Electronic Supplementary Information

for the paper

Captured at Last: Catalyst-Substrate Adduct and Rh-Dihydride Solvate in the Asymmetric Hydrogenation by Rh-Monophosphine Catalyst

by
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Contents:

EXPERIMENTAL DETAILS

General Procedures. All reactions and manipulations were performed under dry argon atmosphere using standard Schlenk-type techniques. NMR experiments were carried out on a Jeol ESX-400 spectrometer. Methanol-d_4 of grade "100%" (99.6% D) packed in sealed ampoules was purchased from Cambridge Isotope Laboratories, Inc. Methylene chloride-d_2 and tetrahydrofuran-d_8 were purchased from Aldrich. Hydrogen (99.9999%, Tanuma Sanso) was used for mechanistic studies. HPLC analysis of **7** was performed at 40 °C on the OJ column, flow rate 1 mL/min, eluent hexane : isopropanol 9 : 1 with UV detector (254 nm); retention times: 14.9 min (*R*), 20.6 min (*S*).

Solvate complex 3: A solution of catalytic precursor **1** (20-40 mg) in 0.5 mL of CD_2Cl_2 was prepared in a 5 mm NMR tube under argon. Then, the sample was degassed by three cycles of freezing, pumping, and warming. The sample was cooled to –20 °C and 2 atm H_2 was admitted, and the temperature was raised to ambient. The sample was intensely shaken manually during the hydrogenation at ambient temperature. The progress of the hydrogenation was monitored by ^{31}P NMR; complete hydrogenation of the coordinated norbornadiene required 5-10 minutes at room temperature. After completion of the reaction, excess hydrogen was removed by

several cycles of freezing, pumping, and warming. The thus-prepared solution of solvate complex **3** in CD_2Cl_2 was stable at ambient temperature.

Catalyst-substrate complex 4: 2 equivalents of solid MAC was added to a solution of **3** in CD_2Cl_2 and the sample was shaken manually until all solid was dissolved.

Hydrogenation of 4. The temperature of the cooling bath was maintained at –90 °C (liquid nitrogen + methanol), and the sample connected to the rubber balloon with dihydrogen was manually kept inside the bath throughout the whole hydrogenation process. To enable the necessary mass transfer, the sample was intensely shaken manually. The condition of the sample was reguraly checked by placing the sample in a pre-cooled probe of the NMR spectrometer. After 30 min of hydrogenation at –90 °C the signals of **4** were not seen any more in the NMR spectra.

Dihydride solvates 6a and 6b: suspension of **1** in a mixture CD_2Cl_2-CD_3OD (1 : 1) or CD_2Cl_2-THF-d_8 (1 : 1) was was prepared in a 5 mm NMR tube under argon. Then, the sample was degassed by three cycles of freezing, pumping, and warming. The sample was cooled to –20 °C and 2 atm H_2 was admitted, and the temperature was raised to ambient. The sample was intensely shaken manually until clear light yellow solution was obtained. The NMR analysis shown clean formation of solvate dihydrides **6a** or **6b** respectively (see figures S18-S22).

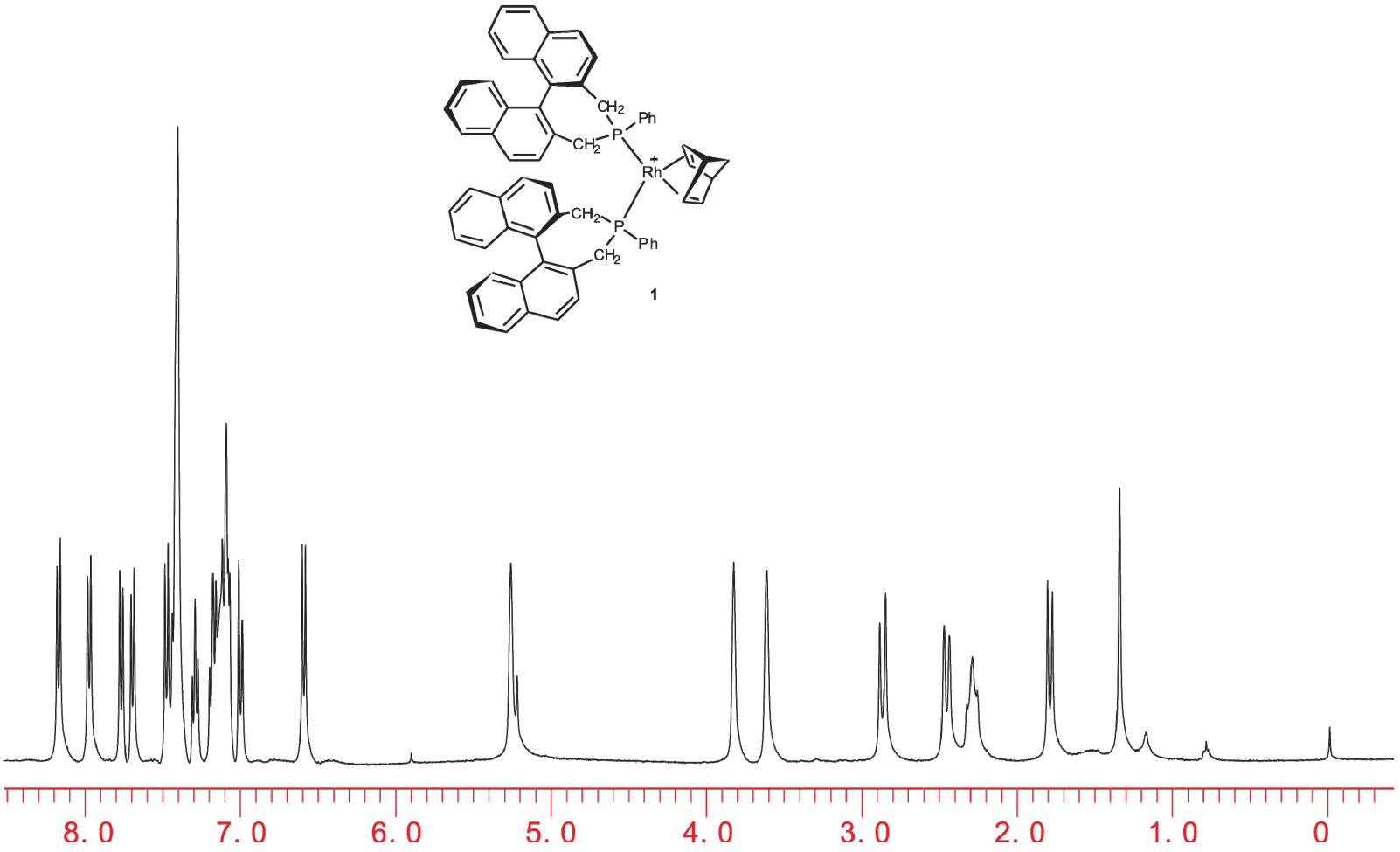


Figure S1. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the catalytic precursor **1**.

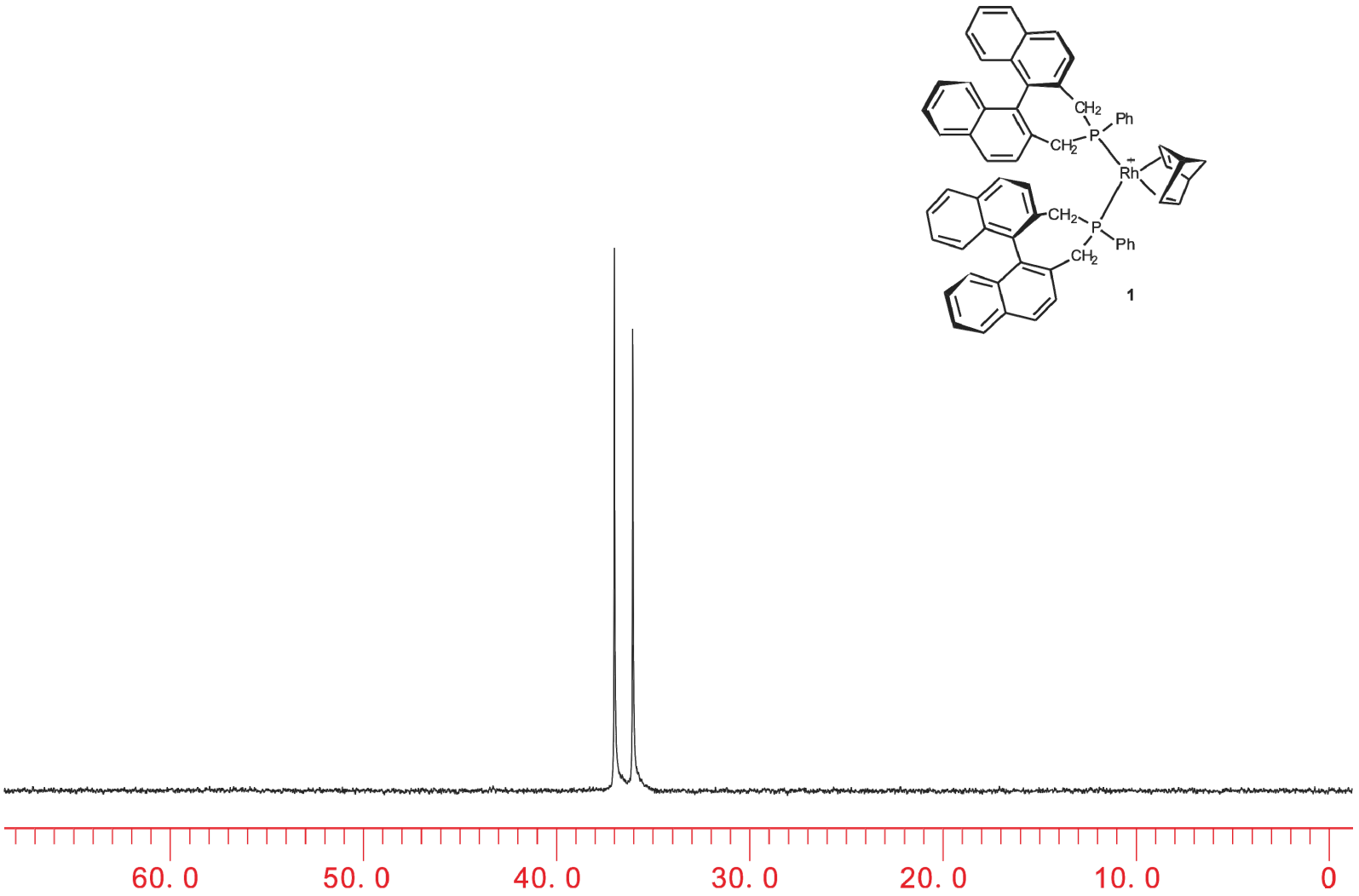


Figure S2. ^{31}P NMR spectrum (162 MHz, CD_2Cl_2, 25 °C) of the catalytic precursor **3**.

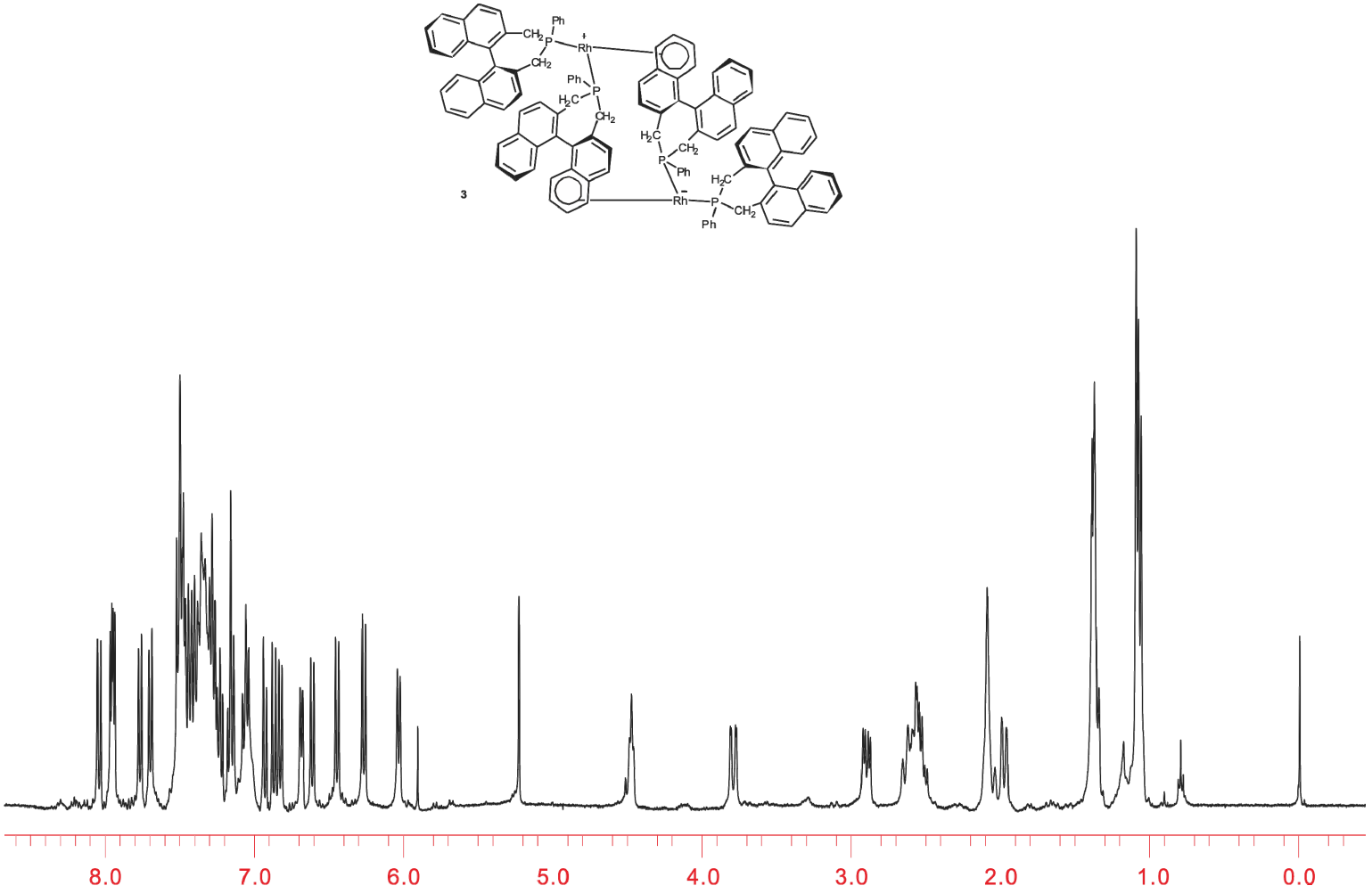


Figure S3. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

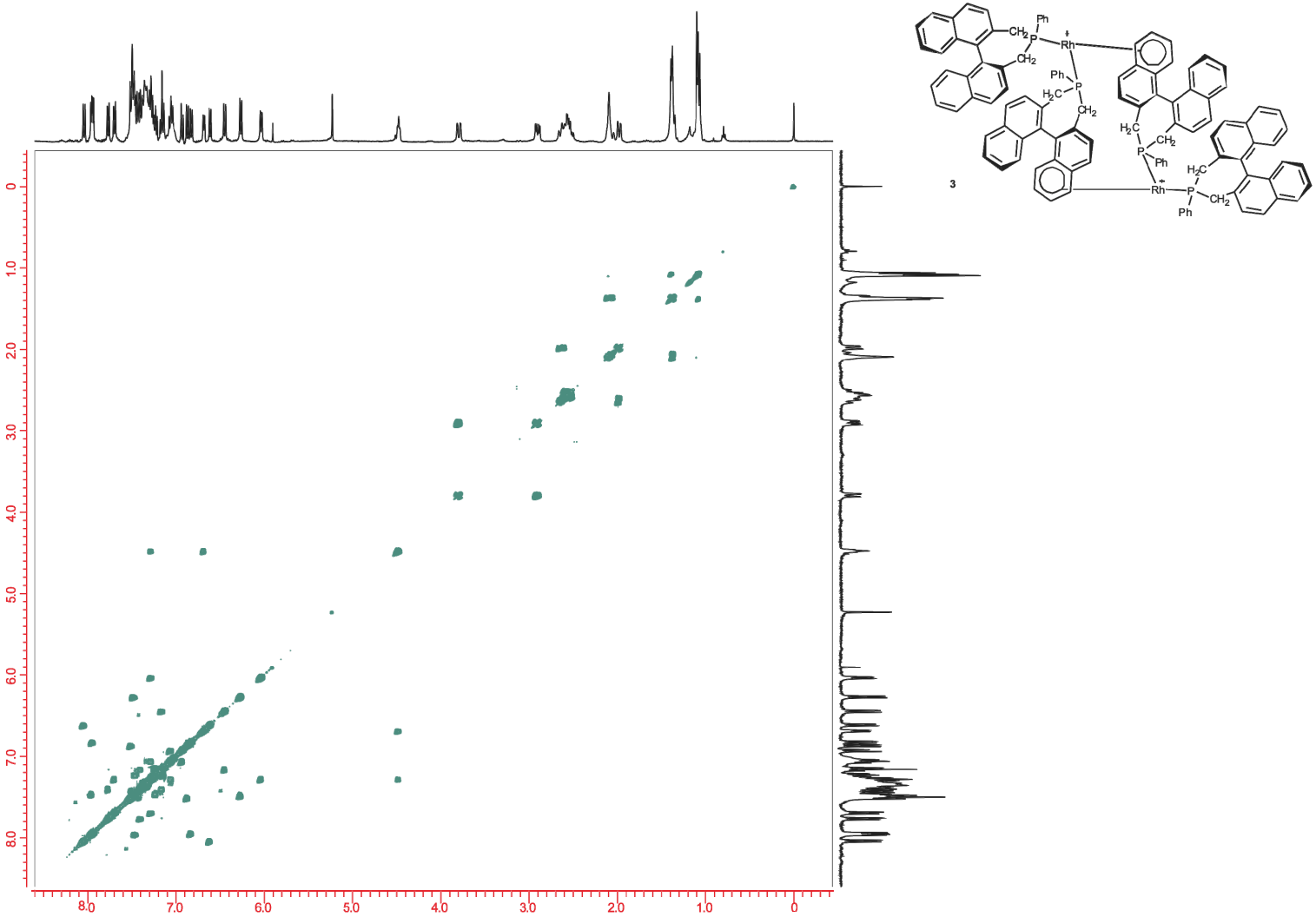


Figure S4. ^{1}H–^{1}H COSY NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

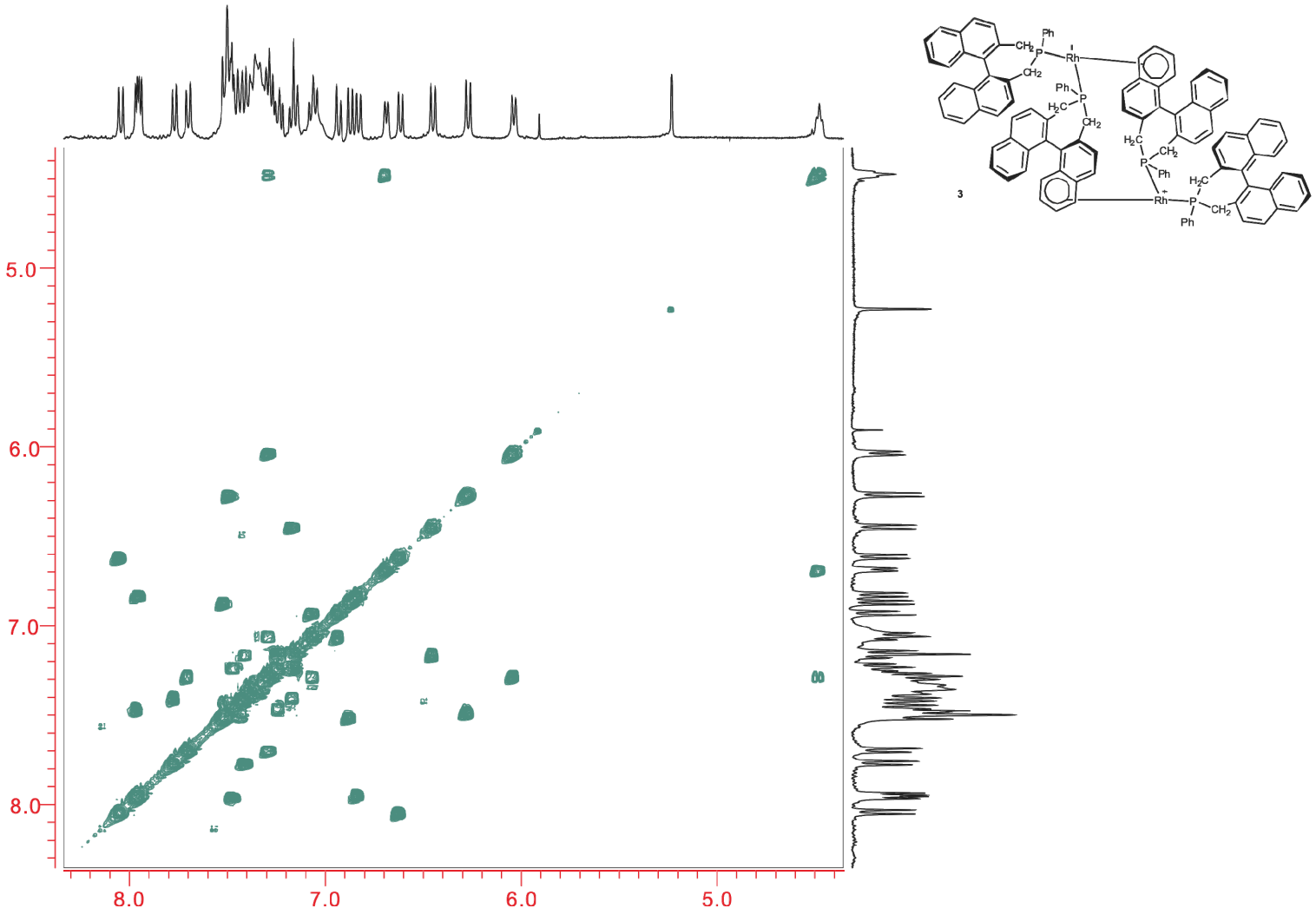


Figure S5. Section plot of the aromatic region in the ^{1}H–^{1}H COSY NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

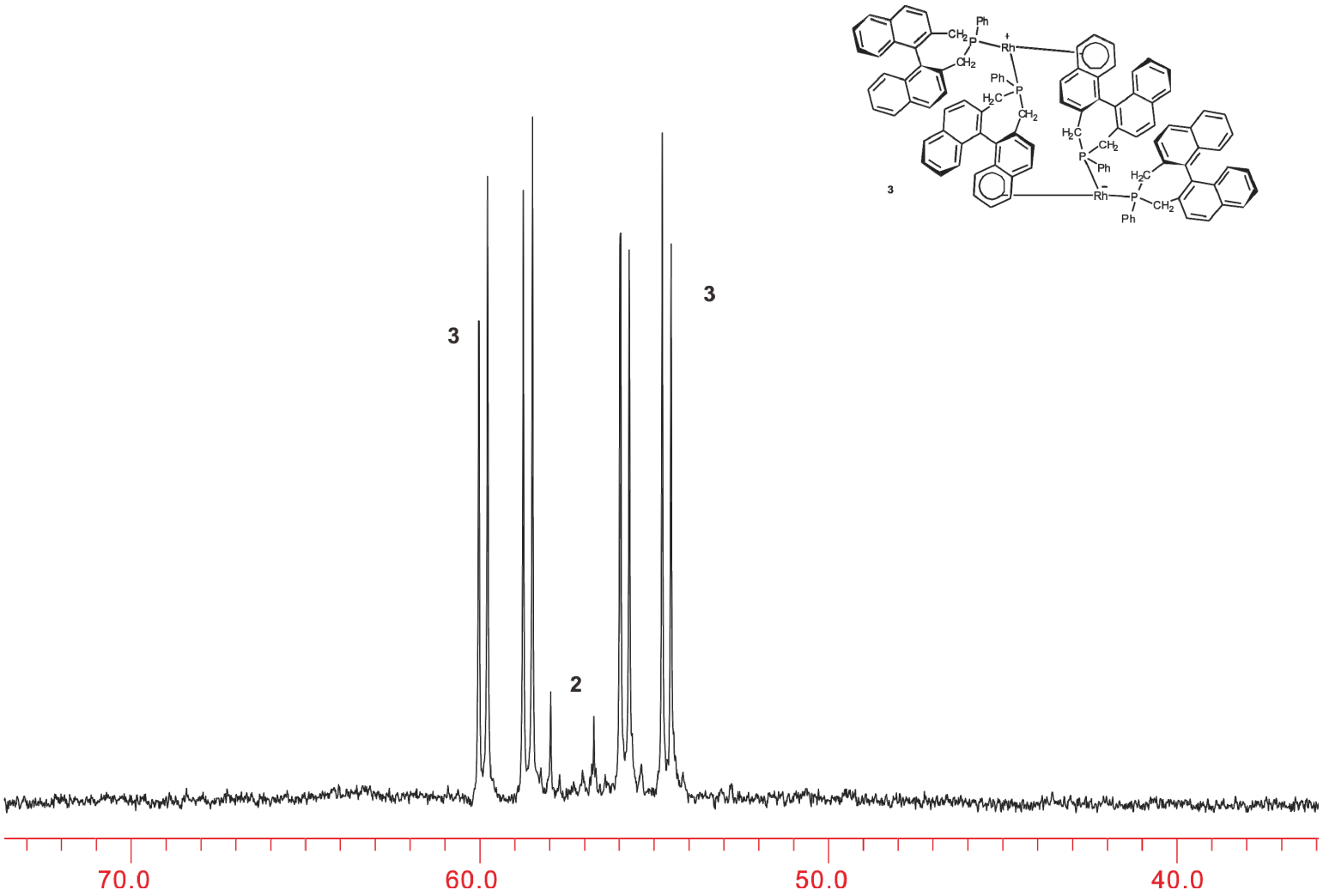


Figure S6. ^{31}P NMR spectrum (162 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

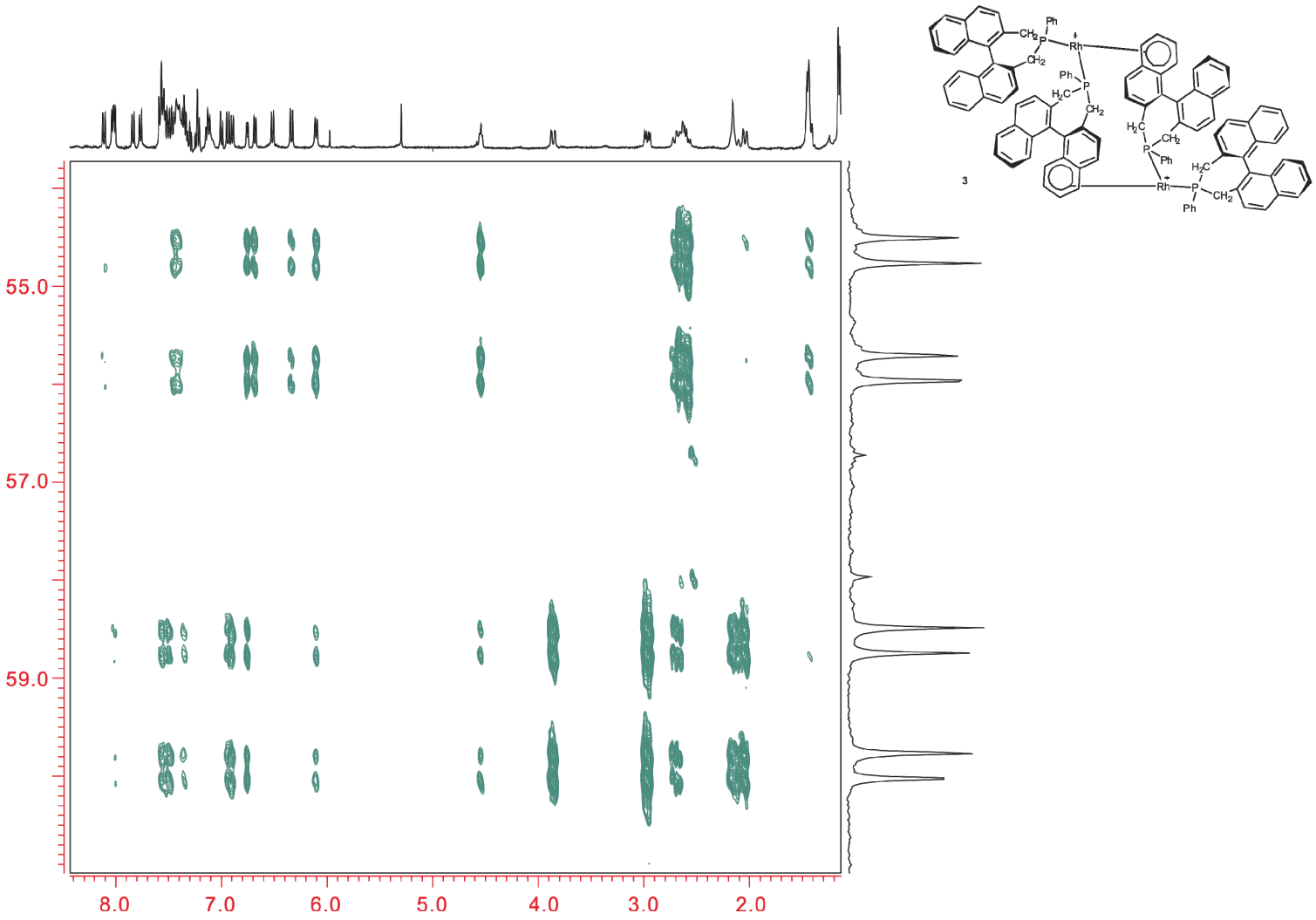


Figure S7. Section plot of 2D ^{1}H–^{31}P correlation NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**

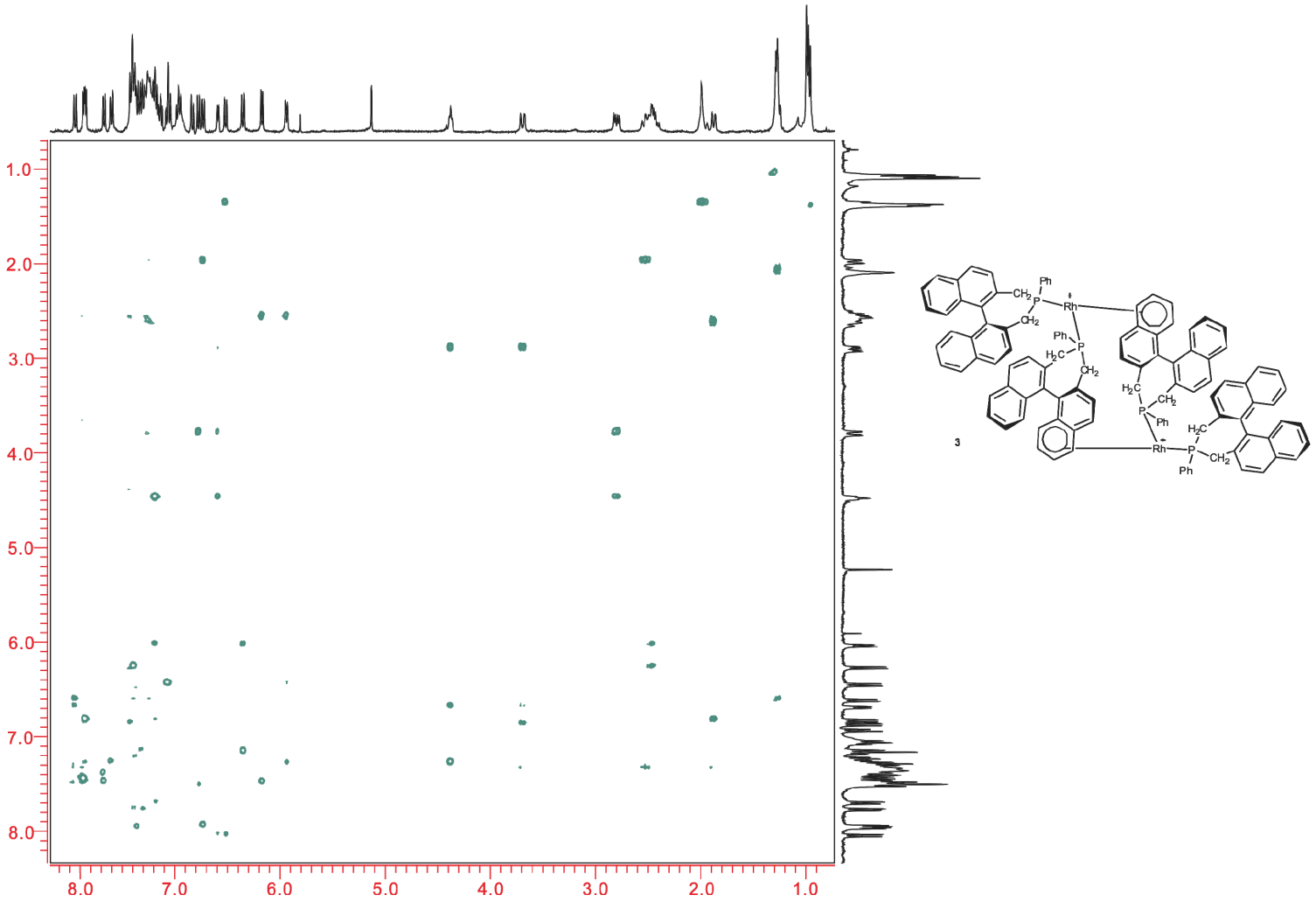


Figure S8. Phase sensitive 2D ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

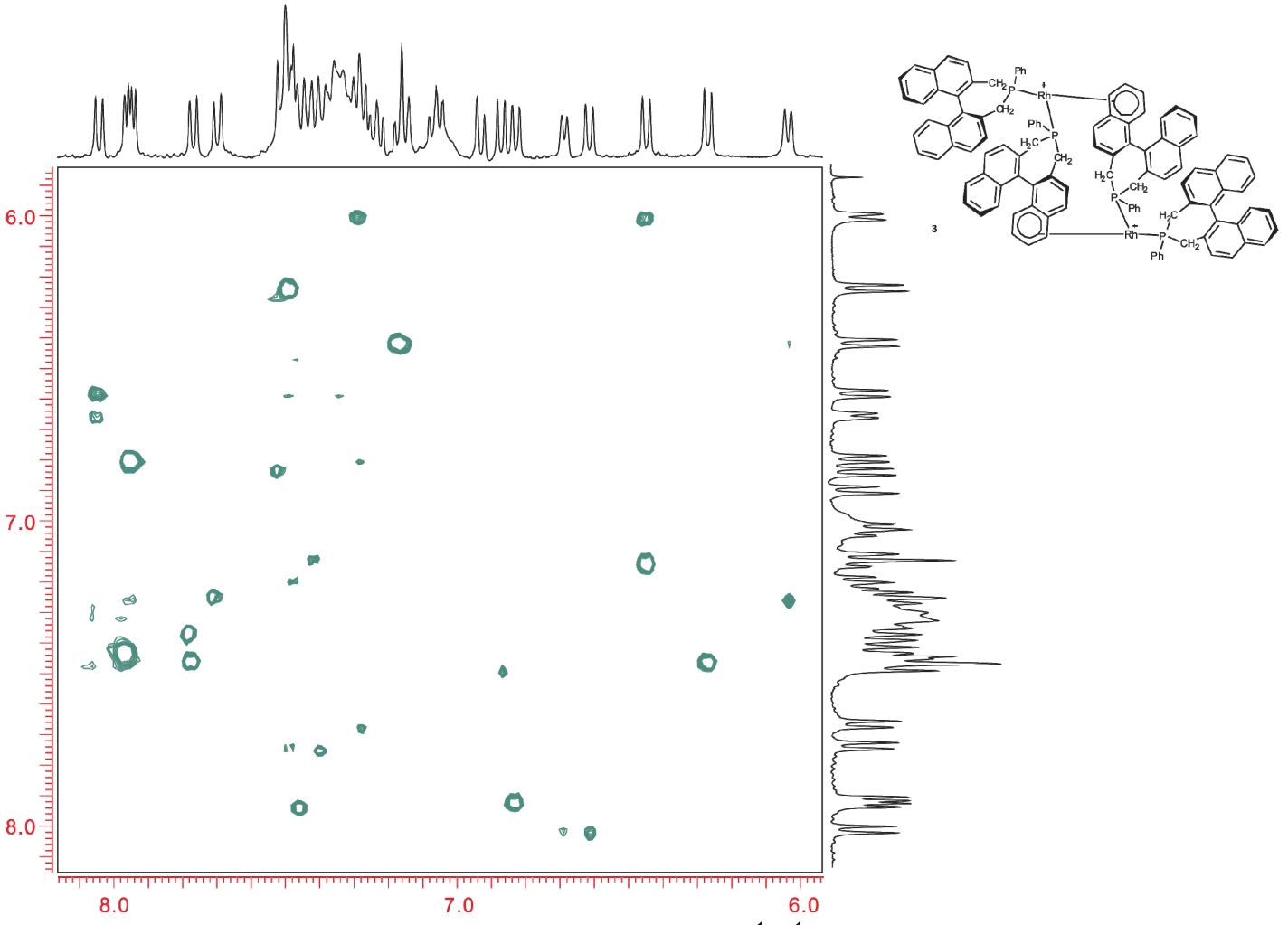


Figure S9. Section plot of the aromatic region in phase sensitive 2D ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

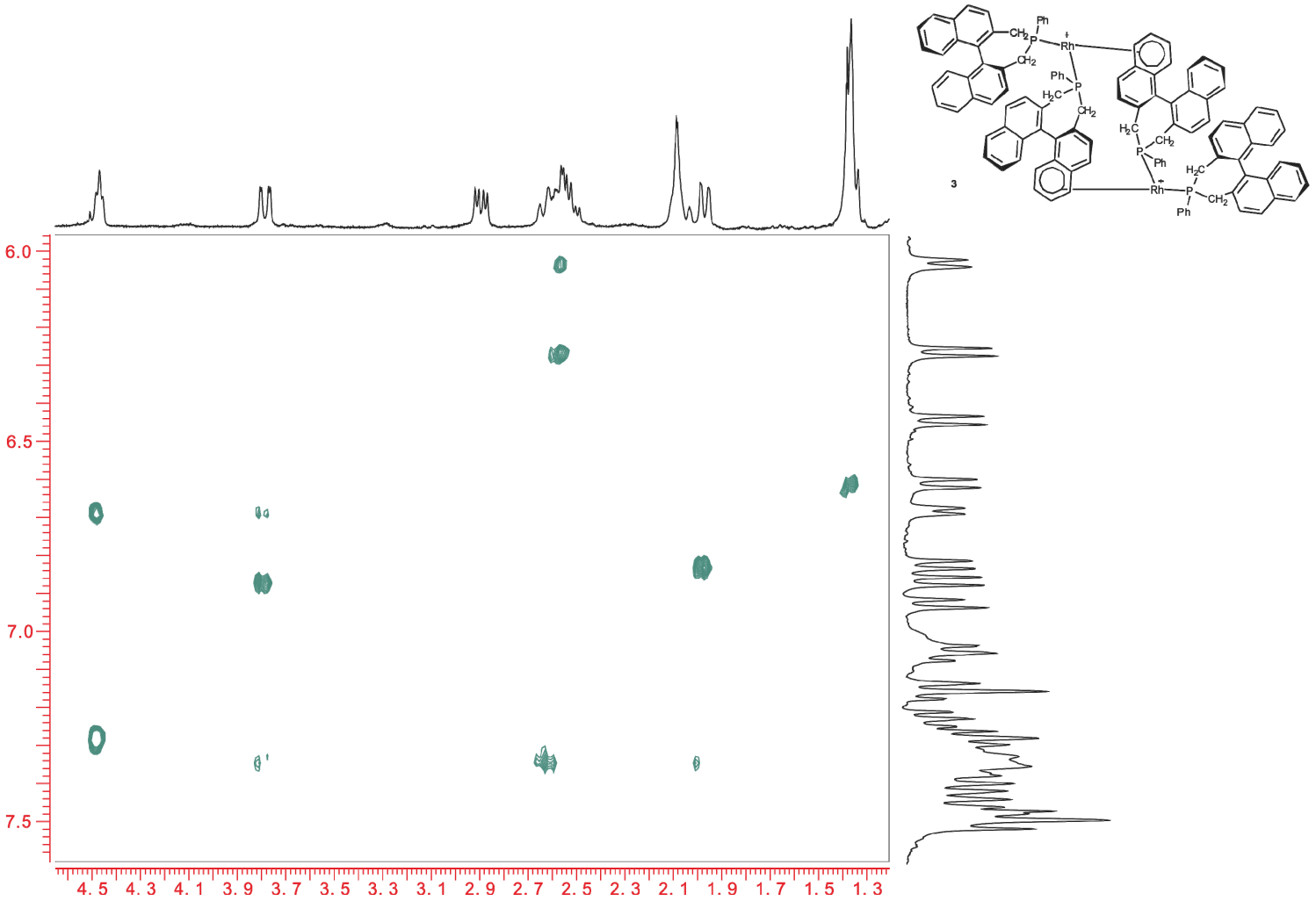


Figure S10. Section plot of the high-field region in phase sensitive 2D ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, CD_2Cl_2, 25 °C) of the dimer **3**.

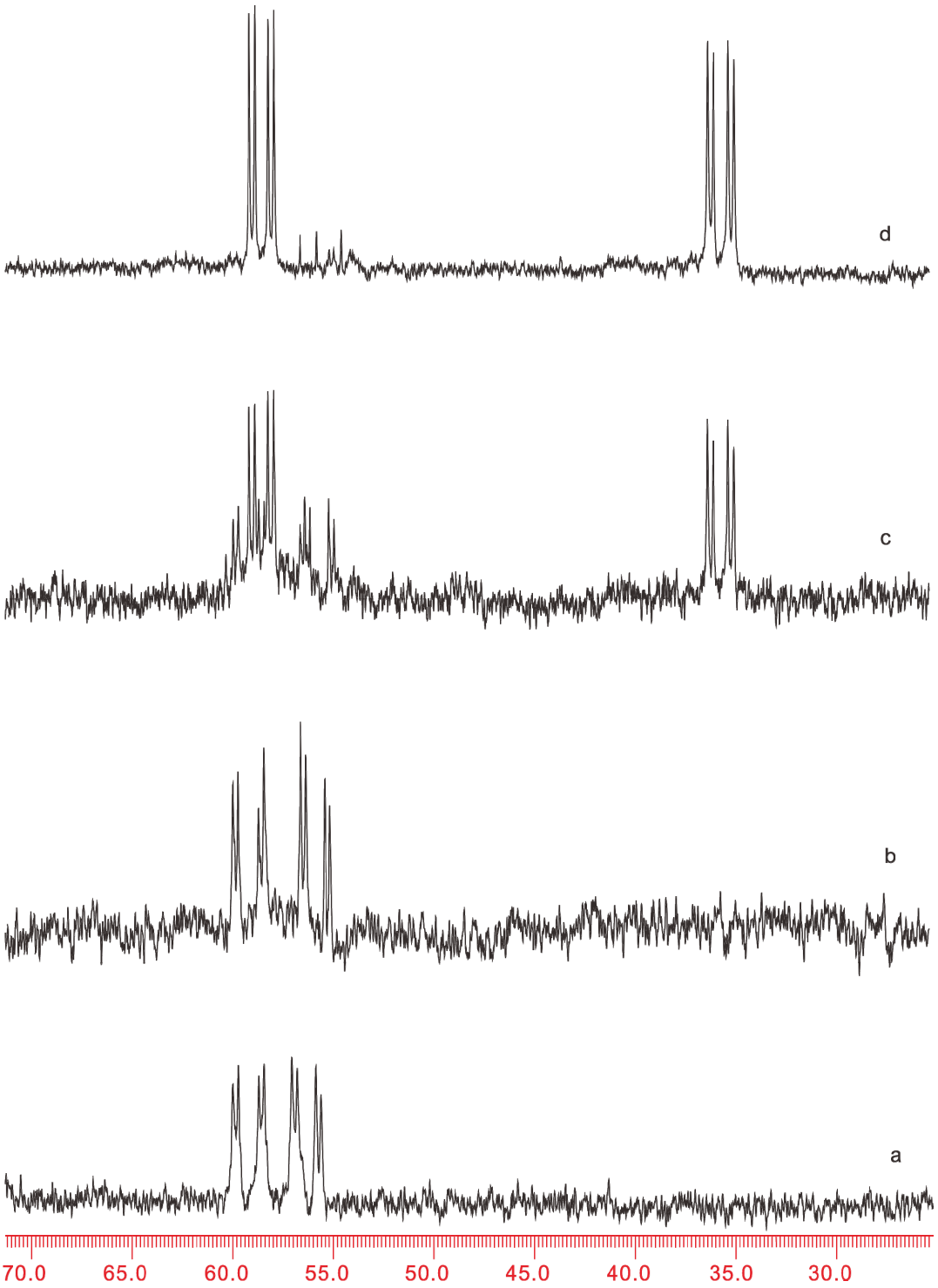


Figure S11. a) ^{31}P NMR spectrum (162 MHz, CD_2Cl_2, –90 °C) of the sample obtained by addition of 2 equivalents of MAC to a solution of dimer **3** precooled to –90 °C; b) Spectrum of the same sample after raising the temperature to –50 °C; c) Spectrum of the same sample after raising the temperature to –30 °C; d) after 30 min at –30 °C.

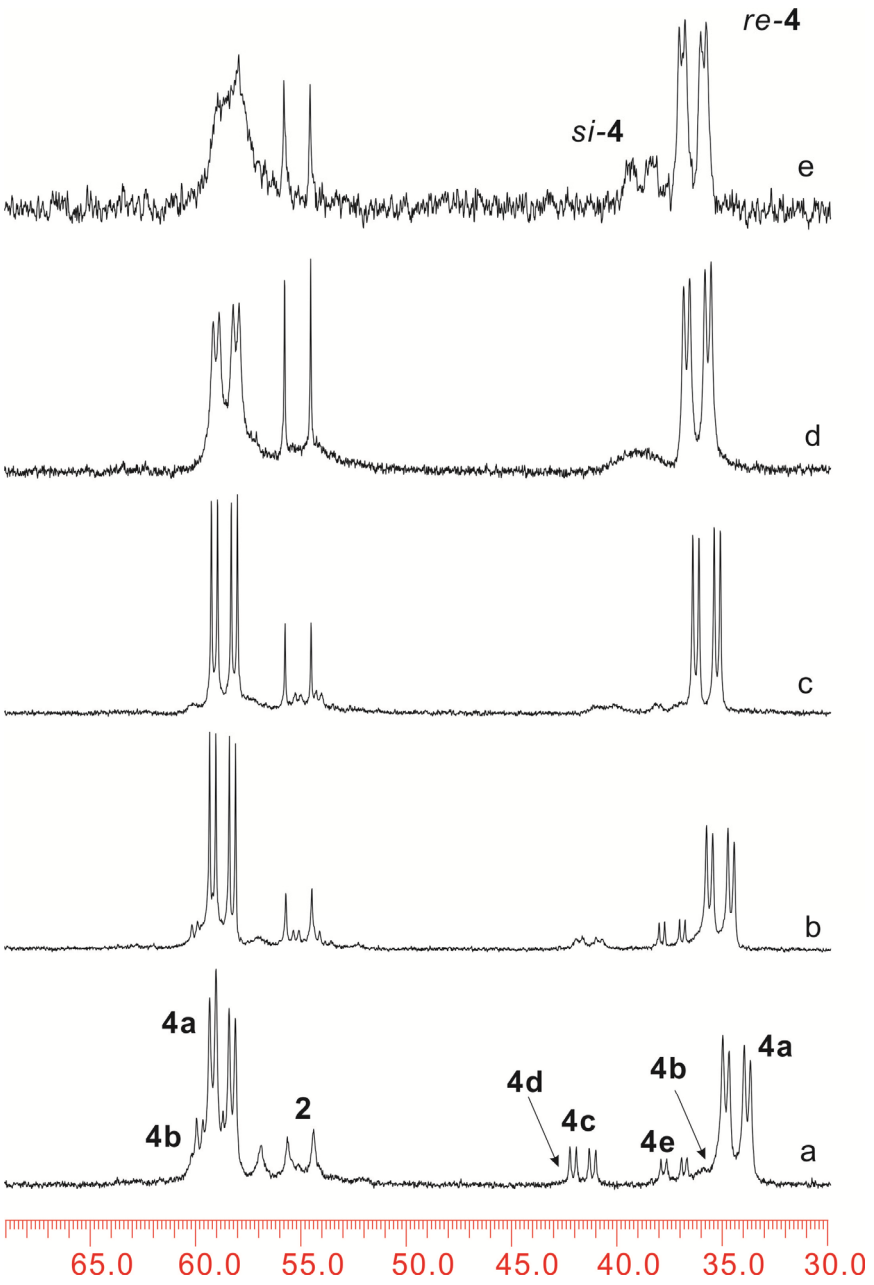


Figure S12. ^{31}P NMR spectra (162 MHz, CD_2Cl_2) of the sample obtained by adding 2 equivalents of MAC to a solution of **3**: a) at –90 °C, due to the rapid exchange between conformations the signals of minor species **4b** and **4d** are merged into background despite the very low temperature; b) at –60 °C, the existence of **4d**, not actually seen in the spectrum, follows from the broadening of the signal **4c,** **4a** and **4b** are exhibiting the averaged signal due to the fast exchange ; c) at –30 °C, the averaged signal of **4c**+**4d** broadened due to exchange with **4e**, while that of **4a**+**4b** sharpened, hence the exchange between *re*- and *si*-coordinated species is still relatively slow at this temperature; d) at 0 °C; e) at 25 °C, high-field multiplets of *re*- and *si*-coordinated species are seen separately, they are broadened due to exchange with **2** and with each other.

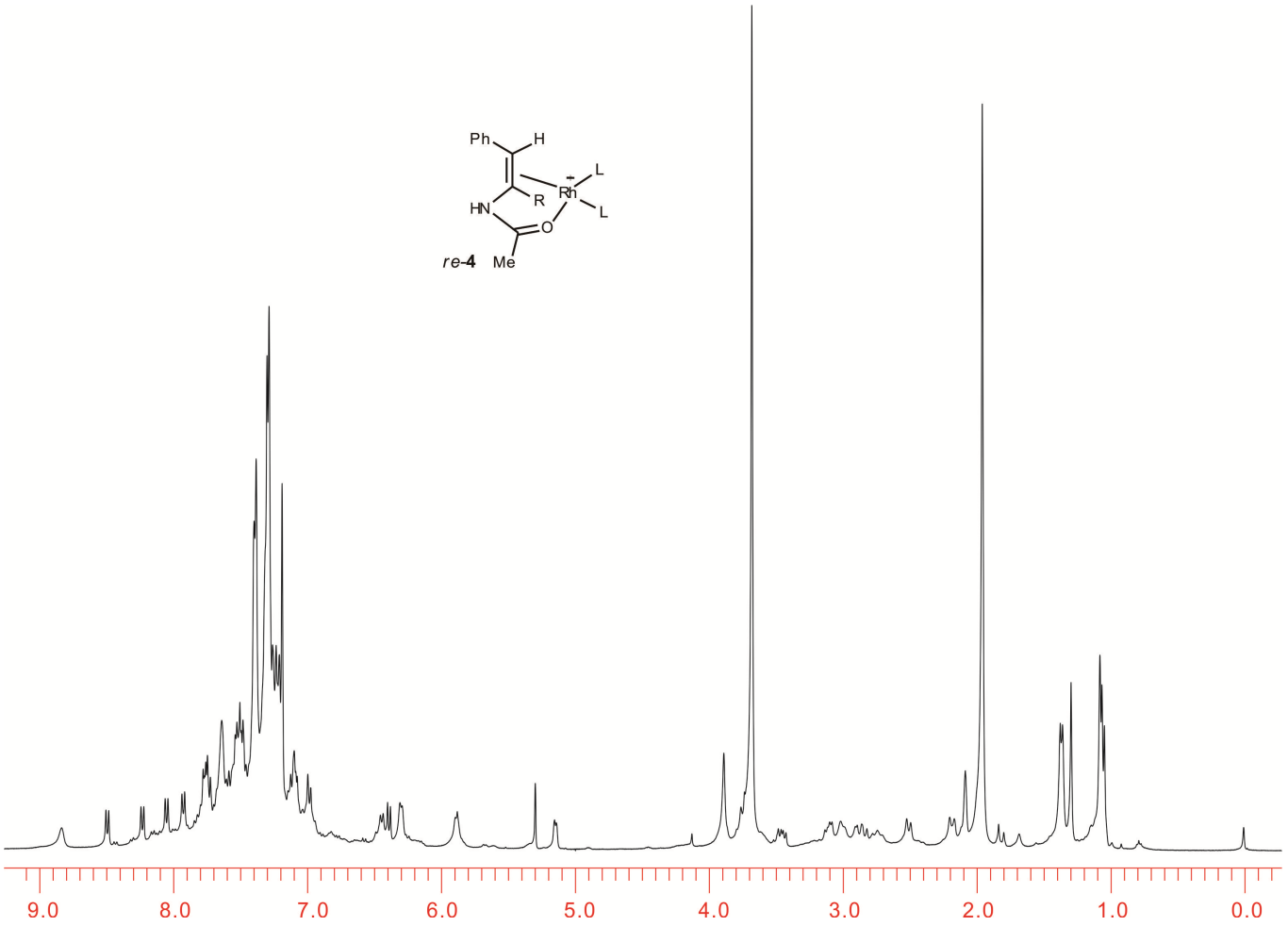


Figure S13. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of the catalyst-substrate complex **4**.

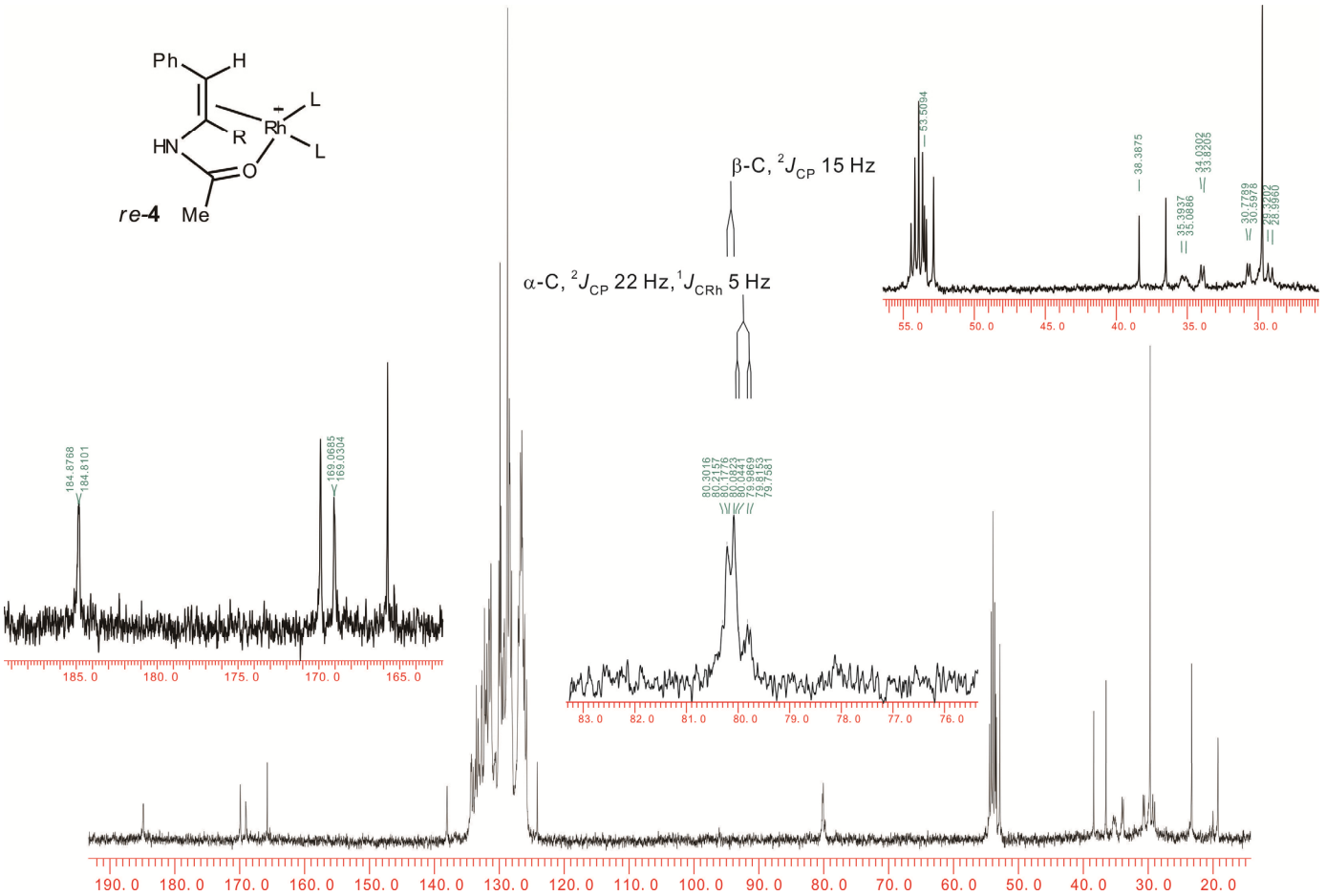


Figure S14. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2, –50 °C) of the catalyst-substrate complex **4**. Due to the broadness of the signals of minor species at this temperature, essentially only the spectrum of the major species is observed.

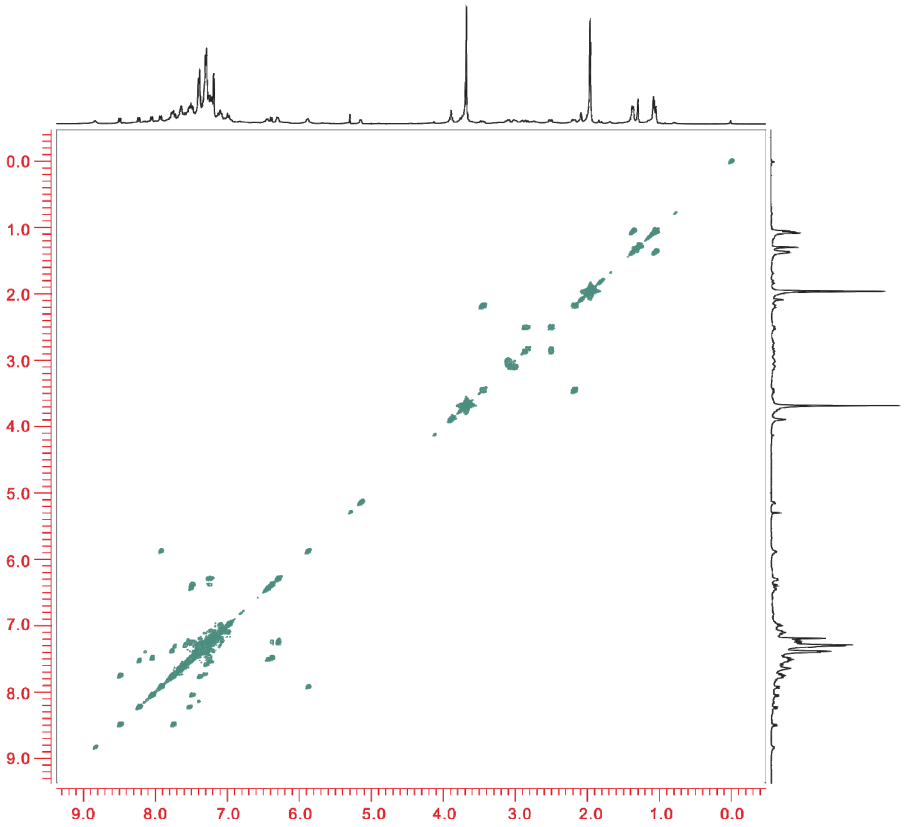


Figure S15. ^{1}H–^{1}H COSY NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of the catalyst-substrate complex **4**.

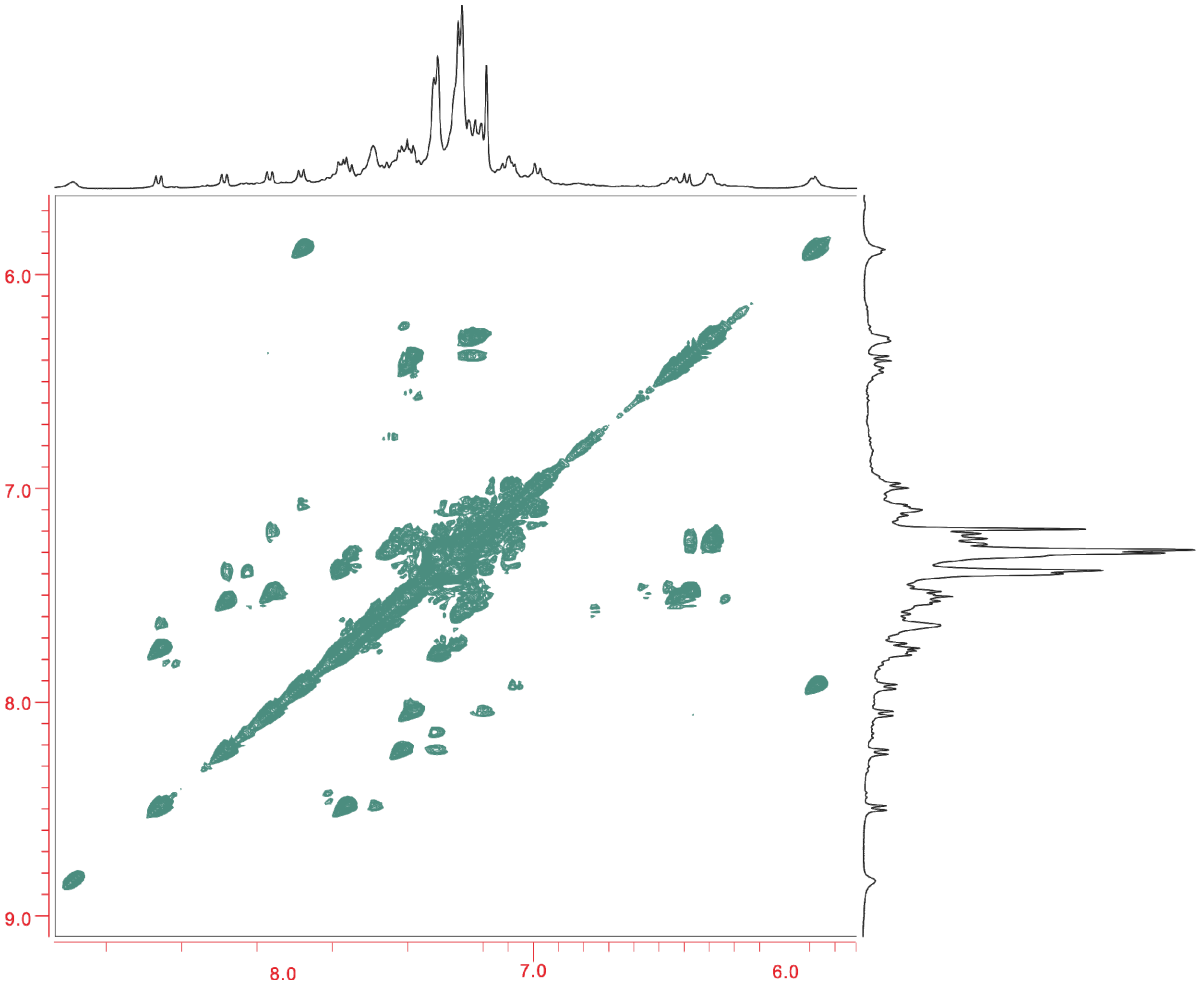


Figure S16. Section plot of the low-field region in the ^{1}H–^{1}H COSY NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of the catalyst-substrate complex **4**.

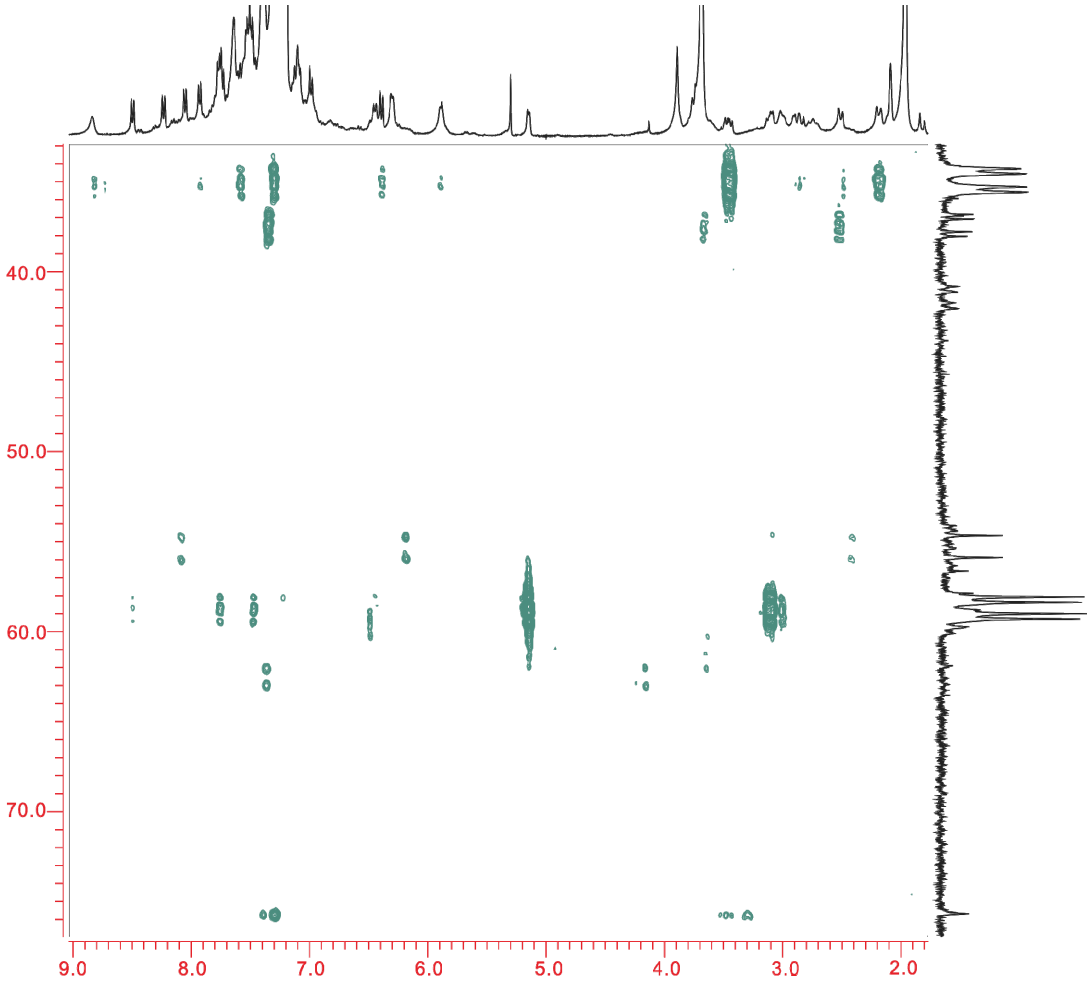


Figure S17. 2D ^{1}H–^{31}P correlation NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of thecatalyst-substrate complex **4**.

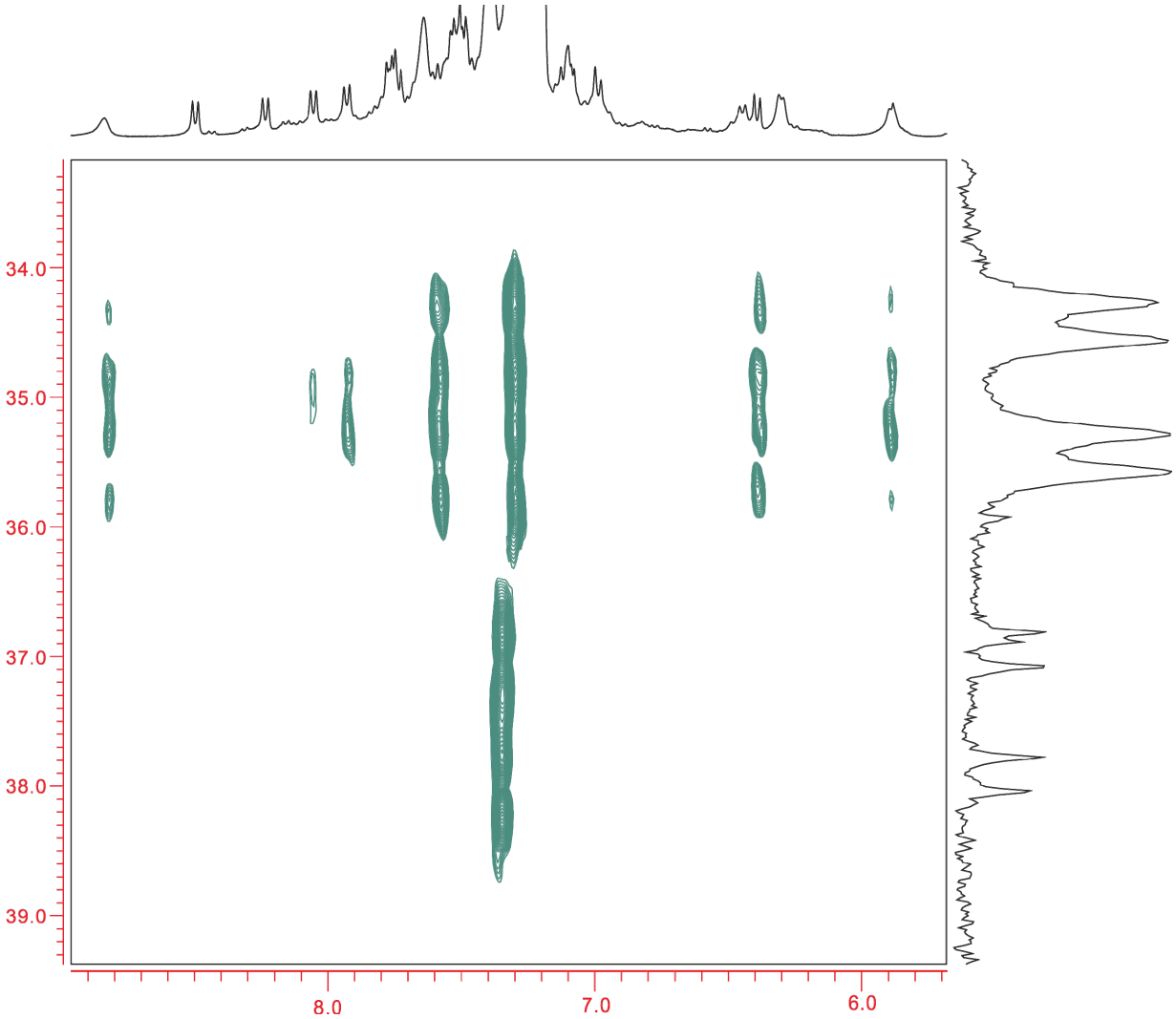


Figure S18. Section plot of the 2D ^{1}H–^{31}P correlation NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of thecatalyst-substrate complex **4**.

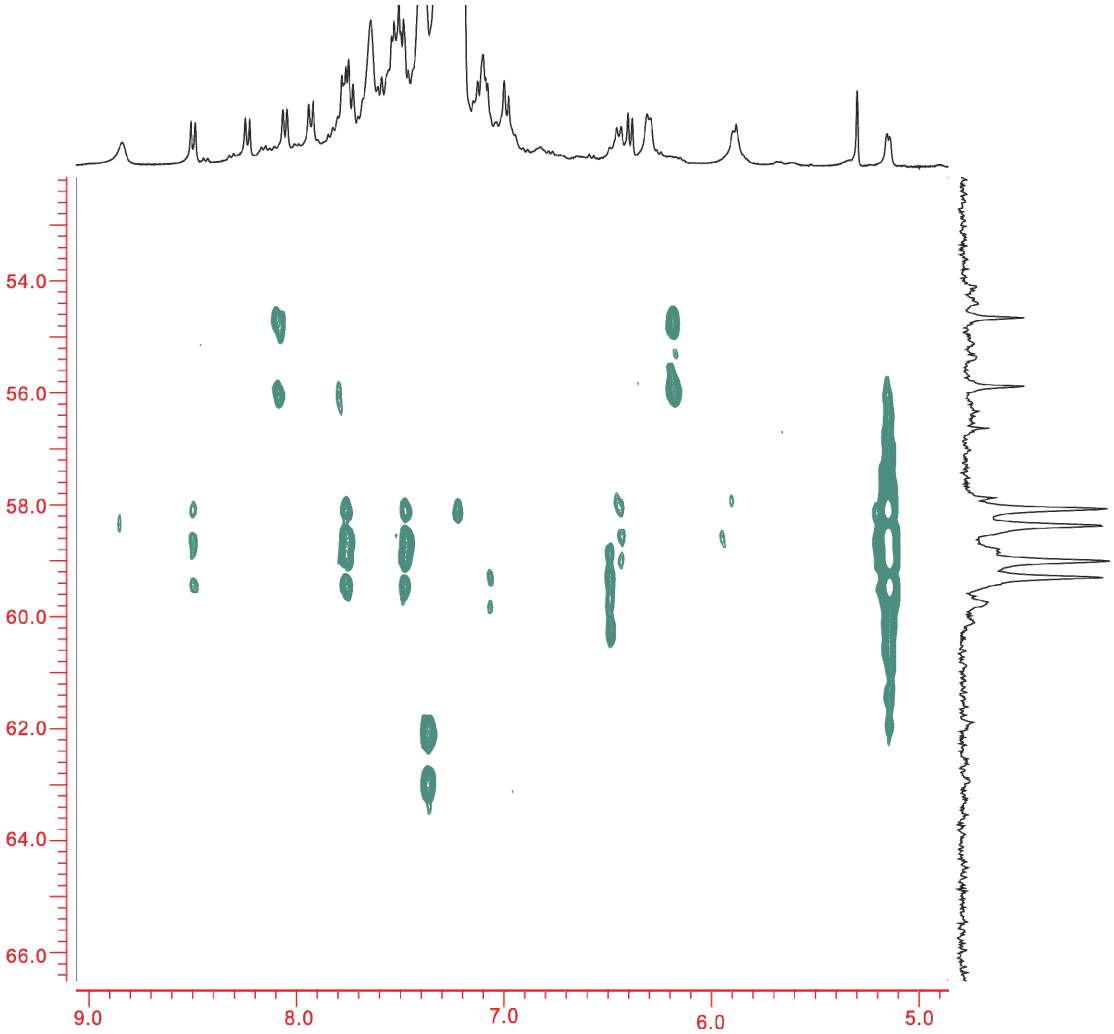


Figure S19. Section plot of the 2D ^{1}H–^{31}P correlation NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of thecatalyst-substrate complex **4**.

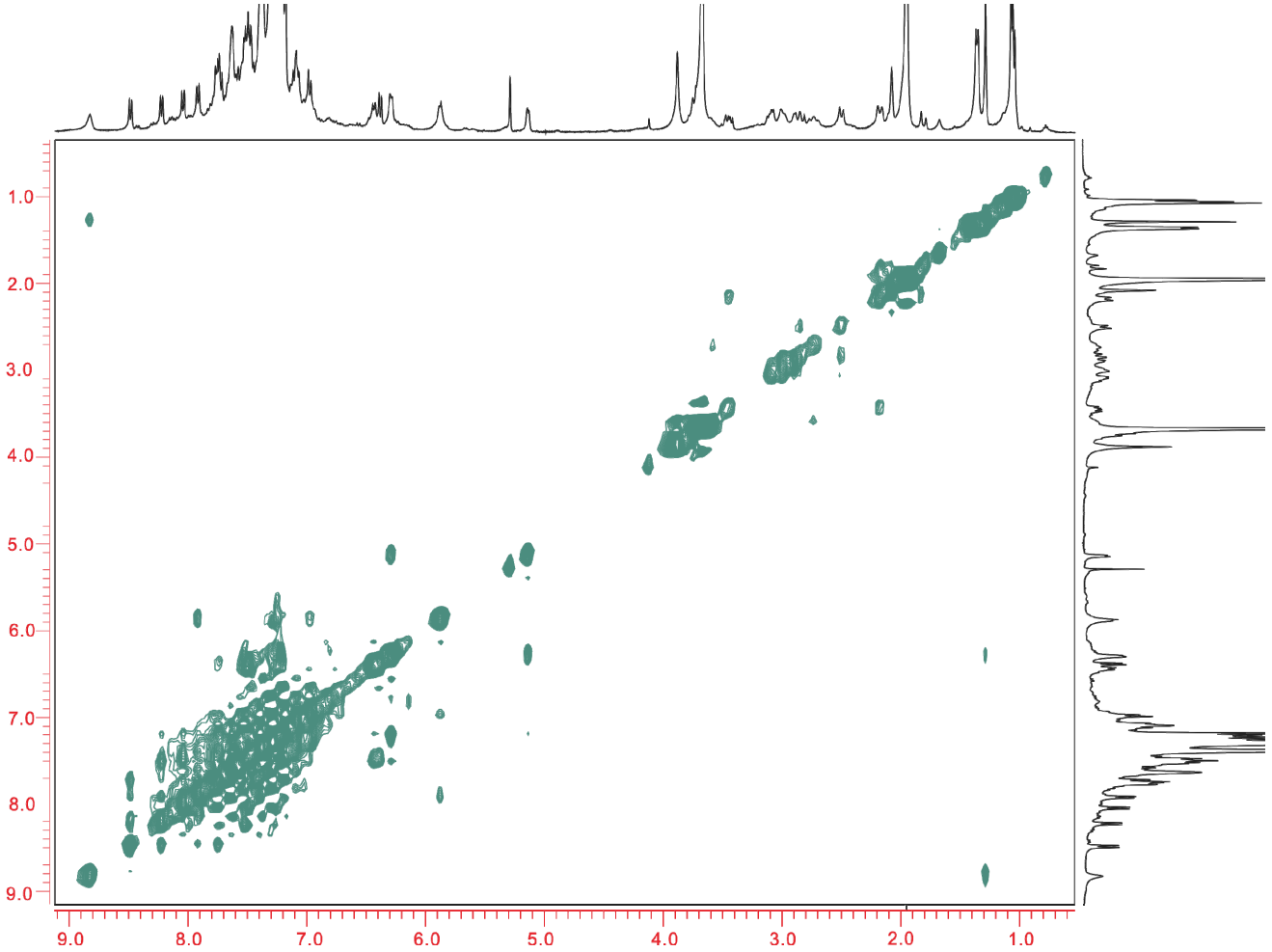


Figure S20. Phase sensitive 2D ^{1}H–^{1}H NOESY NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of thecatalyst-substarate complex **4**. The major species is in a fast exchange with a low concentrated conformer

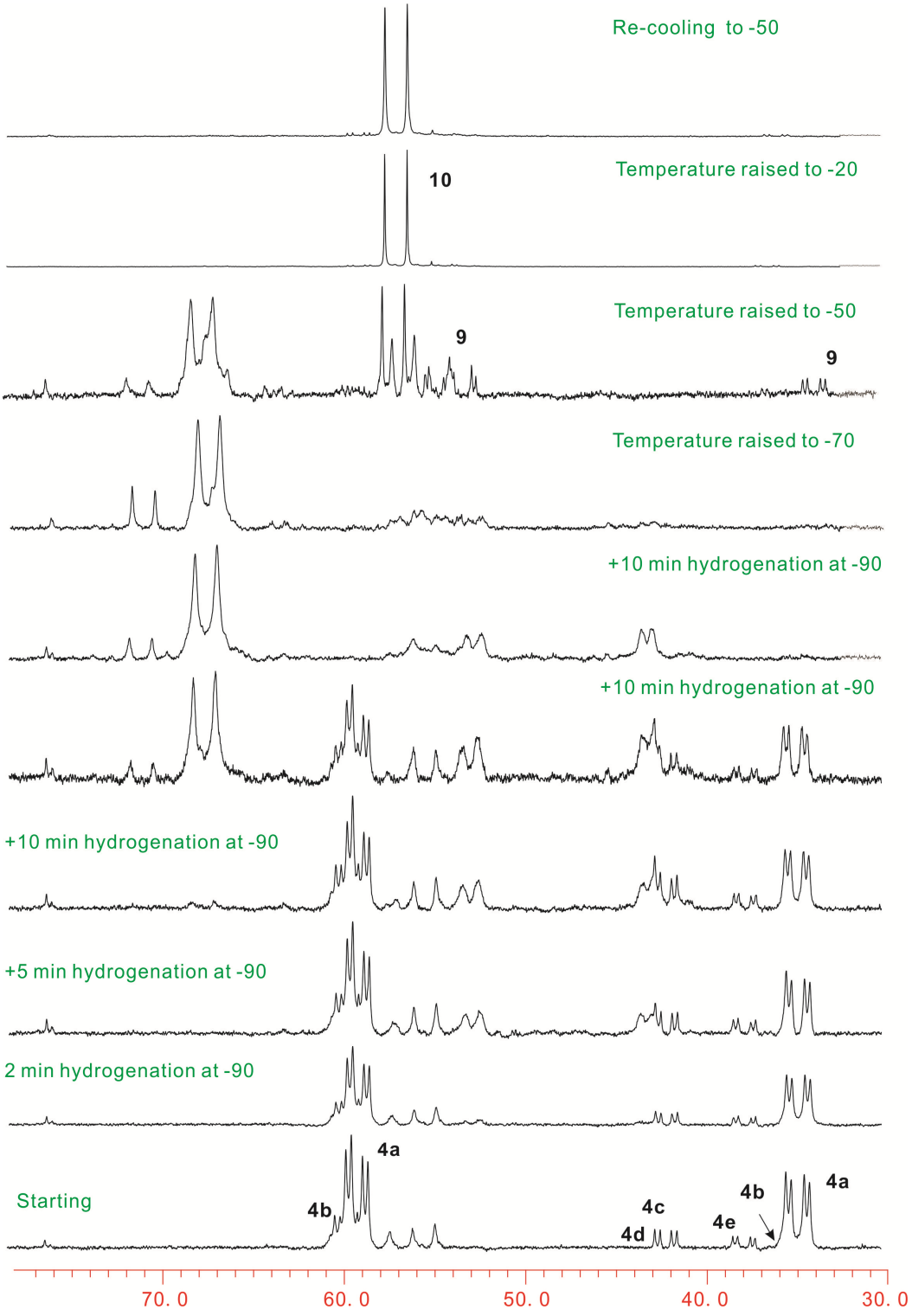


Figure S21. More detailed Figure 3.

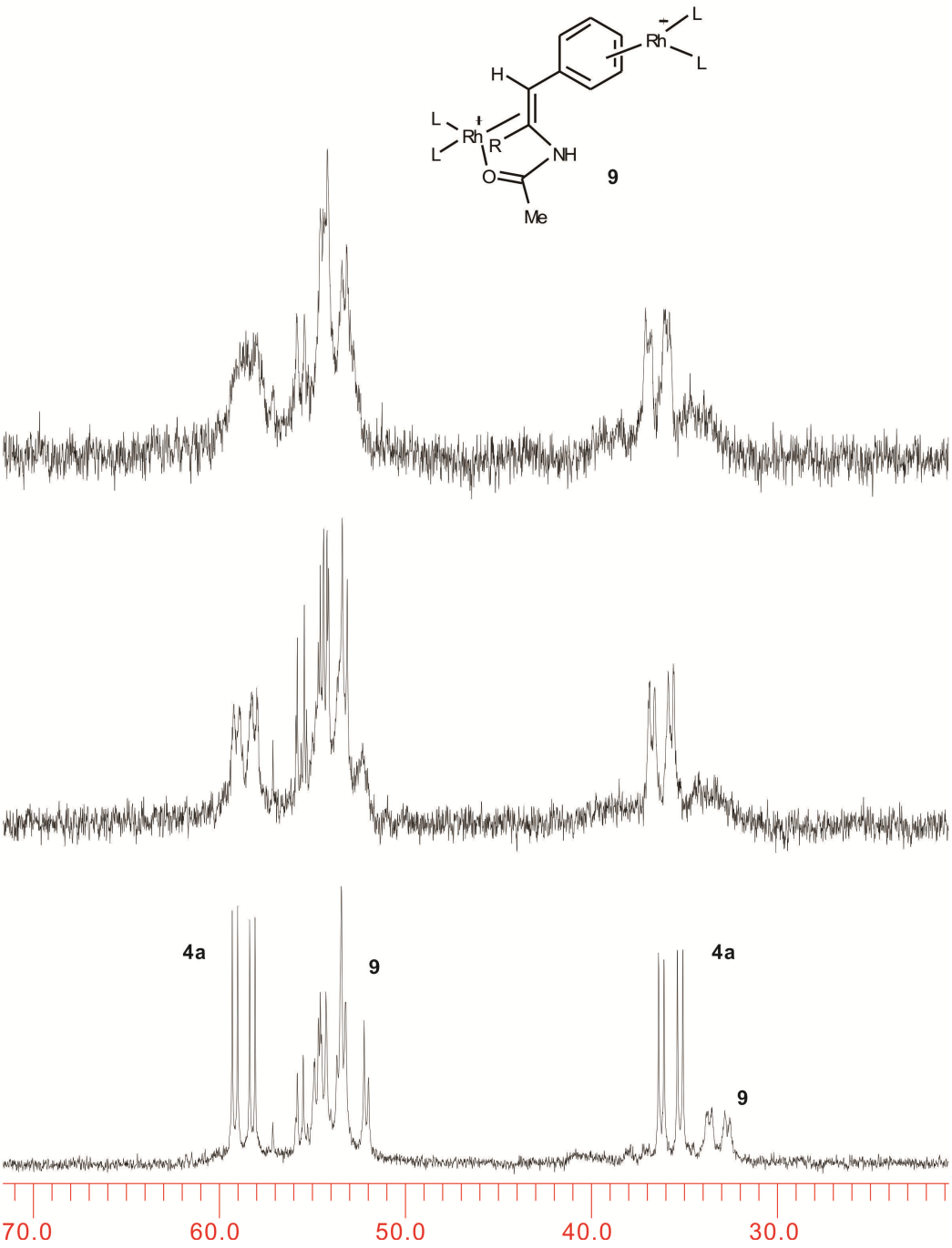


Figure S22. Spectra ^{31}P NMR (162 MHz, CD_2Cl_2) of the sample obtained by the addition of 0.5 equivalents of MAC to the solution of **3**: top, 25 °C; middle, 0 °C; bottom, –50 °C.

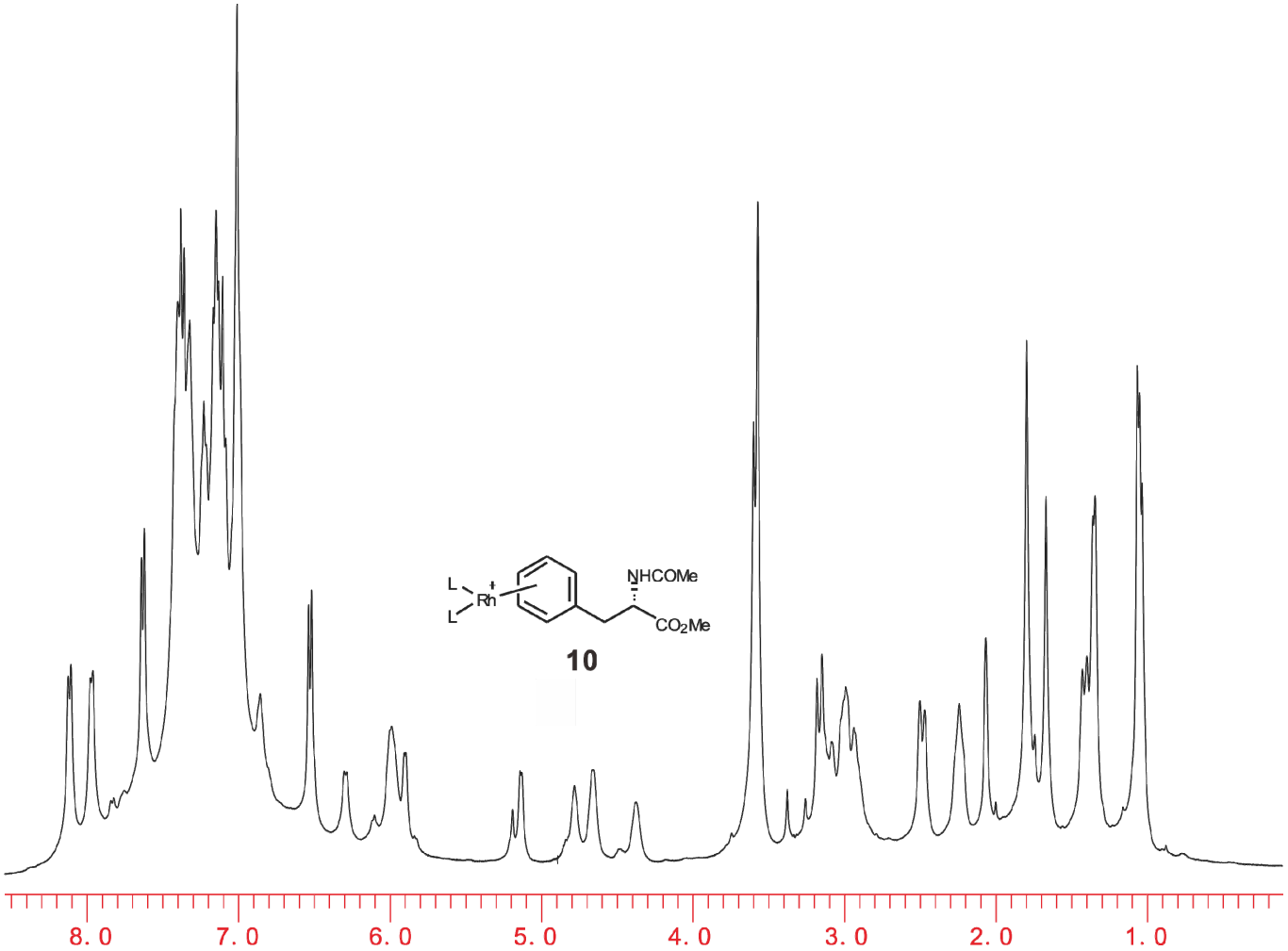


Figure S23. Spectrum ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C) of the reaction mixture after low-temperature hydrogenation experiment containing the catalyst-product complex **10**.

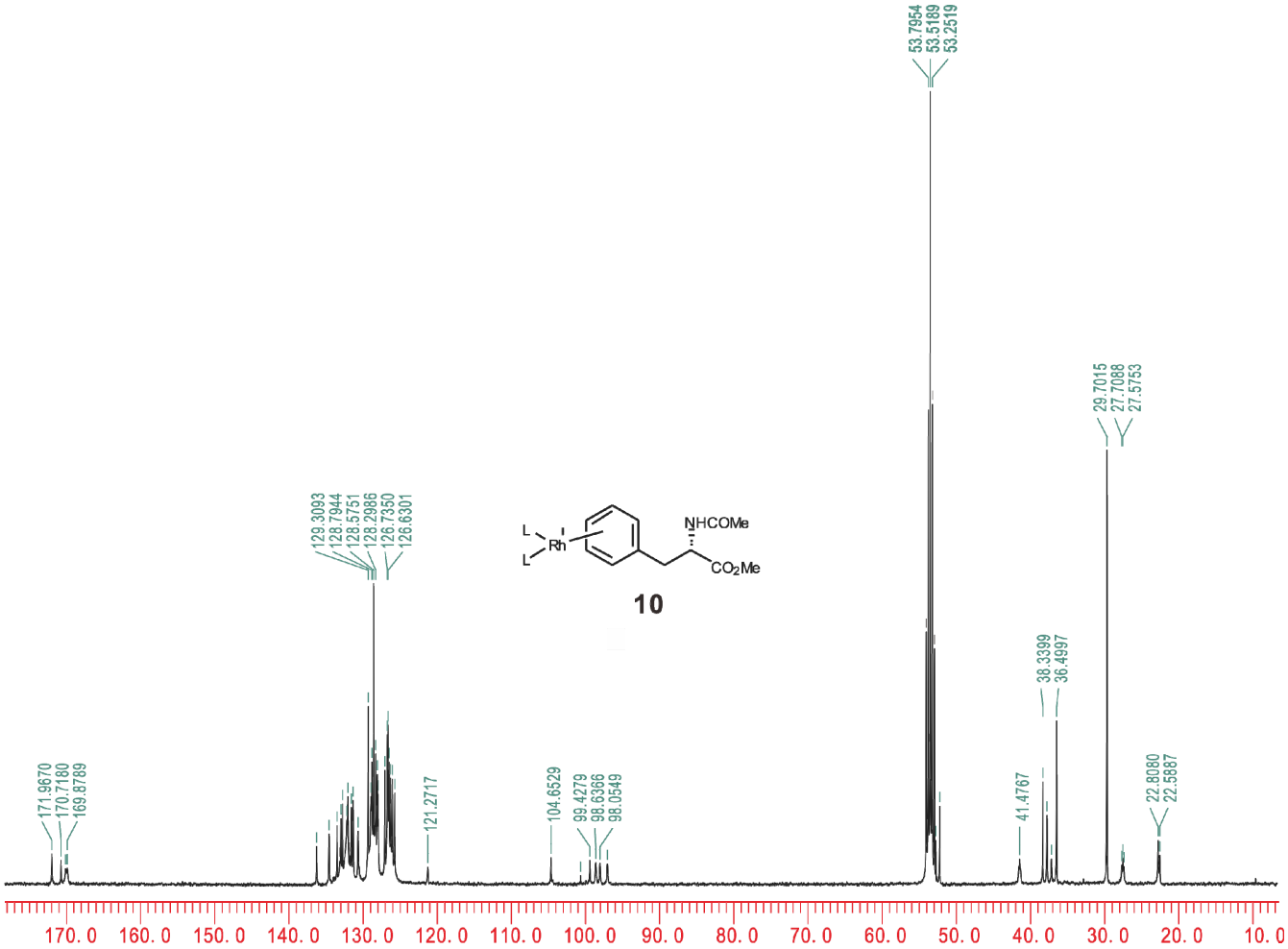


Figure S24. Spectrum ^{13}C NMR (100 MHz, CD_2Cl_2, 25 °C) of the reaction mixture after low-temperature hydrogenation experiment containing the catalyst-product complex **10**.

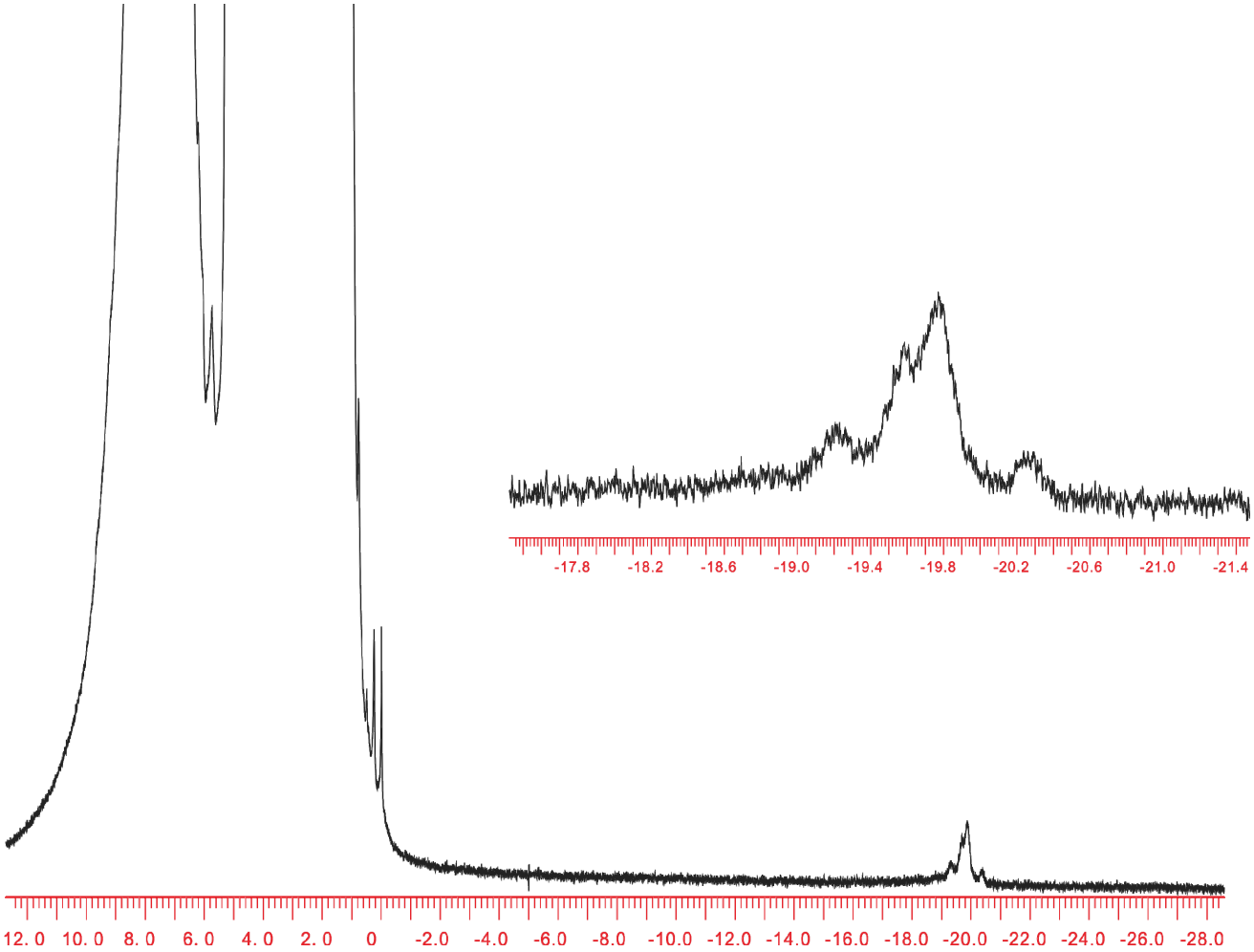


Figure S25. Hydride signals seen in the ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, –90 °C) during the low temperature hydrogenation of the catalyst-substrate complex **4**

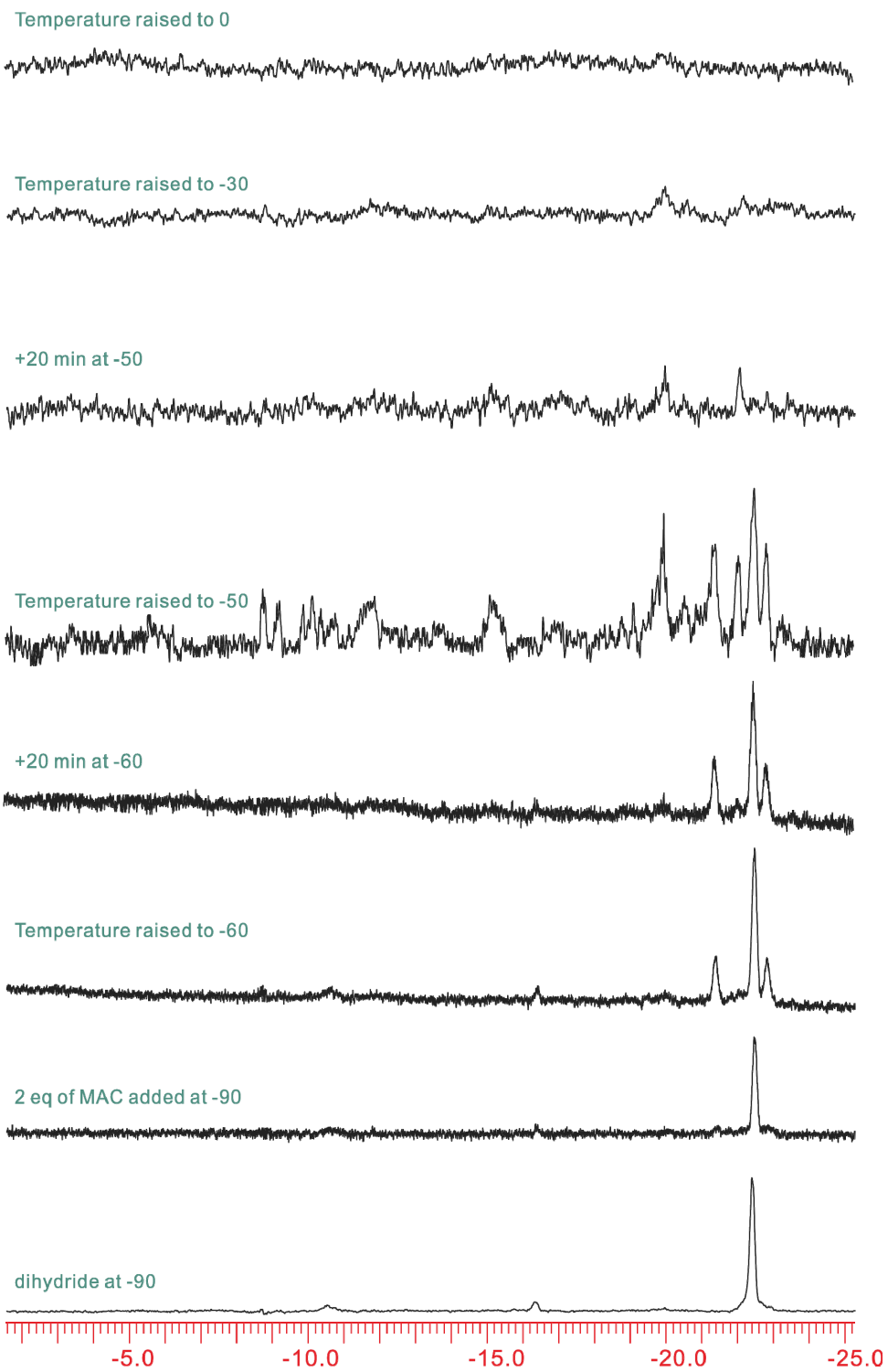


Figure S26. ^{1}H NMR spectra (400 MHz, CD_2Cl_2-THF-d_8 1 : 1): illustrating the reaction of the solvate dihydride **6b** with MAC.

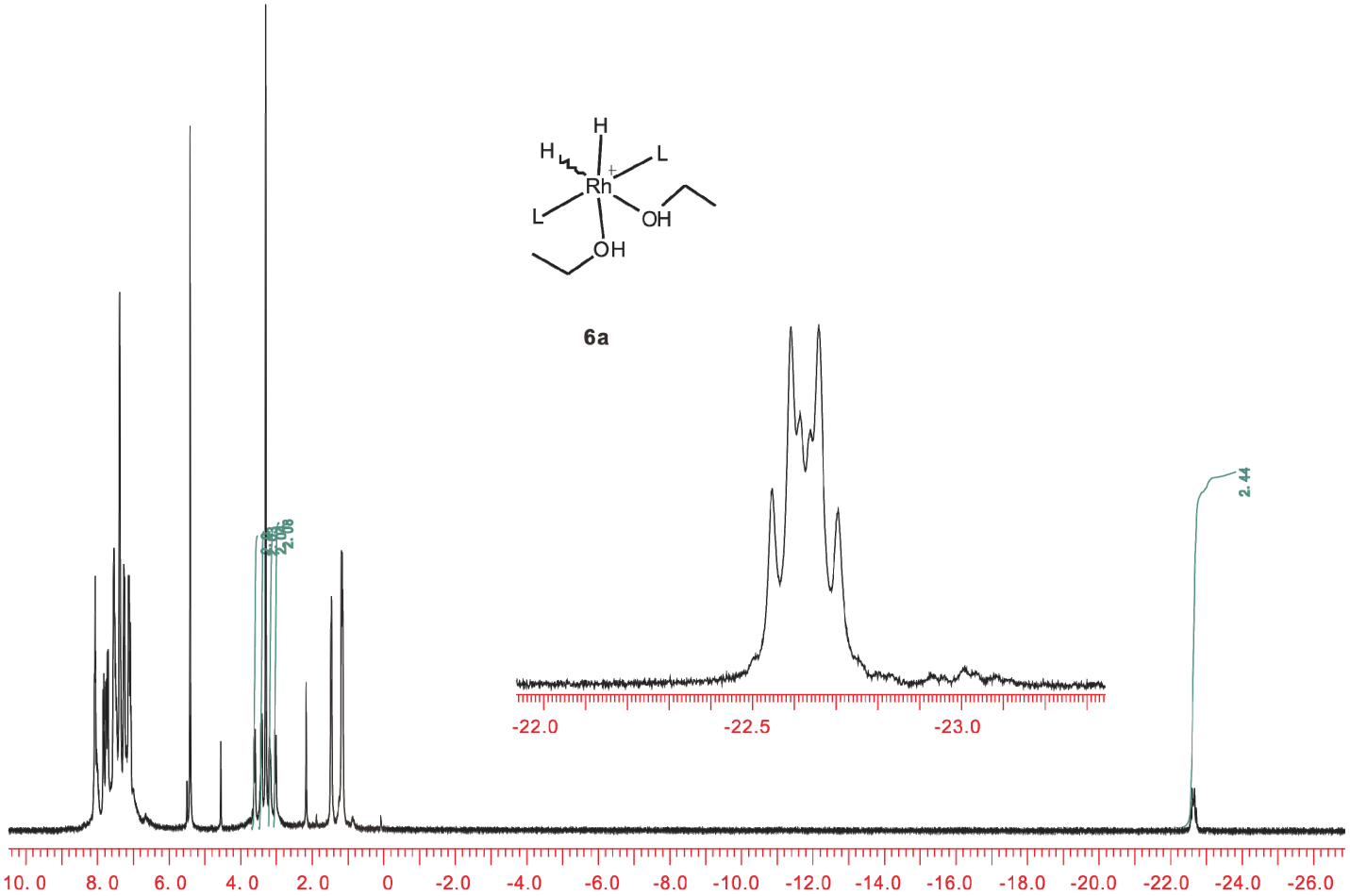
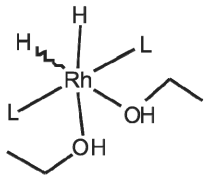


Figure S27. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2-CD_3OD, –50 °C) of the solvate dihydride complex **6a**.



6a

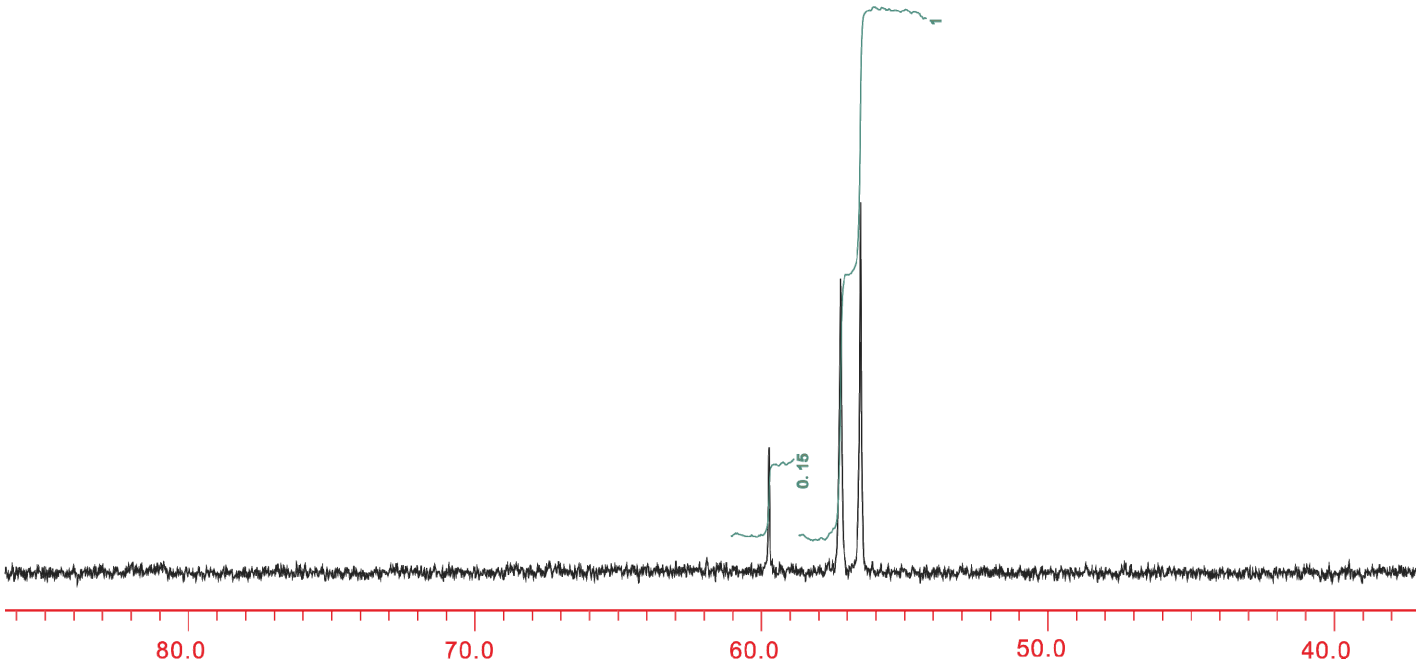
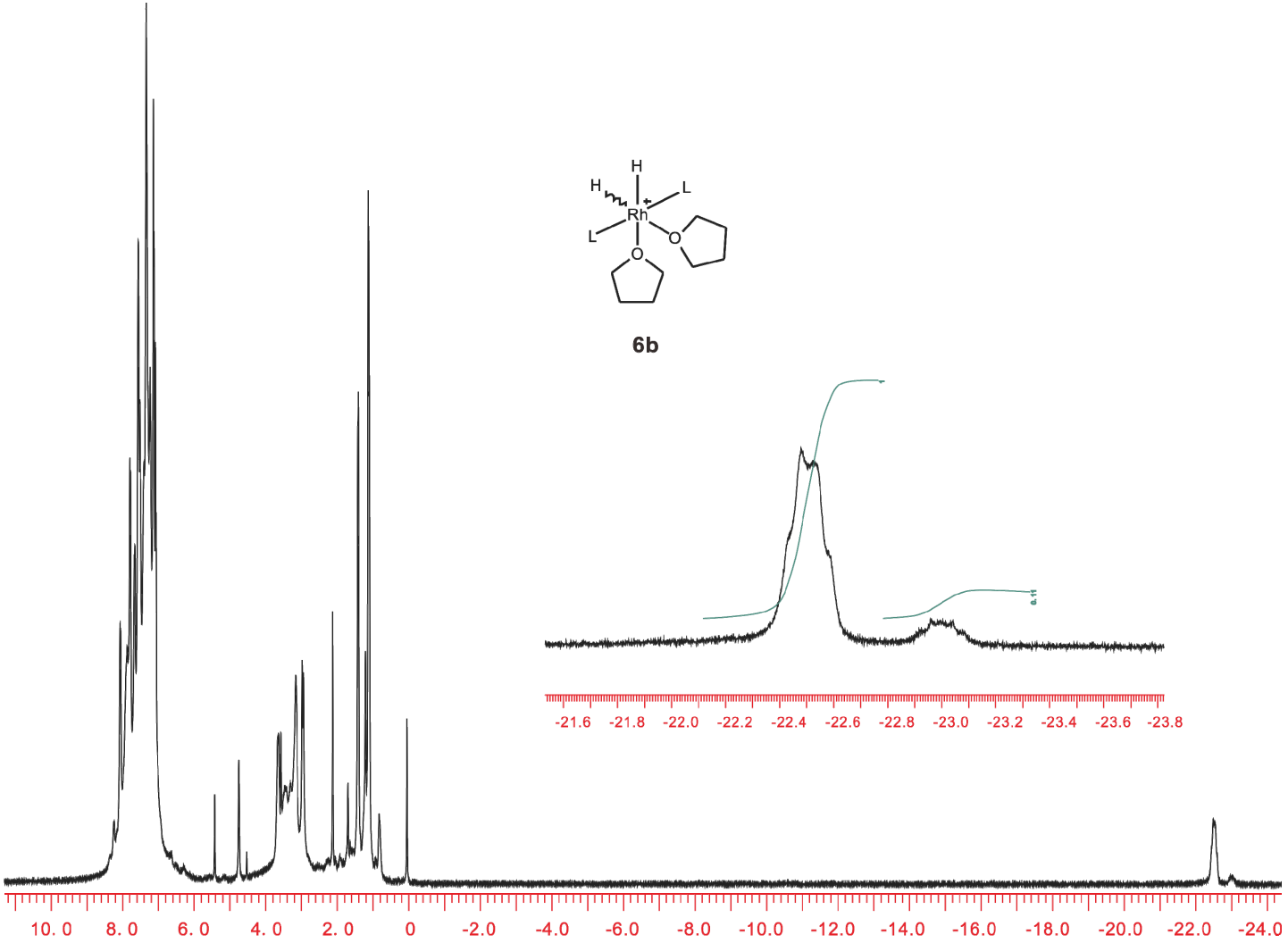


Figure S28. ^{31}P NMR spectrum (162 MHz, CD_2Cl_2-CD_3OD, –50 °C) of the solvate dihydride complex **6a**. The singlet at δ 59.8 is an impurity of the oxidized PhenylBinepine.



6b

Figure S29. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2-THF-d_8, –50 °C) of the solvate dihydride complex **6b**.

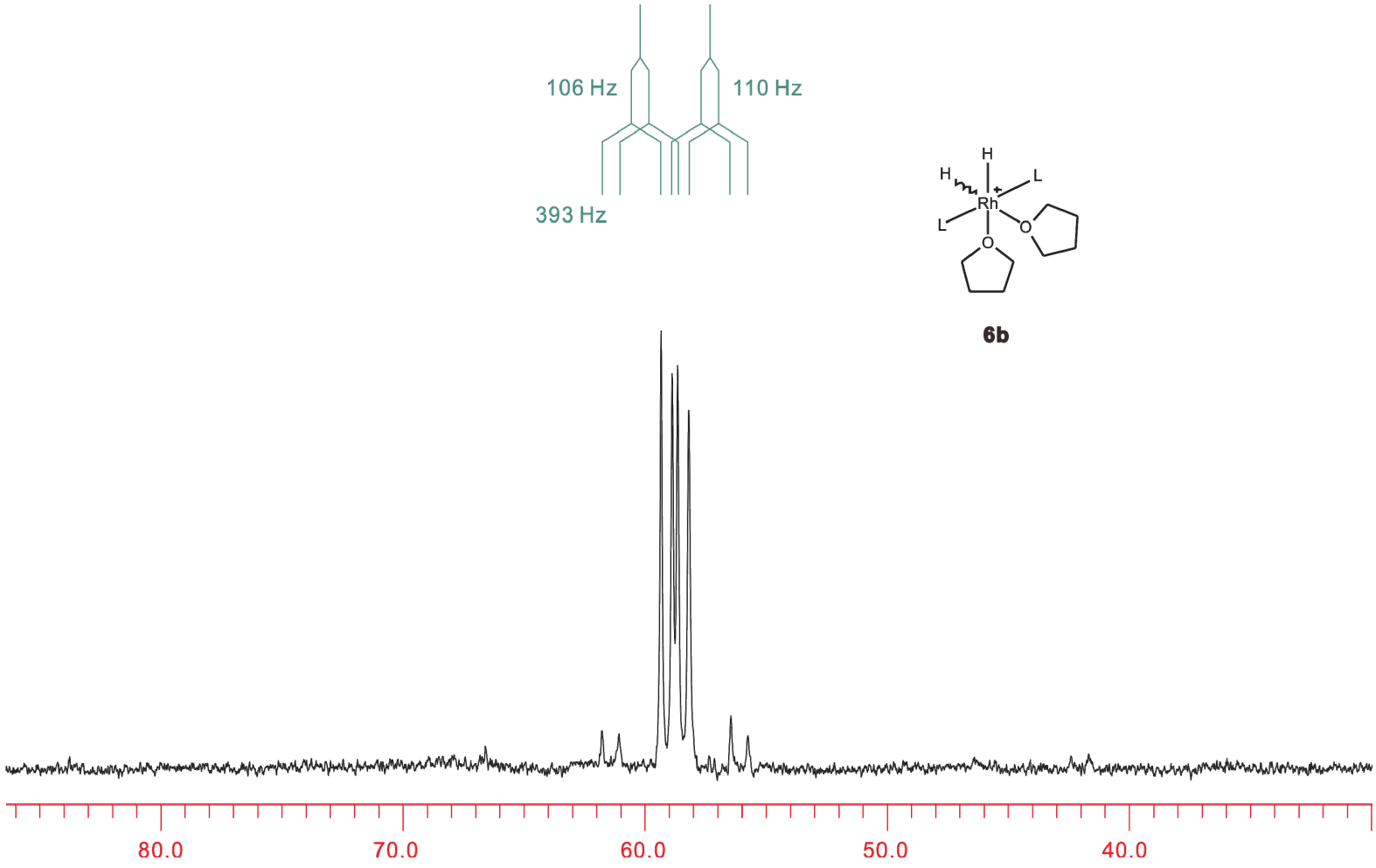


Figure S30. ^{31}P NMR spectrum (162 MHz, CD_2Cl_2-THF-d_8, –50 °C) of the solvate dihydride complex **6b**.

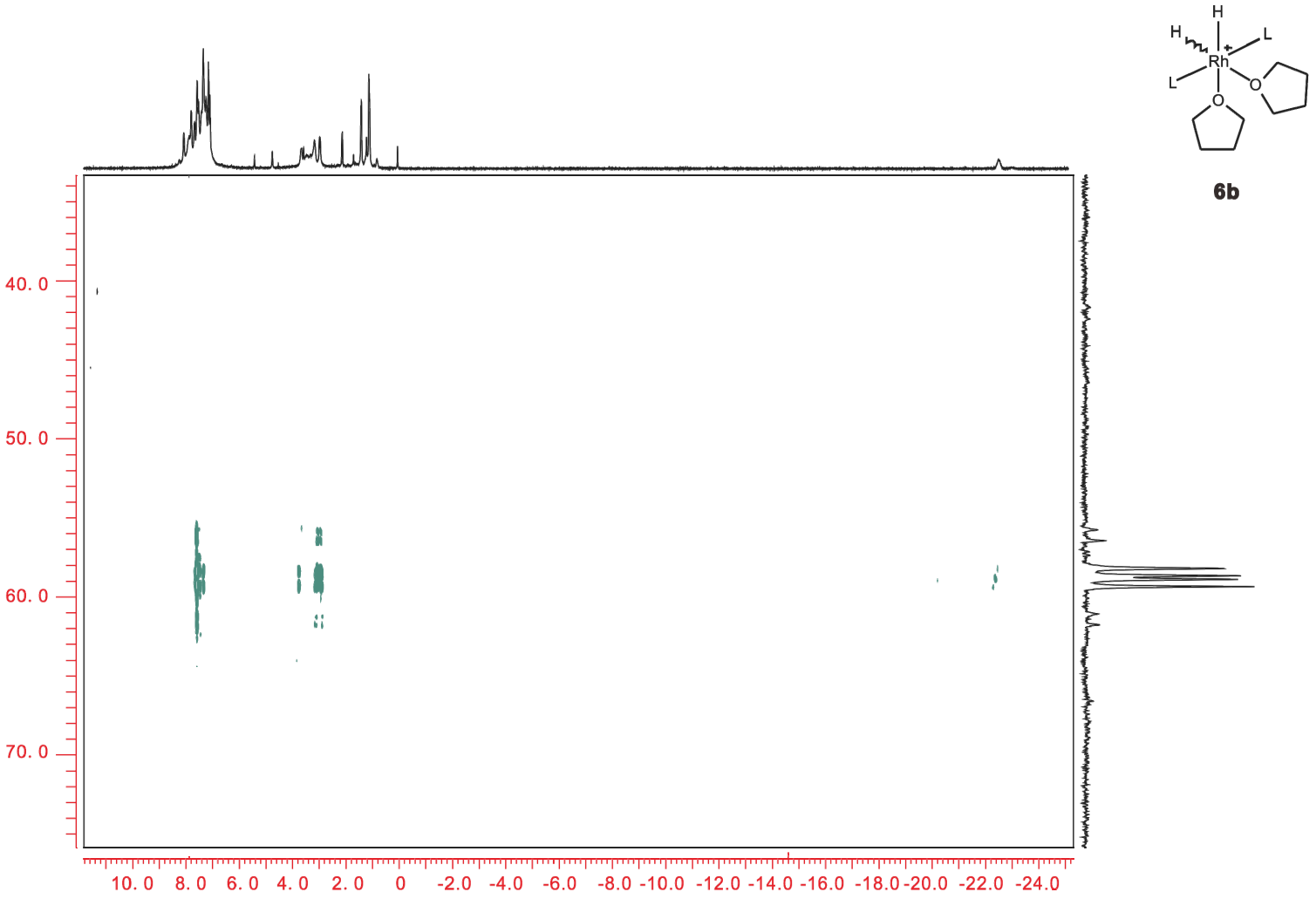
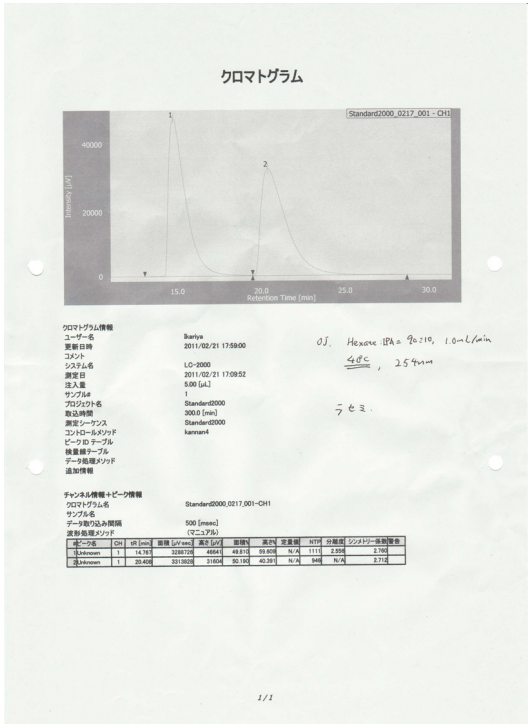


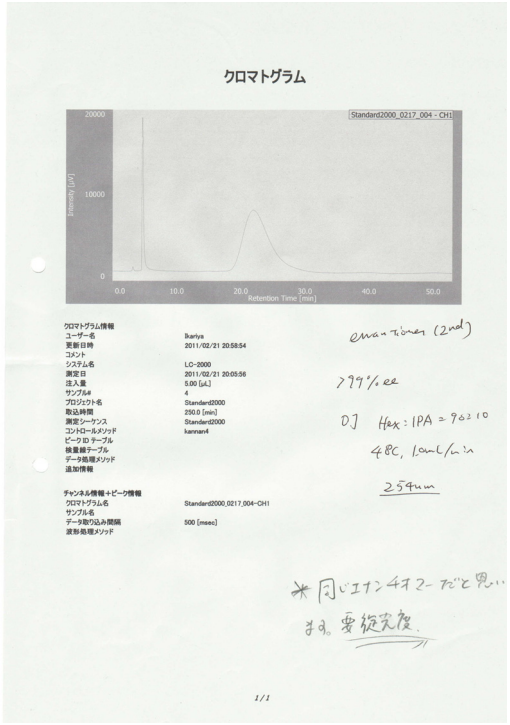
Figure S31. 2D ^{1}H–^{31}P correlation NMR spectrum (400 MHz, CD_2Cl_2, –70 °C) of the solvate dihydride complex **6b**.

HPLC analysis:

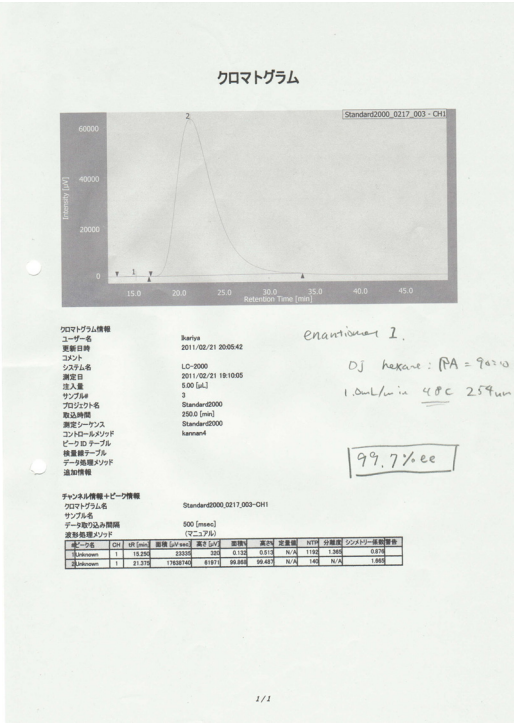
Racemic sample



Sample from LT hydrogenation of **4**.

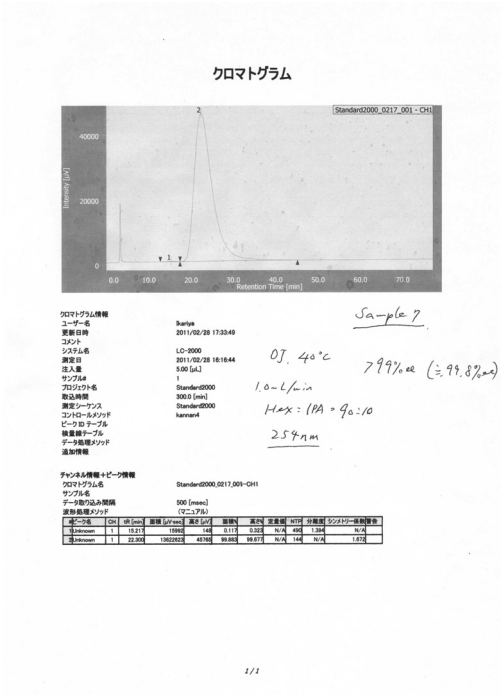


Sample from the reaction of **6a** with MAC

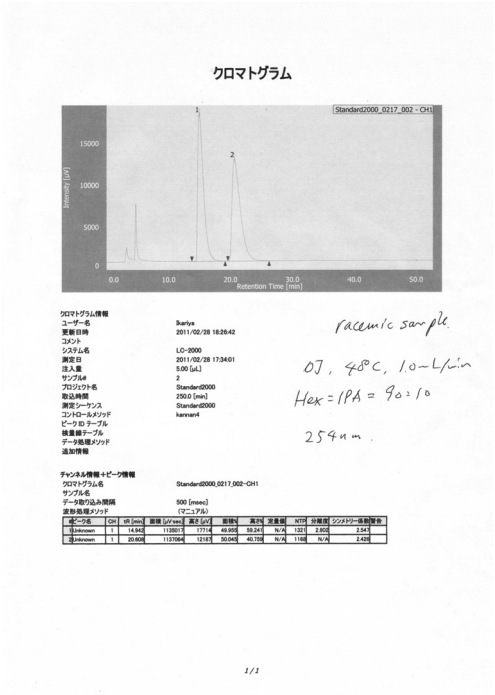


HPLC analysis:

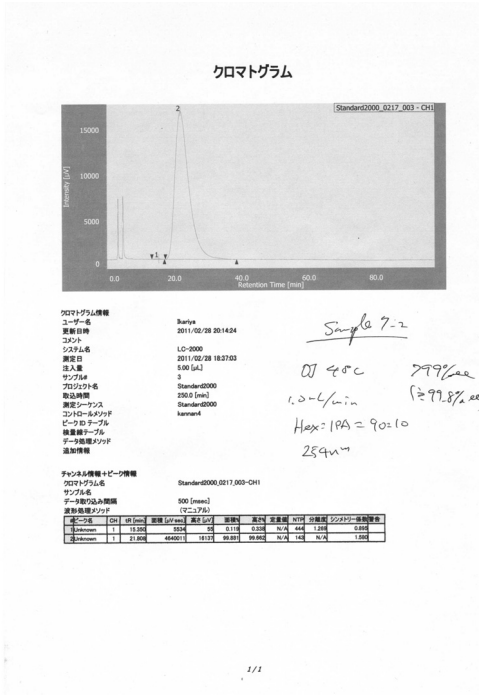
Sample from the reaction of **6b** with MAC



Racemic sample



Sample from the reaction of **6b** with MAC (repeated analysis).



Computational details

All computations were carried out using the hybrid Becke functional (B3)[1] for electron exchange and the correlation functional of Lee, Yang and Parr (LYP),[2] as implemented in the GAUSSIAN 09 software package.[3] For rhodium, the SDD basis set with the associated effective core potential was employed.[4] All other atoms were modeled at the 6-31G(d) level of theory.[5] Geometry optimizations were performed without any symmetry constraints (C_1 symmetry) in a corresponding solvent using CPCM model.

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(2) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

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Compound	*Electronic energy, a.u.*	*Relative electronic energy, kcal/mol*	*Energy, ZPPE corrected, a.u.*	*Relative ZPPE corrected energy, kcal/mol*	*Free energy at 298 K, a. u.*	*Relative Free energy at 298 K, kcal/mol*
4a	-3698.079472	0.0	-3697.031549	0.0	-3697.135005	0.0
4b	-3698.07686	1.6	-3697.029095	1.5	-3697.132591	1.5
4f	-3698.066062	8.4	-3697.018684	8.1	-3697.121954	8.2
4c	-3698.075708	2.4	-3697.027938	2.3	-3697.131708	2.1
4d	-3698.073148	4.0	-3697.025059	4.1	-3697.127596	4.6
4e	-3698.075339	2.6	-3697.027709	2.4	-3697.131262	2.3
5a C_2-symmetric conformation	-3185.176484	5.8	-3184.237917	5.7	-3184.330633	6.2
5a C_S-symmetric conformation	-3185.173114	7.9	-3184.23467	7.8	-3184.328002	7.9
6a C_2-symmetric conformation	-3185.183535	1.3	-3184.245067	1.2	-3184.339378	0.6
6a C_S-symmetric conformation	-3185.184034	1.0	-3184.2457	0.8	-3184.339584	0.6
***Trans*(P)-*trans*(H)-dihydride**	-3185.137533	30.2	-3184.199532	29.8	-3184.291285	30.9

Table S1. Absolute and relative energies for the optimized intermediates.

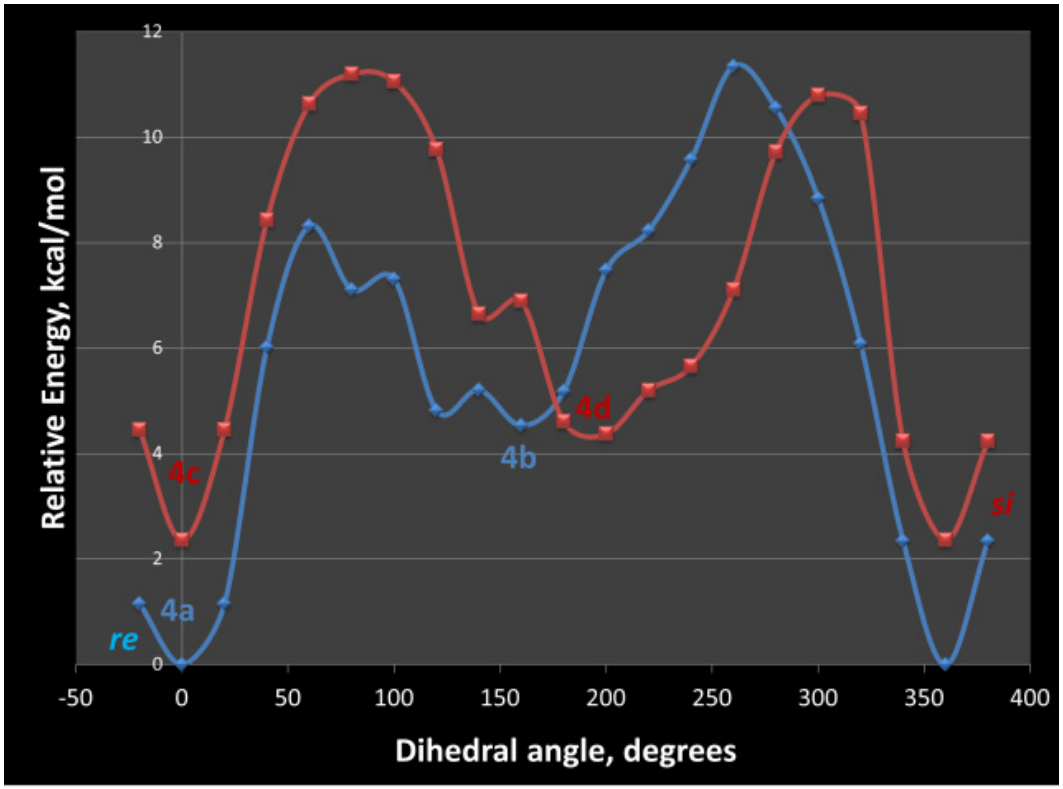

Figure S32. Scans of relative energy (not ZPVE corrected) *vs.* dihedral angle P–Rh–P–Ph for *re*-**4** and *si*-**4**. All points were optimized at the BLYP/SDD(Rh),6-31G* (C,H,N,P)/PCM(CD_2Cl_2) level of theory. The angle values are relative to the angle in the most stable conformation.

4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	−0.042463	1.266464	−0.890684
2	15	0	1.286421	0.389835	0.896521
3	15	0	−2.111916	0.842412	0.037575
4	6	0	−0.515141	2.685051	−2.527370
5	6	0	−0.394537	3.368636	−1.268059
6	6	0	3.039485	1.042914	0.697714
7	6	0	4.062350	0.243101	1.464981
8	6	0	4.606720	0.775517	2.664371
9	6	0	5.523717	0.068700	3.403761
10	6	0	5.927966	−1.231379	3.002549
11	6	0	6.846342	−1.992975	3.776375
12	6	0	7.203556	−3.267512	3.398661
13	6	0	6.646688	−3.836988	2.227439
14	6	0	5.762061	−3.121027	1.450566
15	6	0	5.382321	−1.792684	1.799276
16	6	0	4.460102	−1.016464	1.016510
17	6	0	1.608591	−1.461240	0.865226
18	6	0	2.499078	−1.815084	−0.303366
19	6	0	1.920160	−2.367591	−1.476077
20	6	0	2.688121	−2.647006	−2.580984
21	6	0	4.078419	−2.358968	−2.586413
22	6	0	4.880358	−2.596842	−3.736684
23	6	0	6.220809	−2.283164	−3.742018
24	6	0	6.815296	−1.710925	−2.590853
25	6	0	6.068123	−1.479461	−1.456192
26	6	0	4.681903	−1.804385	−1.407662
27	6	0	3.869425	−1.566480	−0.246461
28	6	0	0.912147	0.779816	2.659284
29	6	0	0.613892	−0.203783	3.615517
30	6	0	0.351839	0.152918	4.941381
31	6	0	0.391209	1.492236	5.331485
32	6	0	0.688546	2.479456	4.387710
33	6	0	0.940478	2.127749	3.060965
34	6	0	−2.168290	−0.501652	1.348875
35	6	0	−3.541202	−1.094425	1.548235
36	6	0	−4.299604	−0.716822	2.688127
37	6	0	−5.562300	−1.216036	2.896236
38	6	0	−6.154952	−2.098349	1.955513
39	6	0	−7.477322	−2.589968	2.134031
40	6	0	−8.059287	−3.411933	1.195791
41	6	0	−7.338981	−3.771181	0.030434
42	6	0	−6.051628	−3.320936	−0.166302
43	6	0	−5.408903	−2.484332	0.791306
44	6	0	−4.070050	−1.990323	0.619022
45	6	0	−3.252520	0.066660	−1.235137
46	6	0	−2.877579	−1.375320	−1.481655
47	6	0	−2.120797	−1.706728	−2.636872
48	6	0	−1.734886	−3.002996	−2.882831
49	6	0	−2.053813	−4.038491	−1.964900
50	6	0	−1.625629	−5.377119	−2.181573
51	6	0	−1.908507	−6.366856	−1.267793
52	6	0	−2.630003	−6.053186	−0.090124
53	6	0	−3.069493	−4.768063	0.143187
54	6	0	−2.811886	−3.721007	−0.787757
55	6	0	−3.251554	−2.368583	−0.577382
56	6	0	−3.074923	2.212267	0.808725
57	6	0	−4.304920	2.663574	0.307294
58	6	0	−4.993964	3.699009	0.944643
59	6	0	−4.466778	4.294500	2.091280
60	6	0	−3.243997	3.850117	2.601605
61	6	0	−2.551423	2.820336	1.963950
62	1	0	−1.359106	3.595804	−0.824746
63	1	0	3.028442	2.089544	1.015359
64	1	0	3.232392	1.029781	−0.376294
65	1	0	4.292730	1.763657	2.989383
66	1	0	5.941994	0.493259	4.312857
67	1	0	7.256091	−1.548873	4.680270
68	1	0	7.903533	−3.841671	3.999030
69	1	0	6.917455	−4.849573	1.941315
70	1	0	5.340422	−3.575665	0.561124
71	1	0	0.651983	−1.985758	0.799079
72	1	0	2.081825	−1.733467	1.813132
73	1	0	0.853866	−2.577022	−1.489717
74	1	0	2.236218	−3.082567	−3.468699
75	1	0	4.409728	−3.026904	−4.617470
76	1	0	6.822875	−2.465416	−4.627669

77	1	0	7.869841	−1.449815	−2.604204
78	1	0	6.536989	−1.035048	−0.585282
79	1	0	0.580712	−1.253185	3.342311
80	1	0	0.122784	−0.621547	5.667672
81	1	0	0.192490	1.766197	6.363516
82	1	0	0.722779	3.524616	4.681826
83	1	0	1.157150	2.910187	2.338585
84	1	0	−1.460118	−1.265809	1.017629
85	1	0	−1.782871	−0.073932	2.276869
86	1	0	−3.861338	−0.028964	3.405954
87	1	0	−6.127979	−0.929793	3.779171
88	1	0	−8.024579	−2.294781	3.025916
89	1	0	−9.071614	−3.778421	1.340297
90	1	0	−7.808039	−4.404918	−0.717057
91	1	0	−4.272717	0.138319	−0.848119
92	1	0	−3.198302	0.647938	−2.155166
93	1	0	−1.173013	−3.248410	−3.780548
94	1	0	−1.060911	−5.601813	−3.082993
95	1	0	−1.573110	−7.385325	−1.441405
96	1	0	−3.615556	−4.544229	1.052819
97	1	0	−4.740901	2.214909	−0.577416
98	1	0	−5.946085	4.034009	0.543244
99	1	0	−5.005410	5.097243	2.586465
100	1	0	−2.827219	4.302732	3.496843
101	1	0	−1.602207	2.490904	2.375842
102	6	0	0.656383	4.278609	−0.756899
103	6	0	0.401079	4.893650	0.489197
104	6	0	1.850045	4.622020	−1.422498
105	6	0	1.306961	5.784508	1.059326
106	1	0	−0.526242	4.666559	1.008090
107	6	0	2.752823	5.520627	−0.853606
108	1	0	2.068592	4.220208	−2.402068
109	6	0	2.494315	6.098571	0.391451
110	1	0	1.081323	6.241531	2.018718
111	1	0	3.660704	5.774829	−1.393422
112	1	0	3.202494	6.795873	0.829542
113	8	0	1.756965	1.246502	−2.071676
114	6	0	1.666989	1.836035	−3.184271
115	7	0	0.592788	2.578373	−3.452065
116	1	0	0.459587	2.950472	−4.385665
117	6	0	2.781699	1.747060	−4.185274
118	1	0	3.646110	2.304618	−3.807609
119	1	0	3.082032	0.701241	−4.291536
120	1	0	2.500065	2.150917	−5.159964
121	6	0	−1.788203	2.652890	−3.294859
122	8	0	−1.850895	2.284472	−4.458784
123	8	0	−2.853385	3.112745	−2.610998
124	6	0	−4.082845	3.212425	−3.362226
125	1	0	−4.796987	3.674790	−2.682663
126	1	0	−3.933289	3.836118	−4.245544
127	1	0	−4.429285	2.222379	−3.668476
128	1	0	−5.518079	−3.600415	−1.067822
129	1	0	−2.836188	−6.833319	0.637344
130	1	0	−1.864260	−0.919100	−3.340577

4b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.164965	0.996876	−0.650807
2	15	0	1.612005	−0.462425	0.565910
3	15	0	−1.609543	−0.474482	−0.684007
4	6	0	−0.646156	2.990831	−1.246210
5	6	0	−0.751642	2.781559	0.171660
6	6	0	3.015757	0.565159	1.276664
7	6	0	4.185055	−0.270380	1.733524
8	6	0	4.386699	−0.478634	3.124387
9	6	0	5.418998	−1.259253	3.584119
10	6	0	6.293693	−1.908541	2.674339
11	6	0	7.340740	−2.755164	3.131376
12	6	0	8.160616	−3.410508	2.240875
13	6	0	7.959262	−3.248758	0.848294
14	6	0	6.960607	−2.426299	0.373766
15	6	0	6.103416	−1.717532	1.264381
16	6	0	5.048566	−0.854581	0.806657
17	6	0	2.578857	−1.730090	−0.430123
18	6	0	3.654197	−1.063457	−1.255703
19	6	0	3.444974	−0.878357	−2.647795
20	6	0	4.378817	−0.238949	−3.426998
21	6	0	5.566770	0.281399	−2.849196
22	6	0	6.524869	0.983571	−3.631269
23	6	0	7.658673	1.511037	−3.055754
24	6	0	7.877313	1.361271	−1.664476
25	6	0	6.973743	0.676028	−0.881372
26	6	0	5.797324	0.101609	−1.443646
27	6	0	4.830556	−0.614614	−0.657037
28	6	0	0.990251	−1.401788	2.021630
29	6	0	0.907591	−2.803004	2.041530
30	6	0	0.404154	−3.467077	3.164265
31	6	0	−0.016274	−2.743311	4.280693
32	6	0	0.062582	−1.347269	4.271174
33	6	0	0.554379	−0.680768	3.148461
34	6	0	−3.130705	0.089079	−1.619813
35	6	0	−4.235019	−0.936572	−1.622600
36	6	0	−4.461927	−1.718436	−2.786408
37	6	0	−5.442330	−2.680134	−2.813163
38	6	0	−6.231820	−2.940386	−1.662263
39	6	0	−7.220534	−3.962307	−1.659019
40	6	0	−7.954225	−4.233494	−0.526286
41	6	0	−7.721349	−3.492450	0.657944
42	6	0	−6.778427	−2.487834	0.683915
43	6	0	−6.012473	−2.166284	−0.473476
44	6	0	−5.016393	−1.130063	−0.484725
45	6	0	−2.425599	−1.246760	0.823179
46	6	0	−3.529529	−0.372686	1.372946
47	6	0	−3.295861	0.372535	2.559335
48	6	0	−4.253610	1.214450	3.072228
49	6	0	−5.495536	1.384447	2.406589
50	6	0	−6.477864	2.291450	2.890608
51	6	0	−7.665012	2.473061	2.218082
52	6	0	−7.915839	1.753353	1.024267
53	6	0	−6.989901	0.856329	0.536906
54	6	0	−5.756716	0.630272	1.213586
55	6	0	−4.763133	−0.288167	0.727719
56	6	0	−1.010332	−1.886860	−1.705998
57	6	0	−0.942737	−3.210274	−1.244071
58	6	0	−0.452859	−4.224811	−2.072230
59	6	0	−0.026273	−3.931770	−3.368506
60	6	0	−0.085731	−2.615924	−3.837717
61	6	0	−0.568566	−1.599972	−3.011942
62	1	0	−1.753170	2.492899	0.474603
63	1	0	2.600214	1.158117	2.096084
64	1	0	3.291959	1.259072	0.480453
65	1	0	3.712879	0.000571	3.829295
66	1	0	5.570099	−1.399259	4.651461
67	1	0	7.475462	−2.881074	4.202889
68	1	0	8.955206	−4.057844	2.600938
69	1	0	8.596701	−3.781324	0.147911
70	1	0	6.816386	−2.320074	−0.695577
71	1	0	1.878759	−2.280540	−1.063716
72	1	0	3.019295	−2.432726	0.283407
73	1	0	2.532741	−1.263392	−3.095372
74	1	0	4.214472	−0.116956	−4.494732

75	1	0	6.339581	1.101240	−4.696181
76	1	0	8.382275	2.048328	−3.662211
77	1	0	8.764903	1.793150	−1.210490
78	1	0	7.153952	0.575690	0.183133
79	1	0	1.229971	−3.389625	1.187976
80	1	0	0.347537	−4.551768	3.163195
81	1	0	−0.402583	−3.261494	5.153488
82	1	0	−0.259957	−0.775943	5.136978
83	1	0	0.593393	0.405170	3.151385
84	1	0	−3.448303	1.014051	−1.137988
85	1	0	−2.810307	0.337846	−2.635704
86	1	0	−3.851582	−1.538803	−3.667164
87	1	0	−5.616026	−3.263482	−3.713782
88	1	0	−7.379519	−4.533219	−2.570528
89	1	0	−8.704242	−5.019273	−0.533781
90	1	0	−8.289587	−3.721172	1.555295
91	1	0	−2.830486	−2.209909	0.499127
92	1	0	−1.658754	−1.435377	1.575649
93	1	0	−4.066279	1.767252	3.989241
94	1	0	−6.267522	2.847493	3.800847
95	1	0	−8.406588	3.172248	2.593770
96	1	0	−7.195105	0.317744	−0.381554
97	1	0	−1.264690	−3.464680	−0.240101
98	1	0	−0.410752	−5.244615	−1.700838
99	1	0	0.349504	−4.722849	−4.010742
100	1	0	0.241888	−2.379604	−4.846052
101	1	0	−0.602451	−0.580250	−3.387864
102	6	0	−0.001863	3.388762	1.296384
103	6	0	−0.414520	3.027048	2.597515
104	6	0	1.037031	4.333115	1.179584
105	6	0	0.205160	3.550496	3.729245
106	1	0	−1.242394	2.333309	2.709742
107	6	0	1.652027	4.863384	2.314144
108	1	0	1.349552	4.688209	0.207244
109	6	0	1.251072	4.468215	3.592417
110	1	0	−0.135869	3.252397	4.716702
111	1	0	2.444597	5.596801	2.194983
112	1	0	1.736004	4.882725	4.471437
113	8	0	1.935353	2.087029	−1.204847
114	6	0	1.718586	3.173574	−1.808000
115	7	0	0.482391	3.671690	−1.845375
116	1	0	0.290758	4.483692	−2.421039
117	6	0	2.848011	3.933888	−2.439562
118	1	0	3.464923	4.378791	−1.650596
119	1	0	3.476500	3.236897	−2.999945
120	1	0	2.496095	4.728628	−3.100839
121	6	0	−1.841841	3.204371	−2.108933
122	8	0	−1.766536	3.442328	−3.305084
123	8	0	−3.007050	3.194669	−1.432690
124	6	0	−4.191454	3.447425	−2.219535
125	1	0	−5.021093	3.388032	−1.516313
126	1	0	−4.135872	4.440853	−2.669149
127	1	0	−4.298774	2.695719	−3.004959
128	1	0	−6.608021	−1.935761	1.601398
129	1	0	−8.846568	1.912128	0.486779
130	1	0	−2.348121	0.246886	3.074826

4f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.004183	−0.825614	−1.587088
2	15	0	−1.498244	0.942710	−0.854384
3	15	0	1.931934	0.201839	−0.835093
4	6	0	0.648405	−2.869794	−2.095955
5	6	0	0.310175	−2.777879	−0.702875
6	6	0	−1.891644	1.026480	0.982303
7	6	0	−3.057636	1.918266	1.342353
8	6	0	−2.803571	3.148915	2.007758
9	6	0	−3.819608	4.018426	2.317435
10	6	0	−5.156518	3.726109	1.942690
11	6	0	−6.213434	4.642848	2.195686
12	6	0	−7.502001	4.362372	1.801329
13	6	0	−7.783233	3.148091	1.129320
14	6	0	−6.782712	2.232834	0.883459
15	6	0	−5.439831	2.480657	1.289720
16	6	0	−4.368046	1.551717	1.040429
17	6	0	−3.247333	0.785231	−1.555643
18	6	0	−4.151152	−0.150182	−0.789067
19	6	0	−4.521397	−1.389569	−1.376970
20	6	0	−5.351834	−2.269207	−0.727770
21	6	0	−5.824359	−1.984123	0.579408
22	6	0	−6.630206	−2.911802	1.294893
23	6	0	−7.046518	−2.644052	2.579415
24	6	0	−6.665771	−1.431229	3.203527
25	6	0	−5.900332	−0.504517	2.529316
26	6	0	−5.463853	−0.738939	1.193353
27	6	0	−4.659268	0.203571	0.459751
28	6	0	−1.085296	2.651634	−1.411564
29	6	0	−1.246652	2.953187	−2.776770
30	6	0	−0.954402	4.227238	−3.262712
31	6	0	−0.490862	5.220923	−2.396125
32	6	0	−0.313363	4.928789	−1.043688
33	6	0	−0.605101	3.652497	−0.554894
34	6	0	3.530325	−0.774964	−0.679519
35	6	0	4.681133	0.078422	−0.204388
36	6	0	5.642744	0.529744	−1.147898
37	6	0	6.688996	1.332919	−0.764844
38	6	0	6.814707	1.763343	0.582045
39	6	0	7.864423	2.633222	0.986002
40	6	0	7.953873	3.078105	2.285571
41	6	0	6.986636	2.672255	3.237183
42	6	0	5.964229	1.820126	2.880035
43	6	0	5.849054	1.324986	1.549240
44	6	0	4.793334	0.441377	1.136345
45	6	0	2.024520	1.177805	0.767530
46	6	0	2.436601	0.309677	1.937173
47	6	0	1.456014	−0.135528	2.863196
48	6	0	1.791273	−0.941038	3.925235
49	6	0	3.128776	−1.378667	4.105896
50	6	0	3.486709	−2.247077	5.173460
51	6	0	4.780862	−2.692826	5.317732
52	6	0	5.772366	−2.290294	4.389880
53	6	0	5.459463	−1.440025	3.351612
54	6	0	4.135334	−0.943110	3.180575
55	6	0	3.771044	−0.057280	2.108523
56	6	0	2.350814	1.365898	−2.202841
57	6	0	2.565079	2.740723	−2.031371
58	6	0	2.903250	3.544079	−3.123389
59	6	0	3.030432	2.987605	−4.396942
60	6	0	2.814090	1.619166	−4.580548
61	6	0	2.473758	0.813868	−3.493638
62	1	0	1.181569	−2.678695	−0.062918
63	1	0	−0.992060	1.334766	1.518944
64	1	0	−2.077448	−0.017937	1.256060
65	1	0	−1.785493	3.390144	2.299198
66	1	0	−3.608153	4.947536	2.840317
67	1	0	−5.980218	5.577158	2.700377
68	1	0	−8.301670	5.071754	1.994513
69	1	0	−8.797435	2.937958	0.801216
70	1	0	−7.016205	1.312545	0.360334
71	1	0	−3.153530	0.463140	−2.593871
72	1	0	−3.647808	1.803687	−1.547511
73	1	0	−4.141859	−1.624770	−2.364796

74	1	0	−5.641316	−3.204180	−1.200489
75	1	0	−6.902864	−3.845156	0.808397
76	1	0	−7.657058	−3.362242	3.119406
77	1	0	−6.978079	−1.231033	4.224736
78	1	0	−5.612720	0.415096	3.026014
79	1	0	−1.606666	2.195883	−3.468159
80	1	0	−1.091854	4.443190	−4.318384
81	1	0	−0.269134	6.214764	−2.774109
82	1	0	0.047133	5.693052	−0.361060
83	1	0	−0.462393	3.456806	0.501189
84	1	0	3.343204	−1.613302	−0.004913
85	1	0	3.742965	−1.186406	−1.667145
86	1	0	5.545246	0.222726	−2.185551
87	1	0	7.425538	1.660999	−1.493836
88	1	0	8.592205	2.948355	0.242332
89	1	0	8.757391	3.746148	2.582356
90	1	0	7.049997	3.039534	4.257721
91	1	0	2.754150	1.978173	0.618394
92	1	0	1.055420	1.643779	0.944965
93	1	0	1.031284	−1.258398	4.634560
94	1	0	2.713204	−2.559333	5.870689
95	1	0	5.043444	−3.359013	6.134530
96	1	0	6.229248	−1.147907	2.646325
97	1	0	2.464444	3.202575	−1.056091
98	1	0	3.066748	4.607196	−2.973520
99	1	0	3.296442	3.615638	−5.242355
100	1	0	2.911543	1.176519	−5.567766
101	1	0	2.312738	−0.249402	−3.651780
102	6	0	−0.836159	−3.351831	0.041115
103	6	0	−0.954455	−3.004541	1.403969
104	6	0	−1.742490	−4.293064	−0.481821
105	6	0	−1.955273	−3.549543	2.203626
106	1	0	−0.239672	−2.307829	1.834011
107	6	0	−2.737979	−4.846577	0.324608
108	1	0	−1.656634	−4.622162	−1.509686
109	6	0	−2.856482	−4.473335	1.664813
110	1	0	−2.023847	−3.265309	3.249963
111	1	0	−3.418785	−5.580202	−0.097976
112	1	0	−3.636260	−4.903950	2.286107
113	8	0	−1.605232	−1.507507	−2.830541
114	6	0	−1.388270	−2.608246	−3.408580
115	7	0	−0.309744	−3.321164	−3.085396
116	1	0	−0.096267	−4.161345	−3.610783
117	6	0	−2.352550	−3.146203	−4.425551
118	1	0	−3.233696	−3.544240	−3.909386
119	1	0	−2.681357	−2.331697	−5.075346
120	1	0	−1.913718	−3.943647	−5.029314
121	6	0	2.020780	−3.220649	−2.571343
122	8	0	2.338051	−3.236248	−3.750623
123	8	0	2.846215	−3.598490	−1.579163
124	6	0	4.168278	−4.016040	−1.981430
125	1	0	4.679798	−4.280422	−1.057054
126	1	0	4.100168	−4.879857	−2.645908
127	1	0	4.692520	−3.204724	−2.491800
128	1	0	5.228272	1.525684	3.619805
129	1	0	6.788856	−2.658665	4.496513
130	1	0	0.425711	0.181676	2.737828

4c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	−0.042463	1.266464	−0.890684
2	15	0	1.286421	0.389835	0.896521
3	15	0	−2.111916	0.842412	0.037575
4	6	0	−0.515141	2.685051	−2.527370
5	6	0	−0.394537	3.368636	−1.268059
6	6	0	3.039485	1.042914	0.697714
7	6	0	4.062350	0.243101	1.464981
8	6	0	4.606720	0.775517	2.664371
9	6	0	5.523717	0.068700	3.403761
10	6	0	5.927966	−1.231379	3.002549
11	6	0	6.846342	−1.992975	3.776375
12	6	0	7.203556	−3.267512	3.398661
13	6	0	6.646688	−3.836988	2.227439
14	6	0	5.762061	−3.121027	1.450566
15	6	0	5.382321	−1.792684	1.799276
16	6	0	4.460102	−1.016464	1.016510
17	6	0	1.608591	−1.461240	0.865226
18	6	0	2.499078	−1.815084	−0.303366
19	6	0	1.920160	−2.367591	−1.476077
20	6	0	2.688121	−2.647006	−2.580984
21	6	0	4.078419	−2.358968	−2.586413
22	6	0	4.880358	−2.596842	−3.736684
23	6	0	6.220809	−2.283164	−3.742018
24	6	0	6.815296	−1.710925	−2.590853
25	6	0	6.068123	−1.479461	−1.456192
26	6	0	4.681903	−1.804385	−1.407662
27	6	0	3.869425	−1.566480	−0.246461
28	6	0	0.912147	0.779816	2.659284
29	6	0	0.613892	−0.203783	3.615517
30	6	0	0.351839	0.152918	4.941381
31	6	0	0.391209	1.492236	5.331485
32	6	0	0.688546	2.479456	4.387710
33	6	0	0.940478	2.127749	3.060965
34	6	0	−2.168290	−0.501652	1.348875
35	6	0	−3.541202	−1.094425	1.548235
36	6	0	−4.299604	−0.716822	2.688127
37	6	0	−5.562300	−1.216036	2.896236
38	6	0	−6.154952	−2.098349	1.955513
39	6	0	−7.477322	−2.589968	2.134031
40	6	0	−8.059287	−3.411933	1.195791
41	6	0	−7.338981	−3.771181	0.030434
42	6	0	−6.051628	−3.320936	−0.166302
43	6	0	−5.408903	−2.484332	0.791306
44	6	0	−4.070050	−1.990323	0.619022
45	6	0	−3.252520	0.066660	−1.235137
46	6	0	−2.877579	−1.375320	−1.481655
47	6	0	−2.120797	−1.706728	−2.636872
48	6	0	−1.734886	−3.002996	−2.882831
49	6	0	−2.053813	−4.038491	−1.964900
50	6	0	−1.625629	−5.377119	−2.181573
51	6	0	−1.908507	−6.366856	−1.267793
52	6	0	−2.630003	−6.053186	−0.090124
53	6	0	−3.069493	−4.768063	0.143187
54	6	0	−2.811886	−3.721007	−0.787757
55	6	0	−3.251554	−2.368583	−0.577382
56	6	0	−3.074923	2.212267	0.808725
57	6	0	−4.304920	2.663574	0.307294
58	6	0	−4.993964	3.699009	0.944643
59	6	0	−4.466778	4.294500	2.091280
60	6	0	−3.243997	3.850117	2.601605
61	6	0	−2.551423	2.820336	1.963950
62	1	0	−1.359106	3.595804	−0.824746
63	1	0	3.028442	2.089544	1.015359
64	1	0	3.232392	1.029781	−0.376294
65	1	0	4.292730	1.763657	2.989383
66	1	0	5.941994	0.493259	4.312857
67	1	0	7.256091	−1.548873	4.680270
68	1	0	7.903533	−3.841671	3.999030
69	1	0	6.917455	−4.849573	1.941315
70	1	0	5.340422	−3.575665	0.561124
71	1	0	0.651983	−1.985758	0.799079
72	1	0	2.081825	−1.733467	1.813132
73	1	0	0.853866	−2.577022	−1.489717
74	1	0	2.236218	−3.082567	−3.468699
75	1	0	4.409728	−3.026904	−4.617470
76	1	0	6.822875	−2.465416	−4.627669

77	1	0	7.869841	−1.449815	−2.604204
78	1	0	6.536989	−1.035048	−0.585282
79	1	0	0.580712	−1.253185	3.342311
80	1	0	0.122784	−0.621547	5.667672
81	1	0	0.192490	1.766197	6.363516
82	1	0	0.722779	3.524616	4.681826
83	1	0	1.157150	2.910187	2.338585
84	1	0	−1.460118	−1.265809	1.017629
85	1	0	−1.782871	−0.073932	2.276869
86	1	0	−3.861338	−0.028964	3.405954
87	1	0	−6.127979	−0.929793	3.779171
88	1	0	−8.024579	−2.294781	3.025916
89	1	0	−9.071614	−3.778421	1.340297
90	1	0	−7.808039	−4.404918	−0.717057
91	1	0	−4.272717	0.138319	−0.848119
92	1	0	−3.198302	0.647938	−2.155166
93	1	0	−1.173013	−3.248410	−3.780548
94	1	0	−1.060911	−5.601813	−3.082993
95	1	0	−1.573110	−7.385325	−1.441405
96	1	0	−3.615556	−4.544229	1.052819
97	1	0	−4.740901	2.214909	−0.577416
98	1	0	−5.946085	4.034009	0.543244
99	1	0	−5.005410	5.097243	2.586465
100	1	0	−2.827219	4.302732	3.496843
101	1	0	−1.602207	2.490904	2.375842
102	6	0	0.656383	4.278609	−0.756899
103	6	0	0.401079	4.893650	0.489197
104	6	0	1.850045	4.622020	−1.422498
105	6	0	1.306961	5.784508	1.059326
106	1	0	−0.526242	4.666559	1.008090
107	6	0	2.752823	5.520627	−0.853606
108	1	0	2.068592	4.220208	−2.402068
109	6	0	2.494315	6.098571	0.391451
110	1	0	1.081323	6.241531	2.018718
111	1	0	3.660704	5.774829	−1.393422
112	1	0	3.202494	6.795873	0.829542
113	8	0	1.756965	1.246502	−2.071676
114	6	0	1.666989	1.836035	−3.184271
115	7	0	0.592788	2.578373	−3.452065
116	1	0	0.459587	2.950472	−4.385665
117	6	0	2.781699	1.747060	−4.185274
118	1	0	3.646110	2.304618	−3.807609
119	1	0	3.082032	0.701241	−4.291536
120	1	0	2.500065	2.150917	−5.159964
121	6	0	−1.788203	2.652890	−3.294859
122	8	0	−1.850895	2.284472	−4.458784
123	8	0	−2.853385	3.112745	−2.610998
124	6	0	−4.082845	3.212425	−3.362226
125	1	0	−4.796987	3.674790	−2.682663
126	1	0	−3.933289	3.836118	−4.245544
127	1	0	−4.429285	2.222379	−3.668476
128	1	0	−5.518079	−3.600415	−1.067822
129	1	0	−2.836188	−6.833319	0.637344
130	1	0	−1.864260	−0.919100	−3.340577

4d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.160529	0.989248	−0.822862
2	15	0	−1.493744	−0.760130	−0.713661
3	15	0	1.549860	0.030993	0.752226
4	6	0	0.119247	2.978503	0.045775
5	6	0	0.894248	3.035264	−1.164218
6	6	0	−3.011712	−0.249353	−1.698904
7	6	0	−4.123537	−1.263617	−1.607534
8	6	0	−4.352059	−2.138674	−2.703686
9	6	0	−5.325696	−3.105932	−2.649598
10	6	0	−6.106621	−3.280212	−1.477110
11	6	0	−7.084843	−4.308154	−1.385253
12	6	0	−7.807734	−4.495848	−0.228960
13	6	0	−7.574356	−3.660649	0.890823
14	6	0	−6.642892	−2.647025	0.828871
15	6	0	−5.888383	−2.410426	−0.356313
16	6	0	−4.902626	−1.368682	−0.455765
17	6	0	−2.320713	−1.345535	0.866577
18	6	0	−3.423715	−0.412758	1.314666
19	6	0	−3.187402	0.467575	2.403411
20	6	0	−4.161311	1.331799	2.842350
21	6	0	−5.420267	1.393478	2.190553
22	6	0	−6.423543	2.313300	2.602650
23	6	0	−7.626457	2.392494	1.938395
24	6	0	−7.871831	1.554135	0.823406
25	6	0	−6.924801	0.643604	0.407490
26	6	0	−5.675682	0.519115	1.081814
27	6	0	−4.663382	−0.417871	0.675876
28	6	0	−0.938668	−2.299680	−1.562792
29	6	0	−0.813440	−3.535944	−0.910408
30	6	0	−0.342557	−4.656553	−1.601645
31	6	0	0.006562	−4.557950	−2.949050
32	6	0	−0.109399	−3.329573	−3.606908
33	6	0	−0.570688	−2.207242	−2.918573
34	6	0	3.098640	0.971300	1.245563
35	6	0	4.143704	0.085625	1.876923
36	6	0	4.321992	0.109043	3.285573
37	6	0	5.250958	−0.698626	3.894970
38	6	0	6.034396	−1.603316	3.131337
39	6	0	6.968858	−2.477658	3.750941
40	6	0	7.696415	−3.378366	3.006485
41	6	0	7.511983	−3.444918	1.603731
42	6	0	6.622647	−2.603242	0.971651
43	6	0	5.864856	−1.646282	1.706422
44	6	0	4.923509	−0.756358	1.084550
45	6	0	2.345997	−1.498658	0.005272
46	6	0	3.481896	−1.121930	−0.917813
47	6	0	3.268006	−1.132619	−2.321957
48	6	0	4.263300	−0.759557	−3.193221
49	6	0	5.523975	−0.323912	−2.707058
50	6	0	6.550210	0.105962	−3.592392
51	6	0	7.756154	0.561410	−3.109548
52	6	0	7.981759	0.611475	−1.712367
53	6	0	7.011991	0.189867	−0.828418
54	6	0	5.758735	−0.305316	−1.290996
55	6	0	4.720946	−0.747529	−0.399611
56	6	0	0.905689	−0.506975	2.395626
57	6	0	0.778489	−1.856174	2.762058
58	6	0	0.305895	−2.205366	4.030666
59	6	0	−0.040180	−1.214560	4.950238
60	6	0	0.080920	0.132098	4.595420
61	6	0	0.543940	0.483167	3.326778
62	1	0	−2.691507	−0.088441	−2.729198
63	1	0	−3.310795	0.723095	−1.297875
64	1	0	−3.745736	−2.027828	−3.598379
65	1	0	−5.498933	−3.760318	−3.500139
66	1	0	−7.243728	−4.951597	−2.247140
67	1	0	−8.549160	−5.287470	−0.168107
68	1	0	−8.133148	−3.823464	1.808279
69	1	0	−6.471682	−2.021787	1.697982
70	1	0	−1.560728	−1.454816	1.641104
71	1	0	−2.728743	−2.337511	0.651681
72	1	0	−2.224029	0.436190	2.902944
73	1	0	−3.972486	1.988488	3.687658
74	1	0	−6.216781	2.961028	3.451066
75	1	0	−8.384573	3.101371	2.259129

76	1	0	−8.814795	1.632621	0.289417
77	1	0	−7.126165	0.014116	−0.451920
78	1	0	−1.076148	−3.641017	0.137266
79	1	0	−0.254142	−5.606624	−1.082549
80	1	0	0.368208	−5.431018	−3.484347
81	1	0	0.160725	−3.243615	−4.655555
82	1	0	−0.644913	−1.256355	−3.440009
83	1	0	3.474972	1.416702	0.325017
84	1	0	2.809542	1.788383	1.910330
85	1	0	3.715480	0.785809	3.880898
86	1	0	5.387863	−0.663266	4.972767
87	1	0	7.090982	−2.425825	4.830017
88	1	0	8.404774	−4.044428	3.490849
89	1	0	8.075062	−4.169201	1.021696
90	1	0	2.712352	−2.108650	0.835463
91	1	0	1.579059	−2.067996	−0.523242
92	1	0	4.093020	−0.786415	−4.266562
93	1	0	6.358908	0.075725	−4.662216
94	1	0	8.531823	0.891212	−3.794767
95	1	0	7.199691	0.239813	0.238303
96	1	0	1.039690	−2.647058	2.066995
97	1	0	0.214277	−3.254354	4.296852
98	1	0	−0.401690	−1.487870	5.937169
99	1	0	−0.185190	0.910640	5.304513
100	1	0	0.624645	1.535801	3.070610
101	1	0	0.750570	2.986932	0.928913
102	6	0	−1.200503	3.592694	0.330040
103	6	0	−1.318601	4.291349	1.549935
104	6	0	−2.320211	3.567577	−0.524068
105	6	0	−2.489251	4.969384	1.885357
106	1	0	−0.472077	4.319766	2.231396
107	6	0	−3.492152	4.243416	−0.185695
108	1	0	−2.296005	2.990866	−1.438885
109	6	0	−3.581512	4.952691	1.014903
110	1	0	−2.546862	5.509319	2.826248
111	1	0	−4.342581	4.207124	−0.860700
112	1	0	−4.497136	5.476333	1.273804
113	6	0	2.340973	3.407626	−1.181049
114	8	0	3.002334	3.464658	−2.205491
115	8	0	2.823947	3.747559	0.028379
116	6	0	4.210988	4.147076	0.061782
117	1	0	4.414661	4.391154	1.103492
118	1	0	4.855443	3.331120	−0.274272
119	1	0	4.364725	5.019563	−0.576298
120	8	0	−0.812493	1.530364	−2.667462
121	6	0	−0.495407	2.664789	−3.126945
122	7	0	0.296675	3.459684	−2.413162
123	1	0	0.604183	4.338496	−2.814085
124	6	0	−1.033682	3.129919	−4.448511
125	1	0	−2.116587	3.270958	−4.366747
126	1	0	−0.576632	4.064655	−4.779033
127	1	0	−0.854903	2.352104	−5.196247
128	1	0	6.488675	−2.671863	−0.102210
129	1	0	8.927967	0.988399	−1.334144
130	1	0	2.305581	−1.462721	−2.703278

4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.246288	−1.992824	−0.321240
2	15	0	−1.336620	−0.804541	1.045724
3	15	0	2.133424	−0.727817	0.091644
4	6	0	0.402486	−2.118910	−2.461787
5	6	0	0.966465	−3.329153	−1.928271
6	6	0	−3.068998	−1.321725	0.534051
7	6	0	−4.152691	−0.637368	1.327380
8	6	0	−4.820517	−1.364952	2.349366
9	6	0	−5.791438	−0.776816	3.122189
10	6	0	−6.127556	0.590511	2.942861
11	6	0	−7.095315	1.227888	3.766917
12	6	0	−7.383727	2.565206	3.615081
13	6	0	−6.705206	3.323806	2.630298
14	6	0	−5.771615	2.732160	1.807330
15	6	0	−5.459843	1.346573	1.921615
16	6	0	−4.486169	0.695372	1.086934
17	6	0	−1.612919	1.047202	1.226139
18	6	0	−2.402000	1.628650	0.077444
19	6	0	−1.723151	2.378409	−0.918825
20	6	0	−2.401122	2.922488	−1.982751
21	6	0	−3.796620	2.711811	−2.133779
22	6	0	−4.505395	3.223081	−3.256123
23	6	0	−5.850335	2.976072	−3.415307
24	6	0	−6.542586	2.199888	−2.453872
25	6	0	−5.887316	1.703440	−1.347930
26	6	0	−4.499775	1.950924	−1.140370
27	6	0	−3.782022	1.444281	−0.002104
28	6	0	−1.156565	−1.406283	2.781144
29	6	0	−0.851021	−0.556188	3.856053
30	6	0	−0.658774	−1.077464	5.138912
31	6	0	−0.769908	−2.449974	5.365523
32	6	0	−1.069997	−3.305502	4.301414
33	6	0	−1.255107	−2.791167	3.017873
34	6	0	2.046745	0.645487	1.366540
35	6	0	3.369456	1.343173	1.559200
36	6	0	4.156936	1.033118	2.699946
37	6	0	5.384832	1.617065	2.892983
38	6	0	5.914561	2.519462	1.933812
39	6	0	7.204514	3.095621	2.094843
40	6	0	7.727775	3.937641	1.139928
41	6	0	6.978716	4.232745	−0.025109
42	6	0	5.720488	3.700198	−0.204792
43	6	0	5.137799	2.840024	0.770012
44	6	0	3.830466	2.260507	0.615613
45	6	0	3.105783	0.157554	−1.249822
46	6	0	2.642511	1.578047	−1.473968
47	6	0	1.882047	1.883803	−2.633785
48	6	0	1.447682	3.163460	−2.883417
49	6	0	1.711683	4.208314	−1.959462
50	6	0	1.225337	5.527494	−2.174203
51	6	0	1.455208	6.524277	−1.253438
52	6	0	2.180312	6.237557	−0.071034
53	6	0	2.676784	4.973056	0.159448
54	6	0	2.474407	3.919561	−0.778188
55	6	0	2.976680	2.588060	−0.571010
56	6	0	3.306314	−1.921449	0.878044
57	6	0	4.623964	−2.131347	0.444704
58	6	0	5.446538	−3.057191	1.093033
59	6	0	4.967013	−3.785468	2.182350
60	6	0	3.657103	−3.583972	2.625324
61	6	0	2.832468	−2.663269	1.978217
62	1	0	−3.118269	−2.407154	0.630577
63	1	0	−3.133732	−1.089967	−0.533950
64	1	0	−4.557434	−2.407145	2.507936
65	1	0	−6.303896	−1.348789	3.891514
66	1	0	−7.597473	0.636826	4.528856
67	1	0	−8.121550	3.043248	4.253147
68	1	0	−6.920684	4.383547	2.525454
69	1	0	−5.257066	3.330895	1.064398
70	1	0	−0.653938	1.554255	1.333163
71	1	0	−2.161234	1.174574	2.164472
72	1	0	−0.652945	2.535995	−0.823678
73	1	0	−1.871588	3.510518	−2.727758
74	1	0	−3.959177	3.807547	−3.992448
75	1	0	−6.381165	3.366957	−4.278664
76	1	0	−7.599904	1.991736	−2.591995

77	1	0	−6.431234	1.105391	−0.625442
78	1	0	−0.761239	0.515340	3.710245
79	1	0	−0.426447	−0.405124	5.959863
80	1	0	−0.624095	−2.851671	6.364079
81	1	0	−1.159068	−4.375152	4.469227
82	1	0	−1.477036	−3.468230	2.197811
83	1	0	1.288700	1.342690	1.004742
84	1	0	1.685792	0.206898	2.301144
85	1	0	3.769286	0.327997	3.429993
86	1	0	5.972619	1.382473	3.776701
87	1	0	7.775126	2.849194	2.986864
88	1	0	8.716134	4.368799	1.271245
89	1	0	7.402140	4.882477	−0.785981
90	1	0	4.149030	0.158665	−0.922923
91	1	0	3.048261	−0.433139	−2.164213
92	1	0	0.887114	3.387014	−3.787505
93	1	0	0.659184	5.731002	−3.079780
94	1	0	1.075308	7.527346	−1.424974
95	1	0	3.224030	4.770084	1.073113
96	1	0	5.029715	−1.579555	−0.395268
97	1	0	6.465047	−3.202364	0.744417
98	1	0	5.609221	−4.502878	2.684864
99	1	0	3.274663	−4.141825	3.475303
100	1	0	1.817713	−2.522344	2.341393
101	1	0	1.144140	−1.384473	−2.760096
102	6	0	−0.878505	−1.970630	−3.206206
103	6	0	−1.460544	−0.690966	−3.297834
104	6	0	−1.486632	−3.028178	−3.907337
105	6	0	−2.625827	−0.482588	−4.033084
106	1	0	−0.996192	0.143315	−2.780447
107	6	0	−2.650597	−2.816218	−4.648775
108	1	0	−1.039497	−4.015145	−3.899792
109	6	0	−3.230708	−1.547773	−4.707496
110	1	0	−3.059506	0.511780	−4.081180
111	1	0	−3.097559	−3.646217	−5.189005
112	1	0	−4.137664	−1.386698	−5.283272
113	6	0	2.386920	−3.725939	−2.128658
114	8	0	2.785479	−4.864003	−1.934360
115	8	0	3.168793	−2.743210	−2.610663
116	6	0	4.516623	−3.131565	−2.958626
117	1	0	4.999265	−2.217722	−3.302777
118	1	0	5.033849	−3.539119	−2.088783
119	1	0	4.493240	−3.876698	−3.756707
120	8	0	−1.240996	−3.556821	−0.338271
121	6	0	−0.914707	−4.571463	−1.017822
122	7	0	0.161229	−4.524212	−1.800547
123	1	0	0.506804	−5.368561	−2.242475
124	6	0	−1.752685	−5.815573	−0.980343
125	1	0	−2.699603	−5.619043	−1.495478
126	1	0	−1.260620	−6.663312	−1.461944
127	1	0	−1.981929	−6.064682	0.059021
128	1	0	5.164747	3.931258	−1.106484
129	1	0	2.343737	7.022205	0.662393
130	1	0	1.664717	1.091816	−3.345427

5a C_2-symmetric conformation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.113742	−0.064842	1.644532
2	15	0	1.676536	−0.732832	0.154040
3	15	0	−1.573897	0.856506	0.070925
4	6	0	3.139942	−1.599712	0.939891
5	6	0	4.299040	−1.773170	−0.008797
6	6	0	4.554560	−3.051798	−0.572882
7	6	0	5.577269	−3.240603	−1.470106
8	6	0	6.386326	−2.149728	−1.882848
9	6	0	7.421041	−2.318145	−2.843787
10	6	0	8.176441	−1.247373	−3.265449
11	6	0	7.919961	0.044254	−2.743941
12	6	0	6.931902	0.238156	−1.803028
13	6	0	6.141515	−0.848374	−1.328877
14	6	0	5.098741	−0.683518	−0.352799
15	6	0	2.544451	0.625867	−0.802492
16	6	0	3.615270	1.292815	0.028993
17	6	0	3.365103	2.579006	0.578561
18	6	0	4.296720	3.206628	1.370091
19	6	0	5.524047	2.567264	1.686556
20	6	0	6.479886	3.180791	2.542531
21	6	0	7.651596	2.537226	2.871014
22	6	0	7.912632	1.243365	2.357199
23	6	0	7.012506	0.627712	1.514720
24	6	0	5.796792	1.268846	1.138864
25	6	0	4.831333	0.653466	0.268909
26	6	0	1.091995	−1.905654	−1.140718
27	6	0	0.879175	−1.496906	−2.467843
28	6	0	0.404506	−2.401379	−3.421695
29	6	0	0.136608	−3.724252	−3.064949
30	6	0	0.343383	−4.141432	−1.747195
31	6	0	0.813299	−3.238748	−0.791994
32	6	0	−3.041617	1.563133	1.013970
33	6	0	−4.248364	1.845147	0.157443
34	6	0	−4.570746	3.189397	−0.170893
35	6	0	−5.647515	3.487575	−0.970042
36	6	0	−6.451487	2.452877	−1.515614
37	6	0	−7.546013	2.742039	−2.376295
38	6	0	−8.296343	1.730613	−2.932083
39	6	0	−7.974316	0.380150	−2.651723
40	6	0	−6.926342	0.067293	−1.813194
41	6	0	−6.138170	1.086809	−1.205097
42	6	0	−5.034170	0.801036	−0.329526
43	6	0	−2.466809	−0.252875	−1.154849
44	6	0	−3.459512	−1.131495	−0.431454
45	6	0	−3.128477	−2.492007	−0.174647
46	6	0	−3.972160	−3.305755	0.548751
47	6	0	−5.186971	−2.796151	1.078238
48	6	0	−6.048353	−3.607957	1.865730
49	6	0	−7.213732	−3.097326	2.391399
50	6	0	−7.561499	−1.745419	2.152349
51	6	0	−6.752888	−0.936294	1.383528
52	6	0	−5.547057	−1.432567	0.810688
53	6	0	−4.674477	−0.613397	0.013782
54	6	0	−0.988701	2.273977	−0.952541
55	6	0	−0.902823	2.217512	−2.352390
56	6	0	−0.405862	3.304887	−3.078347
57	6	0	0.004970	4.463374	−2.418280
58	6	0	−0.074806	4.530327	−1.023728
59	6	0	−0.558652	3.442259	−0.296758
60	1	0	2.788215	−2.557268	1.334225
61	1	0	3.404503	−0.977611	1.799475
62	1	0	3.930452	−3.890445	−0.277143
63	1	0	5.770463	−4.226689	−1.884674
64	1	0	7.598430	−3.312488	−3.246171
65	1	0	8.961903	−1.386808	−4.002817
66	1	0	8.505812	0.890440	−3.092121
67	1	0	6.744611	1.234978	−1.419861
68	1	0	1.789159	1.346838	−1.124365
69	1	0	2.978021	0.162060	−1.693373
70	1	0	2.425342	3.072638	0.347114
71	1	0	4.099242	4.197433	1.771408
72	1	0	6.261114	4.168612	2.940659
73	1	0	8.372672	3.013210	3.529477
74	1	0	8.830047	0.730740	2.632911
75	1	0	7.225080	−0.365781	1.136114
76	1	0	1.078973	−0.474199	−2.770730

77	1	0	0.249510	−2.068730	−4.443948
78	1	0	−0.228529	−4.426792	−3.808309
79	1	0	0.143240	−5.169961	−1.461155
80	1	0	0.969791	−3.586163	0.224584
81	1	0	−3.261478	0.833135	1.797268
82	1	0	−2.690082	2.465769	1.521387
83	1	0	−3.953977	3.989104	0.229949
84	1	0	−5.889655	4.521281	−1.203624
85	1	0	−7.773536	3.782763	−2.593882
86	1	0	−9.127916	1.962964	−3.591309
87	1	0	−8.557250	−0.416650	−3.105410
88	1	0	−2.972957	0.384861	−1.885829
89	1	0	−1.721294	−0.853991	−1.681484
90	1	0	−3.716406	−4.348121	0.720986
91	1	0	−5.763481	−4.640630	2.050571
92	1	0	−7.863681	−3.724086	2.995160
93	1	0	−7.030645	0.098232	1.215771
94	1	0	−1.218108	1.330152	−2.891047
95	1	0	−0.346700	3.242655	−4.161284
96	1	0	0.386016	5.308610	−2.984105
97	1	0	0.242112	5.428150	−0.500604
98	1	0	−0.598154	3.505547	0.787538
99	1	0	−6.689883	−0.972485	−1.616931
100	1	0	−8.473855	−1.341874	2.582563
101	1	0	−2.210092	−2.896831	−0.593892
102	1	0	1.205670	−0.466382	2.724763
103	1	0	0.884982	1.266092	1.574324
104	8	0	−1.138153	−1.925406	2.240315
105	8	0	−1.186906	0.583804	3.328666
106	6	0	−0.636413	−3.094122	2.919856
107	1	0	−1.456518	−3.607567	3.430389
108	1	0	−0.149800	−3.778902	2.219156
109	1	0	0.090896	−2.740087	3.650061
110	6	0	−0.634404	1.237467	4.491176
111	1	0	−0.255324	2.201455	4.152271
112	1	0	−1.425305	1.390493	5.230847
113	1	0	0.182466	0.649692	4.919043
114	1	0	−1.551939	−0.284947	3.581734
115	1	0	−1.823638	−2.197482	1.599763

5a *C*$_S$-symmetric conformation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.151324	−1.424938	−1.812612
2	15	0	−1.365528	−1.221305	0.127345
3	15	0	2.156994	−1.005851	−0.881525
4	6	0	−3.132532	−1.784605	−0.224116
5	6	0	−4.130679	−1.318602	0.805734
6	6	0	−4.625510	−2.242050	1.764863
7	6	0	−5.510785	−1.847135	2.738379
8	6	0	−5.928464	−0.493567	2.829776
9	6	0	−6.811808	−0.058925	3.856074
10	6	0	−7.180275	1.263360	3.959737
11	6	0	−6.670764	2.210864	3.038251
12	6	0	−5.822064	1.819486	2.025606
13	6	0	−5.432174	0.457236	1.875594
14	6	0	−4.545484	0.012557	0.835841
15	6	0	−1.702893	0.526348	0.722968
16	6	0	−2.644904	1.234531	−0.224083
17	6	0	−2.121322	2.153816	−1.172014
18	6	0	−2.940964	2.779627	−2.081159
19	6	0	−4.332147	2.498619	−2.113702
20	6	0	−5.188078	3.103092	−3.075302
21	6	0	−6.529567	2.797630	−3.119626
22	6	0	−7.070845	1.865543	−2.200463
23	6	0	−6.270293	1.271999	−1.248707
24	6	0	−4.880604	1.574281	−1.161903
25	6	0	−4.013346	0.968096	−0.189130
26	6	0	−0.943093	−2.175910	1.649160
27	6	0	−0.657353	−1.576082	2.885680
28	6	0	−0.309852	−2.358879	3.990840
29	6	0	−0.248198	−3.748548	3.878627
30	6	0	−0.528660	−4.356703	2.651453
31	6	0	−0.865935	−3.577671	1.544050
32	6	0	2.218282	−0.292513	0.847929
33	6	0	3.594364	0.187058	1.241411
34	6	0	4.370888	−0.595193	2.137717
35	6	0	5.638451	−0.209611	2.499706
36	6	0	6.218258	0.967224	1.957636
37	6	0	7.545208	1.357365	2.287982
38	6	0	8.113110	2.479154	1.727633
39	6	0	7.373083	3.256220	0.803209
40	6	0	6.080837	2.911125	0.471533
41	6	0	5.452957	1.767684	1.044519
42	6	0	4.109236	1.373170	0.718985
43	6	0	3.232136	0.225790	−1.795985
44	6	0	2.870671	1.646987	−1.432518
45	6	0	2.100100	2.420654	−2.341443
46	6	0	1.720191	3.705742	−2.035829
47	6	0	2.059868	4.280812	−0.782919
48	6	0	1.636691	5.592129	−0.430478
49	6	0	1.939014	6.125786	0.801818
50	6	0	2.675947	5.361231	1.739127
51	6	0	3.111801	4.092817	1.422757
52	6	0	2.834214	3.513710	0.150993
53	6	0	3.268580	2.191890	−0.211975
54	6	0	3.157183	−2.547753	−0.804838
55	6	0	2.924276	−3.487251	0.217538
56	6	0	3.623551	−4.696902	0.240298
57	6	0	4.558852	−4.985524	−0.756475
58	6	0	4.790078	−4.062323	−1.778569
59	6	0	4.091731	−2.853178	−1.807616
60	1	0	−3.117694	−2.876081	−0.299614
61	1	0	−3.393337	−1.383056	−1.208552
62	1	0	−4.299462	−3.277205	1.713774
63	1	0	−5.892217	−2.566095	3.458961
64	1	0	−7.184527	−0.794022	4.565192
65	1	0	−7.852493	1.585051	4.750144
66	1	0	−6.949639	3.256653	3.133560
67	1	0	−5.435899	2.559164	1.333165
68	1	0	−0.749074	1.055536	0.790485
69	1	0	−2.135877	0.471880	1.725733
70	1	0	−1.056158	2.367952	−1.164156
71	1	0	−2.529835	3.491812	−2.792155
72	1	0	−4.757764	3.807714	−3.782754
73	1	0	−7.173341	3.261785	−3.861382
74	1	0	−8.126792	1.614367	−2.249123
75	1	0	−6.699131	0.555689	−0.556815
76	1	0	−0.697286	−0.498086	3.001794

77	1	0	−0.091547	−1.877106	4.939684
78	1	0	0.018082	−4.354629	4.739768
79	1	0	−0.482205	−5.437692	2.553907
80	1	0	−1.063150	−4.063847	0.592370
81	1	0	1.497258	0.530323	0.845257
82	1	0	1.843146	−1.046373	1.544004
83	1	0	3.943450	−1.506482	2.546244
84	1	0	6.217741	−0.809721	3.196676
85	1	0	8.107059	0.744261	2.988320
86	1	0	9.129086	2.765774	1.983977
87	1	0	7.830574	4.130730	0.348916
88	1	0	4.269568	0.004600	−1.527350
89	1	0	3.105779	0.048405	−2.865702
90	1	0	1.146023	4.293419	−2.747543
91	1	0	1.059401	6.162969	−1.153648
92	1	0	1.606688	7.126650	1.062314
93	1	0	3.668619	3.518384	2.154573
94	1	0	2.203672	−3.281812	1.004791
95	1	0	3.437725	−5.408186	1.039625
96	1	0	5.103541	−5.924787	−0.736712
97	1	0	5.514858	−4.280552	−2.557439
98	1	0	4.282364	−2.154255	−2.615818
99	1	0	5.531560	3.513807	−0.242986
100	1	0	2.896566	5.778149	2.717851
101	1	0	1.824266	1.984320	−3.297423
102	1	0	0.083685	0.105836	−1.999240
103	8	0	0.203915	−3.740910	−1.699780
104	6	0	0.352619	−4.487856	−2.926678
105	1	0	1.312169	−4.266166	−3.404078
106	1	0	0.272608	−5.558857	−2.717562
107	1	0	−0.461973	−4.175423	−3.578136
108	1	0	0.933438	−3.991570	−1.106279
109	1	0	1.057475	−1.413047	−3.122525
110	8	0	−1.532212	−1.828005	−3.218969
111	6	0	−1.887415	−0.853007	−4.227045
112	1	0	−2.641091	−1.281009	−4.893246
113	1	0	−2.260620	0.065294	−3.765445
114	1	0	−0.974313	−0.643809	−4.782908
115	1	0	−2.343176	−2.152890	−2.797369

6a C_2-symmetric conformation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.017902	−0.174868	0.868131
2	15	0	2.221430	−0.933871	0.592450
3	15	0	−2.111882	0.818058	0.753856
4	6	0	3.526444	0.130305	1.420206
5	6	0	4.928963	−0.186675	0.965655
6	6	0	5.790270	−0.913524	1.830578
7	6	0	7.062110	−1.257147	1.441609
8	6	0	7.536697	−0.920826	0.146984
9	6	0	8.835481	−1.304557	−0.287090
10	6	0	9.273563	−1.007236	−1.557710
11	6	0	8.420771	−0.315672	−2.452581
12	6	0	7.160766	0.079401	−2.058437
13	6	0	6.679049	−0.193868	−0.745607
14	6	0	5.369386	0.198071	−0.300606
15	6	0	2.877752	−1.008420	−1.156681
16	6	0	3.265892	0.370766	−1.637969
17	6	0	2.400602	1.067664	−2.522985
18	6	0	2.695283	2.340537	−2.948663
19	6	0	3.861519	3.004537	−2.485778
20	6	0	4.159518	4.338479	−2.878630
21	6	0	5.275114	4.985390	−2.397147
22	6	0	6.140074	4.320795	−1.493463
23	6	0	5.885665	3.023817	−1.103333
24	6	0	4.749514	2.316527	−1.591938
25	6	0	4.448537	0.966403	−1.200603
26	6	0	2.487295	−2.619333	1.285549
27	6	0	2.738900	−3.742621	0.481648
28	6	0	2.860804	−5.011167	1.056010
29	6	0	2.727942	−5.177407	2.435503
30	6	0	2.467939	−4.068154	3.245260
31	6	0	2.343095	−2.798799	2.676517
32	6	0	−3.516871	−0.187180	1.488756
33	6	0	−4.889235	0.286462	1.075279
34	6	0	−5.696947	0.978570	2.017572
35	6	0	−6.935637	1.462513	1.674640
36	6	0	−7.428882	1.312070	0.352474
37	6	0	−8.688088	1.848700	−0.032954
38	6	0	−9.141935	1.729394	−1.327028
39	6	0	−8.345236	1.068790	−2.293974
40	6	0	−7.125771	0.527526	−1.948779
41	6	0	−6.629725	0.616653	−0.615910
42	6	0	−5.358822	0.071676	−0.220488
43	6	0	−2.757065	1.109435	−0.983269
44	6	0	−3.280669	−0.170966	−1.589257
45	6	0	−2.490166	−0.860529	−2.547842
46	6	0	−2.909550	−2.050834	−3.092139
47	6	0	−4.134160	−2.640105	−2.681994
48	6	0	−4.563903	−3.892969	−3.200451
49	6	0	−5.736642	−4.471607	−2.770927
50	6	0	−6.528187	−3.818682	−1.794385
51	6	0	−6.145448	−2.598115	−1.281859
52	6	0	−4.947338	−1.959730	−1.714137
53	6	0	−4.514834	−0.688946	−1.198088
54	6	0	−2.232473	2.485427	1.527735
55	6	0	−2.592735	2.646942	2.875814
56	6	0	−2.620476	3.917054	3.457015
57	6	0	−2.284044	5.042918	2.702708
58	6	0	−1.916882	4.893004	1.363170
59	6	0	−1.888975	3.624991	0.779910
60	1	0	3.417704	0.000637	2.500519
61	1	0	3.249217	1.162670	1.185474
62	1	0	5.430444	−1.189489	2.818108
63	1	0	7.716070	−1.802227	2.117439
64	1	0	9.474589	−1.846675	0.405580
65	1	0	10.266232	−1.308343	−1.880284
66	1	0	8.762716	−0.098148	−3.460698
67	1	0	6.518612	0.600555	−2.759533
68	1	0	2.100948	−1.444352	−1.789933
69	1	0	3.743246	−1.677618	−1.160235
70	1	0	1.497908	0.572461	−2.870459
71	1	0	2.032146	2.857830	−3.637370
72	1	0	3.480770	4.841767	−3.562837
73	1	0	5.490574	6.006092	−2.700201
74	1	0	7.010379	4.840388	−1.102257
75	1	0	6.554227	2.531352	−0.406034

76	1	0	2.842523	−3.642248	−0.593790
77	1	0	3.060519	−5.868774	0.420041
78	1	0	2.823936	−6.164609	2.877810
79	1	0	2.362104	−4.187627	4.319636
80	1	0	2.136268	−1.946387	3.318880
81	1	0	−3.327253	−1.212726	1.159645
82	1	0	−3.402045	−0.187709	2.576442
83	1	0	−5.325646	1.113849	3.029228
84	1	0	−7.547182	1.978777	2.410227
85	1	0	−9.283189	2.364759	0.716500
86	1	0	−10.103491	2.146882	−1.611965
87	1	0	−8.697890	0.991752	−3.318780
88	1	0	−3.542643	1.868416	−0.917019
89	1	0	−1.936793	1.515533	−1.580064
90	1	0	−2.302414	−2.560037	−3.836246
91	1	0	−3.940508	−4.389849	−3.939820
92	1	0	−6.053318	−5.430797	−3.170644
93	1	0	−6.758965	−2.115047	−0.529672
94	1	0	−2.852521	1.787485	3.485919
95	1	0	−2.907837	4.022821	4.499231
96	1	0	−2.307460	6.030018	3.155246
97	1	0	−1.653117	5.762701	0.768130
98	1	0	−1.598127	3.532211	−0.262389
99	1	0	−6.526259	0.032246	−2.704292
100	1	0	−7.444043	−4.286818	−1.444394
101	1	0	−1.545691	−0.422732	−2.859240
102	1	0	0.547343	1.207984	0.416476
103	1	0	−0.147287	−0.406560	−0.646357
104	8	0	−0.759436	−2.247407	1.542382
105	1	0	−0.054360	−2.652303	2.079293
106	8	0	0.321108	0.072830	3.162580
107	6	0	0.747149	1.300378	3.792479
108	1	0	−0.007020	2.082511	3.675200
109	1	0	0.945655	1.120846	4.853127
110	1	0	1.667745	1.602251	3.294678
111	1	0	−0.460007	−0.259688	3.633923
112	6	0	−1.167068	−3.219589	0.554676
113	1	0	−1.564792	−4.108035	1.053705
114	1	0	−1.947345	−2.753562	−0.045771
115	1	0	−0.326864	−3.492767	−0.090613

6a *Cs*-symmetric conformation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.026695	−1.674525	0.013106
2	15	0	2.350272	−1.413218	−0.218869
3	15	0	−2.306635	−1.417519	0.095410
4	6	0	3.088804	−0.514073	1.255327
5	6	0	4.487346	−0.011079	1.003166
6	6	0	5.587809	−0.695768	1.585234
7	6	0	6.880084	−0.295197	1.348009
8	6	0	7.150035	0.799210	0.485294
9	6	0	8.482934	1.201372	0.195282
10	6	0	8.736189	2.239393	−0.672678
11	6	0	7.658315	2.916155	−1.294280
12	6	0	6.355142	2.557527	−1.025382
13	6	0	6.052832	1.500031	−0.119364
14	6	0	4.706699	1.093667	0.180749
15	6	0	2.937018	−0.326865	−1.627088
16	6	0	2.706203	1.134513	−1.317595
17	6	0	1.621001	1.813302	−1.933708
18	6	0	1.350901	3.129990	−1.647586
19	6	0	2.133632	3.836962	−0.697579
20	6	0	1.837630	5.183892	−0.349651
21	6	0	2.579719	5.848716	0.600500
22	6	0	3.652074	5.186461	1.247027
23	6	0	3.972338	3.886054	0.922147
24	6	0	3.236646	3.170090	−0.066024
25	6	0	3.535543	1.809759	−0.422145
26	6	0	3.356844	−2.948501	−0.356977
27	6	0	4.021206	−3.312797	−1.539218
28	6	0	4.728960	−4.516061	−1.612410
29	6	0	4.782481	−5.368872	−0.508777
30	6	0	4.119235	−5.018334	0.670911
31	6	0	3.406599	−3.821430	0.745162
32	6	0	−3.000152	−0.480926	−1.370478
33	6	0	−4.430376	−0.042156	−1.179354
34	6	0	−5.467043	−0.736447	−1.858797
35	6	0	−6.785910	−0.397265	−1.678954
36	6	0	−7.148836	0.639132	−0.779604
37	6	0	−8.511250	0.974210	−0.547367
38	6	0	−8.855015	1.955012	0.355271
39	6	0	−7.842315	2.639611	1.070858
40	6	0	−6.512485	2.346079	0.859792
41	6	0	−6.117139	1.349516	−0.078585
42	6	0	−4.740806	1.011611	−0.320472
43	6	0	−3.007888	−0.415962	1.518428
44	6	0	−2.822874	1.065041	1.281282
45	6	0	−1.794008	1.757013	1.974677
46	6	0	−1.564418	3.094392	1.757547
47	6	0	−2.331718	3.812438	0.803413
48	6	0	−2.076231	5.184430	0.529146
49	6	0	−2.801024	5.861980	−0.425409
50	6	0	−3.813431	5.187551	−1.150988
51	6	0	−4.093778	3.861991	−0.898947
52	6	0	−3.375881	3.131769	0.091827
53	6	0	−3.634730	1.746192	0.374838
54	6	0	−3.251559	−2.999932	0.140399
55	6	0	−3.312161	−3.802218	−1.015864
56	6	0	−3.953708	−5.042985	−0.988489
57	6	0	−4.535299	−5.505778	0.194304
58	6	0	−4.474096	−4.722099	1.348590
59	6	0	−3.836015	−3.479797	1.325053
60	1	0	3.051336	−1.199092	2.106213
61	1	0	2.395913	0.304949	1.470100
62	1	0	5.392900	−1.545648	2.233537
63	1	0	7.712547	−0.820795	1.808916
64	1	0	9.301277	0.664206	0.668557
65	1	0	9.758491	2.535773	−0.889974
66	1	0	7.861828	3.723486	−1.992391
67	1	0	5.542538	3.081756	−1.515750
68	1	0	2.400934	−0.627378	−2.531088
69	1	0	4.002416	−0.525314	−1.776989
70	1	0	1.005717	1.274727	−2.649351
71	1	0	0.525570	3.641611	−2.135988
72	1	0	1.002088	5.674859	−0.842237
73	1	0	2.341828	6.875861	0.862269
74	1	0	4.224917	5.708302	2.008648
75	1	0	4.792031	3.391600	1.431614

76	1	0	3.991728	−2.668806	−2.412169
77	1	0	5.239485	−4.781757	−2.533708
78	1	0	5.335696	−6.301869	−0.566567
79	1	0	4.154759	−5.677226	1.533919
80	1	0	2.886248	−3.569036	1.664720
81	1	0	−2.325828	0.370129	−1.505150
82	1	0	−2.886544	−1.118526	−2.251833
83	1	0	−5.202003	−1.542876	−2.536936
84	1	0	−7.568598	−0.928881	−2.214116
85	1	0	−9.279140	0.431432	−1.093115
86	1	0	−9.899194	2.199975	0.527869
87	1	0	−8.117542	3.400830	1.795638
88	1	0	−4.068939	−0.669680	1.603749
89	1	0	−2.509529	−0.728403	2.439586
90	1	0	−0.782622	3.614223	2.305332
91	1	0	−1.286222	5.685313	1.082993
92	1	0	−2.594795	6.908711	−0.630066
93	1	0	−4.867254	3.359689	−1.469259
94	1	0	−2.874236	−3.455689	−1.948606
95	1	0	−3.999412	−5.643120	−1.892529
96	1	0	−5.033505	−6.470502	0.215429
97	1	0	−4.925474	−5.074209	2.271660
98	1	0	−3.803066	−2.889731	2.235479
99	1	0	−5.750631	2.874464	1.421951
100	1	0	−4.371809	5.720200	−1.915815
101	1	0	−1.192492	1.215126	2.699309
102	8	0	0.405787	−2.256800	2.232633
103	6	0	−0.049804	−3.463021	2.878984
104	1	0	0.437951	−3.566457	3.852732
105	1	0	−1.137103	−3.462444	3.003861
106	1	0	0.243660	−4.288908	2.231886
107	1	0	0.220242	−1.500297	2.810314
108	1	0	−0.109330	−1.243186	−1.462071
109	1	0	0.047301	−0.151826	0.295459
110	8	0	−0.077068	−3.934068	−0.425587
111	6	0	0.305907	−4.478451	−1.707236
112	1	0	0.170769	−5.563990	−1.700621
113	1	0	−0.281805	−4.031740	−2.515413
114	1	0	1.359584	−4.243493	−1.847207
115	1	0	−0.999298	−4.199015	−0.260293

***Trans*(P)-*trans*(H)-dihydride**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	−0.040443	−0.019979	−0.525397
2	15	0	−2.215169	−0.932963	−0.586848
3	15	0	2.149946	0.898171	−0.558387
4	6	0	−3.454382	0.166310	−1.460980
5	6	0	−4.886932	−0.237598	−1.217487
6	6	0	−5.606508	−0.894571	−2.251090
7	6	0	−6.901260	−1.311696	−2.060120
8	6	0	−7.543192	−1.124712	−0.808006
9	6	0	−8.867950	−1.588274	−0.579202
10	6	0	−9.467965	−1.437856	0.650568
11	6	0	−8.758966	−0.818985	1.709202
12	6	0	−7.478028	−0.348941	1.516210
13	6	0	−6.830272	−0.471139	0.252895
14	6	0	−5.493474	0.000597	0.015949
15	6	0	−3.085269	−1.227918	1.044522
16	6	0	−3.574898	0.084361	1.611767
17	6	0	−2.835347	0.713451	2.649122
18	6	0	−3.215189	1.936400	3.149458
19	6	0	−4.344920	2.614421	2.619740
20	6	0	−4.729388	3.897615	3.097087
21	6	0	−5.806605	4.560846	2.553915
22	6	0	−6.543085	3.965192	1.500953
23	6	0	−6.203085	2.717593	1.024328
24	6	0	−5.105497	1.993370	1.572493
25	6	0	−4.717089	0.694266	1.095006
26	6	0	−2.271620	−2.540715	−1.479149
27	6	0	−2.666845	−3.739984	−0.864642
28	6	0	−2.645337	−4.941227	−1.578357
29	6	0	−2.227724	−4.963821	−2.910019
30	6	0	−1.826306	−3.777928	−3.531181
31	6	0	−1.842353	−2.575397	−2.821847
32	6	0	3.383941	−0.206556	−1.436432
33	6	0	4.813073	0.221210	−1.217008
34	6	0	5.505901	0.881922	−2.266860
35	6	0	6.795259	1.324538	−2.099812
36	6	0	7.458846	1.161596	−0.855745
37	6	0	8.777462	1.653190	−0.651066
38	6	0	9.398644	1.526108	0.570784
39	6	0	8.717202	0.903787	1.645239
40	6	0	7.443200	0.406560	1.475294
41	6	0	6.774386	0.503406	0.220740
42	6	0	5.443445	0.002248	0.007602
43	6	0	3.016995	1.167630	1.084430
44	6	0	3.556713	−0.127977	1.642725
45	6	0	2.878305	−0.761302	2.718239
46	6	0	3.321938	−1.956293	3.233503
47	6	0	4.453120	−2.607781	2.675739
48	6	0	4.897593	−3.868106	3.162655
49	6	0	5.974127	−4.507682	2.590901
50	6	0	6.649854	−3.910393	1.498591
51	6	0	6.251935	−2.683895	1.012579
52	6	0	5.152483	−1.983907	1.588514
53	6	0	4.706186	−0.706447	1.103585
54	6	0	2.313980	2.517376	−1.421977
55	6	0	2.068303	2.573431	−2.805505
56	6	0	2.160811	3.782217	−3.494640
57	6	0	2.483434	4.958146	−2.810424
58	6	0	2.716429	4.916277	−1.435107
59	6	0	2.635842	3.703783	−0.743661
60	1	0	−3.203086	0.150930	−2.525172
61	1	0	−3.253331	1.174679	−1.090156
62	1	0	−5.118752	−1.057085	−3.208372
63	1	0	−7.445094	−1.802223	−2.863381
64	1	0	−9.396051	−2.073707	−1.396237
65	1	0	−10.479011	−1.799385	0.815417
66	1	0	−9.229030	−0.717567	2.683508
67	1	0	−6.947204	0.114943	2.340044
68	1	0	−2.375836	−1.711439	1.720362
69	1	0	−3.922910	−1.909861	0.871126
70	1	0	−1.963396	0.205712	3.051924
71	1	0	−2.650433	2.401095	3.953753
72	1	0	−4.147956	4.349407	3.897062
73	1	0	−6.088959	5.542626	2.923306
74	1	0	−7.381913	4.499071	1.063044
75	1	0	−6.772579	2.278954	0.212560

76	1	0	−2.992396	−3.751750	0.169959
77	1	0	−2.956677	−5.859179	−1.088415
78	1	0	−2.212619	−5.899582	−3.460916
79	1	0	−1.499715	−3.785624	−4.566945
80	1	0	−1.526634	−1.659882	−3.316373
81	1	0	3.197998	−1.217169	−1.065913
82	1	0	3.121307	−0.203604	−2.498097
83	1	0	5.000209	1.028334	−3.217208
84	1	0	7.317783	1.817706	−2.915540
85	1	0	9.283507	2.141231	−1.480448
86	1	0	10.404729	1.908810	0.717280
87	1	0	9.202870	0.821245	2.613683
88	1	0	3.832298	1.877968	0.919061
89	1	0	2.298154	1.622930	1.770937
90	1	0	2.802217	−2.422341	4.066812
91	1	0	4.361671	−4.321994	3.992673
92	1	0	6.302109	−5.472408	2.967528
93	1	0	6.776085	−2.244322	0.171239
94	1	0	1.790893	1.673105	−3.346367
95	1	0	1.975430	3.806322	−4.564745
96	1	0	2.549555	5.900415	−3.346699
97	1	0	2.964295	5.825157	−0.894350
98	1	0	2.818341	3.700032	0.325674
99	1	0	6.934309	−0.059408	2.311553
100	1	0	7.487775	−4.426416	1.038051
101	1	0	2.000461	−0.279089	3.138146
102	1	0	0.061801	−0.277384	1.107912
103	8	0	0.810514	−1.905433	−0.956580
104	1	0	0.312970	−2.282273	−1.706418
105	6	0	0.960680	−2.923125	0.069459
106	1	0	1.462002	−3.784202	−0.378940
107	1	0	1.576644	−2.483627	0.850690
108	1	0	−0.012110	−3.211501	0.472707
109	1	0	−0.145925	0.240883	−2.175129
110	8	0	−0.997297	1.810184	−0.059846
111	6	0	−1.062436	3.014655	−0.862525
112	1	0	−1.892277	3.621965	−0.492932
113	1	0	−0.125237	3.569576	−0.814385
114	1	0	−1.255159	2.687820	−1.882522
115	1	0	−0.857565	2.025387	0.876743

Dimer 3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	3.567288	0.124786	0.270577
2	15	0	3.089600	1.435808	−1.592059
3	15	0	5.075428	−1.182712	−0.711178
4	6	0	1.765473	2.597629	−0.932623
5	6	0	1.081165	3.418679	−1.993230
6	6	0	1.393667	4.800206	−2.096805
7	6	0	0.811459	5.588445	−3.058544
8	6	0	−0.088397	5.029831	−4.002956
9	6	0	−0.662310	5.826242	−5.031356
10	6	0	−1.497905	5.271107	−5.973591
11	6	0	−1.782548	3.885032	−5.929541
12	6	0	−1.252273	3.088719	−4.937151
13	6	0	−0.405699	3.631611	−3.927465
14	6	0	0.167145	2.837477	−2.870765
15	6	0	2.257196	0.797945	−3.146068
16	6	0	0.816071	0.402766	−2.923337
17	6	0	0.462572	−0.962996	−2.941611
18	6	0	−0.856831	−1.368040	−2.831266
19	6	0	−1.869410	−0.412026	−2.636286
20	6	0	−3.269205	−0.771789	−2.538483
21	6	0	−4.292049	0.197524	−2.567892
22	6	0	−3.932861	1.561587	−2.340382
23	6	0	−2.586825	1.894045	−2.199672
24	6	0	−1.520901	0.968923	−2.533437
25	6	0	−0.177227	1.384630	−2.751590
26	6	0	4.430399	2.536814	−2.203463
27	6	0	4.912129	2.491910	−3.520871
28	6	0	5.963182	3.324439	−3.917576
29	6	0	6.539440	4.212308	−3.008690
30	6	0	6.067575	4.262871	−1.693178
31	6	0	5.027890	3.425339	−1.290247
32	6	0	5.649330	−2.628166	0.346448
33	6	0	6.917992	−3.257711	−0.175817
34	6	0	6.845796	−4.499519	−0.861721
35	6	0	7.972754	−5.088648	−1.380715
36	6	0	9.236934	−4.452476	−1.271276
37	6	0	10.405934	−5.027479	−1.841037
38	6	0	11.620529	−4.384549	−1.762633
39	6	0	11.712971	−3.129657	−1.112581
40	6	0	10.600654	−2.551025	−0.541052
41	6	0	9.330206	−3.194333	−0.586746
42	6	0	8.146371	−2.618314	−0.009860
43	6	0	6.713374	−0.342959	−1.075879
44	6	0	7.533373	−0.207396	0.185358
45	6	0	7.596425	1.051390	0.840514
46	6	0	8.298426	1.206409	2.011828
47	6	0	8.953085	0.099646	2.614034
48	6	0	9.648296	0.232091	3.847331
49	6	0	10.251475	−0.854490	4.439243
50	6	0	10.177199	−2.126041	3.819951
51	6	0	9.521089	−2.285048	2.618578
52	6	0	8.899527	−1.180992	1.967457
53	6	0	8.201613	−1.309594	0.717242
54	6	0	4.593498	−1.999571	−2.289568
55	6	0	5.146099	−1.630541	−3.526512
56	6	0	4.747352	−2.275809	−4.701110
57	6	0	3.800245	−3.299638	−4.654132
58	6	0	3.241979	−3.672790	−3.427337
59	6	0	3.627439	−3.021426	−2.255269
60	1	0	2.239183	3.232863	−0.179515
61	1	0	1.060982	1.947654	−0.404307
62	1	0	2.095533	5.233481	−1.389874
63	1	0	1.045337	6.648242	−3.116393
64	1	0	−0.417451	6.884846	−5.064309
65	1	0	−1.927484	5.887444	−6.757941
66	1	0	−2.419177	3.442716	−6.690628
67	1	0	−1.467385	2.026119	−4.938271
68	1	0	2.838671	−0.047924	−3.520176
69	1	0	2.313442	1.603429	−3.885756
70	1	0	1.240070	−1.705045	−3.092416
71	1	0	−1.117876	−2.420059	−2.904576
72	1	0	−3.526013	−1.818706	−2.663194
73	1	0	−5.326180	−0.076574	−2.740775
74	1	0	−4.701531	2.320788	−2.249592
75	1	0	−2.325502	2.919898	−1.966986
76	1	0	4.479932	1.813127	−4.248356

77	1	0	6.324780	3.278066	−4.940658
78	1	0	7.352627	4.860989	−3.320760
79	1	0	6.510820	4.951399	−0.979556
80	1	0	4.683193	3.463745	−0.260162
81	1	0	5.791910	−2.239061	1.357464
82	1	0	4.831611	−3.352961	0.386013
83	1	0	5.880925	−4.987864	−0.965515
84	1	0	7.906895	−6.044974	−1.893125
85	1	0	10.318727	−5.984804	−2.348847
86	1	0	12.506699	−4.830973	−2.204597
87	1	0	12.669886	−2.617202	−1.067664
88	1	0	7.236973	−0.953426	−1.817547
89	1	0	6.504672	0.633605	−1.518590
90	1	0	8.354384	2.178486	2.495288
91	1	0	9.687394	1.211028	4.318636
92	1	0	10.777127	−0.742959	5.383253
93	1	0	9.469219	−3.266462	2.160586
94	1	0	5.887127	−0.840558	−3.589487
95	1	0	5.185457	−1.979351	−5.649651
96	1	0	3.497960	−3.805296	−5.566445
97	1	0	2.505366	−4.469851	−3.382257
98	1	0	3.171815	−3.313241	−1.312763
99	1	0	10.688330	−1.586566	−0.053624
100	1	0	10.640261	−2.984413	4.298560
101	1	0	7.091138	1.900914	0.389400
102	45	0	−3.551356	0.210546	−0.475622
103	15	0	−3.064493	1.319795	1.531148
104	15	0	−4.906962	−1.384412	0.438943
105	6	0	−1.686237	2.571036	1.250972
106	6	0	−1.139386	3.159291	2.528161
107	6	0	−1.507987	4.484063	2.885206
108	6	0	−1.069556	5.052488	4.056220
109	6	0	−0.266682	4.312731	4.962818
110	6	0	0.154015	4.870048	6.201399
111	6	0	0.893661	4.129762	7.095464
112	6	0	1.235245	2.790480	6.787233
113	6	0	0.854189	2.225795	5.589295
114	6	0	0.108396	2.968124	4.628276
115	6	0	−0.309250	2.415360	3.367871
116	6	0	−2.362417	0.402184	3.008901
117	6	0	−0.907195	0.049238	2.811863
118	6	0	−0.550087	−1.275150	2.477006
119	6	0	0.770447	−1.637285	2.297382
120	6	0	1.794488	−0.676498	2.421791
121	6	0	3.182993	−1.030601	2.224397
122	6	0	4.204368	−0.084914	2.427604
123	6	0	3.845170	1.272638	2.718557
124	6	0	2.524556	1.638003	2.838405
125	6	0	1.453142	0.674875	2.748806
126	6	0	0.086838	1.025943	2.972297
127	6	0	−4.446637	2.322976	2.218587
128	6	0	−5.029085	2.061254	3.468364
129	6	0	−6.098838	2.837085	3.925973
130	6	0	−6.594170	3.883036	3.146831
131	6	0	−6.022376	4.149307	1.898694
132	6	0	−4.963557	3.369669	1.433650
133	6	0	−5.576171	−2.602318	−0.834296
134	6	0	−6.776430	−3.370074	−0.336599
135	6	0	−6.620300	−4.723916	0.063799
136	6	0	−7.683096	−5.446520	0.548655
137	6	0	−8.960498	−4.844764	0.693955
138	6	0	−10.060011	−5.564674	1.236836
139	6	0	−11.284465	−4.960339	1.410805
140	6	0	−11.456878	−3.601202	1.051720
141	6	0	−10.414319	−2.879600	0.512189
142	6	0	−9.137319	−3.475381	0.301695
143	6	0	−8.024186	−2.752864	−0.250051
144	6	0	−6.516145	−0.696989	1.116847
145	6	0	−7.455970	−0.334761	−0.009766
146	6	0	−7.591732	1.026554	−0.391652
147	6	0	−8.409413	1.392166	−1.434136
148	6	0	−9.115960	0.410833	−2.177979
149	6	0	−9.934057	0.767619	−3.284974
150	6	0	−10.587303	−0.194942	−4.020811
151	6	0	−10.441659	−1.561924	−3.680162
152	6	0	−9.665686	−1.939317	−2.605687
153	6	0	−8.988680	−0.970830	−1.809837
154	6	0	−8.166784	−1.326454	−0.684984
155	6	0	−4.286560	−2.519542	1.753210
156	6	0	−3.325881	−3.488527	1.410748
157	6	0	−2.849132	−4.385895	2.367037
158	6	0	−3.309889	−4.317595	3.685325

159	6	0	−4.250657	−3.349804	4.039711
160	6	0	−4.740264	−2.457918	3.080594
161	1	0	−2.079971	3.349344	0.592442
162	1	0	−0.918811	2.031139	0.689641
163	1	0	−2.140316	5.052521	2.209032
164	1	0	−1.347177	6.072276	4.309585
165	1	0	−0.131052	5.893178	6.433096
166	1	0	1.205544	4.563473	8.041158
167	1	0	1.797935	2.200607	7.505305
168	1	0	1.111700	1.193135	5.380923
169	1	0	−2.961581	−0.494693	3.177246
170	1	0	−2.477729	1.057871	3.877121
171	1	0	−1.329339	−2.023149	2.380687
172	1	0	1.031061	−2.665152	2.059603
173	1	0	3.420857	−2.085357	2.128227
174	1	0	5.243807	−0.384240	2.503765
175	1	0	4.628937	2.013505	2.836739
176	1	0	2.276466	2.675733	3.027751
177	1	0	−4.660903	1.256394	4.096001
178	1	0	−6.538836	2.622120	4.895426
179	1	0	−7.421856	4.486933	3.506880
180	1	0	−6.402743	4.960702	1.284888
181	1	0	−4.541739	3.577457	0.453838
182	1	0	−5.830295	−2.015366	−1.719658
183	1	0	−4.761296	−3.276971	−1.110482
184	1	0	−5.642547	−5.188999	−0.025093
185	1	0	−7.554077	−6.485799	0.839841
186	1	0	−9.910726	−6.603413	1.520911
187	1	0	−12.116607	−5.518454	1.830314
188	1	0	−12.419954	−3.122794	1.206432
189	1	0	−6.958224	−1.465180	1.757887
190	1	0	−6.285451	0.174399	1.733672
191	1	0	−8.518713	2.439048	−1.706181
192	1	0	−10.027160	1.819451	−3.543915
193	1	0	−11.207149	0.088334	−4.866676
194	1	0	−9.561103	−2.990628	−2.361911
195	1	0	−2.943947	−3.548979	0.395089
196	1	0	−2.116487	−5.135544	2.082248
197	1	0	−2.937307	−5.014957	4.429814
198	1	0	−4.613441	−3.288449	5.061580
199	1	0	−5.477715	−1.720498	3.380563
200	1	0	−10.562520	−1.838271	0.248962
201	1	0	−10.944958	−2.320018	−4.273706
202	1	0	−7.047908	1.784328	0.165038