Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2012

Coordination chemistry of diphenylphosphinoferrocenyl thioethers on cyclooctadiene and norbornadiene rhodium(I) platforms

Ekaterina M. Kozinets,[a,b] Oleksandr Konev,[a] Oleg A. Filippov,[b] Jean-Claude Daran,[a] Rinaldo Poli,[a,c] Elena S. Shubina,[b] Natalia V. Belkova,*[b] and Eric Manoury*[a]

[a]*CNRS; LCC (Laboratoire de Chimie de Coordination); Université de Toulouse; UPS, INP; F-31077 Toulouse, France ; 205, route de Narbonne, F-31077 Toulouse, France; Fax: (+) 33-561553003; E-mail:* eric.manoury@lcc-toulouse.fr.

[b] *A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilov Street 28, 119991 Moscow, Russia. E-mail:* nataliabelk@ineos.ac.ru.

[c]*Institut Universitaire de France, 103, bd Saint-Michel, 75005 Paris, France*

SUPPORTING INFORMATION

Table S1. Anharmonicity correction on selected low frequency modes for compound $\mathbf{3}^{\mathbf{tBu}}$.

Figure S1. DFT(B3LYP) optimized geometry of $\mathbf{2}^{\mathbf{R}}$ and $\mathbf{4}^{\mathbf{R}}$ (R = Ph, *t*Bu).

Figure S2. DFT(B3LYP) optimized geometry of $\mathbf{1}^{t\mathbf{Bu}}$, $\mathbf{3}^{\mathbf{R}}$ (R = Ph, *t*Bu) and (COD)IrCl(P,S*t*Bu).

Table S2. Selected bond lengths [Å] and angles [°] in the DFT optimized geometries of $\mathbf{1}^{\mathbf{Ph}}$, $\mathbf{1}^{\mathbf{tBu}}$, $\mathbf{3}^{\mathbf{Ph}}$, $\mathbf{3}^{\mathbf{tBu}}$, and Ir(COD)(P,S*t*Bu)Cl.

Figure S3. Calculated IR spectra (lower fingerprint region) for complexes $\mathbf{2}^{\mathbf{R}}$, $\mathbf{3}^{t\mathbf{Bu}}$ and $\mathbf{4}^{\mathbf{R}}$ (R = Ph, *t*Bu).

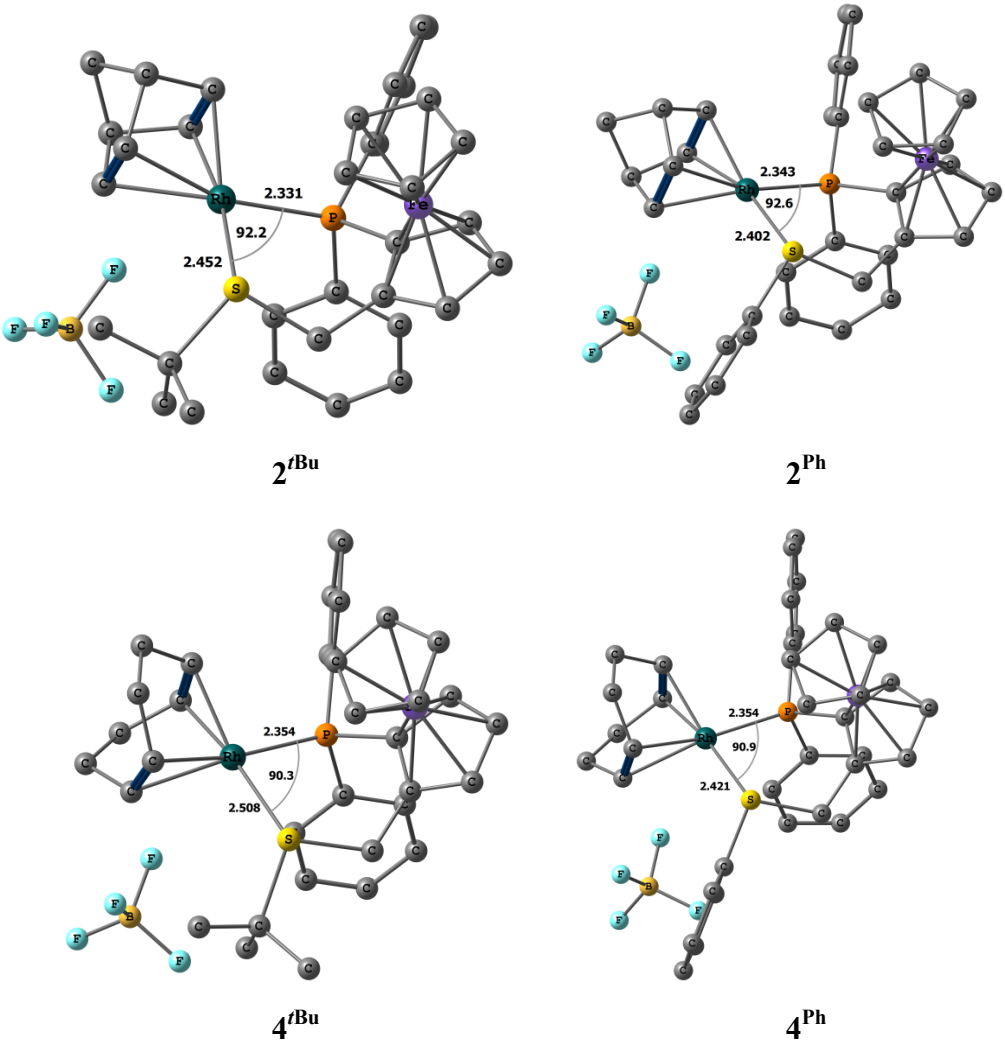
Table S3. Cartesian coordinates of all optimized structures.

Figure S4. NMR spectra for the isolated compounds.

Table S1. Anharmonicity correction on selected low frequency modes for compound $\mathbf{3}^{tBu}$.

Mode #	ν(harm)	ν(anharm)	Intencity	Δν(harm-anharm)	
38	296	275	5	21	
37	288	241	0	47	
36	275	273	18	1	(Rh-Cl stretching mode)
35	270	204	0	66	
34	257	243	5	14	
33	257	245	2	11	
32	253	239	4	13	
31	248	236	3	12	
30	239	223	2	16	

Anharmonicity was taken into account only for a few low frequency modes between 300 and 230 cm^{-1}. For the most intense mode, #36, which corresponds to the Rh-Cl stretch, there is a negligible difference. All other low intensive modes possess a significant contribution of bending modes of the C-H bonds of the tBu and COD groups. The CH vibrations are usually very sensitive to anharmonic corrections.



$\mathbf{2}^{tBu}$ $\mathbf{2}^{Ph}$

$\mathbf{4}^{tBu}$ $\mathbf{4}^{Ph}$

Figure S1. DFT(B3LYP) optimized geometry of $\mathbf{2}^{R}$ and $\mathbf{4}^{R}$ (R = Ph, *t*Bu). Hydrogen atoms are omitted for clarity.

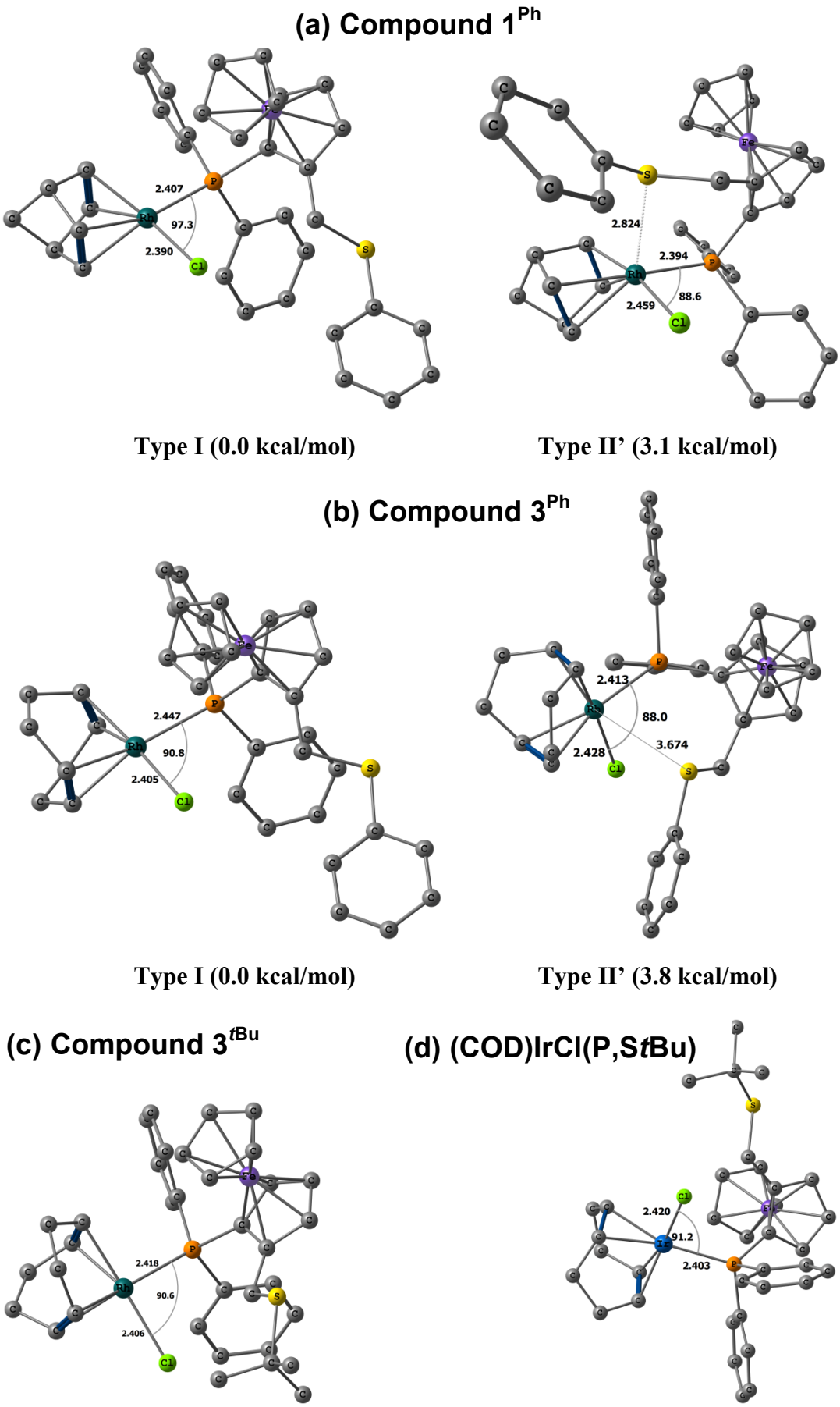


Figure S2. DFT(B3LYP) optimized geometry of $\mathbf{1}^{t\mathrm{Bu}}$, $\mathbf{3}^{\mathrm{R}}$ (R = Ph, *t*Bu) and (COD)IrCl(P,S*t*Bu). Hydrogen atoms are omitted for clarity.

Table S2. Selected bond lengths [Å] and angles [°] in the DFT optimized geometries of **1**^{Ph}, **1**^{tBu}, **3**^{Ph}, **3**^{tBu}, and Ir(COD)(P,S*t*Bu)Cl.

	1^{Ph}		**1**^{tBu}		**3**^{Ph}		**3**^{tBu}	Ir(COD)(P,S*t*Bu)Cl	
								DFT	X-ray[a]
ΔE, kcal mol^{-1}	0	3.1	0	8.2	0	3.8			
Distances									
M-P	2.407	2.394	2.400	2.344	2.447	2.413	2.418	2.403	2.3312(9)
M-Cl	2.390	2.459	2.382	2.572	2.405	2.428	2.406	2.420	2.3625(8)
M-X1[b]	2.098	2.068	2.101	2.198	2.109	2.117	2.120	2.105	2.0859(6)
M-X2[b]	2.014	2.018	2.016	1.969	2..034	2.021	2.029	2.017	1.9988(5)
M···S	5.918	2.824	5.903	2.702	6.269	3.674	5.556	5.533	-
Cl···H[c]	2.451	2.586	2.497	3.491	2.534	2.509	2.759	2.818	
C=C (1)	1.390	1.401	1.389	1.379	1.392	1.390	1.390	1.402	1.392(4)
C=C (2)	1.413	1.418	1.413	1.445	1.412	1.415	1.412	1.428	1.418(4)
Angles									
P-M-X1	168.3	158.9	169.7	163.8	177.1	175.7	175.5	176.0	177.594(17)
P-M-X2	99.3	102.9	100.7	95.0	95.5	97.1	95.8	95.5	93.369(19)
P-M-Cl	97.3	88.6	95.3	96.9	90.8	88.0	90.6	91.2	92.49(2)
Cl-M-X1	92.5	92.7	93.1	94.7	87.3	88.2	87.9	87.7	87.904(18)
Cl-M-X2	163.1	159.0	163.5	134.8	171.8	169.7	169.9	170.0	172.601(17)
X1-M-X2	70.6	70.5	70.6	68.8	86.1	86.4	86.2	86.1	86.434(11)

[a] From Malacea, R.; Manoury, E.; Routaboul, L.; Daran, J.-C.; Poli, R.; Dunne, J. P.; Withwood, A. C.; Godard, C.; Duckett, S. B. *Eur. J. Inorg. Chem.* **2006**, 1803–1816.. [b] X is the center of the C=C bond (X1 for the C=C bond *cis* to the Cl ligand and X2 for the C=C bond *cis* to the P ligand) . [c] Distance to the hydrogen of CH_2SR bridge.

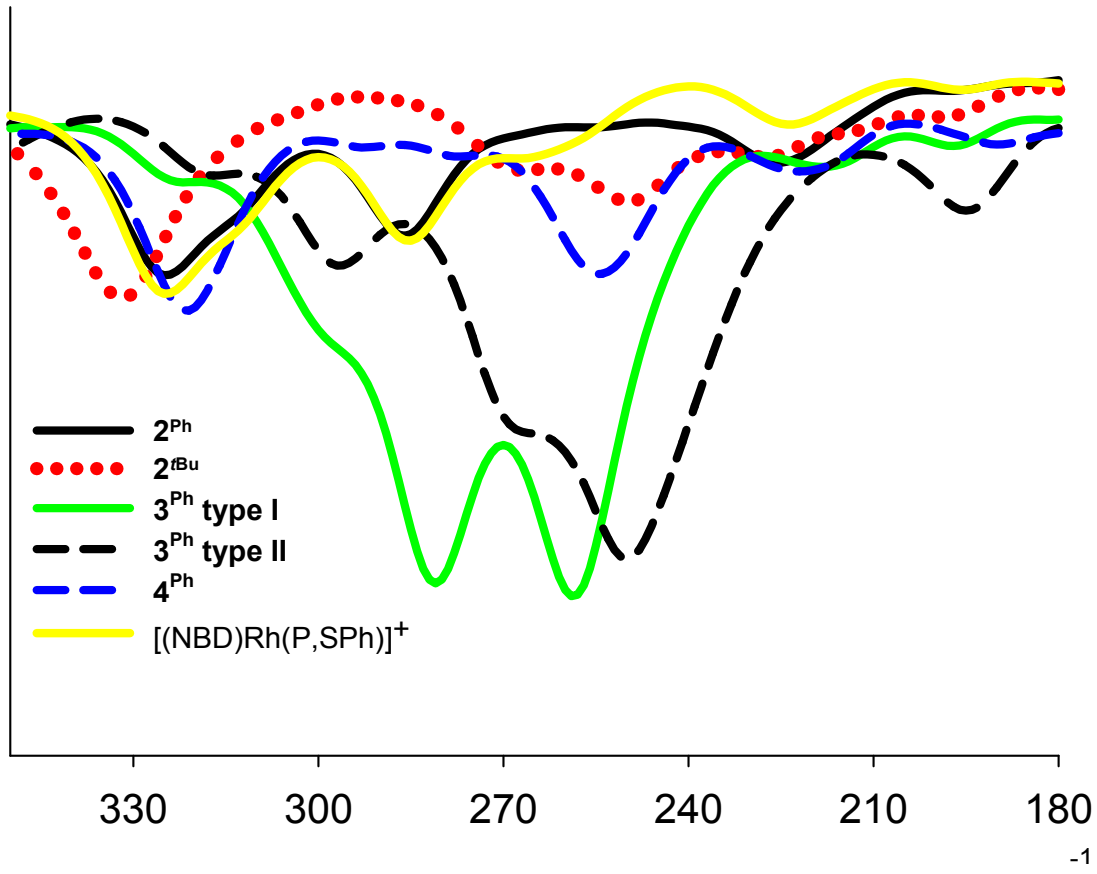


Figure S3. Calculated IR spectra (lower fingerprint region) for complexes $\mathbf{2^R}$, $\mathbf{3^{tBu}}$ and $\mathbf{4^R}$ (R = Ph, *t*Bu).

Table S3. Cartesian coordinates of all optimized structures.

[(NBD)Rh(P,SPh)]$^{+}$
E= -2365.61966953

45	0.778246000	3.369288000	2.344075000
26	-0.137629000	2.608110000	-1.965559000
15	0.076414000	4.936296000	0.742918000
16	-0.903505000	1.789718000	1.685911000
6	-0.692237000	4.195653000	-0.726611000
6	-1.671899000	3.133562000	-0.668223000
6	-2.181693000	2.945457000	-1.992144000
6	-1.528528000	3.865012000	-2.862769000
6	-0.608856000	4.630835000	-2.092698000
1	-2.921439000	2.209505000	-2.278676000
1	-1.675070000	3.939295000	-3.931658000
1	0.057422000	5.395187000	-2.467141000
6	0.141762000	0.722503000	-2.795264000
6	0.855296000	1.701247000	-3.548425000
6	1.797891000	2.327048000	-2.679907000
6	1.667280000	1.732604000	-1.387992000
6	0.643776000	0.740655000	-1.460017000
1	-0.657966000	0.095928000	-3.166045000
1	0.689641000	1.947735000	-4.588323000
1	2.476223000	3.122999000	-2.954780000
1	2.228530000	1.993601000	-0.500435000
1	0.299910000	0.123712000	-0.641971000
6	-2.220427000	2.464540000	0.553709000
1	-2.841694000	1.609628000	0.276900000
1	-2.826372000	3.155296000	1.147752000
6	-2.170822000	6.660058000	0.550468000
6	-3.175359000	7.473610000	1.076132000
6	-3.281649000	7.656714000	2.457382000
6	-2.382233000	7.021542000	3.315502000
6	-1.378325000	6.202811000	2.793672000
6	-1.259594000	6.018662000	1.406367000
1	-2.099322000	6.522265000	-0.523799000
1	-3.875069000	7.964224000	0.406349000
1	-4.064328000	8.290954000	2.862247000
1	-2.461957000	7.161325000	4.389489000
1	-0.685384000	5.699106000	3.461714000
6	1.311726000	7.459662000	0.325879000
6	2.331362000	8.292061000	-0.144403000
6	3.409396000	7.756057000	-0.848539000
6	3.472266000	6.378961000	-1.079440000
6	2.461542000	5.542916000	-0.605928000
6	1.364649000	6.076844000	0.094684000
1	0.474943000	7.892578000	0.863306000
1	2.276785000	9.360849000	0.038671000
1	4.198205000	8.405619000	-1.215079000
1	4.310120000	5.956095000	-1.625871000
1	2.518999000	4.474916000	-0.789612000
6	2.067587000	4.666129000	3.500584000
6	2.069461000	3.843707000	4.809842000
6	3.338258000	2.682662000	3.334165000
6	2.851135000	3.943926000	2.587723000
1	1.831972000	5.722757000	3.446609000
1	3.308651000	4.335023000	1.687076000
6	3.506216000	3.251348000	4.771564000
1	3.671497000	2.473458000	5.524741000
1	4.287077000	4.015758000	4.842479000
6	1.245906000	2.601225000	4.400835000
1	0.342945000	2.263682000	4.895919000
6	2.023022000	1.890278000	3.501002000
1	1.860298000	0.878066000	3.149274000
1	1.745409000	4.362045000	5.711565000
1	4.173644000	2.145523000	2.886822000
6	-1.896992000	1.307293000	3.110753000
6	-2.493259000	2.260215000	3.948891000
6	-2.055851000	-0.060511000	3.363571000
6	-3.256382000	1.834608000	5.036461000
6	-2.814426000	-0.474787000	4.461447000
6	-3.415382000	0.469754000	5.294443000
1	-2.360395000	3.320126000	3.754125000
1	-1.592784000	-0.792139000	2.708719000
1	-3.723523000	2.569329000	5.685188000
1	-2.937531000	-1.534969000	4.659207000
1	-4.007464000	0.144838000	6.144226000

(COD)IrCl(P,StBu)
E= -2786.59820399

77	5.629883000	2.632905000	4.393317000
26	4.478301000	1.625518000	-0.284831000
15	4.868470000	3.941098000	2.526370000
16	1.712804000	-0.243407000	1.747610000
6	4.045660000	3.143335000	1.084803000
6	3.001523000	2.132770000	1.085211000
6	2.454464000	2.085646000	-0.233594000
6	3.145852000	3.019396000	-1.057114000
6	4.121138000	3.671153000	-0.256704000
1	1.680034000	1.402819000	-0.552218000
1	2.986192000	3.175397000	-2.115694000
1	4.811299000	4.431390000	-0.591594000
6	4.557912000	-0.271092000	-1.118792000
6	5.301209000	0.645901000	-1.920976000
6	6.342301000	1.195505000	-1.113581000
6	6.239315000	0.615277000	0.188222000
6	5.136286000	-0.289154000	0.185984000
1	3.680971000	-0.822913000	-1.428417000
1	5.092421000	0.904370000	-2.950425000
1	7.065139000	1.934651000	-1.431619000
1	6.859260000	0.842553000	1.043015000
1	4.770740000	-0.857693000	1.029789000
6	2.527817000	1.329323000	2.265875000
1	1.810440000	1.918108000	2.844473000
1	3.363787000	1.107550000	2.929537000
6	2.691606000	5.745217000	2.123079000
6	1.822355000	6.763937000	2.518747000
6	1.902777000	7.296015000	3.806709000
6	2.851653000	6.800871000	4.702895000
6	3.713359000	5.774173000	4.314658000
6	3.647369000	5.241602000	3.017735000
1	2.619644000	5.342962000	1.118693000
1	1.081620000	7.139198000	1.818314000
1	1.224222000	8.087207000	4.112812000
1	2.911559000	7.198823000	5.711699000
1	4.423647000	5.366057000	5.026274000
6	6.370071000	6.308405000	2.038466000
6	7.428641000	7.043618000	1.499690000
6	8.338193000	6.438631000	0.632001000
6	8.181983000	5.090519000	0.305058000
6	7.127076000	4.353118000	0.844706000
6	6.202527000	4.951448000	1.718121000
1	5.671659000	6.798610000	2.707315000
1	7.536466000	8.092980000	1.758956000
1	9.159908000	7.011847000	0.212736000
1	8.882301000	4.608790000	-0.371684000
1	7.009258000	3.313188000	0.566155000
17	3.400072000	2.579885000	5.331622000
6	0.703755000	-0.722493000	3.251245000
6	0.067254000	-2.065574000	2.854970000
6	-0.395542000	0.312909000	3.529400000
1	0.018185000	1.288106000	3.800993000
1	-1.046205000	0.441550000	2.659564000
1	-1.011609000	-0.022017000	4.373228000
1	-0.573465000	-1.960636000	1.973312000
1	-0.551930000	-2.433812000	3.680971000
1	0.829356000	-2.821307000	2.640205000
6	1.606921000	-0.903837000	4.480069000
1	2.088686000	0.032344000	4.776237000
1	1.005730000	-1.250028000	5.330526000
1	2.384226000	-1.650115000	4.287923000
1	5.601915000	2.236944000	7.067289000
6	6.377321000	1.921199000	6.373606000
6	6.081613000	0.818520000	5.559632000
1	5.111302000	0.348399000	5.708041000
6	7.096242000	-0.025024000	4.812331000
1	7.599968000	-0.715830000	5.505447000
1	6.543994000	-0.652282000	4.104311000
6	8.132859000	0.819713000	4.037579000
1	8.481078000	0.247731000	3.170506000
1	9.023048000	0.996563000	4.651216000
6	7.556266000	2.156284000	3.560569000
6	7.624465000	3.369976000	4.309963000
1	7.674473000	4.290950000	3.731257000
1	7.564290000	2.276331000	2.480502000
6	8.224483000	3.524692000	5.697594000
1	9.322588000	3.578147000	5.636684000
1	7.892171000	4.492731000	6.090467000
6	7.787768000	2.410094000	6.672203000
1	8.489222000	1.570703000	6.634559000
1	7.823624000	2.789069000	7.698883000

1^{Ph} (type I)
E= -2826.02375567

45	1.591928000	3.807527000	2.729403000
26	-0.096005000	2.161975000	-1.202850000
15	0.262834000	4.858635000	1.019891000
16	-4.081892000	3.401853000	1.097518000
6	-0.608160000	3.981659000	-0.352617000
6	-1.708938000	3.042512000	-0.240396000
6	-2.080205000	2.658111000	-1.566668000
6	-1.240093000	3.329768000	-2.495533000
6	-0.337368000	4.145367000	-1.758847000
1	-2.864100000	1.950719000	-1.802729000
1	-1.257578000	3.219677000	-3.571560000
1	0.429384000	4.771987000	-2.186682000
6	0.053300000	0.093312000	-1.285992000
6	0.842607000	0.684198000	-2.319749000
6	1.819422000	1.523371000	-1.701630000
6	1.630079000	1.450572000	-0.287668000
6	0.538051000	0.569051000	-0.030225000
1	-0.788565000	-0.569992000	-1.432626000
1	0.706351000	0.543652000	-3.383712000
1	2.555060000	2.124636000	-2.219346000
1	2.175549000	1.999588000	0.470025000
1	0.131930000	0.351431000	0.948280000
6	-2.425716000	2.570052000	0.987060000
1	-1.845112000	2.769049000	1.885417000
1	-2.608652000	1.493708000	0.933321000
6	-2.025771000	6.540071000	0.945280000
6	-3.018288000	7.329355000	1.524071000
6	-3.086127000	7.463756000	2.913752000
6	-2.160170000	6.805112000	3.723091000
6	-1.160349000	6.018675000	3.145574000
6	-1.080463000	5.885714000	1.752273000
1	-1.991600000	6.425696000	-0.134083000
1	-3.746589000	7.828421000	0.891586000
1	-3.866183000	8.071879000	3.362748000
1	-2.219034000	6.892957000	4.804030000
1	-0.449003000	5.487747000	3.771751000
6	1.153645000	7.469473000	0.262594000
6	2.003939000	8.364564000	-0.393946000
6	3.014099000	7.893027000	-1.231292000
6	3.178097000	6.516426000	-1.403356000
6	2.337528000	5.621860000	-0.740673000
6	1.302368000	6.085110000	0.092471000
1	0.369633000	7.855748000	0.904298000
1	1.869038000	9.432792000	-0.249860000
1	3.670760000	8.589855000	-1.743839000
1	3.964063000	6.137176000	-2.050451000
1	2.480624000	4.554540000	-0.880623000
17	-0.045834000	2.227322000	3.459695000
6	2.944861000	5.428071000	3.021237000
6	3.389448000	5.076634000	4.461325000
6	4.359989000	5.534016000	3.115462000
6	3.550906000	4.465638000	2.182628000
1	2.598859000	6.410408000	2.721829000
1	3.756713000	4.581167000	1.126542000
6	4.822902000	4.537672000	4.205821000
1	5.261040000	4.047530000	5.083228000
1	5.505891000	5.303842000	3.821170000
6	2.620716000	3.756024000	4.679928000
1	1.894390000	3.569680000	5.461417000
6	3.216694000	2.809181000	3.855657000
1	3.045752000	1.739788000	3.866084000
1	3.253180000	5.849523000	5.217923000
1	5.111129000	2.901388000	2.642129000
6	-4.838323000	2.559271000	2.482231000
6	-6.236435000	2.428246000	2.470936000
6	-4.111301000	2.073760000	3.580050000
6	-6.896212000	1.832059000	3.544958000
6	-4.781316000	1.458222000	4.639277000
6	-6.171764000	1.338257000	4.631927000
1	-6.802178000	2.785901000	1.615072000
1	-3.031984000	2.175687000	3.622166000
1	-7.978767000	1.739818000	3.522586000
1	-4.205366000	1.079664000	5.479353000
1	-6.685629000	0.863020000	5.462429000

1^{Ph} (type II')
E= -2826.01873805

45	-0.380391000	4.129509000	3.357878000
26	-1.473489000	3.180117000	-1.437828000
15	-0.858047000	5.403661000	1.387616000
16	-1.459109000	1.860135000	2.068763000
6	-1.857466000	4.612134000	0.064955000
6	-2.753498000	3.484251000	0.194422000
6	-3.491672000	3.381472000	-1.027003000
6	-3.064638000	4.413371000	-1.912844000
6	-2.048894000	5.158506000	-1.252800000
1	-4.228559000	2.618763000	-1.243111000
1	-3.413601000	4.569147000	-2.924951000
1	-1.499777000	5.994081000	-1.664197000
6	-1.294584000	1.571989000	-2.738512000
6	-0.562146000	2.690753000	-3.239254000
6	0.430332000	3.037041000	-2.275504000
6	0.311078000	2.128162000	-1.179546000
6	-0.752647000	1.223482000	-1.465639000
1	-2.136656000	1.095948000	-3.222962000
1	-0.753687000	3.210280000	-4.168727000
1	1.123652000	3.863046000	-2.344065000
1	0.900799000	2.131914000	-0.274054000

1	-1.109241000	0.442391000	-0.809571000
6	-3.010799000	2.606074000	1.385503000
1	-3.671201000	1.783485000	1.101209000
1	-3.468333000	3.188163000	2.191010000
6	-2.973455000	7.331209000	1.107761000
6	-3.648860000	8.497695000	1.479379000
6	-3.179364000	9.275893000	2.536431000
6	-2.035637000	8.877203000	3.233704000
6	-1.370633000	7.706831000	2.875027000
6	-1.823714000	6.927963000	1.797568000
1	-3.354606000	6.735823000	0.286304000
1	-4.545206000	8.792185000	0.940695000
1	-3.705795000	10.181465000	2.824290000
1	-1.672929000	9.467348000	4.070472000
1	-0.509024000	7.376772000	3.447626000
6	0.620393000	7.426767000	-0.012820000
6	1.724513000	7.904709000	-0.724280000
6	2.802472000	7.063885000	-1.001890000
6	2.772355000	5.738157000	-0.562607000
6	1.669850000	5.261558000	0.147543000
6	0.575084000	6.095280000	0.429731000
1	-0.205435000	8.096429000	0.200471000
1	1.739000000	8.938394000	-1.058313000
1	3.661792000	7.438408000	-1.550590000
1	3.609432000	5.076070000	-0.766218000
1	1.659422000	4.231752000	0.485876000
17	-2.645948000	4.641774000	4.165016000
6	1.679968000	4.704230000	3.507773000
6	1.786578000	4.775519000	5.045360000
6	1.619642000	2.575510000	4.534250000
6	1.589752000	3.327940000	3.180629000
1	2.001616000	5.501885000	2.849907000
1	1.855796000	2.866385000	2.236510000
6	2.573917000	3.477975000	5.360144000
1	2.581051000	3.229363000	6.428098000
1	3.598460000	3.493977000	4.969402000
6	0.350571000	4.356045000	5.407811000
1	-0.348088000	4.949115000	5.984080000
6	0.244265000	2.991412000	5.106808000
1	-0.529322000	2.311016000	5.440506000
1	2.142833000	5.715888000	5.466877000
1	1.827995000	1.506044000	4.493983000
6	-2.109256000	0.687636000	3.263283000
6	-3.038403000	1.049110000	4.250663000
6	-1.617820000	-0.625616000	3.214253000
6	-3.479338000	0.090189000	5.164547000
6	-2.050029000	-1.569870000	4.147565000
6	-2.987489000	-1.216595000	5.119765000
1	-3.383750000	2.075480000	4.321437000
1	-0.903763000	-0.903603000	2.444400000
1	-4.201284000	0.374648000	5.924914000
1	-1.663493000	-2.584232000	4.103216000
1	-3.331676000	-1.954325000	5.838807000

1^{tBu} (type I)

E= -2752.23529085

45	-0.613489000	6.094079000	3.013217000
26	0.656851000	3.335107000	-0.483930000
15	-1.467170000	5.895560000	0.779264000
16	-1.836432000	0.677875000	1.008656000
6	-1.036708000	4.519082000	-0.370264000
6	-1.392974000	3.115719000	-0.239807000
6	-0.973480000	2.458822000	-1.437515000
6	-0.359306000	3.410850000	-2.298615000
6	-0.403360000	4.676841000	-1.656154000
1	-1.075400000	1.399304000	-1.624611000
1	0.090948000	3.204975000	-3.260566000
1	-0.016982000	5.598852000	-2.061566000
6	2.002577000	1.810001000	-0.079369000
6	2.628752000	2.818033000	-0.873385000
6	2.579121000	4.045964000	-0.144797000
6	1.920876000	3.793352000	1.098839000
6	1.564202000	2.412706000	1.138747000
1	1.845620000	0.779331000	-0.366810000
1	3.040047000	2.683164000	-1.864810000
1	2.958080000	4.999819000	-0.487561000
1	1.676451000	4.524649000	1.858581000
1	1.010747000	1.920426000	1.926400000
6	-2.183240000	2.486796000	0.876390000
1	-3.250018000	2.616621000	0.663085000
1	-1.972115000	2.972824000	1.830067000
6	-3.991641000	5.516764000	-0.470828000
6	-5.385285000	5.557922000	-0.521701000
6	-6.115408000	5.985300000	0.590737000
6	-5.447804000	6.367309000	1.754742000
6	-4.052720000	6.321315000	1.811287000
6	-3.312296000	5.901274000	0.697246000
1	-3.432103000	5.181075000	-1.338541000
1	-5.900085000	5.254348000	-1.428881000
1	-7.200672000	6.013185000	0.550648000
1	-6.009904000	6.688068000	2.626991000
1	-3.535905000	6.585646000	2.728004000
6	-1.944724000	8.384237000	-0.533758000
6	-1.555398000	9.548748000	-1.201852000
6	-0.222022000	9.744426000	-1.560908000
6	0.725500000	8.768785000	-1.243266000
6	0.340227000	7.610218000	-0.568430000
6	-1.003191000	7.395134000	-0.210852000
1	-2.986973000	8.248294000	-0.267340000
1	-2.301412000	10.300276000	-1.444290000
1	0.077878000	10.648341000	-2.082918000
1	1.767080000	8.909438000	-1.518238000
1	1.088508000	6.860122000	-0.333400000
6	0.044787000	8.120427000	2.905976000
6	0.010684000	8.436520000	4.420166000
6	1.783913000	7.061170000	4.110690000
6	1.151834000	7.264067000	2.713312000
1	-0.428377000	8.739239000	2.153358000
1	1.695182000	7.114889000	1.789423000
6	1.526898000	8.450467000	4.754493000
1	1.729965000	8.469492000	5.831727000
1	2.068205000	9.261672000	4.254069000
6	-0.396130000	7.061036000	4.988210000
1	-1.278987000	6.858589000	5.581836000
6	0.690881000	6.216748000	4.799857000
1	0.823982000	5.226423000	5.217724000
1	-0.596492000	9.288193000	4.727387000
1	2.796920000	6.659131000	4.135055000
17	-1.951100000	4.342445000	3.917678000
6	-3.210342000	0.039077000	2.108259000
6	-2.932803000	-1.471288000	2.201085000
6	-4.587613000	0.274590000	1.470925000
1	-4.826977000	1.339148000	1.393242000
1	-4.643467000	-0.167125000	0.471653000
1	-5.364327000	-0.185493000	2.094546000
1	-2.982010000	-1.950106000	1.217713000
1	-3.684269000	-1.941479000	2.845802000
1	-1.946588000	-1.669158000	2.632750000
6	-3.137900000	0.676800000	3.502926000
1	-3.278349000	1.759993000	3.469791000
1	-3.923669000	0.253986000	4.142310000
1	-2.170832000	0.482313000	3.974886000

1^{tBu} (type II')

E= -2752.22229352

45	0.573577000	3.685269000	2.810000000
26	-0.173670000	2.684992000	-1.719244000
15	-0.058781000	5.100077000	1.051127000
16	-1.029729000	1.714775000	1.889026000
6	-0.726600000	4.269838000	-0.439482000
6	-1.709318000	3.215271000	-0.398996000
6	-2.211691000	3.038924000	-1.726343000
6	-1.549301000	3.959248000	-2.590867000
6	-0.630972000	4.711226000	-1.805341000
1	-2.949970000	2.303412000	-2.018841000
1	-1.687505000	4.042323000	-3.660582000
1	0.033024000	5.482948000	-2.167306000
6	0.051500000	0.791693000	-2.537668000
6	0.764328000	1.752193000	-3.316586000
6	1.741811000	2.363280000	-2.475113000
6	1.630022000	1.780339000	-1.175889000
6	0.587340000	0.808127000	-1.215527000
1	-0.774894000	0.184086000	-2.881303000
1	0.575798000	1.997733000	-4.353077000
1	2.430088000	3.142758000	-2.772409000
1	2.205844000	2.044532000	-0.300143000
1	0.237695000	0.227197000	-0.374642000
6	-2.280030000	2.536804000	0.811772000
1	-2.993831000	1.776082000	0.486118000
1	-2.810460000	3.268181000	1.429250000
6	-2.314273000	6.739277000	0.424160000
6	-3.248395000	7.740285000	0.698513000
6	-3.238175000	8.390878000	1.933486000
6	-2.296737000	8.029186000	2.897868000
6	-1.370411000	7.018472000	2.634676000
6	-1.362830000	6.370697000	1.388844000
1	-2.331801000	6.250026000	-0.543150000
1	-3.981804000	8.010465000	-0.056151000
1	-3.965625000	9.169435000	2.145609000
1	-2.293288000	8.515527000	3.868837000
1	-0.680712000	6.706507000	3.409755000
6	1.474527000	7.480885000	0.754502000
6	2.552300000	8.237879000	0.289503000
6	3.494084000	7.671419000	-0.570019000
6	3.352103000	6.339119000	-0.960925000
6	2.279374000	5.579283000	-0.491686000
6	1.321027000	6.139338000	0.369354000
1	0.746287000	7.944189000	1.410647000
1	2.648730000	9.274980000	0.597927000
1	4.329578000	8.262545000	-0.933592000
1	4.077933000	5.887272000	-1.631556000
1	2.174128000	4.550304000	-0.812735000
6	2.382584000	4.661257000	3.160529000
6	2.767821000	4.108104000	4.549100000
6	3.116309000	2.403326000	3.100133000
6	2.600077000	3.573423000	2.235334000
1	2.472437000	5.714620000	2.918787000
1	2.908110000	3.695891000	1.204759000
6	3.932317000	3.149560000	4.187918000
1	4.234008000	2.503837000	5.022280000
1	4.806319000	3.672078000	3.781940000
6	1.619737000	3.103656000	4.766025000
1	0.857540000	3.178183000	5.529855000
6	1.834250000	2.067492000	3.881291000
1	1.306154000	1.126340000	3.831516000
1	2.921597000	4.838952000	5.342823000
1	3.593306000	1.574949000	2.574566000
17	-1.335525000	4.315846000	4.414489000
6	-2.172568000	0.744466000	3.060936000
6	-1.327118000	0.403493000	4.294599000
6	-2.587637000	-0.541928000	2.329546000
1	-3.149839000	-0.329485000	1.414305000
1	-1.718680000	-1.150779000	2.062916000
1	-3.238351000	-1.138473000	2.981112000
1	-0.438190000	-0.178673000	4.027548000
1	-1.925808000	-0.211191000	4.976829000
1	-1.027447000	1.310889000	4.823939000
6	-3.405883000	1.552416000	3.485551000
1	-4.092090000	1.728304000	2.652048000
1	-3.956499000	0.971787000	4.236131000
1	-3.118070000	2.509393000	3.925559000

2^{Ph}

E= -2790.28707810

45	0.779490000	3.406418000	2.367401000
26	-0.159673000	2.585383000	-1.943332000
15	0.073541000	4.959677000	0.760940000
16	-0.892820000	1.810723000	1.715822000
6	-0.683910000	4.200357000	-0.714794000
6	-1.677314000	3.155913000	-0.631318000
6	-2.198470000	2.949514000	-1.947843000
6	-1.539506000	3.844730000	-2.840390000
6	-0.604525000	4.610963000	-2.087226000
1	-2.949857000	2.217597000	-2.214215000
1	-1.692950000	3.903465000	-3.909491000
1	0.068430000	5.361315000	-2.477742000
6	0.094869000	0.682499000	-2.735566000
6	0.817598000	1.638815000	-3.509967000
6	1.770803000	2.268871000	-2.655043000
6	1.636244000	1.701662000	-1.351157000
6	0.601258000	0.720493000	-1.402097000
1	-0.716028000	0.060949000	-3.090593000
1	0.650562000	1.869407000	-4.553434000
1	2.456993000	3.052784000	-2.945262000
1	2.194311000	1.980240000	-0.466962000
1	0.247212000	0.132581000	-0.567403000
6	-2.215913000	2.513480000	0.611049000
1	-2.872487000	1.678319000	0.355928000
1	-2.783575000	3.230481000	1.212152000
6	-2.092651000	6.763859000	0.454369000
6	-3.117798000	7.577215000	0.933326000
6	-3.339200000	7.691569000	2.310703000
6	-2.533225000	6.994648000	3.209669000
6	-1.499024000	6.181196000	2.735535000
6	-1.272106000	6.061017000	1.356705000
1	-1.935969000	6.670631000	-0.616045000
1	-3.748500000	8.116430000	0.232011000
1	-4.145790000	8.319464000	2.678409000
1	-2.700266000	7.049378000	4.279858000
1	-0.886104000	5.650665000	3.457045000
6	1.380004000	7.452235000	0.414306000
6	2.412313000	8.277483000	-0.040582000
6	3.445637000	7.750815000	-0.815262000
6	3.451079000	6.388972000	-1.128900000
6	2.427562000	5.560220000	-0.669364000
6	1.373005000	6.085503000	0.098095000
1	0.579618000	7.875221000	1.011905000
1	2.403453000	9.333463000	0.212750000
1	4.245189000	8.394666000	-1.169459000
1	4.255752000	5.970732000	-1.727058000
1	2.443948000	4.502605000	-0.910911000
9	-1.430075000	5.681139000	7.631457000
6	2.070519000	4.715055000	3.519540000
6	2.107813000	3.894412000	4.824802000
6	3.354332000	2.746082000	3.316717000
6	2.842083000	4.007588000	2.584383000
1	1.785264000	5.759329000	3.484599000
1	3.281412000	4.405407000	1.677209000
6	3.547538000	3.312980000	4.750694000
1	3.734819000	2.534624000	5.499122000

1	4.325371000	4.083052000	4.806522000
6	1.288762000	2.648516000	4.434180000
1	0.391153000	2.343081000	4.957711000
6	2.045718000	1.944003000	3.512688000
1	1.882393000	0.930372000	3.163983000
1	1.770106000	4.408422000	5.719455000
1	4.181970000	2.214727000	2.845996000
6	-1.883091000	1.267694000	3.120249000
6	-2.321475000	2.166620000	4.099303000
6	-2.188825000	-0.097856000	3.211014000
6	-3.075245000	1.692168000	5.174638000
6	-2.946807000	-0.559045000	4.288482000
6	-3.388698000	0.334787000	5.267556000
1	-2.073945000	3.221599000	4.061091000
1	-1.832808000	-0.787828000	2.451553000
1	-3.384822000	2.398230000	5.937448000
1	-3.184981000	-1.616010000	4.364088000
1	-3.969648000	-0.030047000	6.109463000
5	-1.181659000	5.024928000	6.430044000
9	-0.648734000	3.730526000	6.658726000
9	-2.382990000	4.893271000	5.675036000
9	-0.247881000	5.763942000	5.642819000

2^{tBu}

E= -2716.49423510

45	0.769887000	3.465906000	2.393647000
26	-0.066104000	2.577270000	-1.884545000
15	0.068445000	4.986399000	0.772351000
16	-1.020682000	1.890361000	1.826586000
6	-0.644517000	4.219332000	-0.716376000
6	-1.626862000	3.167929000	-0.637543000
6	-2.104641000	2.924157000	-1.964407000
6	-1.426128000	3.802840000	-2.858397000
6	-0.523433000	4.597275000	-2.095574000
1	-2.841224000	2.179068000	-2.235886000
1	-1.545666000	3.833171000	-3.933037000
1	0.152162000	5.345723000	-2.484431000
6	0.208591000	0.625598000	-2.536847000
6	0.908792000	1.532067000	-3.388386000
6	1.862604000	2.235751000	-2.593338000
6	1.749787000	1.764122000	-1.249976000
6	0.727440000	0.769302000	-1.215457000
1	-0.596880000	-0.031620000	-2.835634000
1	0.726988000	1.682477000	-4.443949000
1	2.536184000	3.003717000	-2.948898000
1	2.317718000	2.109978000	-0.396803000
1	0.386122000	0.245441000	-0.334065000
6	-2.231500000	2.567971000	0.597027000
1	-2.874111000	1.736757000	0.303940000
1	-2.844632000	3.315272000	1.110601000
6	-2.128257000	6.756346000	0.475173000
6	-3.166065000	7.548749000	0.962716000
6	-3.386797000	7.647866000	2.341558000
6	-2.567917000	6.957942000	3.235036000
6	-1.520789000	6.165973000	2.752467000
6	-1.296154000	6.060323000	1.371418000
1	-1.969532000	6.674956000	-0.596198000
1	-3.806276000	8.084328000	0.267188000
1	-4.202989000	8.259846000	2.715096000
1	-2.732309000	6.999268000	4.306787000
1	-0.893619000	5.640147000	3.467168000
6	1.389748000	7.480318000	0.550424000
6	2.414289000	8.327529000	0.120059000
6	3.415085000	7.849482000	-0.726261000
6	3.393604000	6.515017000	-1.138910000
6	2.376796000	5.663711000	-0.705363000
6	1.356926000	6.139672000	0.137057000
1	0.614237000	7.865941000	1.203923000
1	2.424934000	9.362875000	0.447596000
1	4.208653000	8.510792000	-1.061226000
1	4.170817000	6.135074000	-1.796052000
1	2.367473000	4.628655000	-1.030516000
9	-0.868088000	5.382177000	7.746722000
6	2.290870000	4.747441000	3.233834000
6	2.434099000	4.092748000	4.622704000
6	3.364558000	2.644498000	3.148579000
6	2.874817000	3.851480000	2.316824000
1	2.121595000	5.807479000	3.090346000
1	3.250998000	4.099168000	1.331362000
6	3.794140000	3.360255000	4.458795000
1	4.008562000	2.663699000	5.277349000
1	4.638059000	4.045232000	4.317477000
6	1.460653000	2.909003000	4.497523000
1	0.596049000	2.801960000	5.143144000
6	2.023773000	2.019432000	3.600144000
1	1.719491000	0.999041000	3.400366000
1	2.265974000	4.741780000	5.477623000
1	4.072534000	1.974019000	2.660657000
5	-1.076921000	4.930435000	6.448210000
9	-0.940642000	3.507026000	6.390411000
9	-2.361852000	5.281388000	5.978340000
9	-0.103461000	5.493425000	5.566256000
6	-2.195681000	1.288073000	3.209030000
6	-1.304844000	0.512720000	4.188338000
6	-3.215992000	0.328309000	2.576410000
1	-3.939748000	0.844273000	1.940286000
1	-2.730733000	-0.462046000	1.994723000
1	-3.783447000	-0.147365000	3.383803000
1	-0.794114000	-0.323198000	3.698518000
1	-1.938083000	0.104865000	4.983259000
1	-0.569528000	1.157964000	4.667110000
6	-2.890478000	2.461132000	3.904312000
1	-3.490699000	3.057104000	3.210693000
1	-3.574567000	2.063451000	4.663192000
1	-2.188804000	3.115049000	4.422303000

3^{Ph} (type I)

E= -2866.57510086

45	6.260572000	2.429300000	4.144528000
26	4.787013000	0.876001000	0.110033000
15	5.018011000	3.568654000	2.370492000
16	0.496399000	1.973671000	1.723074000
6	4.256571000	2.716610000	0.912467000
6	3.109339000	1.827590000	0.891992000
6	2.879209000	1.454352000	-0.469205000
6	3.846856000	2.090249000	-1.293089000
6	4.694098000	2.864540000	-0.454388000
1	2.094013000	0.786498000	-0.796841000
1	3.946252000	1.983156000	-2.364907000
1	5.525402000	3.461078000	-0.793306000
6	4.861372000	-1.196068000	0.039571000
6	5.774882000	-0.639925000	-0.907818000
6	6.715705000	0.162895000	-0.192594000
6	6.379921000	0.102675000	1.194101000
6	5.233270000	-0.734713000	1.338237000
1	4.012338000	-1.824747000	-0.193219000
1	5.741900000	-0.777833000	-1.980329000
1	7.523325000	0.734362000	-0.630814000
1	6.861479000	0.642523000	2.000507000
1	4.717804000	-0.928071000	2.269206000
6	2.229257000	1.393708000	2.028022000
1	2.591369000	1.785723000	2.974945000
1	2.195675000	0.304483000	2.107473000
6	2.606329000	5.073260000	2.270536000
6	1.565543000	5.807121000	2.839862000
6	1.501186000	5.975209000	4.225453000
6	2.478205000	5.403917000	5.041997000
6	3.521084000	4.668466000	4.475266000
6	3.598522000	4.502810000	3.084469000
1	2.641005000	4.938747000	1.193825000
1	0.799039000	6.236375000	2.201599000
1	0.684962000	6.540212000	4.666362000
1	2.423992000	5.518047000	6.120757000
1	4.267758000	4.198315000	5.108548000
6	5.746452000	6.257782000	1.703725000
6	6.554603000	7.228370000	1.104655000
6	7.646269000	6.853564000	0.322285000
6	7.932447000	5.498128000	0.146159000
6	7.132152000	4.528652000	0.751087000
6	6.018383000	4.892083000	1.530802000
1	4.899585000	6.570461000	2.303865000
1	6.323442000	8.279681000	1.250782000
1	8.270893000	7.609382000	-0.144656000
1	8.781375000	5.193067000	-0.459102000
1	7.369542000	3.479299000	0.603253000
17	4.369855000	1.016400000	4.607157000
1	6.101531000	1.739171000	6.716155000
6	7.024919000	1.952048000	6.183463000
6	7.470383000	0.976869000	5.295729000
1	6.873053000	0.071067000	5.225453000
6	8.851641000	0.894112000	4.680419000
1	9.564474000	0.457314000	5.396549000
1	8.797432000	0.191670000	3.841838000
6	9.365599000	2.256287000	4.166189000
1	10.082669000	2.084722000	3.356020000
1	9.923439000	2.777783000	4.950984000
6	8.239424000	3.152622000	3.650648000
6	7.556515000	4.110199000	4.431048000
1	7.153118000	4.971178000	3.900807000
1	8.280363000	3.347816000	2.583761000
6	7.768989000	4.368490000	5.912172000
1	8.654566000	5.004882000	6.066006000
1	6.912852000	4.950747000	6.272134000
6	7.884754000	3.073682000	6.746102000
1	8.927939000	2.748827000	6.805714000
1	7.572031000	3.277693000	7.775616000
6	-0.416992000	1.126857000	3.004360000
6	0.158933000	0.674089000	4.200974000
6	-1.792442000	0.937842000	2.789265000
1	1.215202000	0.817064000	4.401297000
1	-2.241652000	1.270788000	1.857434000
6	-0.634987000	0.034297000	5.155821000
6	-2.577045000	0.313991000	3.757235000
1	-0.173779000	-0.317386000	6.074679000
1	-3.639316000	0.175082000	3.575200000
6	-2.001790000	-0.146470000	4.944142000
1	-2.612324000	-0.642373000	5.692972000

3^{Ph} (type II')

E= -2866.56907954

45	5.296813000	2.899800000	4.550965000
26	4.468913000	1.549877000	-0.389062000
15	4.766160000	3.928997000	2.433456000
16	3.983867000	-0.114406000	2.911788000
6	3.945248000	2.994135000	1.074217000
6	3.043241000	1.861823000	1.140600000
6	2.419900000	1.740470000	-0.141630000
6	2.914246000	2.762303000	-1.001815000
6	3.862905000	3.522353000	-0.264987000
1	1.708609000	0.969150000	-0.407753000
1	2.653179000	2.904461000	-2.041969000
1	4.434094000	4.361749000	-0.635934000
6	4.735651000	-0.098590000	-1.626444000
6	5.444514000	1.026944000	-2.144476000
6	6.397963000	1.436553000	-1.166830000
6	6.276809000	0.560832000	-0.043189000
6	5.253433000	-0.389292000	-0.330514000
1	3.922935000	-0.618402000	-2.115919000
1	5.263023000	1.510431000	-3.095133000
1	7.063542000	2.283391000	-1.251446000
1	6.838977000	0.613462000	0.878811000
1	4.898053000	-1.155298000	0.342172000
6	2.640308000	1.015809000	2.317974000
1	1.792902000	0.387438000	2.033501000
1	2.348866000	1.658638000	3.151650000
6	2.507639000	5.632420000	1.910312000
6	1.683838000	6.725714000	2.194174000
6	1.951005000	7.543359000	3.291503000
6	3.041498000	7.257508000	4.116672000
6	3.854106000	6.158642000	3.845163000
6	3.605095000	5.340537000	2.730349000
1	2.282591000	5.008173000	1.053520000
1	0.830430000	6.932413000	1.554493000
1	1.308931000	8.391947000	3.509742000
1	3.247958000	7.877638000	4.984240000
1	4.673569000	5.917029000	4.515586000
6	6.204540000	6.149903000	1.320803000
6	7.289433000	6.743426000	0.668857000
6	8.347874000	5.962846000	0.205449000
6	8.315692000	4.579766000	0.397468000
6	7.232547000	3.987486000	1.046929000
6	6.158368000	4.760672000	1.518523000
1	5.392817000	6.775359000	1.673211000
1	7.301310000	7.820126000	0.524930000
1	9.191409000	6.425810000	-0.298303000
1	9.136170000	3.960201000	0.045926000
1	7.218562000	2.913183000	1.179959000
17	2.945924000	3.079213000	5.131487000
1	4.869270000	3.196856000	7.176278000
6	5.736790000	2.707828000	6.741057000
6	5.542511000	1.442074000	6.199977000
1	4.543016000	1.020103000	6.272513000
6	6.632420000	0.462765000	5.815413000
1	7.022086000	-0.045489000	6.710931000
1	6.168779000	-0.312163000	5.198402000
6	7.786423000	1.115066000	5.020953000
1	8.248114000	0.355900000	4.380283000
1	8.578073000	1.452988000	5.698827000
6	7.319966000	2.282161000	4.150869000
6	7.296515000	3.634363000	4.566580000
1	7.409995000	4.386055000	3.787957000
1	7.430394000	2.106023000	3.084505000
6	7.665464000	4.152777000	5.945519000
1	8.759089000	4.245798000	6.040526000
1	7.265532000	5.169974000	6.029923000
6	7.094598000	3.294111000	7.094088000
1	7.791307000	2.491014000	7.353264000
1	6.994150000	3.911630000	7.993129000
6	3.124753000	-1.117590000	4.122461000
6	3.365640000	-2.500774000	4.111116000
6	2.276568000	-0.572295000	5.099326000
1	4.009849000	-2.926379000	3.346959000
1	2.110687000	0.499274000	5.142544000
6	2.774874000	-3.325609000	5.069338000
6	1.670683000	-1.410702000	6.037124000
1	2.971133000	-4.394148000	5.051250000
1	1.011382000	-0.979455000	6.785445000
6	1.919182000	-2.784840000	6.030906000
1	1.449391000	-3.428944000	6.768588000

3^{tBu}

E= -2792.78688826

45	5.656827000	2.617550000	4.393955000
26	4.478935000	1.612777000	-0.280471000
15	4.870237000	3.929153000	2.521666000
16	1.684248000	-0.218504000	1.739606000
6	4.043993000	3.145230000	1.072163000
6	2.990558000	2.144290000	1.068905000
6	2.458586000	2.090292000	-0.255905000
6	3.167504000	3.011025000	-1.079010000
6	4.138857000	3.661323000	-0.272416000
1	1.681068000	1.412212000	-0.577420000
1	3.021217000	3.159924000	-2.140564000
1	4.839534000	4.412414000	-0.605862000
6	4.554026000	-0.291051000	-1.098086000
6	5.312413000	0.614084000	-1.899751000
6	6.348656000	1.163092000	-1.085777000
6	6.227439000	0.594513000	0.219631000
6	5.118130000	-0.302451000	0.212924000
1	3.676482000	-0.839199000	-1.412452000
1	5.116502000	0.865722000	-2.933411000
1	7.080297000	1.894357000	-1.401992000
1	6.841215000	0.823856000	1.078396000
1	4.738264000	-0.860857000	1.057093000
6	2.487392000	1.362593000	2.251697000
1	1.755658000	1.963035000	2.799947000
1	3.303075000	1.153495000	2.942826000
6	2.694303000	5.736816000	2.130233000
6	1.824389000	6.752340000	2.532758000
6	1.903684000	7.274754000	3.824767000
6	2.851808000	6.772865000	4.717975000
6	3.713432000	5.748641000	4.322926000
6	3.649350000	5.226386000	3.021928000
1	2.624071000	5.342470000	1.122503000
1	1.084320000	7.132840000	1.834419000
1	1.224660000	8.063392000	4.136389000
1	2.910213000	7.162557000	5.730095000
1	4.420300000	5.333544000	5.033628000
6	6.356690000	6.307919000	2.027885000
6	7.411070000	7.048603000	1.488320000
6	8.326077000	6.447476000	0.623673000
6	8.179329000	5.097302000	0.300882000
6	7.129010000	4.354376000	0.841941000
6	6.198201000	4.948531000	1.712119000
1	5.653103000	6.796062000	2.692834000
1	7.510844000	8.099664000	1.744057000
1	9.144068000	7.025167000	0.203286000
1	8.883070000	4.618449000	-0.374394000
1	7.018429000	3.312947000	0.564918000
17	3.435176000	2.553620000	5.316176000
6	0.685060000	-0.704774000	3.247692000
6	0.049295000	-2.047834000	2.850168000
6	-0.414656000	0.327130000	3.536691000
1	-0.001038000	1.300585000	3.814440000
1	-1.068532000	0.461187000	2.670050000
1	-1.027385000	-0.014946000	4.380088000
1	-0.598004000	-1.941018000	1.973564000
1	-0.562683000	-2.421485000	3.679119000
1	0.811924000	-2.800596000	2.626716000
6	1.595976000	-0.888411000	4.470475000
1	2.077976000	0.047579000	4.766972000
1	1.000378000	-1.238727000	5.323221000
1	2.373155000	-1.633001000	4.270984000
1	5.614916000	2.214759000	7.045592000
6	6.407894000	1.881675000	6.381239000
6	6.123162000	0.796204000	5.561277000
1	5.139624000	0.344863000	5.670896000
6	7.129050000	-0.022248000	4.778242000
1	7.628149000	-0.747586000	5.439102000
1	6.570835000	-0.614483000	4.045169000
6	8.174604000	0.840324000	4.035447000
1	8.538615000	0.283385000	3.165055000
1	9.053447000	1.008339000	4.667152000
6	7.608302000	2.181834000	3.569463000
6	7.649689000	3.378618000	4.317985000
1	7.647638000	4.306432000	3.749442000
1	7.575310000	2.303539000	2.490700000
6	8.204853000	3.544895000	5.720820000
1	9.300411000	3.653543000	5.686287000
1	7.818624000	4.491437000	6.116578000
6	7.804845000	2.401556000	6.677603000
1	8.529172000	1.583262000	6.621593000
1	7.837920000	2.765876000	7.709849000

4^{Ph}

E= -2830.83838333

45	5.624627000	2.165744000	3.857621000
26	4.606517000	1.301822000	-0.462617000
15	4.947078000	3.705487000	2.211264000
16	3.865492000	0.636395000	3.203603000
6	4.160439000	2.952520000	0.745874000
6	3.118516000	1.960439000	0.845664000
6	2.584272000	1.757589000	-0.465296000
6	3.280816000	2.609031000	-1.372169000
6	4.253252000	3.341364000	-0.633069000
1	1.799070000	1.057281000	-0.718686000
1	3.126217000	2.660535000	-2.441482000
1	4.956081000	4.055558000	-1.037636000
6	4.775309000	-0.620838000	-1.228817000
6	5.538407000	0.291595000	-2.017463000
6	6.519757000	0.890930000	-1.172293000
6	6.361545000	0.349712000	0.139970000
6	5.284337000	-0.585859000	0.103693000
1	3.937375000	-1.211264000	-1.574081000
1	5.379923000	0.514819000	-3.063859000
1	7.239537000	1.640143000	-1.473100000
1	6.931033000	0.620135000	1.019228000
1	4.903072000	-1.143423000	0.946970000
6	2.561452000	1.369820000	2.103651000
1	1.871428000	0.554440000	1.874542000
1	2.027372000	2.123304000	2.690701000
6	2.834816000	5.565440000	1.887892000
6	1.825734000	6.406030000	2.353511000
6	1.587000000	6.524367000	3.727611000
6	2.358163000	5.802832000	4.637563000
6	3.374168000	4.960481000	4.174869000
6	3.621734000	4.836833000	2.800014000
1	3.005418000	5.471450000	0.819718000
1	1.221435000	6.964185000	1.643796000
1	0.793731000	7.174710000	4.084861000
1	2.183032000	5.861439000	5.705680000
1	3.955927000	4.403666000	4.901541000
6	6.274402000	6.180901000	1.801763000
6	7.294905000	6.991873000	1.297554000
6	8.290182000	6.448206000	0.485683000
6	8.268965000	5.084135000	0.183482000
6	7.257199000	4.269673000	0.692001000
6	6.240770000	4.811454000	1.498736000
1	5.502137000	6.618116000	2.425587000
1	7.306466000	8.050076000	1.541239000
1	9.080503000	7.080939000	0.092856000
1	9.043763000	4.652703000	-0.443952000
1	7.252831000	3.210166000	0.457955000
9	2.676512000	4.144377000	9.219674000
5	3.041628000	3.798568000	7.922299000
9	3.795064000	2.592553000	7.917049000
9	1.888175000	3.610171000	7.109864000
9	3.834940000	4.825328000	7.333017000
1	4.945032000	1.005763000	6.246226000
6	5.964760000	1.222279000	5.939005000
6	6.543188000	0.414322000	4.974894000
1	5.972146000	-0.449151000	4.636587000
6	8.009351000	0.383979000	4.592768000
1	8.572155000	-0.240110000	5.303130000
1	8.088352000	-0.118175000	3.622003000
6	8.651210000	1.785094000	4.490968000
1	9.509913000	1.730885000	3.813145000
1	9.052213000	2.092339000	5.460956000
6	7.691280000	2.855926000	3.976726000
6	6.898284000	3.681947000	4.789435000
1	6.618666000	4.649158000	4.372938000
1	7.933237000	3.241087000	2.989746000
6	6.761433000	3.612631000	6.294027000
1	7.586626000	4.173535000	6.760344000
1	5.841239000	4.127218000	6.584398000
6	6.715955000	2.173627000	6.850252000
1	7.724797000	1.790221000	7.031424000
1	6.192100000	2.196048000	7.808326000
6	2.845295000	0.065153000	4.575529000
6	2.611438000	-1.314225000	4.674884000
6	2.300154000	0.954161000	5.508051000
1	3.046340000	-1.994388000	3.948397000
1	2.494668000	2.019696000	5.467167000
6	1.818976000	-1.800145000	5.716014000
6	1.507529000	0.455733000	6.543818000
1	1.636924000	-2.867628000	5.799282000
1	1.111348000	1.157240000	7.269682000
6	1.266841000	-0.915678000	6.646378000
1	0.655787000	-1.298014000	7.458712000

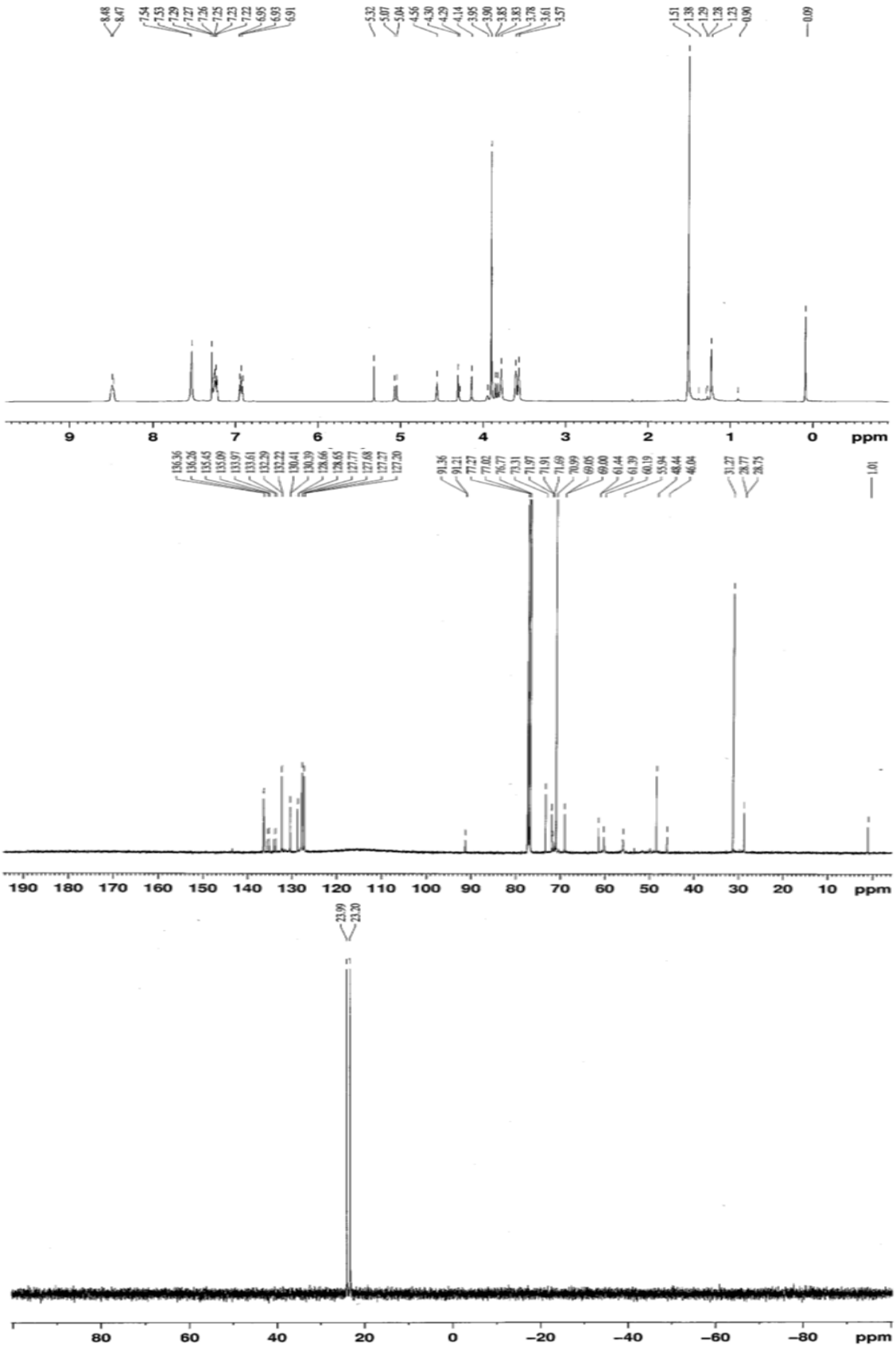
4^{tBu}

E= -2757.04176008

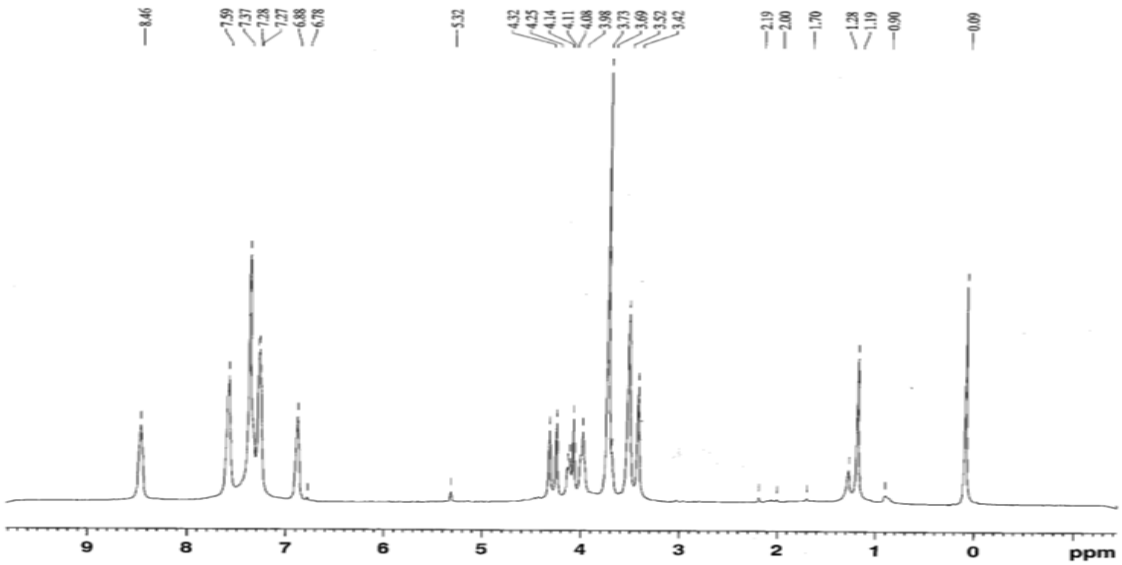
45	5.642355000	2.105939000	3.814710000
26	4.792620000	1.287437000	-0.424131000
15	4.923235000	3.688990000	2.227318000
16	3.698333000	0.627974000	3.241528000
6	4.226928000	2.950769000	0.714141000
6	3.210773000	1.933206000	0.767336000
6	2.766608000	1.692663000	-0.571479000
6	3.498939000	2.544779000	-1.448554000
6	4.401435000	3.317192000	-0.662767000
1	2.014770000	0.969837000	-0.860554000
1	3.413319000	2.573082000	-2.526465000
1	5.107330000	4.044685000	-1.036175000
6	5.061653000	-0.658293000	-1.099498000
6	5.852741000	0.243223000	-1.872823000
6	6.757814000	0.904508000	-0.989151000
6	6.523950000	0.412365000	0.331155000
6	5.476072000	-0.554337000	0.262145000
1	4.264950000	-1.285868000	-1.475504000
1	5.761096000	0.418698000	-2.936207000
1	7.480331000	1.657400000	-1.273789000
1	7.013994000	0.742630000	1.236877000
1	5.045575000	-1.081149000	1.101557000
6	2.552019000	1.380980000	1.993546000
1	1.861301000	0.591387000	1.696920000
1	1.984502000	2.171781000	2.495241000
6	2.651712000	5.366062000	1.970534000
6	1.592210000	6.119024000	2.474026000
6	1.392733000	6.216662000	3.856221000
6	2.254765000	5.565257000	4.738004000
6	3.320859000	4.810740000	4.237573000
6	3.525621000	4.704914000	2.853891000
1	2.795758000	5.288531000	0.896839000
1	0.919636000	6.626330000	1.787888000
1	0.560655000	6.798608000	4.242297000
1	2.111687000	5.608258000	5.812502000
1	3.976393000	4.311973000	4.944275000
6	6.106098000	6.256106000	1.993051000
6	7.071008000	7.161281000	1.543754000
6	8.089220000	6.739482000	0.688461000
6	8.144651000	5.403435000	0.285045000
6	7.187274000	4.494803000	0.737212000
6	6.150558000	4.912279000	1.590553000
1	5.317637000	6.599362000	2.654361000
1	7.021753000	8.197520000	1.864731000
1	8.836589000	7.445784000	0.339431000
1	8.935419000	5.066356000	-0.379117000
1	7.239684000	3.459458000	0.416375000
9	3.655290000	4.199371000	9.378046000
5	3.556533000	3.871722000	8.029409000
9	4.082500000	2.560376000	7.802857000
9	2.215071000	3.905716000	7.586403000
9	4.315106000	4.786218000	7.238116000
6	2.452265000	0.148399000	4.626014000
6	3.166572000	-0.903878000	5.486507000
6	1.227299000	-0.509194000	3.970129000
1	0.592622000	0.209305000	3.446834000
1	1.506053000	-1.313458000	3.281037000
1	0.618428000	-0.949721000	4.766869000
1	3.438950000	-1.787714000	4.900611000
1	2.481379000	-1.219954000	6.280532000
1	4.058562000	-0.514506000	5.976058000
6	2.047150000	1.372487000	5.447882000
1	1.593254000	2.153060000	4.830788000
1	1.298933000	1.070919000	6.190154000
1	2.880335000	1.809430000	5.998407000
1	5.142901000	1.083142000	6.280322000
6	6.140910000	1.195568000	5.869261000
6	6.568686000	0.328223000	4.879085000
1	5.917016000	-0.499582000	4.608233000
6	7.990998000	0.197092000	4.373456000
1	8.580074000	-0.432108000	5.057225000
1	7.957023000	-0.343292000	3.421130000
6	8.693081000	1.556798000	4.161354000
1	9.471611000	1.437950000	3.399984000
1	9.209844000	1.867066000	5.074015000
6	7.740004000	2.665775000	3.717415000
6	7.081005000	3.556077000	4.585964000
1	6.825094000	4.531628000	4.176287000
1	7.913120000	3.023766000	2.706040000
6	7.101677000	3.529180000	6.096838000
1	7.999904000	4.053194000	6.459551000
1	6.241700000	4.096983000	6.461424000
6	7.035403000	2.106421000	6.686446000
1	8.032869000	1.666135000	6.776224000
1	6.611914000	2.169304000	7.691687000

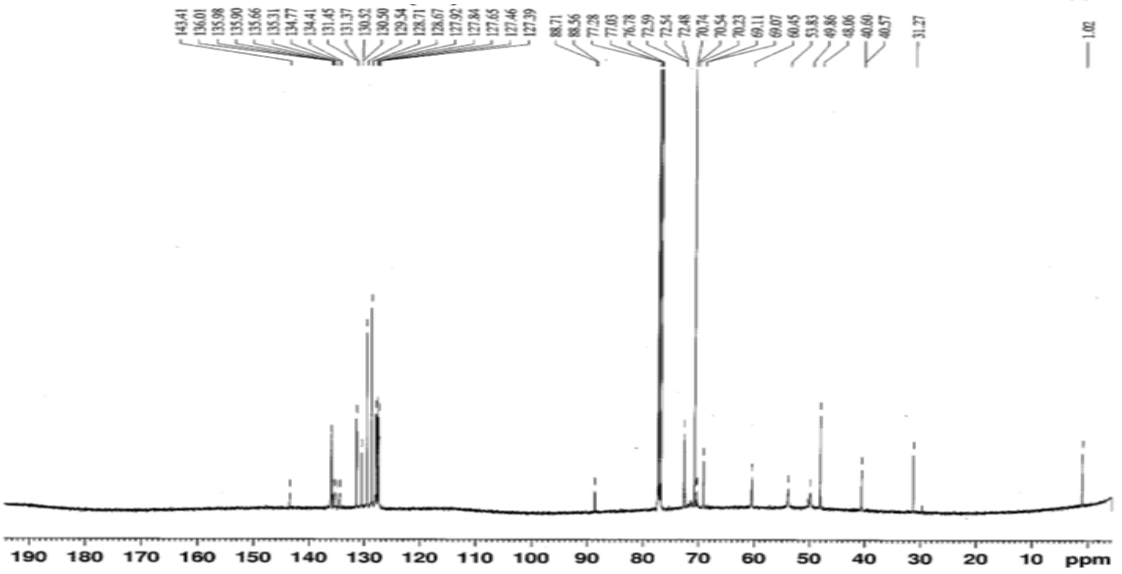
Figure S4. NMR spectra for the isolated compounds (for each compound, spectra are shown in the order: ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$.

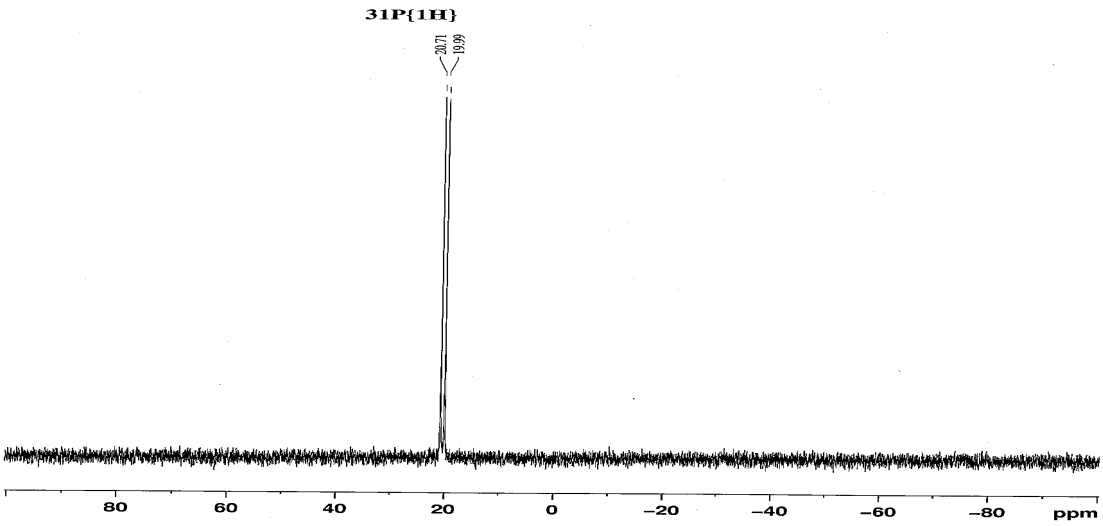
RhCl(NBD)(P,S*t*Bu) **(1^{tBu})**



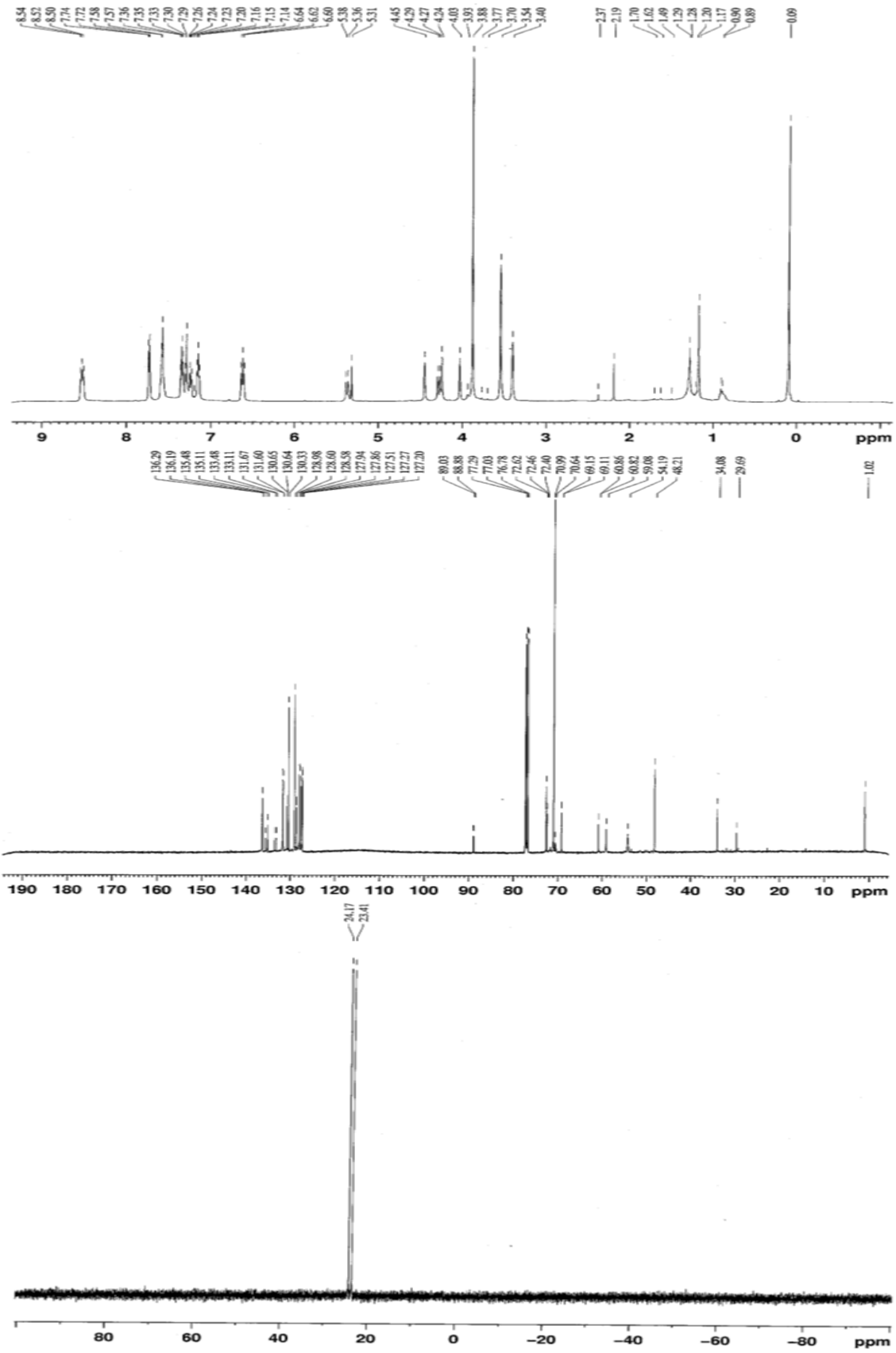
RhCl(NBD)(P,SBz) (**1**^{Bz})



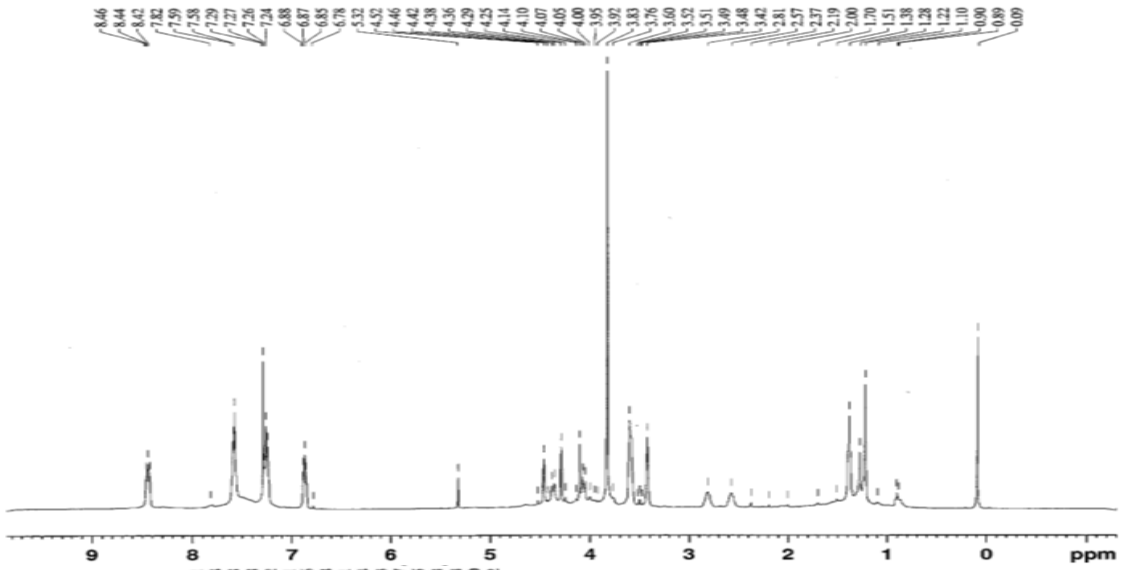


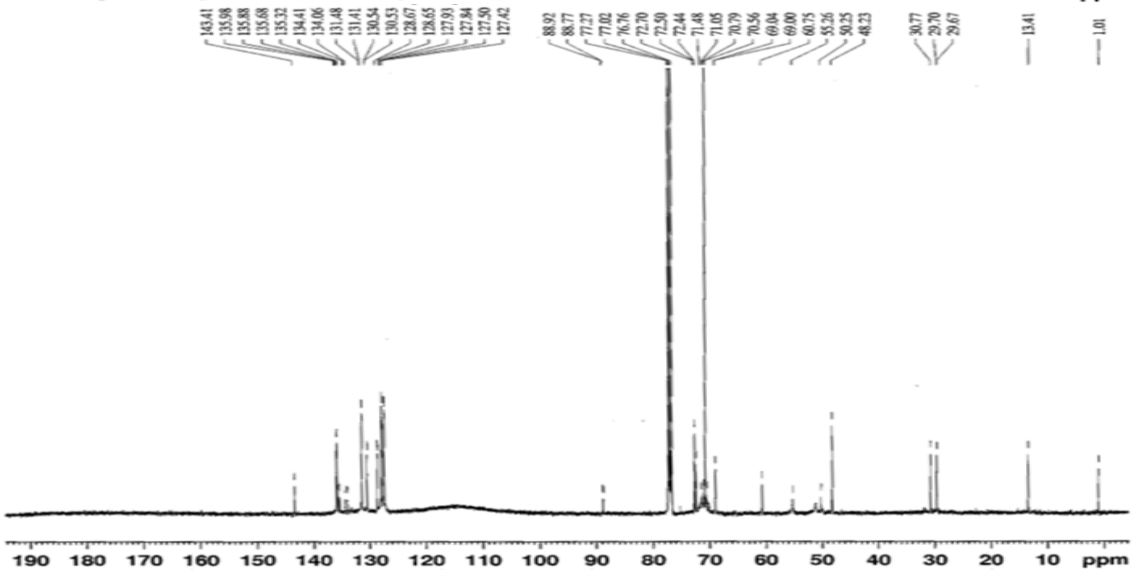


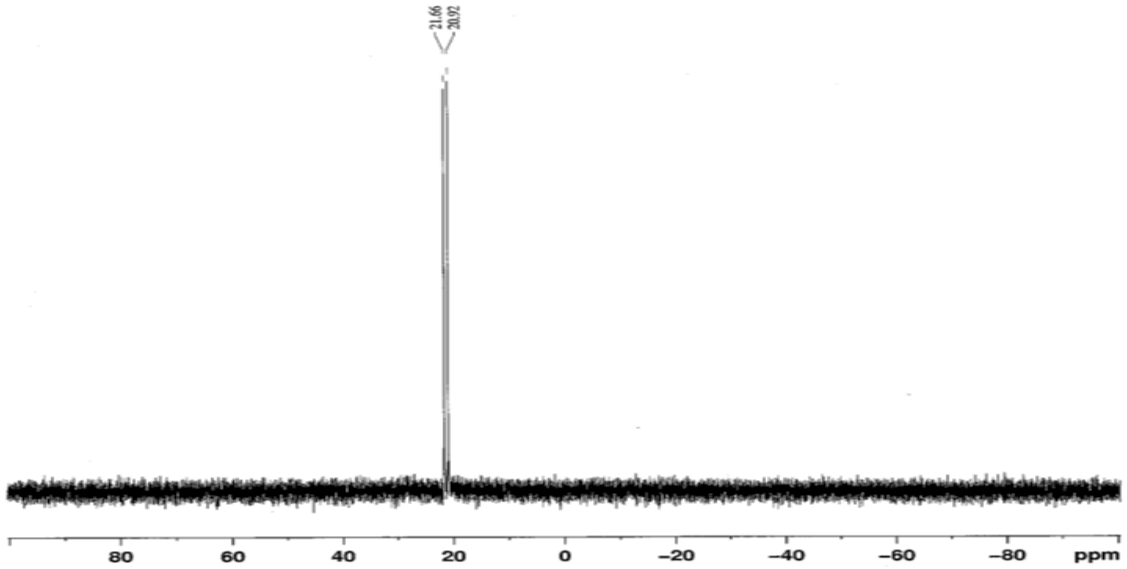
RhCl(NBD)(P,SPh) **(1^{Ph})**



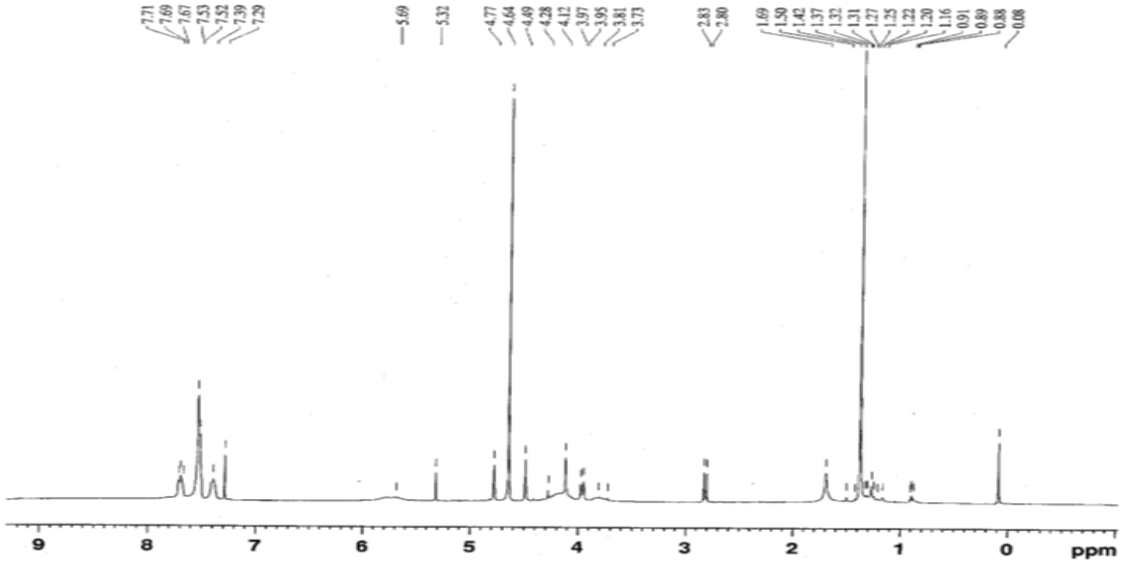
RhCl(NBD)(P,SEt) **(1^{Et})**

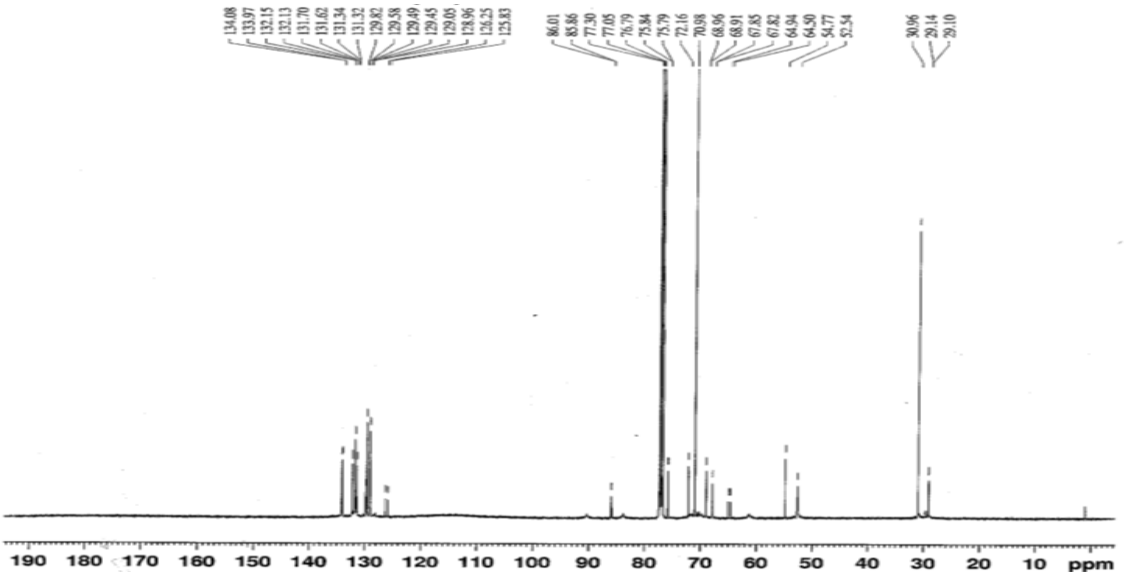


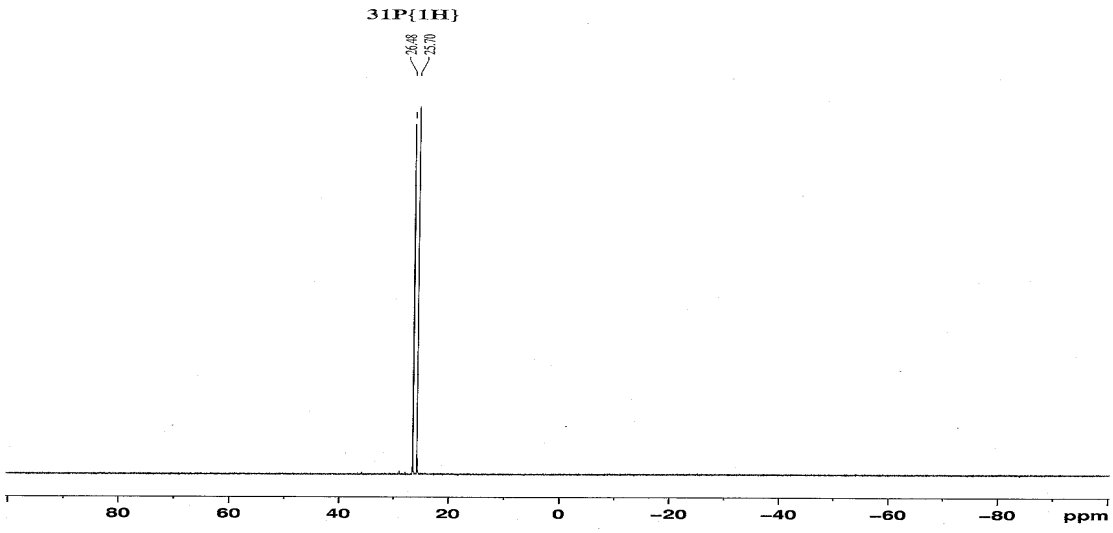




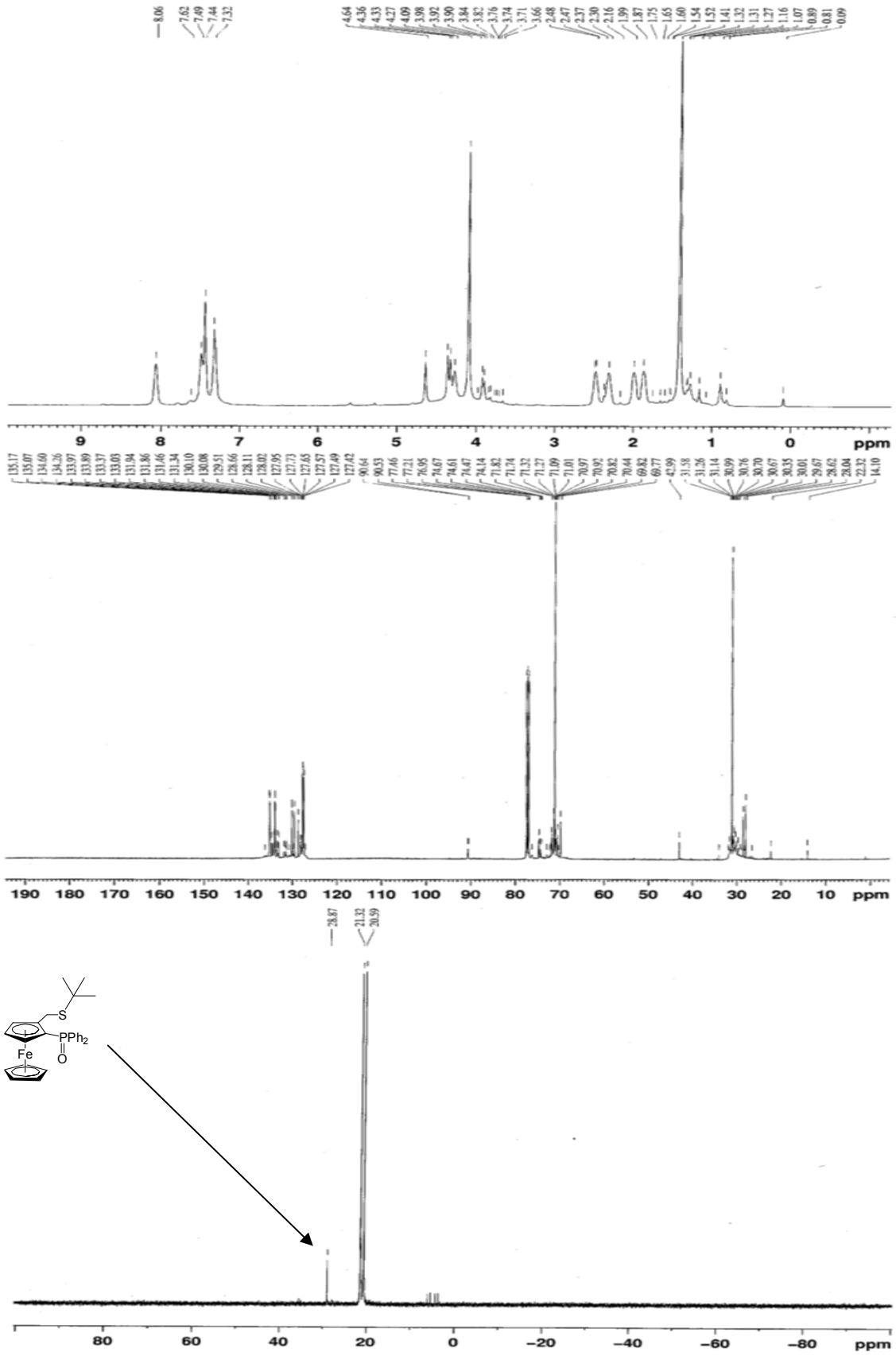
Rh(NBD)(P,S*t*Bu)BF_4 **(2^{tBu})**



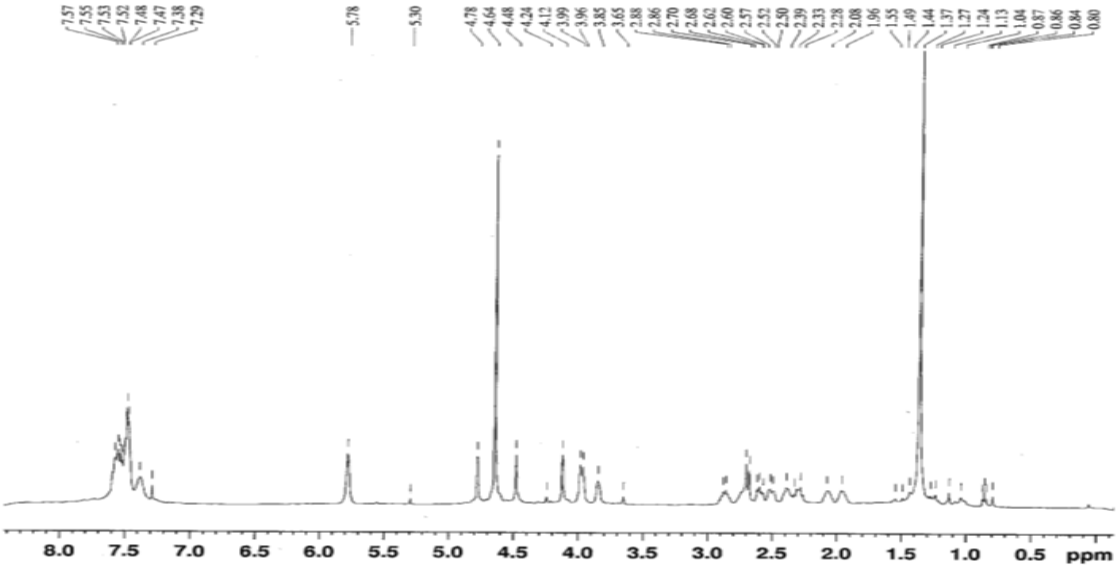


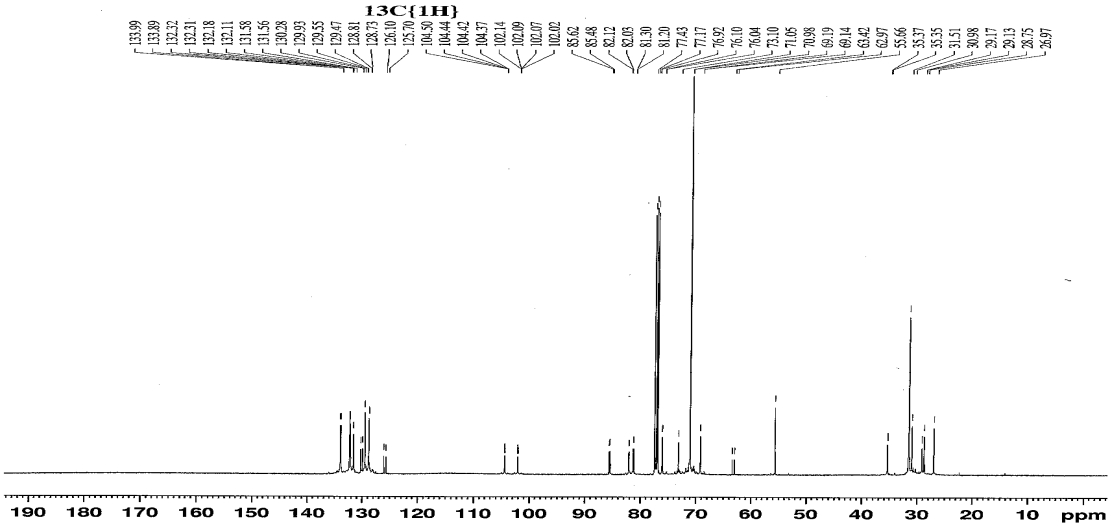


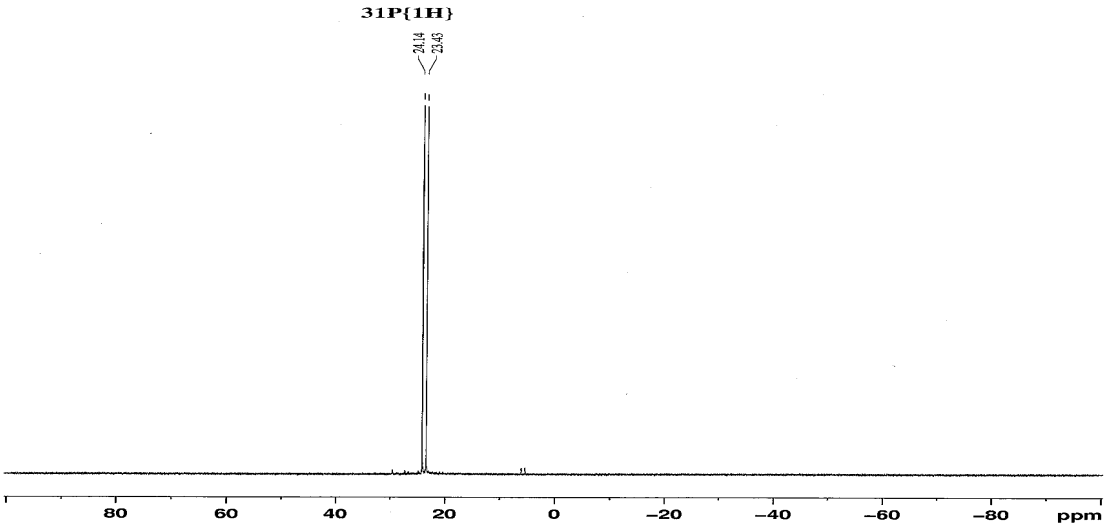
RhCl(COD)(P,S*t*Bu) **(3^{tBu})**



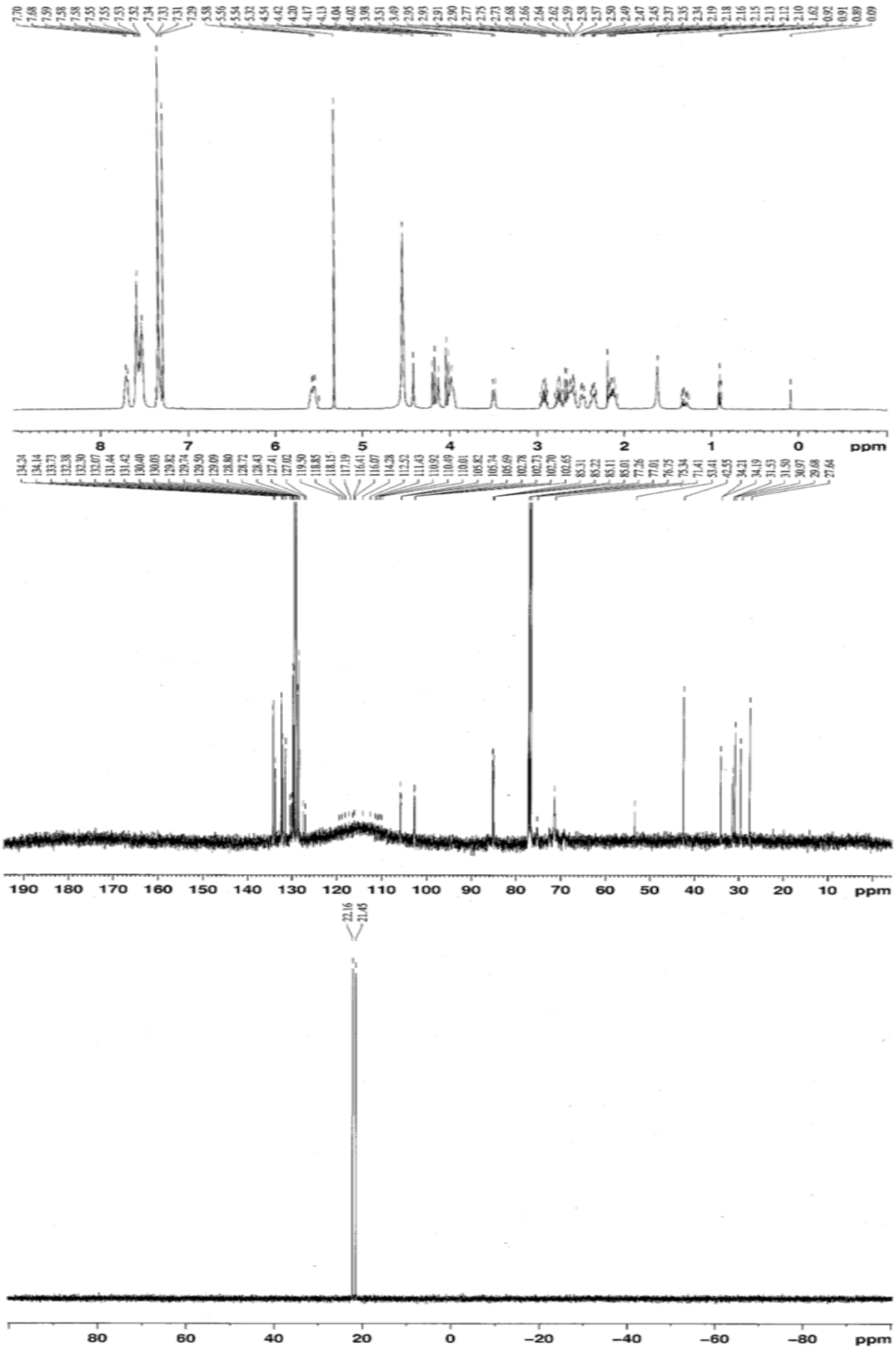
Rh(COD)(P,S*t*Bu)BF_4 **(4^{tBu})**



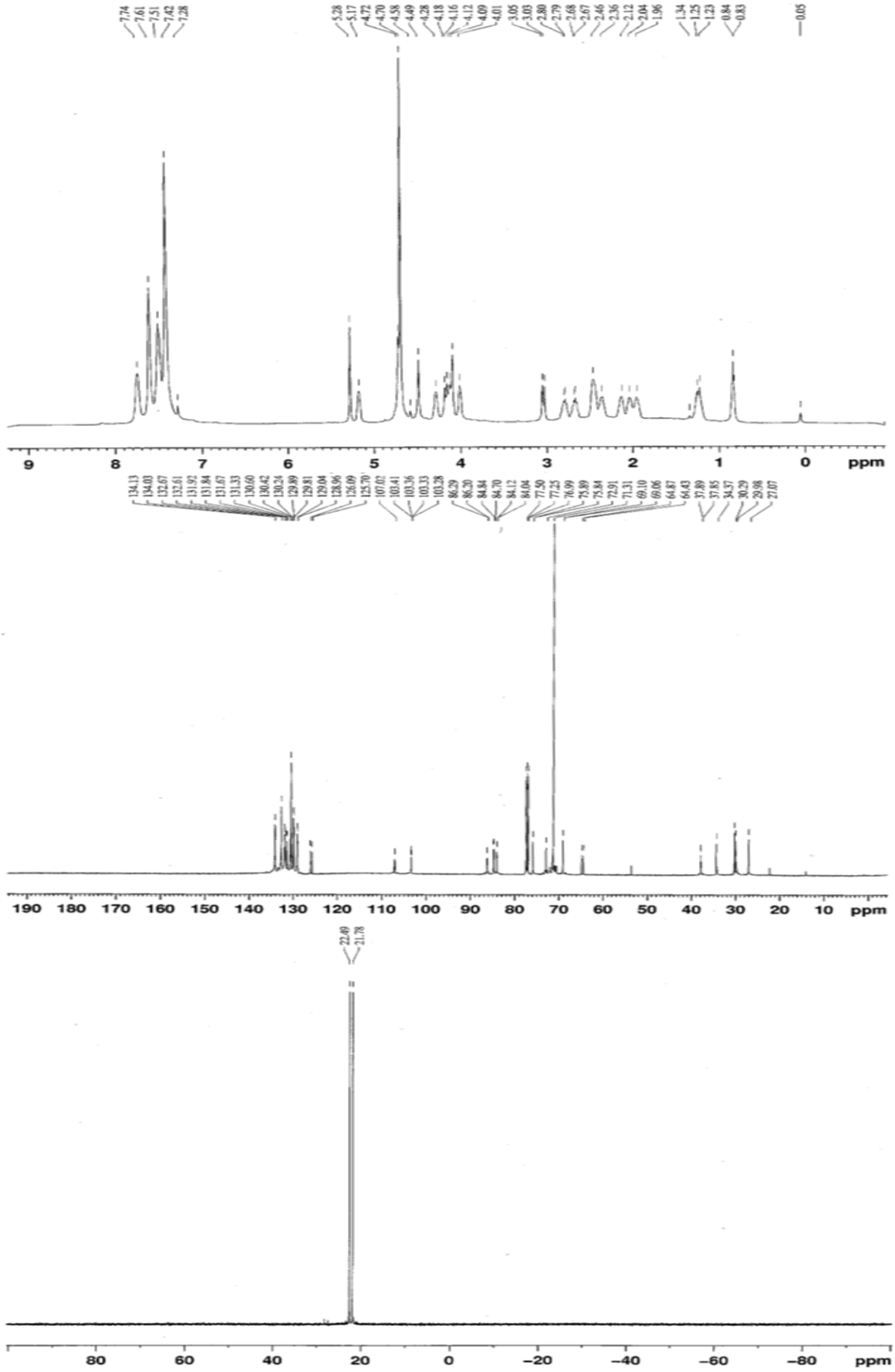
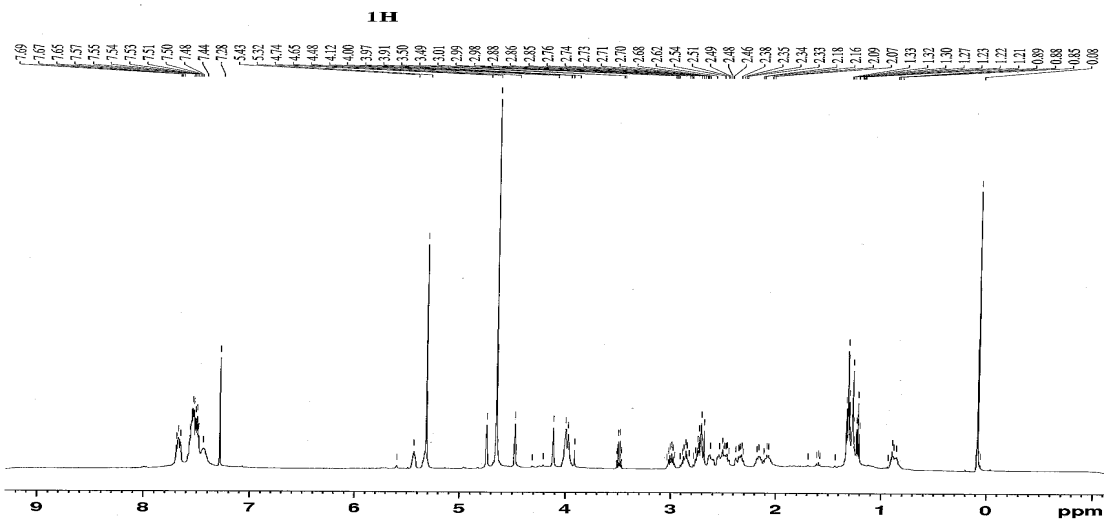
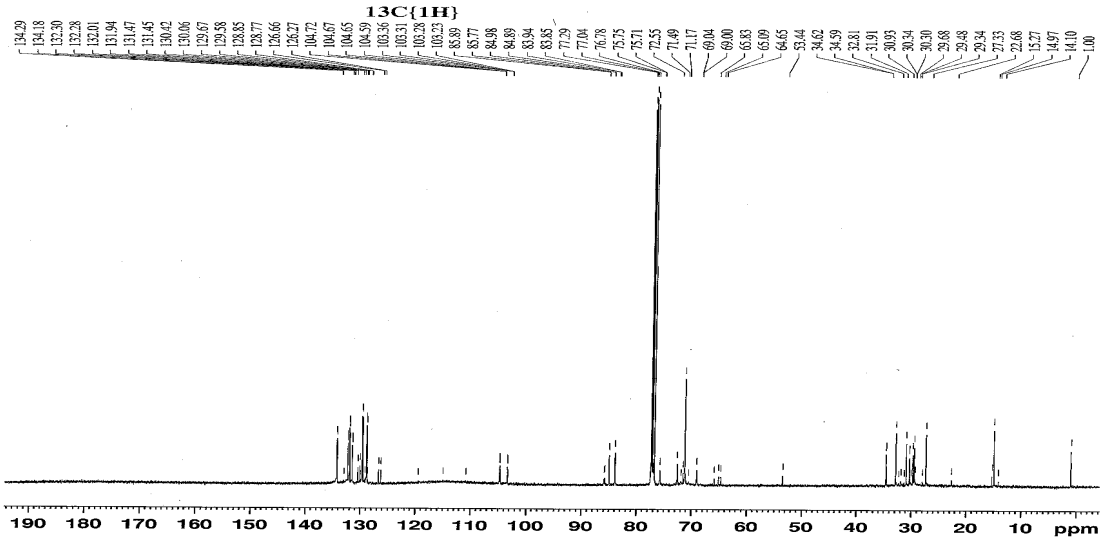
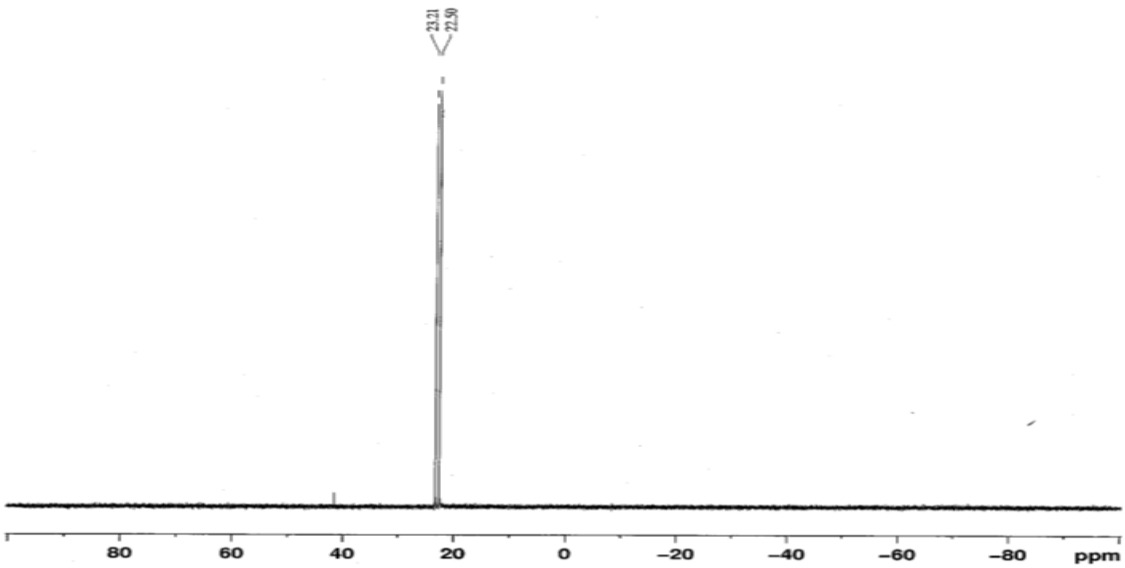




Rh(COD)(P,SBz)BF_4 **(4^{Bz})**



Rh(COD)(P,SPh)BF_4 **(4^{Ph})**



Rh(COD)(P,SEt)BF_4 (**4^{Et}**)