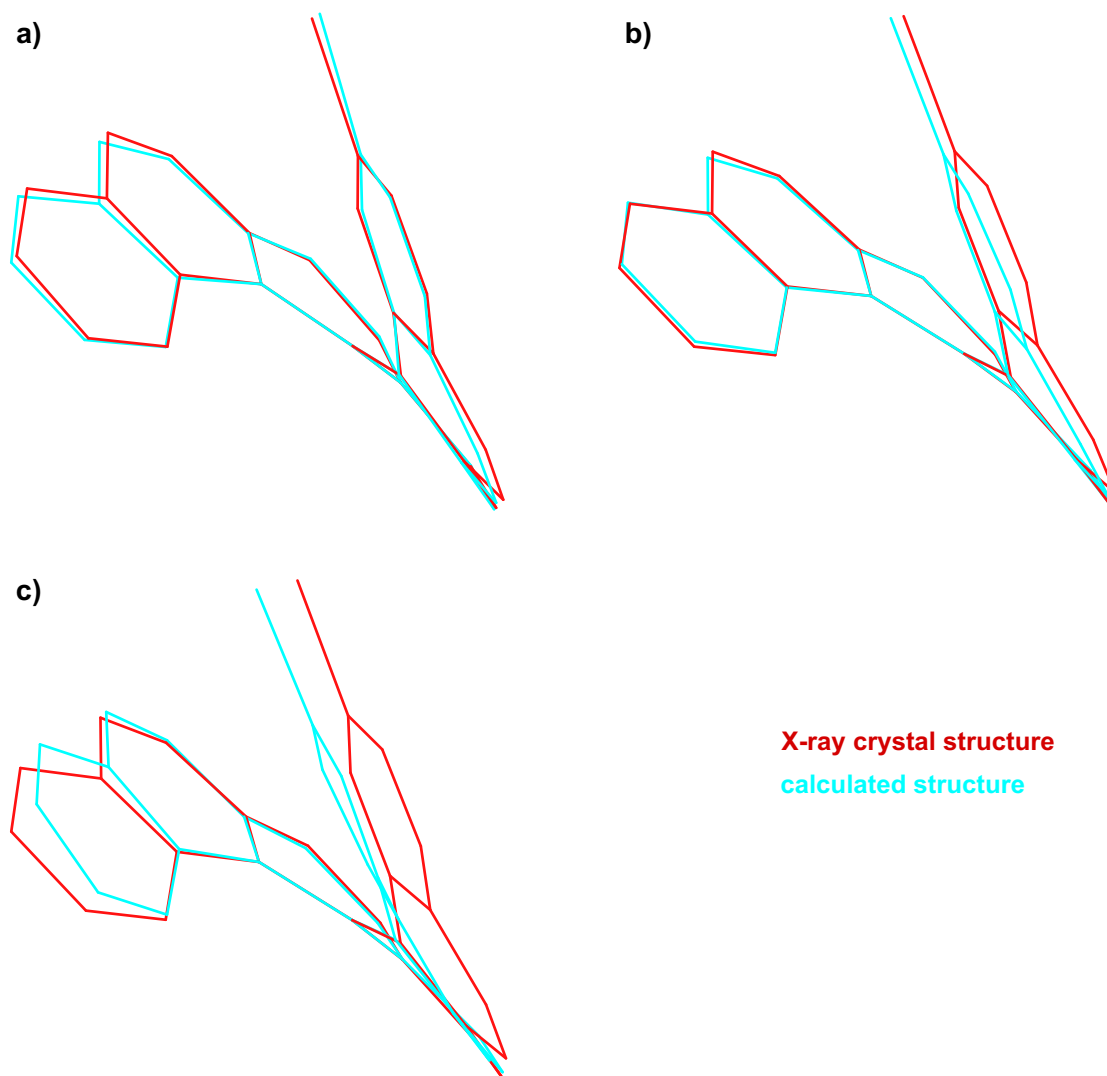


Figure S2: Overlay of X-ray crystal structure of 2-bromo[6]helicene, **41** (red) and corresponding geometry (blue) optimized with DFT (panel **a**), DFT-D2 (panel **b**) and DFT-D3 **c**). Hydrogen atoms are omitted for clarity. X-ray crystal structure taken from Ref. [144].