Supporting Information

(Diphenylphosphine)alkylaldehyde to afford hydride- or alkyl-[(diphenylphosphine)alkylacyl]rhodium(III) or (diphenylphosphine)alkylester complexes. Theoretical and experimental diastereoselectivity

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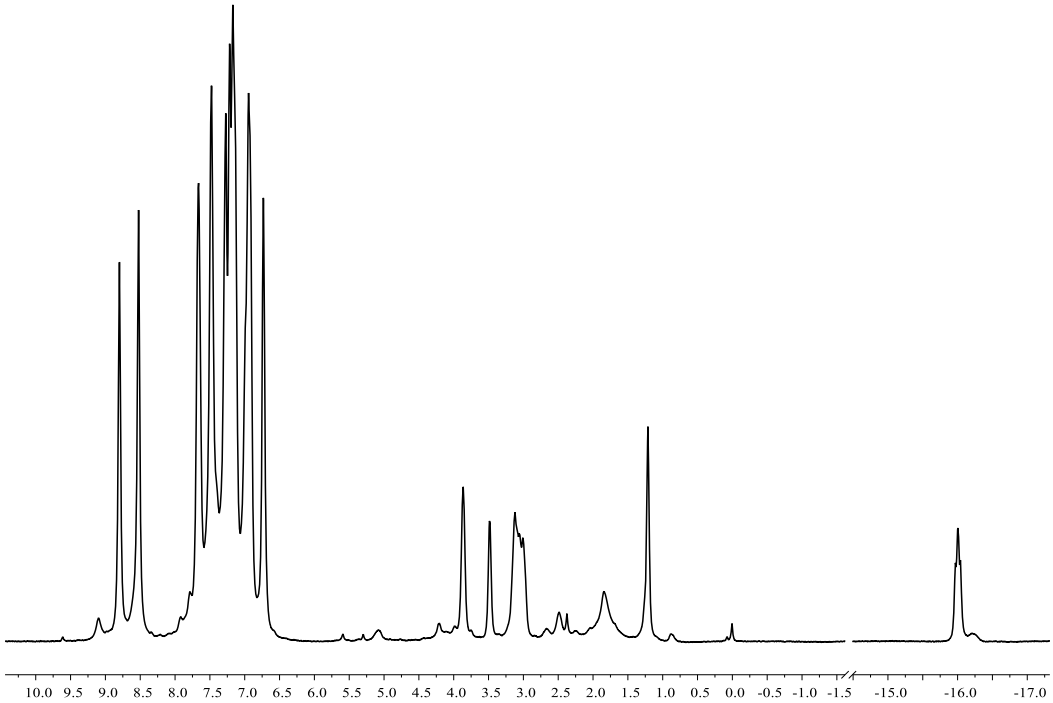
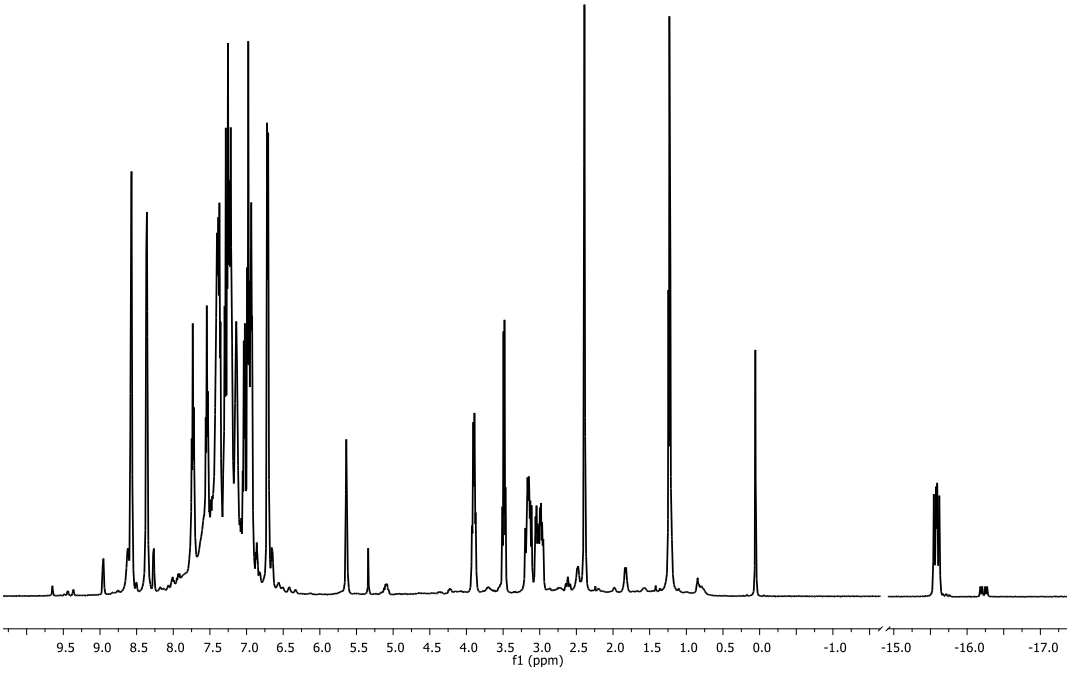
1. NMR SPECTRA

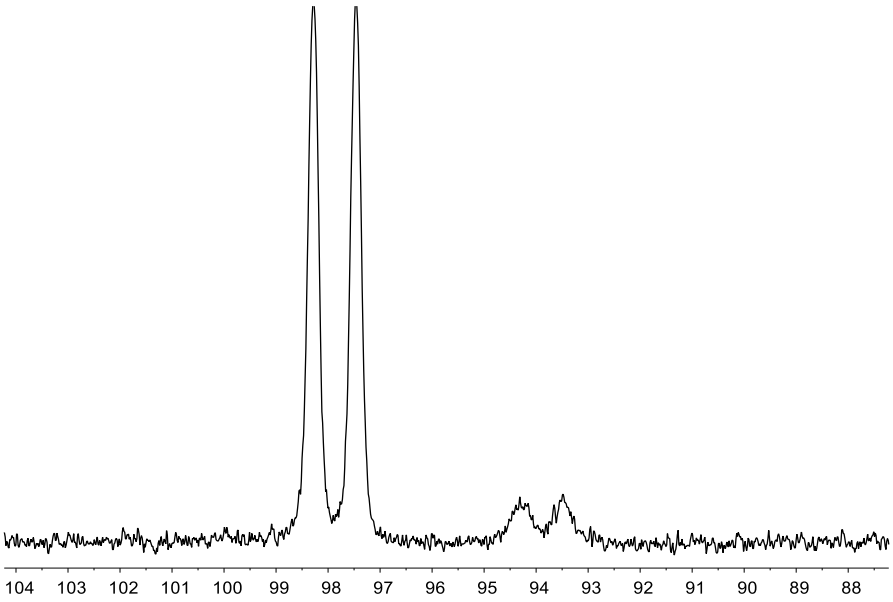
a)



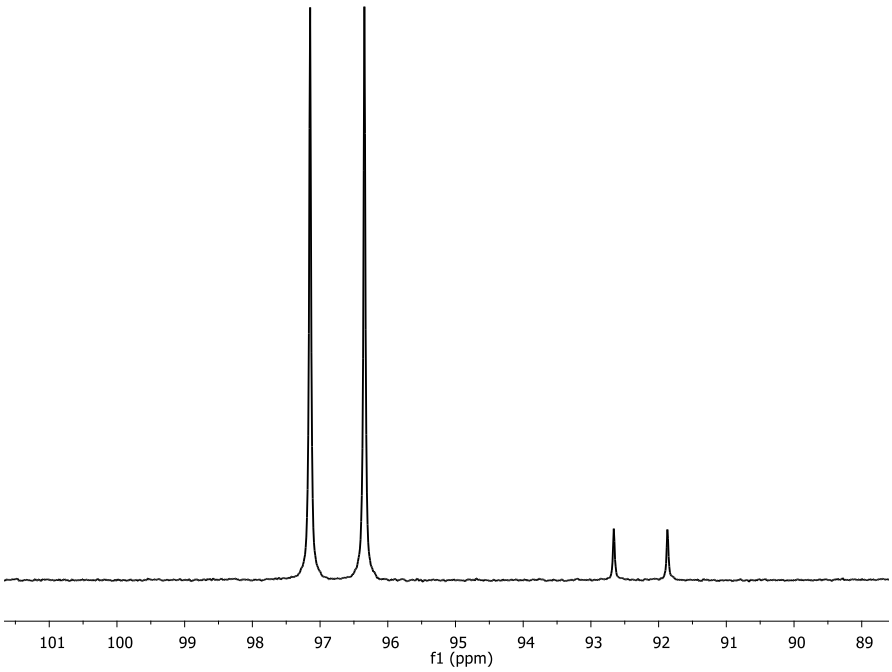
b)



c)


104 103 102 101 100 99 98 97 96 95 94 93 92 91 90 89 88

d)


101 100 99 98 97 96 95 94 93 92 91 90 89
f1 (ppm)

e)

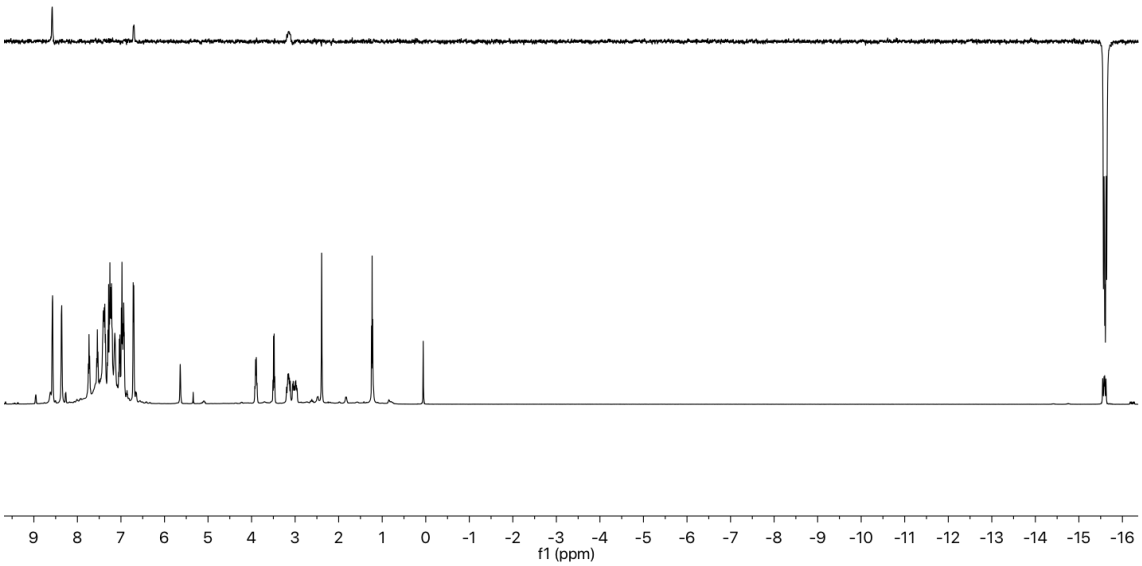


Figure SI-1. a) ^{1}H NMR of complex $[Rh(Cl)H(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**1**) at room temperature in $CDCl_3$. b) ^{1}H NMR of complex $[Rh(Cl)H(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**1**) at -50 ºC $CDCl_3$. c) $^{31}P\{^{1}H\}$ NMR of complex $[Rh(Cl)H(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**1**) at room temperature in $CDCl_3$. d) $^{31}P\{^{1}H\}$ NMR of complex $[Rh(Cl)H(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**1**) at -50 ºC in $CDCl_3$. e) NOE experiment with selective irradiation of the hydrido signal (-15.58 ppm) at -50 ºC in $CDCl_3$.

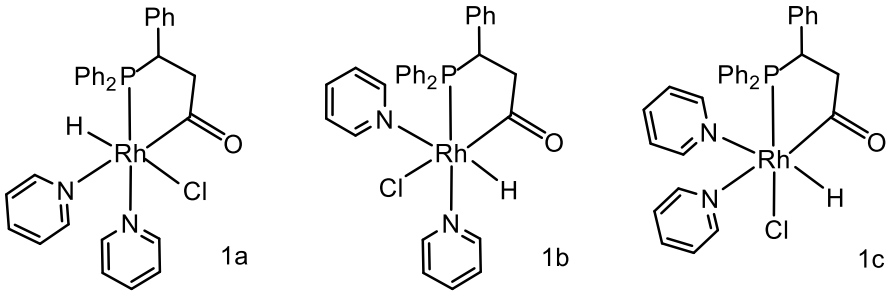


Figure SI-2. Geometric isomers for **1**.

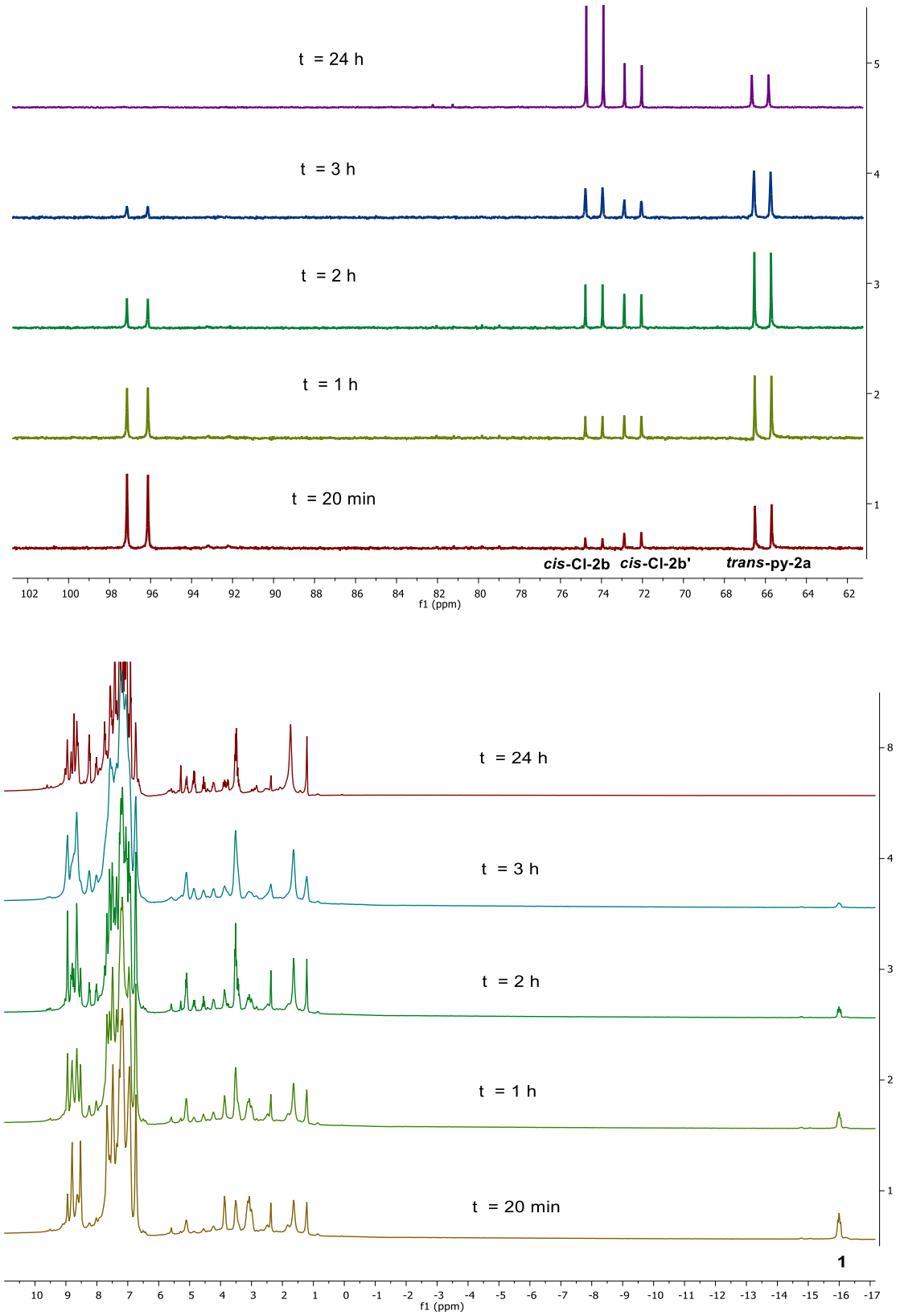


Figure SI-3. $^{31}P\{^{1}H\}$ (top) and ^{1}H (bottom) NMR spectra of the transformation of **1** into **2** in $CDCl_3$.

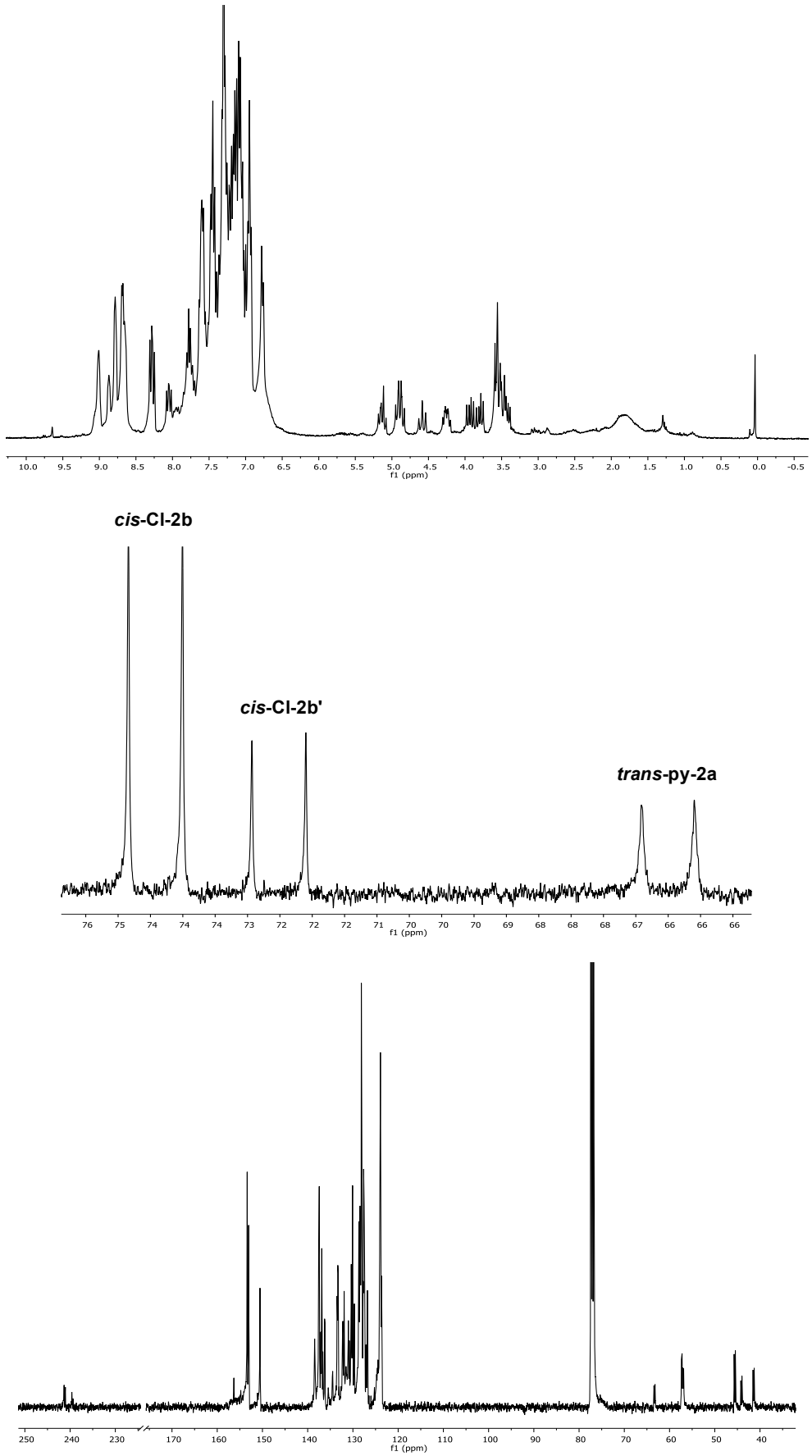


Figure SI-4. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{31}C\{^{1}H\}$ (bottom) NMR of $[RhCl_2(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**2**) in $CDCl_3$.

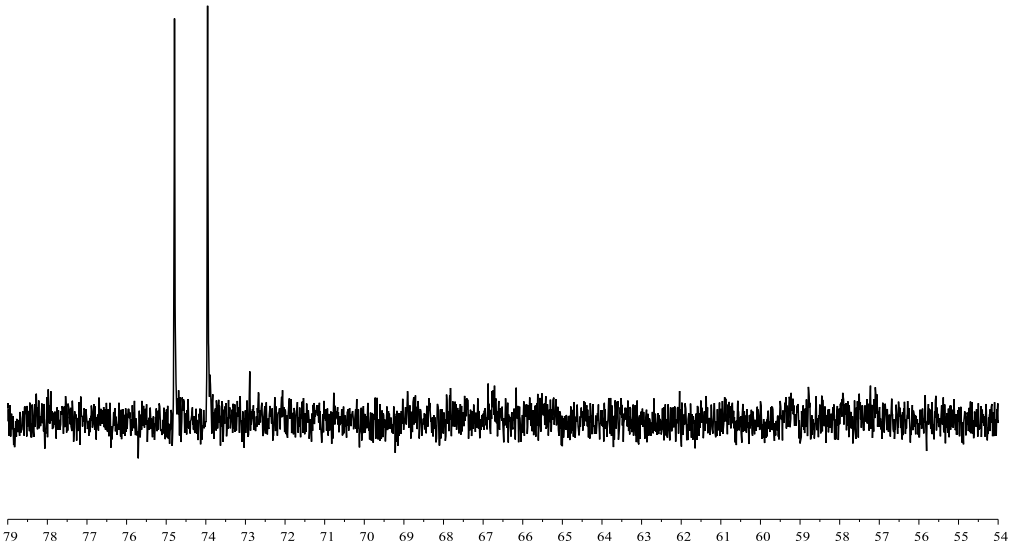


Figure SI-5. $^{31}P\{^{1}H\}$ NMR spectrum of the obtained crystals of $[RhCl_2(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**2**) in $CDCl_3$.

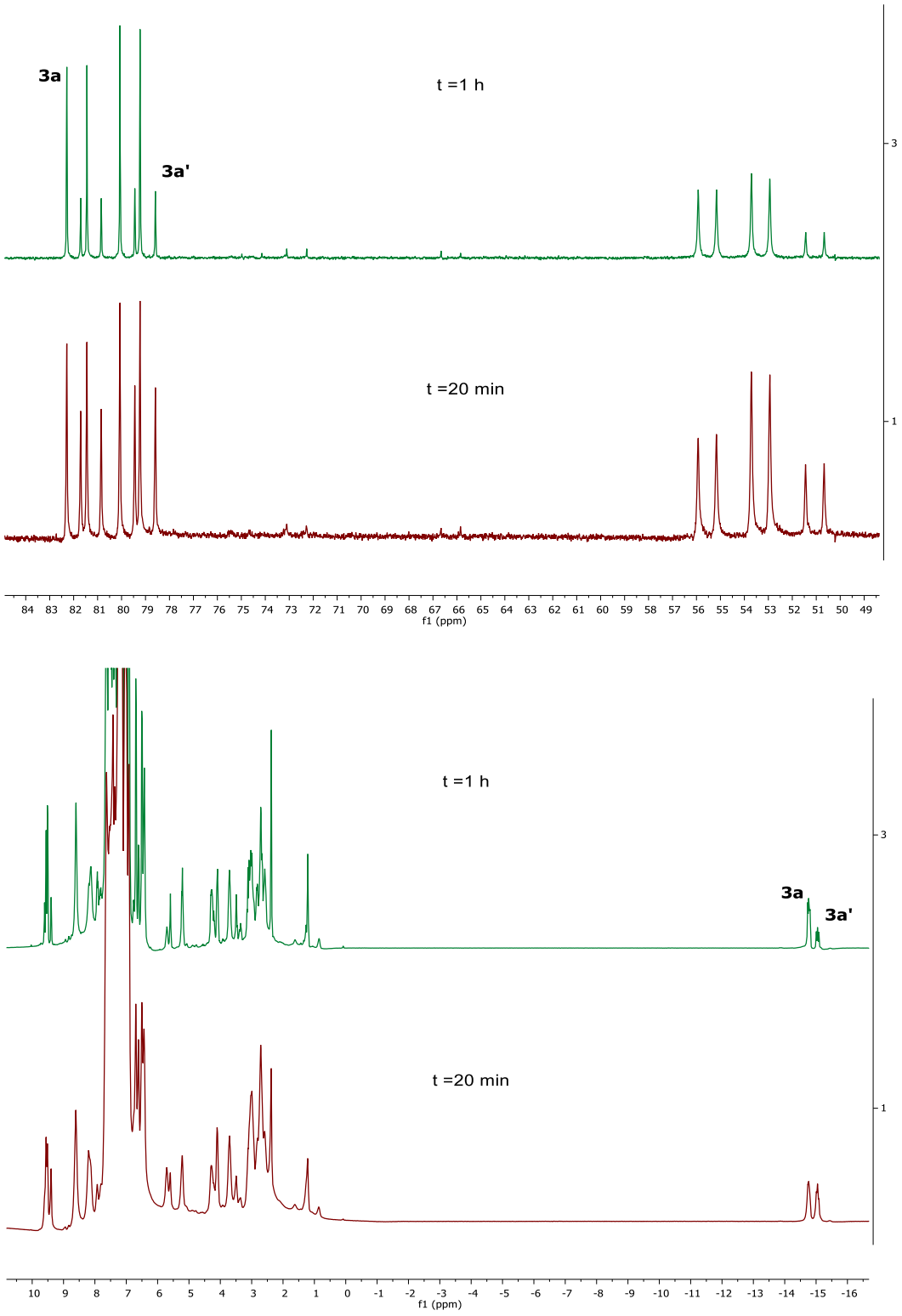


Figure SI-6. $^{31}P\{^{1}H\}$ (top) and ^{1}H (bottom) NMR spectra of the reaction of **1** with $PPh_2CH(Ph)CH_2CHO$ in $CDCl_3$.

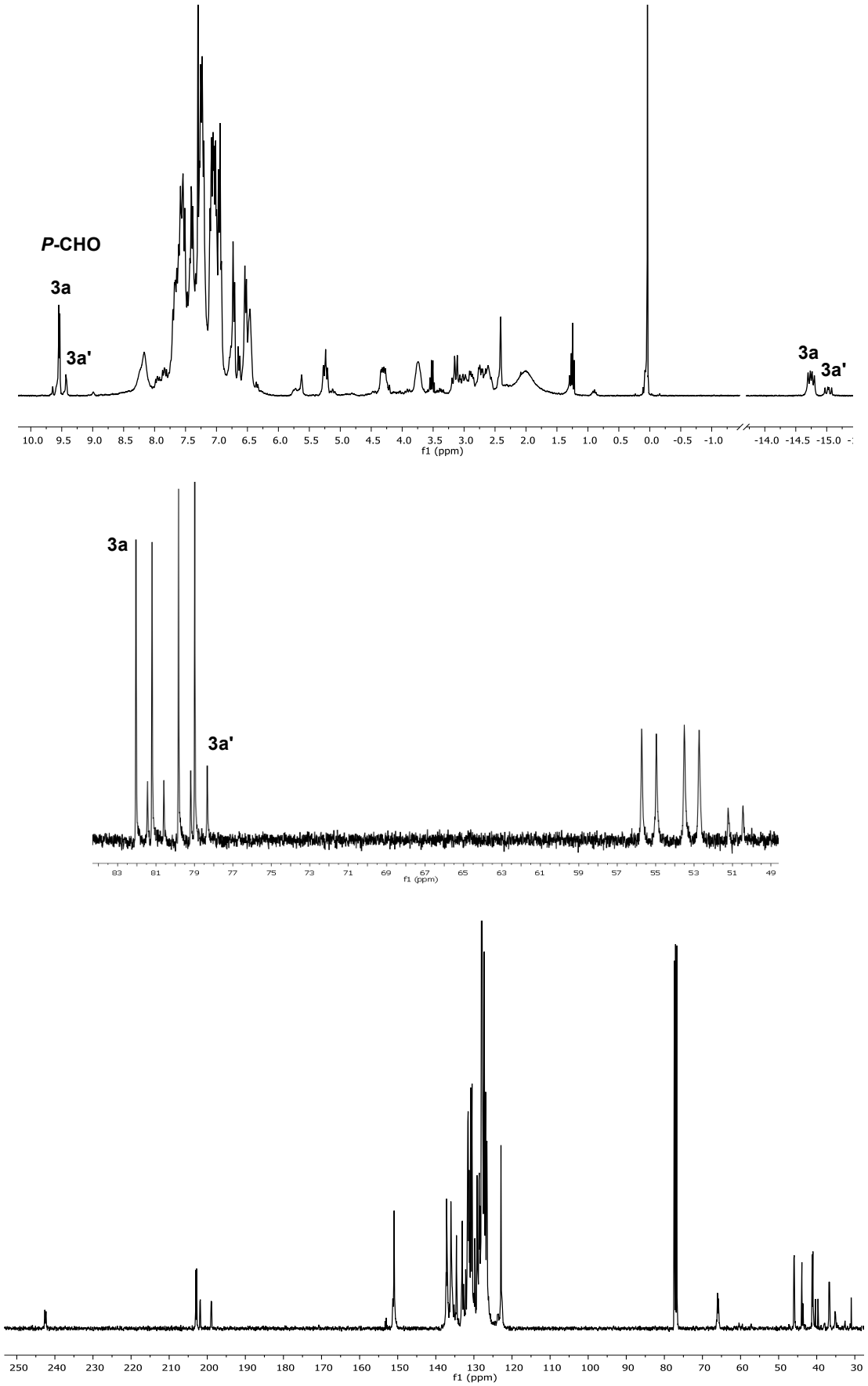


Figure SI-7. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of $[RhHCl(PPh_2CH(Ph)CH_2CO)(PPh_2CH(Ph)CH_2CHO)(Py)]$ (**3**) in $CDCl_3$

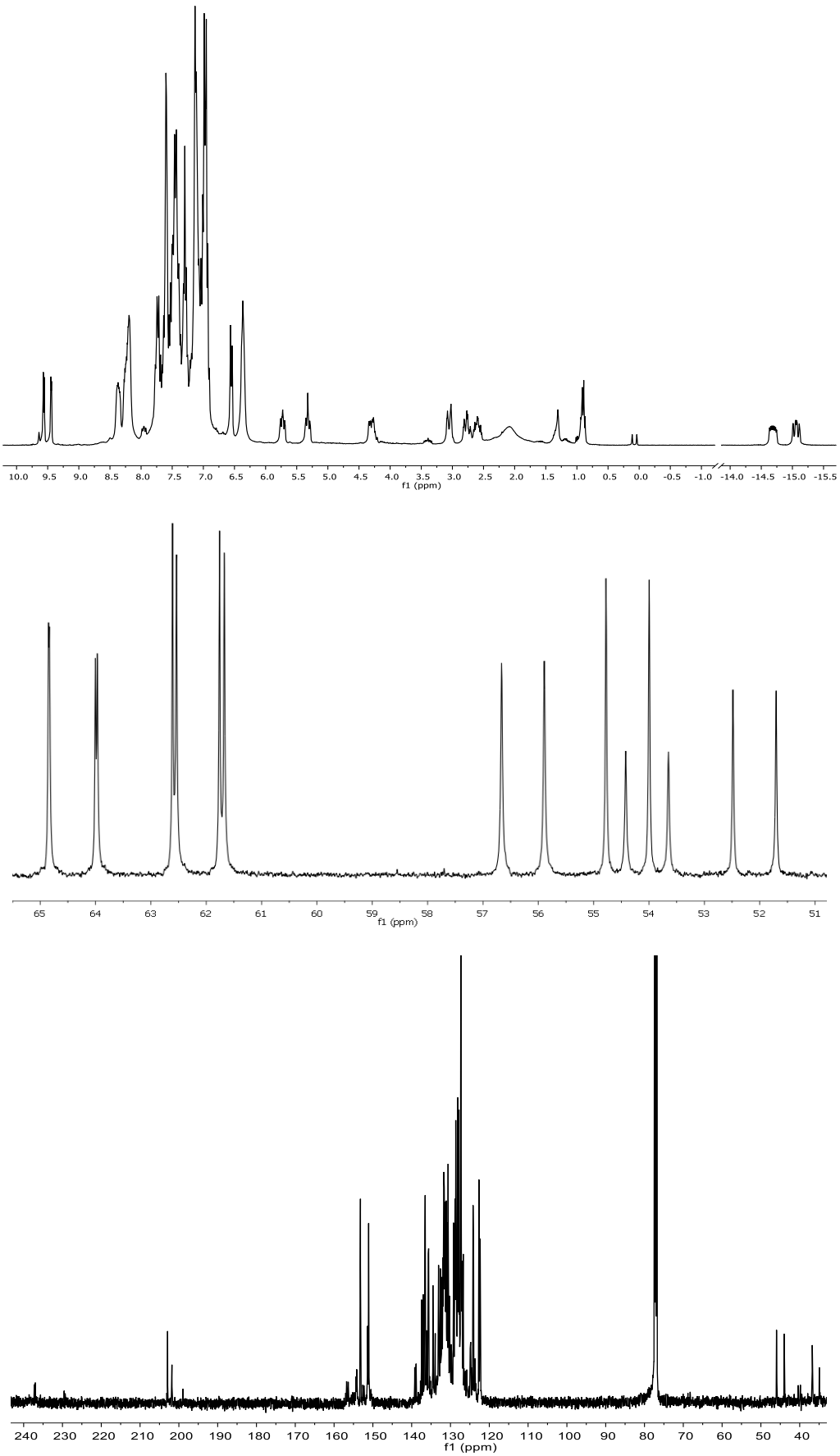


Figure SI-8. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhHCl(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(Py)] (**4**) in $CDCl_3$.

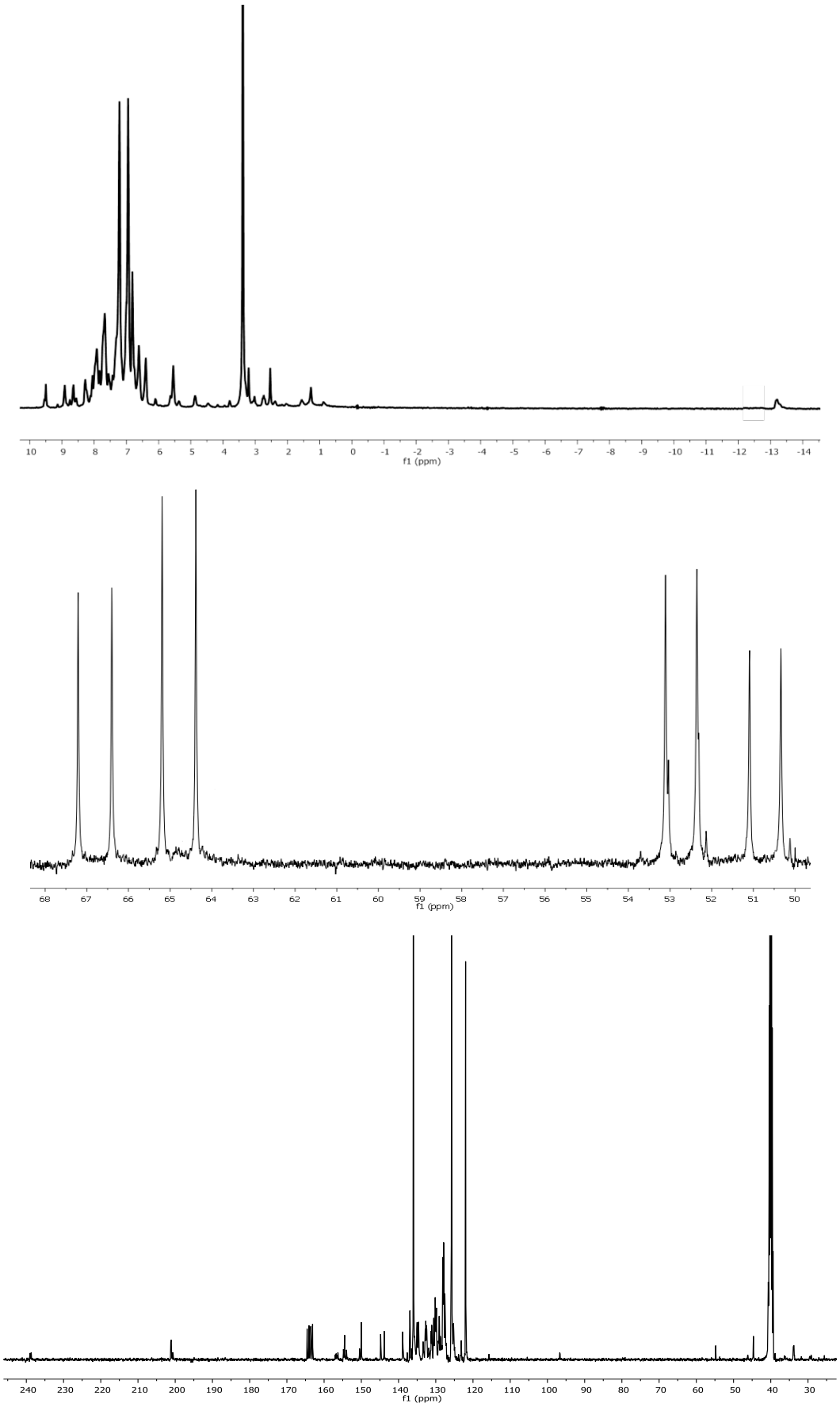


Figure SI-9. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhH(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(phen)]BPh_4 (**5a**) in DMSO-d_6.

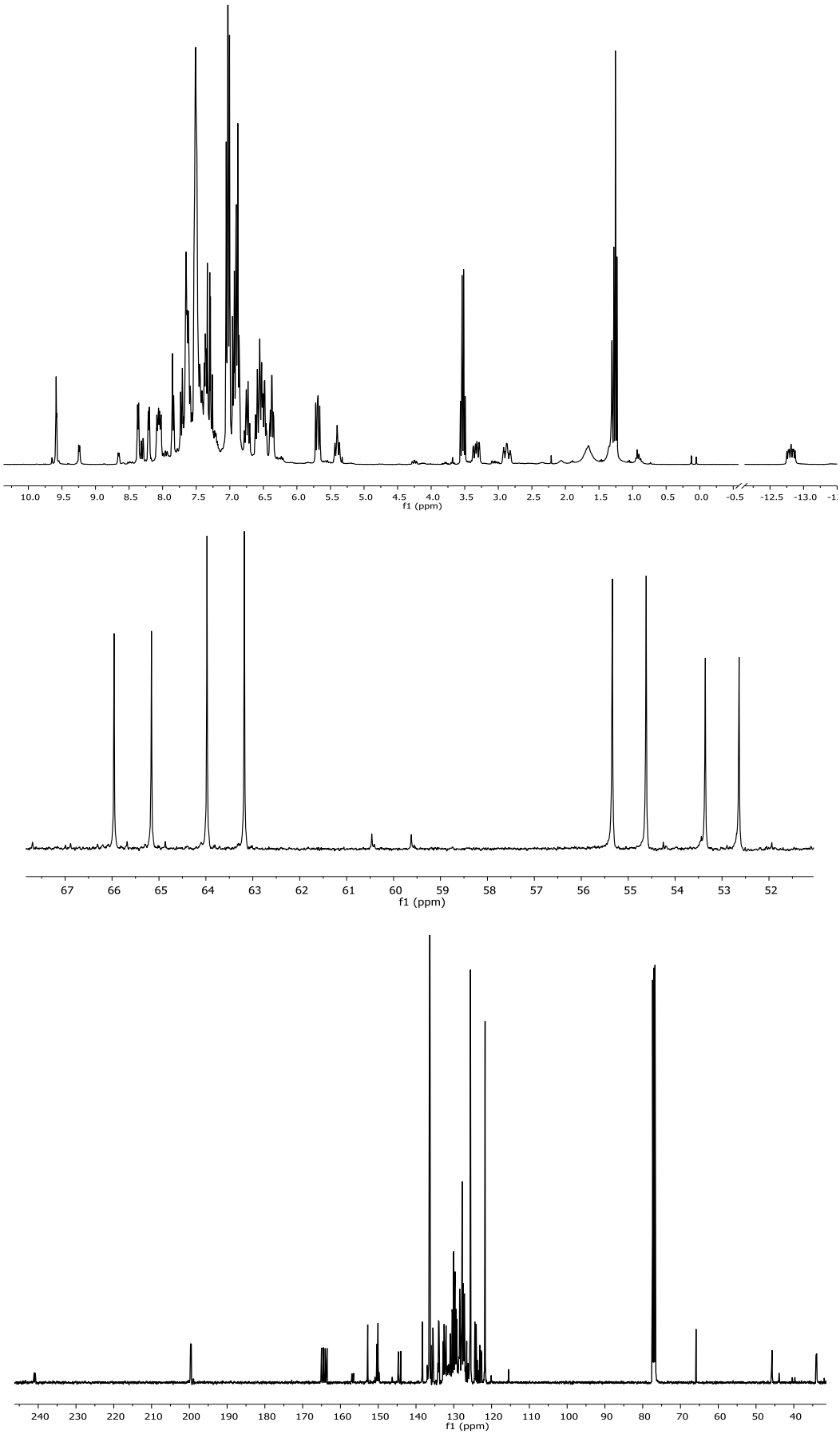


Figure SI-10. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhH(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(phen)]BPh_4 (**5a'**) in $CDCl_3$.

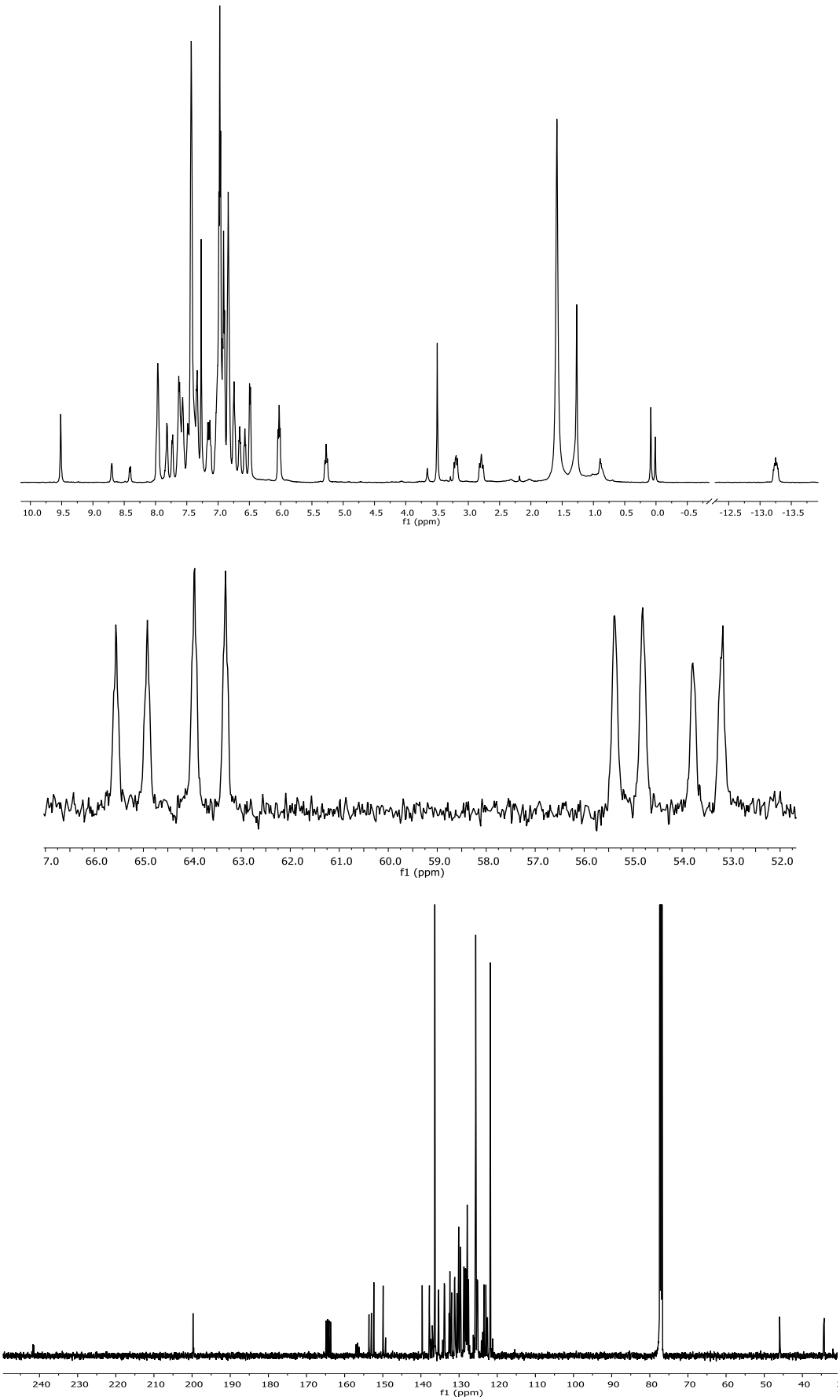


Figure SI-11. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhH(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(bipy)]BPh_4 (**6a**) in $CDCl_3$.

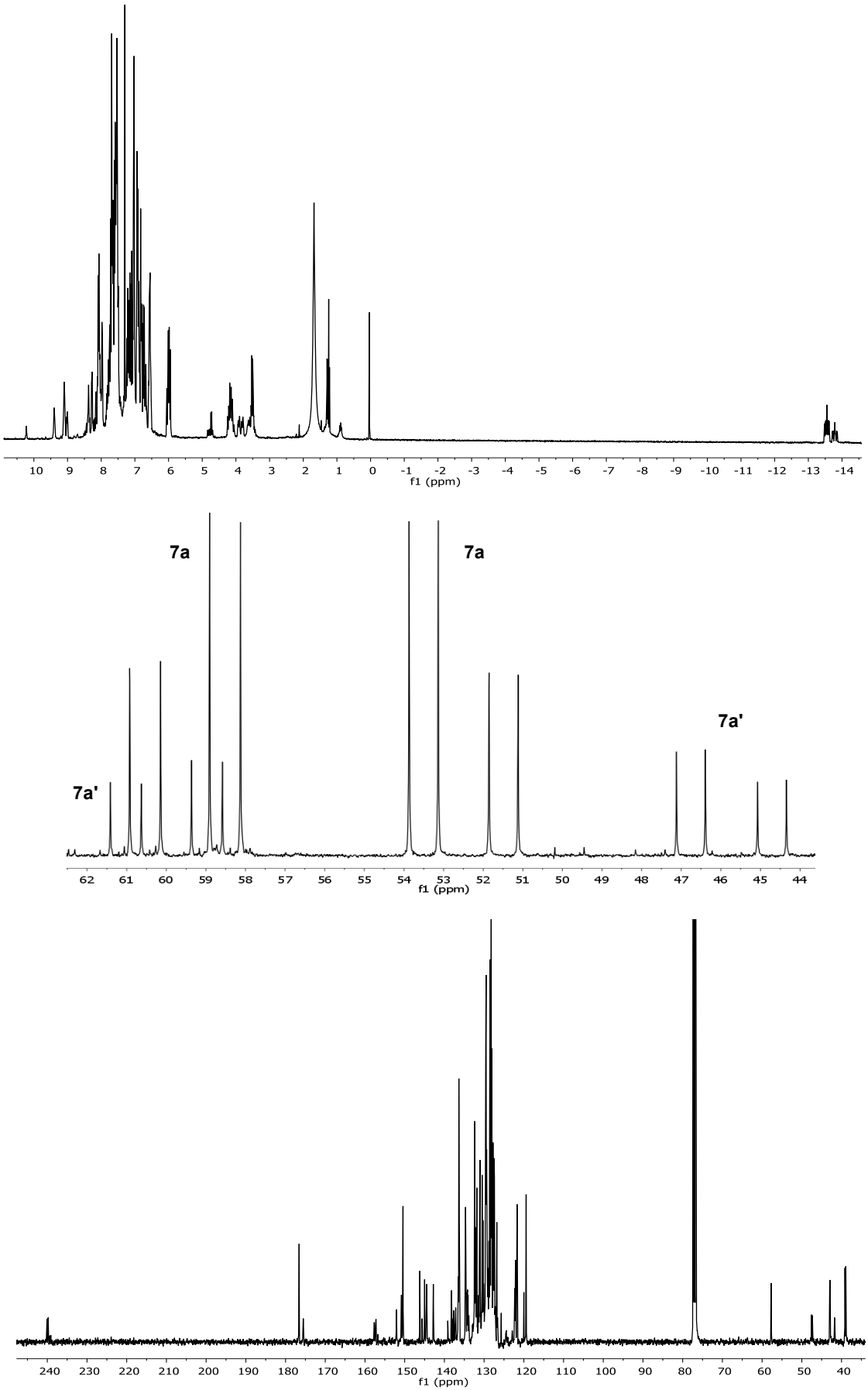


Figure SI-12. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhH(PPh_2(*o*-C_6H_4CO))(κ^3-*P,N,N*-$PPh_2CH(Ph)CH_2CNC_9H_6N$)]BF_4 (**7**) in $CDCl_3$.

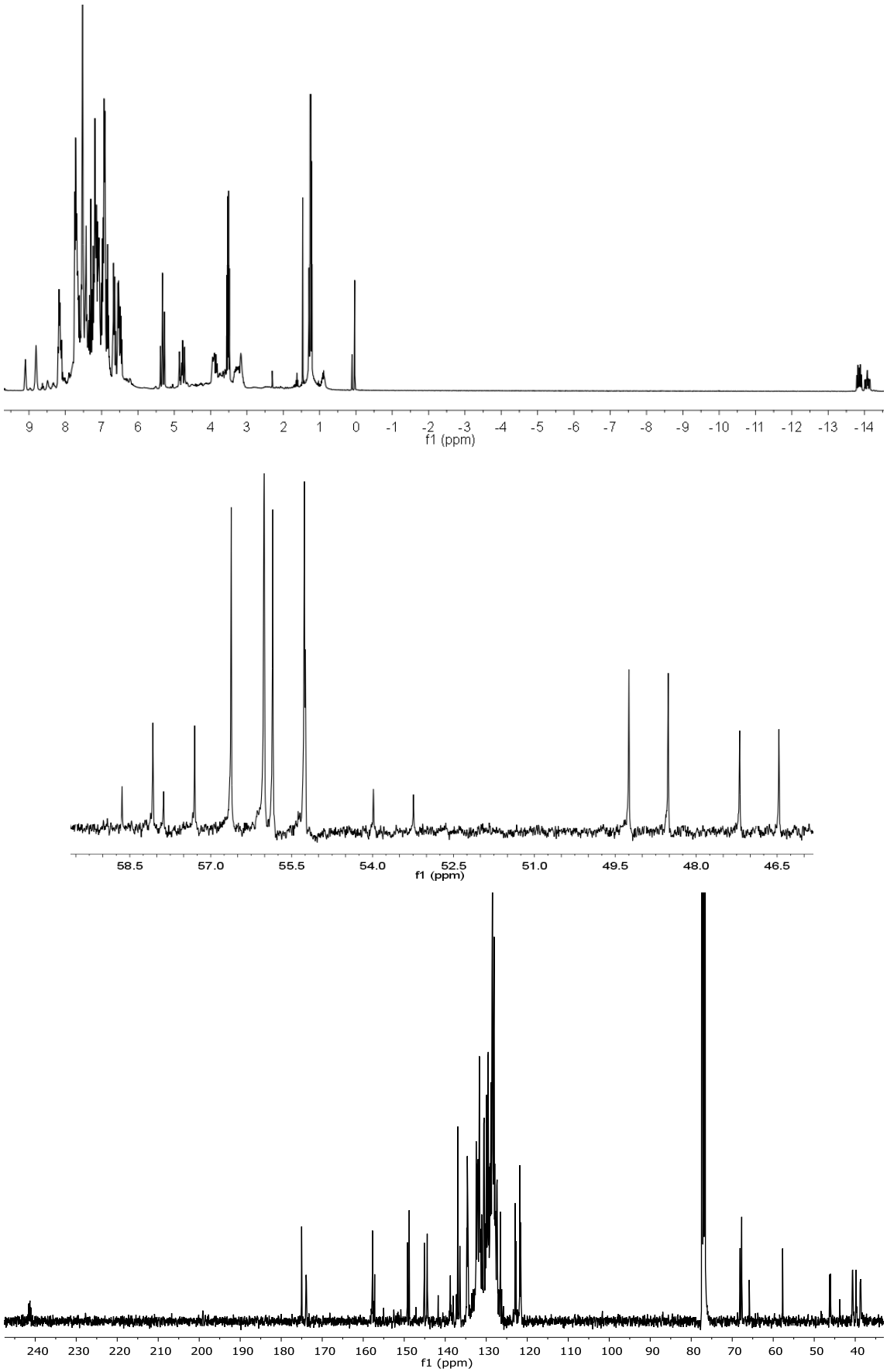


Figure SI-13. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhH(PPh_2(*o*-C_6H_4CO))(κ^3-*P,N,N*-$PPh_2CH(Ph)CH_2CNCH_2C_5H_4N$)]$BF_4$ (**8**) in $CDCl_3$.

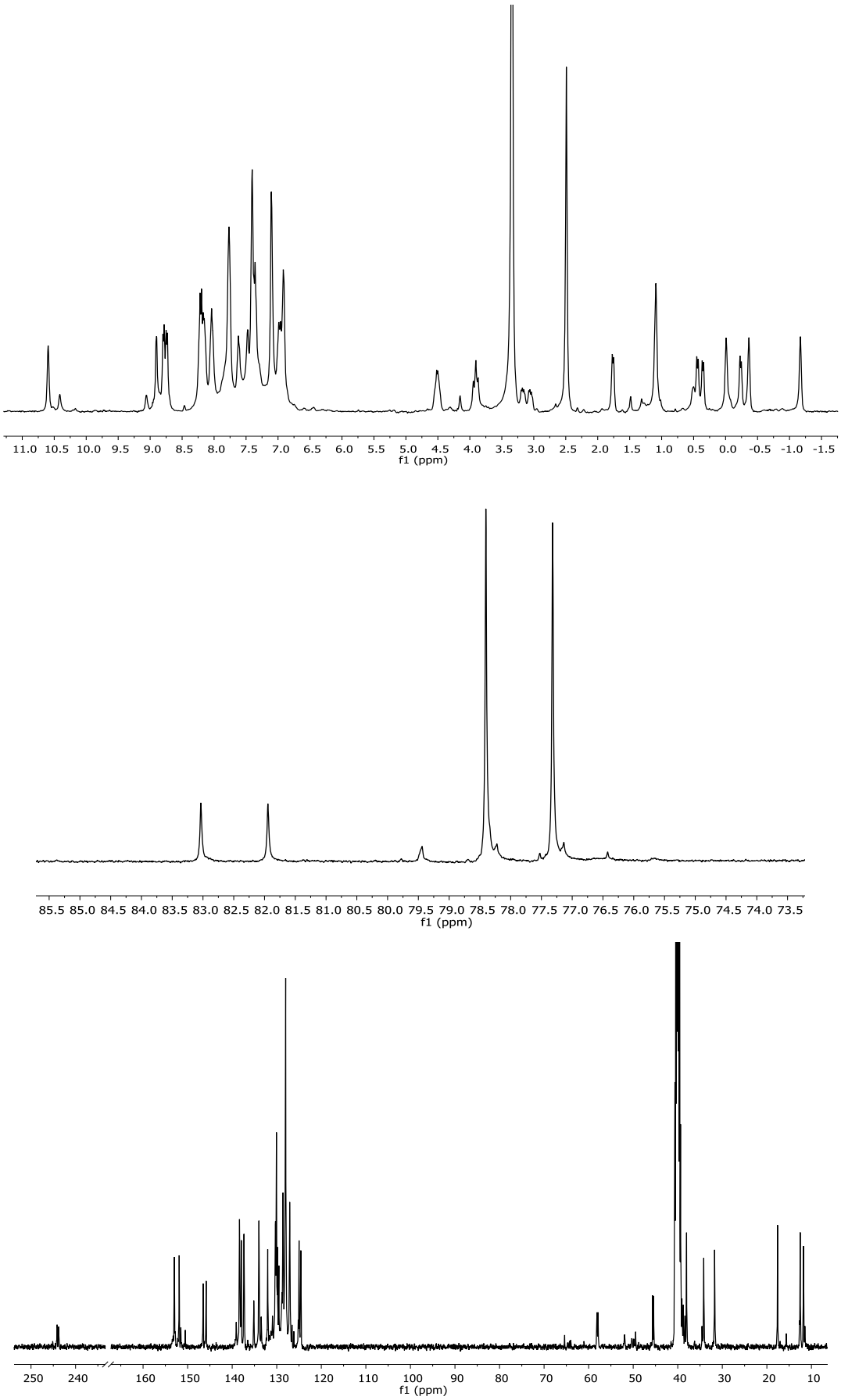


Figure SI-14. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhCl(Ntyl)($PPh_2CH(Ph)CH_2CO$)(phen)] (**9**) in DMSO-d_6.

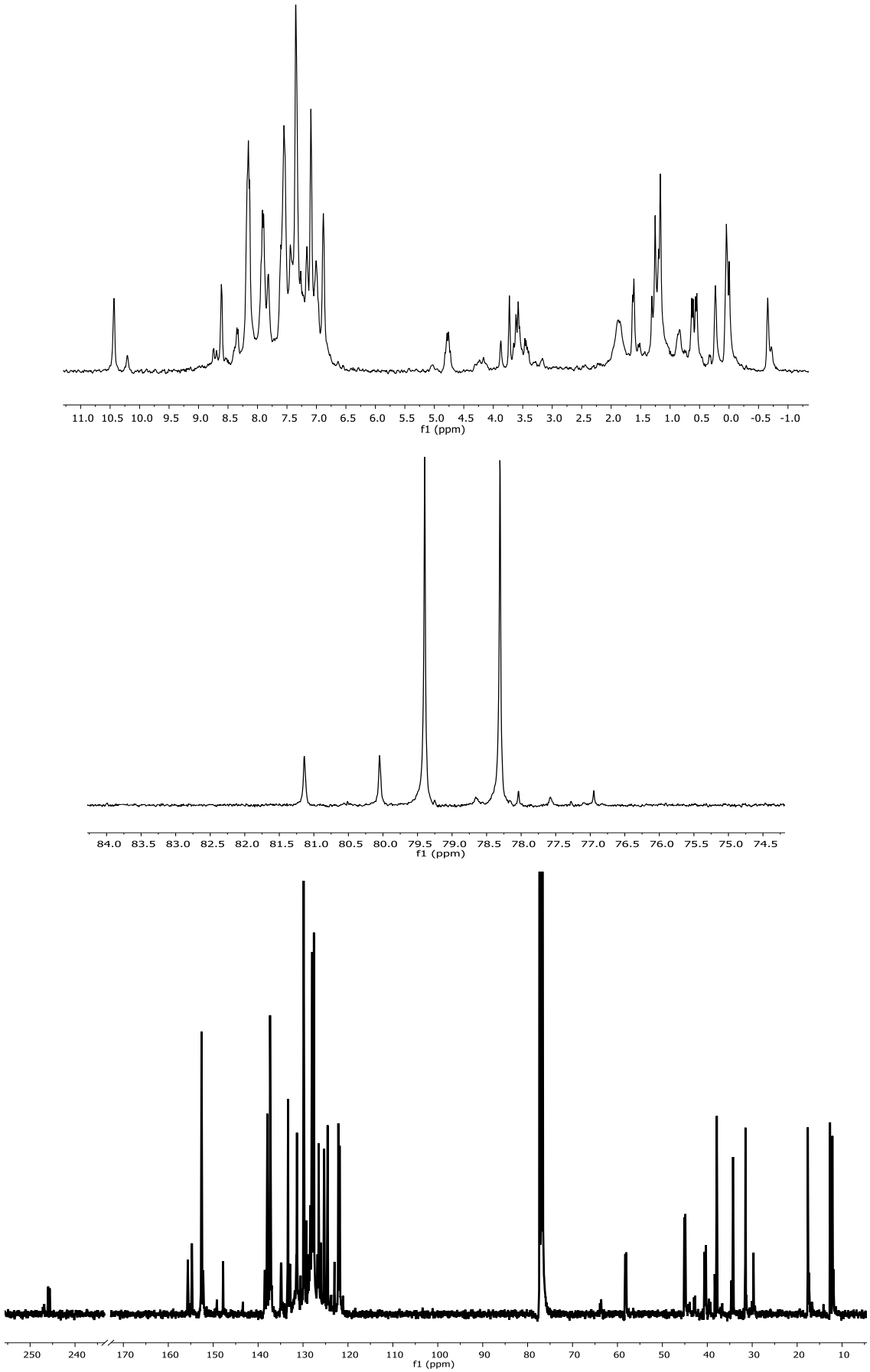


Figure SI-15. ^{1}H (top), $^{31}P\{^{1}H\}$ (middle) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhCl(Ntyl)($PPh_2CH(Ph)CH_2CO$)(bipy)] (**10**) in $CDCl_3$.

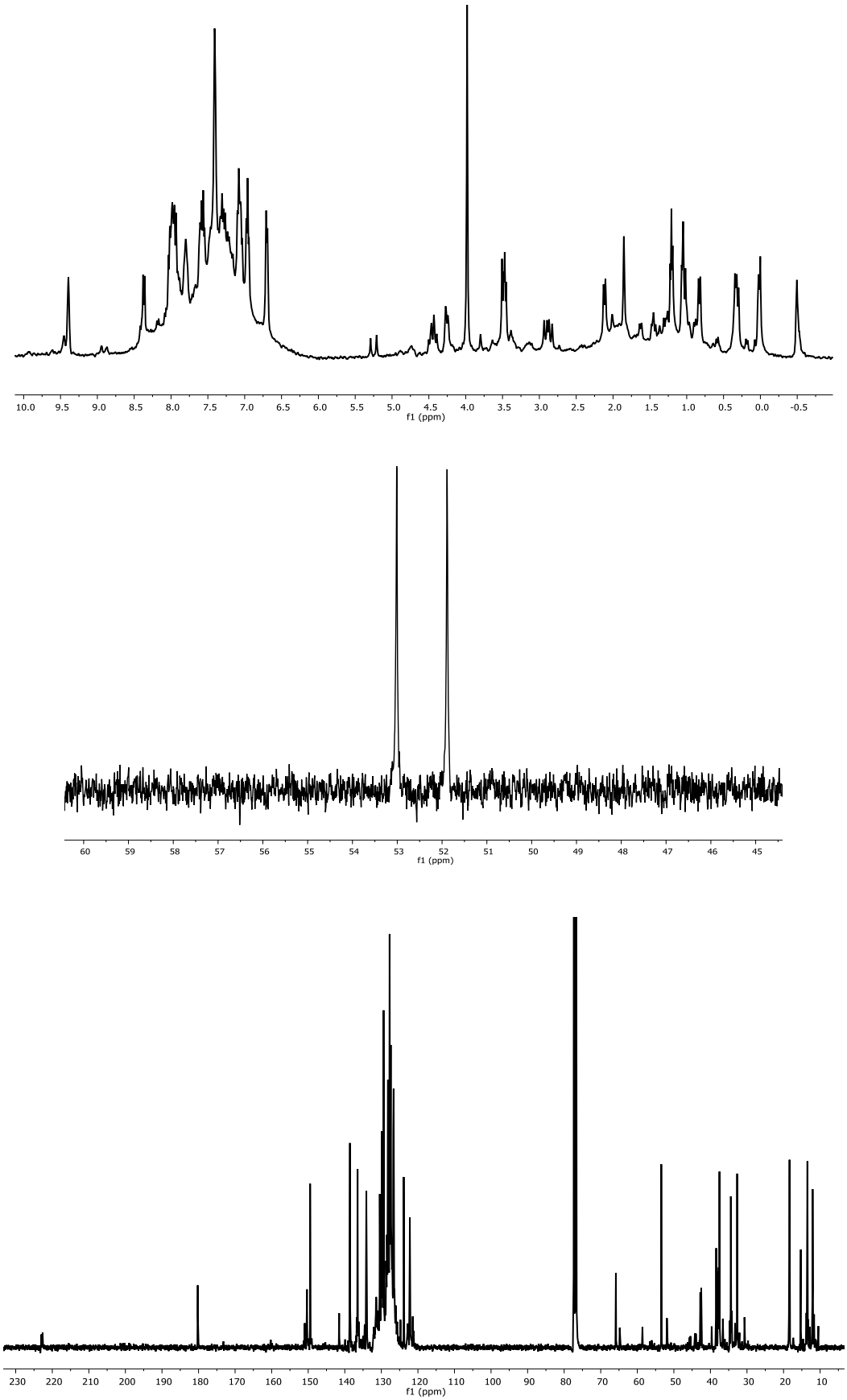


Figure SI-16. ^{1}H (top) and $^{13}C\{^{1}H\}$ (bottom) NMR of [RhCl(Ntyl)(C_9H_6NCO)($PPh_2CH(Ph)CH_2CO(OCH_3)$)] (**11**) in $CDCl_3$, and $^{31}P\{^{1}H\}$ (middle) in CD_3OD.

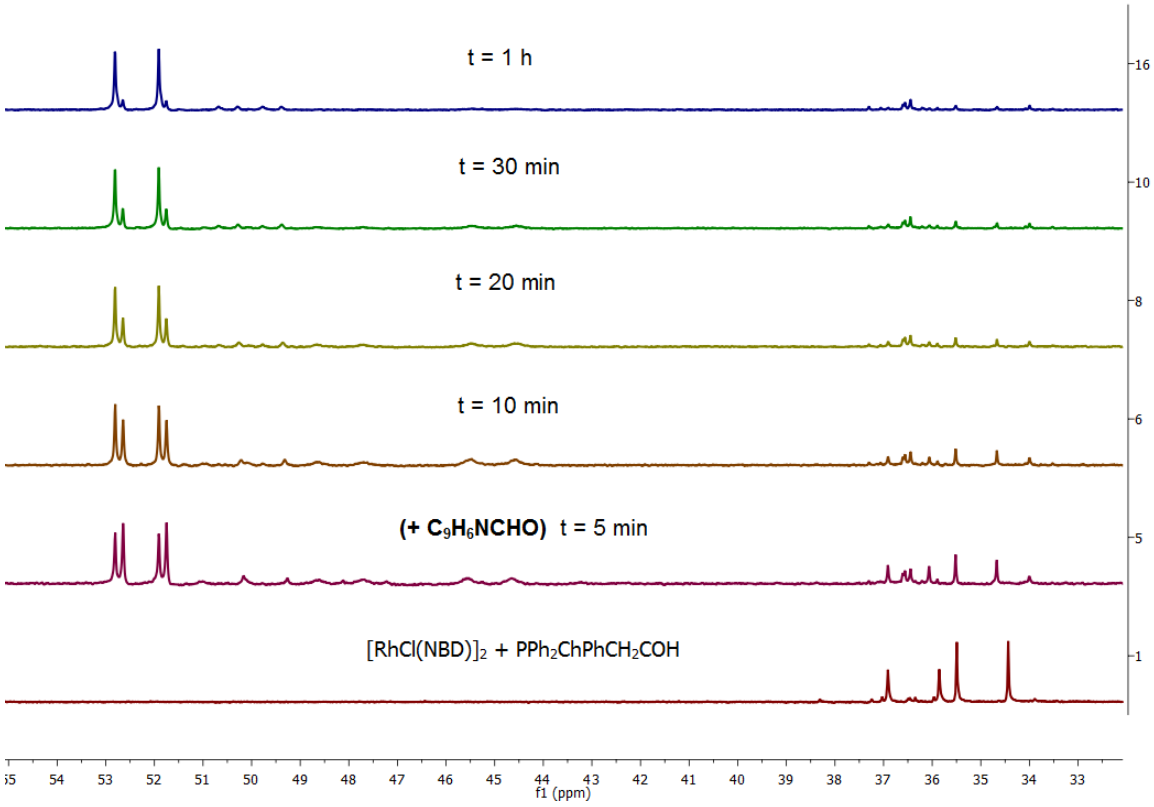


Figure SI-17. $^{31}P\{^{1}H\}$ NMR spectra of the reaction of $[RhCl(NBD)]_2$ with $PPh_2CHPhCH_2CHO$ and C_9H_6NCHO in CD_3OD to afford **11**.

2. X-RAY CRISTALLOGRAPHY

Table **SI.1** . Crystallographic Data and Refinement Details for ***cis*-Cl-2b, 5a, 7a, 10a** and **11**

Compound	**cis-Cl-2b**	**5a**	**7a**	**10a**	**11**
Empirical formula	$C_{31}H_{28}Cl_2N_2OPRh$	$C_{159}H_{131}B_2Cl_{21}N_4O_4P_4Rh_2$	$C_{57}H_{60}BF_4N_2O_3P_2Rh$	$C_{43}H_{47}Cl_3N_2O_2PRh$	$C_{43}H_{44}ClNO_4PRh$
Mr	649.33	3257.45	1072.73	864.05	808.12
Temperature K	100(2)	100(2)	100(2)	100(2)	100(2)
crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
space group	*P*-1 (No. 2)	*P*-1 (No. 2)	*P*21/c (No. 14)	*P*21/c (No. 14)	*P*21/n (No. 14)
a / Å	9.6045(10)	15.671(3)	10.689(6)	10.8421(17)	9.9698(7)
b /Å	12.0456(12)	15.668(3)	29.0982(17)	9.8845(12)	17.4017(12)
c / Å	13.9271(14)	16.235(4)	20.4783(10)	34.895(2)	21.2563(14)
α / °	64.4480(10)	108.514(3)	-	-	-
β / °	72.5590(10)	93.226(3)	111.262(3)	92.883(3)	92.159(8)
γ / °	75.9930(10)	94.916(3)	-	-	-
V /Å^3,	1374.9(2)	3751.2(14)	5935.8(6)	3734.9(8)	3685.2(4)
Z	2	1	4	4	4
F(000)	660	1690	2224	1784	1672
ρ /g·cm^{-3}	1.568	1.442	1.200	1.537	1.457
μ / mm^{-1}	0.902	0.693	0.394	0.756	0.624
data collected	(-12,-15,-17) to (12,15,18)	(-19,-20,-21) to(19,20,21)	(-14,-39,-26) to (13,35,27)	(-14,-12,-46) to (14,13,47)	(-13,-23,-28) to (13,23,28)
θ range / °	1.663 to 28.12	1.309 to 28.200	2.056 to 28.727	2.164 to 28.885	1.513 to 28.527
Reflections collec.	15975	43841	86756	76565	43008
Independent refls.	6150	16840	14864	9432	8853
Refls.obsd. (I)>2σ(I)	5402	12698	10155	6899	7559
R_1 (*) [(I)>2σ(I)]	0.0334	0.0626	0.0698	0.0535	0.0365
wR_2 (**) (all refls)	0.0885	0.1570	0.1945	0.1265	0.0924
Largest diff. Peak and hole eÅ^{-3}	0.809 and -0.524	1.372 and -0.979	1.421 and -0.803	1.620 and -1.301	1.112 and -1.003

(*) $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$

(**)$wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

3. ESI - MS SPECTRA

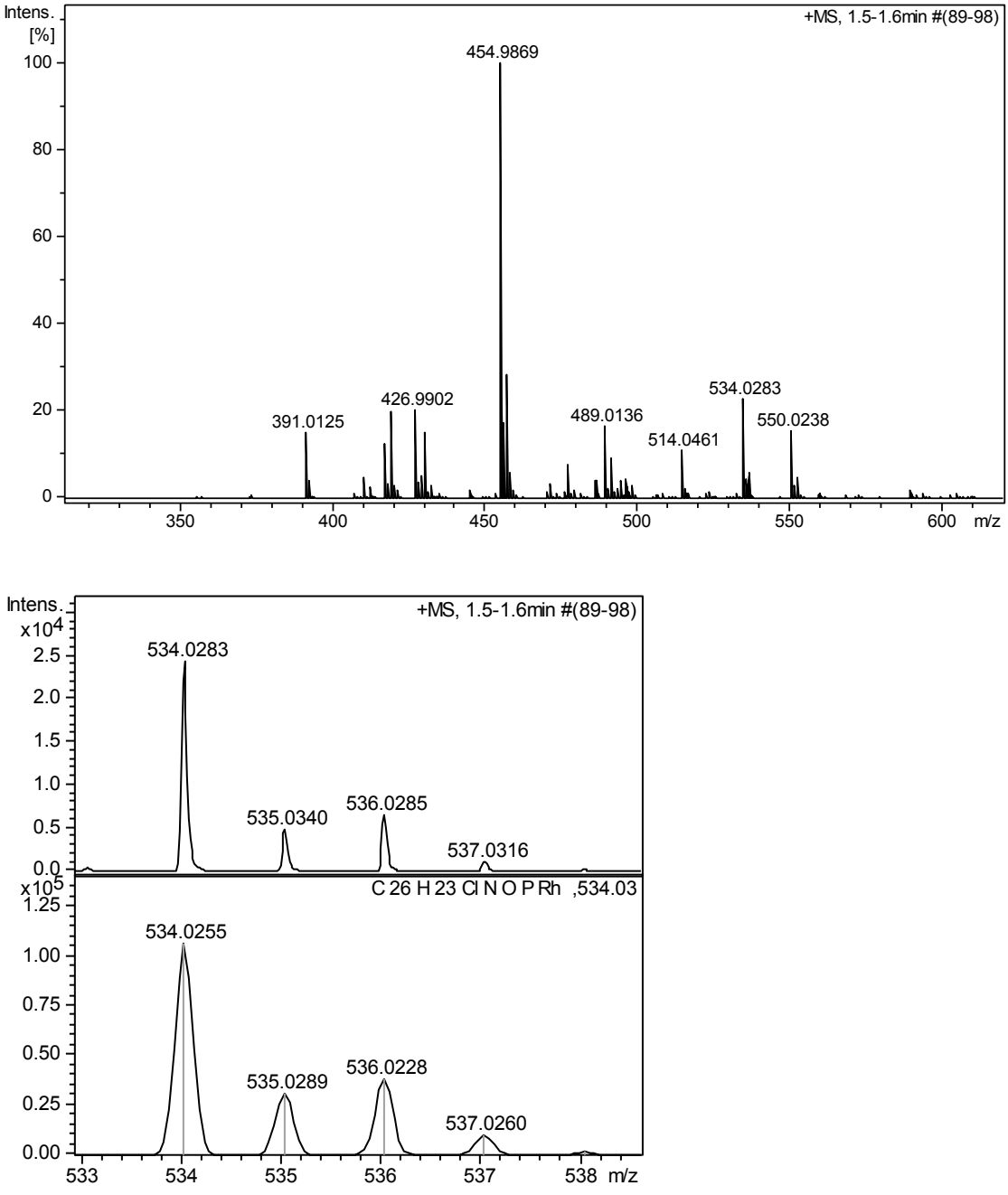


Figure SI-18. ESI-MS of [RhHCl($PPh_2CH(Ph)CH_2CO$)$(Py)_2$] (**1**).

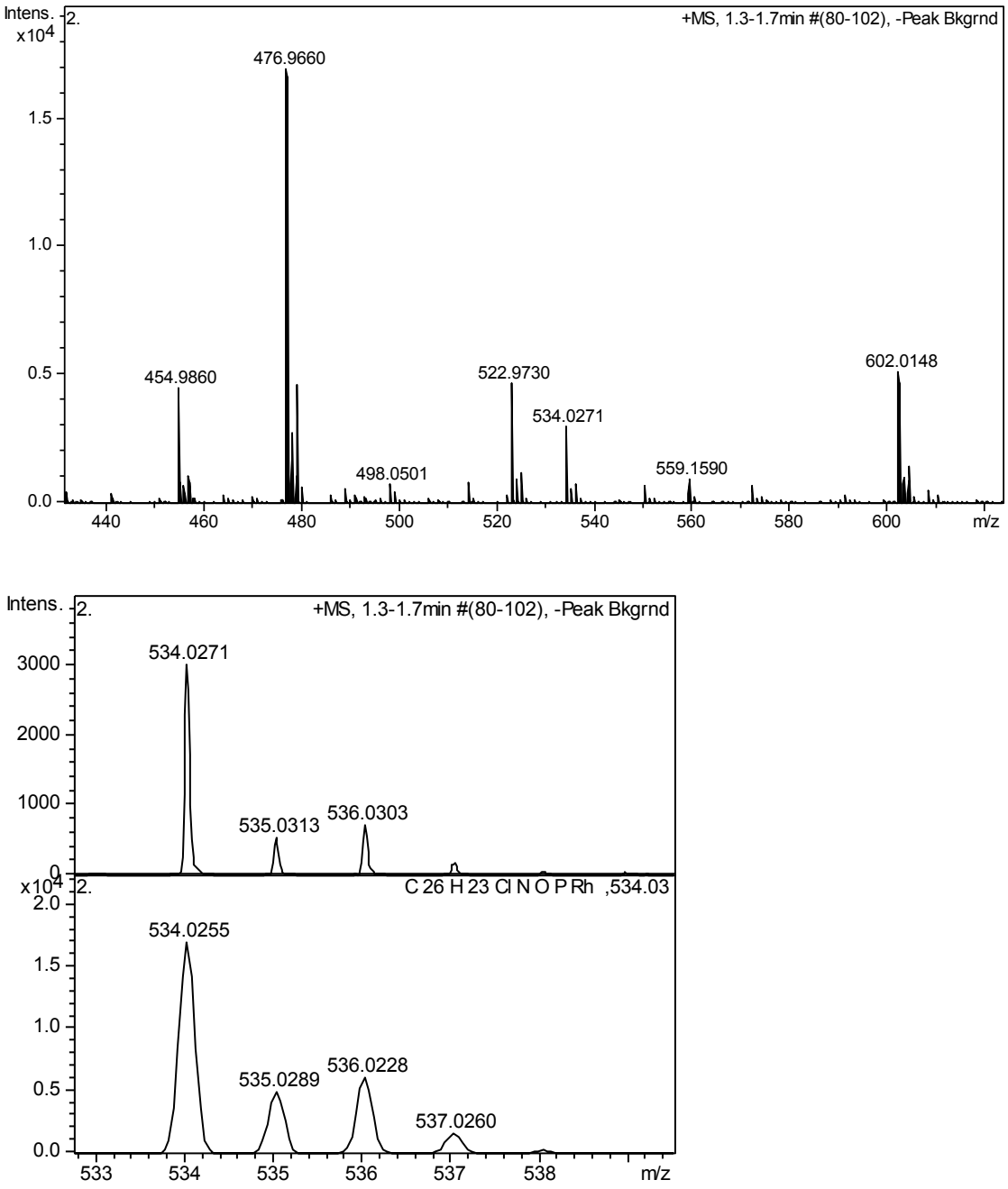


Figure SI-19. ESI-MS of $[RhCl_2(PPh_2CH(Ph)CH_2CO)(Py)_2]$ (**2**).

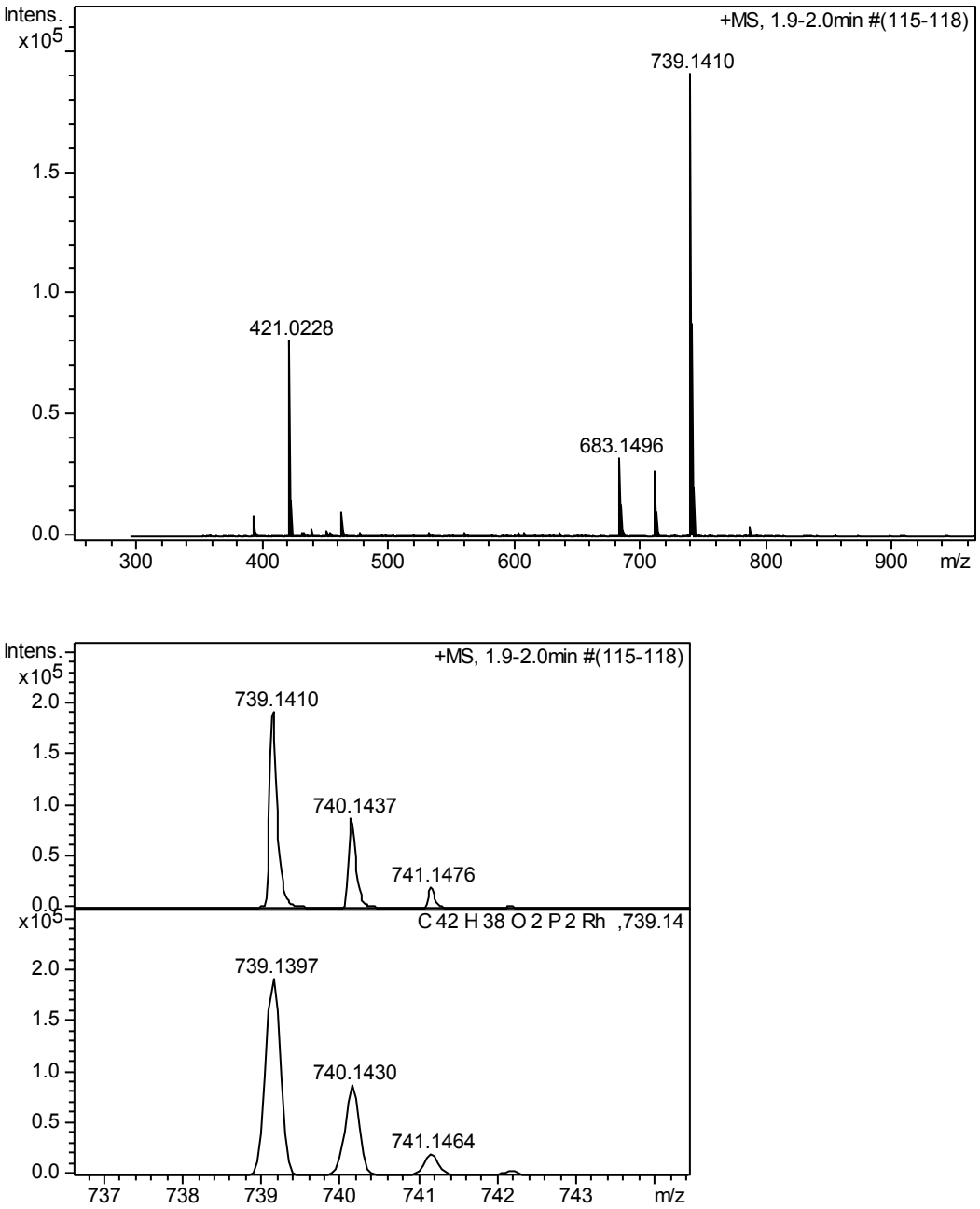


Figure SI-20. ESI-MS of [RhHCl($PPh_2CH(Ph)CH_2CO$)($PPh_2CH(Ph)CH_2CHO$)(Py)] (**3**).

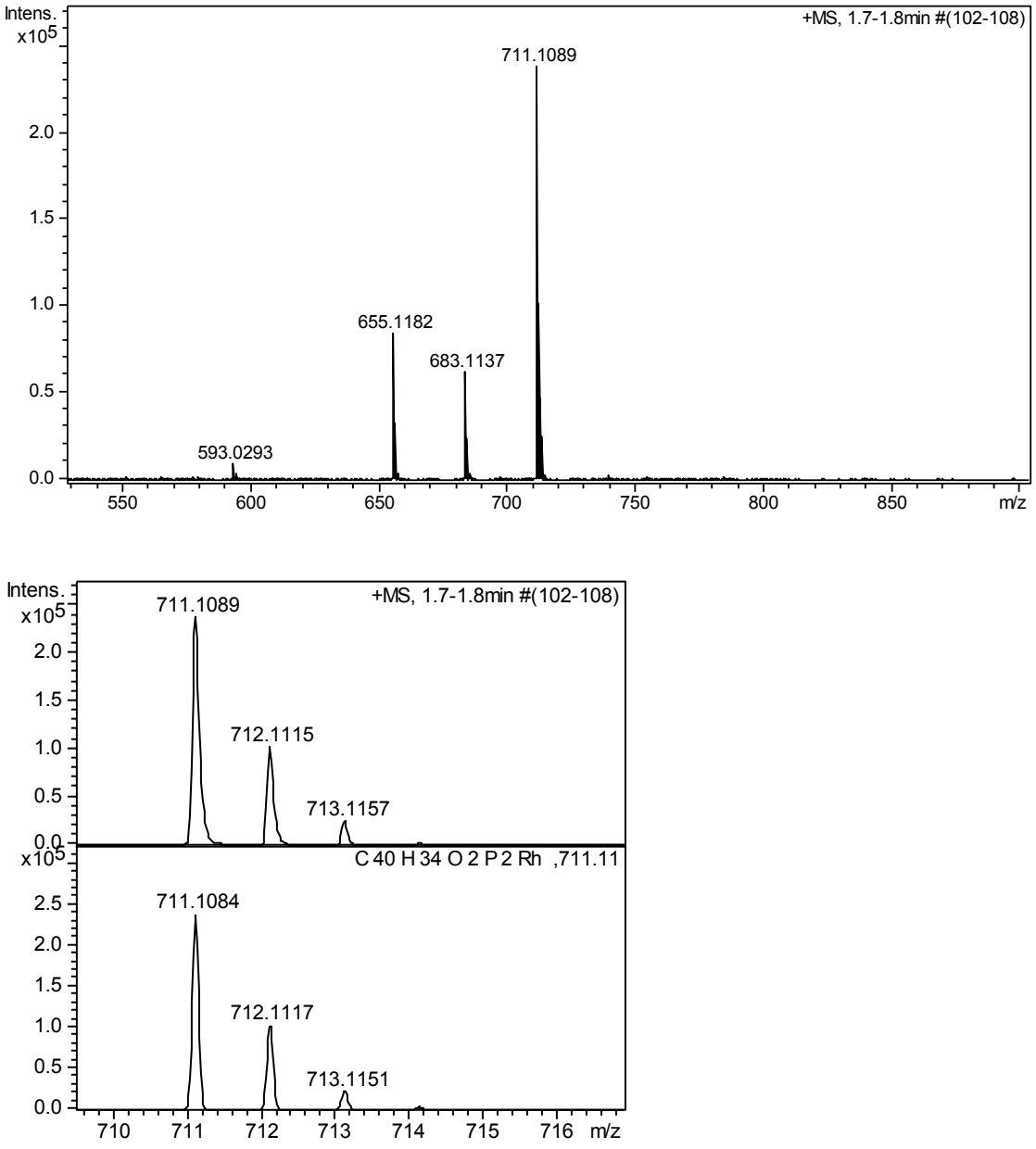


Figure SI-21. ESI-MS of [RhHCl(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(Py)] (**4**).

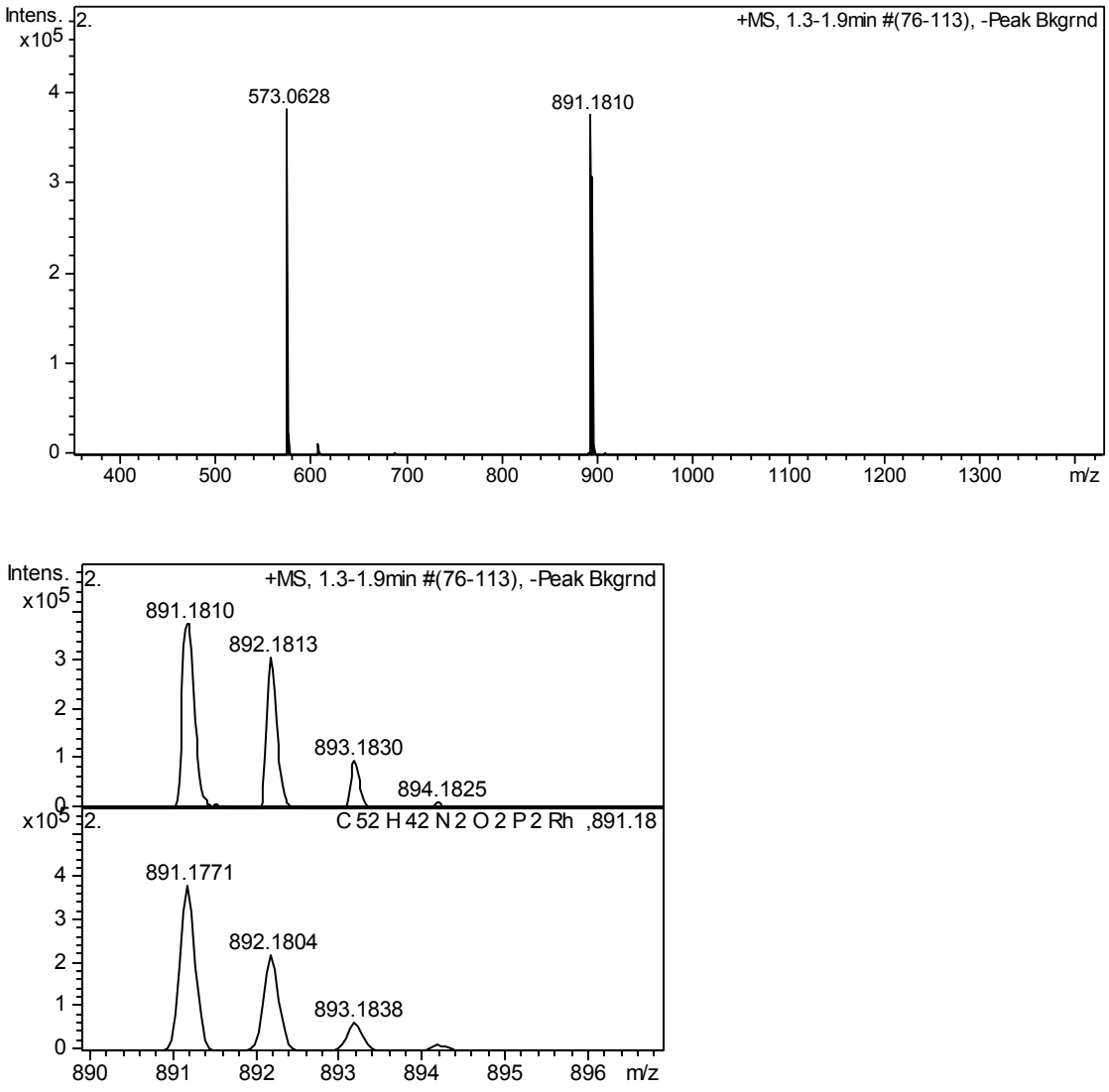


Figure SI-22. ESI-MS of [RhH(PPh$_2$(*o*-C$_6$H$_4$CO))(PPh$_2$CH(Ph)CH$_2$CHO)(phen)]BPh$_4$ (**5**).

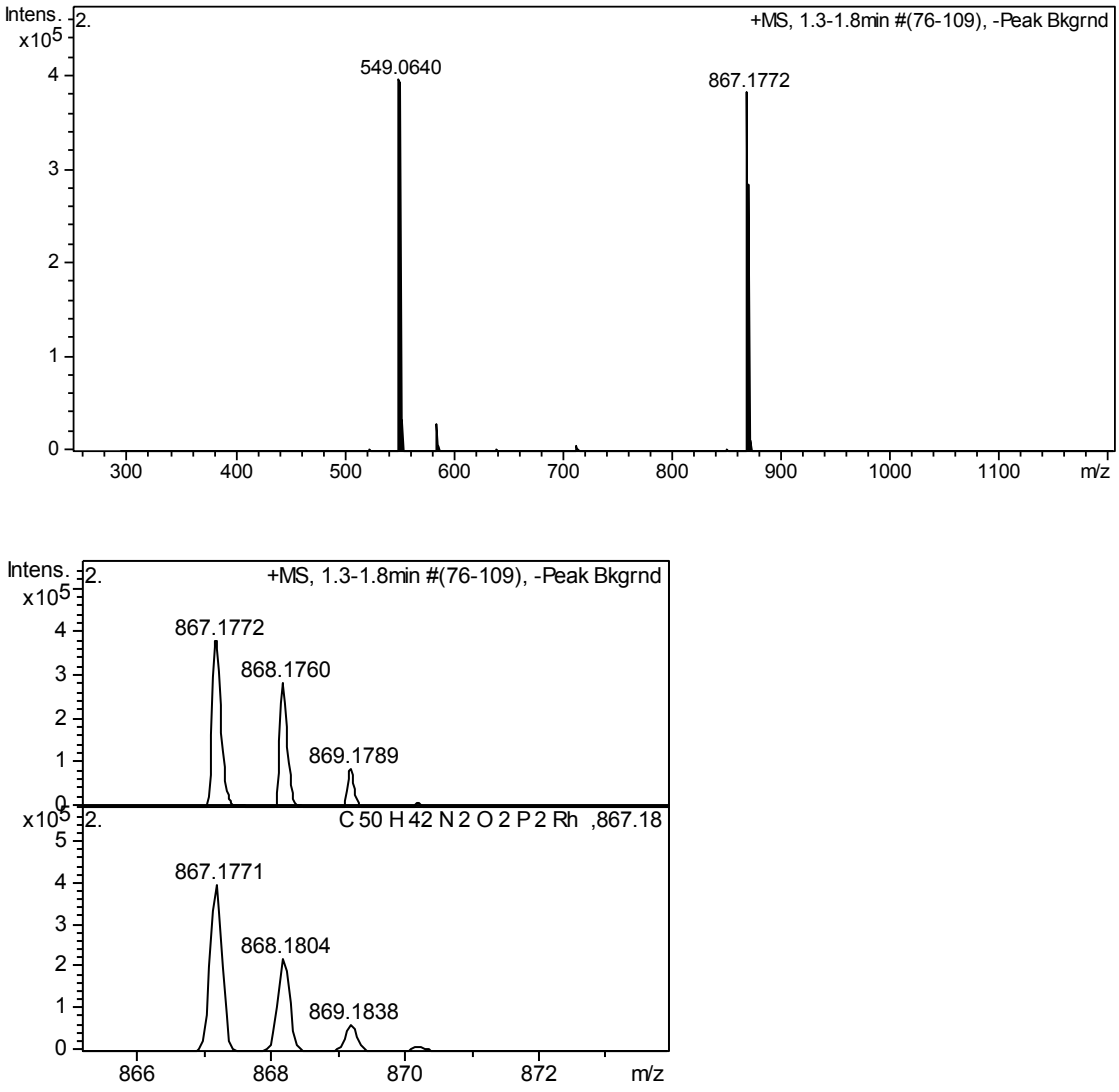


Figure SI-23. ESI-MS of [RhH(PPh_2(*o*-C_6H_4CO))($PPh_2CH(Ph)CH_2CHO$)(bipy)]BPh_4 (**6**).

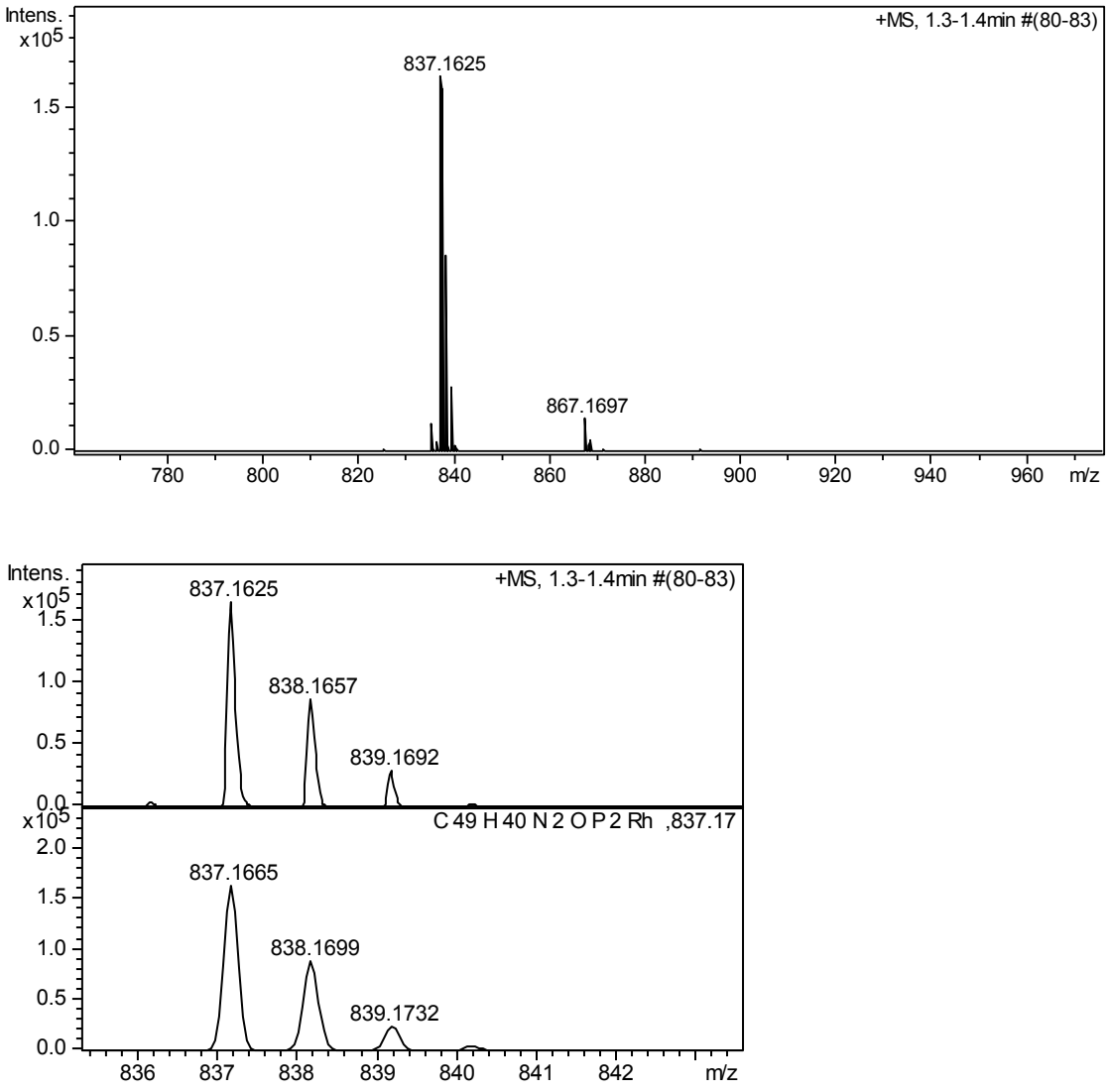


Figure SI-24. ESI-MS of [RhH(PPh_2(*o*-C_6H_4CO))(κ^3-*P,N,N*-$PPh_2CH(Ph)CH_2CNC_9H_6N$)]BF_4 (**7**).

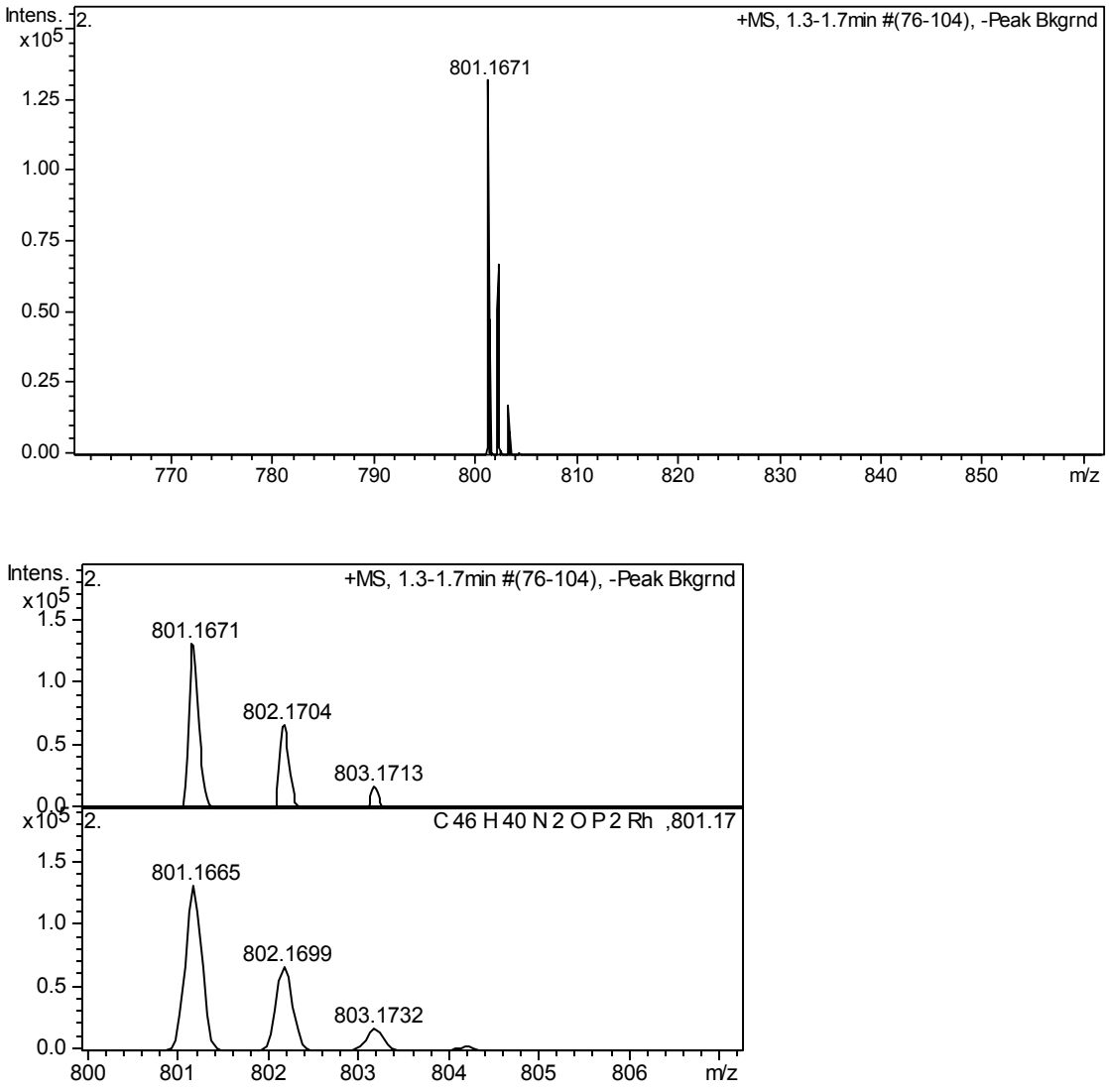


Figure SI-25. ESI-MS of [RhH(PPh$_2$(*o*-C$_6$H$_4$CO))(κ^3-*P*,*N*,*N*-PPh$_2$CH(Ph)CH$_2$CNCH$_2$C$_5$H$_4$N)]BF$_4$ (**8**).

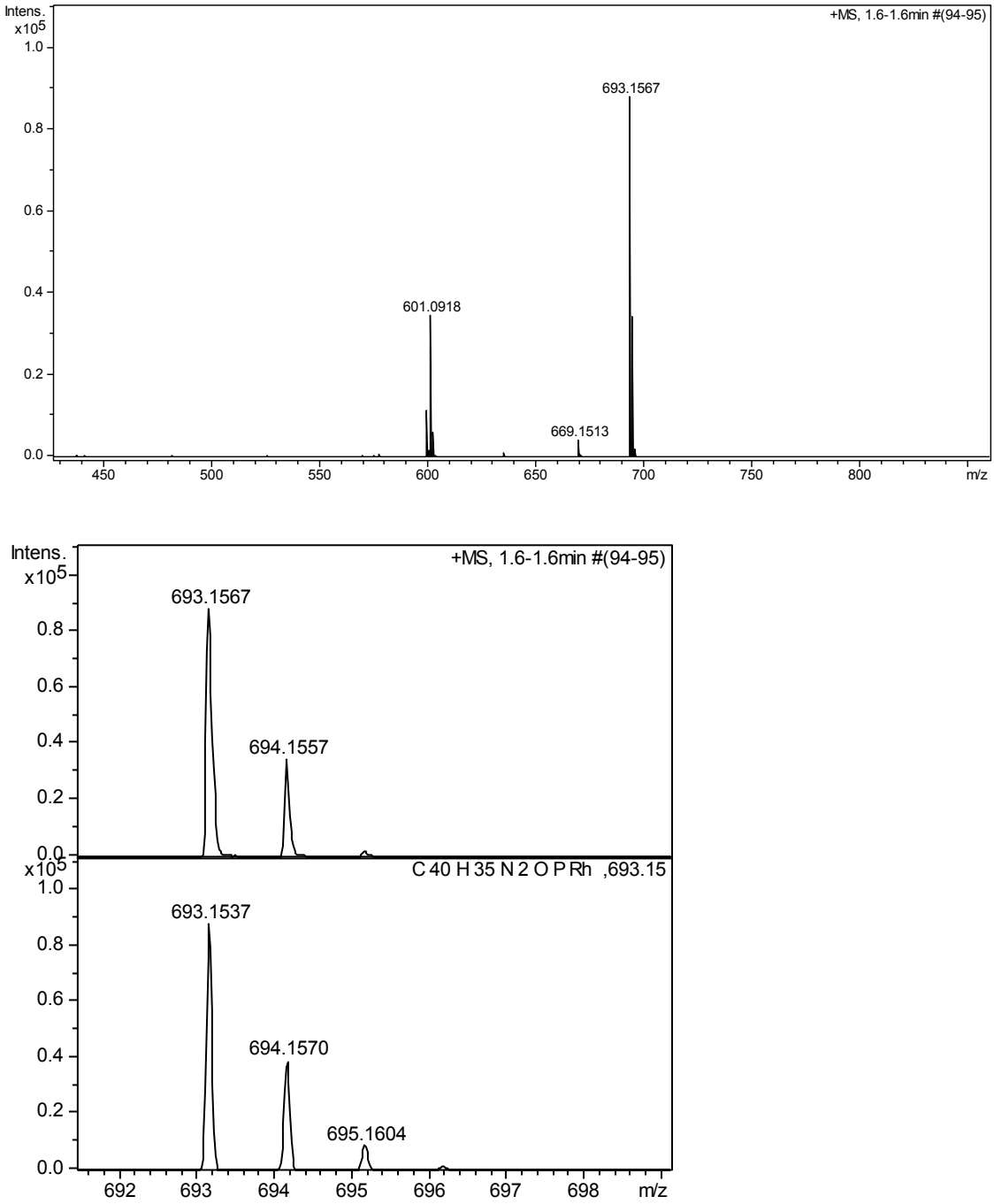


Figure SI-26. ESI-MS of [RhCl(Ntyl)($PPh_2CH(Ph)CH_2CO$)(phen)] (**9**).

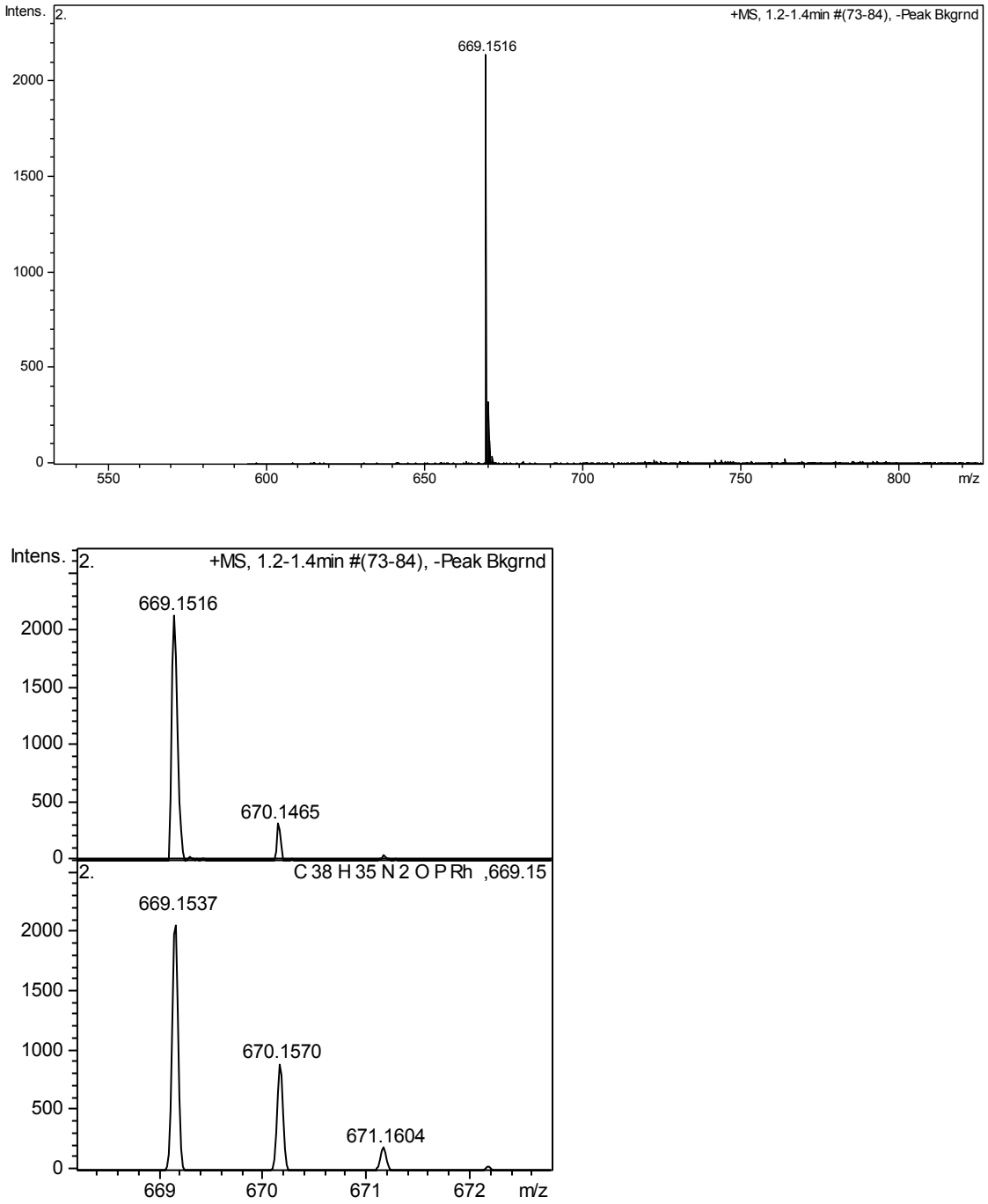


Figure SI-27. ESI-MS of [RhCl(Ntyl)($PPh_2CH(Ph)CH_2CO$)(bipy)] (**10**).

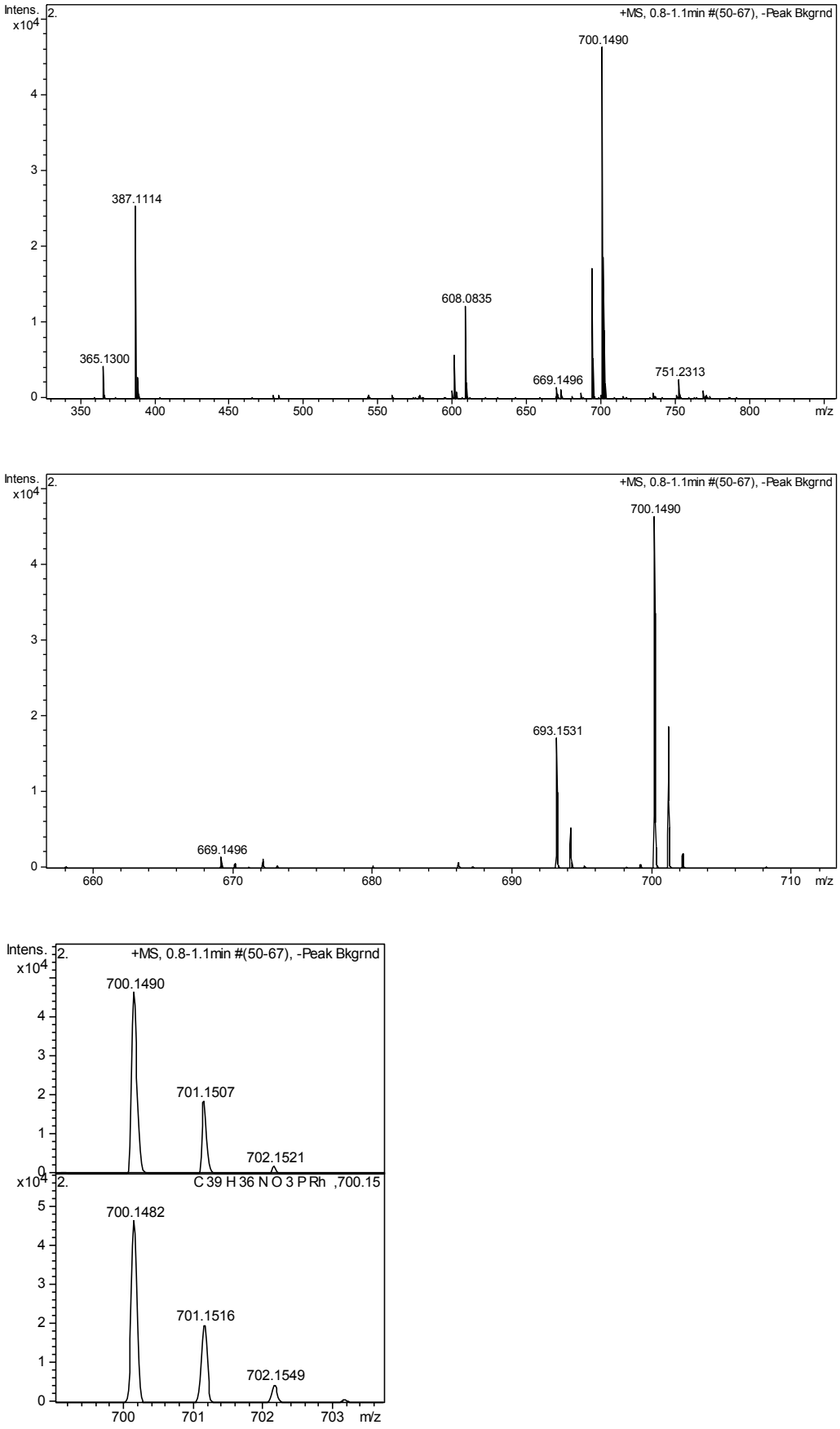


Figure SI-28. ESI-MS of [RhCl(Ntyl)(C_9H_6NCO)($PPh_2CH(Ph)CH_2CO(OCH_3)$)] (**11**).

4. DFT CALCULATIONS

Scheme SI-1. Representation of the three geometric isomers of **1** compatible with the experimental spectroscopic data (hydrido *trans* to chloride or pyridine; only one enantiomer has been represented).

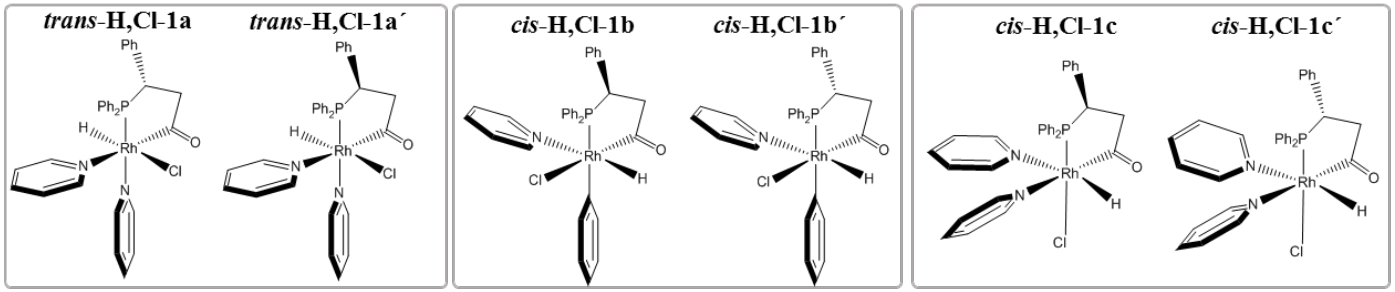


Table SI-2. Calculated electronic enthalpies in vacuum (ε°, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies (ε°+ZPVE, Hartree), the sum of electronic and thermal energies (ε°+E_{tot}, Hartree), the sum of electronic and thermal enthalpies (ε° + H_{corr}, Hartree), the sum of electronic and thermal free energies (ε° + G_{corr}, Hartree), enthropies (S, cal/mol·K), Gibss free energy values in solution (Gs, kcal/mol, dichloromethane) and relative Gibss free energy values in solution (ΔG_s, kcal/mol, dichloromethane) for the geometric isomers and corresponding pairs of diastereomers of **1** compatible with the experimental spectroscopic data.

Geometric Isomer	Diastereomer	ε°	ZPVE	ε°+ZPVE	ε° +E_{tot}	ε° + H_{corr}	ε° + G_{corr}	S	G_s	ΔG_s
***trans*-H,Cl-1a**	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2294.3106	0.524856	-2293.785737	-2293.751143	-2293.750198	-2293.856536	223.81	-1439401.86	0.00
***trans*-H,Cl-1a´**	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2294.3110	0.525573	-2293.785398	-2293.750954	-2293.750010	-2293.854366	219.64	-1439400.50	1.36
***cis*-H,Cl-1b**	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2294.3126	0.526117	-2293.786435	-2293.752243	-2293.751299	-2293.854018	216.19	-1439400.28	1.58
***cis*-H,Cl-1b´**	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2294.3083	0.526458	2293.781862	-2293.747551	-2293.746607	-2293.850711	219.11	-1439398.20	3.66
***cis*-H,Cl-1c**	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2294.2989	0.526142	-2293.772791	-2293.738481	-2293.737537	-2293.843273	222.54	-1439393.54	8.32
***cis*-H,Cl-1c´**	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2294.3046	0.526239	-2293.778313	-2293.743951	-2293.743007	-2293.847149	219.19	-1439395.97	5.89

Scheme SI-2. Representation of the species of **2** compatible with the experimental spectroscopic data.

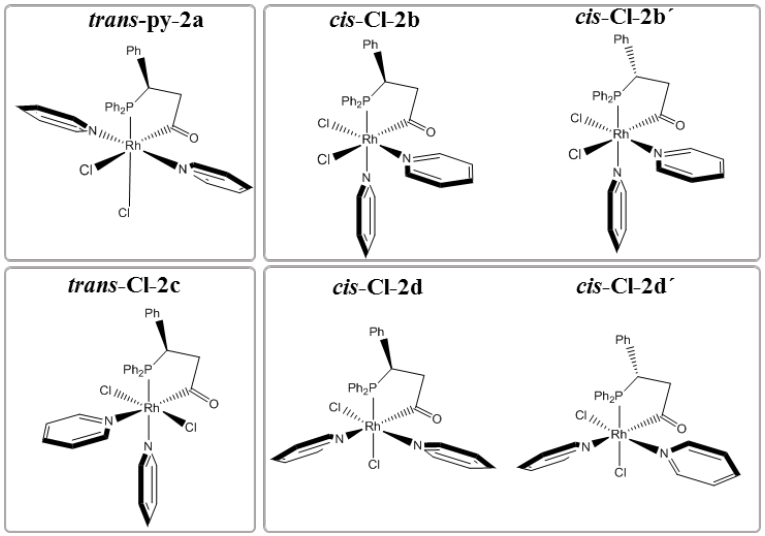


Table SI-3. Calculated electronic enthalpies in vacuum (ε°, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies (ε°+ZPVE, Hartree), the sum of electronic and thermal energies (ε°+E_{tot}, Hartree), the sum of electronic and thermal enthalpies (ε° + H_{corr}, Hartree), the sum of electronic and thermal free energies (ε° + G_{corr}, Hartree), enthropies (S, cal/mol·K) and Gibss free energy values in solution (Gs) and difference in Gibss free energy values in vacuum and in solution (ΔG_v and ΔG_s, kcal/mol, chloroform) for all stable conformers identified for the geometric isomers and diastereomers of **2** compatible with the experimental spectroscopic data.

Geometric Isomer	Diastereomer	ε°v	ε°s	ZPVE	ε°+ZPVE	ε° +E_{tot}	ε° + H_{corr}	ε° + G_{corr}	S	G_s	ΔG_s	ΔG_v
***Trans*-py-2a**	-	-2753.909791	-2753.9469	0.52051	-2753.43446	-2753.39932	-2753.39838	-2753.50195	218.0	-1727830.7	1.28	7.10
***cis*-Cl-2b**	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2753.931421	-2753.9594	0.520313	-2753.44493	-2753.40963	-2753.40869	-2753.51308	219.7	-1727837.7	0.00	0.00
***cis*-Cl-2b'**	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2753.931897	-2753.9591	0.520859	-2753.4443	-2753.40914	-2753.4082	-2753.51219	218.9	-1727837.2	1.03	0.56
***trans*-Cl-2c**	-	-2753.932966	-2753.9537	0.51931	-2753.43876	-2753.40301	-2753.40207	-2753.50924	225.6	-1727835.3	6.98	2.45
***cis*-Cl-2d**	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2753.914725	-2753.9453	0.520293	-2753.43191	-2753.3965	-2753.39556	-2753.50049	220.8	-1727829.8	6.26	8.03
***cis*-Cl-2d´**	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2753.911961	-2753.9433	0.52126	-2753.42924	-2753.39413	-2753.39318	-2753.49648	217.4	-1727827.3	8.31	10.58

Scheme SI-3. Representation of the two pairs of diastereomers of **4** compatible with the experimental spectroscopic data (hydride *trans* to chloride or pyridine; enantiomers omitted).

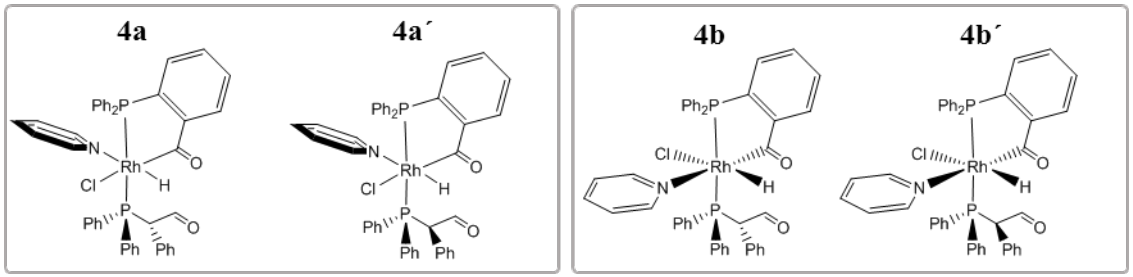


Table SI-4. Calculated electronic enthalpies in vacuum (ε°, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies (ε°+ZPVE, Hartree), the sum of electronic and thermal energies (ε°+E_{tot}, Hartree), the sum of electronic and thermal enthalpies (ε° + H_{corr}, Hartree), the sum of electronic and thermal free energies (ε° + G_{corr}, Hartree), enthropies (S, cal/mol·K) and Gibss free energy values in solution (Gs) and difference in Gibss free energy values in solution (ΔG_s, kcal/mol, dichloromethane) for all stable conformers identified for the geometric isomers and diastereomers of **4** compatible with the experimental spectroscopic data.

Geometric Isomer	Diastereomer	ε°	ZPVE	ε°+ZPVE	ε° +E_{tot}	ε° + H_{corr}	ε° + G_{corr}	S	G_s	ΔG_s
4a	$C_{Rh}S_c$+ $A_{Rh}R_c$	-3156.2622038	0.692449	-3155.569754	-3155.523223	-3155.522279	-3155.652276	273.60	-1980181.27	0.00
4a´	$C_{Rh}R_c$+ $A_{Rh}S_c$	-3156.2600671	0.692630	-3155.567437	-3155.520844	-3155.519899	-3155.650268	274.39	-1980180.01	1.26
4b	$C_{Rh}R_c$+ $A_{Rh}S_c$	-3156.2574321	0.692206	-3155.565226	-3155.518425	-3155.517481	-3155.649402	277.65	-1980179.47	1.80
4b´	$C_{Rh}S_c$+ $A_{Rh}R_c$	-3156.2512527	0.691554	-3155.559699	-3155.512860	-3155.511916	-3155.643018	275.93	-1980175.46	5.81

Scheme SI-4. Representation of the pair of diastereomers of **10** and **11.**

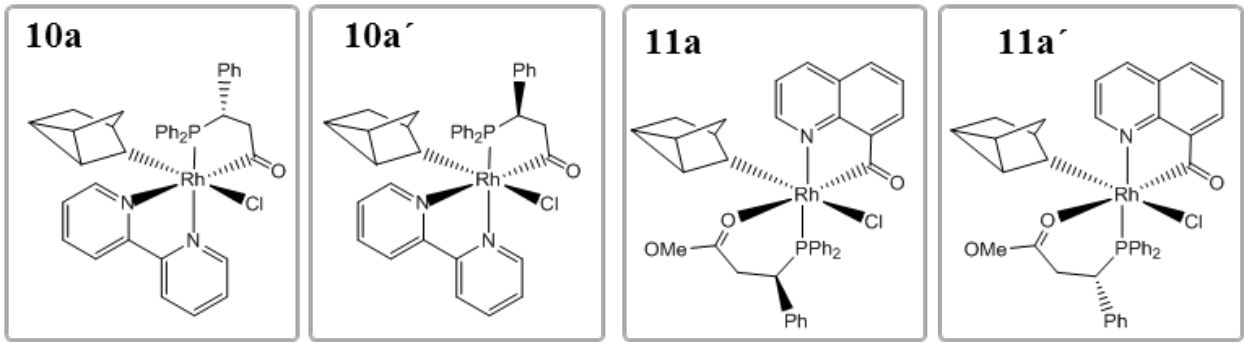


Table SI-5. Calculated electronic enthalpies in vacuum (ε°, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies (ε°+ZPVE, Hartree), the sum of electronic and thermal energies (ε°+E_{tot}, Hartree), the sum of electronic and thermal enthalpies (ε° + H_{corr}, Hartree), the sum of electronic and thermal free energies (ε° + G_{corr}, Hartree), enthropies (S, cal/mol·K) and Gibss free energy values in solution (Gs) and difference in Gibss free energy values in solution ΔG_s, kcal/mol, dichloromethane for **10** and methanol for **11**) for all stable conformers identified for the geometric isomers and diastereomers of **10 and 11,** compatible with the experimental spectroscopic data.

Geometric Isomer	Diastereomer	ε°$_v$	ε°$_s$	ZPVE	ε°+ZPVE	ε° +E_{tot}	ε° + H_{corr}	ε° + G_{corr}	S	ΔG_s	ΔG_v
10a	$A_{Rh}S_c$+ $C_{Rh}R_c$	-2562.982870	-2563.004488	0.616199	-2562.366671	-2562.326793	-2562.325848	-2562.440588	241.5	0.00	0.00
10a´	$A_{Rh}R_c$+ $C_{Rh}S_c$	-2562.974019	-2562.992786	0.617110	-2562.356909	-2562.317286	-2562.316342	-2562.429581	238.3	8.70	7.02
11a	$C_{Rh}R_c$+ $A_{Rh}S_c$	-2697.305824	-2697.328349	0.635605	-2696.670219	-2696.627645	-2696.626701	-2696.746682	252.5	0.00	0.00
11a´	$C_{Rh}S_c$+ $A_{Rh}R_c$	-2697.295811	-2697.322716	0.636179	-2696.659632	-2696.617154	-2696.616209	-2696.736093	252.3	3.90	6.75

XYZ coordinates of the minimum energy geometries of all the calculated structures of 1, 2, 4, 10 and 11.

***trans*-H,Cl-1a**

66

N	1.560520	1.210764	1.335518
C	0.983298	1.219425	2.542633
C	1.148987	2.255329	3.451215
C	1.954966	3.329778	3.093928
C	2.564533	3.321239	1.846152
C	2.339867	2.244370	0.997103
Rh	1.033794	-0.458388	-0.226465
Cl	2.153964	0.906715	-2.195334
C	0.573446	-1.833981	-1.559119
O	1.247394	-2.811789	-1.759607
C	-0.656226	-1.558790	-2.452894
C	-1.835638	-0.954537	-1.689575
C	-2.659364	-1.944112	-0.899837
C	-4.005666	-1.659874	-0.651200
C	-4.777042	-2.500097	0.139376
C	-4.213572	-3.647633	0.693291
C	-2.880906	-3.948166	0.439357
C	-2.106694	-3.102752	-0.352996
P	-1.059210	0.300347	-0.532725
C	-1.118408	1.930020	-1.348081
C	-0.787110	3.051845	-0.580303
C	-0.724203	4.307585	-1.168491
C	-0.987369	4.454545	-2.528594
C	-1.313525	3.342669	-3.295197
C	-1.376632	2.081555	-2.708671
C	-2.205367	0.470983	0.882224
C	-2.132754	-0.437080	1.942170
C	-3.075289	-0.403345	2.962426
C	-4.099847	0.538121	2.935019
C	-4.179428	1.444301	1.883067
C	-3.239281	1.410902	0.858241
N	3.030968	-1.339878	0.203856
C	3.424756	-1.484946	1.474219
C	4.656995	-2.017840	1.821740
C	5.520568	-2.412617	0.807437
C	5.116299	-2.257493	-0.511572
C	3.863189	-1.719187	-0.771212
H	-0.937417	-2.478476	-2.971155
H	-0.289993	-0.837783	-3.193693
H	-2.504435	-0.414722	-2.362570
H	-1.347681	-1.184186	1.962978
H	-3.010102	-1.115363	3.776384
H	-4.834163	0.565230	3.731334
H	-4.976528	2.177495	1.854735
H	-3.318862	2.115481	0.038589
H	-0.582033	2.942927	0.480737
H	-0.465912	5.170939	-0.566905
H	-0.933406	5.434079	-2.988296
H	-1.513436	3.451137	-4.354257
H	-1.612529	1.226023	-3.330420
H	-4.813171	-4.304529	1.312221
H	-5.817939	-2.261303	0.323813
H	-4.444947	-0.760940	-1.072115
H	-1.070269	-3.358468	-0.539400
H	-2.436914	-4.844260	0.856625
H	2.721854	-1.158081	2.231772
H	4.925424	-2.117475	2.864967
H	6.491275	-2.832929	1.041396
H	5.755379	-2.546113	-1.335451
H	3.503236	-1.576174	-1.781319
H	0.361434	0.363986	2.782334
H	0.653692	2.213872	4.412313
H	2.105341	4.156777	3.777305
H	3.201833	4.134560	1.524837
H	2.774977	2.198406	0.004652
H	0.410261	-1.375212	0.811158

trans-H,Cl-1a'

66

N	1.924317	1.480016	-0.580169
C	2.242519	2.353993	0.381145
C	2.387996	3.713647	0.144239
C	2.190061	4.188506	-1.146933
C	1.857755	3.285440	-2.147928
C	1.733972	1.940319	-1.820844
Rh	1.250816	-0.691716	0.044323
Cl	1.671248	-1.490875	-2.433384
C	0.571413	-2.421967	0.690763
O	1.292436	-3.363925	0.898609
C	-0.950868	-2.577638	0.876553
C	-1.623801	-1.268671	1.297294
P	-0.900824	-0.012244	0.116494
C	-2.056664	-0.051284	-1.291436
C	-3.272723	0.641728	-1.239576
C	-4.213611	0.470419	-2.245208
C	-3.955720	-0.400299	-3.302268
C	-2.752818	-1.093879	-3.354429
C	-1.800258	-0.921195	-2.352068
C	-3.129557	-1.262113	1.340168
C	-3.902878	-2.084321	0.517815
C	-5.290349	-1.987741	0.523210
C	-5.928259	-1.069130	1.349641
C	-5.167776	-0.251362	2.180649
C	-3.781089	-0.350923	2.176264
C	-1.043037	1.664447	0.825801
C	-1.206750	2.766753	-0.016759
C	-1.129713	4.057881	0.495806
C	-0.894323	4.259551	1.851236
C	-0.725124	3.165572	2.694492
C	-0.786699	1.874758	2.183020
N	3.385067	-1.165262	0.435897
C	3.780476	-1.805682	1.541548
C	5.117483	-2.025747	1.838963
C	6.084254	-1.566742	0.953462
C	5.675378	-0.903721	-0.196114
C	4.316984	-0.722938	-0.416028
H	-1.147468	-3.380678	1.590527
H	-1.317123	-2.904646	-0.104434
H	-1.234421	-0.986020	2.279941
H	-3.430042	-2.796009	-0.148370
H	-5.873594	-2.630756	-0.125492
H	-7.009035	-0.993929	1.350933
H	-5.653159	0.462903	2.835245
H	-3.193291	0.291910	2.823939
H	-1.382856	2.621534	-1.076706
H	-1.249050	4.904598	-0.169527
H	-0.835479	5.265504	2.249213
H	-0.534489	3.315784	3.750292
H	-0.613287	1.036425	2.848641
H	-3.492519	1.299664	-0.406185
H	-5.153103	1.007927	-2.198376
H	-4.694779	-0.535769	-4.083233
H	-2.548069	-1.769569	-4.176118
H	-0.853985	-1.448869	-2.399906
H	2.992874	-2.160363	2.192637
H	5.385840	-2.550312	2.746265
H	7.136829	-1.725285	1.154744
H	6.389428	-0.530781	-0.918406
H	3.947080	-0.220618	-1.301571
H	2.375722	1.941000	1.375600
H	2.642951	4.379191	0.958516
H	2.290585	5.244634	-1.366898
H	1.692957	3.608936	-3.167390
H	1.477475	1.192942	-2.565137
H	1.115609	-0.281448	1.502992

cis-H,Cl-1b

66

C	-3.645385	-2.430472	0.614225
N	-3.167698	-1.596559	-0.319640
C	-3.952155	-1.256229	-1.349392
C	-5.247746	-1.740909	-1.487007
C	-5.743049	-2.614261	-0.525912
C	-4.925641	-2.966240	0.542353
Rh	-1.150637	-0.725684	-0.058076
P	0.965565	0.017939	0.164542
C	1.107563	1.807379	0.519418
C	0.245715	2.334447	1.490253
C	0.260292	3.698768	1.760046
C	1.137118	4.541646	1.079486
C	2.013611	4.016486	0.134570
C	1.999519	2.651708	-0.146246
N	-2.127029	1.379241	-0.325006
C	-0.678926	-0.883997	-1.964174
C	0.784627	-1.234043	-2.271012
C	1.691741	-0.211354	-1.563469
C	3.160021	-0.536055	-1.677765
C	3.676541	-1.742013	-1.189409
C	5.030981	-2.031701	-1.303294
C	5.895179	-1.124457	-1.913429
C	5.392149	0.070850	-2.416108
C	4.034129	0.358034	-2.301100
O	-1.445666	-0.638978	-2.870039
C	2.078731	-0.761715	1.375493
C	3.377340	-0.265872	1.545250
C	4.250263	-0.887953	2.427761
C	3.827112	-1.999998	3.155157
C	2.529617	-2.479628	3.006975
C	1.649423	-1.862707	2.119468
Cl	-1.651381	-0.586071	2.492421
H	0.957251	-1.220357	-3.351612
H	0.980854	-2.240779	-1.885773
H	1.511274	0.761519	-2.039854
H	3.016700	-2.449189	-0.693284
H	5.413474	-2.967288	-0.908282
H	6.952797	-1.351253	-2.000243
H	6.053602	0.779610	-2.904152
H	3.644205	1.285007	-2.715318
H	-0.438692	1.669813	2.016576
H	-0.419889	4.103322	2.502963
H	1.142388	5.606505	1.290555
H	2.709107	4.666678	-0.386727
H	2.694670	2.249996	-0.877698
H	3.710506	0.597920	0.975134
H	5.258820	-0.506202	2.547828
H	4.509069	-2.484263	3.847372
H	2.193434	-3.330479	3.590382
H	0.623438	-2.204416	2.026132
H	-3.503358	-0.592631	-2.081379
H	-5.847073	-1.435484	-2.336820
H	-6.749193	-3.013471	-0.607299
H	-5.268269	-3.639634	1.319318
H	-2.979433	-2.635104	1.446130
H	-0.535613	-2.109312	0.101947
C	-2.952630	1.846342	0.618847
C	-3.374595	3.172156	0.649044
C	-2.913555	4.045950	-0.328852
C	-2.066585	3.557656	-1.318028
C	-1.708641	2.216073	-1.281067
H	-3.236163	1.131751	1.387641
H	-4.039986	3.505810	1.437094
H	-3.209768	5.090328	-0.322145
H	-1.683031	4.199156	-2.102811
H	-1.060623	1.788056	-2.041188

cis-H,Cl-1b'

66

C	-1.149973	-2.470702	-1.102896
C	-1.955747	-1.584543	-1.819222
C	-3.001055	-2.101132	-2.586898
C	-3.241976	-3.470587	-2.631199
C	-2.436297	-4.345226	-1.909363
C	-1.388505	-3.839945	-1.146336
C	-1.704209	-0.091421	-1.832831
C	-0.498300	0.245217	-2.728382
C	0.817754	-0.059500	-1.995836
O	1.689297	-0.689304	-2.541158
P	-1.262277	0.676913	-0.184291
C	-2.254064	-0.130196	1.125321
C	-1.855119	0.070564	2.449436
C	-2.612003	-0.451504	3.493239
C	-3.772293	-1.169532	3.223687
C	-4.182918	-1.354668	1.907161
C	-3.430996	-0.835609	0.859160
C	-2.038573	2.338578	-0.252653
C	-3.392232	2.459804	-0.583606
C	-3.995621	3.709884	-0.613540
C	-3.256862	4.847522	-0.295744
C	-1.918414	4.728884	0.058270
C	-1.306385	3.478117	0.080230
Rh	1.019110	0.658633	-0.175859
N	3.216334	0.850495	-0.413974
C	4.018194	0.564644	0.619126
C	5.399213	0.676785	0.546848
C	5.974249	1.113814	-0.638943
C	5.143722	1.421295	-1.708925
C	3.773509	1.271190	-1.555631
N	1.526558	-1.370887	0.865565
C	2.242487	-2.269547	0.176504
C	2.634360	-3.486431	0.715611
C	2.270015	-3.786820	2.023080
C	1.535942	-2.853611	2.742691
C	1.189484	-1.657269	2.127258
Cl	1.318343	1.825969	2.216301
H	-2.592131	0.411974	-2.219502
H	-0.536992	-0.314145	-3.665227
H	-0.486995	1.318148	-2.948429
H	-0.960789	0.649240	2.659593
H	-2.294274	-0.292555	4.516794
H	-4.359662	-1.578775	4.036999
H	-5.090998	-1.904852	1.691733
H	-3.767581	-0.990023	-0.158473
H	-3.984356	1.579142	-0.811382
H	-5.042170	3.796088	-0.879669
H	-3.728965	5.822500	-0.317636
H	-1.344564	5.609491	0.320962
H	-0.267812	3.382821	0.374735
H	3.093852	1.492210	-2.367658
H	5.541893	1.772576	-2.651566
H	7.049126	1.216643	-0.726842
H	6.001759	0.427525	1.410176
H	3.523082	0.250855	1.529737
H	0.822107	1.985786	-0.883065
H	0.638342	-0.891022	2.657608
H	1.235288	-3.038318	3.765553
H	2.557772	-4.729138	2.473623
H	3.213151	-4.177743	0.117432
H	2.497961	-1.990301	-0.840787
H	-3.633871	-1.424488	-3.152379
H	-4.060091	-3.852551	-3.230310
H	-2.624379	-5.411594	-1.940280
H	-0.755068	-4.509927	-0.576333
H	-0.340172	-2.094373	-0.490082

cis-H,Cl-1c

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C	-1.631596	2.326703	0.312327
C	-1.814555	1.011017	0.742174
C	-2.843028	0.721728	1.644573
C	-3.689345	1.729862	2.087918
C	-3.509727	3.037744	1.645726
C	-2.476056	3.335453	0.764902
P	-0.779180	-0.330708	0.046038
C	-1.845153	-1.287290	-1.190840
C	-3.304104	-0.904830	-1.189808
C	-3.713927	0.357720	-1.629550
C	-5.050877	0.727280	-1.576717
C	-6.005781	-0.163654	-1.090719
C	-5.613005	-1.428943	-0.672139
C	-4.270425	-1.795887	-0.724112
Rh	1.035781	0.257659	-1.122340
N	2.692875	-1.110732	-0.275556
Cl	2.742306	1.038676	-2.854429
N	1.798785	2.016410	0.370498
C	2.595895	2.985551	-0.098578
C	2.999267	4.071348	0.668885
C	2.561301	4.166149	1.982517
C	1.732337	3.167701	2.477058
C	1.377852	2.121118	1.637118
H	0.007202	1.185543	-1.754405
C	0.362551	-1.111502	-2.365499
O	1.091903	-1.887495	-2.917728
C	-0.557085	-1.488967	1.451738
C	0.622776	-1.437052	2.199164
C	0.812364	-2.295964	3.276914
C	-0.171406	-3.217716	3.616637
C	-1.349497	-3.277134	2.878512
C	-1.541093	-2.418768	1.802305
C	-1.158441	-1.157406	-2.559881
H	-1.426322	-1.997969	-3.203611
H	-1.451716	-0.225132	-3.048256
H	-1.749117	-2.329054	-0.872941
H	-2.980717	1.066411	-2.000758
H	-5.349037	1.713201	-1.912932
H	-7.048978	0.125672	-1.048108
H	-6.348901	-2.135858	-0.307493
H	-3.976771	-2.792524	-0.410918
H	1.409473	-0.743978	1.925699
H	1.735384	-2.250100	3.842322
H	-0.019926	-3.891743	4.451069
H	-2.120580	-3.992490	3.137336
H	-2.467990	-2.475965	1.243709
H	-2.997120	-0.289883	2.000355
H	-4.490258	1.492974	2.777742
H	-4.171312	3.822641	1.992474
H	-2.324142	4.352913	0.425606
H	-0.828121	2.563936	-0.374405
H	2.917309	2.873631	-1.127432
H	3.643801	4.823776	0.233698
H	2.856516	5.000822	2.606835
H	1.357606	3.192873	3.491743
H	0.715949	1.343177	2.000019
C	3.865597	-0.571413	0.070948
C	4.925045	-1.325259	0.557287
C	4.764625	-2.699464	0.679224
C	3.552679	-3.266290	0.305249
C	2.546640	-2.434711	-0.165863
H	3.951785	0.501596	-0.057593
H	5.853121	-0.838367	0.825929
H	5.571493	-3.318514	1.052348
H	3.382119	-4.332443	0.373965
H	1.587816	-2.839182	-0.469543

cis-H,Cl-1c'

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C	-2.419250	-0.471205	2.064992
C	-1.427949	-0.867968	1.162423
C	-1.006231	-2.201399	1.149646
C	-1.560389	-3.119913	2.035200
C	-2.536284	-2.714364	2.939880
C	-2.964674	-1.390378	2.953465
P	-0.832599	0.253301	-0.150141
Rh	1.137940	-0.152387	-1.110963
Cl	3.181426	-0.459395	-2.631126
C	-2.010862	-0.075262	-1.563853
C	-1.456977	-1.347433	-2.214442
C	0.074568	-1.508661	-2.070235
O	0.587839	-2.508822	-2.500641
C	-3.474448	-0.101568	-1.197229
C	-4.270672	1.014412	-1.468236
C	-5.618748	1.034971	-1.125895
C	-6.196077	-0.066871	-0.504926
C	-5.415421	-1.186176	-0.232261
C	-4.068270	-1.204236	-0.573698
C	-1.087181	1.938943	0.482048
C	-1.470010	2.971343	-0.376653
C	-1.482581	4.287493	0.073925
C	-1.099117	4.583004	1.378097
C	-0.708899	3.558865	2.236045
C	-0.701998	2.242164	1.791704
N	2.508201	1.466504	-0.053978
C	2.156710	2.748795	0.081747
C	3.004560	3.715461	0.608238
C	4.278459	3.337101	1.009813
C	4.657274	2.009263	0.855455
C	3.745358	1.113131	0.315608
N	2.096452	-1.649158	0.349018
C	2.635836	-2.776270	-0.127070
C	3.222277	-3.726501	0.700615
C	3.255035	-3.494627	2.069092
C	2.702381	-2.318550	2.564007
C	2.133778	-1.426538	1.667698
H	-1.831964	0.756818	-2.248352
H	0.568235	0.860842	-2.102965
H	-1.887454	-2.246533	-1.765225
H	-1.699907	-1.377203	-3.279403
H	-0.249998	-2.529291	0.445764
H	-1.226427	-4.150311	2.016903
H	-2.964421	-3.429871	3.631882
H	-3.733167	-1.072899	3.647756
H	-2.782270	0.549996	2.063229
H	-0.388230	1.452450	2.466271
H	-0.404709	3.784350	3.250906
H	-1.102503	5.609271	1.724842
H	-1.783144	5.081403	-0.598650
H	-1.732347	2.765277	-1.407147
H	1.160895	3.015000	-0.252465
H	2.663144	4.738865	0.693391
H	4.966531	4.063262	1.425938
H	5.643492	1.667106	1.139985
H	4.010800	0.075378	0.151935
H	1.693751	-0.494568	2.008608
H	2.707007	-2.093052	3.622166
H	3.704509	-4.216130	2.740763
H	3.643290	-4.626004	0.271299
H	2.578165	-2.903789	-1.202024
H	-3.478779	-2.082560	-0.334916
H	-5.855057	-2.050769	0.250957
H	-7.246528	-0.056332	-0.239515
H	-6.216429	1.909945	-1.352372
H	-3.835511	1.873956	-1.966321

***trans*-py-2a**

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N	2.434574	1.189401	0.125243
C	2.204115	1.937756	1.213920
C	2.752568	3.198560	1.373549
C	3.580488	3.699531	0.376823
C	3.844232	2.909034	-0.732685
C	3.256532	1.655857	-0.823172
Rh	1.494420	-0.690416	-0.070806
Cl	2.213384	-1.193651	2.449166
C	0.994821	-0.369824	-1.974453
O	1.803610	-0.067517	-2.799516
C	-0.484589	-0.516681	-2.384165
C	-1.472376	-0.558672	-1.214784
P	-0.624672	0.255904	0.237282
C	-0.615662	2.072957	0.012732
C	-1.092560	2.914343	1.020118
C	-0.963842	4.295859	0.901831
C	-0.358737	4.849224	-0.217990
C	0.119554	4.017069	-1.228073
C	-0.001078	2.640399	-1.112180
C	-2.864452	-0.086107	-1.550733
C	-3.104525	1.177028	-2.098755
C	-4.405318	1.603286	-2.341882
C	-5.483013	0.771826	-2.049357
C	-5.251893	-0.494092	-1.521678
C	-3.950782	-0.918277	-1.274793
C	-1.699005	-0.017702	1.684653
C	-1.189247	-0.561553	2.864560
C	-2.025815	-0.746543	3.962690
C	-3.365070	-0.385592	3.890733
C	-3.870870	0.183451	2.724127
C	-3.044109	0.376584	1.625892
N	0.676925	-2.650319	-0.237059
C	0.879673	-3.366468	-1.353517
C	0.388296	-4.652498	-1.507550
C	-0.327163	-5.227943	-0.465824
C	-0.511276	-4.497986	0.700379
C	0.008941	-3.215690	0.778787
Cl	3.685000	-1.683738	-0.765604
H	-0.566185	-1.427024	-2.985190
H	-0.692607	0.318995	-3.056666
H	-1.548727	-1.590518	-0.859825
H	-2.277835	1.840216	-2.326800
H	-4.576167	2.587613	-2.761235
H	-6.495572	1.107435	-2.238003
H	-6.083498	-1.151395	-1.297836
H	-3.775935	-1.900047	-0.846834
H	-0.139092	-0.823205	2.933523
H	-1.621806	-1.168575	4.874827
H	-4.014232	-0.532297	4.745712
H	-4.909202	0.487529	2.670527
H	-3.443621	0.854911	0.740138
H	-1.548932	2.501726	1.910769
H	-1.332729	4.935062	1.694497
H	-0.252810	5.923880	-0.305103
H	0.600000	4.439227	-2.102246
H	0.414607	2.021865	-1.898042
H	1.469229	-2.894689	-2.129729
H	0.576105	-5.185400	-2.429568
H	-0.724893	-6.230952	-0.557804
H	-1.044786	-4.906635	1.547704
H	-0.092499	-2.620986	1.675771
H	1.564897	1.502005	1.971107
H	2.526609	3.767486	2.265196
H	4.019220	4.685573	0.469313
H	4.496106	3.246641	-1.526922
H	3.426617	1.001057	-1.667166

***cis*-Cl-2b**

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N	1.725970	1.462130	0.338496
C	1.362945	2.046049	1.490251
C	1.660754	3.369553	1.772308
C	2.360057	4.116166	0.833655
C	2.754686	3.502936	-0.348278
C	2.423865	2.173476	-0.558056
Rh	1.218282	-0.558991	-0.046464
N	3.366633	-0.916423	-0.428196
C	3.776136	-1.667111	-1.456617
C	5.117493	-1.914340	-1.708319
C	6.070611	-1.358435	-0.865125
C	5.645365	-0.581557	0.204549
C	4.284817	-0.388873	0.391087
C	0.829205	-0.223931	-1.964843
O	1.698797	0.128116	-2.709497
C	-0.595435	-0.431776	-2.511930
C	-1.640789	-0.814886	-1.465246
P	-1.043316	-0.206130	0.193055
C	-1.450900	1.562082	0.386755
C	-2.017648	2.060721	1.560384
C	-2.185204	3.433324	1.728202
C	-1.788700	4.314803	0.731098
C	-1.209917	3.825155	-0.438357
C	-1.033835	2.459838	-0.604037
C	-3.077003	-0.492142	-1.790411
C	-3.479674	0.764178	-2.251840
C	-4.823485	1.033863	-2.487429
C	-5.785556	0.052051	-2.269888
C	-5.394834	-1.205513	-1.821885
C	-4.051172	-1.473162	-1.585331
C	-2.054027	-1.118616	1.392233
C	-1.505293	-2.181021	2.112342
C	-2.319482	-2.936512	2.951066
C	-3.672555	-2.640426	3.068678
C	-4.222734	-1.584106	2.346851
C	-3.419120	-0.823309	1.507845
Cl	0.771895	-2.901983	-0.533545
Cl	1.771346	-1.041809	2.535520
H	-0.517981	-1.211993	-3.273834
H	-0.850929	0.491592	-3.038386
H	-1.562159	-1.893195	-1.305334
H	-2.749025	1.544687	-2.427395
H	-5.118790	2.013985	-2.842386
H	-6.831707	0.264578	-2.454829
H	-6.134716	-1.979782	-1.657071
H	-3.750312	-2.452176	-1.227103
H	-0.450133	-2.406792	2.021958
H	-1.889959	-3.757130	3.512612
H	-4.301594	-3.232927	3.722636
H	-5.277651	-1.353760	2.433031
H	-3.855942	-0.007439	0.941790
H	-2.314582	1.387150	2.354868
H	-2.622686	3.809021	2.645140
H	-1.919305	5.381841	0.865769
H	-0.882334	4.506814	-1.213863
H	-0.540067	2.101982	-1.500877
H	2.999335	-2.082689	-2.084966
H	5.398539	-2.531398	-2.551196
H	7.126148	-1.531557	-1.036254
H	6.348675	-0.133722	0.893784
H	3.904987	0.187529	1.225938
H	0.830382	1.421574	2.194553
H	1.339087	3.795807	2.713017
H	2.599213	5.155549	1.022764
H	3.312657	4.036545	-1.105729
H	2.712774	1.651172	-1.461555

***cis*-Cl-2b´**

66

C	-3.554150	0.663642	1.106038
C	-2.313840	0.023220	1.225047
C	-2.101849	-0.908650	2.238951
C	-3.136069	-1.207858	3.122944
C	-4.370938	-0.584472	2.994846
C	-4.579208	0.357290	1.988061
P	-1.041693	0.366926	-0.023847
C	-0.967245	2.188708	-0.141333
C	-1.295064	2.995867	0.949756
C	-1.092041	4.371537	0.884831
C	-0.558883	4.947345	-0.262436
C	-0.224115	4.145761	-1.351609
C	-0.422398	2.773462	-1.290024
Rh	1.040674	-0.604231	0.085616
Cl	1.329164	-0.306439	2.742495
N	2.070447	1.240576	-0.147367
C	1.932466	2.210775	0.769878
C	2.614792	3.413440	0.683655
C	3.476519	3.623601	-0.383805
C	3.634268	2.611067	-1.321224
C	2.918959	1.433552	-1.167522
N	3.029170	-1.564584	0.059479
C	3.256418	-2.676497	-0.648533
C	4.495479	-3.298441	-0.677770
C	5.539059	-2.746465	0.053214
C	5.301675	-1.595685	0.793500
C	4.032233	-1.038336	0.772871
C	0.769090	-0.874331	-1.862248
C	-0.665510	-1.121348	-2.339624
C	-1.698337	-0.180370	-1.706492
H	-1.731228	0.740689	-2.291438
Cl	0.048778	-2.809770	0.379176
O	1.694549	-0.919788	-2.620255
H	-0.882481	-2.158176	-2.070468
H	-0.678159	-1.036184	-3.427626
C	-3.097593	-0.742908	-1.651734
H	-1.138234	-1.390279	2.335584
H	-2.970992	-1.932182	3.911246
H	-5.173608	-0.825245	3.681879
H	-5.539477	0.848787	1.889098
H	-3.719819	1.395936	0.323257
H	-1.697568	2.554060	1.854049
H	-1.350108	4.989882	1.736007
H	-0.399756	6.017937	-0.308538
H	0.200221	4.587513	-2.245054
H	-0.122488	2.160814	-2.134825
H	2.412626	-3.078280	-1.194629
H	4.628597	-4.198537	-1.262751
H	6.519087	-3.207882	0.049951
H	6.079664	-1.132644	1.385410
H	3.793409	-0.155069	1.352869
H	1.267478	1.998538	1.594608
H	2.461597	4.164013	1.447454
H	4.020344	4.555368	-0.480013
H	4.303930	2.717899	-2.163826
H	3.018942	0.614951	-1.868329
C	-4.157623	-0.020038	-2.195975
C	-5.462518	-0.497186	-2.103690
C	-5.718312	-1.703757	-1.463002
C	-4.662659	-2.433525	-0.919893
C	-3.361192	-1.959311	-1.015573
H	-3.963377	0.927243	-2.688840
H	-6.276237	0.075328	-2.532922
H	-6.733067	-2.075267	-1.385216
H	-4.854966	-3.372613	-0.414668
H	-2.546457	-2.518735	-0.565091

***trans*-Cl-2c**

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C	1.897201	-1.104402	2.418739
C	1.783687	0.066384	1.662641
C	2.176910	1.280985	2.230499
C	2.712826	1.314829	3.514478
C	2.863636	0.139753	4.240004
C	2.450182	-1.070703	3.690696
P	1.012132	0.018599	0.007923
C	1.722743	-1.367140	-1.021168
C	3.224429	-1.486896	-1.047676
C	3.949480	-2.117434	-0.033141
C	5.338826	-2.163938	-0.080255
C	6.025850	-1.588801	-1.144754
C	5.313322	-0.973965	-2.169276
C	3.924998	-0.926820	-2.119863
Rh	-1.208389	-0.566389	-0.077443
Cl	-1.325982	-1.035582	2.299383
N	-3.348356	-1.114963	-0.232605
C	-4.208155	-0.662693	0.688189
C	-5.567848	-0.930318	0.631593
C	-6.054814	-1.697711	-0.418446
C	-5.162165	-2.166873	-1.373263
C	-3.816945	-1.852886	-1.243899
Cl	-1.196836	-0.209788	-2.489982
C	-0.561707	-2.400632	-0.449149
O	-1.325696	-3.318927	-0.484365
C	1.592311	1.552501	-0.790491
C	0.711217	2.423840	-1.431545
C	1.194664	3.575035	-2.046775
C	2.555610	3.856586	-2.033357
C	3.439965	2.989779	-1.396224
C	2.962914	1.845714	-0.770864
C	0.941597	-2.636813	-0.683554
N	-2.020497	1.606199	0.344420
C	-2.854320	2.193203	-0.520271
C	-3.230361	3.524635	-0.409244
C	-2.714474	4.276600	0.639852
C	-1.854190	3.666374	1.544026
C	-1.537597	2.326536	1.360685
H	1.035443	-3.369309	-1.488792
H	1.309882	-3.121213	0.225680
H	1.392228	-1.043157	-2.012994
H	3.438235	-2.578055	0.803008
H	5.884003	-2.655356	0.716875
H	7.107984	-1.626628	-1.178970
H	5.836167	-0.530606	-3.008398
H	3.373744	-0.439054	-2.917336
H	-0.345676	2.198459	-1.464417
H	0.502799	4.248415	-2.538087
H	2.929213	4.752377	-2.515057
H	4.501285	3.206081	-1.380587
H	3.656706	1.187725	-0.259327
H	2.068832	2.206433	1.678166
H	3.014854	2.263115	3.942126
H	3.288215	0.166936	5.236340
H	2.539301	-1.987916	4.259740
H	1.521119	-2.043592	2.034376
H	-3.084827	-2.194144	-1.963329
H	-5.492383	-2.768314	-2.209682
H	-7.111120	-1.926790	-0.490935
H	-6.222748	-0.543151	1.400581
H	-3.779398	-0.075767	1.491111
H	-3.212161	1.568200	-1.332748
H	-3.908528	3.956442	-1.133441
H	-2.980931	5.320567	0.751978
H	-1.431164	4.211513	2.377451
H	-0.878832	1.800989	2.046046

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C	1.156899	-2.460167	0.714689
C	1.186873	-1.130616	1.154351
C	1.320136	-0.868897	2.519517
C	1.446241	-1.918899	3.425464
C	1.436123	-3.233637	2.977941
C	1.290646	-3.503665	1.618524
P	0.807135	0.189239	-0.044742
C	1.872412	0.019605	-1.564130
C	3.343077	-0.151716	-1.279579
C	3.908420	-1.386314	-0.950209
C	5.262586	-1.487929	-0.651224
C	6.074281	-0.357732	-0.677520
C	5.523946	0.875036	-1.011642
C	4.169857	0.974978	-1.310108
Rh	-1.276930	-0.093361	-0.957295
N	-1.838811	-1.706887	0.304732
Cl	-3.464223	-0.506175	-2.157217
N	-2.447712	1.504363	0.459598
C	-3.447530	2.173485	-0.129272
C	-4.119352	3.221269	0.488195
C	-3.743734	3.599684	1.769378
C	-2.700948	2.918323	2.384092
C	-2.086006	1.886822	1.689745
Cl	-0.805639	1.749960	-2.479964
C	-0.271273	-1.293454	-2.194448
O	-0.792486	-2.234561	-2.712425
C	1.368741	1.754050	0.692295
C	0.652690	2.934339	0.478718
C	1.148147	4.142334	0.958643
C	2.360601	4.180570	1.638580
C	3.087973	3.010164	1.834821
C	2.598523	1.799028	1.362531
C	1.213882	-1.003343	-2.490704
H	1.252338	-0.651056	-3.524766
H	1.716927	-1.972783	-2.467090
H	1.724723	1.009421	-2.001981
H	3.298527	-2.281342	-0.926837
H	5.683740	-2.453965	-0.399724
H	7.129367	-0.439560	-0.445718
H	6.147612	1.760611	-1.042017
H	3.742800	1.939809	-1.564191
H	-0.277216	2.911101	-0.075285
H	0.586011	5.053324	0.793777
H	2.743630	5.123517	2.010603
H	4.039071	3.038005	2.352301
H	3.179836	0.894996	1.507520
H	1.315020	0.150039	2.887717
H	1.548704	-1.703416	4.481960
H	1.532894	-4.048593	3.685015
H	1.267051	-4.526693	1.263598
H	0.998819	-2.693504	-0.333186
H	-3.709417	1.849149	-1.128865
H	-4.919705	3.726215	-0.036562
H	-4.248271	4.412638	2.277562
H	-2.358923	3.179526	3.376691
H	-1.243830	1.369590	2.138982
C	-2.254382	-2.865767	-0.225246
C	-2.639583	-3.940901	0.562098
C	-2.613337	-3.814101	1.943241
C	-2.214378	-2.601878	2.491027
C	-1.836591	-1.579302	1.638068
H	-2.270330	-2.915571	-1.304640
H	-2.956901	-4.857654	0.083760
H	-2.905845	-4.639601	2.580387
H	-2.185158	-2.440574	3.560075
H	-1.513072	-0.629375	2.034490

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C	3.920490	0.045726	-1.989374
C	3.379216	-0.835883	-1.054847
C	4.177877	-1.258882	0.012319
C	5.474723	-0.786750	0.164219
C	6.000892	0.109683	-0.762357
C	5.223300	0.514945	-1.841227
C	1.952673	-1.333631	-1.108215
C	1.234523	-1.291322	-2.464456
C	-0.284586	-1.144520	-2.309490
O	-1.051721	-1.836557	-2.910513
P	0.792759	-0.572522	0.180197
C	1.525496	0.649186	1.312904
C	0.880961	0.847289	2.541331
C	1.274286	1.878904	3.384022
C	2.309918	2.727839	3.007072
C	2.945449	2.543449	1.783743
C	2.553739	1.516002	0.931889
C	0.422599	-2.051442	1.200917
C	1.048021	-2.292313	2.426794
C	0.822903	-3.487940	3.103249
C	-0.011924	-4.455821	2.558071
C	-0.609176	-4.237255	1.319566
C	-0.390580	-3.045231	0.642639
Rh	-0.900170	0.294320	-1.077898
Cl	0.784519	1.830621	-1.953544
N	-2.424510	-0.879629	-0.218686
C	-2.597267	-0.868093	1.111618
C	-3.611345	-1.571838	1.736540
C	-4.482286	-2.321377	0.954963
C	-4.310734	-2.323245	-0.422096
C	-3.275025	-1.584681	-0.976492
N	-1.664046	2.081209	0.312497
C	-0.837099	3.003052	0.815408
C	-1.282613	4.089270	1.558724
C	-2.644632	4.231031	1.784544
C	-3.511277	3.287186	1.245721
C	-2.978170	2.235699	0.514979
Cl	-2.635370	1.141224	-2.721644
H	1.545378	-0.428411	-3.052281
H	1.433290	-2.201045	-3.033017
H	1.971709	-2.375554	-0.780221
H	0.064642	0.202201	2.846942
H	0.765637	2.021633	4.329433
H	2.616632	3.534097	3.662442
H	3.745921	3.206758	1.479909
H	3.032019	1.416142	-0.031514
H	1.720502	-1.559839	2.855718
H	1.309075	-3.661205	4.055552
H	-0.187334	-5.383929	3.088355
H	-1.246498	-4.993790	0.878329
H	-0.854273	-2.898483	-0.326531
H	7.011228	0.483226	-0.647772
H	6.074527	-1.118099	1.003432
H	3.770927	-1.957478	0.738262
H	3.328711	0.400532	-2.822822
H	5.626594	1.205756	-2.572139
H	0.217677	2.869436	0.603715
H	-0.566934	4.802901	1.946112
H	-3.025700	5.065336	2.361238
H	-4.582400	3.361632	1.379456
H	-3.623249	1.493778	0.056996
H	-3.096827	-1.549930	-2.042016
H	-4.968054	-2.883747	-1.072922
H	-5.283242	-2.888754	1.412767
H	-3.705820	-1.529400	2.813053
H	-1.901862	-0.264534	1.681544

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Rh	-0.427859	-0.181446	-0.127440
Cl	-0.262414	0.252445	-2.741478
H	-0.228642	-1.690331	-0.263394
P	-2.666864	-0.681919	-0.198403
C	-5.179123	3.168676	-0.012622
C	-4.342982	2.900728	-1.095860
C	-3.632978	1.709853	-1.146441
C	-3.758512	0.776234	-0.111482
C	-4.593324	1.045358	0.971448
C	-5.305137	2.242768	1.015716
H	-5.727384	4.102358	0.029488
H	-4.233635	3.627023	-1.892437
H	-2.951829	1.510647	-1.969455
H	-4.683675	0.334730	1.785182
H	-5.952798	2.451146	1.858921
C	-4.426258	-3.418394	-3.451778
C	-3.059373	-3.429559	-3.190824
C	-2.527356	-2.585547	-2.222670
C	-3.368174	-1.729989	-1.508339
C	-4.738930	-1.711067	-1.780412
C	-5.264889	-2.558316	-2.749321
H	-4.837287	-4.074697	-4.209590
H	-2.404667	-4.087797	-3.748846
H	-1.460360	-2.571557	-2.033429
H	-5.391627	-1.030661	-1.243908
H	-6.327723	-2.542564	-2.958058
C	-2.915296	-2.732241	3.897659
C	-3.976745	-2.933454	3.015310
C	-3.963624	-2.345481	1.754342
C	-2.872050	-1.566941	1.378898
C	-1.803076	-1.375125	2.255187
C	-1.831697	-1.944925	3.526062
H	-2.935378	-3.196553	4.876324
H	-4.816122	-3.550939	3.311691
H	-4.790641	-2.498316	1.068882
H	-0.998931	-1.777422	4.199049
C	-0.624105	-0.526010	1.804986
O	0.108808	-0.051092	2.640224
C	-1.405454	4.800581	0.478845
C	-1.738036	3.880813	1.465512
C	-1.404396	2.548462	1.272482
N	-0.783069	2.102747	0.174274
C	-0.464449	2.992234	-0.771510
C	-0.752326	4.346381	-0.658444
H	-1.651009	5.849380	0.595589
H	-2.250098	4.180256	2.370523
H	-1.649891	1.809852	2.026891
H	0.027146	2.593265	-1.650500
H	-0.466944	5.021488	-1.454670
C	2.818156	-0.764251	-1.522672
P	1.960095	-0.028592	-0.009504
C	2.874397	4.476231	0.248091
C	2.439274	3.760533	1.362566
C	2.227548	2.391976	1.272630
C	2.462007	1.721888	0.065139
C	2.874780	2.444728	-1.051947
C	3.085832	3.818751	-0.957018
H	3.037458	5.545037	0.319296
H	2.255495	4.271335	2.300309
H	1.856567	1.837182	2.129253
H	3.017168	1.954949	-2.005886
H	3.409741	4.371628	-1.830684
C	4.202493	-2.259033	3.338801
C	3.040062	-2.791333	2.786584
C	2.342856	-2.081562	1.816316
C	2.816327	-0.842420	1.378968
C	3.982874	-0.313668	1.933168
C	4.668598	-1.018198	2.916739
H	4.741466	-2.810006	4.100462
H	2.671715	-3.754759	3.117835
H	1.428782	-2.490247	1.398127
H	4.367032	0.638490	1.585206
H	5.573721	-0.602328	3.342783
H	2.457042	-0.129686	-2.338218
C	7.131568	-0.827647	-1.534292
C	6.430812	0.039132	-2.365708
C	5.040759	0.048623	-2.346343
C	4.324907	-0.796779	-1.493262
C	5.040343	-1.676622	-0.672877
C	6.430738	-1.688234	-0.695899
H	8.214896	-0.838768	-1.546343
H	6.963188	0.703161	-3.036198
H	4.506971	0.707278	-3.022349
H	4.510066	-2.360873	-0.025322
H	6.967455	-2.376506	-0.053404
C	2.149882	-2.115591	-1.736708
O	2.611536	-3.167747	-1.380972
H	1.172138	-2.051941	-2.242625

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C	2.211253	-2.355422	-1.710176
C	2.841841	-1.191120	-1.265322
C	4.151904	-0.919982	-1.675543
C	4.811354	-1.793611	-2.531456
C	4.177602	-2.953088	-2.968083
C	2.880515	-3.235819	-2.552793
P	1.968417	-0.141134	-0.059022
C	2.817838	-0.622532	1.568689
C	4.323715	-0.594650	1.509869
C	4.975829	0.589016	1.872247
C	6.360280	0.690822	1.806459
C	7.119279	-0.397808	1.387395
C	6.481483	-1.582692	1.037193
C	5.094650	-1.682471	1.088364
C	2.516248	1.576872	-0.349058
C	2.315706	2.514409	0.670976
C	2.561900	3.861630	0.442098
C	2.994993	4.290539	-0.810908
C	3.164816	3.368375	-1.836086
C	2.919128	2.015825	-1.611640
C	2.166026	-1.928226	1.976905
O	2.545513	-3.023778	1.654440
O	0.221961	0.565258	2.590984
C	-0.582644	-0.048072	1.921716
C	-1.785003	-0.662784	2.619305
C	-2.890681	-1.039673	1.856048
C	-4.000461	-1.625008	2.458884
C	-3.995098	-1.832276	3.835023
C	-2.897111	-1.442890	4.602289
C	-1.794314	-0.849204	4.000307
P	-2.704855	-0.637028	0.090991
Rh	-0.454038	-0.229270	-0.037045
Cl	-0.477330	-0.474599	-2.665387
C	-3.484980	-1.978968	-0.856127
C	-4.861823	-1.974097	-1.094984
C	-5.451572	-3.038585	-1.767763
C	-4.670536	-4.102497	-2.208737
C	-3.297467	-4.102799	-1.981608
C	-2.701771	-3.042172	-1.308875
C	-3.742013	0.835433	-0.199081
C	-3.619554	1.449768	-1.450749
C	-4.272233	2.648584	-1.700552
C	-5.050192	3.240864	-0.706649
C	-5.176996	2.629416	0.534510
C	-4.521122	1.427391	0.793698
N	-0.722059	2.065345	-0.320232
C	-0.375555	2.671166	-1.460423
C	-0.586783	4.025262	-1.686291
C	-1.192294	4.784179	-0.694682
C	-1.557588	4.158958	0.491254
C	-1.299543	2.803814	0.634343
H	-0.311820	-1.730029	0.213860
H	-5.552698	4.181020	-0.900903
H	-4.164424	3.127564	-2.666525
H	-2.982795	1.002188	-2.209017
H	-4.610106	0.967491	1.771469
H	-5.780453	3.088199	1.308586
H	-5.132201	-4.928172	-2.737154
H	-2.686978	-4.924034	-2.336670
H	-1.629742	-3.023910	-1.152213
H	-5.469836	-1.138069	-0.766254
H	-6.518888	-3.033026	-1.952399
H	-2.902991	-1.611008	5.672433
H	-4.848172	-2.299436	4.312080
H	-4.856784	-1.921618	1.862204
H	-0.932185	-0.542674	4.581099
H	-1.378212	5.841371	-0.842219
H	-0.280812	4.464370	-2.627015
H	0.071362	2.036655	-2.216209
H	-1.575759	2.289274	1.547750
H	-2.038140	4.701861	1.294678
H	3.185258	5.342305	-0.988974
H	2.405333	4.579189	1.238797
H	1.934411	2.193843	1.635294
H	3.026467	1.311030	-2.427614
H	3.482371	3.697410	-2.818260
H	2.455910	0.136435	2.264431
H	1.259095	-1.811066	2.594877
H	8.199204	-0.323196	1.338036
H	6.845020	1.617962	2.088405
H	4.392111	1.438656	2.209128
H	7.063803	-2.436448	0.710360
H	4.665676	-0.035606	-1.315404
H	5.824726	-1.573236	-2.845081
H	4.695026	-3.635553	-3.632162
H	2.383280	-4.136114	-2.892768
H	1.190138	-2.559800	-1.411331
H	4.607176	-2.600556	0.792074

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Rh	0.466541	0.310952	0.077832
H	0.427289	0.836520	-1.343012
P	2.751013	0.467026	0.001446
C	4.791306	-2.740186	2.592535
C	4.377454	-3.032401	1.295350
C	3.805669	-2.040625	0.509001
C	3.643441	-0.748166	1.018911
C	4.046977	-0.461857	2.322284
C	4.627368	-1.457005	3.102487
H	5.237532	-3.513873	3.205837
H	4.498505	-4.032045	0.895427
H	3.486847	-2.272564	-0.503121
H	3.897557	0.528906	2.735103
H	4.940933	-1.229284	4.114038
C	5.022737	0.586583	-4.022460
C	3.675337	0.926650	-3.966518
C	2.990402	0.865329	-2.757807
C	3.648608	0.461760	-1.594421
C	5.005119	0.125113	-1.655618
C	5.686169	0.188434	-2.865860
H	5.555140	0.630102	-4.965012
H	3.153555	1.236839	-4.863749
H	1.941243	1.133855	-2.719320
H	5.529783	-0.194718	-0.762491
H	6.736024	-0.076199	-2.903976
C	3.163781	4.671260	1.788621
C	4.335684	3.959273	1.528162
C	4.270826	2.681194	0.987007
C	3.025097	2.116040	0.718132
C	1.851713	2.827657	0.966927
C	1.925525	4.112717	1.504300
H	3.223965	5.667425	2.210512
H	5.299165	4.404273	1.745725
H	5.181080	2.128253	0.779154
H	1.006845	4.655151	1.691905
C	0.498111	2.211423	0.627773
O	-0.486111	2.912906	0.732750
Cl	0.498785	-0.465336	2.576431
C	-2.984364	1.189400	1.204483
P	-1.953572	0.194865	-0.029800
C	-3.898649	1.951035	-3.834128
C	-2.698760	2.456951	-3.344617
C	-2.105262	1.880894	-2.226007
C	-2.714617	0.801703	-1.581603
C	-3.934914	0.316123	-2.062195
C	-4.514821	0.880571	-3.192368
H	-4.356549	2.393854	-4.710675
H	-2.220805	3.296967	-3.834181
H	-1.172516	2.277659	-1.840592
H	-4.441193	-0.492010	-1.545247
H	-5.457266	0.493586	-3.561309
C	-2.848811	-4.312038	0.391428
C	-2.716846	-3.514643	1.523006
C	-2.506780	-2.145524	1.395564
C	-2.456292	-1.554963	0.129360
C	-2.570342	-2.365885	-1.004506
C	-2.764751	-3.735968	-0.872438
H	-3.004649	-5.379569	0.493474
H	-2.766091	-3.956749	2.510920
H	-2.367391	-1.547455	2.288005
H	-2.491739	-1.933102	-1.995462
H	-2.844232	-4.352710	-1.759994
C	-2.447014	1.050882	2.614835
O	-3.042961	0.538967	3.527178
H	-1.446471	1.487760	2.753042
H	-2.675678	2.195629	0.898009
C	0.772391	-4.473450	-1.655907
C	0.789207	-3.388053	-2.524322
C	0.697889	-2.110245	-1.991176
N	0.596305	-1.877659	-0.676917
C	0.581011	-2.923510	0.156025
C	0.663482	-4.235813	-0.292531
H	0.839646	-5.485228	-2.037514
H	0.871421	-3.521121	-3.595049
H	0.702896	-1.235373	-2.632349
H	0.498164	-2.684790	1.210855
H	0.639856	-5.048183	0.422078
C	-7.218194	0.781722	0.544139
C	-6.520675	1.878633	0.048804
C	-5.156994	1.998598	0.287474
C	-4.467988	1.031053	1.023858
C	-5.178977	-0.062033	1.527077
C	-6.543784	-0.183663	1.285640
H	-8.280983	0.681475	0.357984
H	-7.034907	2.638491	-0.527734
H	-4.611516	2.845334	-0.117926
H	-4.669469	-0.812041	2.114739
H	-7.081636	-1.036767	1.682259

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Rh	-0.252701	-0.314517	-0.014742
H	-0.206098	-0.009301	-1.504405
P	-2.462806	-0.733337	-0.297331
C	-4.883232	-0.022193	3.552815
C	-4.571158	1.041059	2.709243
C	-3.877149	0.811515	1.528646
C	-3.489951	-0.487938	1.185032
C	-3.795701	-1.549292	2.036164
C	-4.496785	-1.314238	3.214634
H	-5.423219	0.158607	4.474503
H	-4.865538	2.050425	2.970956
H	-3.641731	1.645595	0.873953
H	-3.476032	-2.554980	1.789537
H	-4.732354	-2.142536	3.871669
C	-4.821871	1.174520	-3.786173
C	-3.450509	0.965888	-3.895642
C	-2.740489	0.422747	-2.831464
C	-3.396749	0.082162	-1.645905
C	-4.776852	0.284066	-1.545502
C	-5.482926	0.830498	-2.612107
H	-5.373268	1.603551	-4.614236
H	-2.930245	1.227660	-4.808948
H	-1.672962	0.261268	-2.924963
H	-5.304486	0.020087	-0.636713
H	-6.551124	0.986696	-2.522368
C	-2.214881	-5.192279	-1.307927
C	-3.482655	-4.609236	-1.266237
C	-3.621806	-3.260680	-0.962512
C	-2.481820	-2.502964	-0.699549
C	-1.214581	-3.077643	-0.745838
C	-1.082515	-4.432667	-1.049254
H	-2.116093	-6.244510	-1.546647
H	-4.360851	-5.208556	-1.474126
H	-4.605590	-2.803979	-0.929127
H	-0.091788	-4.869549	-1.079995
C	0.017736	-2.222022	-0.466884
O	1.093709	-2.768290	-0.449898
Cl	-0.263467	-1.117383	2.473744
C	3.184424	0.548200	1.472762
P	2.118267	0.552737	-0.099378
C	5.521001	-0.742964	-2.959885
C	4.501176	-1.633001	-2.646508
C	3.450366	-1.237279	-1.820892
C	3.417320	0.058167	-1.307171
C	4.446690	0.951659	-1.625261
C	5.491692	0.552271	-2.447989
H	6.338744	-1.054475	-3.599110
H	4.521497	-2.643049	-3.038300
H	2.672006	-1.939447	-1.552787
H	4.435162	1.962192	-1.230804
H	6.284578	1.250973	-2.687418
C	1.467551	4.970992	-1.329816
C	1.748214	4.678068	-0.000678
C	1.988105	3.364633	0.398663
C	1.939034	2.331281	-0.536232
C	1.644718	2.629750	-1.871516
C	1.418699	3.942046	-2.266963
H	1.284665	5.994399	-1.635521
H	1.781665	5.472575	0.735832
H	2.183258	3.150076	1.442355
H	1.595690	1.832896	-2.607487
H	1.200511	4.160036	-3.305958
H	3.832304	1.426576	1.387307
C	2.370971	0.700870	2.749968
O	1.936777	1.754758	3.140467
H	2.233738	-0.221219	3.334246
C	5.524204	-3.059610	1.418058
C	4.149252	-3.122592	1.621100
C	3.390555	-1.956660	1.656197
C	4.008554	-0.715626	1.491556
C	5.388103	-0.657051	1.293085
C	6.143528	-1.823335	1.254414
H	6.111667	-3.969646	1.386095
H	3.660599	-4.082180	1.742713
H	2.312541	-2.011857	1.779108
H	5.868151	0.306064	1.154160
H	7.213879	-1.767186	1.095000
C	-1.772756	4.385730	1.324643
C	-1.737658	3.992160	-0.008875
C	-1.269788	2.722847	-0.313389
N	-0.854973	1.858167	0.620684
C	-0.893885	2.237064	1.901923
C	-1.340065	3.493421	2.295494
H	-2.129060	5.371348	1.599499
H	-2.060858	4.652013	-0.803304
H	-1.220011	2.378094	-1.340189
H	-0.558985	1.502790	2.625094
H	-1.347535	3.753349	3.346055

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N	-1.946613	-1.434390	0.877546
C	-3.223637	-1.741613	0.535319
C	-3.969088	-2.676910	1.275260
C	-3.393157	-3.299795	2.381234
C	-2.082153	-2.969135	2.733446
C	-1.404236	-2.032509	1.952083
C	-3.780057	-1.011519	-0.626376
C	-5.064441	-1.276065	-1.128420
C	-5.554884	-0.541649	-2.206619
C	-4.742327	0.447479	-2.761330
C	-3.469748	0.653071	-2.226205
N	-2.992322	-0.050714	-1.184144
Rh	-0.925626	0.032736	-0.506147
P	1.295144	-0.127529	0.092630
C	1.945898	-1.736588	0.745460
C	1.386366	-2.936673	0.263501
C	1.896380	-4.168573	0.688551
C	2.956932	-4.221297	1.601705
C	3.517691	-3.031674	2.081562
C	3.021079	-1.794745	1.653790
Cl	-0.645179	-1.828397	-2.252893
C	-1.333033	1.489510	0.993163
C	-2.793583	1.673947	1.384600
C	-3.308311	2.949104	0.736686
C	-2.154934	3.518110	-0.081472
C	-1.006614	2.996382	0.819127
C	-1.444814	3.553949	2.205776
C	-2.859704	2.980227	2.191650
C	-0.204031	1.240707	-1.935025
O	-0.896438	1.973834	-2.632005
C	1.308009	1.232319	-2.258128
C	2.092404	0.093645	-1.603801
C	3.600804	0.125001	-1.734810
C	4.341594	-1.055413	-1.519954
C	5.731742	-1.074490	-1.662539
C	6.420303	0.085397	-2.038740
C	5.698692	1.257952	-2.283455
C	4.306134	1.275471	-2.136484
C	1.986497	1.095085	1.291327
C	1.651308	0.968207	2.655215
C	2.091144	1.908630	3.591596
C	2.870344	2.997675	3.182262
C	3.207435	3.135097	1.832131
C	2.766163	2.194222	0.893428
H	-0.773253	1.092372	1.857981
H	-3.463114	0.850967	1.633422
H	-4.355964	3.070731	0.458704
H	-3.567147	3.107183	3.012173
H	-0.824437	3.161100	3.027920
H	-1.427987	4.657130	2.244411
H	0.014233	3.246406	0.506279
H	-2.105216	3.125033	-1.104337
H	-2.172176	4.621040	-0.121987
H	1.411540	1.202583	-3.355149
H	1.666577	2.226493	-1.936058
H	1.720891	-0.842632	-2.064997
H	3.816675	-1.974267	-1.249564
H	6.278201	-2.005248	-1.490131
H	7.506399	0.070149	-2.156757
H	6.217935	2.165007	-2.603432
H	3.766145	2.197302	-2.366384
H	1.054898	0.117946	2.996179
H	1.821814	1.790415	4.644109
H	3.213114	3.733775	3.913281
H	3.821182	3.976793	1.501894
H	3.054874	2.314247	-0.149850
H	0.568357	-2.893595	-0.465163
H	1.458125	-5.091674	0.300431
H	3.349401	-5.185650	1.934702
H	4.353353	-3.062133	2.785387
H	3.480595	-0.875958	2.022132
H	-2.775998	1.393380	-2.634357
H	-5.072147	1.051885	-3.607912
H	-6.550910	-0.745086	-2.605941
H	-5.676978	-2.061288	-0.685710
H	-4.996640	-2.912514	0.998193
H	-3.963437	-4.028052	2.961976
H	-1.585769	-3.425388	3.591493
H	-0.374002	-1.756097	2.182541

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N	1.855405	0.859779	1.335401
C	2.874974	1.705401	1.034244
C	3.382193	2.606960	1.983175
C	2.842240	2.626191	3.268969
C	1.814779	1.732908	3.580618
C	1.355066	0.873237	2.580343
C	3.437815	1.570840	-0.328652
C	4.605867	2.233973	-0.735897
C	5.115585	2.021094	-2.015675
C	4.453785	1.127594	-2.860994
C	3.300371	0.494138	-2.397431
N	2.795181	0.713825	-1.169358
Rh	0.874708	-0.000496	-0.533502
P	-1.344112	-0.435399	-0.024829
C	-1.968092	0.439420	1.474006
C	-2.309067	1.803632	1.450927
C	-2.673910	2.458046	2.633338
C	-2.685267	1.774357	3.853778
C	-2.313428	0.424833	3.892723
C	-1.953135	-0.236623	2.713441
Cl	0.204656	2.485100	-0.767334
C	1.556517	-1.992625	-0.282022
C	1.333684	-2.614238	1.088587
C	2.647540	-2.561112	1.860046
C	3.671588	-1.883990	0.955999
C	3.068029	-2.345989	-0.390655
C	3.009135	-3.885930	-0.165530
C	2.243231	-3.849446	1.156117
C	0.183352	-0.382460	-2.369685
O	0.807247	-0.995331	-3.227384
C	-1.164442	0.276835	-2.720953
C	-2.258095	0.032802	-1.666428
H	-2.729265	-0.934844	-1.897927
C	-2.087116	-2.142866	0.140562
C	-3.228872	-2.413905	0.920196
C	-3.840094	-3.673371	0.877219
C	-3.333727	-4.679083	0.046953
C	-2.220265	-4.410413	-0.756867
C	-1.607463	-3.153974	-0.714531
H	1.039004	-2.558845	-1.069906
H	0.371731	-2.614854	1.601871
H	2.673309	-2.491314	2.948178
H	1.954936	-4.744378	1.708608
H	2.460283	-4.403680	-0.969250
H	4.011139	-4.339546	-0.071822
H	3.585369	-2.024855	-1.301814
H	3.696044	-0.793593	1.072321
H	4.691090	-2.278841	1.107623
H	-0.932638	1.351421	-2.792564
H	-1.492558	-0.085794	-3.708376
H	-3.658856	-1.638128	1.555572
H	-4.723458	-3.862335	1.492683
H	-3.811469	-5.661339	0.016628
H	-1.824307	-5.179592	-1.424509
H	-0.755890	-2.957011	-1.366964
H	-2.259878	2.362311	0.518329
H	-2.944530	3.515969	2.594423
H	-2.974829	2.291045	4.772352
H	-2.304173	-0.118899	4.840990
H	-1.658771	-1.287794	2.761559
H	2.733722	-0.211677	-3.011169
H	4.814423	0.918907	-3.869448
H	6.019892	2.539411	-2.341881
H	5.119171	2.909641	-0.051779
H	4.182051	3.299702	1.720180
H	3.219923	3.329293	4.014561
H	1.362806	1.702233	4.573417
H	0.542302	0.173023	2.775577
C	-5.567557	2.835140	-1.468741
C	-5.758513	1.473885	-1.203669
C	-4.677562	0.589218	-1.270897
C	-3.383035	1.041948	-1.593817
C	-3.205110	2.411627	-1.861893
C	-4.287813	3.296377	-1.800187
H	-6.410440	3.529235	-1.424187
H	-6.753435	1.096674	-0.953492
H	-4.839626	-0.476080	-1.079032
H	-2.207525	2.795480	-2.087407
H	-4.126114	4.356476	-2.012191

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C	-4.405882	1.708910	0.340365
C	-3.812216	0.670826	1.085734
C	-4.659437	-0.273293	1.694166
C	-6.049806	-0.193611	1.555888
C	-6.624060	0.841784	0.810188
C	-5.795166	1.794992	0.206893
C	-2.309791	0.597302	1.274812
P	-1.329292	-0.163427	-0.193105
C	-1.852923	-1.936392	-0.236558
C	-2.228175	-2.660352	0.908905
C	-2.526200	-4.026400	0.825991
C	-2.439084	-4.692877	-0.400125
C	-2.038480	-3.987546	-1.541733
C	-1.742971	-2.623382	-1.463176
C	-1.737180	1.974408	1.677441
C	-0.408394	1.916580	2.404854
O	0.245018	0.887805	2.565127
Rh	0.942389	0.224550	0.192382
C	1.128849	-1.675542	1.107864
C	2.228238	-1.778428	2.152687
C	3.392666	-2.544938	1.545202
C	2.997225	-2.877305	0.109868
C	1.470039	-2.981554	0.346118
C	1.430609	-4.012426	1.511673
C	2.398404	-3.278444	2.437323
O	0.050168	3.045720	2.985452
C	-0.524767	4.326522	2.638855
C	-2.130521	0.496730	-1.724218
C	-3.391283	0.015510	-2.133320
C	-3.996187	0.515046	-3.290190
C	-3.354360	1.501547	-4.049854
C	-2.105074	1.984183	-3.646075
C	-1.490497	1.484478	-2.491047
C	1.558128	-0.310238	-1.581169
C	2.997305	0.110173	-1.787127
C	3.678351	0.642547	-0.665553
C	5.032494	1.077156	-0.756783
C	5.685629	0.954919	-2.015258
C	5.010519	0.435917	-3.108547
C	3.662638	0.011566	-3.000186
C	5.622225	1.616136	0.417710
C	4.869030	1.705968	1.574163
C	3.529100	1.252477	1.576464
N	2.960786	0.723365	0.497643
Cl	0.805717	2.749764	-0.347761
O	0.927330	-0.860414	-2.470733
H	-2.085371	-0.101121	2.097587
H	0.148066	-1.774420	1.602004
H	2.360738	-1.052073	2.953595
H	4.423726	-2.375198	1.857922
H	2.673088	-3.639292	3.429178
H	0.420056	-4.120834	1.936956
H	1.796046	-5.009133	1.209404
H	0.855237	-3.216655	-0.529097
H	3.274932	-2.096033	-0.610703
H	3.423829	-3.834194	-0.236707
H	-2.470491	2.465969	2.341507
H	-1.607638	2.638458	0.806352
H	-3.900970	-0.755670	-1.552543
H	-4.972671	0.131583	-3.596573
H	-3.827060	1.888493	-4.956487
H	-1.594739	2.751097	-4.234144
H	-0.521135	1.872867	-2.171154
H	-2.286751	-2.171688	1.882918
H	-2.822904	-4.569191	1.727038
H	-2.673028	-5.758327	-0.464274
H	-1.948984	-4.501860	-2.501837
H	-1.406446	-2.088567	-2.353274
H	2.896601	1.329127	2.464175
H	5.285587	2.128994	2.489757
H	6.658476	1.963966	0.392869
H	-0.411306	4.501614	1.558573
H	-1.580725	4.391392	2.944595
H	0.061959	5.062734	3.200395
H	6.724435	1.283102	-2.108100
H	5.521820	0.352804	-4.070618
H	3.130642	-0.397336	-3.862269
H	-4.228337	-1.078534	2.293412
H	-6.684694	-0.939286	2.040891
H	-7.709517	0.908876	0.704634
H	-6.230536	2.609028	-0.377885
H	-3.776877	2.453864	-0.152536

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C	1.803547	1.290160	-0.819224
C	3.287495	1.217663	-0.527574
O	1.360305	2.135395	-1.585149
C	3.738135	0.108221	0.226970
C	5.114880	-0.059086	0.554476
C	5.469113	-1.211002	1.306683
C	4.482307	-2.103654	1.683080
C	3.136819	-1.860177	1.319583
N	2.779073	-0.794109	0.610827
Rh	0.855315	-0.072463	0.213791
P	-1.255966	0.924230	0.087592
C	-2.220646	1.069564	-1.488979
C	-3.598589	1.357327	-1.475334
C	-4.296903	1.536970	-2.672233
C	-3.625541	1.446804	-3.898757
C	-2.251537	1.188397	-3.919197
C	-1.550082	1.001259	-2.720643
Cl	1.171279	1.127018	2.443775
C	0.542588	-1.339420	-1.471663
C	0.869808	-2.804868	-1.209381
C	2.198683	-3.129961	-1.879006
C	2.696671	-1.845509	-2.530288
C	1.308078	-1.229888	-2.823534
C	0.642946	-2.390703	-3.619574
C	0.897850	-3.487394	-2.585694
C	-1.780062	-0.458461	2.574683
C	-2.482038	0.070416	1.289373
H	-3.121326	0.901263	1.630878
C	-1.331109	2.692652	0.649187
C	-1.093978	3.705075	-0.298459
C	-1.119848	5.050551	0.082286
C	-1.385865	5.405676	1.409377
C	-1.611982	4.403993	2.358986
C	-1.575924	3.056204	1.984989
H	-0.532814	-1.233577	-1.690043
H	0.529109	-3.344441	-0.326641
H	2.865855	-3.899604	-1.488891
H	0.579133	-4.521967	-2.718291
H	-0.429029	-2.210489	-3.804581
H	1.141703	-2.585652	-4.584791
H	1.315614	-0.249885	-3.315720
H	3.317370	-1.226731	-1.870361
H	3.261396	-2.035939	-3.459234
H	-2.543432	-0.558889	3.357856
H	-1.008253	0.265117	2.915805
H	-0.873466	3.443404	-1.334130
H	-0.930758	5.823782	-0.666516
H	-1.408664	6.457742	1.704295
H	-1.801417	4.667274	3.402522
H	-1.713985	2.297619	2.755467
H	-4.134871	1.453518	-0.529407
H	-5.367480	1.755150	-2.646521
H	-4.172440	1.589091	-4.834196
H	-1.715892	1.136057	-4.870384
H	-0.473327	0.834484	-2.735475
H	2.329755	-2.533995	1.614743
H	4.718442	-2.995747	2.265569
H	6.513682	-1.377456	1.583344
C	-1.003317	-1.737297	2.378697
O	-0.099550	-1.849940	1.556065
O	-1.243408	-2.822352	3.153701
C	-2.334619	-2.848776	4.099428
H	-2.171921	-2.128833	4.915647
H	-3.297197	-2.661245	3.600758
H	-2.327768	-3.866476	4.507696
C	6.027966	0.937253	0.108748
C	5.577936	2.023883	-0.624093
H	7.088092	0.833527	0.355345
H	6.289296	2.783404	-0.957364
C	4.206155	2.166101	-0.950625
H	3.851680	3.019523	-1.533276
C	-5.169668	-2.971872	-0.262531
C	-3.809899	-3.017568	-0.590542
C	-2.931215	-2.037199	-0.115655
C	-3.398242	-0.986151	0.693918
C	-4.768418	-0.952661	1.017022
C	-5.647667	-1.934319	0.546187
H	-5.853357	-3.736835	-0.638245
H	-3.425278	-3.819274	-1.225806
H	-1.875209	-2.091781	-0.385191
H	-5.152029	-0.139929	1.642807
H	-6.707889	-1.883431	0.806858