

Supporting Information

Mechanistic Implications For The Ni-Catalyzed Kumada Cross-Coupling Reaction

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X-ray Data Collection and Structure Solution Refinement. Single crystals suitable for X-ray structure analysis were coated with Paratone N oil, mounted on a fiber loop, and placed in a cold, gaseous dinitrogen stream on the diffractometer. For all measurements Oxford XCalibur diffractometer performing ϕ and ω scans at 170(2) K were used. Diffraction intensities were measured using graphite-monochromatic Mo K α radiation ($\lambda = 0.71073$ Å). Data collection, indexing, initial cell refinements, frame integration, final cell refinements, and absorption corrections were accomplished with the program CrysAlisPro,^[1] Space groups were assigned by analysis of the metric symmetry and systematic absences (determined by WinGX^[2]) and were further checked by PLATON^[3,4] for additional symmetry. Structures were solved by direct methods and refined against all data in the reported 2θ ranges by full-matrix least squares on F² with the SHELXL program suite^[5] using the OLEX2 or shelXle interface.^[6,7] Crystallographic data as well as refinement parameters are presented in Table S2.

Table S1. Cell Parameters of complex **1** and of crystals obtained from the stoichiometric reactions solutions of **1** with 1 equiv. phenylmagnesium bromide, and of **2**, **3** or **4** with both 1 equiv. phenylmagnesium bromide and 1 equiv. 4-iodotoluene.

Cell Parameters (Å and °)		
Complex 1	a = 20.70(2)	$\alpha = 90$
	b = 10.259(11)	$\beta = 90$
	c = 16.853(16)	$\gamma = 90$
Complex 1 + phenyl Grignard	a = 20.59(5)	$\alpha = 90$
	b = 10.283(9)	$\beta = 90$
	c = 16.73(4)	$\gamma = 90$
Complex 2 + phenyl Grignard + 4-iodotoluene	a = 20.620(13)	$\alpha = 90$
	b = 10.185(7)	$\beta = 90$
	c = 16.932(13)	$\gamma = 90$
Complex 3 + phenyl Grignard + 4-iodotoluene	a = 20.571(17)	$\alpha = 90$
	b = 10.163(10)	$\beta = 90$
	c = 17.085(17)	$\gamma = 90$
Complex 4 + phenyl Grignard + 4-iodotoluene	a = 20.509(15)	$\alpha = 90$
	b = 10.31(6)	$\beta = 90$
	c = 16.922(13)	$\gamma = 90$
	a = 20.5259(16)	$\alpha = 90$
	b = 17.0858(10)	$\beta = 90$
	c = 20.7340(12)	$\gamma = 90$

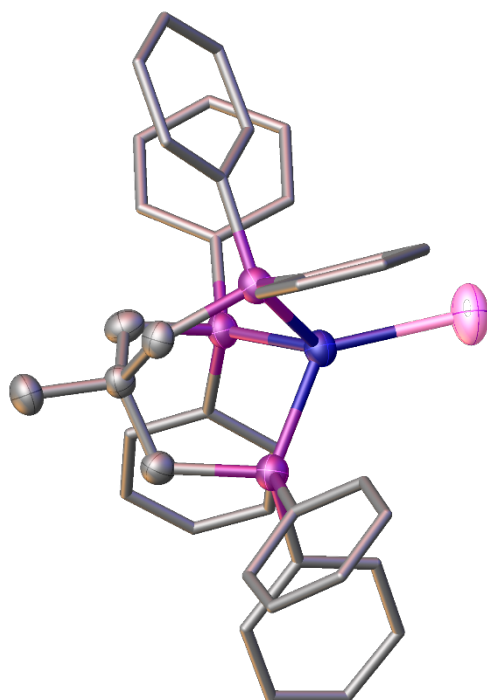


Figure S1. Structure of the asymmetric unit of compound 1. Probability level at 50%. Hydrogens and Carbons of the phenyl rings are omitted for clarity. Grey: Carbon; Purple: Phosphorus; Blue: Nickel; Pink: Iodine

Table S2. Crystal Data and Structure Refinement of [(Triphos)Ni^II].

Property	Value
Identification code	LI274
Empirical formula	C ₄₁ H ₃₉ INiP ₃
Formula weight	810.24
Temperature/K	170
Crystal system	orthorhombic
Space group	Pna2 ₁
a/Å	20.5260(16)
b/Å	10.3670(6)
c/Å	17.0858(10)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3635.7(4)
Z	4
ρ _{calc} /g/cm ³	1.480
μ/mm ⁻¹	1.543
F(000)	1644.0
Crystal size/mm ³	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.074 to 73.248
Index ranges	-30 ≤ h ≤ 29, -16 ≤ k ≤ 15, -28 ≤ l ≤ 25
Reflections collected	109489
Independent reflections	14073 [R _{int} = 0.1807, R _{sigma} = 0.1939]
Data/restraints/parameters	14073/1/417
Goodness-of-fit on F ²	0.941
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0787, wR ₂ = 0.1646
Final R indexes [all data]	R ₁ = 0.2132, wR ₂ = 0.2167
Largest diff. peak/hole / e Å ⁻³	1.54/-1.36
Flack parameter	-0.09(3)
CCDC Reference	1578308

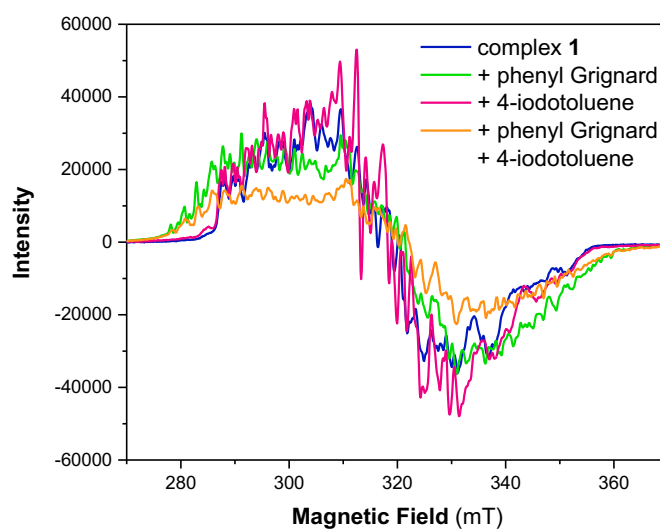


Figure S2. EPR Spectrum of complex **1** (blue) and its reaction solutions with 1 equiv. phenyl Grignard (green), 1 equiv. 4-iodotoluene (red) and with both 1 equiv. phenyl Grignard and 1 equiv. 4-iodotoluene (orange) in THF. Experimental conditions: T = 10 K, frequency 9.63 GHz, microwave power 2 mW, modulation amplitude 0.3 mT.

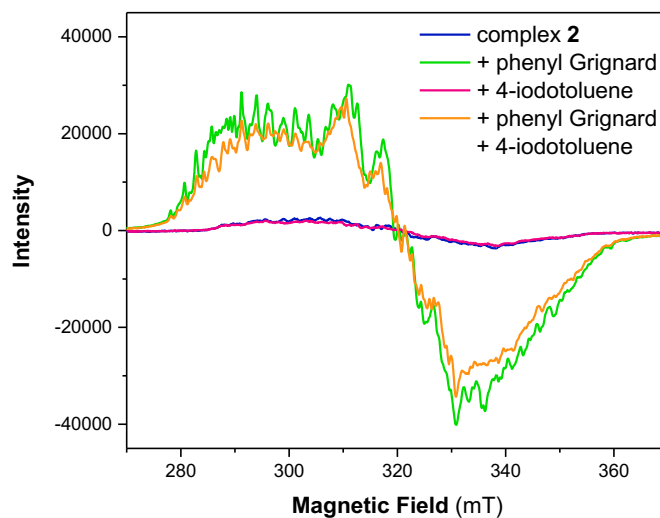


Figure S3. EPR Spectrum of complex **2** (blue) and its reaction solutions with 1 equiv. phenyl Grignard (green), 1 equiv. 4-iodotoluene (red) and with both 1 equiv. phenyl Grignard and 1 equiv. 4-iodotoluene (orange) in THF. Experimental conditions: T = 10 K, frequency 9.63 GHz, microwave power 2 mW, modulation amplitude 0.3 mT.

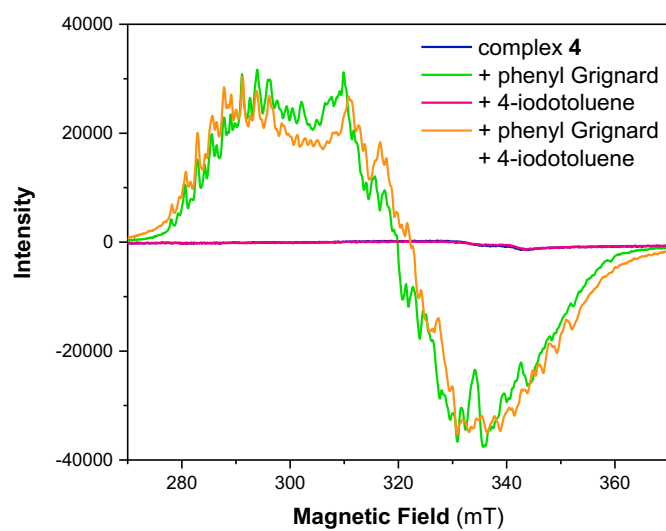


Figure S4. EPR Spectrum of complex **4** (blue) and its reaction solutions with 1 equiv. phenyl Grignard (green), 1 equiv. 4-iodotoluene (red) and with both 1 equiv. phenyl Grignard and 1 equiv. 4-iodotoluene (orange) in THF. Experimental conditions: T = 10 K, frequency 9.63 GHz, microwave power 2 mW, modulation amplitude 0.3 mT.

NMR- and GC-MS-Data for Kumada coupling products

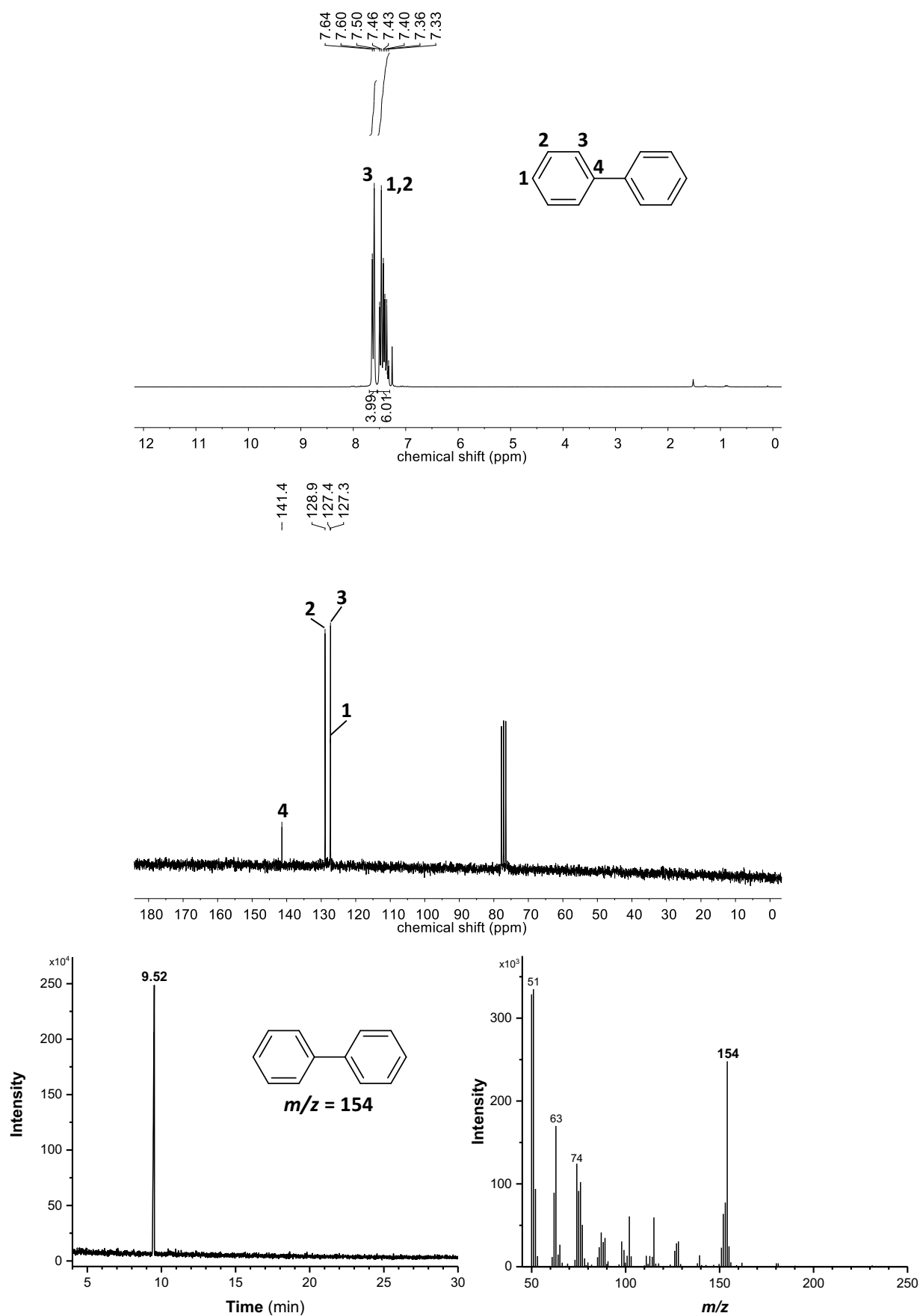


Figure S5. ¹H NMR (200 MHz) and ¹³C NMR (50 MHz) spectra and GC-MS of 1,1'-biphenyl (P1).

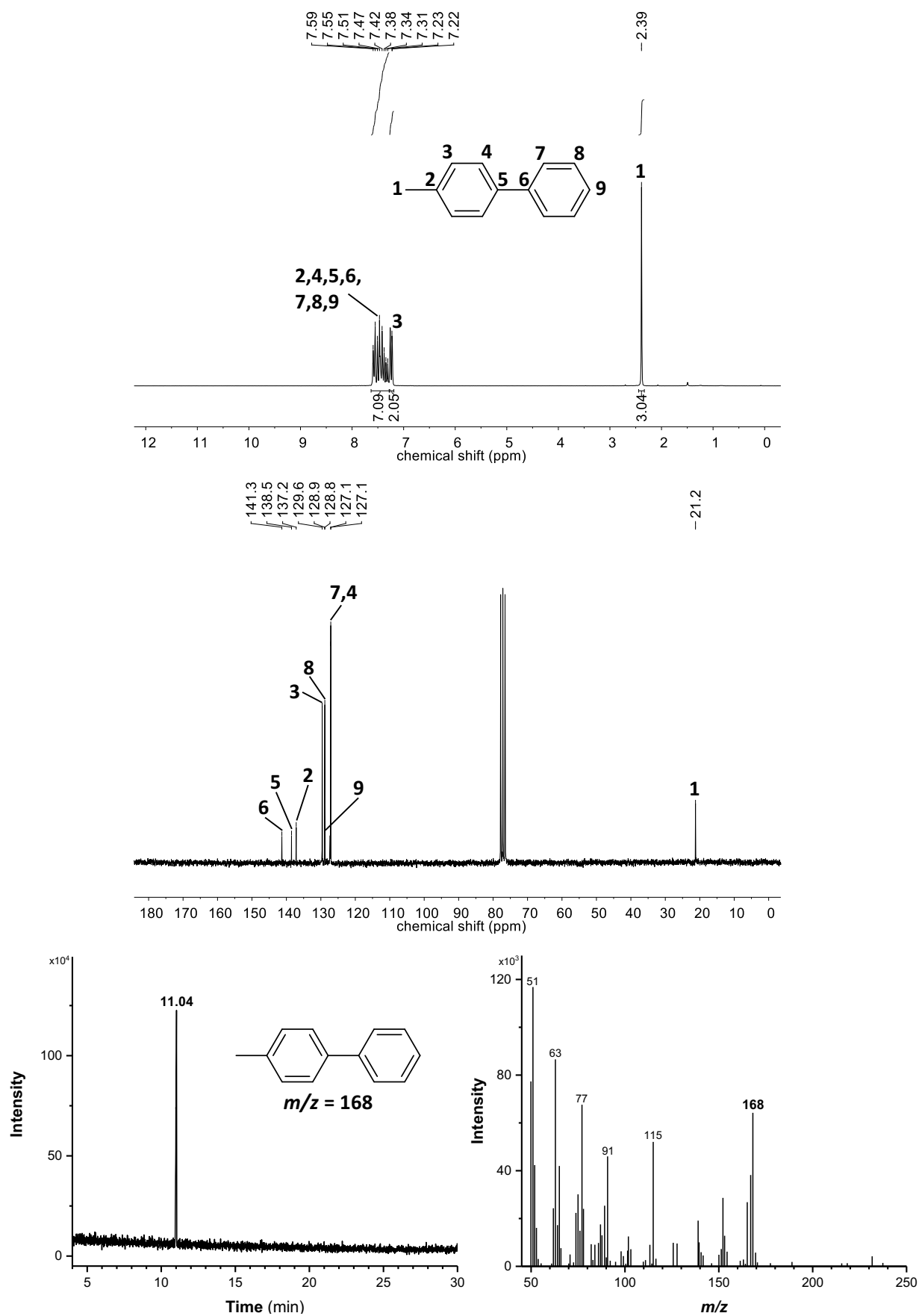


Figure S6. ^1H NMR (200 MHz) and ^{13}C NMR (50 MHz) spectra and GC-MS of 4-methyl-1,1'-biphenyl (**P2**).

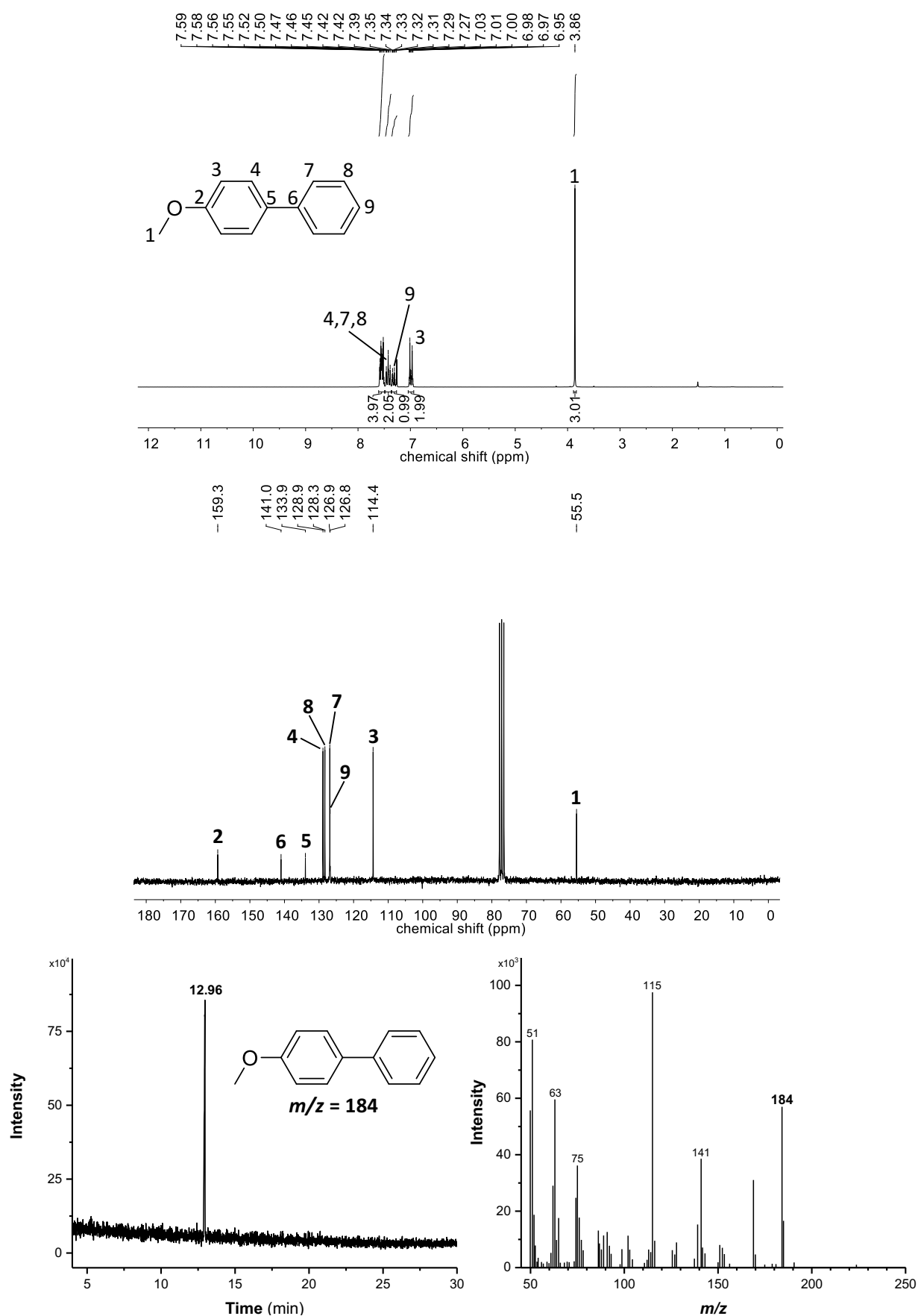


Figure S7. ^1H NMR (200 MHz) and ^{13}C NMR (50 MHz) spectra and GC-MS of 4-methoxy-1,1'-biphenyl (**P3**).

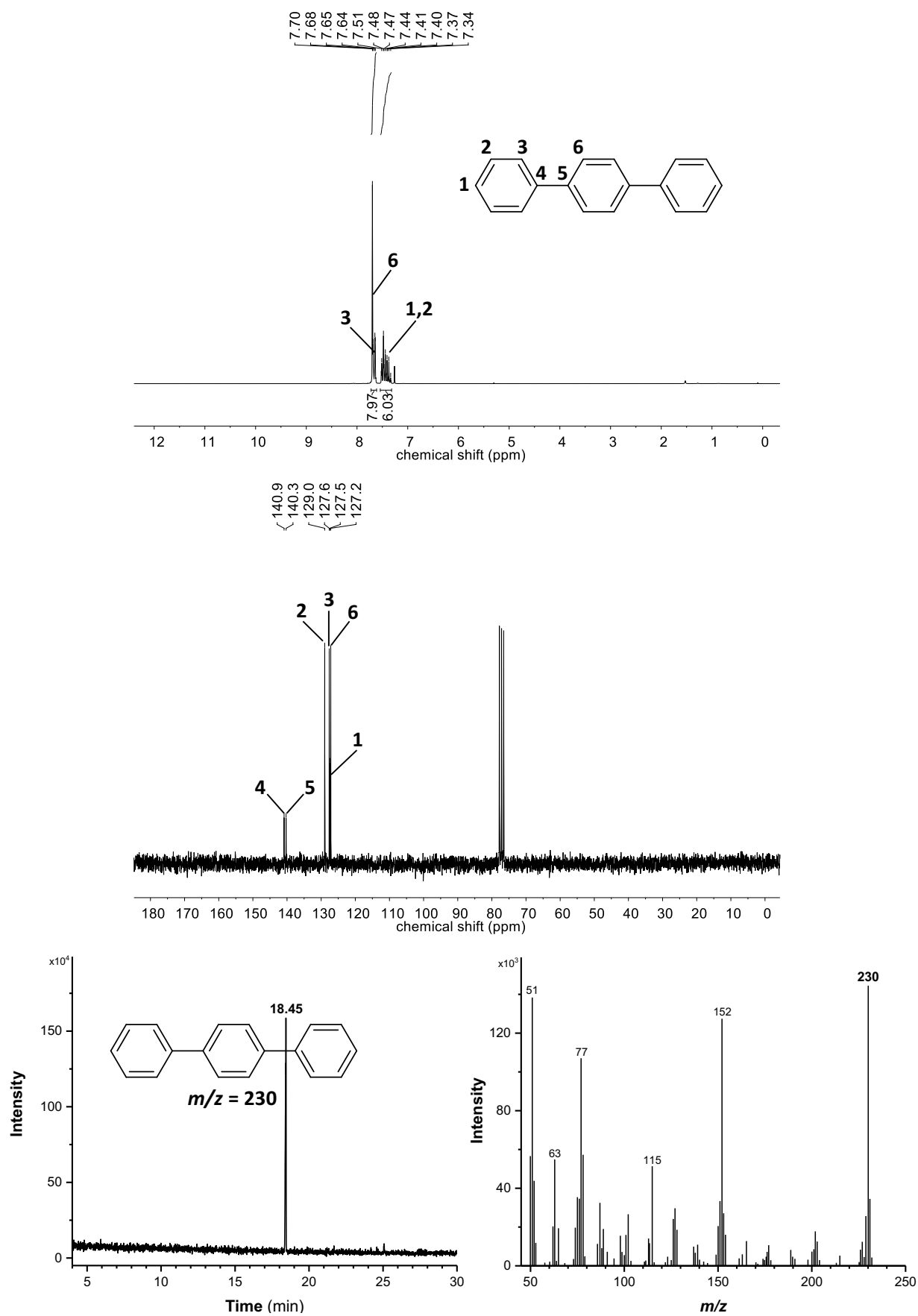
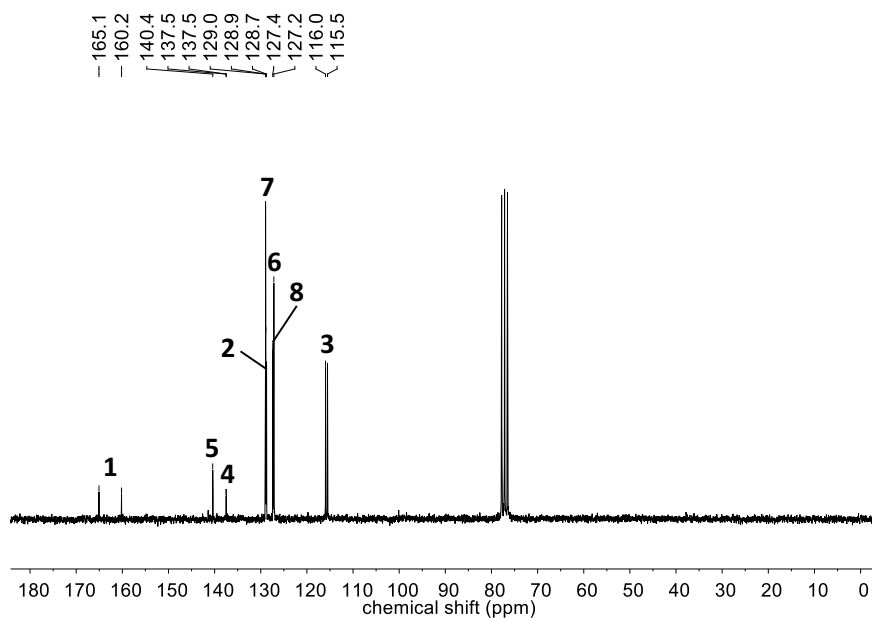
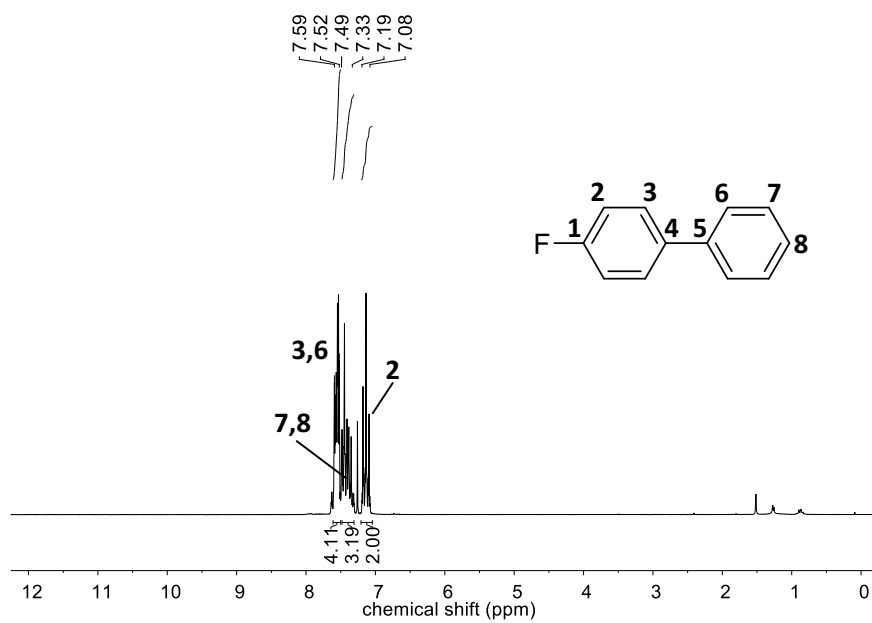


Figure S10. ^1H NMR (200 MHz) and ^{13}C NMR (50 MHz) and GC-MS of 1,4-biphenylbenzene (**P4**).



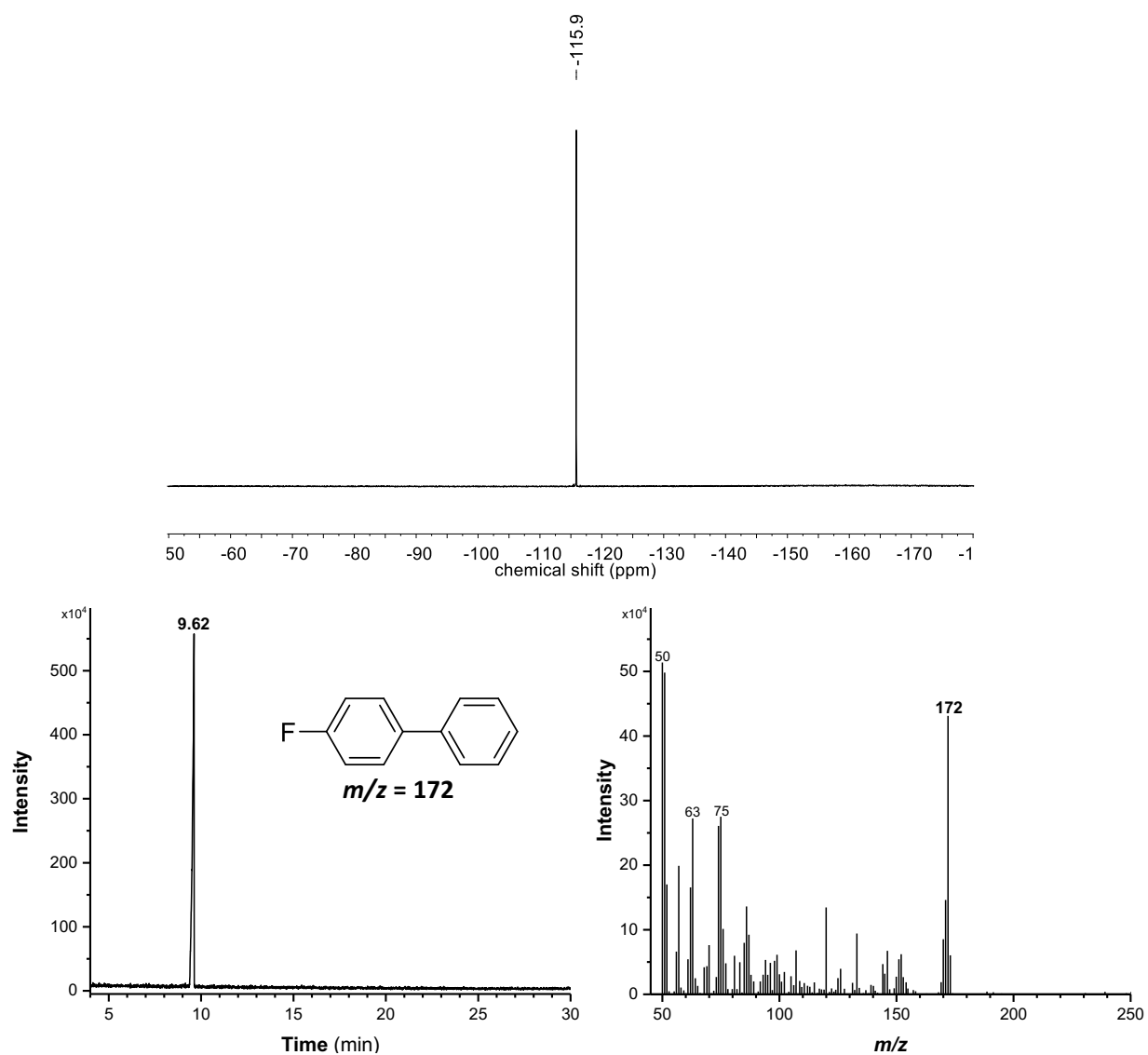


Figure S8. ^1H NMR (200 MHz), ^{13}C NMR (50 MHz) and ^{19}F NMR (235 MHz) spectra and GC-MS of 4-fluoro-1,1'-biphenyl (**P5**).

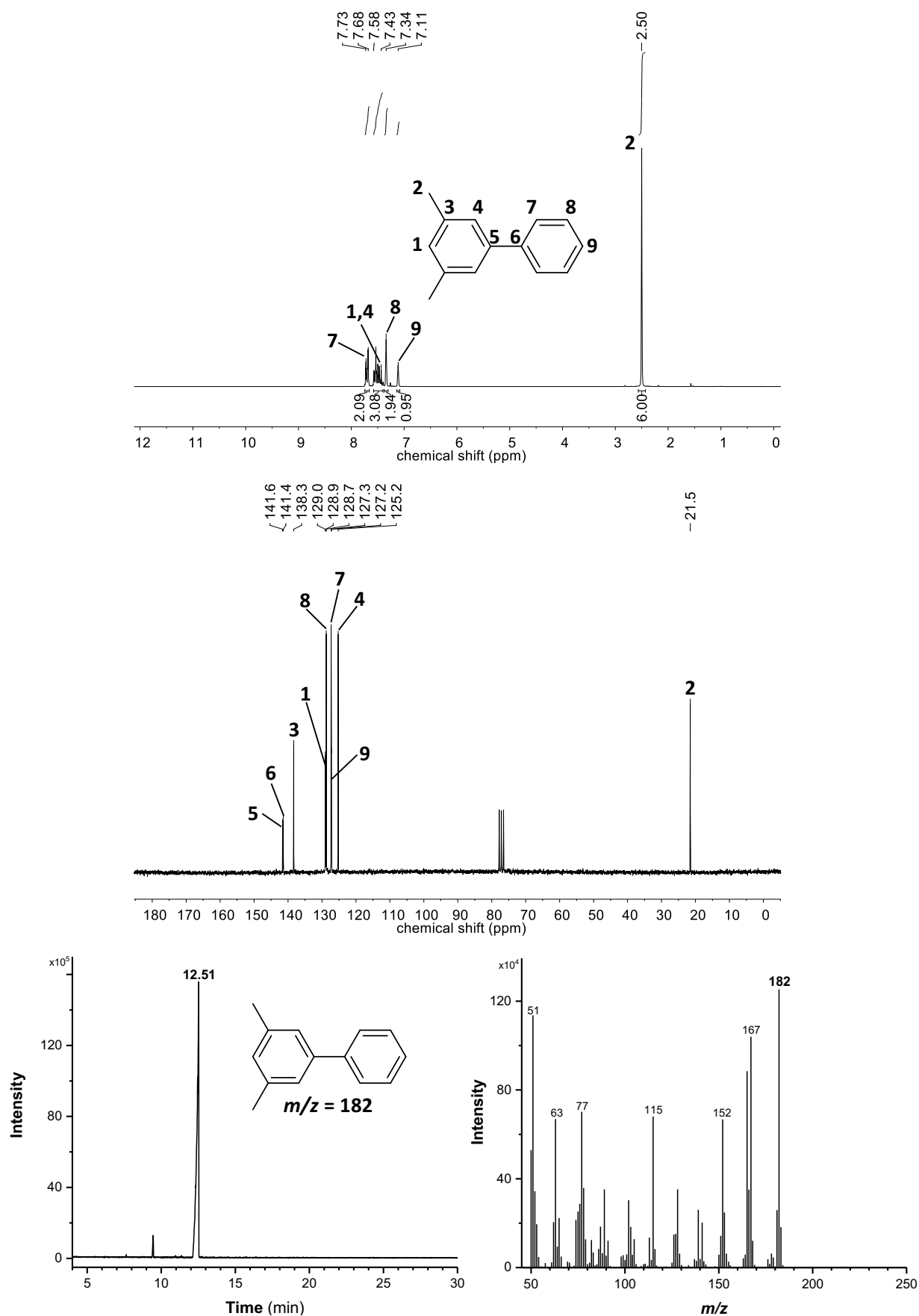


Figure S9. ^1H NMR (200 MHz) and ^{13}C NMR (50 MHz) and GC-MS of 3,5-dimethyl-1,1'-biphenyl (P6).

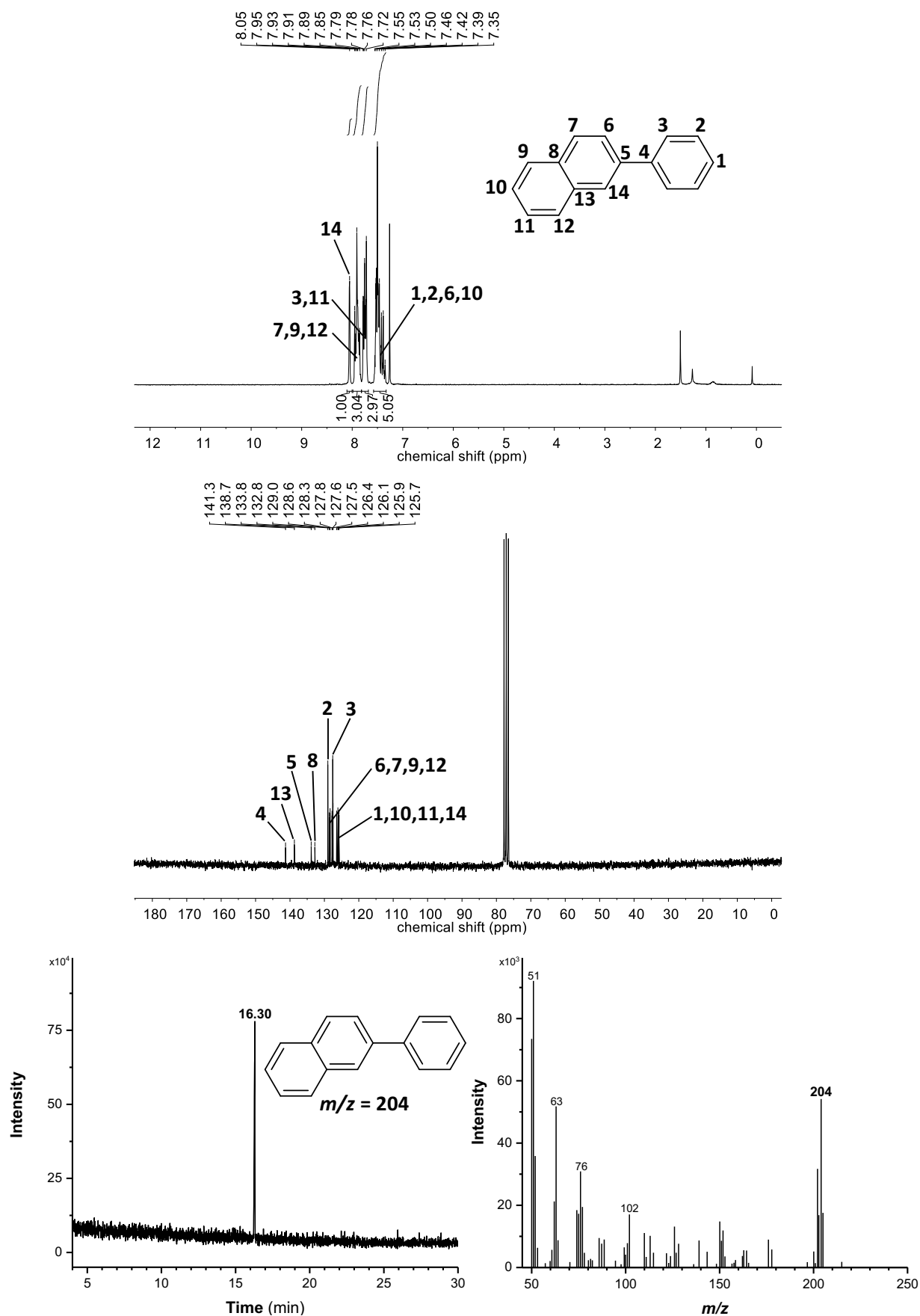


Figure S11. ^1H NMR (200 MHz) and ^{13}C NMR (50 MHz) and GC-MS of 2-phenylnaphthalene (P7).

Cartesian coordinates [Angstrom] of geometry-optimized models used in the calculations

[TriphosNiCl]

Ni	9.22961673484519	0.76513251222575	0.64387181601814
P	11.32242516543792	1.37551328381263	0.50753786938042
P	9.50819890254801	-0.15138385630870	2.61483881539301
P	8.54954222836968	2.75948880416634	1.28619541372941
C	12.59522682609535	0.14665595641284	-0.04904717279704
C	9.80710671588861	3.45581585295896	2.49381729271549
H	10.41644806862734	4.19402902427379	1.93055386448467
H	9.28762694290967	4.02873167942564	3.29086327632570
C	8.10088147875377	6.55463804232356	-0.47076614586301
H	8.37407439847083	7.60132545524166	-0.26185372210310
C	11.91175111478222	1.98401021935903	2.17423948990070
H	12.48654921245941	1.15870938303795	2.64401878392166
H	12.62038683238389	2.82584159036368	2.02931491315304
C	7.42090203378373	3.88266314170866	-0.99579168124347
H	7.17636146532167	2.82864547426944	-1.21121489590149
C	10.78247443366500	2.43037694979660	3.15790500553600
C	8.14341215137669	4.19772827411509	0.17900271328200
C	14.80520119618387	-0.89341236804092	-0.03273311038041
H	15.81243598170299	-0.97457038408055	0.40505958305687
C	6.94826794212630	2.69269239173984	2.24332193862396
C	12.22922721865199	-0.68534438513761	-1.13158703211184
H	11.20914744801828	-0.61885097423246	-1.54551998872133
C	10.04153243936215	1.20840342190899	3.79721510242417
H	9.11794648334623	1.57468910230806	4.29232514766474
H	10.68031254493970	0.78499817460416	4.59956267138621
C	10.77123026727588	2.95011396691443	-1.74459122617985
H	9.85664581765243	2.33687304955365	-1.77754398846583
C	8.48233623839621	5.54439954679821	0.43148820964192
H	9.04050006041146	5.82530612272394	1.33775450223630
C	12.85615558890582	3.54381260685777	-0.63255304509470
H	13.59513673791643	3.39684154510953	0.17174411770225
C	11.48213698260577	3.18102031218113	4.32020317011617
H	11.95971647969507	4.11502849375419	3.95879745462580
H	12.26871469027036	2.54939883656366	4.78290020035300
H	10.75041157493065	3.45238436573325	5.10836705478663
C	13.09797396564927	4.52129632128604	-1.61307943852337
H	14.01131630210335	5.13460376961584	-1.55867750458019
C	6.58582657168674	3.64049696313797	3.22581311653270
H	7.27339765128691	4.45814095330266	3.49573577657459
C	13.14894221509418	-1.60046537634110	-1.66794950808274
H	12.85384241749052	-2.23845445681898	-2.51581549852859
C	4.77465640965943	1.60784658284284	2.52902001155099
H	4.06852832210592	0.80952324229262	2.25178716985018
C	12.51719615437921	-3.72372411465788	3.04139819759612
H	13.20295908095622	-4.58234927817826	3.11756178849580
C	6.03164590206915	1.67402814998859	1.90268580784912
H	6.31348244647395	0.93376285797442	1.13595637844285
C	11.47196786126689	-1.76152856944422	4.04279116291150

H	11.34172651781384	-1.10825784368398	4.92050708649958
C	7.37057519943789	6.23448990794859	-1.62862227110812
H	7.06927823222722	7.02795168309606	-2.33017490877845
C	11.80650332783266	-3.49008971834552	1.85094445856185
H	11.93514292096583	-4.16267299000690	0.98820475473033
C	13.89053785297062	0.03333586506650	0.49894200875830
H	14.20341473345248	0.66592754317019	1.34410574364156
C	10.75867307130807	-1.51661721927130	2.84898575132333
C	11.68750429243354	2.75238312894245	-0.69013999180173
C	7.02939442537240	4.89370653911451	-1.88743293353140
H	6.46362462618260	4.63136953169716	-2.79536930927180
C	14.43992547762861	-1.70730265992357	-1.11865089395378
H	15.16117062421262	-2.42739205144179	-1.53584280595038
C	4.42480650783484	2.54913542398359	3.51213211189101
H	3.44304315117376	2.49404576877452	4.00773362646797
C	11.02032985268346	3.92034197436903	-2.73113332505997
H	10.29727856746663	4.06586111699450	-3.54878607807853
C	12.18162816302516	4.70920311868249	-2.66526407072114
H	12.37512944027536	5.47354448168444	-3.43450779935367
C	5.33442374063769	3.56474801424339	3.86121271700601
H	5.06632473773853	4.30847170403576	4.62853835945764
C	12.35054968672877	-2.85519821981651	4.13535370826894
H	12.90193788621408	-3.03364340222017	5.07212882361548
C	7.14812930217577	-1.64797552979144	2.64374014043210
H	7.29013580543462	-1.63685513267571	1.54926003028758
C	7.85408234064596	-0.92686316337374	4.86159572178064
H	8.55047472748476	-0.38999393172809	5.52434141117687
C	5.86274264077336	-2.31113848061190	4.60511946834825
H	5.00691900570734	-2.84161526790291	5.05159212663006
C	6.06107274470684	-2.33331739797532	3.21302157038524
H	5.35852199893320	-2.87917309429439	2.56334442582771
C	6.75877668530477	-1.60364044644772	5.42657452827617
H	6.60799111458193	-1.58083707821991	6.51798770279450
C	8.05865342320817	-0.94553675180671	3.46456580071564
C	10.94022137063726	-2.38869361545808	1.75320531239888
H	10.39415437968600	-2.18579097747309	0.81786002051832
Cl	7.98242480277101	-0.28951614177713	-0.90139322587009

[BrMgPh]

C	7.01103561974184	-1.89737578251604	2.56343372917841
H	7.09088593172200	-1.97444259578793	1.46331030436776
C	7.77632023843227	-1.08864574619987	4.70187268867968
H	8.47508640714087	-0.50980662122703	5.33337248337556
C	5.80846452695581	-2.52415941495458	4.59005831132593
H	4.98429978159767	-3.06019075110609	5.08834275234555
C	5.95360395776097	-2.58548479790656	3.19228814289930
H	5.23998695391667	-3.17307161742882	2.59033077103518
C	6.72511129582131	-1.77164364451248	5.34623380623540
H	6.62001292971250	-1.71709524693008	6.44328614104112
C	7.95760518143448	-1.12660852511999	3.29211549876002
Mg	9.56145166055455	-0.12106256162219	2.34924708129476
Br	11.43394675420910	1.05908017831166	1.33576413946133

BrMgCl

Mg	7.67348780139508	-1.20526581434906	-4.32241003672183
Br	5.96359395400313	-0.05447264471406	-5.57571941264637
Cl	9.27357353760179	-2.28405416593688	-3.16097143863179

Iodobenzene

C	-0.75533517640803	-0.00006184380112	-2.98822006998653
C	-1.91834407640854	-0.35633867329729	-2.28279997192997
C	0.40765554614598	0.35628398793179	-2.28280180156846
H	-2.83411459457273	-0.63747391987430	-2.82620742450466
H	1.32331922099330	0.63775958540950	-2.82620663295795
C	-1.92798840738217	-0.35948660372789	-0.87532724621978
C	0.41727323836999	0.35951678490158	-0.87532905795245
H	-2.83995187857718	-0.64029853120903	-0.32859937990013
H	1.32932687173166	0.64003728707613	-0.32859379539437
C	-0.75536203192533	0.00002925885623	-0.18773037438645
H	-0.75533961441554	-0.00006349686251	-4.08931295356282
I	-0.75538560155140	0.00009616459691	1.94956892836356

[TriphosNiPh]

Ni	9.22675716351875	0.73719060156183	0.44115840390732
P	11.36732270847740	1.33989637099098	0.43476121474174
P	9.40929211419596	-0.26212622201077	2.41201585954010
P	8.53657140875227	2.72286649516774	1.11412423866603
C	12.69118600957686	0.14914009667419	-0.10259662413393
C	9.75896405273396	3.35118373407497	2.40383460831582
H	10.39825484902464	4.10175879870924	1.89500265154590
H	9.21008165684236	3.90447853333561	3.19469418910176
C	8.50504588059857	6.58193004663888	-0.59333430238679
H	8.96775288875177	7.56570817002521	-0.41628860695281
C	11.88736212457836	1.89866047857681	2.14429416074168
H	12.43567425551806	1.06079318536634	2.62233369852090
H	12.60302961606114	2.74337918562915	2.05912543694947
C	7.33682110015582	4.07089703346295	-1.02236112474395
H	6.87412309098763	3.08653595566083	-1.20030130209642
C	10.70642145744664	2.30839723276248	3.07865416443122
C	8.22846723083264	4.23849081511121	0.06460510113613
C	14.84984278935494	-0.98513841927235	0.07525624328244
H	15.78543949012310	-1.15901569776163	0.62975294021780
C	6.88428990458387	2.72231418703618	1.99351476241992
C	12.45769933966637	-0.53553968451940	-1.31770725325213
H	11.51098887859515	-0.37347245581732	-1.85991945483435
C	9.95151670231532	1.06513357105211	3.63981630469185
H	9.03602814668347	1.41711039678366	4.15832189018230
H	10.57832943098752	0.58509329096479	4.41954347862932
C	10.92325947324516	3.14654381720213	-1.68589823717941
H	9.95300465389566	2.62950608470229	-1.74480173093405
C	8.80888127578874	5.50978729410414	0.26630574100012
H	9.50241904376470	5.68858596838081	1.10185800129750
C	13.06974936461045	3.43638142387134	-0.57855566293414

H	13.80277638184784	3.14448947801521	0.19082338580589
C	11.34196784536552	3.02351019680702	4.30017290321951
H	11.83015898842534	3.97247143280163	3.99505398145829
H	12.11025791900343	2.38086128949240	4.77837732259283
H	10.57139712738627	3.26308845290095	5.06151751864393
C	13.39116279076491	4.46852502360348	-1.47566865673851
H	14.36084024603104	4.98395811831874	-1.39157106070876
C	6.54521262956159	3.63760884962370	3.01515459321960
H	7.27616318051306	4.38245517628577	3.36773517739478
C	13.41295765388643	-1.42416624678918	-1.83522257527589
H	13.21714624658885	-1.94417411031868	-2.78575251974670
C	4.61875047871554	1.80352666721464	2.11370716302239
H	3.86773362676476	1.08210015622964	1.75542143215697
C	12.57224420055064	-3.71409811980242	2.70315233111894
H	13.30202466871040	-4.53791508963918	2.75050534914223
C	5.90899250310590	1.80062141377158	1.55425375513506
H	6.17926476158282	1.06990785221151	0.77518455835105
C	11.32617098215450	-1.93446020572271	3.80836188057909
H	11.07535515733843	-1.39188480519570	4.73392274202923
C	7.61415341608856	6.40511457023154	-1.66477740329006
H	7.37455130854705	7.24690175380293	-2.33318744751384
C	11.95003290778264	-3.39087243880243	1.48570567820443
H	12.19076323539315	-3.95691273369671	0.57284196362199
C	13.89770878488475	-0.08565614979223	0.58923108200933
H	14.11424815112448	0.42900787357877	1.53737873499364
C	10.70320555546642	-1.59431668863225	2.58633518325669
C	11.82779695637143	2.76894660678014	-0.67374264764531
C	7.02817767286520	5.14230931826255	-1.87478448849974
H	6.32696835371167	4.98889267720583	-2.71060870381294
C	14.61359716303243	-1.65355691885510	-1.13740743134893
H	15.36329514033132	-2.35372176665805	-1.53811535041644
C	4.29293688012427	2.71067054528203	3.13643989750890
H	3.28592982123529	2.70693958412369	3.58203173440889
C	11.24733543548440	4.17357505388029	-2.59017723388361
H	10.52681769914453	4.45883239706934	-3.37224521629289
C	12.48058913232583	4.83817111494058	-2.48437649931782
H	12.73487049739570	5.64684979818103	-3.18769156235364
C	5.26208571227431	3.62467479297949	3.58970526981261
H	5.01668096984742	4.34050872556531	4.39049642354833
C	12.26033070258727	-2.98216159311990	3.86428230482618
H	12.74158535090701	-3.23465982842208	4.82221862850304
C	7.86894727821912	-2.48406246215251	3.32957140459321
H	8.61510756402715	-3.10472831657308	2.81079000870206
C	7.03473364848097	-0.31702422438121	4.03383981570640
H	7.09528124046213	0.78146543389223	4.06062462542628
C	5.82428213985242	-2.34426056019776	4.65132403982206
H	4.97732978675546	-2.83474565970249	5.15620401133540
C	6.78599779075021	-3.11029577164069	3.96837159360845
H	6.69874260732853	-4.20838590496780	3.93594613390408
C	5.95606191524867	-0.94509574985760	4.68052565054597
H	5.21016976128043	-0.32972566421430	5.20807739805770
C	8.01749925503694	-1.07514567025924	3.35531164272057
C	11.02726759902022	-2.33189425411398	1.42800077970807

H	10.54496680761290	-2.06064462063275	0.47548873305867
C	7.89141456184783	-0.16644287996385	-0.64079216743247
C	7.70283370774655	0.29640372856379	-1.97790669155103
C	7.22559436449516	-1.38462098323938	-0.32604135241745
C	6.95879156862187	-0.42009349027021	-2.93669707624994
C	6.46752457492538	-2.10675089868894	-1.26843123977259
C	6.33316604328800	-1.63086484184417	-2.58635518703383
H	8.15824611917098	1.25080643658946	-2.29596362088765
H	7.30642931100671	-1.79354977585186	0.69562876282310
H	6.85879911029776	-0.02473288464944	-3.96210535109202
H	5.98284925231560	-3.05267820088572	-0.97265064348165
H	5.74302904031921	-2.19195662013606	-3.32896290268345

[κ^2 -TriphosNiPh₂l]

Ni	8.09182161107628	0.56270796339273	0.62433454402369
P	12.13675382974076	0.82964622707819	0.36135899828292
P	10.43403481471363	-1.21010390941653	3.24621967097944
P	7.92392037648696	2.71124526526263	1.72736367994454
C	13.67692449053112	0.37828875407413	1.23526880525476
C	9.29564554341989	2.84682261159322	2.95841042160264
H	9.78443694931966	3.83062671974607	2.76929423644303
H	8.86935562218157	2.88128848914638	3.98524909764704
C	8.73517269624455	6.42696674321685	0.10641869998130
H	9.02102527998632	7.42215691208821	0.48505054638965
C	10.48700427009471	1.40912602846134	1.32982985777572
H	9.94247600067825	0.50710067165302	0.95604261859483
H	10.24956532539128	2.30458273806512	0.68545630410194
C	8.02091312254030	3.88188324788842	-0.83942356552751
H	7.71552603708315	2.90575279685710	-1.22211715443314
C	10.32599456352249	1.67239702225503	2.84677392352422
C	8.17284974364009	4.08688948636523	0.53866631198092
C	15.89989294249281	0.80050638494664	2.12169488099846
H	16.65322096387340	1.51296566761784	2.47800901750920
C	6.39703819844419	3.12023700401055	2.65668275675390
C	13.97000316861027	-1.00728089994391	1.21409536771209
H	13.21667774687351	-1.70844210249653	0.82915235539874
C	9.65925395186519	0.45583283689091	3.56123149520719
H	8.61270026845821	0.35579940087034	3.19076389735190
H	9.58327197407140	0.67536949502626	4.64517265536652
C	13.09229033443747	2.34994611086384	-1.73295934397113
H	13.10424434311297	1.36100329101460	-2.22529451674658
C	8.51953350082945	5.37480991595774	1.01631847769824
H	8.63072847463815	5.57087666988069	2.09517338626957
C	12.58533299307439	3.74247950171232	0.21556453372736
H	12.23132481289616	3.86151606852184	1.25652800225897
C	11.61833723925852	2.08512740352138	3.57074153744615
H	12.10641057063202	2.96909550177624	3.11401987653735
H	12.35817795063064	1.26628757705349	3.59347967124923
H	11.36991688706880	2.35230548862702	4.60741327546425
C	13.01665296792081	4.87269262076595	-0.50185747550322
H	12.98568405830943	5.86407246648239	-0.02504288588412
C	6.27235530265031	2.81065756191075	4.02498847659064
H	7.10139647503146	2.34365922884435	4.58412291433660
C	15.23524286591931	-1.47851656257121	1.60726702841777
H	15.46887552111725	-2.55232975302973	1.54789774448418

C	4.13971626636857	4.07229387225650	2.68590941528358
H	3.30899023017029	4.57581726776086	2.15790050833681
C	13.59182743782183	-1.91678752941857	6.59931418305996
H	14.34637297464839	-2.09159239331484	7.37749247315088
C	5.32072069601553	3.75421721474362	1.98945376579424
H	5.40070988436603	4.01734484145312	0.92564194697837
C	11.39146795713810	-1.09512522023340	5.94187196295434
H	10.43271683973757	-0.63826853555792	6.22555789917132
C	8.59690819617681	6.20855580216291	-1.27374366031291
H	8.77040030837696	7.03467513984774	-1.98433072041488
C	13.85246115131875	-2.30021938023936	5.28074412782380
H	14.80910812529891	-2.77160201341739	5.01277430310839
C	14.65718710370444	1.28267312621168	1.68634800756422
H	14.47787027609074	2.37020580372554	1.67972579544641
C	11.65258776554007	-1.46048695538960	4.60707903967779
C	12.62903494503497	2.46201038259569	-0.39356376639478
C	8.23082221857002	4.93962449013963	-1.74235663253886
H	8.11914620511497	4.75787385889230	-2.81215522135910
C	16.19767118386776	-0.57487817171827	2.07390047165002
H	17.18759203342060	-0.93929124412146	2.39026076144310
C	4.02161117474704	3.76188535744029	4.04826240558416
H	3.09790671558592	4.01857904813886	4.59304106090167
C	13.52367768078355	3.48622597074908	-2.43730916305377
H	13.87722102886548	3.37843961194782	-3.47644807363371
C	13.49382132838062	4.74706623078988	-1.82593191461900
H	13.83501561535262	5.63791503154539	-2.37653054024248
C	5.09015006049224	3.13161223460527	4.71661170064610
H	5.01229364528907	2.89635333443729	5.78637287910146
C	12.36193912532358	-1.31994501341508	6.92851807362147
H	12.15092274403746	-1.02874533066359	7.96374217021688
C	9.49221367710955	-3.76881713078812	3.86134650602657
H	10.55634872770432	-4.05895299267098	3.77321497710065
C	7.72870358794172	-2.08963666877383	3.81134575245435
H	7.38256482077000	-1.05596655193629	3.71469540358107
C	7.16758014197765	-4.40274749422447	4.25996470545712
H	6.41804318846168	-5.17308058067744	4.47993603143072
C	8.53267739273962	-4.74756680569098	4.14488054535603
H	8.85596926748231	-5.78774718957135	4.27699676477907
C	6.76755957924746	-3.07383981172257	4.08344859306838
H	5.70481845152548	-2.78869406288270	4.17382259285697
C	9.10424488157994	-2.41928845358622	3.70209709806549
C	12.87938108766492	-2.07704846118902	4.28660667130726
H	13.08699994601275	-2.37987921794763	3.25614319899764
C	6.25576502734035	0.48797805397496	0.20892940721047
C	5.97945078732413	0.72763380965711	-1.15263768247393
C	5.24480416344618	0.45216200807937	1.16175446316364
C	4.65332612045078	0.94585088813277	-1.55342547744252
C	3.91438373016553	0.67784105163129	0.74587016364568
C	3.62240189615569	0.93906739025799	-0.59733672893035
H	6.82519217423419	0.73878796687838	-1.83792816680572
H	5.44569109888622	0.26956838378750	2.22498797344678
H	4.40889402211192	1.13270462967877	-2.61063609098686
H	3.11516957171496	0.66775353294654	1.49422696202115
H	2.58512548149561	1.14685889517281	-0.90852224882185
C	8.44215048409469	-0.98967898075428	-0.37710232336160
C	9.06506239834358	-0.77207446939217	-1.64090490223588
C	8.12103776257797	-2.31110039350764	0.03376711148803

C	9.32862362489982	-1.85735263983678	-2.50371819949132
C	8.35516705143909	-3.38356544973480	-0.84212001887414
C	8.96669298975252	-3.16087898986690	-2.11164713387726
H	9.34283106988791	0.25258433958912	-1.95790368255016
H	7.67862251873779	-2.53356198243596	1.02477964796007
H	9.80081902610158	-1.68006334379374	-3.48747313224055
H	8.08457354263049	-4.40650155619285	-0.52908052129614
H	9.18553323115645	-4.02106519841738	-2.76587495734101
I	4.40413443826524	-1.72801360431535	-12.53612656823601

Biphenyl

C	11.45985196853259	-9.39049674046563	3.41372949266598
C	10.29579750585618	-9.74290124461156	4.11553090905987
C	12.55169475083343	-8.77426191608192	4.07378769277053
H	9.46381943681825	-10.22842091484977	3.58121870846780
C	10.19406867877880	-9.48755574435306	5.49478723154583
C	12.43383660686097	-8.52560202510742	5.46352586503687
H	9.28086353149940	-9.76414786244334	6.04449129782857
H	13.25790000529076	-8.02786221416373	5.99779990138615
C	11.26916532565209	-8.87676085027428	6.16517677656304
H	11.19816336552186	-8.66196763071449	7.24310401526753
H	11.53318775660332	-9.62028245788049	2.33937397530356
C	13.78526212868275	-8.39592761932519	3.32830422490202
C	15.06058764239857	-8.47088103604683	3.94070942703243
C	13.71748678885938	-7.94726222482258	1.98592332784422
C	16.22213227196756	-8.11000742845230	3.23890279305585
C	14.87887032031031	-7.58556569511460	1.28447206158101
C	16.13732713910982	-7.66462358253248	1.90758895343305
H	15.14701414579060	-8.84025101242229	4.97414645434086
H	12.73745263003925	-7.85692459655882	1.49212039320109
H	17.20270872775046	-8.18535050437678	3.73486748804441
H	14.79826430842683	-7.22962503219012	0.24571798260489
H	17.04792762841680	-7.37933221521231	1.35856223906445

[TriphosNil]

Ni	9.29728992705462	0.90189590225093	0.87346462297441
P	11.39802072198985	1.42659554645966	0.56623940215150
P	9.55890296290085	-0.18961335707514	2.73084858861738
P	8.53898867101910	2.89021600239832	1.34678183894842
C	12.65243119299725	0.18988682702694	0.01403614002826
C	9.84383499665598	3.49809770333661	2.56141631165736
H	10.47293524169404	4.22859966297072	2.01151734356238
H	9.32043504891091	4.07061645819637	3.35606305544720
C	8.32522285690962	6.71363370047423	-0.35194541844656
H	8.69625804706276	7.72902537100476	-0.14354498207819
C	11.93869273934344	2.00191096967280	2.25961457068990
H	12.48993205729385	1.16207403578535	2.73027733191917
H	12.66496985277567	2.83175464962980	2.13336231373349
C	7.38895642849436	4.11892741795134	-0.87241787945301
H	7.02380102772643	3.10086178112157	-1.08611904628471
C	10.79610687481468	2.45052132273184	3.22425827978268
C	8.20060266182488	4.35190092391596	0.26166218244003
C	14.79725869279085	-0.96683779817515	0.15542168485961
H	15.75142618284979	-1.13363686176230	0.67835646887657

C	6.96407052215431	2.83065527046883	2.32836621481483
C	12.35995964968164	-0.52892443488979	-1.16832675000239
H	11.40455959074900	-0.36604603229854	-1.69419419918141
C	10.04456264775150	1.23352109560312	3.86071359177828
H	9.10194128034784	1.59879234964338	4.31755527336708
H	10.66002486178921	0.82563709863286	4.68881511892080
C	10.78785295795080	3.11698398719287	-1.59484193224872
H	9.83383907983046	2.56741631020086	-1.60758147797661
C	8.66677018721195	5.65957343401742	0.51491018443973
H	9.29669444520425	5.87691333541444	1.39049320055468
C	12.96422491814759	3.53217456536352	-0.57477366798895
H	13.73429850392279	3.29900718082530	0.17790291835434
C	11.48802458147739	3.19257462222854	4.39955341541180
H	11.97142693986531	4.12668029408948	4.04798537163818
H	12.26795422231902	2.55482177411004	4.86369089209876
H	10.74902791672969	3.45995857053931	5.18135658425893
C	13.21274545865167	4.53682996759149	-1.52388467156338
H	14.16403168867665	5.09034286005688	-1.49533440484429
C	6.50742536820082	3.93833402258811	3.07847512764664
H	7.09323892366107	4.87124233019134	3.11316962499543
C	13.28125674143669	-1.45392840453469	-1.68317192153208
H	13.04380954666283	-2.00490466861746	-2.60547661634441
C	4.95533701194908	1.59217061348683	2.97056507271051
H	4.35188194057615	0.67309136588046	2.92126023957567
C	12.71159350756064	-3.60574970077227	3.20428149437054
H	13.43467001778999	-4.43032228601871	3.30292182995596
C	6.17864992000804	1.66046239722740	2.28024108460700
H	6.52814392679957	0.79369823657914	1.69690455880845
C	11.46343144461756	-1.76660586559222	4.20475641966116
H	11.20655222720924	-1.17568806011670	5.09806614897718
C	7.51413573135438	6.47507352842277	-1.47398624434451
H	7.24759249562740	7.30227905311679	-2.14956726235004
C	12.11040853174847	-3.34010047326325	1.96239429120157
H	12.36259573390659	-3.95040609745072	1.08208781744578
C	13.87922612085806	-0.03622622886306	0.67322466291753
H	14.13891392950001	0.50863833076374	1.59287889059860
C	10.86096486280316	-1.48967669177233	2.95710317556632
C	11.74406227715135	2.81941659297451	-0.60220566695994
C	7.04439686982109	5.17386061813721	-1.73138889470975
H	6.41118822576524	4.97726864889576	-2.61012454000648
C	14.50236875566683	-1.67610656381290	-1.02063992235732
H	15.22515948553209	-2.40261570501797	-1.42262179154045
C	4.51082635527083	2.69433428241814	3.71955603863705
H	3.55294400674875	2.64470777019961	4.25931639782599
C	11.04395988869214	4.11608155669606	-2.55026706705314
H	10.28961677988686	4.34195552141774	-3.31925255722073
C	12.25408473043717	4.82883820468538	-2.51309686997354
H	12.45386973849425	5.61531244055449	-3.25734568367050
C	5.28961349546256	3.86659228319930	3.77372301481412
H	4.94176863958883	4.73530745165777	4.35380671791993
C	12.38893582382258	-2.81639914850879	4.32390583198228
H	12.85497931878954	-3.02392180069399	5.29939521734781
C	7.31105288764473	-1.84654939496374	2.79893239597406
H	7.529444648903396	-1.98229187812275	1.72692036036923
C	7.82032175870984	-0.81219857803328	4.94647314559152
H	8.43185380128238	-0.15133439540156	5.57856932009660
C	5.93448509343031	-2.34584655255648	4.74387600837202

H	5.08148974708497	-2.87155306177345	5.19953793223552
C	6.22787253710851	-2.52566981194471	3.38014892181288
H	5.60616588495805	-3.19188986742662	2.76271670812738
C	6.73126024963150	-1.48898519370238	5.52310015172833
H	6.50588335152622	-1.34346865067721	6.59109700417675
C	8.11852793052973	-0.98657316008027	3.57764528582355
C	11.19272664628965	-2.28325862210989	1.83856317058159
H	10.73227897470326	-2.06109748818105	0.86338208921746
I	1.98995571309689	-6.59136206078870	-10.69294593086707

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