Table S3 Atoms' cartesian coordinates (in Angström) in the principal axis orientation (x,y,z = a,b,c) corresponding to the calculated equilibrium geometry of naphthalene at the B97-1/ANO-DZP level.

atom	x	y	z
C	2.423247	0.705674	0.000000
C	1.239335	1.396987	0.000000
C	0.000000	0.713185	0.000000
C	0.000000	-0.713185	0.000000
C	1.239335	-1.396987	0.000000
C	2.423247	-0.705674	0.000000
H	-1.237376	2.476742	0.000000
H	3.361100	1.238312	0.000000
H	1.237376	2.476742	0.000000
C	-1.239335	1.396987	0.000000
C	-1.239335	-1.396987	0.000000
H	1.237376	-2.476742	0.000000
H	3.361100	-1.238312	0.000000
C	-2.423247	-0.705674	0.000000
C	-2.423247	0.705674	0.000000
H	-1.237376	-2.476742	0.000000
H	-3.361100	-1.238312	0.000000
H	-3.361100	1.238312	0.000000

Table S4 Naphthalene's calculated harmonic and anharmonic frequencies at the B97-1/cc-pVTZ level and excited states' rotational constants at the B97-1/cc-pVTZ//ANO-DZP level.[a]

symmetry	mode	harmonic	anharmonic	A	B	C
A_g	1	3182.522	3044.149	0.104100	0.041125	0.029487
	2	3156.392	3031.492	0.104103	0.041123	0.029486
	3	1606.891	1569.649	0.104023	0.041101	0.029440
	4	1487.282	1455.844	0.104086	0.041124	0.029479
	5	1394.614	1361.220	0.103939	0.041083	0.029450
	6	1179.968	1167.839	0.104205	0.041133	0.029487
	7	1041.753	1029.251	0.104056	0.041137	0.029480
	8	770.544	757.982	0.104083	0.041124	0.029479
	9	517.194	512.159	0.104156	0.041128	0.029485
A_u	10	990.476	992.974	0.104039	0.041117	0.029491
	11	849.168	837.341	0.104117	0.041146	0.029493
	12	635.047	641.653	0.104090	0.041127	0.029498
	13	185.967	179.699	0.104103	0.041117	0.029510
B_{1g}	14	958.440	950.555	0.103947	0.041116	0.029493
	15	729.317	715.278	0.104101	0.041123	0.029495
	16	394.051	389.182	0.104058	0.041138	0.029505
B_{1u}	17	3169.430	3037.079	0.104103	0.041124	0.029487
	18	3150.967	3000.345	0.104104	0.041124	0.029486
	19	1633.449	1599.582	0.104080	0.041093	0.029474
	20	1414.959	1388.789	0.104156	0.041113	0.029495
	21	1283.942	1255.674	0.104108	0.041119	0.029486
	22	1146.910	1132.891	0.104185	0.041125	0.029453
	23	805.258	795.108	0.104209	0.041098	0.029481
	24	361.486	361.883	0.104316	0.041139	0.029487
B_{2g}	25	996.351	995.383	0.104038	0.041116	0.029491
	26	897.809	888.796	0.104081	0.041118	0.029493
	27	786.185	791.675	0.104110	0.041121	0.029495
	28	477.908	472.640	0.104067	0.041134	0.029504
B_{2u}	29	3181.672	3043.105	0.104100	0.041125	0.029487
	30	3153.740	3028.881	0.104103	0.041123	0.029486
	31	1542.703	1507.046	0.104060	0.041105	0.029460
	32	1385.956	1360.483	0.104058	0.041096	0.029451
	33	1229.155	1210.413	0.104125	0.041087	0.029456
	34	1164.060	1147.203	0.104130	0.041129	0.029506
	35	1031.596	1015.165	0.104059	0.041133	0.029482
	36	629.705	623.348	0.104147	0.041135	0.029483
B_{3g}	37	3168.604	3042.087	0.104102	0.041125	0.029487
	38	3149.709	3005.389	0.104104	0.041124	0.029486
	39	1662.414	1622.646	0.104047	0.041080	0.029484
	40	1486.145	1460.425	0.104142	0.041098	0.029475
	41	1265.524	1242.722	0.104121	0.041124	0.029474
	42	1168.111	1152.150	0.104151	0.041133	0.029487
	43	949.168	935.235	0.104302	0.041132	0.029479
	44	514.723	508.138	0.104159	0.041136	0.029484
B_{3u}	45	974.958	974.916	0.104087	0.041114	0.029492
	46	799.957	782.764	0.103997	0.041127	0.029495
	47	484.877	483.901	0.104134	0.041130	0.029504
	48	171.881	167.856	0.103907	0.041165	0.029523

[a] All values are in cm^{-1}