Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Dimerization of Substituted 4-Aryl-1,3-diacetylenes – Quantum Chemical Calculations and Kinetic Studies

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1. Additional Figure and Table

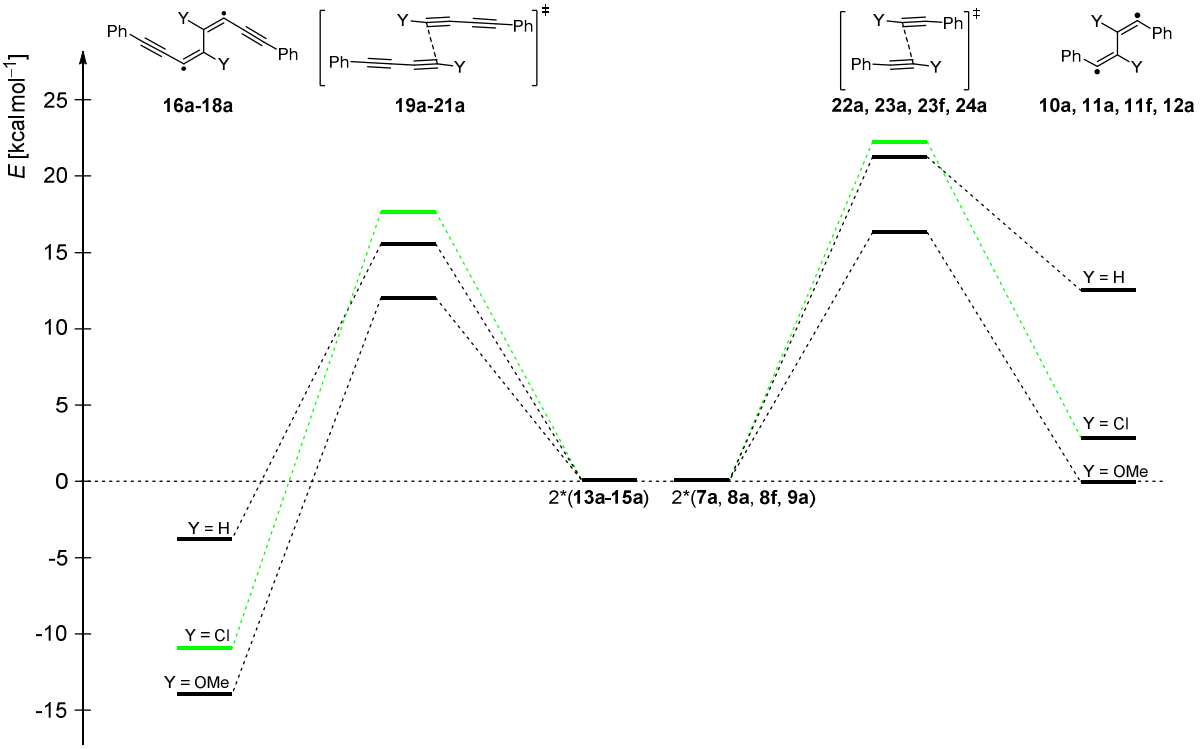


Figure S1. Energy profiles for the dimerization of **7a**, **8a**, **8f**, **9a** and **13a-15a** calculated by means of UB3LYP/6-31G*//B2PLYPD/6-31G*.

Table S1. Summary of the Energies (ΔE in kcal/mol) calculated by means of B2PLYPD/6-31G*, the distances between the atoms C1, C2 and C3 and the angles between C1-C2-C3 of the diradical intermediates **16a**, **17a-e** and **18a**.

	X	Y	ΔE^a	C1-C2 [Å]	C2-C3 [Å]	C3-C4 [Å]	C1-C2-C3 [°]
13a	H	H	0.00	1.219	1.367	1.224	
19a	H	H	14.89	1.261	1.347	1.233	
16a	H	H	2.99	1.336	1.310	1.254	162
14a	H	Cl	0.00	1.220	1.363	1.224	
20a	H	Cl	13.24	1.260	1.342	1.233	
17a	H	Cl	-8.18	1.325	1.302	1.254	175
14b	Me	Cl	0.00	1.220	1.363	1.225	
20b	Me	Cl	12.97	1.260	1.342	1.234	
17b	Me	Cl	-8.68	1.325	1.302	1.254	175
14c	OH	Cl	0.00	1.220	1.363	1.225	
20c	OH	Cl	12.64	1.260	1.342	1.234	
17c	OH	Cl	-9.09	1.324	1.303	1.254	175
14d	OMe	Cl	0.00	1.220	1.363	1.225	
20d	OMe	Cl	12.56	1.260	1.342	1.234	
17d	OMe	Cl	-9.34	1.324	1.302	1.254	175
14e	NH_2	Cl	0.00	1.220	1.363	1.225	
20e	NH_2	Cl	12.16	1.260	1.342	1.235	
17e	NH_2	Cl	-10.07	1.324	1.302	1.255	175
15a	H	OMe	0.00	1.220	1.365	1.225	
21a	H	OMe	7.64	1.255	1.350	1.231	
18a	H	OMe	-14.54	1.330	1.313	1.250	165

[a] B2PLYPD/6-31G*

2. Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S2. Absolute energies [au] calculated by means of different methods.

	E^a	E^b	E^c	E^d
13a	-384.1356001	-384.551195	-384.2841868	
19a	-768.2474666	-769.0775664	-768.5407822	
16a	-768.2664304	-769.1082540	-768.5560834	
14a	-843.5692965	-844.13904200	-843.7395162	-844.1391376
20a	-1687.1174998	-1688.2500129	-1687.4561936	-1688.2504005
17a	-1687.1516250	-1688.2953942	-1687.4884097	-1688.2968984
14b	-882.8375237	-883.45758180	-883.0255663	-883.4577147
20b	-1765.654384	-1766.8875333	-1766.0287804	-1766.887976
17b	-1765.6888869	-1766.9330488	-1766.061381	-1766.934622
14c	-918.7271007	-919.3562541	-918.9366947	
20c	-1837.4340549	-1838.685577	-1837.851541	
17c	-1837.468688	-1838.730864	-1837.884234	
14d	-957.9823267	-958.6628675	-958.2041016	-958.6630500
20d	-1915.9446441	-1917.2988867	-1916.3865503	-1917.2994179
17d	-1915.9795361	-1917.3442766	-1916.4195416	-1917.3459963
14e	-898.8707893	-899.4945517	-899.0699636	
20e	-1797.7221953	-1798.963053	-1798.118986	
17e	-1797.7576195	-1799.008839	-1798.152496	
15a	-498.5365622	-499.06627220	-498.7360388	
21a	-997.0609558	-998.1135100	-997.4578427	
18a	-997.0962882	-998.1546406	-997.4896739	
7a	-308.0525583	-308.393534		
22a	-616.0741403	-616.753288		
10a	-616.0807615	-616.7672491		
8a	-767.4861481	-767.981170		
23a	-1534.9450022	-1535.926971		
11a	-1534.9639868	-1535.957935		
8f	-998.2974353	-998.5270788		-999.0389615
23f	-1996.5695101	-1997.028164		-1998.0446683
11f	-1996.5903420	-1997.047721		-1998.0788115
9a	-422.4517964	-422.9067523		
24a	-844.8867588	-845.7876121		
12a	-844.9079879	-845.8135369		
25	-1036.3228212	-1037.1004706	-1036.5631508	-1037.1006421
28	-2072.6265103	-2074.1744055	-2073.1055555	-2074.1749530
31	-2072.6632632	-2074.2217343	-2073.1403153	-2074.2232480
26	-1203.5290092	-1204.2143662	-1203.7112445	-1204.2145411
29	-2407.0395967	-2408.4035599	-2407.4025900	-2408.4040536
32	-2407.0773259	-2408.4521307	-2407.4384477	-2408.4535588
27				-1114.515292
30				-2229.003521
33				-2229.050503

[a] B2PLYPD/6-31G*. [b] UB3LYP/6-31G*//B2PLYPD/6-31G*. [c] B2PLYPD/def2-TZVP//B2PLYPD/6-31G*. [d] UB3LYP/6-31G*

Cartesian coordinates of the optimized geometry for **13a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-3.61884600	0.00000300	0.00000100
C	-4.83762100	-0.00001000	-0.00000300
C	0.39598800	0.00000700	0.00000000
C	1.10686100	1.21539300	0.00000000
C	1.10684500	-1.21538800	0.00000000
C	2.49958800	1.20979500	0.00000000
H	0.55732000	2.15057800	0.00000000
C	2.49957200	-1.20980800	0.00000000
H	0.55729200	-2.15056600	0.00000000
C	3.19910100	-0.00001100	0.00000000
H	3.04025600	2.15082000	0.00000000
H	3.04022800	-2.15084000	0.00000000
H	4.28438000	-0.00001800	-0.00000100
H	-5.90308000	-0.00003300	0.00000500
C	-2.25227100	0.00001500	0.00000100
C	-1.02861700	0.00001500	0.00000100

Cartesian coordinates of the optimized geometry for **19a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.35860700	-0.00015700	0.90432000
C	-0.35860700	0.00015700	-0.90431900
H	0.51988400	0.00026500	-1.52107700
H	-0.51988400	-0.00026400	1.52107800
C	1.61709100	-0.00017200	0.99691000
C	-1.61709100	0.00017200	-0.99691000
C	2.92935000	-0.00012000	0.69442600
C	-2.92935000	0.00011900	-0.69442600
C	4.14362100	-0.00008200	0.47827100
C	-4.14362100	0.00008200	-0.47827100
C	5.53253000	-0.00003400	0.19799600
C	6.23319400	1.21674700	0.05841900
C	6.23319200	-1.21676700	0.05799500
C	7.59778700	1.21017800	-0.21536000
H	5.69483600	2.15218700	0.16700900
C	7.59778600	-1.21010400	-0.21578100
H	5.69483300	-2.15224400	0.16625900
C	8.28429400	0.00006000	-0.35345900
H	8.12817600	2.15114800	-0.32147800
H	8.12817400	-2.15103800	-0.32222700
H	9.34835800	0.00009700	-0.56689400
C	-5.53253000	0.00003400	-0.19799600
C	-6.23319000	1.21676700	-0.05798700
C	-6.23319600	-1.21674700	-0.05842800
C	-7.59778400	1.21010400	0.21579000
H	-5.69483000	2.15224400	-0.16624400
C	-7.59778900	-1.21017700	0.21535100
H	-5.69483900	-2.15218700	-0.16702400
C	-8.28429400	-0.00006000	0.35345900
H	-8.12817000	2.15103900	0.32224200
H	-8.12818000	-2.15114800	0.32146200
H	-9.34835800	-0.00009600	0.56689300

Cartesian coordinates of the optimized geometry for **16a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.33136500	0.00022200	-0.65510300

C	1.66011900	0.00042900	-0.78942300
C	-1.66014300	-0.00018300	0.78958000
C	-0.33138800	0.00006900	0.65526200
H	-0.31787300	0.00028700	-1.52496800
H	0.31784900	-0.00003700	1.52512600
C	2.94027600	0.00045700	-0.51261000
C	4.18576200	0.00044600	-0.36467900
C	-2.94029300	-0.00027600	0.51273900
C	-4.18577300	-0.00033700	0.36475400
C	5.57463600	0.00016100	-0.15045000
C	6.28709100	1.21892800	-0.04388200
C	6.28663000	-1.21889300	-0.04406200
C	7.66189500	1.21027100	0.16426500
H	5.74521900	2.15517200	-0.12614200
C	7.66143900	-1.21079000	0.16407200
H	5.74440300	-2.15492000	-0.12646100
C	8.35505100	-0.00039800	0.26917600
H	8.19718500	2.15117200	0.24527100
H	8.19637400	-2.15190500	0.24493200
H	9.42814700	-0.00061400	0.43153900
C	-5.57463600	-0.00016900	0.15044700
C	-6.28673100	1.21882600	0.04407500
C	-6.28697900	-1.21899500	0.04379000
C	-7.66152800	1.21061100	-0.16413300
H	-5.74459100	2.15489700	0.12654500
C	-7.66177200	-1.21044900	-0.16443000
H	-5.74502900	-2.15519500	0.12604000
C	-8.35502900	0.00016400	-0.26932700
H	-8.19654200	2.15168300	-0.24498000
H	-8.19697500	-2.15139300	-0.24550500
H	-9.42811600	0.00029200	-0.43174800

Cartesian coordinates of the optimized geometry for **14a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	2.34481000	0.00023400	0.00046500
C	3.56426500	-0.00039800	0.01556900
C	-1.66662900	0.00006100	-0.00078300
C	-2.37752600	-1.21552600	-0.00078300
C	-2.37765700	1.21556900	-0.00077900
C	-3.77018300	-1.20990900	-0.00044300
H	-1.82801000	-2.15072400	-0.00094000
C	-3.77031300	1.20980500	-0.00044300
H	-1.82824100	2.15082600	-0.00093600
C	-4.46974200	-0.00008900	-0.00026300
H	-4.31082200	-2.15093700	-0.00028300
H	-4.31105200	2.15077600	-0.00028200
H	-5.55500700	-0.00014800	0.00001000
Cl	5.20799900	0.00003600	-0.00480000
C	0.98174400	0.00005100	0.00335300
C	-0.24257700	0.00013600	-0.00188800

Cartesian coordinates of the optimized geometry for **20a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	-0.40570800	0.95216600	-0.00003900
C	0.40570700	-0.95216400	-0.00009100
Cl	-0.88274800	-2.04131800	-0.00013700
Cl	0.88274700	2.04132000	-0.00005200
C	-1.66489100	0.96234100	-0.00000800
C	1.66489100	-0.96233900	-0.00007900
C	-2.98037700	0.69689500	0.00001900
C	2.98037700	-0.69689400	-0.00005700
C	-4.19867000	0.50425200	0.00004600

C	4.19867000	-0.50425100	-0.00003800
C	-5.59312700	0.25879600	0.00007600
C	-6.29598300	0.13600000	1.21756200
C	-6.29604500	0.13605200	-1.21738000
C	-7.66661400	-0.10462600	1.21088200
H	-5.75431000	0.23075700	2.15251800
C	-7.66667500	-0.10457500	-1.21064000
H	-5.75441900	0.23084900	-2.15235900
C	-8.35551500	-0.22557500	0.00013600
H	-8.19988100	-0.19848400	2.15142400
H	-8.19999000	-0.19839300	-2.15116000
H	-9.42442000	-0.41325900	0.00015900
C	5.59312700	-0.25879700	-0.00001600
C	6.29600000	-0.13605600	1.21746700
C	6.29602900	-0.13599800	-1.21747600
C	7.66663000	0.10456900	1.21077900
H	5.75433900	-0.23085500	2.15242500
C	7.66666000	0.10462700	-1.21074300
H	5.75439100	-0.23075300	-2.15245200
C	8.35551600	0.22557300	0.00002900
H	8.19990900	0.19838500	2.15131900
H	8.19996200	0.19848800	-2.15126500
H	9.42442100	0.41325600	0.00004700

Cartesian coordinates of the optimized geometry for **17a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.44438600	-0.57722700	0.00051700
C	1.76813200	-0.52755600	0.00044900
C	-1.76813100	0.52760600	-0.00005000
C	-0.44438100	0.57726400	0.00000700
Cl	-0.36568600	-2.14206900	0.00080600
Cl	0.36574700	2.14208700	-0.00044900
C	3.06210700	-0.37819500	0.00034000
C	4.31091600	-0.26805200	0.00023200
C	-3.06212300	0.37824900	-0.00006300
C	-4.31093300	0.26810600	-0.00007100
C	5.70842700	-0.13109500	0.00002200
C	6.42307900	-0.06268000	-1.22013300
C	6.42334000	-0.06169600	1.21997100
C	7.80677000	0.07172900	-1.21159000
H	5.87658000	-0.11572300	-2.15566900
C	7.80703200	0.07268000	1.21102400
H	5.87704100	-0.11398400	2.15566600
C	8.50378400	0.13984500	-0.00038500
H	8.34585300	0.12394600	-2.15217500
H	8.34631700	0.12564100	2.15145200
H	9.58396900	0.24479200	-0.00054300
C	-5.70844800	0.13110100	-0.00011300
C	-6.42313000	0.06150100	-1.22018400
C	-6.42333500	0.06284600	1.21991600
C	-7.80682100	-0.07291300	-1.21148000
H	-5.87665400	0.11366300	-2.15578200
C	-7.80702100	-0.07160600	1.21112800
H	-5.87701600	0.11604500	2.15554800
C	-8.50380600	-0.13991900	-0.00019700
H	-8.34592600	-0.12602800	-2.15200300
H	-8.34628300	-0.12370000	2.15161800
H	-9.58398800	-0.24489600	-0.00023000

Cartesian coordinates of the optimized geometry for **14b** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	2.89867100	-0.00000100	0.00164900

C	4.11815200	0.00000000	0.02281000
C	-1.11202800	-0.00000500	-0.00331500
C	-1.82792300	-1.21209600	-0.00648600
C	-1.82792100	1.21209000	-0.00648600
C	-3.21916500	-1.20328200	-0.01019500
H	-1.28339400	-2.15035500	-0.00961100
C	-3.21916100	1.20327900	-0.01019600
H	-1.28338800	2.15034600	-0.00961000
C	-3.93786500	-0.00000200	-0.00996600
H	-3.75897500	-2.14619000	-0.01630500
H	-3.75896800	2.14618900	-0.01630500
Cl	5.76217400	0.00000400	-0.00291100
C	1.53567100	-0.00000400	0.00453400
C	0.31113200	-0.00000600	-0.00449700
C	-5.44521800	0.00001000	0.02152700
H	-5.85095400	0.88645800	-0.47431300
H	-5.81638500	0.00031600	1.05314200
H	-5.85095700	-0.88672500	-0.47379600

Cartesian coordinates of the optimized geometry for **14b** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 0):

C	-2.89809400	-0.00001400	0.00075600
C	-4.11357200	0.00006000	0.00200800
C	1.10584200	0.00001600	-0.00260200
C	1.82618700	1.21117000	-0.00541500
C	1.82617000	-1.21115200	-0.00541500
C	3.21653500	1.20247000	-0.00934900
H	1.28337900	2.15131300	-0.00858800
C	3.21651500	-1.20247500	-0.00934900
H	1.28334500	-2.15128500	-0.00858800
C	3.93816000	-0.00000600	-0.00796000
H	3.75422500	2.14779800	-0.01514500
H	3.75419100	-2.14781100	-0.01514700
Cl	-5.75847500	-0.00002400	0.00365400
C	-1.53643900	0.00001300	-0.00062500
C	-0.31605400	0.00002700	-0.00196600
C	5.44771700	-0.00002500	0.02026900
H	5.85837300	-0.88636200	-0.47468500
H	5.82438200	-0.00031900	1.05211700
H	5.85838500	0.88657700	-0.47419500

Cartesian coordinates of the optimized geometry for **20b** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.39490300	0.95969300	-0.00005700
C	-0.39490300	-0.95969300	0.00006900
Cl	0.90957100	-2.02994200	0.00012900
Cl	-0.90957100	2.02994200	-0.00011400
C	1.65375800	0.98687200	-0.00007000
C	-1.65375800	-0.98687200	0.00007900
C	2.97243400	0.73839900	-0.00006600
C	-2.97243400	-0.73839900	0.00007100
C	4.19344800	0.56180200	-0.00006600
C	-4.19344800	-0.56180200	0.00006800
C	5.58993000	0.33541500	-0.00006500
C	6.29906400	0.21869400	-1.21409700
C	6.29908700	0.21884800	1.21396900
C	7.67074100	-0.00643900	-1.20432400
H	5.76045800	0.30210600	-2.15205100
C	7.67076400	-0.00628700	1.20419800
H	5.76049900	0.30237800	2.15192200
C	8.38041200	-0.12068500	-0.00006200
H	8.20341400	-0.09888200	-2.14676800

H	8.20345400	-0.09861100	2.14664400
C	-5.58993000	-0.33541500	0.00006300
C	-6.29908300	-0.21884800	-1.21397300
C	-6.29906700	-0.21869400	1.21409300
C	-7.67076000	0.00628700	-1.20420700
H	-5.76049200	-0.30237800	-2.15192500
C	-7.67074500	0.00643900	1.20431500
H	-5.76046500	-0.30210600	2.15204800
C	-8.38041200	0.12068500	0.00005200
H	-8.20344700	0.09861100	-2.14665500
H	-8.20342000	0.09888200	2.14675800
C	9.87300400	-0.32960800	-0.00006300
H	10.19478800	-0.88304400	0.88673100
H	10.40331000	0.63009000	-0.00013500
H	10.19477000	-0.88316700	-0.88678800
C	-9.87300400	0.32960800	0.00004700
H	-10.19477600	0.88314600	0.88678200
H	-10.40331000	-0.63009000	0.00009200
H	-10.19478200	0.88306500	-0.88673600

Cartesian coordinates of the optimized geometry for **20b** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 1):

C	0.44215400	-0.94925300	0.00012300
C	-0.44215400	0.94925200	-0.00000900
Cl	0.82329100	2.07130400	-0.00004900
Cl	-0.82329100	-2.07130400	0.00021000
C	1.69352200	-0.92844800	0.00011600
C	-1.69352100	0.92844800	-0.00003300
C	3.01488900	-0.69433400	0.00009300
C	-3.01488900	0.69433400	-0.00004600
C	4.23116300	-0.51787500	0.00007400
C	-4.23116300	0.51787500	-0.00006100
C	5.62908500	-0.30887100	0.00005000
C	6.34409900	-0.19937100	1.21323400
C	6.34408400	-0.19954700	-1.21315900
C	7.71723000	0.00970600	1.20362400
H	5.80617600	-0.27627200	2.15293300
C	7.71721500	0.00953100	-1.20359600
H	5.80614900	-0.27658400	-2.15284000
C	8.43117000	0.11489400	0.00000200
H	8.24906200	0.09513000	2.14836300
H	8.24903500	0.09481800	-2.14835500
C	-5.62908500	0.30887100	-0.00008000
C	-6.34411700	0.19952700	1.21310800
C	-6.34406600	0.19939200	-1.21328500
C	-7.71724700	-0.00955200	1.20350500
H	-5.80620700	0.27654800	2.15280500
C	-7.71719700	-0.00968500	-1.20371500
H	-5.80611800	0.27630800	-2.15296800
C	-8.43117000	-0.11489400	-0.00011400
H	-8.24909300	-0.09485400	2.14824800
H	-8.24900400	-0.09509300	-2.14847100
C	9.92774800	0.30972300	-0.00002200
H	10.26107000	0.85906700	-0.88673500
H	10.45197600	-0.65569400	0.00002200
H	10.26108700	0.85915800	0.88662800
C	-9.92774800	-0.30972200	-0.00013400
H	-10.26106300	-0.85914200	-0.88680200
H	-10.45197600	0.65569400	-0.00017500
H	-10.26109400	-0.85908300	0.88656000

Cartesian coordinates of the optimized geometry for **17b** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.43981400	0.58020200	-0.00493600
C	1.76374900	0.54315300	-0.00541400
C	-1.76386200	-0.54433500	-0.00509800
C	-0.43991000	-0.58130600	-0.00492300
Cl	-0.38515800	2.13884300	-0.00498200
Cl	0.38505200	-2.13993500	-0.00508500
C	3.05888700	0.40584800	-0.00320200
C	4.30910000	0.30765900	-0.00154500
C	-3.05893700	-0.40646100	-0.00296900
C	-4.30912000	-0.30788800	-0.00130800
C	5.70609000	0.18181700	0.00061500
C	6.42522700	0.12174800	1.21838100
C	6.42878200	0.12044300	-1.21501200
C	7.80855400	0.00189700	1.20868800
H	5.88212700	0.17329600	2.15612000
C	7.81205200	0.00061800	-1.20115300
H	5.88838600	0.17098100	-2.15436500
C	8.52709000	-0.06290300	0.00486200
H	8.34646100	-0.03990600	2.15189500
H	8.35273300	-0.04218000	-2.14272800
C	-5.70607400	-0.18162400	0.00070300
C	-6.42529700	-0.12136700	1.21843100
C	-6.42863700	-0.11999900	-1.21496400
C	-7.80857000	-0.00112400	1.20863000
H	-5.88226700	-0.17308800	2.15620100
C	-7.81189300	0.00021900	-1.20121400
H	-5.88819400	-0.17066500	-2.15428300
C	-8.52699800	0.06390600	0.00472700
H	-8.34655300	0.04079700	2.15179100
H	-8.35247900	0.04321200	-2.14283200
C	10.02453700	-0.22945700	0.00707300
H	10.47455200	0.22693100	-0.87923800
H	10.30126000	-1.29059200	0.00767400
H	10.47200000	0.22728400	0.89449300
C	-10.02439900	0.23087600	0.00692600
H	-10.47428400	-0.22308600	-0.88068800
H	-10.30082400	1.29208300	0.01025600
H	-10.47224700	-0.22804100	0.89303700

Cartesian coordinates of the optimized geometry for **14c** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	2.87201600	-0.00113900	0.00153800
C	4.09157200	-0.00358800	0.02363900
C	-1.13755000	0.00400600	-0.00041800
C	-1.85577700	-1.20577100	-0.00089600
C	-1.85592400	1.21777500	-0.00089300
C	-3.24686200	-1.20372700	-0.00089400
H	-1.31477700	-2.14577200	-0.00091300
C	-3.24375600	1.22270300	-0.00090700
H	-1.31054100	2.15526900	-0.00089900
C	-3.94396800	0.00998800	-0.00092200
H	-3.79293100	-2.14393800	-0.00086100
H	-3.80372800	2.15105200	-0.00088500
Cl	5.73577600	-0.00456100	-0.00806500
C	1.50907000	0.00039300	0.00633900
C	0.28433900	0.00238900	-0.00199100
O	-5.30712000	0.07811000	-0.00075200
H	-5.66822500	-0.82212900	-0.00087700

Cartesian coordinates of the optimized geometry for **20c** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.39896400	-0.96045400	0.00686700
C	1.65790000	-0.98829100	0.00501300
C	-1.65790000	0.98829100	-0.00500800
C	-0.39896400	0.96045400	-0.00686000
Cl	-0.90525800	-2.03172200	0.01772800
Cl	0.90525800	2.03172200	-0.01771800
C	2.97599200	-0.73754800	0.00140400
C	4.19712000	-0.55989800	-0.00138900
C	-2.97599200	0.73754800	-0.00140200
C	-4.19712000	0.55989800	0.00139000
C	5.59152800	-0.33075100	-0.00350000
C	6.30548700	-0.22755000	-1.21923800
C	6.30153800	-0.20319500	1.20829300
C	7.67381600	-0.00396500	-1.22332400
H	5.76808400	-0.32455900	-2.15628900
C	7.67296600	0.02095400	1.20532300
H	5.76542900	-0.28067700	2.14787300
C	8.36292400	0.12114400	-0.00953300
H	8.22886500	0.07744200	-2.15108500
H	8.21123000	0.11887700	2.14495200
O	9.70700800	0.34030700	-0.07773000
C	-5.59152800	0.33075100	0.00349800
C	-6.30153600	0.20319700	-1.20829700
C	-6.30548900	0.22754900	1.21923400
C	-7.67296400	-0.02095300	-1.20532800
H	-5.76542600	0.28068000	-2.14787500
C	-7.67381800	0.00396300	1.22331800
H	-5.76808700	0.32455700	2.15628700
C	-8.36292400	-0.12114500	0.00952700
H	-8.21122700	-0.11887500	-2.14495900
H	-8.22886800	-0.07744500	2.15107800
O	-9.70700800	-0.34030800	0.07772100
H	-10.06303100	-0.40838200	-0.82213800
H	10.06303200	0.40838300	0.82212800

Cartesian coordinates of the optimized geometry for **17c** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.43983800	-0.58111500	0.00146400
C	1.76346300	-0.54712800	-0.00086600
C	-1.76346300	0.54712600	0.00104600
C	-0.43983800	0.58111200	-0.00118300
Cl	-0.38913300	-2.13963600	0.00843400
Cl	0.38913300	2.13963300	-0.00831800
C	3.05835900	-0.40561400	-0.00315200
C	4.30843200	-0.30422800	-0.00532300
C	-3.05835900	0.40561400	0.00320600
C	-4.30843300	0.30423000	0.00528200
C	5.70363800	-0.17551700	-0.00584100
C	6.42860600	-0.11495800	-1.22356800
C	6.42516100	-0.10597000	1.20954700
C	7.80777400	0.01051300	-1.22415000
H	5.88695100	-0.16728500	-2.16179500
C	7.80757200	0.01988900	1.20617200
H	5.88524200	-0.15099400	2.14913000
C	8.50402600	0.07846400	-0.00866600
H	8.36817000	0.05822900	-2.15119300
H	8.35135100	0.07327600	2.14635500
O	9.85968800	0.20167800	-0.07579700
C	-5.70363800	0.17551900	0.00577600
C	-6.42513500	0.10591500	-1.20962500
C	-6.42863200	0.11501600	1.22349000
C	-7.80754600	-0.01994400	-1.20627300

H	-5.88519600	0.15089600	-2.14919700
C	-7.80780100	-0.01045500	1.22404800
H	-5.88699800	0.16738600	2.16172700
C	-8.50402600	-0.07846300	0.00855300
H	-8.35130400	-0.07337400	-2.14646500
H	-8.36821700	-0.05812900	2.15108200
O	-9.85968900	-0.20167300	0.07566000
H	-10.22029300	-0.23884000	-0.82436800
H	10.22031000	0.23880200	0.82422500

Cartesian coordinates of the optimized geometry for **14d** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	1.30167400	1.36274100	-0.00092600
C	2.68579700	1.41346300	-0.00098900
C	3.43730000	0.22710400	-0.00079700
C	2.78408700	-1.01246200	-0.00049200
C	1.39080100	-1.05693100	-0.00046500
C	0.62751700	0.12216800	-0.00017100
H	3.34320100	-1.93953800	-0.00028900
H	0.88410600	-2.01611700	-0.00024700
O	4.78913300	0.38974500	-0.00069500
C	-0.79322800	0.06813400	-0.00174100
C	-2.01724800	0.02463100	0.00700200
C	-3.37926900	-0.02506200	0.00193000
C	-4.59797900	-0.06962300	0.02468500
H	3.21480400	2.36001700	-0.00114800
H	0.72381900	2.28063700	-0.00108300
C	5.59166500	-0.78495200	-0.00106800
H	5.40653600	-1.39091100	0.89292000
H	6.62395100	-0.43700200	-0.00149800
H	5.40567600	-1.39093400	-0.89484700
Cl	-6.24128500	-0.12937600	-0.00882800

Cartesian coordinates of the optimized geometry for **14d** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 0):

C	-1.29856400	1.35970800	0.00015100
C	-2.68183600	1.41082500	-0.00005100
C	-3.43548400	0.22498500	-0.00006400
C	-2.77983600	-1.01397400	0.00011500
C	-1.38779200	-1.05898800	0.00031700
C	-0.62026700	0.11965200	0.00034200
H	-3.33956700	-1.94200100	0.00010100
H	-0.88239600	-2.01970300	0.00045200
O	-4.78635900	0.38630300	-0.00027300
C	0.79915400	0.06601600	0.00059100
C	2.01923700	0.02335100	0.00036800
C	3.37993900	-0.02565900	0.00010000
C	4.59483400	-0.06917100	-0.00036500
H	-3.20944700	2.35926300	-0.00020400
H	-0.72161800	2.27911000	0.00015600
C	-5.60754900	-0.77260800	-0.00037400
H	-5.43881900	-1.38519600	-0.89543800
H	-6.63626500	-0.40869900	-0.00059200
H	-5.43916600	-1.38510400	0.89481900
Cl	6.23924300	-0.12781800	-0.00022800

Cartesian coordinates of the optimized geometry for **20d** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.38933000	0.95875500	0.11561200
C	1.64740500	1.00381300	0.08735100

C	-1.64740400	-1.00381600	-0.08729700
C	-0.38932900	-0.95875800	-0.11555000
Cl	-0.92633500	2.00179500	0.28896800
Cl	0.92633400	-2.00180000	-0.28890400
C	2.96755700	0.77363500	0.02137300
C	4.19024900	0.61455700	-0.03125100
C	-2.96755700	-0.77363800	-0.02133300
C	-4.19025000	-0.61455900	0.03127300
C	5.58626900	0.40711000	-0.09726700
C	6.33149600	0.14260500	1.06774600
C	6.26906300	0.46350100	-1.33546900
C	7.70771800	-0.06168200	1.01083300
H	5.81969500	0.09708300	2.02309700
C	7.63653700	0.26121500	-1.39675400
H	5.70704700	0.66662800	-2.24060300
C	8.36695500	-0.00282700	-0.22538500
H	8.25134800	-0.26396700	1.92500000
H	8.17041100	0.30101100	-2.33975700
C	-5.58627000	-0.40711000	0.09726700
C	-6.26908600	-0.46350800	1.33545700
C	-6.33147700	-0.14259700	-1.06775800
C	-7.63656000	-0.26122100	1.39672000
H	-5.70708500	-0.66664100	2.24059900
C	-7.70770000	0.06169000	-1.01086700
H	-5.81966000	-0.09707200	-2.02309900
C	-8.36695800	0.00282900	0.22534000
H	-8.17045100	-0.30102100	2.33971300
H	-8.25131400	0.26398100	-1.92504200
O	9.70350300	-0.18616600	-0.39821200
C	10.48617700	-0.45752300	0.75909400
H	11.50956200	-0.56926600	0.40312500
H	10.16137800	-1.38291100	1.24750600
H	10.43206100	0.36970200	1.47544900
O	-9.70350800	0.18616900	0.39814500
C	-10.48616300	0.45753400	-0.75917300
H	-11.50955400	0.56927600	-0.40322100
H	-10.43203500	-0.36968800	-1.47553200
H	-10.16135400	1.38292400	-1.24757400

Cartesian coordinates of the optimized geometry for **20d** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 1):

C	0.43854100	-0.95111000	-0.09929300
C	1.68961000	-0.94693200	-0.06552800
C	-1.68961000	0.94693300	0.06556200
C	-0.43854200	0.95111000	0.09933700
Cl	-0.83839900	-2.04902900	-0.26166000
Cl	0.83839800	2.04902700	0.26171800
C	3.01234500	-0.72968700	-0.00522800
C	4.23018000	-0.56838900	0.04451400
C	-3.01234500	0.72968800	0.00524900
C	-4.23017900	0.56839000	-0.04450400
C	5.62743100	-0.37663100	0.10490700
C	6.37774600	-0.13661300	-1.06466600
C	6.31589600	-0.42009800	1.34250600
C	7.75482400	0.05350500	-1.01259500
H	5.86598100	-0.10005300	-2.02119400
C	7.68449300	-0.23173000	1.39892200
H	5.75415300	-0.60362900	2.25284200
C	8.41764600	0.00690300	0.22286300
H	8.29965800	0.23611600	-1.93151000
H	8.21855900	-0.26325300	2.34322200
C	-5.62743000	0.37663200	-0.10491100
C	-6.31588300	0.42010000	-1.34251700
C	-6.37775600	0.13661200	1.06465300

C	-7.68447900	0.23173200	-1.39894700
H	-5.75413000	0.60363200	-2.25284800
C	-7.75483400	-0.05350600	1.01256900
H	-5.86600100	0.10005200	2.02118700
C	-8.41764300	-0.00690300	-0.22289600
H	-8.21853600	0.26325600	-2.34325300
H	-8.29967700	-0.23611800	1.93147800
O	9.75539600	0.17843800	0.38953900
C	10.55755700	0.42474900	-0.75759000
H	11.57922400	0.52858600	-0.38892100
H	10.25819000	1.35045700	-1.26542000
H	10.51015600	-0.41087100	-1.46749200
O	-9.75539200	-0.17843800	-0.38958600
C	-10.55756400	-0.42475000	0.75753600
H	-11.57922700	-0.52858700	0.38885600
H	-10.51017100	0.41086900	1.46743900
H	-10.25820300	-1.35045900	1.26536700

Cartesian coordinates of the optimized geometry for **17d** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.43698300	0.58157500	0.04557000
C	1.76029300	0.55836800	0.00839100
C	-1.76025300	-0.55797800	-0.00868700
C	-0.43694100	-0.58120200	-0.04583200
Cl	-0.39997600	2.12680400	0.21993300
Cl	0.40003800	-2.12643600	-0.22013200
C	3.05545500	0.42930200	-0.03842700
C	4.30599800	0.33926800	-0.07902600
C	-3.05542200	-0.42898400	0.03816000
C	-4.30597100	-0.33904500	0.07884000
C	5.70099400	0.22355100	-0.12824800
C	6.45684100	0.04603100	1.05241600
C	6.39442600	0.28497300	-1.36590300
C	7.84243900	-0.06768000	1.00959300
H	5.94152900	-0.00277700	2.00578500
C	7.77110800	0.17213900	-1.40929000
H	5.82903500	0.42095500	-2.28151600
C	8.50780200	-0.00491900	-0.22407200
H	8.39063400	-0.20382800	1.93341200
H	8.31002100	0.21686600	-2.34935200
C	-5.70097800	-0.22350300	0.12819200
C	-6.39429100	-0.28504900	1.36590900
C	-6.45695800	-0.04605200	-1.05239600
C	-7.77098700	-0.17238100	1.40942200
H	-5.82879700	-0.42100900	2.28146200
C	-7.84256900	0.06751000	-1.00944500
H	-5.94174100	0.00284300	-2.00581200
C	-8.50781600	0.00465000	0.22427500
H	-8.30980900	-0.21721200	2.34953100
H	-8.39086600	0.20357800	-1.93321500
O	9.85417500	-0.10418000	-0.38227700
C	10.64464400	-0.28554300	0.78794800
H	11.67574700	-0.33997000	0.44112200
H	10.37809400	-1.21451500	1.30383400
H	10.52975900	0.55895300	1.47628600
O	-9.85419100	0.10379400	0.38261200
C	-10.64483400	0.28489600	-0.78753200
H	-11.67590700	0.33922800	-0.44060000
H	-10.52990500	-0.55967000	-1.47578300
H	-10.37848800	1.21383500	-1.30358400

Cartesian coordinates of the optimized geometry for **14e** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	2.88421300	0.00001700	-0.00292000
C	4.10396300	0.00001100	-0.02669100
C	-1.12445600	0.00001000	-0.00744100
C	-1.84671400	1.20975300	-0.00608600
C	-1.84670600	-1.20974100	-0.00609700
C	-3.23444200	1.20978700	-0.00384000
H	-1.30539100	2.14989300	-0.00561800
C	-3.23443000	-1.20978900	-0.00385100
H	-1.30537300	-2.14987600	-0.00563700
C	-3.95145500	-0.00000200	0.00020600
H	-3.77640100	2.15152300	-0.00757700
H	-3.77638800	-2.15152400	-0.00760300
N	-5.34245100	-0.00003800	-0.05892600
Cl	5.74868000	-0.00001500	0.01657800
C	1.52143600	0.00001500	-0.01151400
C	0.29617000	0.00001600	-0.00369000
H	-5.78618100	0.83770700	0.29415300
H	-5.78615200	-0.83766200	0.29447700

Cartesian coordinates of the optimized geometry for **20e** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.40523400	-0.96389200	0.00001900
C	1.66409800	-0.98948200	0.00002100
C	-1.66409800	0.98948200	0.00000300
C	-0.40523400	0.96389200	0.00001200
Cl	-0.89973500	-2.03511200	0.00001900
Cl	0.89973500	2.03511200	0.00001900
C	2.98140000	-0.73569900	0.00002100
C	4.20288000	-0.55613600	0.00002100
C	-2.98140000	0.73569900	-0.00000700
C	-4.20288000	0.55613600	-0.00001600
C	5.59534800	-0.32575700	0.00002100
C	6.31186400	-0.21089100	-1.21177800
C	6.31186300	-0.21088600	1.21182000
C	7.68033000	0.00951900	-1.21113300
H	5.77686000	-0.29789500	-2.15146600
C	7.68033000	0.00952400	1.21117500
H	5.77685900	-0.29788600	2.15150900
C	8.38891500	0.12034800	0.00002100
H	8.21557800	0.10048500	-2.15235000
H	8.21557600	0.10049400	2.15239200
N	9.75013800	0.40015900	0.00002100
C	-5.59534800	0.32575700	-0.00002800
C	-6.31185300	0.21088600	-1.21183200
C	-6.31187400	0.21089200	1.21176500
C	-7.68032000	-0.00952400	-1.21119900
H	-5.77684100	0.29788500	-2.15151700
C	-7.68034000	-0.00951800	1.21111000
H	-5.77687800	0.29789500	2.15145800
C	-8.38891500	-0.12034800	-0.00005000
H	-8.21555900	-0.10049500	-2.15242000
H	-8.21559500	-0.10048400	2.15232200
N	-9.75013800	-0.40015900	-0.00006100
H	10.24769700	0.13338100	-0.83917600
H	10.24769600	0.13338500	0.83921900
H	-10.24768900	-0.13338500	-0.83926400
H	-10.24770400	-0.13338100	0.83913200

Cartesian coordinates of the optimized geometry for **17e** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.44393800	-0.57804800	-0.00031900
C	1.76689900	-0.54003200	-0.00026300
C	-1.76690000	0.54004300	0.00025000
C	-0.44393900	0.57805800	0.00035200
Cl	-0.38030700	-2.14289900	-0.00121600
Cl	0.38030800	2.14290800	0.00117900
C	3.06134100	-0.39723500	-0.00017800
C	4.31208600	-0.29405300	-0.00011800
C	-3.06134200	0.39724000	0.00015900
C	-4.31208600	0.29405300	0.00009800
C	5.70491100	-0.16581500	-0.00006500
C	6.43318800	-0.10140100	-1.21472600
C	6.43328500	-0.10347700	1.21464700
C	7.81220100	0.01896800	-1.21214600
H	5.89401400	-0.14838300	-2.15493400
C	7.81229600	0.01691800	1.21216200
H	5.89418700	-0.15206700	2.15481600
C	8.52774200	0.07645900	0.00002900
H	8.35308600	0.07163900	-2.15321300
H	8.35325500	0.06799600	2.15327400
N	9.90402100	0.25527100	0.00012700
C	-5.70491100	0.16581200	0.00006000
C	-6.43329600	0.10345300	-1.21464400
C	-6.43317700	0.10141700	1.21472800
C	-7.81230700	-0.01694400	-1.21214500
H	-5.89420600	0.15202800	-2.15481900
C	-7.81219000	-0.01895500	1.21216200
H	-5.89399500	0.14841600	2.15493100
C	-8.52774200	-0.07646700	-0.00000500
H	-8.35327400	-0.06803900	-2.15325100
H	-8.35306700	-0.07161100	2.15323500
N	-9.90402100	-0.25528200	-0.00008700
H	10.38405600	-0.03731500	-0.84060400
H	10.38412100	-0.03873300	0.84032500
H	-10.38413000	0.03870800	-0.84028600
H	-10.38404900	0.03731800	0.84064200

Cartesian coordinates of the optimized geometry for **15a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-2.32946800	0.00367300	-0.29858200
C	-3.54583500	0.00477700	-0.38451500
C	1.67600400	0.00039000	-0.03857100
C	2.38918700	1.21398300	0.01066200
C	2.38757800	-1.21435400	0.00523000
C	3.77907600	1.20797900	0.10144300
H	1.84145000	2.14968700	-0.02371900
C	3.77746900	-1.21060100	0.09610100
H	1.83860500	-2.14916900	-0.03336600
C	4.47717600	-0.00187600	0.14454600
H	4.31899500	2.14891900	0.13836400
H	4.31613800	-2.15241100	0.12885700
H	5.56025600	-0.00275100	0.21512900
C	-0.96775800	0.00256500	-0.21179200
C	0.25413700	0.00154100	-0.13101500
O	-4.84472300	0.00623300	-0.49715800
C	-5.55134100	-0.00910700	0.76816000
H	-6.60861800	-0.00581300	0.50913500
H	-5.29331700	-0.91247500	1.32549600
H	-5.29308100	0.88033200	1.34736100

Cartesian coordinates of the optimized geometry for **21a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	-0.33553200	-1.00027900	0.00014100
C	-1.58966200	-1.04049800	0.00014900
C	1.58966200	1.04049800	-0.00015200
C	0.33553200	1.00027900	-0.00014500
C	-2.90709800	-0.74844400	0.00011000
C	-4.12121600	-0.54428700	0.00008400
C	2.90709800	0.74844400	-0.00011200
C	4.12121600	0.54428700	-0.00008400
C	-5.51472600	-0.27496300	0.00005000
C	-6.21844000	-0.14034400	1.21519000
C	-6.21844600	-0.14068300	-1.21512500
C	-7.58565200	0.12234900	1.20972700
H	-5.67846800	-0.24378700	2.15035600
C	-7.58565800	0.12201100	-1.20972800
H	-5.67847900	-0.24438700	-2.15026400
C	-8.27372300	0.25441000	-0.00001700
H	-8.11681400	0.22451400	2.15088600
H	-8.11682400	0.22391400	-2.15091300
H	-9.33965500	0.45898700	-0.00004300
C	5.51472600	0.27496300	-0.00004800
C	6.21844400	0.14068300	1.21512800
C	6.21844200	0.14034500	-1.21518700
C	7.58565600	-0.12201200	1.20973300
H	5.67847600	0.24438600	2.15026600
C	7.58565400	-0.12234800	-1.20972200
H	5.67847200	0.24378800	-2.15035300
C	8.27372300	-0.25441000	0.00002300
H	8.11682100	-0.22391500	2.15091900
H	8.11681700	-0.22451300	-2.15088100
H	9.33965500	-0.45898600	0.00005100
O	0.80940400	-1.65820400	0.00023200
C	0.64375800	-3.09068400	0.00043600
O	-0.80940400	1.65820400	-0.00023800
C	-0.64375800	3.09068400	-0.00044300
H	-1.65293400	3.50095500	-0.00050100
H	-0.09803100	3.40276800	0.89396700
H	-0.09803200	3.40251300	-0.89494200
H	1.65293400	-3.50095500	0.00049300
H	0.09802900	-3.40276800	-0.89397300
H	0.09803300	-3.40251300	0.89493600

Cartesian coordinates of the optimized geometry for **18a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-0.34122900	-0.65336200	0.00007700
C	-1.66749400	-0.75036100	0.00013100
C	1.66749300	0.75035800	-0.00008200
C	0.34122900	0.65335900	-0.00010800
C	-2.95695300	-0.50429500	0.00018600
C	-4.19827100	-0.35614400	0.00016600
C	2.95695300	0.50429300	0.00004300
C	4.19827100	0.35614300	0.00006600
C	-5.59143100	-0.15378700	0.00004400
C	-6.30506600	-0.05231200	1.21781900
C	-6.30492200	-0.05275900	-1.21785300
C	-7.68185800	0.14449000	1.21046600
H	-5.76122100	-0.12893200	2.15339900
C	-7.68171500	0.14404600	-1.21073500
H	-5.76096600	-0.12972200	-2.15334000
C	-8.37577400	0.24330800	-0.00019400
H	-8.21791000	0.22173700	2.15130000
H	-8.21765600	0.22094700	-2.15166100
H	-9.45024500	0.39691500	-0.00028600
C	5.59143200	0.15378700	0.00000100
C	6.30506600	0.05265700	1.21780500

C	6.30492200	0.05241700	-1.21786700
C	7.68185800	-0.14414700	1.21050800
H	5.76122000	0.12954000	2.15336300
C	7.68171600	-0.14438400	-1.21069300
H	5.76096700	0.12911700	-2.15337600
C	8.37577500	-0.24330400	-0.00012400
H	8.21791000	-0.22112800	2.15136400
H	8.21765700	-0.22155000	-2.15159800
H	9.45024600	-0.39691000	-0.00017200
O	0.53468600	-1.69804000	0.00029400
C	-0.07056000	-2.99180600	0.00054300
O	-0.53468600	1.69803700	-0.00018900
C	0.07056000	2.99180300	-0.00030700
H	-0.75750200	3.70029000	-0.00035400
H	0.69106100	3.13077300	0.89108400
H	0.69103500	3.13062200	-0.89174000
H	0.75750200	-3.70029200	0.00069700
H	-0.69103500	-3.13087800	-0.89085000
H	-0.69106100	-3.13052300	0.89197400

Cartesian coordinates of the optimized geometry for **7a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	2.02225900	-0.00031700	-0.00022400
C	3.23703300	0.00015000	-0.00035100
C	0.59135000	-0.00014800	-0.00006600
C	-0.11949900	-1.21357600	-0.00013900
C	-0.11922500	1.21344100	0.00016100
C	-1.51284800	-1.20895000	0.00001300
H	0.42974800	-2.14897800	-0.00031600
C	-1.51257500	1.20913400	0.00031200
H	0.43023300	2.14872000	0.00021700
C	-2.21289600	0.00017100	0.00023900
H	-2.05311900	-2.15028400	-0.00004500
H	-2.05263300	2.15059000	0.00048800
H	-3.29822300	0.00029400	0.00035700
H	4.30240300	0.00022300	-0.00036600

Cartesian coordinates of the optimized geometry for **22a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.34369200	-0.00044400	-0.86537700
C	-0.34369200	-0.00044400	0.86538000
C	1.60312600	-0.00032100	-0.95740200
C	-1.60312600	-0.00032000	0.95740300
C	-2.93848800	-0.00011100	0.49714200
C	2.93848800	-0.00011100	-0.49714100
C	3.62210900	1.21726400	-0.26919700
C	4.93787800	1.21040000	0.18197600
C	5.60214900	0.00033800	0.40892500
C	4.93829800	-1.20994800	0.18193600
C	3.62253200	-1.21725600	-0.26923700
C	-3.62253200	-1.21725600	0.26923700
C	-4.93829700	-1.20994800	-0.18193700
C	-5.60214800	0.00033700	-0.40892700
C	-4.93787700	1.21040000	-0.18197700
C	-3.62210900	1.21726400	0.26919700
H	-3.10284600	2.15313300	0.44743200
H	-5.44954700	2.15151600	-0.35812100
H	-6.62944100	0.00051000	-0.75897400
H	-5.45029500	-2.15089200	-0.35805100
H	-3.10359600	-2.15330000	0.44750300
H	3.10284600	2.15313300	-0.44743200
H	5.44954700	2.15151600	0.35811900

H	6.62944200	0.00051000	0.75897200
H	5.45029500	-2.15089200	0.35805000
H	3.10359600	-2.15330000	-0.44750300
H	-0.51106100	-0.00049500	-1.51852400
H	0.51106000	-0.00049500	1.51852600

Cartesian coordinates of the optimized geometry for **10a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.23058800	-0.00036100	-0.73334600
C	1.50952000	-0.00038500	-1.01573000
C	-1.50952400	-0.00035500	1.01574100
C	-0.23059100	-0.00034600	0.73335700
C	2.82870300	-0.00015900	-0.52232600
C	-2.82870500	-0.00014300	0.52233000
C	3.51539100	-1.21883800	-0.28781200
C	4.82380000	-1.21099200	0.18118600
C	5.48461600	0.00036600	0.41664700
C	4.82303600	1.21146200	0.18200500
C	3.51461800	1.21879700	-0.28698300
C	-3.51462900	1.21880400	0.28697300
C	-4.82304400	1.21145300	-0.18202200
C	-5.48461200	0.00034900	-0.41665800
C	-4.82378700	-1.21100100	-0.18118200
C	-3.51538000	-1.21883100	0.28782300
H	2.99881400	-2.15508300	-0.47308400
H	5.33421100	-2.15145500	0.36504500
H	6.50754100	0.00056500	0.77957000
H	5.33284700	2.15212500	0.36650300
H	2.99744400	2.15483900	-0.47162200
H	-2.99746400	2.15485200	0.47160600
H	-5.33286400	2.15211000	-0.36653100
H	-6.50753500	0.00053600	-0.77958700
H	-5.33418800	-2.15147000	-0.36503600
H	-2.99879500	-2.15507000	0.47310700
H	-0.57232600	-0.00045000	-1.46255300
H	0.57232300	-0.00041800	1.46256500

Cartesian coordinates of the optimized geometry for **8a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-0.89572300	0.00000900	-0.00009100
C	-2.11086700	-0.00002100	-0.00021500
C	0.53334800	0.00000800	0.00005400
C	1.24442400	1.21373900	-0.00002400
C	1.24441500	-1.21373300	0.00027600
C	2.63744000	1.20895700	0.00011700
H	0.69557400	2.14944400	-0.00019600
C	2.63742900	-1.20896300	0.00041700
H	0.69555300	-2.14943100	0.00033600
C	3.33789500	-0.00000500	0.00033800
H	3.17707500	2.15055600	0.00005500
H	3.17705900	-2.15056500	0.00058800
H	4.42311800	-0.00001100	0.00044800
Cl	-3.76109100	0.00000400	-0.00038000

Cartesian coordinates of the optimized geometry for **23a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.45773500	0.88255600	-0.00035900
C	-0.45773400	-0.88255500	-0.00048600
Cl	0.74742900	-2.08281400	-0.00084800
Cl	-0.74742900	2.08281400	-0.00055000

C	1.71246400	0.83671500	-0.00019400
C	-1.71246400	-0.83671400	-0.00031600
C	-3.07523700	-0.48042000	0.00002100
C	3.07523600	0.48042000	0.00009100
C	3.77406100	0.31761600	1.21864300
C	5.12620700	-0.00620600	1.21160100
C	5.80774700	-0.16929400	0.00067800
C	5.12674400	-0.00614800	-1.21053800
C	3.77460100	0.31767700	-1.21815800
C	-3.77460300	-0.31750600	-1.21820400
C	-5.12674700	0.00631700	-1.21053600
C	-5.80774700	0.16929300	0.00070400
C	-5.12620500	0.00603600	1.21160400
C	-3.77405900	-0.31778700	1.21859700
H	-3.23843400	-0.44343300	2.15346300
H	-5.65283400	0.13267200	2.15219700
H	-6.86320700	0.42196800	0.00097000
H	-5.65379500	0.13317000	-2.15086500
H	-3.23939600	-0.44293700	-2.15333900
H	3.23843900	0.44313100	2.15352800
H	5.65283800	-0.13297500	2.15217600
H	6.86320700	-0.42196900	0.00090600
H	5.65379000	-0.13286900	-2.15088600
H	3.23939100	0.44323900	-2.15327400

Cartesian coordinates of the optimized geometry for **11a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.43046400	0.61430400	-0.00101200
C	1.73121100	0.62023900	-0.00072600
C	-1.73120700	-0.62021800	-0.00129200
C	-0.43046100	-0.61428500	-0.00086800
Cl	-0.48565400	2.12714100	-0.00152500
Cl	0.48565700	-2.12712300	-0.00039000
C	3.09112900	0.34406800	0.00006500
C	-3.09112900	-0.34406500	-0.00044600
C	3.80822900	0.22328100	-1.22287100
C	5.17504000	-0.01513700	-1.21114800
C	5.86605200	-0.13450600	0.00159900
C	5.17379800	-0.01450000	1.21357600
C	3.80697700	0.22392500	1.22378900
C	-3.80674000	-0.22322500	1.22334900
C	-5.17356400	0.01518400	1.21326200
C	-5.86605700	0.13447900	0.00135000
C	-5.17528100	0.01441300	-1.21146200
C	-3.80846700	-0.22399200	-1.22331000
H	3.26771400	0.31439900	-2.15904600
H	5.70992400	-0.10988200	-2.15099200
H	6.93525100	-0.32041000	0.00219800
H	5.70772400	-0.10874300	2.15401500
H	3.26550700	0.31554000	2.15936400
H	-3.26508400	-0.31429000	2.15887000
H	-5.70730700	0.10996800	2.15375000
H	-6.93525800	0.32037100	0.00205000
H	-5.71035000	0.10860400	-2.15125600
H	-3.26813800	-0.31564900	-2.15953900

Cartesian coordinates of the optimized geometry for **8f** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-4.63680500	-1.14316800	0.38728600
C	-5.33961500	-0.00008400	-0.00016600
C	-4.63692700	1.14309600	-0.38757100
C	-3.24266300	1.14297500	-0.38838600

C	-2.52472700	0.00015100	0.00007600
C	-3.24253600	-1.14282500	0.38829300
C	-1.04546800	0.00013100	0.00005000
C	-0.32402000	-1.14154600	-0.38746200
C	1.06636500	-1.14720200	-0.38767200
C	1.78226900	-0.00010300	0.00018600
C	1.06652500	1.14708500	0.38808500
C	-0.32386100	1.14166000	0.38776600
C	3.21023300	-0.00025100	0.00034300
C	4.42543300	-0.00017900	0.00019700
Cl	6.07506700	0.00010700	-0.00035500
H	-5.17467600	-2.03333400	0.69835300
H	-6.42494200	-0.00018000	-0.00024200
H	-5.17488700	2.03314600	-0.69881500
H	-2.70191700	2.02503300	-0.71692800
H	-2.70168200	-2.02487800	0.71668300
H	-0.86245900	-2.02496500	-0.71538800
H	1.61053400	-2.03308300	-0.69745900
H	1.61082400	2.03286100	0.69794600
H	-0.86215900	2.02513800	0.71574000

Cartesian coordinates of the optimized geometry for **23f** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	9.47894400	-0.87953200	-0.59083800
C	10.06053800	0.32776300	-0.19684700
C	9.25401400	1.34652400	0.31576100
C	7.87755000	1.16018500	0.43285300
C	7.28009100	-0.04966200	0.04028500
C	8.10264800	-1.06681000	-0.47304100
C	5.82177000	-0.24703700	0.16392700
C	5.10772800	-0.98579800	-0.79850600
C	3.73825800	-1.17482600	-0.68901300
C	3.02196100	-0.61892100	0.39692200
C	3.73739900	0.12035300	1.36800700
C	5.10716600	0.29984700	1.24655900
C	1.63817400	-0.82829100	0.52799700
C	0.38421900	-0.78307700	0.49718600
Cl	-0.92157100	-1.70328200	1.07715100
H	10.09899900	-1.68033600	-0.98157300
H	11.13214500	0.47332400	-0.28830600
H	9.69607500	2.29146700	0.61593200
H	7.25320800	1.96636300	0.80501600
H	7.66121700	-2.01776200	-0.75421100
H	5.63606600	-1.39117800	-1.65549300
H	3.19791300	-1.73531000	-1.44451700
H	3.19992300	0.54094000	2.21128200
H	5.64401900	0.84961700	2.01298900
C	-9.25401400	-1.34652300	-0.31576700
C	-10.06053900	-0.32776100	0.19683900
C	-9.47894500	0.87953300	0.59083000
C	-8.10264900	1.06681100	0.47303600
C	-7.28009100	0.04966200	-0.04028800
C	-7.87755000	-1.16018500	-0.43285600
C	-5.82177000	0.24703700	-0.16392900
C	-5.10716500	-0.29984800	-1.24655800
C	-3.73739700	-0.12035500	-1.36800400
C	-3.02196000	0.61892100	-0.39691900
C	-3.73826000	1.17482700	0.68901500
C	-5.10773000	0.98579900	0.79850500
C	-1.63817300	0.82829000	-0.52799200
C	-0.38421700	0.78307600	-0.49717900
Cl	0.92157200	1.70328200	-1.07714300
H	-9.69607500	-2.29146600	-0.61593800
H	-11.13214700	-0.47332300	0.28829700

H	-10.09900100	1.68033800	0.98156300
H	-7.66121800	2.01776300	0.75420500
H	-7.25320800	-1.96636300	-0.80501800
H	-5.64401700	-0.84961900	-2.01298900
H	-3.19992000	-0.54094300	-2.21127900
H	-3.19791500	1.73531100	1.44451900
H	-5.63606900	1.39118000	1.65549200

Cartesian coordinates of the optimized geometry for **11f** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-9.38966100	-0.86969300	1.01815600
C	-10.16884900	-0.26766100	0.02725500
C	-8.00436300	-0.71789700	1.01071300
C	-7.36843400	0.04025700	0.01155600
C	-8.16480700	0.64092100	-0.97953500
C	-9.55005400	0.48808000	-0.97146700
C	-5.90311200	0.20028800	0.00329500
C	-5.17410000	0.27886900	1.20880800
C	-3.79958900	0.42768800	1.21277000
C	-3.07516200	0.50124600	-0.01237700
C	-3.81270600	0.42492300	-1.22945700
C	-5.18720300	0.27637300	-1.21024300
H	-9.86061900	-1.46690100	1.79274300
H	-7.40394000	-1.21403400	1.76664400
H	-10.14804400	0.96757800	-1.74019500
H	-11.24764000	-0.38626200	0.03325400
H	-7.69483900	1.25440300	-1.74166500
H	-5.70797500	0.24963300	2.15337800
H	-3.25495900	0.49636200	2.14858500
H	-5.72509700	0.18707000	-2.14878200
H	-3.27557600	0.46705000	-2.17117700
C	-1.70653100	0.68454800	-0.01889000
C	-0.40713200	0.62877500	-0.02050200
Cl	0.56587000	2.10827900	-0.02251500
C	0.40712400	-0.62872000	-0.02073600
Cl	-0.56587600	-2.10821600	-0.02336600
C	1.70652400	-0.68446600	-0.01914600
C	3.07515600	-0.50120600	-0.01256400
C	3.81268800	-0.42431400	-1.22961700
C	3.79960100	-0.42823500	1.21260900
C	5.18718800	-0.27579700	-1.21034700
C	5.90311400	-0.20030200	0.00321700
C	5.17411400	-0.27944000	1.20870100
H	3.27554500	-0.46598100	-2.17134900
H	5.72507100	-0.18605700	-2.14885100
H	3.25498000	-0.49733800	2.14839900
H	5.70800000	-0.25065900	2.15327900
C	7.36843800	-0.04029600	0.01153700
C	8.16479100	-0.64049000	-0.97985500
C	9.55004100	-0.48767100	-0.97173000
C	8.00439000	0.71736700	1.01105300
H	7.69480600	-1.25359700	-1.74227600
C	10.16885800	0.26757800	0.02735100
H	10.14801500	-0.96680400	-1.74069700
C	9.38968900	0.86914000	1.01855200
H	7.40398200	1.21314600	1.76723000
H	11.24765100	0.38616200	0.03339400
H	9.86066500	1.46596800	1.79342300

Cartesian coordinates of the optimized geometry for **9a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-0.87089400	-0.25527600	-0.00002100

C	-2.07595300	-0.41295600	-0.00001800
C	0.54954100	-0.10118200	-0.00000800
C	1.39090000	-1.22962900	0.00001100
C	1.13162700	1.18014800	-0.00001900
C	2.77565800	-1.07572200	0.00001800
H	0.94673800	-2.21939200	0.00002000
C	2.51746900	1.32521400	-0.00000500
H	0.48781600	2.05356100	-0.00003700
C	3.34536100	0.20000100	0.00001200
H	3.41203800	-1.95527800	0.00003100
H	2.95202700	2.32011000	-0.00001000
H	4.42445400	0.31612500	0.00002000
O	-3.37245600	-0.59927000	-0.00003900
C	-4.13746500	0.62626000	0.00004600
H	-3.90944100	1.20920900	0.89600200
H	-5.18215500	0.31925800	-0.00007300
H	-3.90930000	1.20942500	-0.89573400

Cartesian coordinates of the optimized geometry for **24a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	0.37377100	-0.94113000	-0.00008300
C	1.62544100	-0.93063100	-0.00003900
C	-1.62544100	0.93063000	-0.00001200
C	-0.37377100	0.94113000	-0.00005600
C	2.98339500	-0.52679900	0.00001100
C	-2.98339500	0.52679900	0.00002700
C	3.67915000	-0.33713600	1.21417400
C	5.01908200	0.03898100	1.20962900
C	5.69520000	0.22816400	0.00010200
C	5.01906500	0.03932800	-1.20947100
C	3.67913500	-0.33679000	-1.21410700
C	-3.67915200	0.33687600	-1.21409500
C	-5.01908200	-0.03924300	-1.20946800
C	-5.69520100	-0.22816400	0.00010100
C	-5.01906500	-0.03906600	1.20963300
C	-3.67913400	0.33705100	1.21418600
H	3.14838100	-0.48204100	2.14927300
H	5.53978500	0.18550100	2.15107200
H	6.74067500	0.52027000	0.00013700
H	5.53975600	0.18611900	-2.15087900
H	3.14835300	-0.48142700	-2.14923900
H	-3.14838200	0.48157800	-2.14922400
H	-5.53978500	-0.18596700	-2.15087900
H	-6.74067500	-0.52027000	0.00013000
H	-5.53975500	-0.18565300	2.15107300
H	-3.14835200	0.48189000	2.14928800
O	0.73313100	1.68192000	-0.00009700
O	-0.73313100	-1.68192000	-0.00014700
C	-0.46016400	-3.09221100	-0.00015700
H	0.10881000	-3.36700700	-0.89327700
H	-1.43438700	-3.58107700	-0.00020100
H	0.10874200	-3.36703200	0.89299900
C	0.46016400	3.09221100	-0.00006600
H	-0.10874200	3.36700600	0.89309700
H	-0.10881000	3.36703300	-0.89317800
H	1.43438700	3.58107700	-0.00009600

Cartesian coordinates of the optimized geometry for **12a** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	-0.32481400	0.68018300	0.00013700
C	-1.62923900	0.80776000	-0.00003600
C	1.62923900	-0.80783000	-0.00064000

C	0.32484200	-0.68016300	-0.00051800
C	-2.97308800	0.41992500	0.00003600
C	2.97308600	-0.41997300	-0.00026200
C	-3.68215100	0.24848600	1.21865400
C	-5.02837300	-0.09369600	1.21149800
C	-5.71003800	-0.26455400	0.00031700
C	-5.02900700	-0.09214100	-1.21100000
C	-3.68278600	0.25003700	-1.21842300
C	3.68260200	-0.24862000	-1.21862300
C	5.02880600	0.09362800	-1.21099000
C	5.70999700	0.26462700	0.00043600
C	5.02851900	0.09228300	1.21151200
C	3.68231400	-0.24996400	1.21845300
H	-3.14823400	0.37938700	2.15427100
H	-5.55356900	-0.22870600	2.15228400
H	-6.76263100	-0.52987200	0.00042200
H	-5.55469500	-0.22594400	-2.15168300
H	-3.14935800	0.38213200	-2.15415200
H	3.14904500	-0.37963200	-2.15443000
H	5.55434900	0.22858600	-2.15158800
H	6.76257800	0.52999300	0.00071200
H	5.55384900	0.22619000	2.15238000
H	3.14853500	-0.38200700	2.15399000
O	-0.61215200	-1.67659300	-0.00075900
O	0.61206800	1.67653800	0.00072000
C	0.06736700	2.99434300	0.00039700
H	-0.54794300	3.16213100	-0.89034700
H	0.92515600	3.66728700	0.00041500
H	-0.54822900	3.16250800	0.89087300
C	-0.06722000	-2.99431700	-0.00092500
H	0.54771300	-3.16250500	0.88999600
H	0.54874700	-3.16188100	-0.89124900
H	-0.92497100	-3.66732200	-0.00171500

Cartesian coordinates of the optimized geometry for **25** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.98097800	-0.58134400	0.00155700
C	4.75686300	-0.09063900	-0.02292500
Cl	6.38696500	0.12038900	0.00794400
C	-0.42824200	-0.76516600	0.00016500
C	-1.31479700	0.36672100	0.00046200
C	-0.95805500	-2.04853600	0.00077000
C	-0.82311700	1.69662200	0.00004300
C	-2.72925600	0.14221700	0.00058900
C	-2.35110500	-2.25180100	0.00085700
C	-1.68874400	2.76894600	-0.00000900
C	-3.59108300	1.27258600	0.00043000
C	-3.24135000	-1.19473300	0.00085400
H	-2.73394600	-3.26832300	0.00098000
C	-3.08541900	2.55475600	0.00017100
C	2.19589800	-0.42055100	-0.00604200
C	3.54728300	-0.24796600	-0.00130800
H	-4.66441800	1.11993400	0.00049800
H	-3.76174300	3.40380300	0.00005300
H	-1.29704500	3.78119200	-0.00029300
H	0.25014400	1.85475400	-0.00022800
H	-0.28596500	-2.90020800	0.00086700
C	-4.72643900	-1.44964100	0.00102900
H	-5.20728100	-1.01162800	0.88263700
H	-4.93123000	-2.52300100	0.00124700
H	-5.20742100	-1.01196700	-0.88067300

Cartesian coordinates of the optimized geometry for **25** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 0):

C	-3.60867900	1.25527400	-0.00003800
C	-3.12110100	2.54362900	-0.00002200
C	-1.72780300	2.77568100	0.00002100
C	-0.85022100	1.71398800	0.00004300
C	-1.32154300	0.37693800	0.00002100
C	-2.73443800	0.13364300	-0.00002000
H	-4.68110500	1.09057400	-0.00006700
H	-3.80948500	3.38440700	-0.00003700
H	-1.34817800	3.79372500	0.00003900
H	0.22153800	1.88646500	0.00007800
C	-3.22915800	-1.21232900	-0.00003300
C	-2.32231900	-2.25527600	-0.00000300
C	-0.93283500	-2.03318500	0.00003500
C	-0.41624800	-0.74378600	0.00005100
H	-2.68821100	-3.27891300	-0.00000700
H	-0.25116400	-2.87788200	0.00006100
C	-4.71137300	-1.49542700	-0.00007600
H	-5.20658200	-1.06996800	-0.88207500
H	-5.20663900	-1.06994100	0.88187800
H	-4.89987800	-2.57281300	-0.00006600
C	0.99049400	-0.54802700	0.00011200
C	2.20247700	-0.39768900	0.00007700
C	3.55368900	-0.23245800	0.00009200
C	4.76040700	-0.08519000	0.00000700
Cl	6.39303600	0.11409600	-0.00008300

Cartesian coordinates of the optimized geometry for **28** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	-4.15126600	-0.57471900	0.57328300
C	-0.38857700	-0.05525800	0.97016500
C	4.15126500	0.57471800	-0.57328400
Cl	0.91222000	0.12374700	2.02790100
Cl	-0.91222000	-0.12375100	-2.02790200
C	5.53157700	0.76078100	-0.34653000
C	6.41251500	-0.36955900	-0.19573500
C	6.05527400	2.04916100	-0.26990100
C	5.93038800	-1.70002000	-0.26335900
C	7.80745000	-0.13930500	0.03033100
C	7.42746200	2.25534800	-0.04734900
C	6.78783300	-2.76949200	-0.11543700
H	4.87121000	-1.86218300	-0.43336800
C	8.66137000	-1.26585200	0.17795400
C	8.30933600	1.19973000	0.10304800
H	7.80423100	3.27265600	0.00769400
C	8.16548500	-2.55014800	0.10696200
H	6.40337600	-3.78302800	-0.16954200
H	9.72027400	-1.10903500	0.34955200
H	8.83517000	-3.39654300	0.22264600
C	-5.53157700	-0.76078100	0.34653000
C	-6.41251400	0.36956000	0.19573500
C	-6.05527500	-2.04916000	0.26990000
C	-5.93038700	1.70002100	0.26336000
C	-7.80745000	0.13930700	-0.03033000
C	-7.42746400	-2.25534700	0.04734800
C	-6.78783100	2.76949300	0.11543900
C	-8.66136900	1.26585400	-0.17795300
C	-8.30933600	-1.19972800	-0.10304800
H	-7.80423300	-3.27265400	-0.00769500
C	-8.16548400	2.55015000	-0.10696000
C	2.94086200	0.40496000	-0.75098600
C	1.63537300	0.22746200	-0.99901200
C	0.38857700	0.05525500	-0.97016600

H	5.38956400	2.89820400	-0.38389100
C	-2.94086200	-0.40496100	0.75098500
C	-1.63537300	-0.22746400	0.99901100
H	-9.72027400	1.10903800	-0.34955000
H	-8.83516900	3.39654500	-0.22264300
H	-6.40337400	3.78302900	0.16954400
H	-4.87120900	1.86218200	0.43336900
H	-5.38956600	-2.89820300	0.38389000
C	9.77389200	1.46045900	0.34006800
H	10.39142200	1.01784100	-0.44933300
H	10.10755400	1.03020900	1.29084300
H	9.97344400	2.53446600	0.36501800
C	-9.77389300	-1.46045600	-0.34006800
H	-10.39142300	-1.01783800	0.44933400
H	-9.97344600	-2.53446200	-0.36501900
H	-10.10755600	-1.03020600	-1.29084200

Cartesian coordinates of the optimized geometry for **28** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 1):

C	4.19841600	-0.52414100	-0.53314800
C	0.44100700	-0.02976700	-0.95908600
C	-4.19841200	0.52413200	0.53315200
Cl	-0.81865200	0.16249500	-2.06945300
Cl	0.81865000	-0.16254700	2.06946000
C	-5.57873700	0.72902800	0.32756700
C	-6.48527800	-0.38451600	0.17380100
C	-6.08438700	2.02649800	0.27059400
C	-6.02946100	-1.72467300	0.22191200
C	-7.87992400	-0.12697000	-0.03305000
C	-7.45425200	2.25986400	0.06705900
C	-6.90565400	-2.77798100	0.07335500
H	-4.97099500	-1.90801600	0.37826400
C	-8.75338400	-1.23910500	-0.18201400
C	-8.35905100	1.22379300	-0.08509900
H	-7.81021100	3.28622700	0.02854900
C	-8.28109700	-2.53237700	-0.13049300
H	-6.53756000	-3.79942500	0.11291100
H	-9.81241700	-1.06354900	-0.33940100
H	-8.96814300	-3.36608300	-0.24713000
C	5.57874300	-0.72902500	-0.32756500
C	6.48527500	0.38452700	-0.17380300
C	6.08440400	-2.02649000	-0.27059100
C	6.02944700	1.72468000	-0.22191500
C	7.87992400	0.12699300	0.03304600
C	7.45427200	-2.25984500	-0.06705900
C	6.90563200	2.77799600	-0.07336100
C	8.75337500	1.23913500	0.18200600
C	8.35906200	-1.22376600	0.08509600
H	7.81023900	-3.28620500	-0.02854800
C	8.28107700	2.53240300	0.13048400
C	-2.99149900	0.36304100	0.70872200
C	-1.68195900	0.18908500	0.94032300
C	-0.44100800	0.02972700	0.95909200
H	-5.40391300	2.86413300	0.38584500
C	2.99150100	-0.36306000	-0.70871600
C	1.68195900	-0.18911500	-0.94031700
H	9.81241000	1.06358800	0.33939200
H	8.96811600	3.36611600	0.24711900
H	6.53752900	3.79943700	-0.11291800
H	4.97097900	1.90801400	-0.37826500
H	5.40393600	-2.86413100	-0.38583900
C	-9.82190300	1.52153800	-0.30161600
H	-10.44626100	1.08705800	0.48937100
H	-10.18266800	1.11382700	-1.25443800

H	-10.00061600	2.60047100	-0.31209200
C	9.82191700	-1.52149900	0.30161000
H	10.44627000	-1.08701500	-0.48937800
H	10.00063900	-2.60043000	0.31208700
H	10.18268100	-1.11378300	1.25443100

Cartesian coordinates of the optimized geometry for **31** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	4.27748000	-0.57955000	-0.29333600
C	0.44350500	-0.05380300	-0.57452900
C	-4.27747300	0.57953400	0.29334700
Cl	-0.35267100	0.07469700	-2.14410500
Cl	0.35265000	-0.07471400	2.14424500
C	-5.65520900	0.76291200	0.17513800
C	-6.55223200	-0.36997500	0.09392300
C	-6.18975400	2.05667600	0.13645400
C	-6.06758100	-1.69883600	0.12712400
C	-7.95869500	-0.13791300	-0.02406900
C	-7.57258500	2.25921200	0.02044900
C	-6.93468100	-2.76929800	0.04781300
H	-4.99845300	-1.86244500	0.21576400
C	-8.82222900	-1.26305700	-0.10335100
C	-8.46491000	1.20268700	-0.06000200
H	-7.95334500	3.27634700	-0.00697400
C	-8.32397500	-2.54890800	-0.06833400
H	-6.54734700	-3.78282800	0.07444600
H	-9.89105500	-1.10523000	-0.19313800
H	-9.00195800	-3.39430600	-0.13054300
C	5.65522300	-0.76291700	-0.17516100
C	6.55223200	0.36998000	-0.09394300
C	6.18978700	-2.05667200	-0.13653300
C	6.06756000	1.69883600	-0.12707900
C	7.95870200	0.13793500	0.02399900
C	7.57262600	-2.25919100	-0.02057600
C	6.93464500	2.76930800	-0.04776100
C	8.82222100	1.26309100	0.10328900
C	8.46494000	-1.20265700	0.05987200
H	7.95340100	-3.27632200	0.00680600
C	8.32394600	2.54893500	0.06833300
C	-3.03577400	0.40809800	0.39177900
C	-1.75509200	0.23441800	0.52203000
C	-0.44352100	0.05375700	0.57466500
H	-5.51813900	2.90667600	0.19705900
C	3.03577100	-0.40814200	-0.39169400
C	1.75507900	-0.23450000	-0.52192400
H	9.89105200	1.10527700	0.19303500
H	9.00191800	3.39434200	0.13054900
H	6.54729500	3.78283300	-0.07434400
H	4.99842600	1.86243000	-0.21567900
H	5.51818300	-2.90668100	-0.19713700
C	-9.94278400	1.46360200	-0.18372400
H	-10.49801300	1.02236100	0.65160900
H	-10.34920500	1.03185300	-1.10523000
H	-10.14350000	2.53763900	-0.19496100
C	9.94282200	-1.46355400	0.18353500
H	10.49801700	-1.02227900	-0.65180400
H	10.14355400	-2.53758900	0.19473000
H	10.34927000	-1.03182900	1.10504000

Cartesian coordinates of the optimized geometry for **26** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	3.64050800	-0.07363600	0.00240900

S	2.19083300	-1.03391700	-0.00054100
C	1.17046200	0.39445900	-0.00138200
C	-0.22967900	0.29301300	-0.00012000
C	-1.45046000	0.17718100	-0.00813900
C	-2.80685200	0.06668600	-0.00243000
C	-4.02192600	-0.04350200	-0.02502500
C	3.33710300	1.26733000	0.00281500
C	1.94548700	1.53898400	0.00102200
H	1.51127000	2.53131700	0.00161900
H	4.10196200	2.03592300	0.00419000
C	4.99732800	-0.71066200	0.00243400
H	5.15192800	-1.33536400	-0.88349100
H	5.14931700	-1.34105100	0.88476200
H	5.76360100	0.06889400	0.00604100
Cl	-5.66019100	-0.16918600	0.00976600

Cartesian coordinates of the optimized geometry for **26** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 0):

C	3.64158400	-0.07410700	-0.00001200
S	2.18568500	-1.03539300	0.00010000
C	1.16333900	0.40281400	-0.00000700
C	-0.23399900	0.30074100	0.00002000
C	-1.45074400	0.18303900	0.00002900
C	-2.80518000	0.06778600	0.00003100
C	-4.01682400	-0.03650700	0.00014100
C	3.33823100	1.26548400	-0.00003000
C	1.94585300	1.54117500	0.00005000
H	1.51919500	2.53761200	0.00007500
H	4.10211400	2.03648500	-0.00006500
C	4.99643900	-0.71673300	-0.00014600
H	5.14970000	-1.34736300	-0.88433100
H	5.14942000	-1.34838300	0.88335200
H	5.77203400	0.05531100	0.00041700
Cl	-5.65503600	-0.17467800	-0.00008800

Cartesian coordinates of the optimized geometry for **29** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 1):

C	7.99102400	0.11437300	-0.07113600
S	6.55651500	-0.05279800	-1.03749500
C	5.55715200	-0.33308700	0.38353400
C	4.18684700	-0.56153500	0.27710100
C	2.96947900	-0.74087300	0.15840100
C	1.66015300	-0.99366100	0.04043500
C	0.40443200	-0.96837300	-0.05207700
C	7.70212200	-0.03929100	1.26666400
C	6.33594800	-0.29192300	1.53129300
H	5.91516200	-0.44125800	2.51815400
H	8.46336800	0.03011800	2.03575700
C	9.32428800	0.39232900	-0.69613200
H	9.32303600	1.33781600	-1.24862200
H	9.61767200	-0.39953800	-1.39327700
H	10.08555000	0.45641100	0.08565000
Cl	-0.89464800	-2.02523800	-0.23987700
H	-9.32303600	-1.33779800	1.24863200
H	-9.61768500	0.39955700	1.39324600
S	-6.55651800	0.05279900	1.03749000
C	-9.32429100	-0.39232400	0.69612000
C	-7.99102400	-0.11437100	0.07112800
H	-10.08554700	-0.45642900	-0.08566500
Cl	0.89464800	2.02523600	0.23988800
C	-0.40443200	0.96837000	0.05208600
C	-1.66015300	0.99365900	-0.04042800

C	-2.96947900	0.74087100	-0.15839700
C	-5.55715200	0.33308800	-0.38353600
C	-4.18684600	0.56153500	-0.27710000
C	-7.70211900	0.03929200	-1.26667200
C	-6.33594400	0.29192300	-1.53129700
H	-8.46336300	-0.03011800	-2.03576600
H	-5.91515500	0.44125700	-2.51815700

Cartesian coordinates of the optimized geometry for **29** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 1):

C	8.04275800	-0.11186900	0.07215800
S	6.60110500	0.05367500	1.03788000
C	5.59661100	0.30772400	-0.39608300
C	4.22584500	0.51862700	-0.29257300
C	3.01334100	0.70075800	-0.17396500
C	1.70098500	0.93792000	-0.05774800
C	0.45305400	0.96042500	0.03840000
C	7.75221100	0.02243200	-1.26623900
C	6.38303900	0.25797600	-1.53750000
H	5.96784500	0.38925200	-2.53000100
H	8.51321900	-0.04793700	-2.03682500
C	9.37734600	-0.36620600	0.70547900
H	9.38607600	-1.30245100	1.27685600
H	9.66290900	0.43923300	1.39309600
H	10.14770800	-0.43702800	-0.06845800
Cl	-0.80816500	2.06890700	0.21735900
H	-9.38605100	1.30246000	-1.27694000
H	-9.66288400	-0.43922500	-1.39318600
S	-6.60108600	-0.05367200	-1.03791600
C	-9.37733200	0.36621300	-0.70556300
C	-8.04275500	0.11187400	-0.07221900
H	-10.14770800	0.43703600	0.06836000
Cl	0.80816700	-2.06891400	-0.21726800
C	-0.45305500	-0.96043100	-0.03833200
C	-1.70098700	-0.93792500	0.05779700
C	-3.01334500	-0.70076100	0.17399200
C	-5.59661700	-0.30772200	0.39606500
C	-4.22585000	-0.51862800	0.29257900
C	-7.75223200	-0.02242600	1.26618300
C	-6.38306500	-0.25797300	1.53746800
H	-8.51325400	0.04794400	2.03675600
H	-5.96788900	-0.38924900	2.52997700

Cartesian coordinates of the optimized geometry for **32** at B2PLYPD/6-31G* level of theory (number of imaginary frequencies = 0):

C	8.14135300	-0.07192900	0.08159100
S	6.68916100	0.00134100	1.03746200
C	5.67703200	0.16614500	-0.40476900
C	4.30978800	0.28272600	-0.31863900
C	3.05760100	0.38008800	-0.20897800
C	1.77333800	0.50709200	-0.10826800
C	0.45146500	0.56939200	-0.00419800
C	7.85347400	0.02546500	-1.26376000
C	6.47922500	0.15952600	-1.54924700
H	6.05918600	0.24959800	-2.54363900
H	8.62697600	-0.00063300	-2.02361900
C	9.48629600	-0.22434800	0.72290200
H	9.55548000	-1.15173400	1.30152500
H	9.70748400	0.60685500	1.40097800
H	10.25809400	-0.24735000	-0.05086800
Cl	-0.33086900	2.14319200	0.15007700
H	-9.56085000	1.15312600	-1.28487200

H	-9.71175400	-0.60532900	-1.38844200
S	-6.69304100	-0.00159800	-1.03311000
C	-9.48907300	0.22427300	-0.70889900
C	-8.14197400	0.07136400	-0.07225600
H	-10.25842600	0.24463600	0.06737700
Cl	0.33109000	-2.14251100	-0.15993300
C	-0.45110400	-0.56871400	-0.00520100
C	-1.77292100	-0.50632100	0.09887600
C	-3.05704500	-0.37983700	0.20201100
C	-5.67596500	-0.16653600	0.40556100
C	-4.30899200	-0.28292800	0.31487600
C	-7.84942600	-0.02622600	1.27209200
C	-6.47421000	-0.16020800	1.55283100
H	-8.62031900	-0.00035900	2.03460700
H	-6.05071300	-0.25040500	2.54574800

Cartesian coordinates of the optimized geometry for **27** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 0):

C	0.58002400	-1.15129500	0.37222200
C	-0.80864000	-1.14461000	0.37012500
C	-1.53514800	0.00127100	-0.00238300
C	-0.80753200	1.14671400	-0.37398200
C	0.58116100	1.15262400	-0.37410100
C	1.30230600	0.00048500	-0.00042400
H	-1.34069300	2.03744700	-0.69314600
H	1.12385300	2.04406800	-0.67284800
C	-3.01758100	0.00121900	-0.00280600
C	2.72320700	0.00009100	0.00052600
C	3.94380900	-0.00027100	0.00131800
C	5.30522300	-0.00064300	0.00214600
C	6.52076900	-0.00093700	0.00288400
Cl	8.16544700	-0.00125600	0.00389400
H	-1.34285300	-2.03508000	0.68831200
H	1.12182100	-2.04305900	0.67163900
C	-3.74567100	1.14381900	0.36921800
C	-3.74487000	-1.14040700	-0.37948200
C	-5.13738800	-1.13678700	-0.38246800
C	-5.86257900	0.00158300	-0.00693600
C	-5.13817400	1.14144800	0.36554100
H	-3.21415700	-2.03078600	-0.70520100
H	-5.67138200	-2.03243000	-0.69244900
H	-5.67286200	2.04036800	0.66469600
H	-3.21571900	2.03699500	0.68846200
C	-7.37269100	-0.00765100	0.01979000
H	-7.75135400	-0.32637700	1.00040500
H	-7.78271200	-0.69774300	-0.72529900
H	-7.78388500	0.98802600	-0.17790300

Cartesian coordinates of the optimized geometry for **30** at UB3LYP/6-31G* (guess=mix) level of theory (number of imaginary frequencies = 1):

C	-4.20752100	0.58526600	0.35221100
C	-0.40514800	0.83370900	0.49933500
C	4.20712200	-0.58377100	-0.34772600
Cl	0.90465200	1.75203800	1.04594500
Cl	-0.90508400	-1.75066000	-1.04069500
C	5.61039700	-0.44920200	-0.26812600
C	6.33213000	-1.00586300	0.81176700
C	6.33006100	0.24540700	-1.26640900
C	7.71058100	-0.86956600	0.88405500
C	7.70860400	0.37344800	-1.18222000
C	8.43289700	-0.17883500	-0.10811200
H	8.24182900	0.88732700	-1.97657000

C	-5.61076300	0.45057400	0.27225900
C	-6.33233700	1.00766500	-0.80753900
C	-6.33055900	-0.24453700	1.27007700
C	-7.71072300	0.87114500	-0.88018300
C	-7.70908200	-0.37281000	1.18552700
C	-8.43316200	0.17966600	0.11140600
H	-8.24230400	-0.88698200	1.97966900
C	2.98466000	-0.69576700	-0.41384100
C	1.65581500	-0.85420400	-0.50764500
C	0.40472000	-0.83223600	-0.49424100
H	5.79100900	0.67001300	-2.10747100
C	-2.98507400	0.69729200	0.41857400
C	-1.65624600	0.85572800	0.51260600
H	-5.79164500	-0.66934800	2.11112300
C	9.90498100	-0.03798400	-0.02555600
C	-9.90506500	0.03818100	0.02672600
H	8.23883700	-1.28135700	1.73888900
H	5.79239600	-1.53350300	1.59185200
H	-5.79251600	1.53582400	-1.58721300
H	-8.23899700	1.28336800	-1.73481800
C	-10.55132400	-1.12845000	0.47007900
C	-11.93533100	-1.25762900	0.39083300
C	-12.73289500	-0.23180900	-0.13327800
H	-9.96140600	-1.95423800	0.85796300
H	-12.40483300	-2.17607900	0.73634200
C	-14.23086000	-0.38717600	-0.24612900
H	-14.74088100	0.57925900	-0.17302700
H	-14.62713700	-1.04003000	0.53886700
H	-14.51300300	-0.83090900	-1.21053600
C	10.55030300	1.13001800	-0.46682000
C	11.93394000	1.26131000	-0.38461800
C	12.73255500	0.23412900	0.13527300
C	12.08999800	-0.92949800	0.57822700
C	10.70657400	-1.06557800	0.50048600
H	9.95911100	1.95825400	-0.84748100
H	12.40199700	2.18369700	-0.72145800
H	12.68314800	-1.74588100	0.98449400
H	10.24398900	-1.99208200	0.82910100
C	-12.09014100	0.93378100	-0.57083900
C	-10.70634600	1.06774500	-0.49605900
H	-12.68365900	1.75459600	-0.96749600
H	-10.24387500	1.99716300	-0.81650500
C	14.23587100	0.36646500	0.19281200
H	14.70341400	-0.00668100	-0.72846700
H	14.65786500	-0.20683000	1.02511400
H	14.54222000	1.41129400	0.31090500

Cartesian coordinates of the optimized geometry for **33** at UB3LYP/6-31G* (guess=mix)level of theory (number of imaginary frequencies = 0):

C	4.36186800	-0.22203400	0.15827400
C	0.50407100	-0.42440200	0.31291000
C	-4.36199600	0.21721600	-0.16882600
Cl	-0.17537400	-1.74378800	1.31304300
Cl	0.17527100	1.73827200	-1.32519200
C	-5.75998400	0.16664600	-0.12948800
C	-6.48891800	0.87402900	0.86097900
C	-6.49029700	-0.59338700	-1.07907800
C	-7.87233400	0.81816300	0.89218600
C	-7.87371300	-0.63778800	-1.03254900
C	-8.60178600	0.06371200	-0.04965400
H	-8.40898300	-1.20418600	-1.78886200
C	5.75990500	-0.16972600	0.12293200
C	6.49268900	-0.87611600	-0.86539000
C	6.48640700	0.59132400	1.07463800

C	7.87611900	-0.81839800	-0.89254700
C	7.86989100	0.63757800	1.03215400
C	8.60179200	-0.06294900	0.05140700
H	8.40217400	1.20469000	1.79003800
C	-3.11404700	0.26293100	-0.20461600
C	-1.80912100	0.29473200	-0.22998600
C	-0.50421600	0.41885800	-0.32506600
H	-5.94997000	-1.13249200	-1.85072600
C	3.11391100	-0.26819400	0.19327800
C	1.80896200	-0.30028100	0.21768500
H	5.94309400	1.12969600	1.84469800
C	-10.08004500	0.00992600	-0.00720700
C	10.08011100	-0.00715900	0.01329200
H	-8.40401500	1.34587000	1.67844900
H	-5.94653700	1.45206500	1.60241300
H	5.95326600	-1.45489000	-1.60840600
H	8.41080100	-1.34539200	-1.67725300
C	10.77501800	1.16032000	0.37465000
C	12.16578300	1.20909700	0.33923100
C	12.92300800	0.09885500	-0.05750100
H	10.21940200	2.04867600	0.66168000
H	12.67326000	2.12988200	0.61842100
C	14.43024800	0.16479200	-0.12387000
H	14.83466500	0.86246900	0.61719000
H	14.77006000	0.50667900	-1.11090300
H	14.88273000	-0.81690200	0.05206300
C	-10.77759600	-1.15653400	-0.36678600
C	-12.16830700	-1.20342700	-0.32730400
C	-12.92285700	-0.09221900	0.07184800
C	-12.22920100	1.07270400	0.42558300
C	-10.83849700	1.12491300	0.39033000
H	-10.22402200	-2.04557800	-0.65562200
H	-12.67785100	-2.12347300	-0.60517100
H	-12.78753500	1.95731600	0.72392700
H	-10.33517300	2.05427900	0.64177200
C	12.23197200	-1.06709500	-0.41301400
C	10.84125300	-1.12118700	-0.38182500
H	12.79237800	-1.95101100	-0.70953800
H	10.33994600	-2.05130200	-0.63452900
C	-14.42999100	-0.15617400	0.14259800
H	-14.83769700	-0.85088600	-0.59946000
H	-14.88156900	0.82672800	-0.02879500
H	-14.76729300	-0.50079200	1.12954300

3. Kinetic Studies

Dimerization of 14b. Chlorodiacetylene **14b** (29.0 mg, 0.166 mmol) and maleic anhydride (118.4 mg, 1.21 mmol) were solved in 1,2-dichlorobenzene (5 mL) containing 30% $C_6D_4Cl_2$. As internal standard cyclodecane (4.5 mM) was used. The reaction mixture was heated to 70-90 °C for 11-13 h. The decrease in the concentration of **14b** was monitored by NMR spectroscopy.

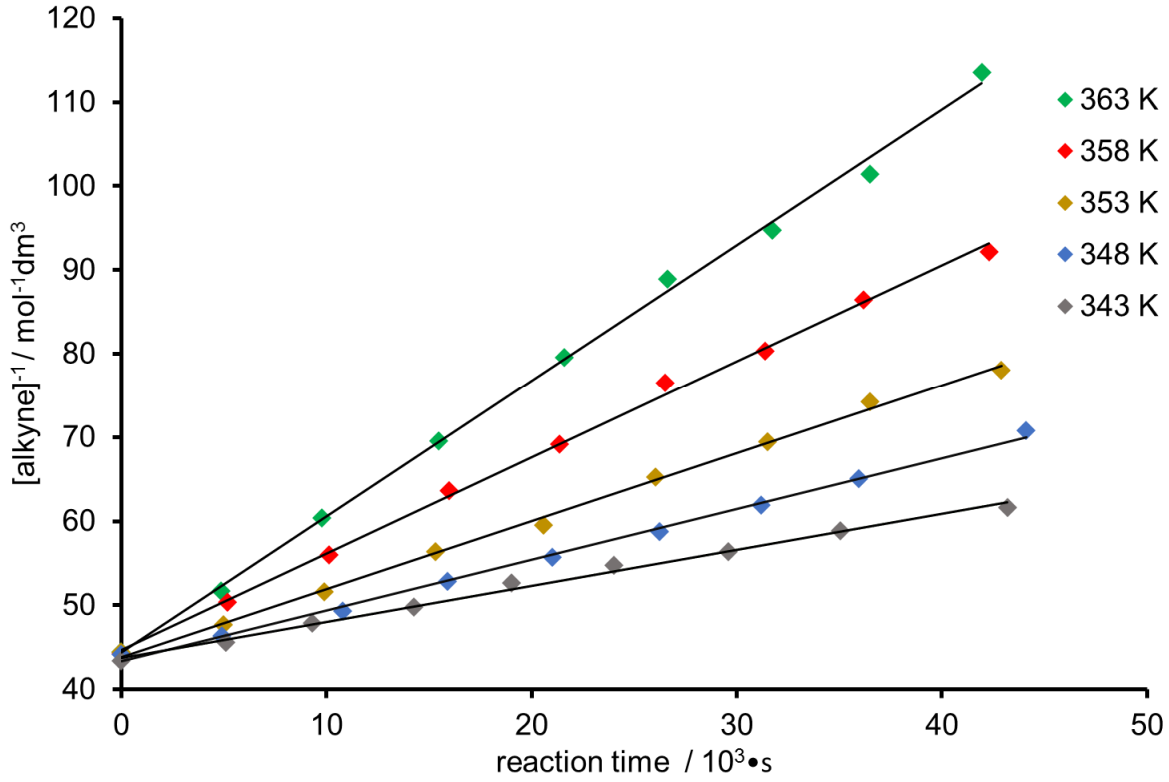


Figure S2. Plot of the reciprocal concentration of **14b** as a function of the reaction time ([**14b**] = 33.2 mM). The dimerization was performed in 1,2-dichlorobenzene as solvent. As internal standard cyclodecane (4.5 mM) was used.

Dimerization of 14d. Chlorodiacetylene **14d** (24.1 mg, 0.126 mmol) and maleic anhydride (114.4 mg, 1.167 mmol) were solved in 1,2-dichlorobenzene (5 mL) containing 30% $C_6D_4Cl_2$. As internal standard cyclodecane (4.4 mM) was used. The reaction mixture was heated to 65-85 °C for 10-13 h. The decrease in the concentration of **14d** was monitored by NMR spectroscopy.

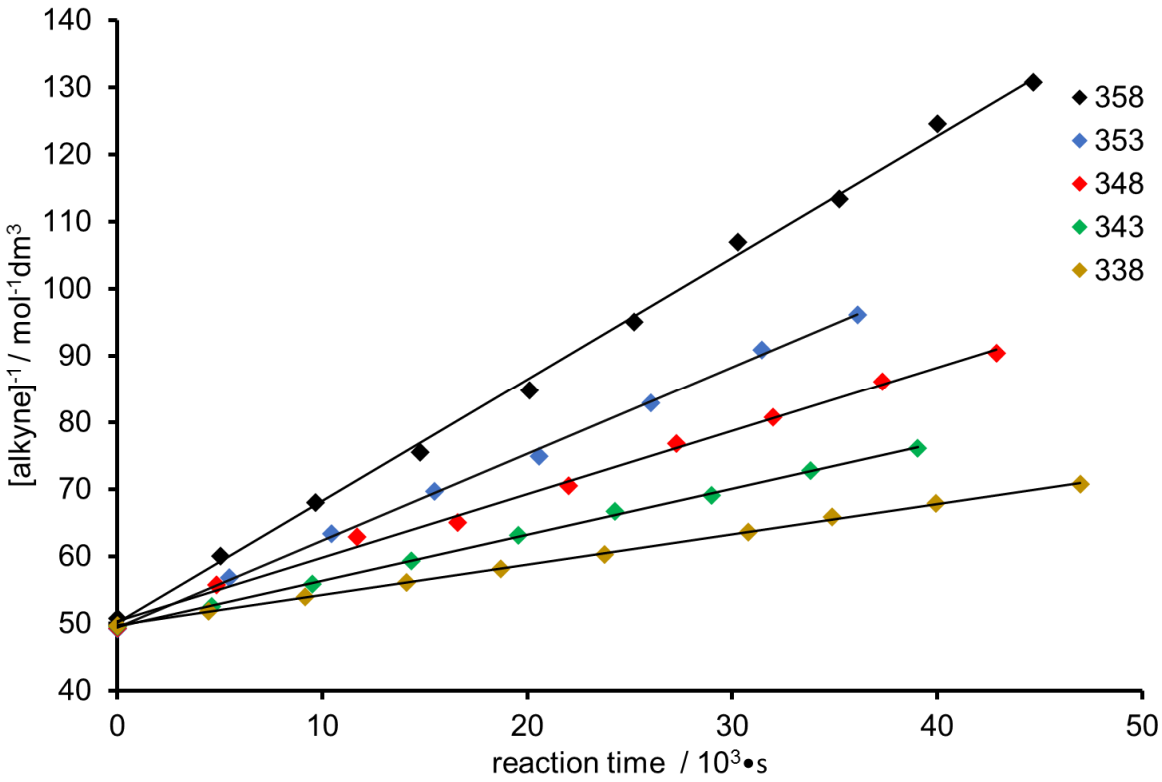


Figure S3. Plot of the reciprocal concentration of **14d** as a function of the reaction time ([**14d**] = 25.3 mM). The dimerization was performed in 1,2-dichlorobenzene as solvent. As internal standard cyclodecane (4.4 mM) was used.

Dimerization of 25. Chlorodiacetylene **25** (35.1 mg, 1.42 mmol) and maleic anhydride (109.8 mg, 1.119 mmol) were solved in 1,2-dichlorobenzene (5 mL) containing 30% $C_6D_4Cl_2$. As internal standard cyclodecane (4.5 mM) was used. The reaction mixture was heated to 70-90 °C for 11-13 h. The decrease in the concentration of **25** was monitored by NMR spectroscopy.

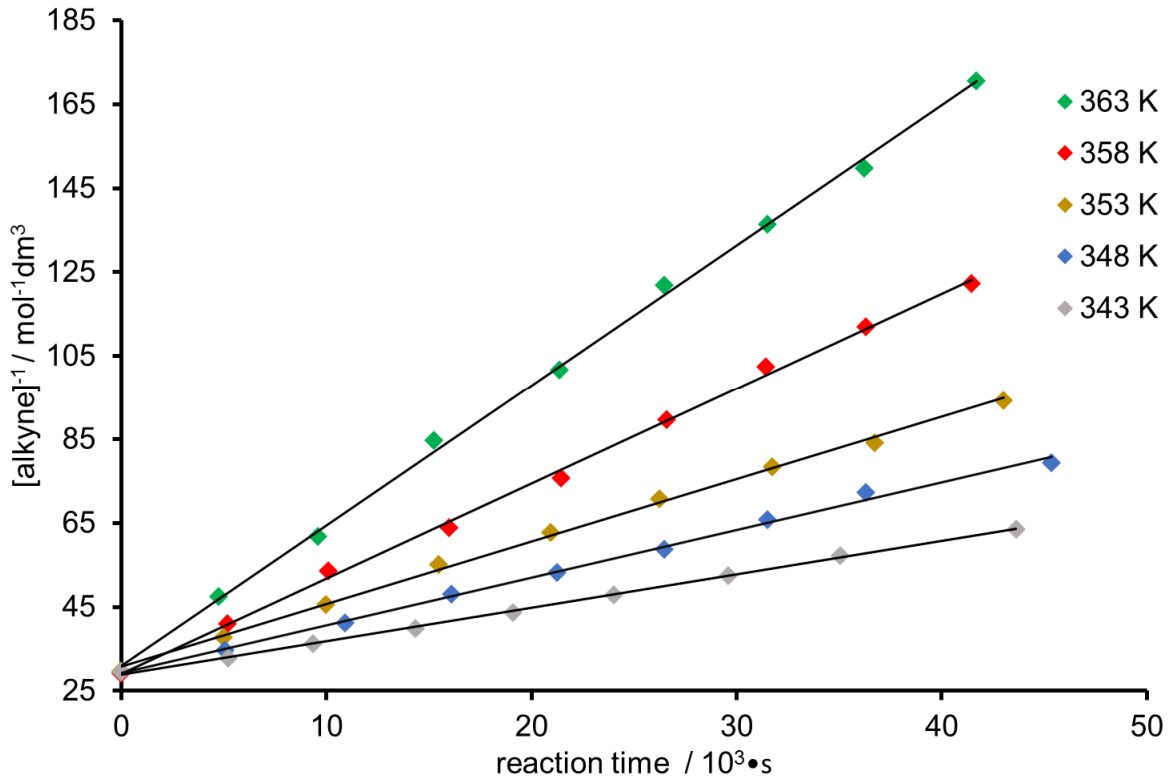


Figure S4. Plot of the reciprocal concentration of **25** as a function of the reaction time ([**25**] =28.4 mM). The dimerization was performed in 1,2-dichlorobenzene as solvent. As internal standard cyclodecane (4.5 mM) was used.

Dimerization of 26. Chlorodiacetylene **26** (33.2 mg, 0.184 mmol) and maleic anhydride (115.8 mg, 1.181 mmol) were solved in 1,2-dichlorobenzene (5 mL) containing 30% $C_6D_4Cl_2$. As internal standard cyclodecane (4.4 mM) was used. The reaction mixture was heated to 60-80 °C for 10-13 h. The decrease in the concentration of **26** was monitored by NMR spectroscopy.

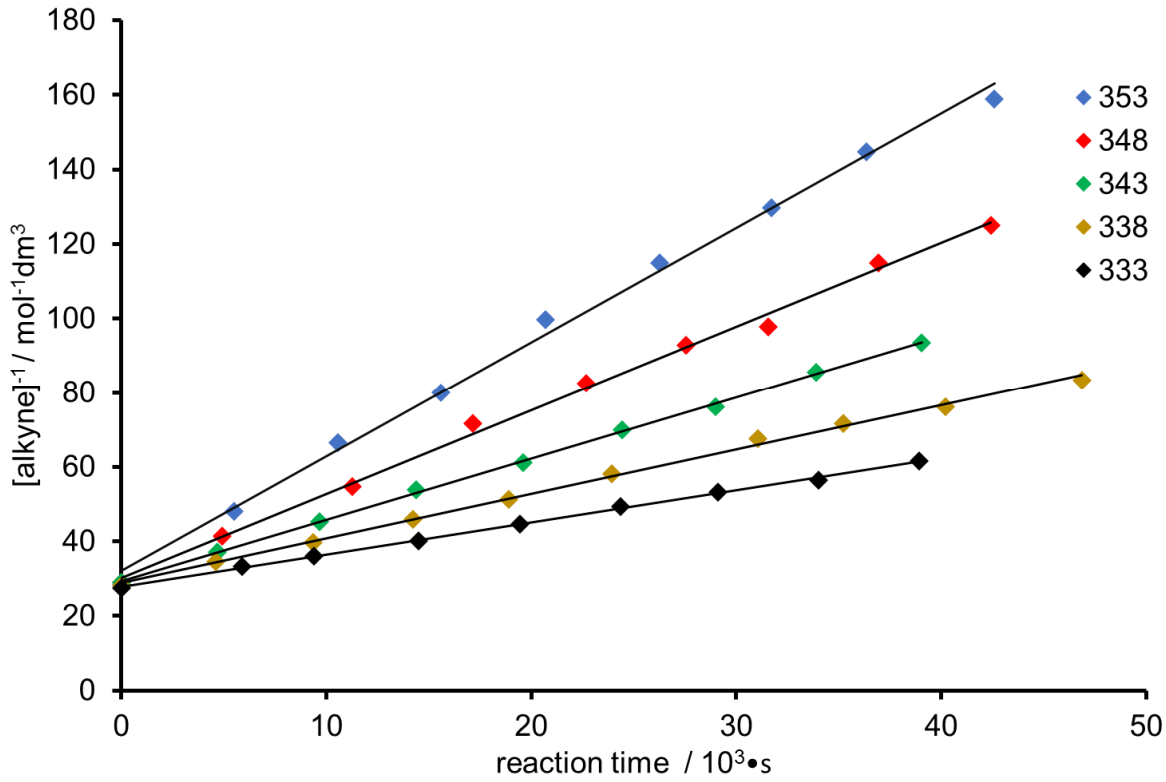


Figure S5. Plot of the reciprocal concentration of **26** as a function of the reaction time ([**26**] = 36.8 mM). The dimerization was performed in 1,2-dichlorobenzene as solvent. As internal standard cyclodecane (4.4 mM) was used.

Dimerization of 27. Chlorodiacetylene **27** (38.1 mg, 0.152 mmol) and maleic anhydride (109.7 mg, 1.118 mmol) were solved in 1,2-dichlorobenzene (5 mL) containing 30% $C_6D_4Cl_2$. As internal standard cyclodecane (4.5 mM) was used. The reaction mixture was heated to 70-90 °C for 11-13 h. The decrease in the concentration of **27** was monitored by NMR spectroscopy.

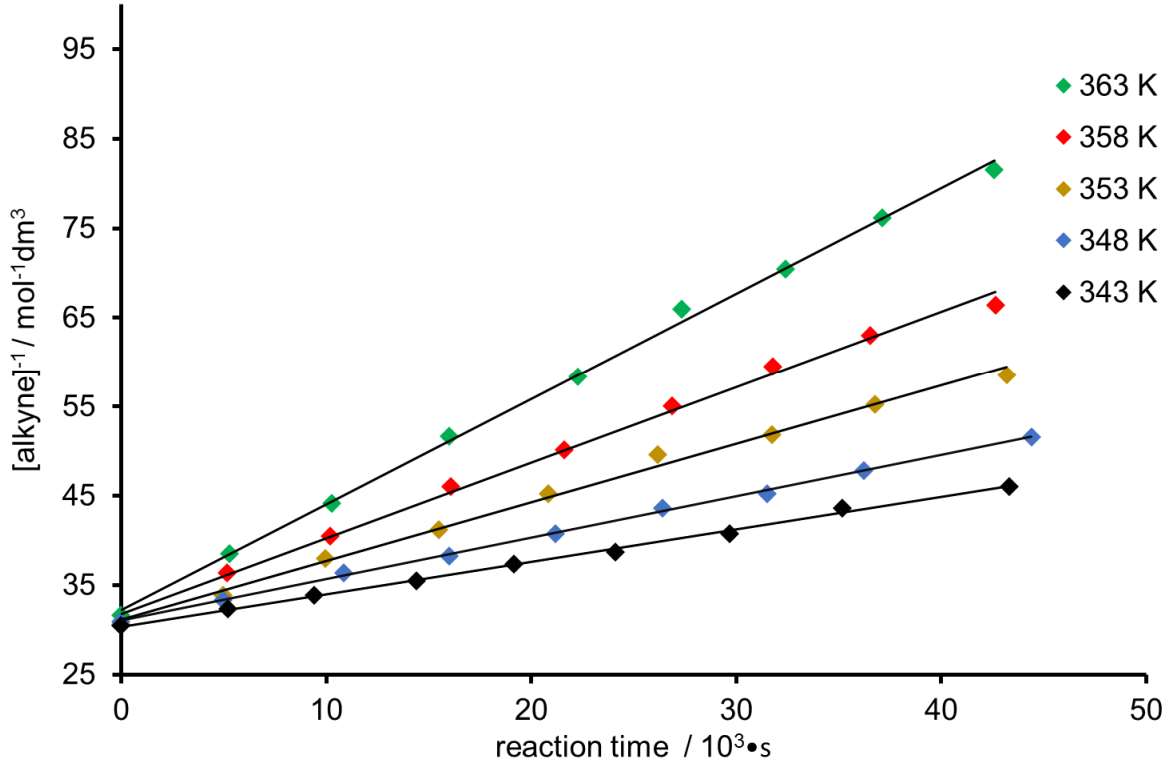
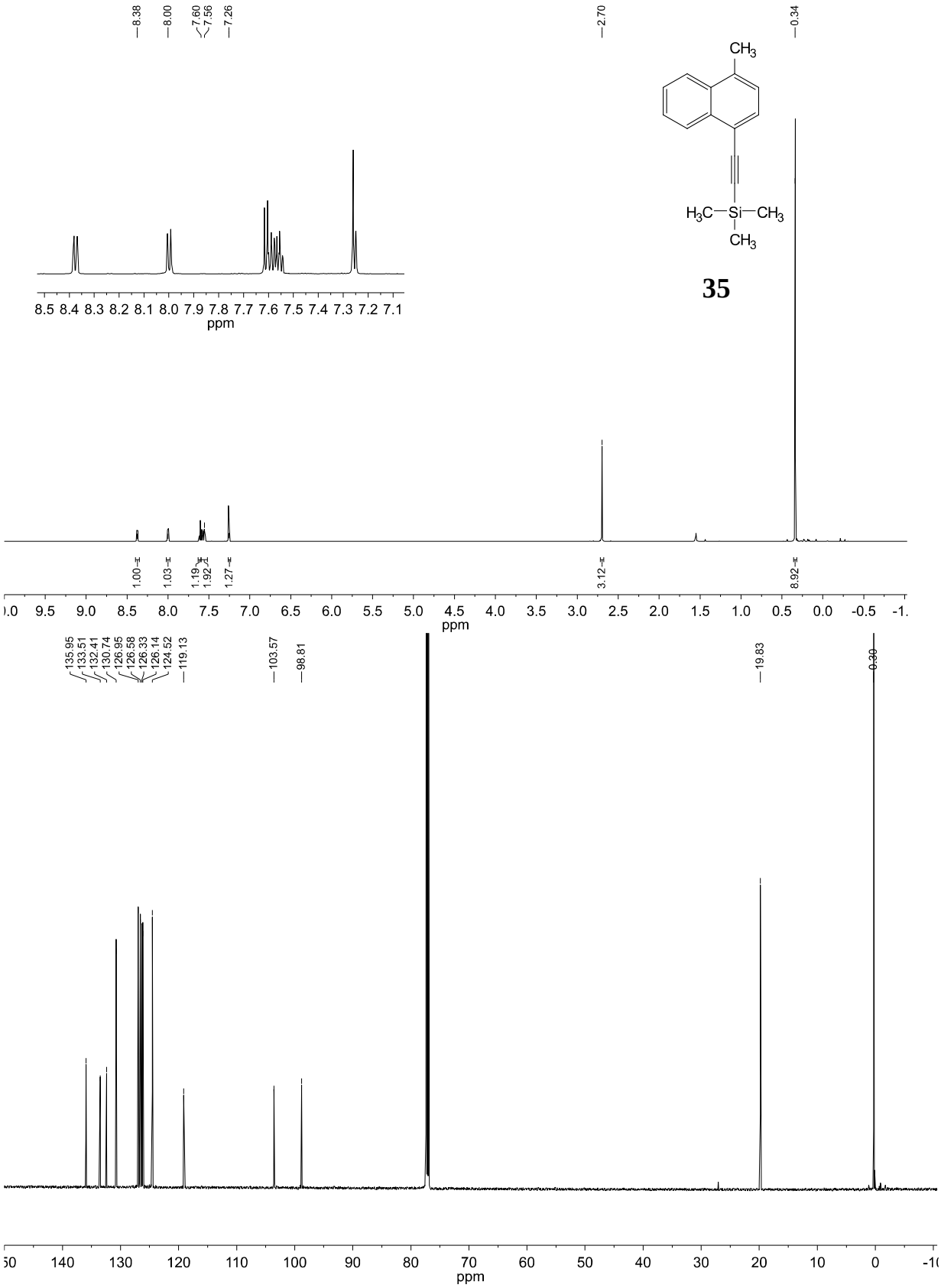


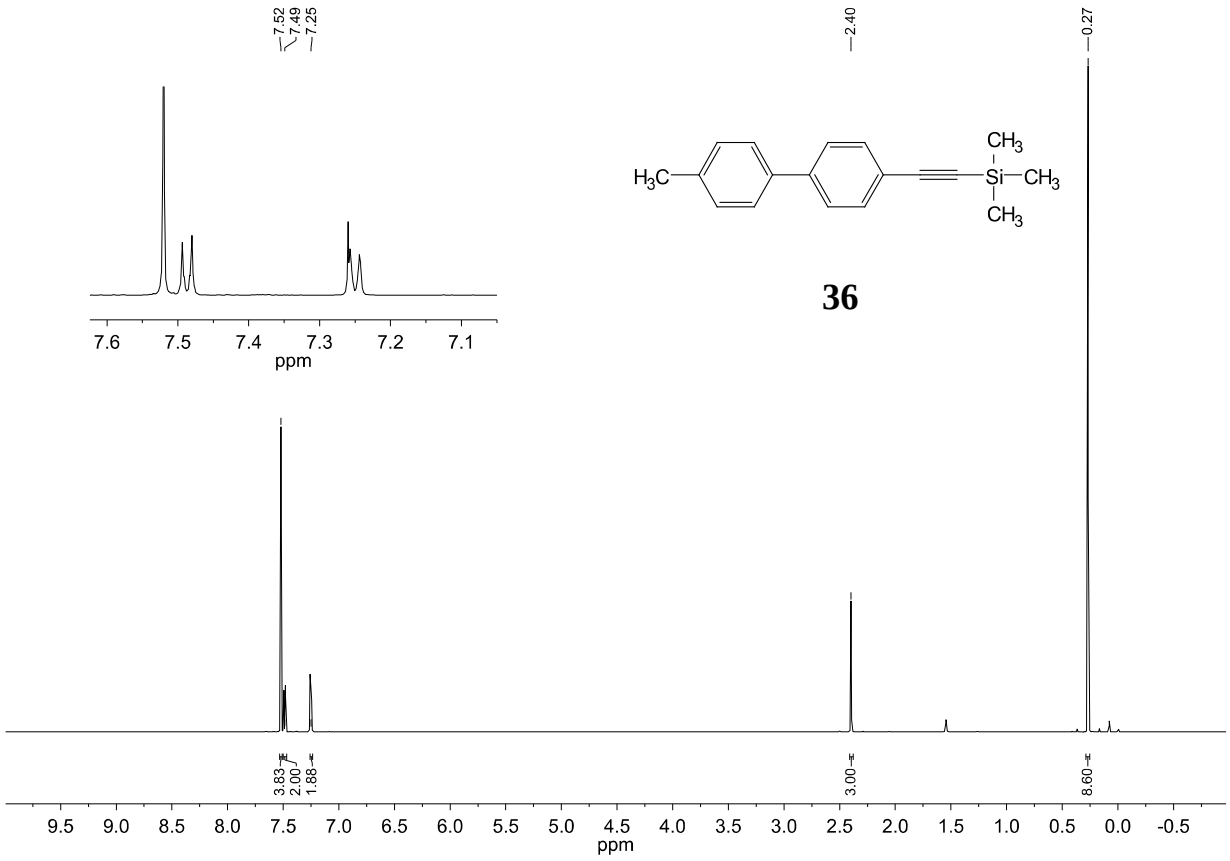
Figure S6. Plot of the reciprocal concentration of **27** as a function of the reaction time ([**27**] =30.4 mM). The dimerization was performed in 1,2-dichlorobenzene as solvent. As internal standard cyclodecane (4.5 mM) was used.

Table S3. Reaction rates (k_{obs}) for the dimerization of the chloroacetylenes**14b**, **14d**, and **25**-**27**.

Compd.	Temp. [K]	k_{obs} [$s^{-1}M^{-1}$]	*R*
14b	343	4.29×10^{-4}	0.997
	348	6.05×10^{-4}	0.998
	353	8.09×10^{-4}	0.999
	358	1.15×10^{-3}	0.999
	363	1.62×10^{-3}	0.999
14d	338	4.52×10^{-4}	0.999
	343	6.86×10^{-4}	0.999
	348	9.47×10^{-4}	0.998
	353	1.30×10^{-3}	0.999
	358	1.82×10^{-3}	0.999
25	343	7.96×10^{-4}	0.999
	348	1.14×10^{-3}	0.998
	353	1.49×10^{-3}	0.999
	358	2.27×10^{-3}	0.999
	363	3.35×10^{-3}	0.999
26	333	8.62×10^{-4}	0.999
	338	1.19×10^{-3}	0.999
	343	1.65×10^{-3}	0.999
	348	2.25×10^{-3}	0.998
	353	3.08×10^{-3}	0.998
27	343	3.62×10^{-4}	0.999
	348	4.63×10^{-4}	0.999
	353	6.56×10^{-4}	0.998
	358	8.47×10^{-4}	0.998
	363	1.18×10^{-3}	0.999

4. ^{1}H NMR and ^{13}C NMR Spectra of the New Compounds

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7.6
7.5
7.4
7.3
7.2
7.1
ppm
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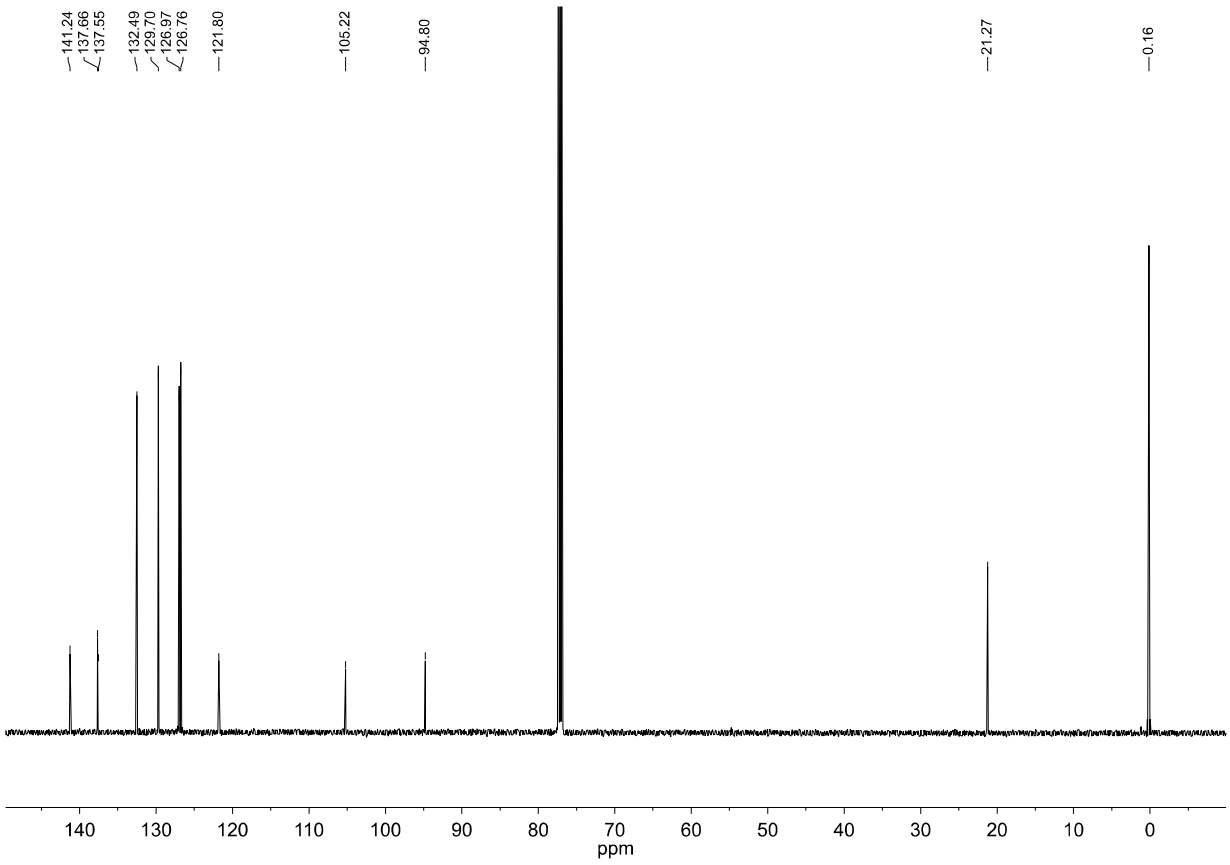
2.00
1.88
3.00
8.60
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm

H3C
CH3
Si
CH3
CH3

36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137.55
132.49
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126.97
126.76
121.80
105.22
94.80
21.27
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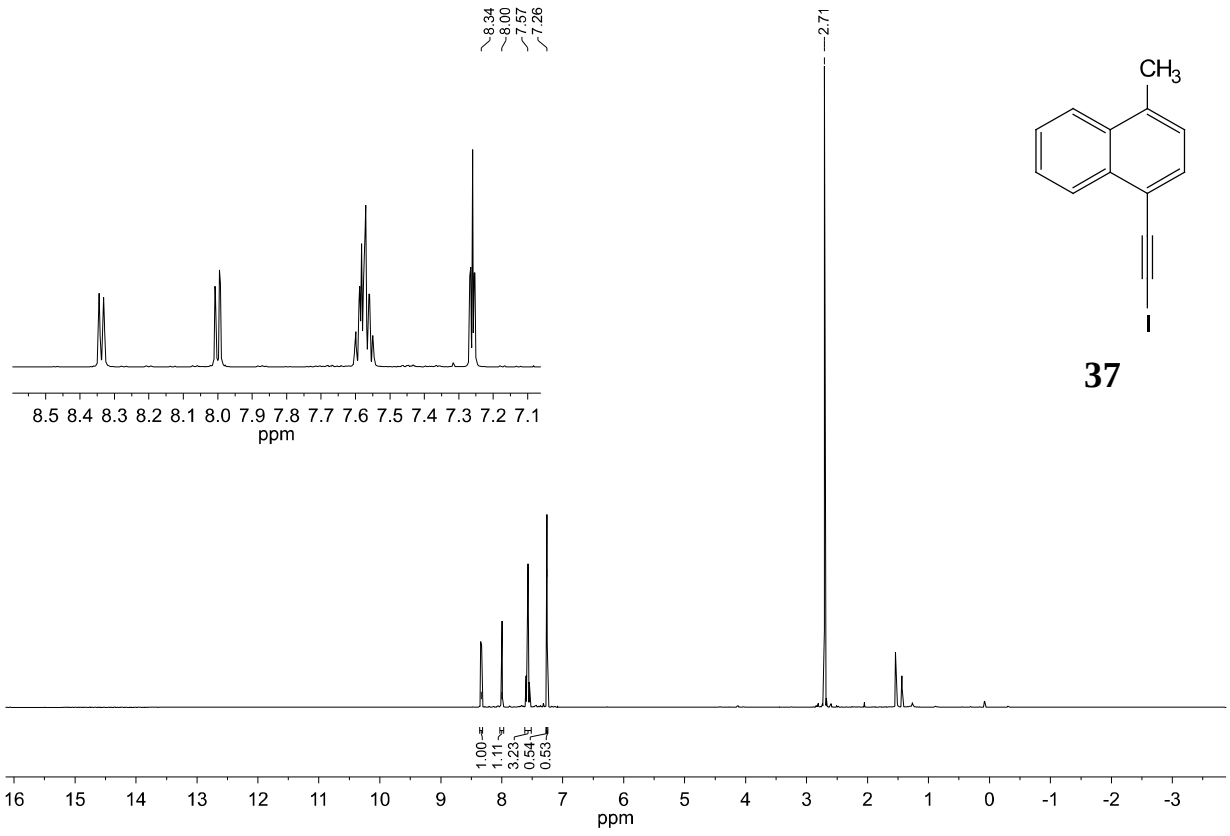
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.00
7.57
7.26
2.71
CH3
I
37
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ppm
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1.11
3.23
0.54
0.53
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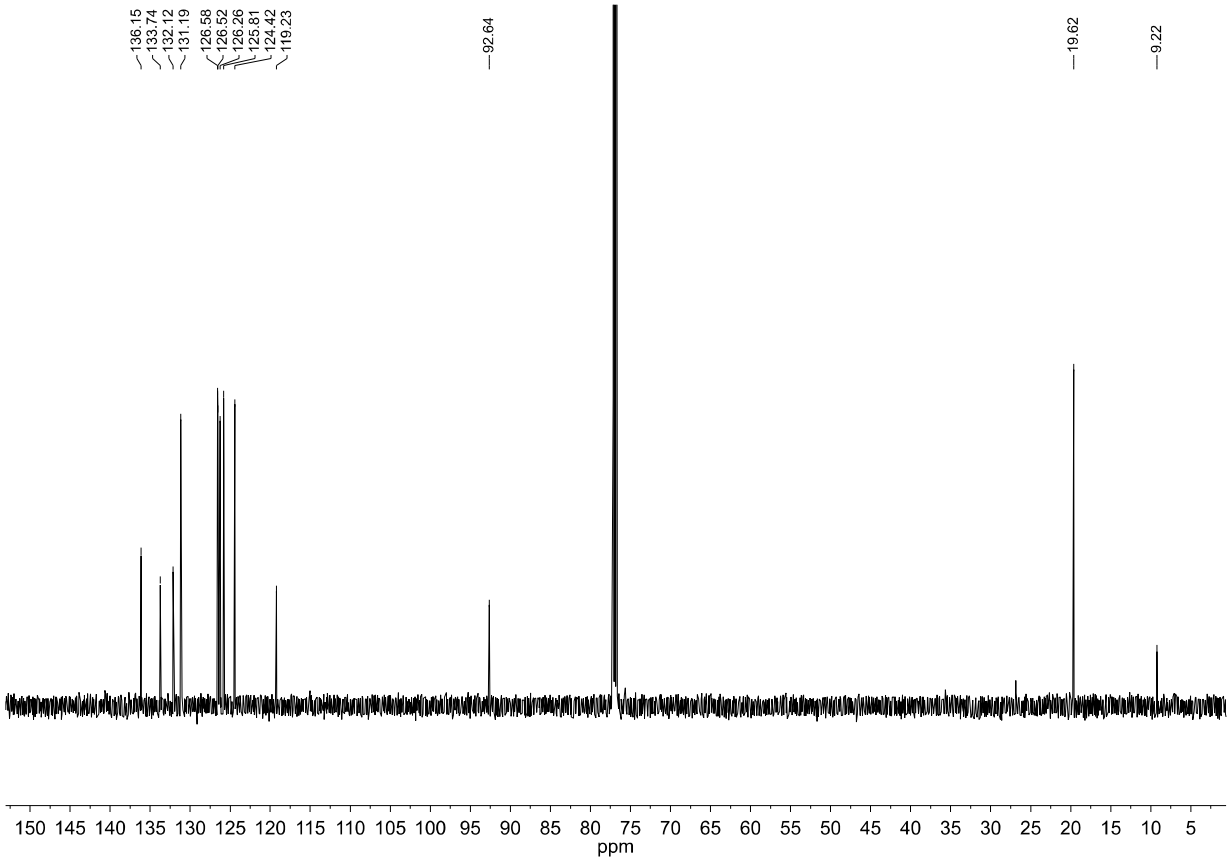
ppm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133.74
132.12
131.19
126.58
126.52
126.26
125.81
124.42
119.23
92.64
19.62
9.22
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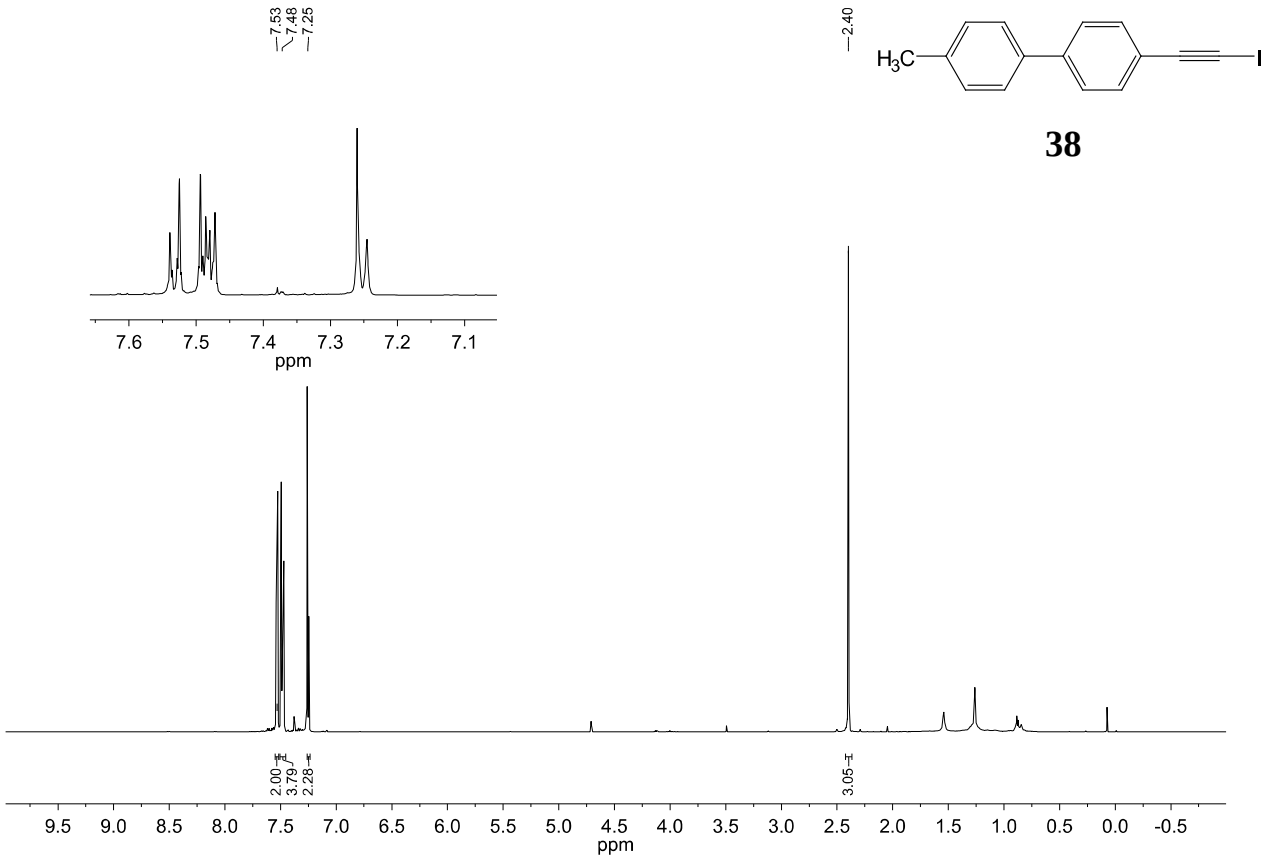
ppm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7.48
7.25
2.40
H3C
I
38
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7.5
7.4
7.3
7.2
7.1
ppm
2.00
3.79
2.28
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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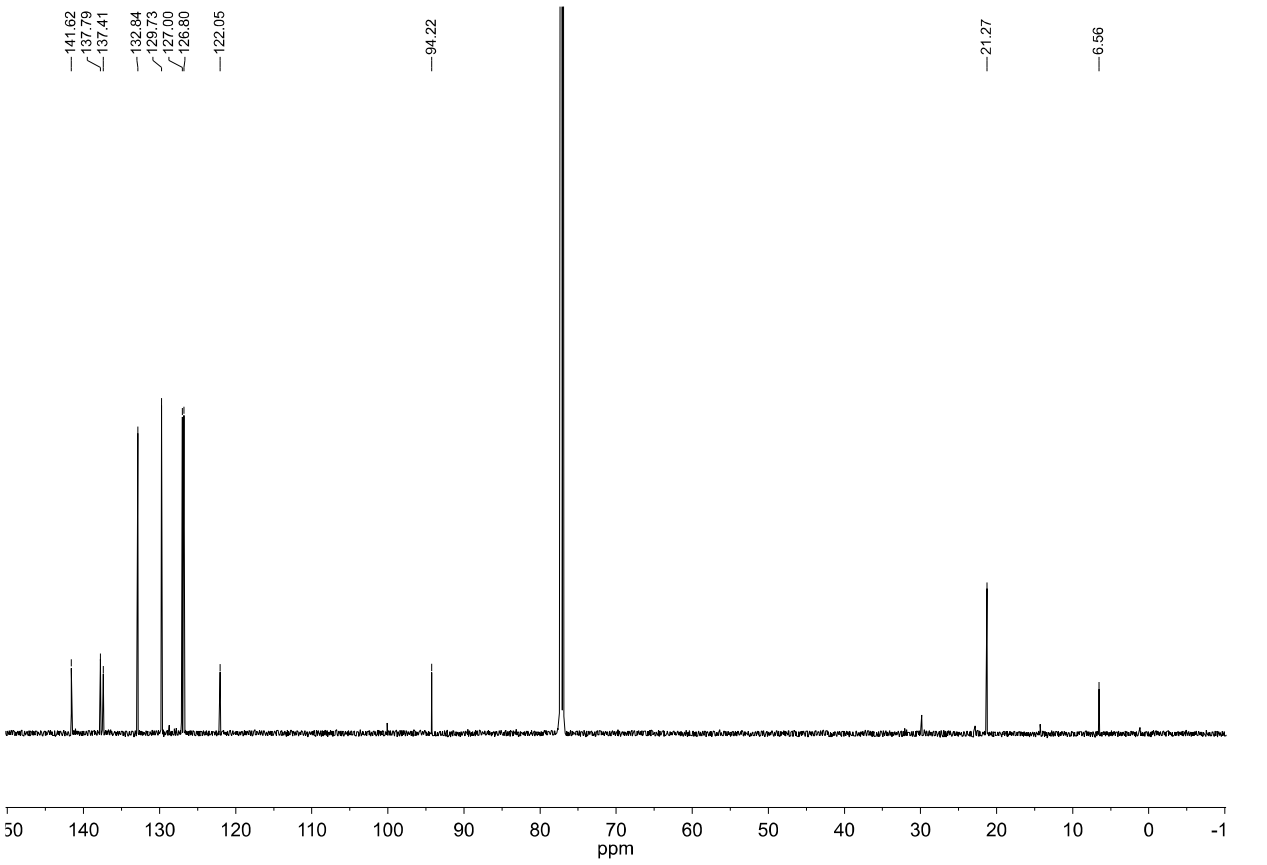
0.0
-0.5
ppm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122.05
94.22
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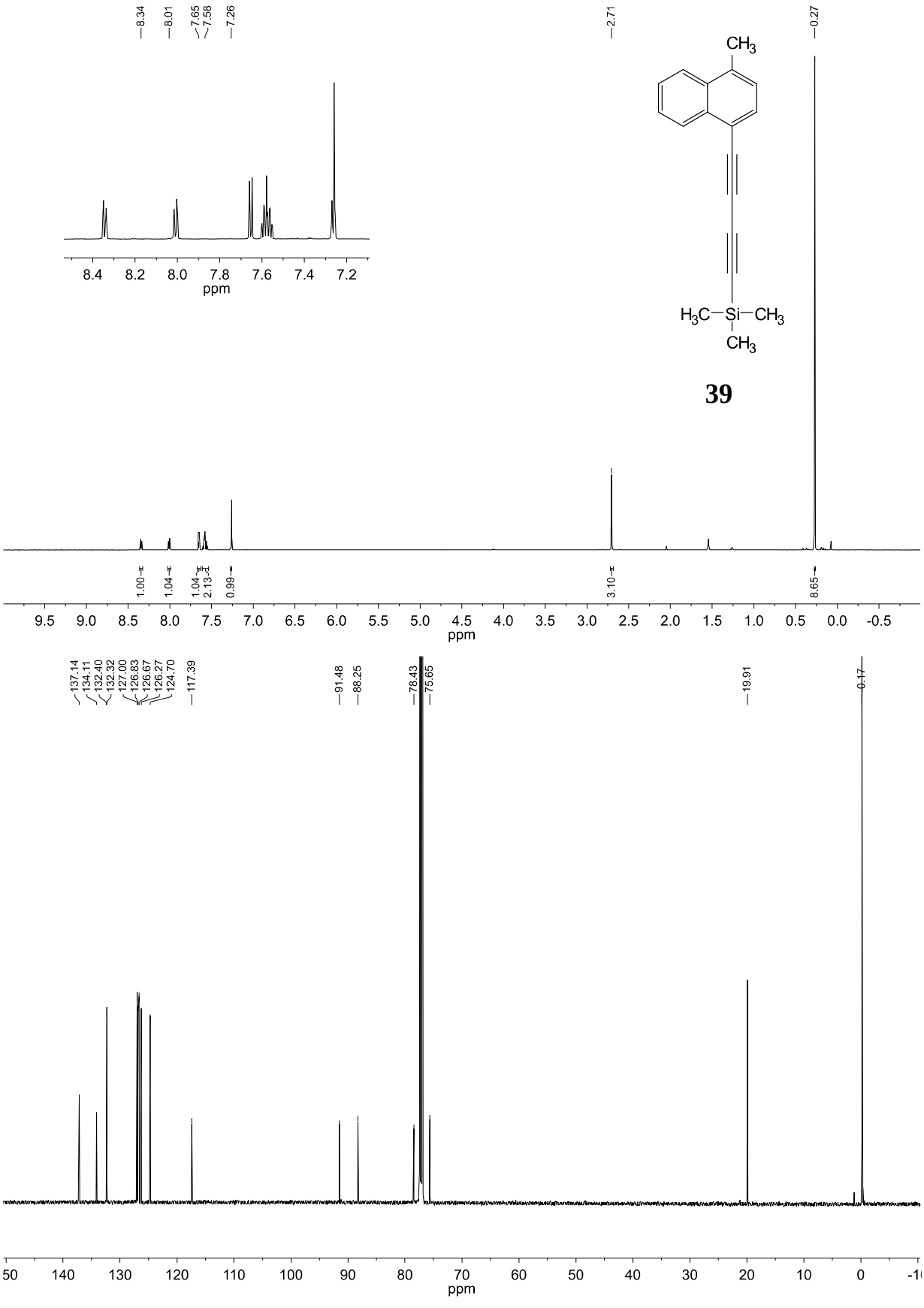
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
ppm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7.58
7.26
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H3C—Si—CH3
CH3
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1.04
1.04
2.13
0.99
3.10
8.65
ppm
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134.11
132.40
132.32
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126.27
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19.91
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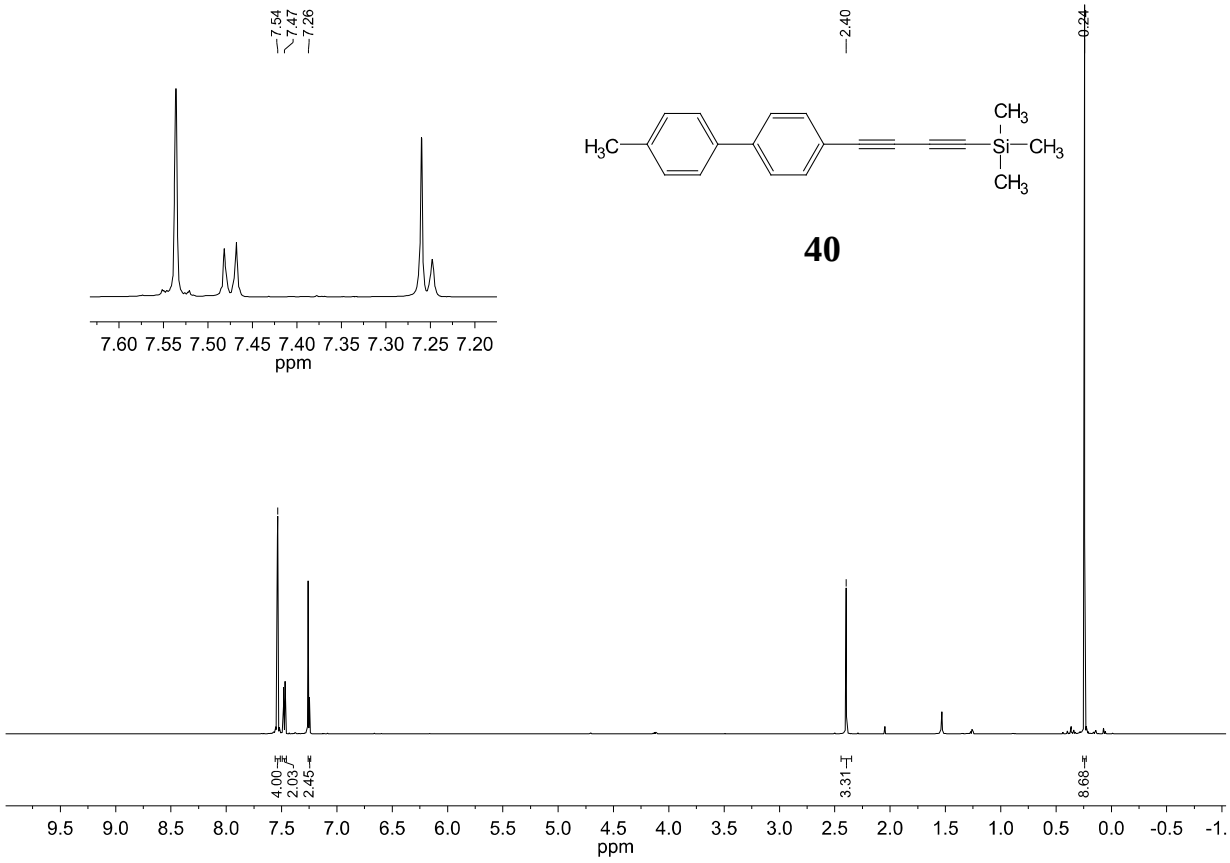
ppm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7.26
2.40
0.24
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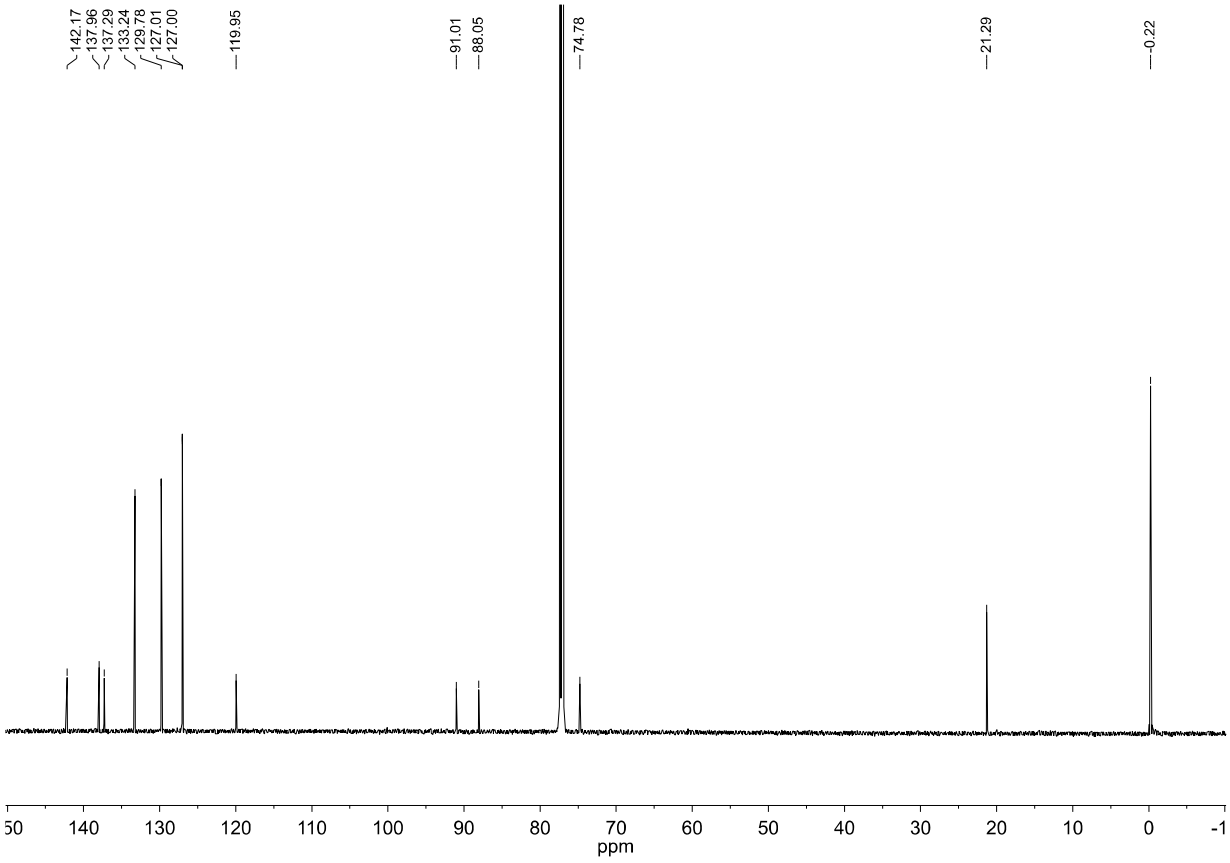
ppm
H3C
CH3
Si
CH3
CH3
40
4.00
2.03
2.45
3.31
8.68
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
ppm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133.24
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127.00
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74.78
21.29
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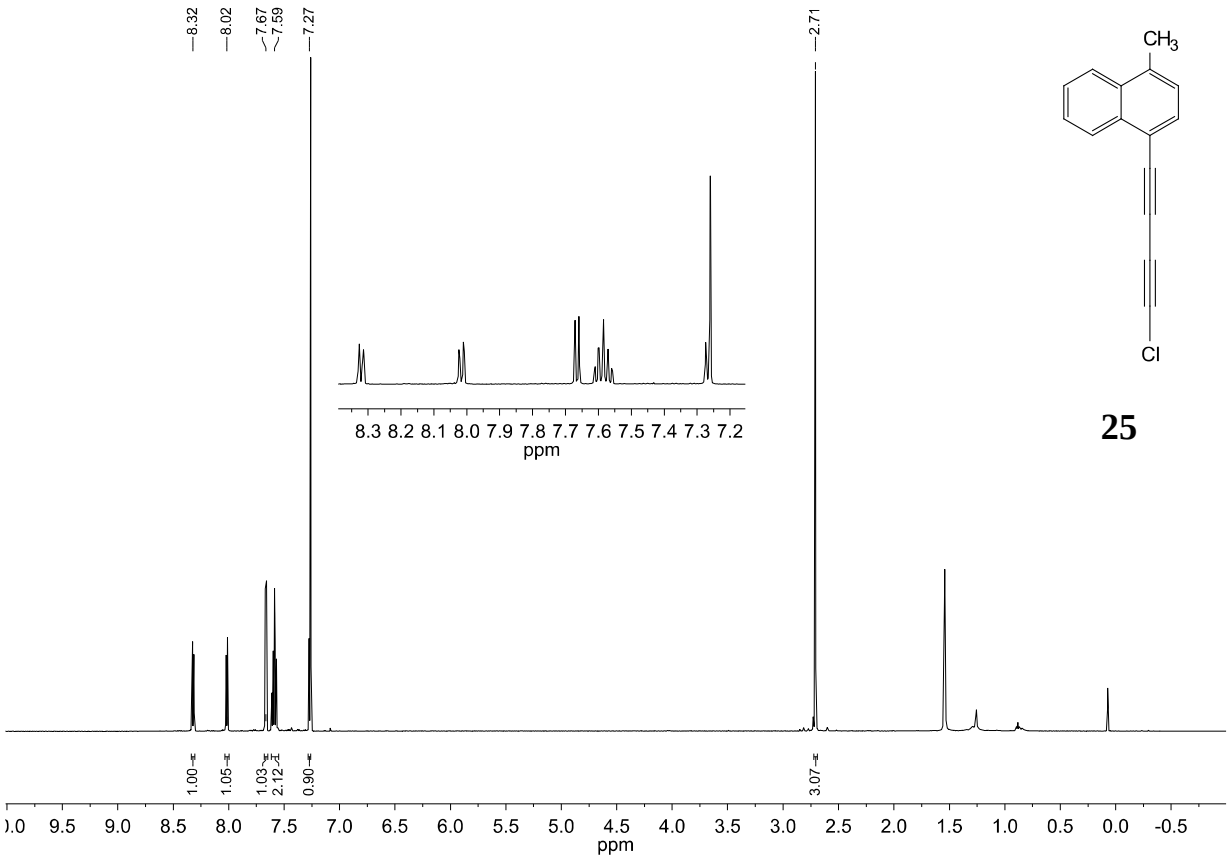
ppm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7.27
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1.00
1.05
1.03
2.12
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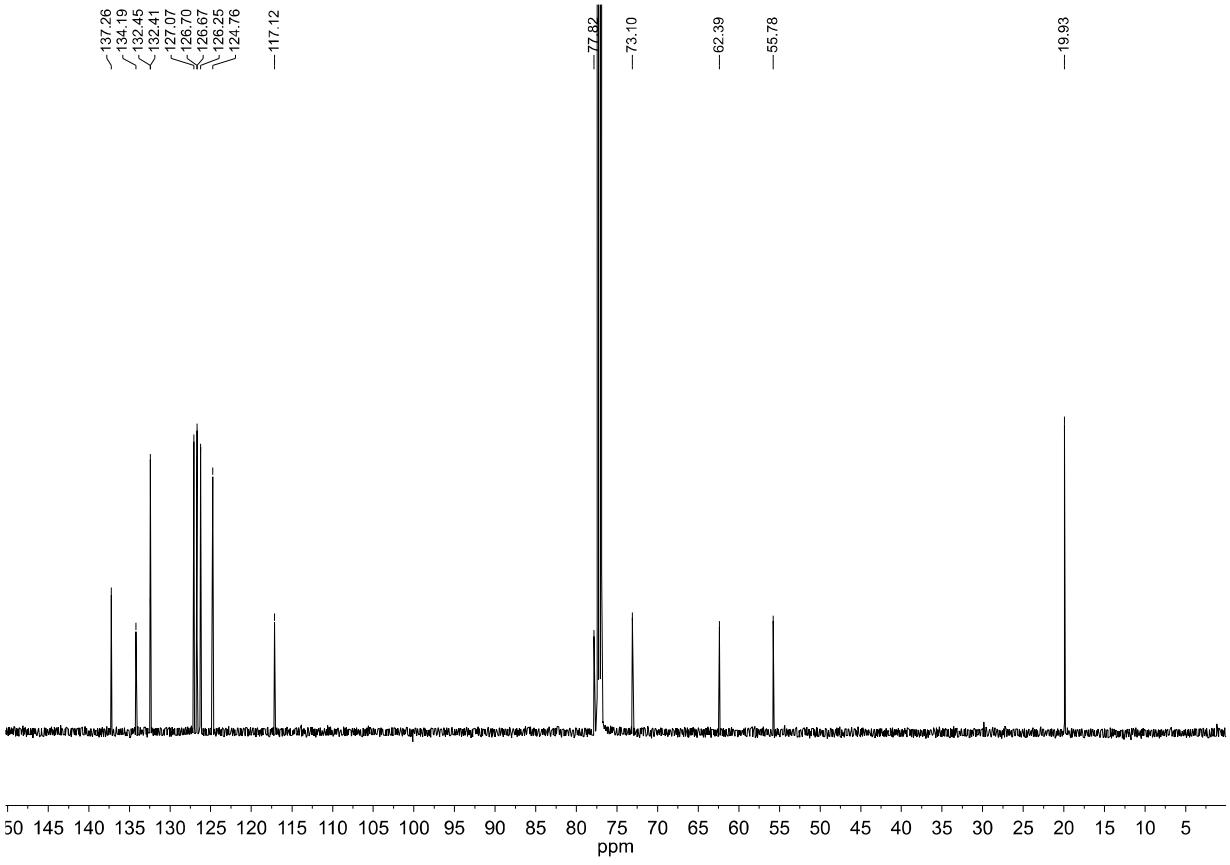
ppm
ppm
CH3
Cl

25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19.93
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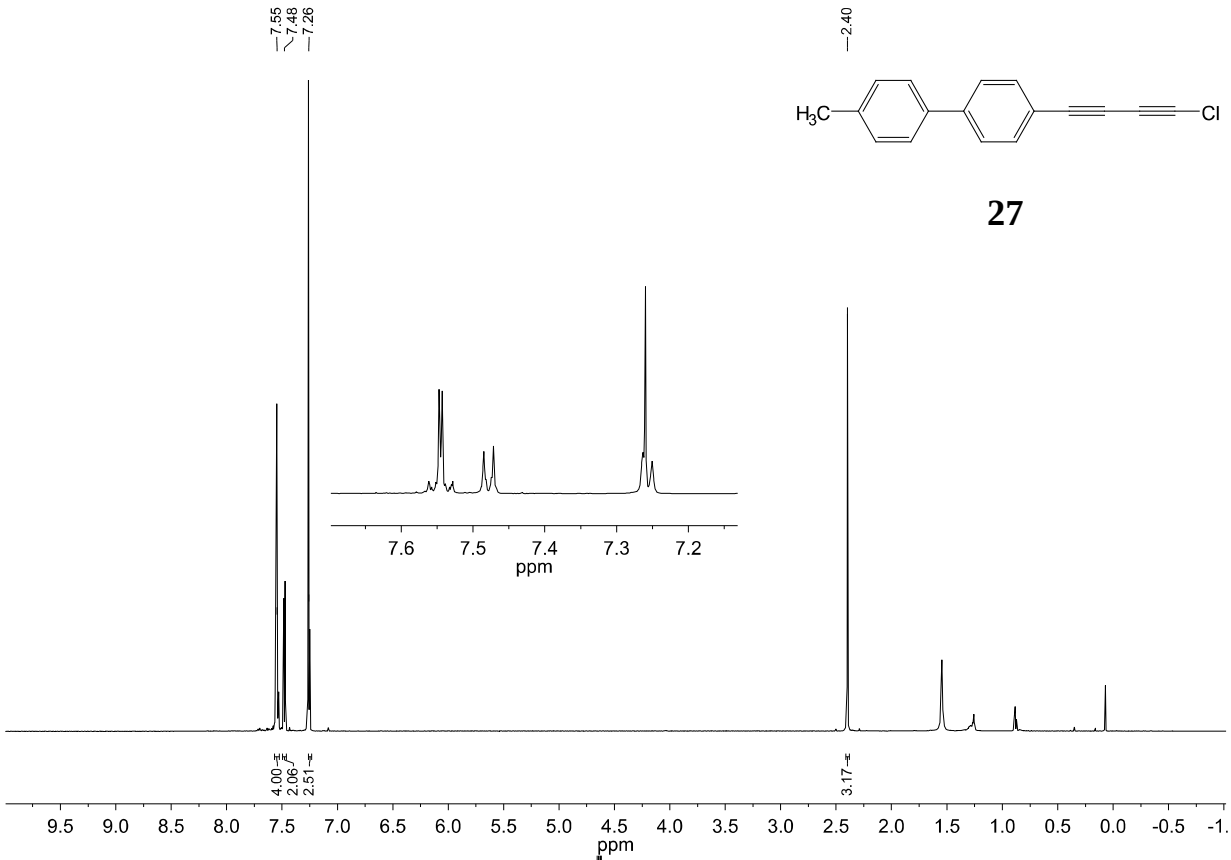
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H3C
Cl
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7.5
7.4
7.3
7.2
ppm
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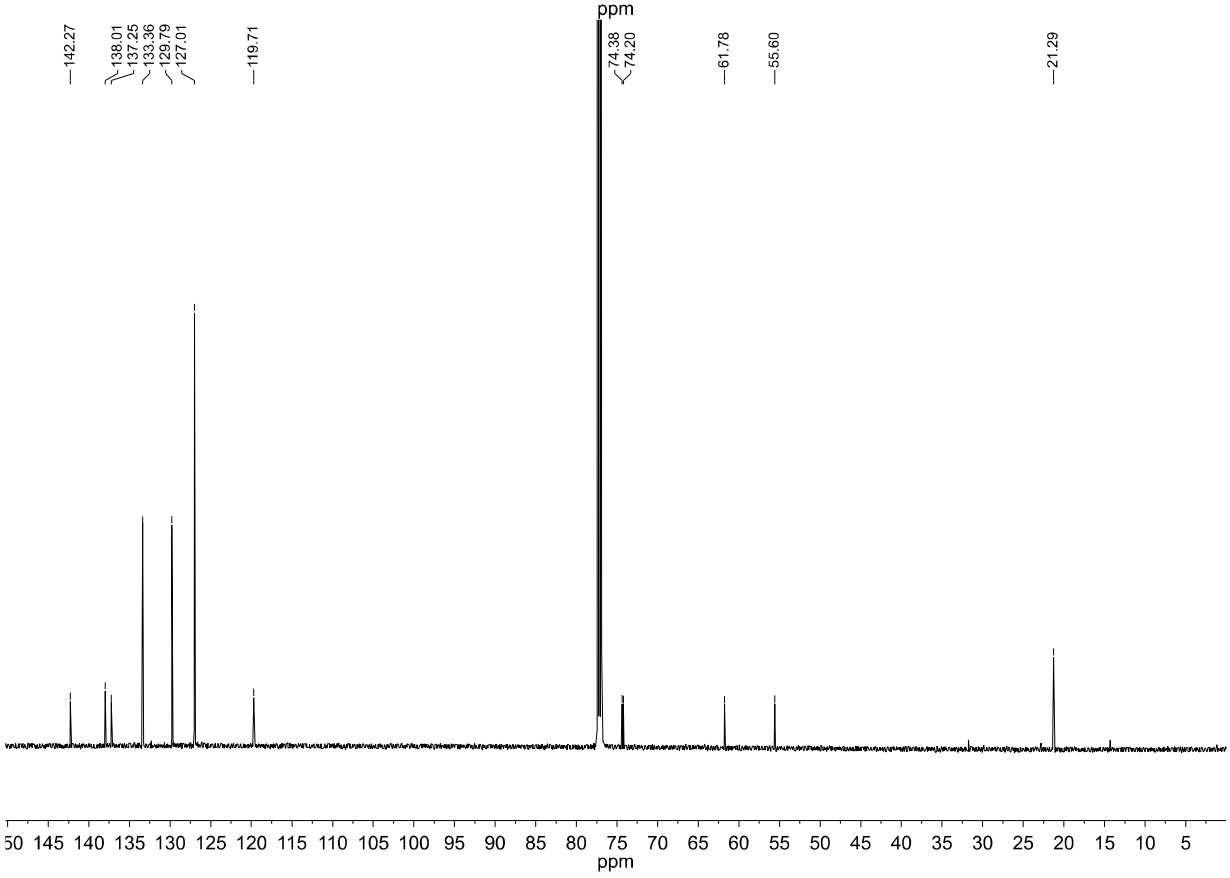
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

27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127.01
119.71
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74.20
61.78
55.60
21.29
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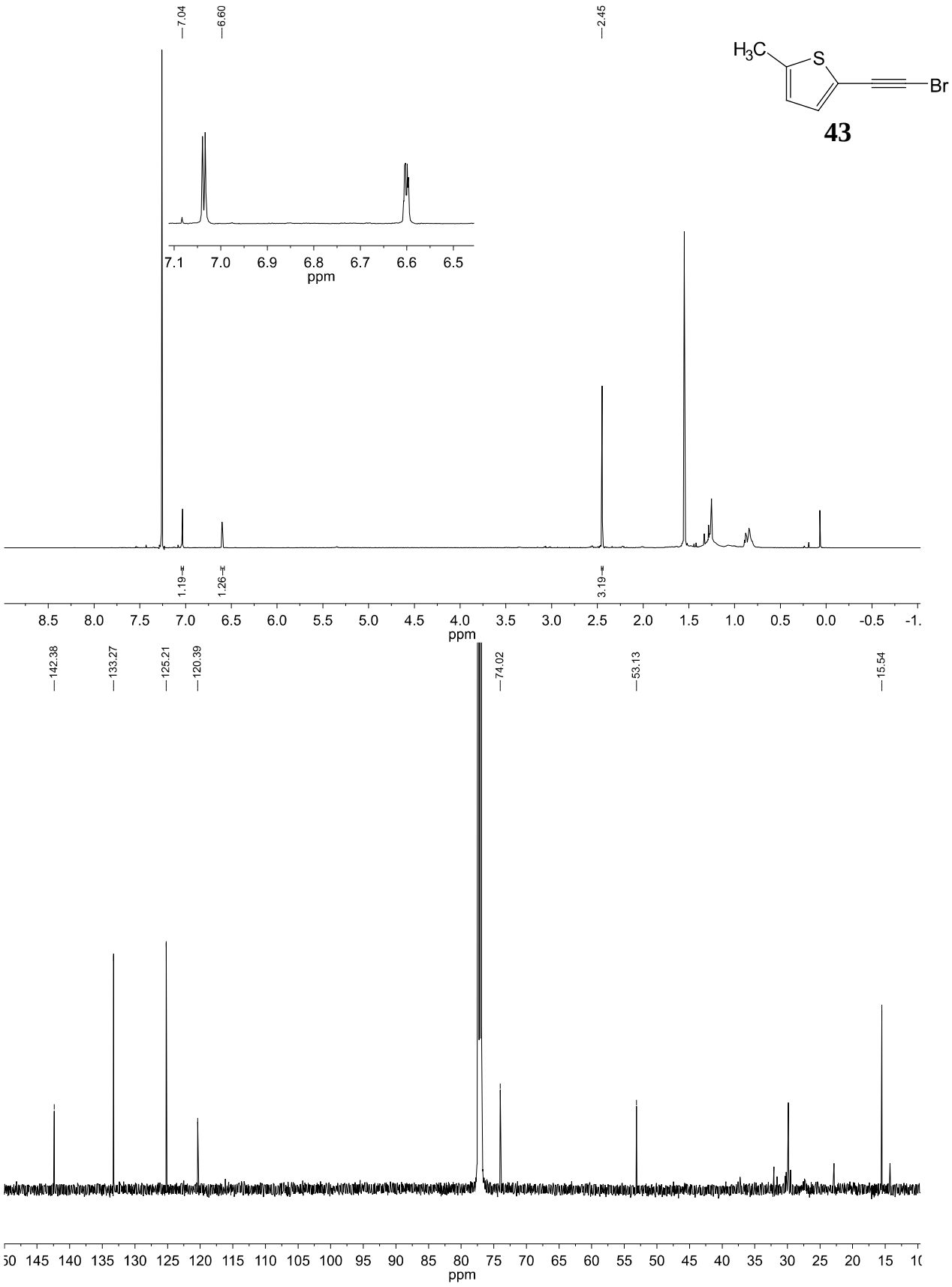
ppm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H3C
S
Br
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3.19
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm
142.38
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74.02
53.13
15.54
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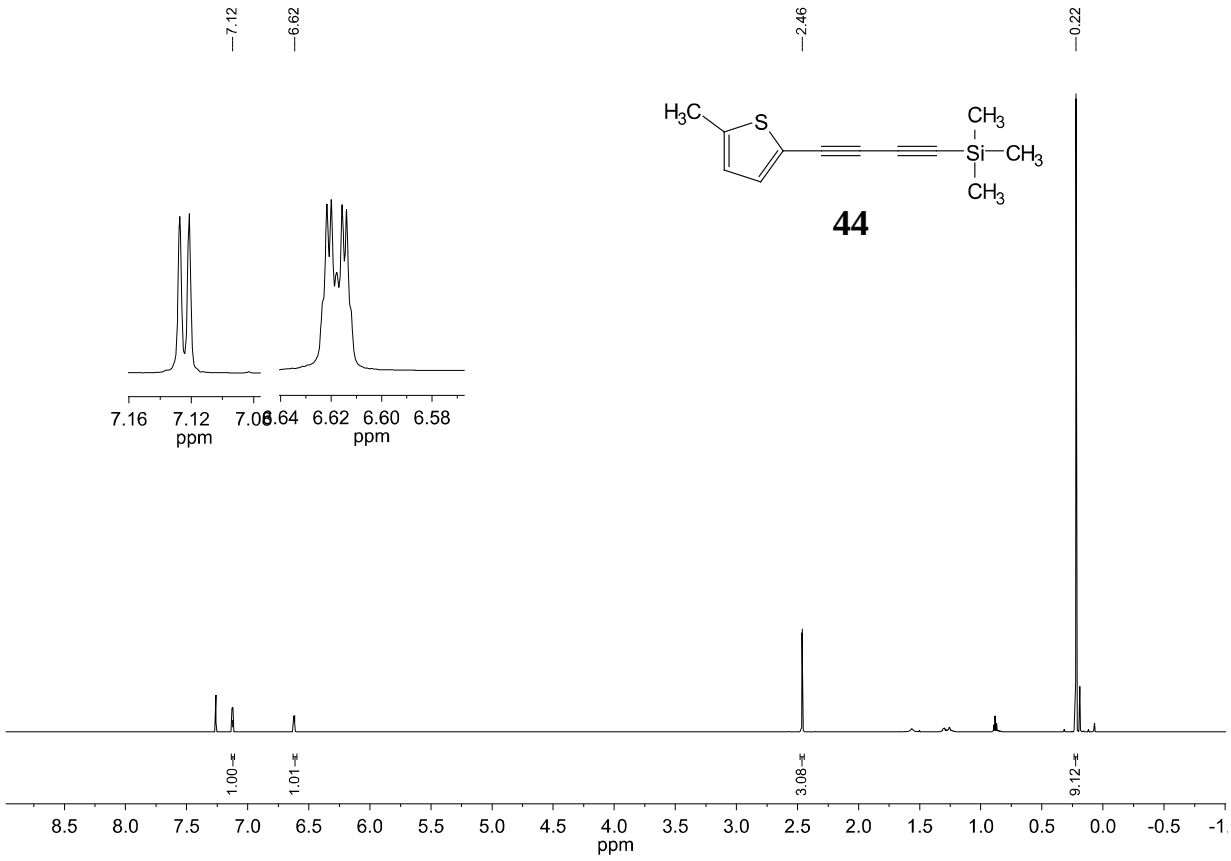
ppm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Si
CH3
CH3
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ppm
6.64
6.62
6.60
6.58
ppm
1.00
1.01
3.08
9.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
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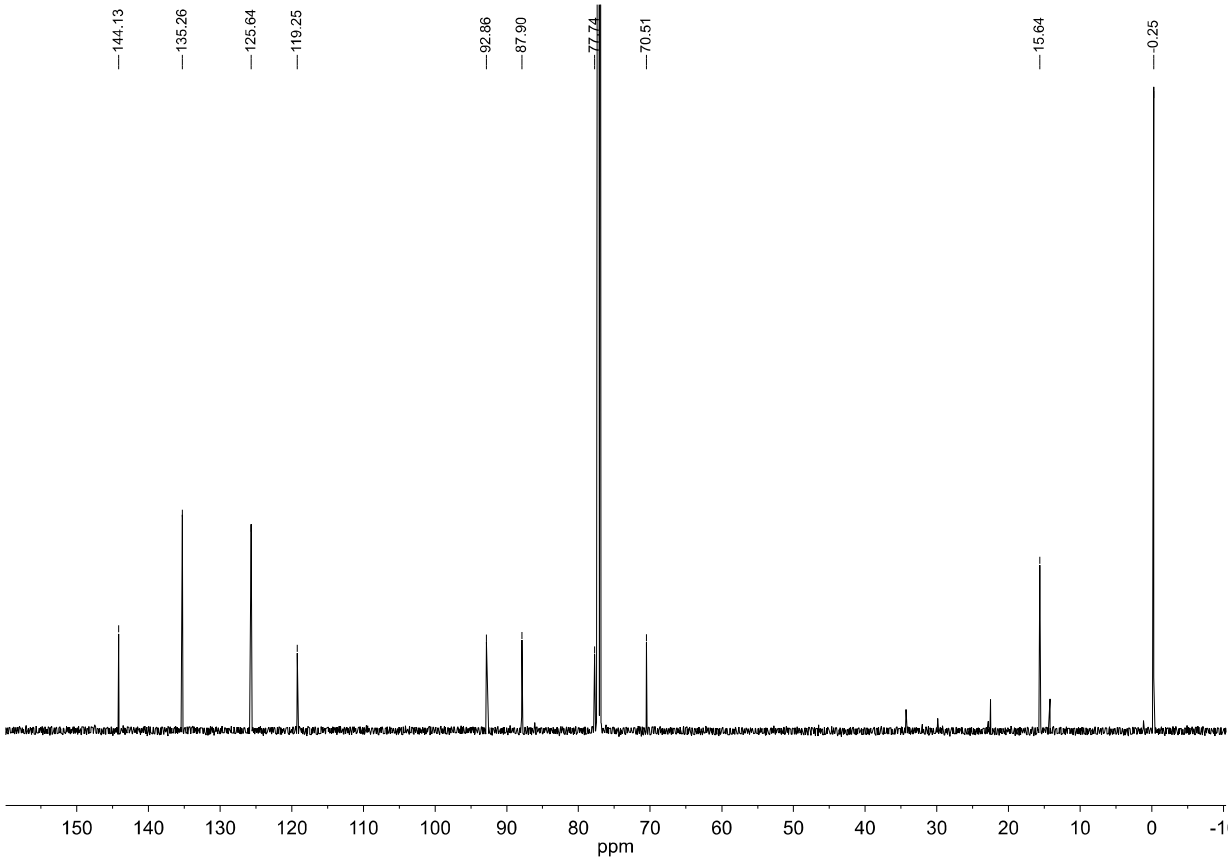
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130
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60
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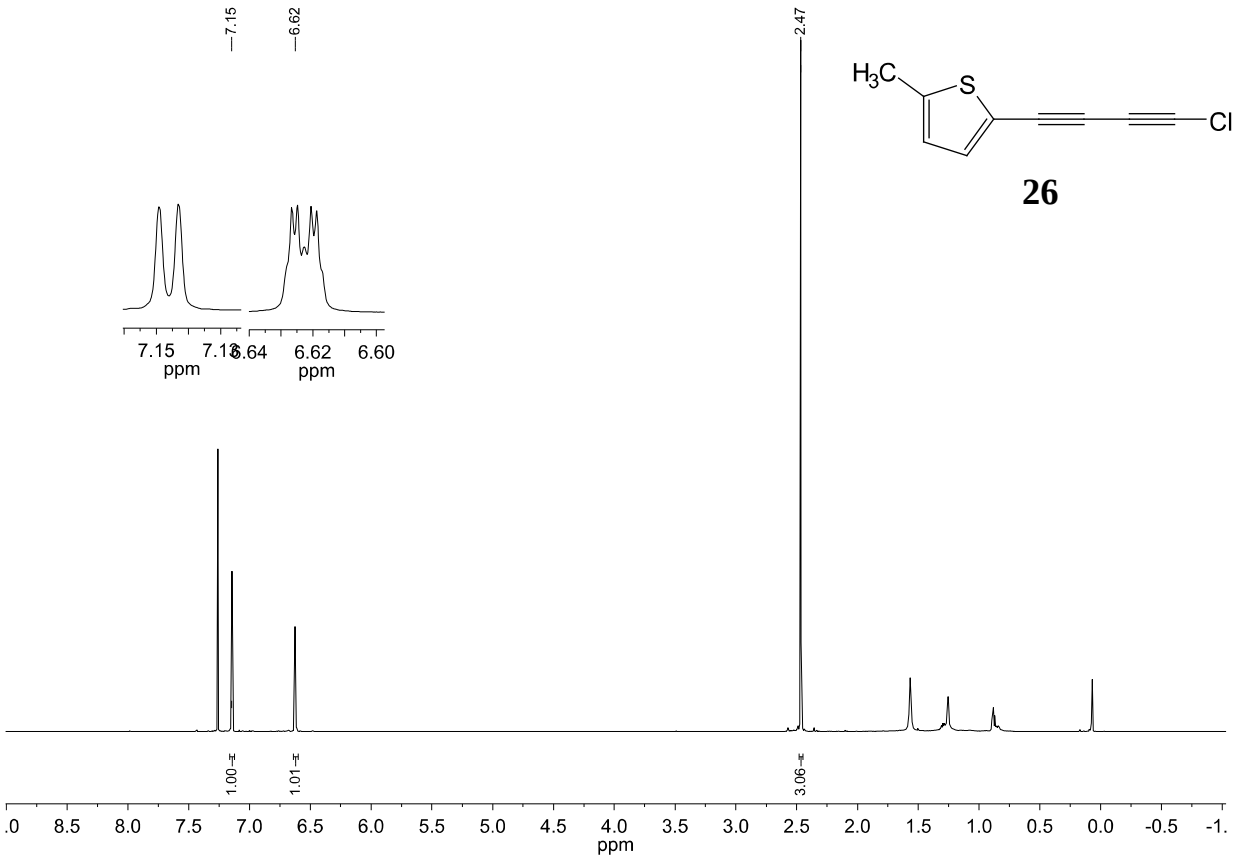
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H3C
S
Cl
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6.62
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ppm
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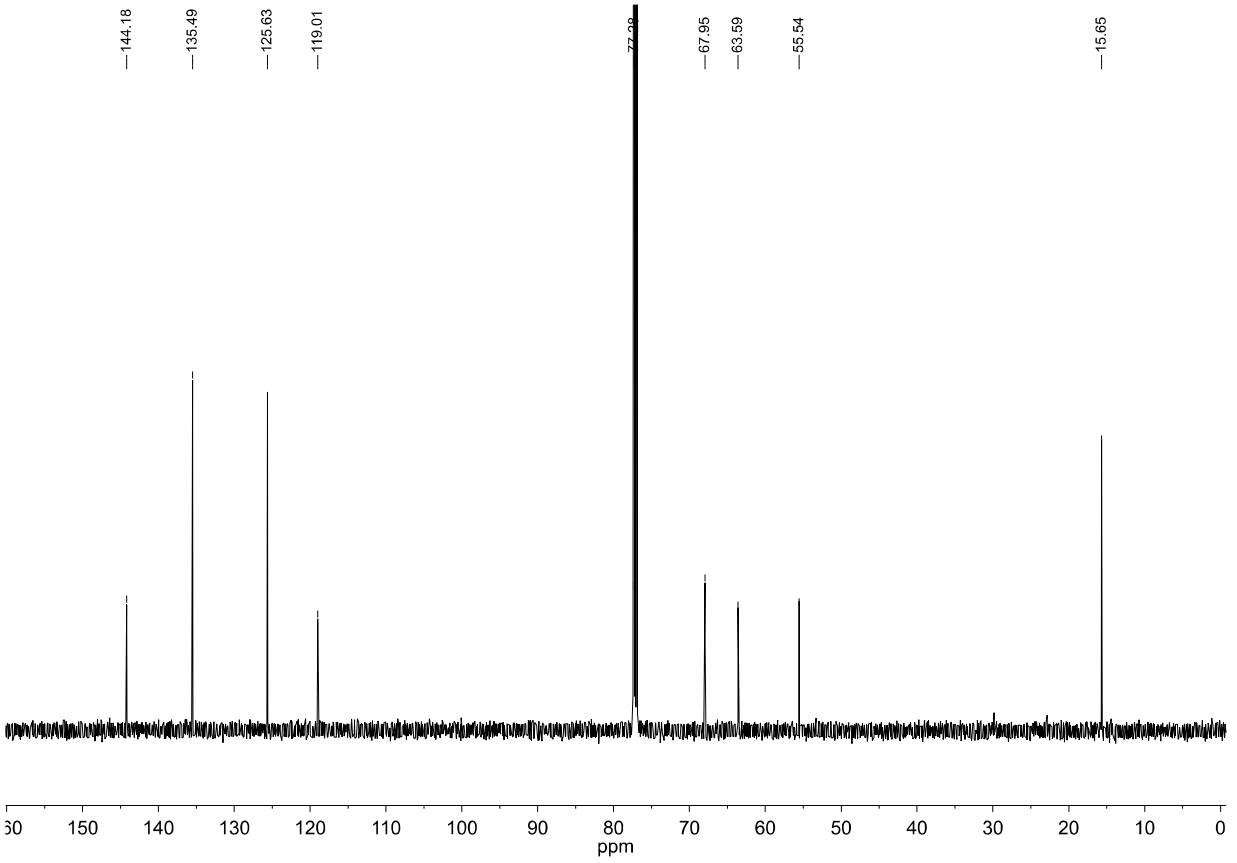
1.01
3.06
ppm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55.54
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ppm