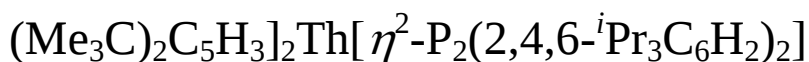


Supporting Information for

Experimental and computational studies on a three-membered

diphosphido thorium metallaheterocycle[η^5 -1,3-



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1. Figure

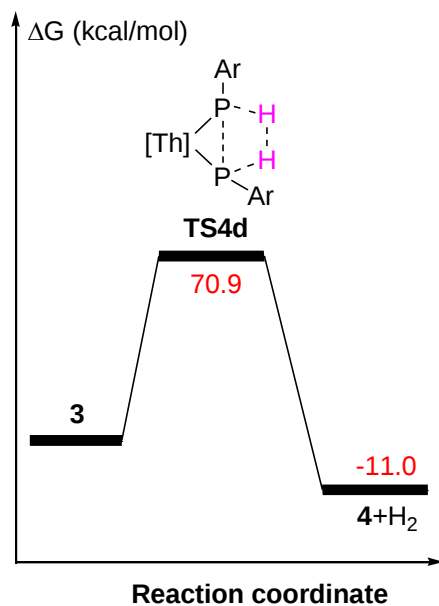


Figure S1. Energy profile (kcal/mol) for the formation of **4+H₂** (computed at $T = 298$ K). [Th] = [η^5 -1,3-(Me₃C)₂C₅H₃]₂Th. Ar = 2,4,6-*i*Pr₃C₆H₂.

2. Crystal parameters

Table S1. Crystal Data and Experimental Parameters for Compounds 2, 3 and 5

Compound	2 0.5C ₆ H ₆	3	5
Formula	C ₄₄ H ₆₉ ClPTh	C ₅₆ H ₉₀ P ₂ Th	C ₆₃ H ₉₈ N ₂ P ₂ Th
Fw	896.45	1057.25	1177.41
crystal system	triclinic	monoclinic	monoclinic
space group	<i>P</i> (-1)	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	10.314(1)	25.307(1)	12.522(1)
<i>b</i> (Å)	14.179(1)	10.110(1)	24.733(1)
<i>c</i> (Å)	16.462(1)	22.290(1)	20.331(1)
α (deg)	70.74(1)	90	90
β (deg)	80.70(1)	105.27(1)	104.56(1)
γ (deg)	70.86(1)	90	90
<i>V</i> (Å ³)	2143.32(17)	5501.5(3)	6094.53(10)
<i>Z</i>	2	4	4
<i>D</i> _{calc} (g/cm ³)	1.389	1.276	1.283
μ (Mo/ <i>K</i> α) _{calc} (cm ⁻¹)	12.329	9.514	8.653
size (mm)	0.20 × 0.20 × 0.15	0.35 × 0.30 × 0.25	0.20 × 0.10 × 0.10
<i>F</i> (000)	910	2184	2440
2 θ range (deg)	6.91 to 146.32	7.24 to 146.56	8.12 to 143.99
no. of reflns, collected	15319	22837	24544
no of obsd reflns	8345	10736	11679
no of variables	474	578	639
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.53	1.00, 0.03	1.00, 0.81
<i>R</i>	0.061	0.087	0.025
<i>R</i> _w	0.179	0.196	0.056
<i>R</i> _{all}	0.073	0.106	0.031
Gof	1.10	1.05	1.02
CCDC	1899192	1899193	1899195

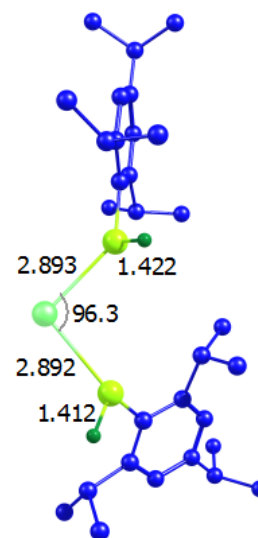
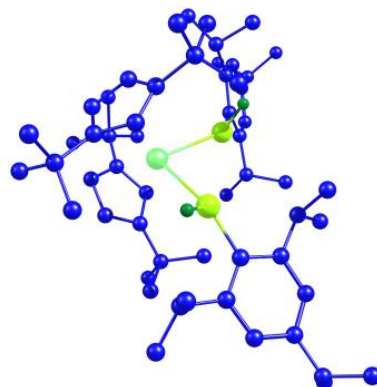
Table S2. Crystal Data and Experimental Parameters for Compounds 9 and 10

Compound	9 C ₆ H ₆ 0.5C ₆ H ₁₄	10 0.5C ₆ H ₆
Formula	C ₇₂ H ₁₀₆ NP ₂ Th	C ₇₃ H ₁₀₁ Cl ₂ O ₂ P ₂ Th
Fw	1279.55	1375.41
crystal system	monoclinic	triclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> (-1)
<i>a</i> (Å)	19.969(1)	11.551(1)
<i>b</i> (Å)	18.077(1)	13.815(1)
<i>c</i> (Å)	18.990(1)	21.174(1)
α (deg)	90	85.75(1)
β (deg)	102.57(1)	83.05(1)
γ (deg)	90	84.31(1)
<i>V</i> (Å ³)	6690.76(17)	3330.90(11)
<i>Z</i>	4	2
<i>D</i> _{calc} (g/cm ³)	1.270	1.371
μ (Mo/K α) _{calc} (cm ⁻¹)	7.920	8.735
size (mm)	0.25 × 0.25 × 0.20	0.22 × 0.18 × 0.15
<i>F</i> (000)	2660	1418
2 θ range (deg)	7.60 to 146.45	7.74 to 144.28
no. of reflns, collected	27849	24342
no of obsd reflns	13109	12761
no of variables	698	745
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.66	1.00, 0.75
<i>R</i>	0.039	0.026
<i>R</i> _w	0.097	0.065
<i>R</i> _{all}	0.046	0.028
Gof	1.08	1.03
CCDC	1899194	1899191

3. Computational details

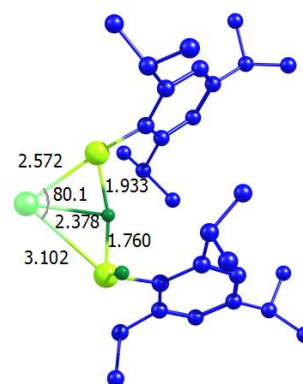
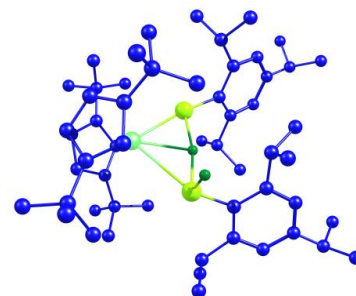
Table S3. The optimized Cartesian Coordinates (in Å) of stationary points for the formation of 4+H₂, obtained with B3PW91-PCM method.

Species	Cartesian coordinates			
3	Th	3.405682	3.646652	11.227222
	P	4.578017	6.144571	12.096646
	H	4.329408	7.007859	10.994576
	P	0.659936	4.553031	11.262227
	H	-0.115205	3.843352	10.319552
	C	5.428718	2.277933	12.748482
	C	4.645446	2.972080	13.710629
	H	5.016097	3.753121	14.361655
	C	3.343328	2.398630	13.783931
	C	3.298124	1.387149	12.790799
	H	2.456667	0.734763	12.588922
	C	4.570177	1.318550	12.155300
	H	4.855418	0.592895	11.404685
	C	6.935024	2.385986	12.523825
	C	7.559521	0.999958	12.783814
	H	7.340627	0.654753	13.800753
	H	8.649453	1.050428	12.667841
	H	7.182743	0.246247	12.083235
	C	7.564299	3.389341	13.498018
	H	7.165004	4.398583	13.358003
	H	8.647678	3.435849	13.336233
	H	7.396639	3.090065	14.539398
	C	7.263503	2.816818	11.085145
	H	6.871037	2.103342	10.351851
	H	8.349592	2.875825	10.941238
	H	6.840745	3.806061	10.869852
	C	2.329100	2.646030	14.892961
	C	2.117311	4.145451	15.142020
	H	3.055124	4.648036	15.399330
	H	1.419672	4.295303	15.974881
	H	1.692031	4.641367	14.262706
	C	0.979417	1.996349	14.569183
	H	0.555970	2.410389	13.648034
	H	0.270129	2.188729	15.382464
	H	1.068795	0.908779	14.459231
	C	2.891990	2.002929	16.179044
	H	3.060676	0.928506	16.041339
	H	2.185990	2.134309	17.008860
	H	3.844746	2.460910	16.467801
	C	2.802320	2.028796	8.921967
	C	2.242151	3.294862	8.593570
	H	1.189843	3.478189	8.411551
	C	3.277703	4.244224	8.364197
	C	4.495156	3.582306	8.666682
	H	5.488232	4.012301	8.604548
	C	4.205251	2.227241	9.000667
	H	4.947232	1.462674	9.190746
	C	2.049324	0.701550	8.867752
	C	2.880448	-0.465970	9.415752
	H	3.840316	-0.561967	8.895296
	H	2.335542	-1.406528	9.272928
	H	3.077412	-0.361635	10.486933
	C	0.715518	0.765148	9.626193
	H	0.866587	0.962097	10.693622
	H	0.181450	-0.188196	9.529209
	H	0.063338	1.552463	9.233809
	C	1.752029	0.416797	7.378221
	H	1.132859	1.206836	6.939554
	H	1.215705	-0.534935	7.273045

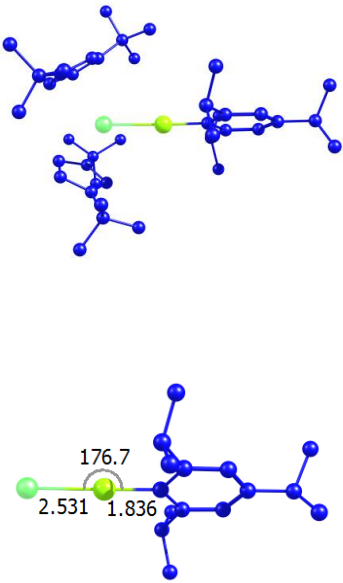


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C	2.712151	5.243384	6.184955
H	3.469839	4.613614	5.704308
H	2.612927	6.166099	5.599308
H	1.754657	4.712203	6.143433
C	4.419554	6.366950	7.615488
H	4.754074	6.612801	8.627968
H	4.277786	7.308351	7.071989
H	5.219334	5.811027	7.112287
C	2.009140	6.453454	8.257808
H	1.051753	5.926429	8.321826
H	1.863340	7.351461	7.644166
H	2.270517	6.773965	9.271376
C	6.174995	6.856729	12.721798
C	7.241304	7.210446	11.847717
C	8.401631	7.782294	12.373645
H	9.200652	8.056835	11.688760
C	8.573887	8.017829	13.738112
C	7.524215	7.665896	14.580629
H	7.628987	7.854866	15.647706
C	6.333023	7.100214	14.110747
C	7.151884	7.053897	10.338500
H	6.355477	6.326519	10.140115
C	6.751670	8.389859	9.691964
H	5.796867	8.757824	10.084437
H	6.657360	8.289022	8.604039
H	7.510611	9.155341	9.895603
C	8.432755	6.511631	9.691469
H	9.254159	7.237127	9.723100
H	8.248597	6.284372	8.634421
H	8.774953	5.594605	10.182938
C	9.844257	8.643079	14.285336
H	9.720834	8.722511	15.374627
C	10.060672	10.062441	13.741296
H	10.210012	10.053224	12.654843
H	10.948664	10.519388	14.194880
H	9.198791	10.704376	13.954419
C	11.073208	7.761275	14.023205
H	10.937603	6.757539	14.441043
H	11.969733	8.202451	14.475623
H	11.261920	7.653420	12.948244
C	5.236059	6.840980	15.133971
H	4.431134	6.301868	14.621740
C	5.708243	5.985876	16.317185
H	6.169453	5.049359	15.983989
H	4.862120	5.737898	16.969600
H	6.446734	6.513252	16.932680
C	4.642944	8.167851	15.630154
H	5.398868	8.767258	16.152607
H	3.815281	7.987296	16.326870
H	4.260601	8.763462	14.794557
C	-0.635541	4.965022	12.512666
C	-0.572236	6.219162	13.179110
C	-1.569149	6.561018	14.094999
H	-1.508441	7.523334	14.596420
C	-2.647397	5.720857	14.377443
C	-2.703552	4.502774	13.705063
H	-3.540763	3.838597	13.908852
C	-1.727026	4.098362	12.788122
C	0.507875	7.245855	12.857520
H	1.406551	6.709170	12.528136
C	0.929010	8.110692	14.049393
H	0.142422	8.812139	14.353282
H	1.805469	8.708588	13.776367
H	1.194016	7.499652	14.919180
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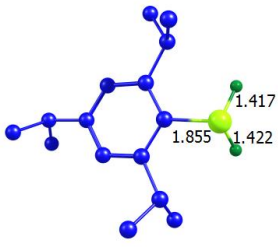
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	H	-3.850498	8.233330	14.849921	
	H	-5.313781	7.588105	15.610870	
	H	-4.943986	7.198793	13.917872	
	C	-3.157717	6.317494	16.782874	
	H	-2.636855	5.419609	17.133835	
	H	-3.959895	6.547739	17.494838	
	H	-2.442949	7.148900	16.806555	
	C	-1.910575	2.761464	12.082663	
	H	-0.916339	2.424744	11.763530	
	C	-2.495327	1.655406	12.970733	
	H	-1.943340	1.557156	13.911350	
	H	-2.446807	0.694060	12.445172	
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	C	-2.777458	2.931699	10.823737	
	H	-3.789469	3.253992	11.098665	
	H	-2.861723	1.985377	10.274410	
	H	-2.364759	3.685878	10.144707	
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	H	3.816863	5.629356	11.674765	
	P	2.152004	5.112271	11.435794	
	H	2.079414	5.878494	10.251513	
	C	6.983177	2.119407	12.142046	
	C	6.117214	2.371402	13.238371	
	H	6.356571	3.009229	14.078727	
	C	4.919762	1.618985	13.090444	
	C	5.027510	0.928315	11.851061	
	H	4.300014	0.239185	11.437770	
	C	6.288902	1.232661	11.277402	
	H	6.680778	0.809276	10.360789	
	C	8.446045	2.528350	12.010698	
	C	9.307160	1.270509	12.252754	
	H	9.113849	0.848840	13.245908	
	H	10.373927	1.520936	12.190501	
	H	9.097001	0.492868	11.509520	
	C	8.828313	3.590585	13.049519	
	H	8.210407	4.489557	12.943982	
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	H	8.713956	3.209857	14.071381	
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	H	9.810506	3.328288	10.513958	
	H	8.164055	3.978456	10.403713	
	C	3.894195	1.368127	14.188975	
	C	3.726258	2.595764	15.094222	
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	H	3.003814	2.381551	15.890406	
	H	3.361647	3.466860	14.537330	
	C	2.526385	0.969998	13.620137	
	H	2.084517	1.777248	13.024646	
	H	1.830025	0.743213	14.436278	
	H	2.591312	0.075980	12.989725	
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	H	3.725429	-0.024973	15.864223	
	H	5.397153	0.443271	15.485980	
	C	3.441777	2.412710	8.617334	
	C	3.426105	3.831610	8.438564	
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	C	4.744412	4.302845	8.200562	
	C	5.602186	3.178401	8.358563	
	H	6.676712	3.171899	8.215774	
	C	4.797872	2.026549	8.584965	
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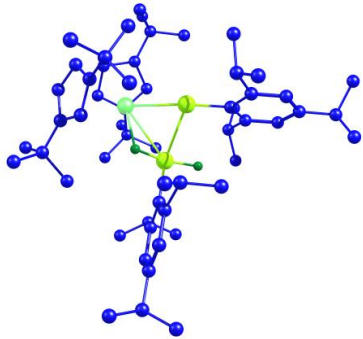
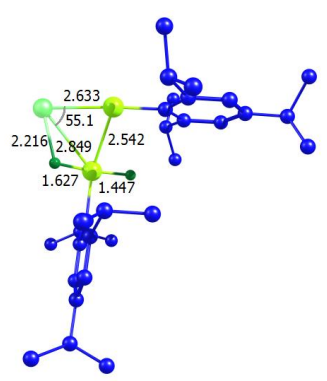


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C	1.385337	1.642397	9.896969
H	1.948466	1.306828	10.776062
H	0.479236	1.025502	9.835086
H	1.080539	2.679931	10.067689
C	1.342536	1.847659	7.404097
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H	0.486681	1.163575	7.343687
H	1.909065	1.769500	6.469135
C	5.117779	5.633647	7.560742
C	4.759988	5.525078	6.061065
H	5.295919	4.694327	5.587530
H	5.031871	6.450251	5.536637
H	3.685879	5.357732	5.922271
C	6.622320	5.906009	7.679524
H	6.938638	5.917192	8.727357
H	6.863514	6.880107	7.237587
H	7.212409	5.150589	7.147362
C	4.333962	6.804753	8.165712
H	3.252377	6.662955	8.058698
H	4.594861	7.739296	7.653758
H	4.562634	6.917297	9.230804
C	6.222912	7.328624	12.800794
C	6.961541	8.346796	12.131523
C	7.377271	9.474537	12.839663
H	7.948088	10.236533	12.314012
C	7.092972	9.657506	14.194430
C	6.373714	8.652297	14.836979
H	6.150086	8.770054	15.896321
C	5.938939	7.494614	14.183425
C	7.370428	8.217037	10.673689
H	6.702986	7.471433	10.226788
C	7.218785	9.511317	9.866172
H	6.213526	9.934465	9.969513
H	7.394159	9.310379	8.802479
H	7.939768	10.279989	10.169999
C	8.803738	7.675377	10.565748
H	9.519668	8.373152	11.018252
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C	7.552300	10.894192	14.945094
H	7.214412	10.784137	15.985250
C	6.911640	12.171994	14.384653
H	7.220055	12.347713	13.347006
H	7.211629	13.046951	14.974389
H	5.818105	12.106752	14.401300
C	9.082877	11.012600	14.967717
H	9.543873	10.115242	15.395172
H	9.395506	11.876743	15.566691
H	9.485848	11.146005	13.956446
C	5.216730	6.446273	15.015513
H	4.870407	5.669363	14.324271
C	6.185740	5.785173	16.006508
H	7.034639	5.329744	15.484068
H	5.676670	5.004099	16.585016
H	6.587342	6.516672	16.718819
C	3.986901	7.005786	15.740298
H	4.262864	7.753690	16.493881
H	3.454600	6.199961	16.260183
H	3.289159	7.473635	15.038792
C	1.426249	6.326368	12.634504
C	1.598822	7.730744	12.499523
C	0.926000	8.584861	13.377751
H	1.055966	9.657336	13.259019
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C	-0.054322	6.737144	14.517913

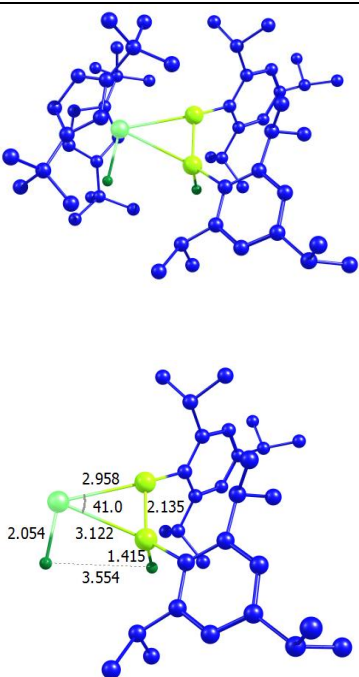
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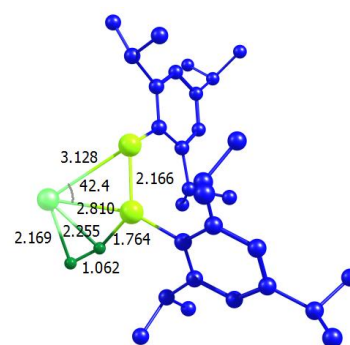
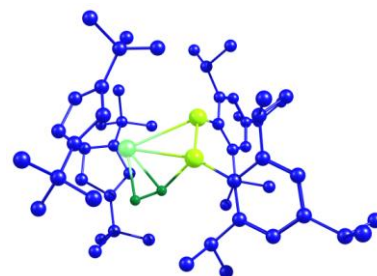
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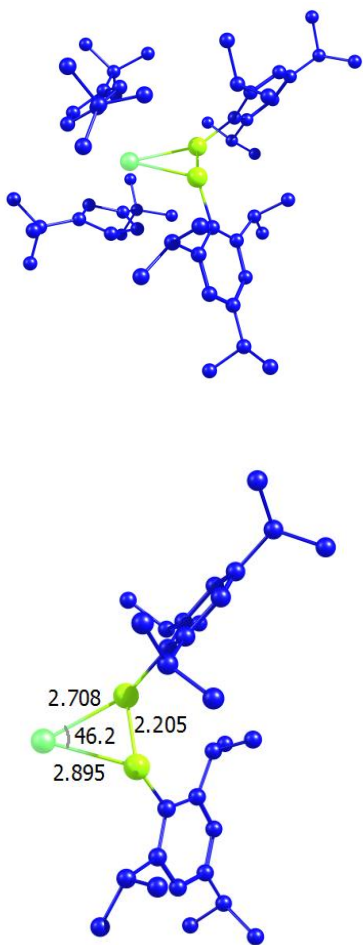
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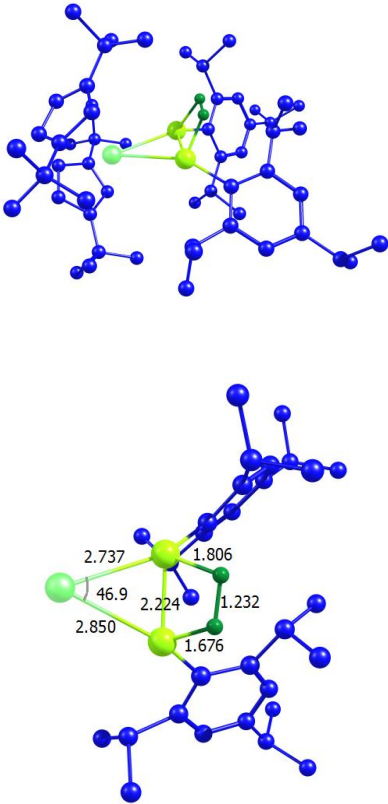
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	H	-4.452857	1.286151	-6.637081
	C	-1.569822	2.993281	-7.614770

	H -0.932513 3.767543 -7.173261 H -1.975123 3.380375 -8.557605 H -0.933254 2.133189 -7.854958 C 0.070849 -0.632009 -3.991835 H 0.450849 -0.782083 -2.976572 C -0.668268 -1.913596 -4.397461 H -1.491420 -2.123583 -3.707757 H 0.014574 -2.771852 -4.378387 H -1.079252 -1.834098 -5.411826 C 1.276371 -0.387018 -4.912030 H 0.976970 -0.283113 -5.961693 H 1.974564 -1.230995 -4.858443 H 1.816118 0.524877 -4.632362 P -0.738366 -1.400442 -0.601862 P -0.650088 0.749504 -1.082724 Th 1.199319 0.212503 0.821043	
H₂	H -2.275303 0.236709 -1.969303 H -2.275303 0.821231 -1.510481	
TS4d	Th -0.407193 -1.895667 -0.754237 P 0.084041 0.742412 -0.214811 H -0.692436 1.869169 -1.392875 P -2.102245 0.333142 -0.221736 H -1.879527 1.539590 -1.363908 C 2.012949 -2.905436 0.392199 C 1.140298 -2.730794 1.501666 H 1.279984 -2.005311 2.292001 C 0.087323 -3.683274 1.436924 C 0.290113 -4.429032 0.243148 H -0.314228 -5.260405 -0.101157 C 1.465280 -3.955428 -0.390350 H 1.893348 -4.361935 -1.299663 C 3.374708 -2.256867 0.169418 C 4.454027 -3.339385 0.380282 H 4.390675 -3.762401 1.389382 H 5.456026 -2.910461 0.251600 H 4.341653 -4.160402 -0.336863 C 3.624797 -1.116357 1.163281 H 2.868606 -0.328706 1.071314 H 4.607517 -0.666531 0.977563 H 3.619769 -1.480724 2.197181 C 3.498045 -1.706972 -1.260349 H 3.323287 -2.485755 -2.011613 H 4.503858 -1.303088 -1.431605 H 2.786371 -0.890259 -1.434608 C -0.927123 -4.009687 2.522266 C -1.114513 -2.833804 3.488218 H -0.182594 -2.600183 4.014151 H -1.866629 -3.083823 4.245673 H -1.444399 -1.929135 2.963680 C -2.280055 -4.379667 1.899222 H -2.670713 -3.554621 1.287945 H -3.021109 -4.595446 2.677664 H -2.202232 -5.268758 1.264066 C -0.399734 -5.222094 3.318552 H -0.268793 -6.095024 2.669128 H -1.102091 -5.492542 4.117462 H 0.568984 -4.995278 3.777837 C -2.012572 -3.216035 -2.823272 C -1.877740 -1.861702 -3.252371 H -2.694505 -1.159136 -3.367351 C -0.531089 -1.606452 -3.618878 C 0.194088 -2.795710 -3.317213 H 1.249157 -2.960872 -3.508746 C -0.715511 -3.781537 -2.859528 H -0.455123 -4.800503 -2.602356 C -3.327124 -3.969072 -2.667716	

C	-3.116561	-5.346441	-2.025173
H	-2.457659	-5.978460	-2.631364
H	-4.076233	-5.867906	-1.929038
H	-2.682205	-5.262955	-1.022620
C	-4.339013	-3.172773	-1.836545
H	-3.989652	-3.035553	-0.807610
H	-5.300040	-3.700004	-1.794055
H	-4.521598	-2.179990	-2.260408
C	-3.908778	-4.178526	-4.083112
H	-4.111003	-3.219471	-4.572608
H	-4.850667	-4.739726	-4.031053
H	-3.210341	-4.739421	-4.714456
C	-0.027714	-0.451230	-4.476026
C	-0.030532	-0.947026	-5.939792
H	0.638949	-1.805062	-6.071192
H	0.303409	-0.146755	-6.612832
H	-1.036791	-1.253595	-6.247474
C	1.404405	-0.044826	-4.105119
H	1.448615	0.342324	-3.081858
H	1.759321	0.745729	-4.777617
H	2.103506	-0.884949	-4.188370
C	-0.945705	0.771986	-4.372529
H	-1.960497	0.540802	-4.716721
H	-0.561912	1.579891	-5.007747
H	-1.007878	1.150680	-3.345622
C	0.864831	2.089964	0.802223
C	1.654752	3.064837	0.126963
C	2.242752	4.098003	0.860550
H	2.840095	4.833973	0.326031
C	2.096688	4.217989	2.242174
C	1.362126	3.228884	2.889751
H	1.261069	3.284486	3.972302
C	0.759283	2.159642	2.216067
C	1.954205	3.030832	-1.368210
H	1.460353	2.152054	-1.789919
C	1.379169	4.250801	-2.098173
H	0.292605	4.300135	-1.970878
H	1.592744	4.190467	-3.172509
H	1.810280	5.187804	-1.724660
C	3.459602	2.881953	-1.635272
H	4.025328	3.755046	-1.288774
H	3.645261	2.774194	-2.711036
H	3.867525	1.999677	-1.129293
C	2.728019	5.359119	3.018879
H	2.450801	5.222487	4.073631
C	2.184638	6.723312	2.571456
H	2.439984	6.928248	1.524808
H	2.611424	7.528400	3.181985
H	1.093891	6.765564	2.663719
C	4.260727	5.324831	2.936538
H	4.655866	4.365544	3.288816
H	4.698806	6.121468	3.550154
H	4.605842	5.470633	1.905853
C	0.076679	1.108080	3.080890
H	-0.344498	0.347412	2.414102
C	1.106803	0.418096	3.989064
H	1.932170	-0.008336	3.409744
H	0.632659	-0.386591	4.563434
H	1.540713	1.123121	4.708659
C	-1.069391	1.676524	3.927374
H	-0.706949	2.411225	4.657633
H	-1.557420	0.870150	4.488673
H	-1.827077	2.160015	3.305628
C	-3.260236	1.285141	0.905858
C	-3.212741	2.705395	1.066690
C	-4.098243	3.325897	1.952441
H	-4.033555	4.403799	2.068525
C	-5.071378	2.632013	2.668846
C	-5.152844	1.263230	2.449338

	H	-5.935844	0.704189	2.956970	
	C	-4.288598	0.575615	1.589082	
	C	-2.319574	3.631956	0.253287	
	H	-1.438808	3.077257	-0.073259	
	C	-1.801147	4.856221	1.018701	
	H	-2.584698	5.597773	1.217658	
	H	-1.032706	5.356357	0.418520	
	H	-1.344079	4.571835	1.971946	
	C	-3.066496	4.078981	-1.013634	
	H	-3.376417	3.218549	-1.615408	
	H	-2.420776	4.710686	-1.636560	
	H	-3.962264	4.657852	-0.753544	
	C	-6.024499	3.334420	3.617882	
	H	-6.695314	2.565891	4.027522	
	C	-6.896659	4.367648	2.891031	
	H	-6.287793	5.178187	2.473066	
	H	-7.619609	4.817431	3.582425	
	H	-7.452517	3.907765	2.066441	
	C	-5.280854	3.974510	4.798472	
	H	-4.687486	3.231342	5.342468	
	H	-5.990171	4.428221	5.501475	
	H	-4.598416	4.762547	4.457925	
	C	-4.617563	-0.894983	1.371130	
	H	-3.783941	-1.347961	0.823999	
	C	-4.795418	-1.681103	2.676300	
	H	-3.922043	-1.579513	3.328301	
	H	-4.936510	-2.745989	2.457623	
	H	-5.675306	-1.351329	3.240570	
	C	-5.875405	-1.017975	0.496099	
	H	-6.742288	-0.564626	0.992233	
	H	-6.113597	-2.070306	0.300630	
	H	-5.741609	-0.512843	-0.466736	

Table S4. Frequencies of the stationary points optimized for the formation of **4**+H₂.

Species	Frequencies (cm ⁻¹)												
3	8	14	17	18	24	28	30	32	34	37	43	46	51
	54	55	60	62	64	64	69	70	76	77	81	82	87
	89	92	93	98	103	124	129	130	132	135	139	147	
	150	160	173	176	180	189	192	195	200	201	222	224	
	228	232	233	236	237	238	240	243	244	245	249	250	
	255	257	261	263	265	265	267	269	271	273	278	283	
	283	287	290	292	297	300	302	305	307	310	313	323	
	330	332	336	340	342	348	353	355	356	366	367	367	
	369	378	385	390	391	401	405	413	414	420	424	442	
	443	444	449	449	484	485	485	492	505	506	523	526	
	559	561	574	577	609	613	617	620	636	637	649	651	
	656	656	669	673	685	691	764	767	784	806	827	828	
	830	834	835	840	845	852	857	857	861	867	877	897	
	901	903	903	907	911	912	933	936	936	937	937	938	
	939	941	942	948	948	950	954	955	958	958	960	962	
	962	962	966	967	969	970	972	974	975	975	976	976	
	978	980	1050	1051	1053	1053	1055	1056	1057	1058	1060		
	1073	1083	1083	1085	1087	1098	1098	1116	1120	1132	1133		
	1135	1135	1139	1139	1141	1143	1168	1170	1191	1192	1201		
	1202	1204	1205	1215	1217	1228	1230	1236	1238	1240	1246		
	1247	1248	1272	1275	1279	1281	1286	1288	1288	1292	1298		
	1307	1332	1333	1337	1346	1348	1355	1357	1357	1359	1361		
	1375	1379	1394	1395	1400	1402	1404	1408	1409	1413	1414		
	1414	1415	1415	1415	1416	1417	1419	1420	1422	1425	1426		
	1432	1434	1435	1435	1436	1437	1446	1446	1448	1450	1472		
	1472	1476	1477	1478	1482	1495	1498	1500	1501	1502	1503		
	1503	1504	1505	1507	1507	1508	1508	1508	1508	1509	1510		
	1510	1511	1511	1512	1512	1513	1515	1520	1520	1522	1522		
	1523	1523	1524	1525	1526	1527	1527	1527	1528	1529	1529		
	1530	1530	1531	1533	1533	1535	1540	1541	1549	1552	1592		
	1610	1613	1661	1663	2404	2474	3040	3043	3044	3045	3046		
	3047	3048	3048	3048	3048	3049	3049	3050	3052	3052	3052		
	3052	3053	3053	3054	3054	3054	3058	3060	3060	3061	3062		
	3062	3065	3071	3117	3117	3120	3120	3121	3121	3121	3122		
	3123	3123	3124	3124	3124	3125	3125	3126	3126	3126	3126		
	3127	3128	3130	3131	3131	3131	3132	3132	3132	3133	3133		
	3133	3134	3135	3135	3135	3136	3138	3138	3138	3139	3140		
	3142	3143	3148	3148	3152	3154	3154	3182	3193	3194	3205		
	3251	3253	3255	3268	3271	3274							
	TS4a	-742	6	14	20	25	27	30	34	37	38	43	45
47		49	53	57	60	61	64	69	70	70	74	79	
82		84	86	88	92	97	108	121	130	133	134	136	
137		147	149	167	172	181	182	182	192	200	202	214	
225		228	231	234	237	238	241	241	246	246	248	253	
254		255	256	260	262	262	264	266	267	269	270	276	
277		278	281	295	299	301	305	305	307	311	313	319	
325		330	332	338	341	343	346	353	357	362	365	366	
367		380	382	382	388	393	406	411	417	421	434	439	
444		448	449	455	458	481	485	488	502	504	508	525	
529		559	561	576	581	611	614	618	623	639	648	649	
650		658	659	662	671	685	692	766	771	772	786	827	
828		831	832	836	837	842	854	858	858	864	869	889	
898		900	903	904	910	910	933	935	937	937	937	939	

	940	940	941	944	947	950	951	953	954	956	958	960
	960	962	963	965	966	968	968	968	969	973	974	975
	976	977	980	1048	1049	1050	1051	1052	1052	1054	1055	
	1059	1061	1083	1084	1084	1086	1098	1103	1121	1123	1133	
	1133	1134	1138	1140	1140	1141	1144	1165	1170	1192	1192	
	1201	1201	1204	1206	1217	1219	1226	1229	1236	1238	1239	
	1242	1245	1246	1272	1274	1274	1280	1286	1288	1289	1290	
	1299	1307	1314	1335	1337	1344	1346	1350	1352	1357	1358	
	1359	1371	1376	1379	1395	1398	1401	1402	1403	1407	1411	
	1411	1412	1412	1413	1415	1415	1417	1417	1417	1417	1418	
	1421	1423	1433	1434	1436	1437	1438	1439	1442	1445	1445	
	1447	1472	1473	1474	1479	1482	1486	1500	1500	1501	1502	
	1504	1505	1505	1507	1507	1507	1508	1508	1509	1509	1510	
	1510	1511	1511	1512	1513	1513	1514	1514	1515	1522	1522	
	1523	1523	1523	1523	1524	1524	1525	1525	1527	1528	1528	
	1529	1529	1530	1531	1531	1532	1536	1537	1541	1544	1550	
	1554	1581	1605	1614	1660	1661	2478	3043	3043	3044	3044	
	3044	3045	3045	3046	3047	3047	3048	3049	3049	3050	3050	
	3050	3050	3051	3051	3052	3054	3055	3056	3056	3057	3058	
	3072	3077	3079	3089	3115	3116	3117	3119	3120	3121	3121	
	3121	3121	3122	3122	3122	3123	3123	3124	3124	3124	3126	
	3126	3126	3127	3127	3128	3128	3128	3129	3129	3130	3131	
	3132	3133	3133	3133	3134	3134	3134	3135	3135	3135	3137	
	3137	3138	3138	3141	3148	3148	3149	3151	3178	3194	3197	
	3205	3242	3249	3250	3260	3274	3281					
INT4a	11 16	23	28	32	35	40	44	53	57	60	72	80
	82	83	87	92	102	105	120	127	128	130	139	145
	147	177	190	199	201	207	212	226	230	231	235	238
	241	243	245	248	249	254	258	260	262	263	266	272
	278	290	296	300	307	311	316	318	325	337	342	351
	352	356	360	367	368	371	378	380	384	404	414	417
	436	443	446	448	452	457	465	489	494	503	505	509
	527	560	563	580	617	617	621	646	649	654	670	677
	691	694	771	779	794	831	832	835	838	840	847	856
	857	859	873	901	902	912	935	936	937	941	942	943
	947	947	950	954	955	957	959	960	960	961	965	971
	972	973	973	974	975	976	1051	1053	1054	1055	1055	
	1056	1064	1066	1073	1081	1084	1086	1102	1125	1126	1132	
	1140	1141	1144	1165	1191	1201	1203	1206	1219	1221	1225	
	1241	1241	1243	1244	1246	1248	1272	1275	1275	1288	1289	
	1289	1299	1342	1345	1350	1358	1364	1365	1374	1397	1398	
	1400	1405	1407	1412	1414	1414	1415	1415	1416	1418	1418	
	1423	1426	1430	1433	1433	1435	1443	1448	1452	1456	1472	
	1476	1481	1486	1500	1501	1504	1505	1506	1507	1508	1508	
	1509	1510	1510	1511	1511	1511	1512	1515	1515	1517	1521	
	1522	1522	1522	1524	1524	1525	1525	1527	1528	1530	1536	
	1537	1541	1544	1548	1552	1564	1582	1591	1605	1660	3035	
	3039	3042	3042	3042	3044	3045	3046	3047	3047	3048	3049	
	3051	3053	3053	3053	3054	3054	3055	3058	3061	3110	3111	
	3111	3113	3116	3117	3117	3119	3120	3121	3122	3123	3124	
	3124	3124	3125	3125	3127	3129	3129	3130	3131	3131	3131	
	3131	3132	3133	3133	3134	3136	3138	3138	3139	3141	3141	
	3141	3169	3175	3234	3236	3252	3260	3267	3277			
ArPH₂	25 34	53	78	87	128	140	155	170	188	227	235	241
	249	256	258	264	270	302	319	338	354	370	386	399
	440	481	521	573	604	634	649	658	747	822	850	855

	860	901	903	913	936	938	940	963	968	974	977	983
	1063	1085	1100	1130	113 1	1139	1145	1147	1175	1191	1211	
	1232	1284	1294	1317	1337	1345	1356	1364	1383	1399	1416	
	1417	1420	1436	1437	1440	1475	1487	1506	1507	1508	1511	
	1513	1516	1523	1525	1527	1529	1530	1535	1621	1665	2413	
	2452	3038	3045	3049	3049	3050	3052	3053	3056	3057	3123	
	3124	3125	3127	3128	3130	3131	3131	3134	3135	3137	3140	
	3197	3210										
TS4b	-200	11	18	20	26	27	30	37	38	40	45	47
	53	54	55	59	62	65	68	71	75	77	80	81
	85	87	88	93	97	102	109	125	129	130	131	133
	147	151	154	168	174	180	186	187	190	200	208	213
	218	225	226	227	230	231	233	237	239	242	252	252
	253	253	254	255	258	261	264	265	267	267	268	270
	272	275	276	287	292	298	301	306	307	310	314	316
	331	334	335	341	344	349	354	359	360	365	368	369
	372	380	384	389	389	406	416	426	427	434	445	447
	448	450	479	480	483	488	504	505	513	519	527	557
	557	567	569	579	601	612	616	623	624	640	647	648
	652	659	661	662	666	682	691	769	772	774	783	829
	830	831	833	835	838	840	844	852	857	858	858	899
	899	903	904	910	911	934	935	937	938	938	940	940
	941	941	946	946	948	954	956	957	958	958	959	961
	962	964	964	970	972	973	973	974	974	975	975	975
	976	1047	1051	1051	1052	1053	1054	1054	1057	1058	1067	
	1069	1084	1084	1084	1092	1095	1099	1117	1124	1132		
	1132	1134	1134	1138	1139	1140	1141	1165	1171	1191		
	1192	1199	1199	1203	1205	1217	1219	1226	1228	1238	1240	
	1240	1241	1244	1246	1252	1274	1275	1275	1282	1287	1288	
	1289	1290	1298	1306	1339	1342	1343	1344	1346	1349	1350	
	1357	1357	1364	1369	1372	1381	1394	1397	1400	1401	1407	
	1408	1410	1411	1413	1414	1414	1415	1416	1416	1416	1417	
	1420	1421	1425	1426	1433	1434	1435	1436	1436	1438	1442	
	1446	1446	1452	1468	1472	1475	1483	1483	1486	1496	1499	
	1500	1503	1503	1504	1504	1505	1505	1507	1507	1508	1508	
	1509	1510	1510	1511	1511	1511	1512	1512	1513	1514	1514	
	1520	1522	1522	1522	1523	1523	1523	1524	1525	1525	1525	
	1527	1527	1529	1529	1530	1530	1531	1532	1535	1538	1541	
	1543	1551	1553	1604	1609	1618	1660	1662	2183	3043	3043	
	3044	3045	3045	3046	3048	3048	3049	3049	3049	3049	3050	
	3051	3051	3052	3052	3052	3053	3053	3054	3055	3056	3057	
	3057	3058	3058	3070	3073	3088	3116	3117	3118	3120	3120	
	3120	3122	3122	3122	3122	3122	3123	3123	3124	3125	3126	
	3126	3127	3127	3127	3127	3129	3129	3130	3132	3132	3133	
	3133	3133	3133	3134	3135	3135	3135	3136	3136	3137	3137	
	3138	3138	3138	3139	3140	3141	3142	3143	3144	3147	3184	
	3185	3199	3203	3240	3244	3253	3258	3263	3279			
INT4b	8	13	15	22	24	27	30	34	40	42	43	50
	54	55	61	63	63	66	69	78	80	85	86	87
	91	93	100	103	106	113	129	130	131	134	137	146
	157	167	171	175	176	186	196	200	204	212	218	222
	228	229	231	235	235	237	239	240	242	246	250	252
	253	255	257	261	262	264	265	266	267	268	269	272
	289	290	292	294	300	302	308	317	317	322	328	333
	333	337	344	349	352	354	356	365	366	368	369	378
	382	388	391	396	402	412	425	426	440	441	447	448

	450	472	485	487	489	506	507	516	527	532	557	560
	578	582	605	609	616	619	624	633	638	641	648	650
	656	660	673	676	678	691	695	768	771	780	791	829
	829	831	833	833	834	839	841	854	858	859	862	899
	901	903	904	913	916	935	937	937	938	938	938	939
	940	941	946	948	949	954	954	955	956	959	959	962
	963	963	966	969	969	970	972	972	974	975	976	976
	976	989	1044	1049	1052	1052	1053	1053	1055	1056	1058	
	1070	1083	1083	1086	1089	1097	1099	1119	1120	1132	1133	
	1135	1136	1139	1139	1139	1141	1166	1169	1192	1193	1200	
	1201	1202	1206	1216	1218	1226	1229	1237	1238	1239	1244	
	1246	1249	1273	1274	1276	1280	1285	1288	1290	1290	1300	
	1316	1339	1344	1347	1347	1355	1358	1358	1358	1364	1371	
	1372	1376	1393	1397	1399	1401	1406	1410	1410	1411	1412	
	1414	1415	1416	1416	1416	1417	1417	1417	1418	1422	1426	
	1435	1436	1436	1437	1437	1438	1439	1440	1445	1452	1470	
	1470	1476	1479	1483	1485	1486	1501	1501	1502	1503	1503	
	1504	1505	1506	1506	1507	1507	1508	1508	1509	1510	1510	
	1512	1512	1512	1512	1512	1513	1513	1516	1520	1521	1522	
	1522	1523	1523	1523	1524	1524	1525	1525	1526	1527	1527	
	1529	1530	1531	1531	1532	1537	1538	1544	1545	1551	1553	
	1572	1611	1619	1661	1664	2428	3043	3044	3045	3045	3045	
	3045	3046	3048	3048	3048	3050	3050	3050	3050	3050	3052	
	3053	3053	3053	3054	3054	3054	3056	3056	3058	3058	3059	
	3064	3085	3102	3117	3118		3118	3119	3119	3120	3120	
	3121	3122	3122	3123	3123	3124	3124	3124	3124	3126	3127	
	3127	3127	3128	3128	3128	3131	3132	3132	3134	3134	3134	
	3134	3134	3135	3135	3135	3136	3136	3137	3138	3140	3140	
	3141	3142	3143	3144	3146	3147	3150	3151	3181	3193	3197	
	3197	3241	3242	3252	3252	3260	3264					
TS4c	-856	11	14	23	24	29	29	34	36	38	46	50
	52	57	59	61	63	63	68	69	71	72	79	80
	81	85	87	90	100	105	108	112	129	133	136	137
	144	145	167	171	173	175	178	181	190	192	209	216
	218	223	227	229	233	236	240	241	242	243	247	249
	251	254	255	256	257	260	263	266	267	268	269	278
	279	283	285	289	290	291	299	301	305	309	310	317
	319	331	336	336	338	341	345	349	352	356	365	366
	368	371	380	387	389	391	400	413	424	426	429	441
	442	448	450	457	474	478	482	488	501	504	506	527
	532	556	559	579	583	611	612	616	621	626	640	647
	650	654	660	661	667	687	691	766	769	772	793	829
	831	832	833	834	835	840	852	856	858	858	859	898
	898	903	903	909	917	921	934	936	936	938	938	939
	940	940	941	941	946	947	955	955	956	957	958	958
	960	963	965	966	968	968	969	971	974	974	974	975
	977	977	1036	1044	1049	1052	1052	1052	1053	1055	1055	
	1060	1080	1083	1084	1088	1093	1097	1115	1123		1131	
	1132	1133	1135	1138	1140	1141	1141	1141	1165	1167	1192	
	1194	1200	1201	1202	1205	1213	1219	1228	1229	1236	1238	
	1239	1240	1244	1247	1272	1274	1275	1278	1288	1289	1290	
	1291	1297	1302	1332	1338	1339	1341	1343	1344	1356	1356	
	1357	1360	1375	1375	1392	1395	1397	1399	1403	1407	1409	
	1411	1412	1413	1415	1415	1416	1416	1417	1417	1418	1418	
	1419	1422	1423	1433	1434	1436	1436	1437	1440	1442	1445	
	1445	1446	1464	1469	1476	1479	1480	1485	1499	1500	1500	
	1502	1502	1503	1504	1505	1506	1507	1508	1508	1508	1509	

	1509	1510	1510	1511	1511	1512	1512	1513	1513	1514	1521	
	1521	1522	1523	1523	1523	1523	1524	1525	1525	1526	1526	
	1528	1528	1528	1530	1531	1531	1533	1534	1535	1537	1541	
	1544	1551	1552	1605	1611	1619	1661	1664	3040	3043	3046	
	3046	3046	3046	3047	3048	3048	3050	3050	3051	3051	3052	
	3052	3053	3053	3053	3054	3054	3056	3057	3058	3059	3060	
	3062	3069	3089	3090	3096	3116	3119	3120	3121	3121	3121	
	3122	3122	3123	3123	3123	3124	3124	3124	3125	3125	3127	
	3127	3128	3128	3130	3130	3132	3132	3132	3133	3134	3134	
	3134	3134	3135	3135	3136	3136	3137	3138	3140	3140	3141	
	3141	3142	3142	3146	3146	3147	3148	3150	3151	3182	3191	
	3198	3202	3237	3241	3255	3256	3261	3269				
4	13 16	17	26	31	32	37	39	43	48	49	50	54
	57	60	64	66	70	77	81	84	85	86	86	91
	94	98	103	106	110	117	131	134	134	139	141	143
	157	170	172	180	185	187	191	205	206	210	216	222
	225	231	236	236	237	244	245	245	249	252	253	254
	256	256	258	261	264	268	272	273	275	278	287	287
	292	293	294	297	300	302	303	317	318	319	330	338
	340	342	346	349	353	356	362	365	366	369	372	380
	384	387	390	404	413	419	426	430	441	448	448	451
	462	472	481	484	494	501	502	510	526	529	557	562
	578	582	607	614	617	619	621	642	642	651	654	660
	666	669	685	686	766	770	775	789	826	831	832	833
	835	836	838	845	855	858	886	893	895	900	902	903
	903	914	933	933	935	936	938	939	939	940	942	946
	948	950	953	954	954	956	959	959	960	962	964	965
	966	971	973	973	974	975	975	975	977	985	1040	
	1044	1049	1050	1052	1054	1055	1057	1057	1078	1081	1082	
	1084	1086	1098	1100	1114	1122	1131	1132	1134	1138	1140	
	1140	1142	1143	1167	1168	1191	1192	1199	1200	1201	1207	
	1214	1218	1228	1230	1231	1239	1240	1244	1244	1251	1272	
	1272	1275	1279	1285	1286	1287	1288	1296	1302	1336	1336	
	1344	1346	1347	1349	1352	1358	1358	1360	1372	1373	1390	
	1393	1396	1399	1402	1404	1412	1413	1413	1414	1414	1415	
	1415	1416	1417	1418	1419	1422	1424	1430	1431	1433	1434	
	1435	1436	1436	1445	1448	1448	1459	1463	1471	1474	1475	
	1480	1486	1499	1501	1502	1502	1503	1503	1505	1506	1506	
	1507	1508	1508	1508	1509	1510	1510	1511	1511	1511	1511	
	1512	1512	1513	1516	1521	1522	1522	1522	1523	1523	1524	
	1524	1525	1525	1526	1527	1528	1529	1530	1531	1534	1535	
	1536	1537	1538	1543	1546	1550	1551	1607	1610	1610	1661	
	1662	3041	3042	3044	3046	3046	3046	3046	3047	3048	3048	
	3048	3049	3049	3050	3050	3051	3052	3052	3053	3053	3053	
	3055	3056	3058	3060	3063	3064	3067	3082	3098	3117	3118	
	3118	3118	3119	3120	3121	3122	3122	3123	3123	3123	3124	
	3124	3124	3125	3125	3126	3127	3127	3128	3128	3129	3130	
	3130	3131	3131	3132	3132	3133	3134	3134	3135	3135	3135	
	3136	3136	3137	3139	3139	3140	3140	3140	3141	3143	3146	
	3148	3150	3186	3196	3199	3205	3231	3237	3250	3261	3268	
	3277											
H₂	4444											
TS4d	-1578	12	15	22	28	32	38	39	40	42	45	49
	55	57	64	65	66	73	74	77	78	81	86	88
	90	92	98	98	101	106	111	116	130	131	133	134
	140	148	153	169	173	178	181	184	193	199	203	213

	219	221	227	232	236	237	238	241	244	246	248	252
	254	255	255	256	258	261	264	267	271	272	275	277
	281	282	296	305	309	311	312	316	320	321	325	327
	336	337	340	344	348	352	354	359	366	368	368	370
	379	381	386	390	400	402	409	424	431	432	445	449
	451	452	463	475	479	487	498	500	506	526	527	530
	559	567	576	583	611	617	619	622	630	633	646	649
	652	659	660	661	669	690	692	756	770	775	779	787
	830	831	833	836	838	840	844	847	852	858	859	861
	899	903	903	904	908	916	936	937	938	940	940	941
	942	942	944	947	950	951	954	955	957	957	958	960
	962	962	964	965	967	972	974	975	975	975	976	977
	979	983	1035	1043	1050	1051	1052	1053	1056	1058	1063	
	1074	1081	1083	1084	1085	1089	1101	1105	1115	1120	1134	
	1134	1136	1139	1140	1140	1142	1143	1165	1167	1177	1193	
	1194	1201	1203	1203	1208	1214	1217	1227	1230	1237	1240	
	1243	1247	1248	1253	1269	1274	1275	1277	1289	1291	1292	
	1295	1296	1301	1322	1339	1343	1345	1348	1351	1355	1357	
	1359	1369	1373	1375	1380	1399	1400	1403	1407	1409	1411	
	1412	1413	1413	1414	1415	1415	1417	1417	1418	1420	1420	
	1423	1426	1429	1433	1434	1435	1436	1438	1438	1445	1448	
	1449	1456	1468	1470	1473	1480	1486	1488	1498	1501	1503	
	1503	1504	1504	1506	1506	1507	1508	1508	1509	1509	1509	
	1509	1510	1511	1511	1512	1512	1513	1513	1513	1516	1522	
	1523	1523	1523	1523	1524	1524	1525	1525	1526	1527	1528	
	1530	1530	1531	1531	1532	1534	1535	1540	1543	1545	1546	
	1551	1552	1610	1610	1657	1660	1662	3041	3043	3044	3044	
	3046	3047	3047	3047	3048	3049	3050	3050	3050	3050	3050	
	3051	3053	3053	3054	3054	3055	3055	3057	3057	3058	3061	
	3070	3084	3104	3112	3114	3117	3119	3119	3120	3121	3121	
	3123	3123	3123	3123	3123	3124	3125	3125	3126	3127	3127	
	3128	3128	3128	3131	3131	3132	3132	3134	3134	3134	3134	
	3135	3135	3136	3136	3136	3136	3137	3138	3138	3139	3139	
	3139	3141	3143	3146	3146	3148	3148	3163	3181	3188	3190	
	3212	3235	3239	3255	3259	3265	3270					

Table S5. The energies (with ZPE correction), enthalpies and free energies (in au at 298K) and corresponding relative values (in kcal/mol) for the formation of **4**+H₂, obtained with B3PW91-PCM method

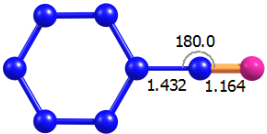
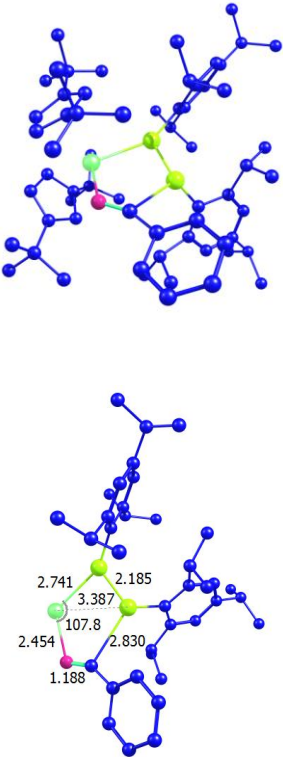
Species	E	H	G
3	-3276.560545	-3276.485692	-3276.643840
TS4a	-3276.530005(19.2)	-3276.455895(18.7)	-3276.612240(19.8)
INT4a	-2349.163426	-2349.110486	-2349.227260
ArPH₂	-927.380338	-927.360081	-927.413460
INT4a+ArPH₂	-3276.543764(10.5)	-3276.470567(9.5)	-3276.640720(2.0)
TS4b	-3276.515994(28.0)	-3276.441360(27.8)	-3276.599440(27.9)
INT4b	-3276.553361(4.5)	-3276.479083 (4.1)	-3276.636140(4.8)
TS4c	-3276.519174(26.0)	-3276.445082 (25.5)	-3276.601080(26.8)
4	-3275.413200	-3275.339967	-3275.497220
H₂	-1.164478	-1.161173	-1.164170
4+H₂	-3276.577678(-10.8)	-3276.501140 (-9.7)	-3276.661390(-11.0)
TS4d	-3276.450090(69.3)	-3276.376872(68.3)	-3276.530780(70.9)

^a : The relative energies in parentheses are with respect to the corresponding energy of **3**.

Table S6. The optimized Cartesian Coordinates (in Å) of stationary points for 4+PhCN, obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
4	C	3.511110	-0.973191	-0.443054	
	C	3.172823	0.141513	-1.259661	
	H	2.828188	0.080469	-2.283855	
	C	3.423802	1.351183	-0.554096	
	C	3.879354	0.976159	0.738807	
	H	4.182415	1.653468	1.531226	
	C	3.928028	-0.439038	0.807646	
	H	4.301911	-1.011426	1.647399	
	C	3.691430	-2.416555	-0.899398	
	C	3.420975	-3.411803	0.237732	
	H	4.086177	-3.247728	1.092726	
	H	3.590007	-4.437112	-0.112773	
	H	2.383674	-3.352340	0.588763	
	C	5.164151	-2.569876	-1.340849	
	H	5.401173	-1.880444	-2.158987	
	H	5.353467	-3.592840	-1.690423	
	H	5.850049	-2.359542	-0.512165	
	C	2.785392	-2.758546	-2.087872	
	H	1.725981	-2.638925	-1.835018	
	H	2.949154	-3.798626	-2.394848	
	H	3.005924	-2.123903	-2.952682	
	C	3.401298	2.769145	-1.113567	
	C	4.860417	3.256045	-1.232347	
	H	5.353093	3.282256	-0.253785	
	H	4.892287	4.267330	-1.657230	
	H	5.440984	2.593483	-1.884197	
	C	2.752322	2.811713	-2.502843	
	H	3.326021	2.222460	-3.227370	
	H	2.720244	3.844348	-2.870054	
	H	1.726865	2.425308	-2.483015	
	C	2.638580	3.717703	-0.175603	
	H	1.577502	3.441089	-0.112497	
	H	2.680332	4.748904	-0.546954	
	H	3.057426	3.713237	0.837725	
	C	1.443258	-0.237183	3.706215	
	C	1.194185	1.154555	3.549913	
	H	1.862571	1.945506	3.873316	
	C	-0.138821	1.355576	3.075215	
	C	-0.682199	0.066891	2.849476	
	H	-1.673050	-0.160491	2.474845	
	C	0.287510	-0.904163	3.215304	
	H	0.123255	-1.975211	3.192137	
	C	2.549568	-0.859479	4.551395	
	C	2.881382	-2.290020	4.104911	
	H	2.003369	-2.942950	4.156704	
	H	3.649036	-2.721552	4.758416	
	H	3.260669	-2.319525	3.078658	
	C	2.011274	-0.924080	5.999818	
	H	1.767765	0.076708	6.373647	
	H	2.762169	-1.366094	6.667378	
	H	1.103139	-1.534483	6.054094	
	C	3.828668	-0.009705	4.559858	
	H	4.264377	0.092050	3.561209	
	H	4.581709	-0.474501	5.207372	
	H	3.640314	0.996459	4.950921	
	C	-0.904372	2.673518	3.120701	
	C	-1.162336	2.994288	4.609542	
	H	-1.713422	2.180586	5.094262	
	H	-1.755406	3.912999	4.703536	
	H	-0.222753	3.138272	5.155158	
	C	-0.108204	3.833346	2.505075	

	H	0.895010	3.918902	2.938772
	H	-0.625504	4.783909	2.684527
	H	-0.007370	3.721642	1.419734
	C	-2.255787	2.553565	2.406108
	H	-2.127195	2.241503	1.363312
	H	-2.774840	3.519448	2.418541
	H	-2.904826	1.822975	2.901759
	C	-2.186219	-2.019462	0.428578
	C	-1.955757	-3.240058	1.136166
	C	-2.976127	-3.808353	1.901874
	H	-2.773659	-4.733343	2.435252
	C	-4.244547	-3.238796	2.002708
	C	-4.475054	-2.080932	1.266642
	H	-5.468335	-1.640488	1.303652
	C	-3.496421	-1.470567	0.471269
	C	-0.647350	-4.015783	1.011513
	H	0.157461	-3.282411	0.874218
	C	-0.280100	-4.863494	2.235576
	H	-0.350168	-4.295362	3.170602
	H	0.747832	-5.232151	2.136569
	H	-0.924595	-5.744996	2.334691
	C	-0.674039	-4.903229	-0.244460
	H	-1.464983	-5.658735	-0.158678
	H	0.282471	-5.425477	-0.373770
	H	-0.865043	-4.311074	-1.145247
	C	-5.340107	-3.862800	2.848188
	H	-6.219336	-3.207539	2.769522
	C	-4.951516	-3.935106	4.331424
	H	-4.084919	-4.590133	4.483189
	H	-5.778853	-4.334713	4.930959
	H	-4.693807	-2.944335	4.722226
	C	-5.749258	-5.245683	2.320826
	H	-6.065973	-5.191269	1.273377
	H	-6.579242	-5.656671	2.908939
	H	-4.915191	-5.955488	2.380391
	C	-3.922687	-0.297257	-0.400547
	H	-3.061238	0.369518	-0.504377
	C	-5.073078	0.537745	0.172252
	H	-6.030816	0.003509	0.145189
	H	-5.201553	1.447851	-0.423604
	H	-4.882856	0.838073	1.209027
	C	-4.282959	-0.802750	-1.806452
	H	-3.443162	-1.341059	-2.257619
	H	-4.541414	0.032942	-2.467878
	H	-5.141073	-1.485901	-1.762537
	C	-1.220781	1.262368	-2.774831
	C	-2.040107	2.420900	-2.885048
	C	-2.486933	2.827198	-4.146462
	H	-3.109338	3.715948	-4.222523
	C	-2.176499	2.135058	-5.314017
	C	-1.358727	1.013141	-5.190907
	H	-1.087009	0.458804	-6.087135
	C	-0.859239	0.571192	-3.962525
	C	-2.410067	3.286885	-1.689272
	H	-2.350764	2.646628	-0.801032
	C	-1.385575	4.416666	-1.510071
	H	-0.372248	4.018242	-1.394020
	H	-1.620987	5.021286	-0.625268
	H	-1.384058	5.080657	-2.383753
	C	-3.828204	3.867569	-1.749676
	H	-3.918837	4.666368	-2.495803
	H	-4.092161	4.305003	-0.779655
	H	-4.570848	3.099408	-1.990104
	C	-2.704776	2.597061	-6.660018
	H	-3.310178	3.496076	-6.477112
	C	-3.621732	1.546261	-7.301773
	H	-3.072149	0.624123	-7.525615
	H	-4.040802	1.921571	-8.243425
	H	-4.452857	1.286151	-6.637081

	C -1.569822 2.993281 -7.614770 H -0.932513 3.767543 -7.173261 H -1.975123 3.380375 -8.557605 H -0.933254 2.133189 -7.854958 C 0.070849 -0.632009 -3.991835 H 0.450849 -0.782083 -2.976572 C -0.668268 -1.913596 -4.397461 H -1.491420 -2.123583 -3.707757 H 0.014574 -2.771852 -4.378387 H -1.079252 -1.834098 -5.411826 C 1.276371 -0.387018 -4.912030 H 0.976970 -0.283113 -5.961693 H 1.974564 -1.230995 -4.858443 H 1.816118 0.524877 -4.632362 P -0.738366 -1.400442 -0.601862 P -0.650088 0.749504 -1.082724 Th 1.199319 0.212503 0.821043	
PhCN	C -1.349158 -7.094892 1.739016 C -2.497248 -7.447135 2.440891 C -0.189158 -6.738996 2.444546 H -3.396219 -7.722946 1.897191 C -2.494214 -7.446204 3.836597 C -0.185026 -6.737728 3.848118 H -3.393843 -7.722217 4.379894 H 0.717418 -6.460851 4.384144 C -1.340177 -7.092137 4.537199 H -1.339515 -7.091934 5.623399 H -1.341731 -7.092613 0.653507 C 0.996119 -6.375344 1.728742 N 1.959650 -6.079726 1.146855	
TS9	C 0.449948 8.298682 3.137114 C 1.295995 9.435528 3.057581 H 1.046094 10.423487 3.422265 C 2.453591 9.124762 2.284318 C 2.348660 7.751302 1.947760 H 3.048071 7.192756 1.339840 C 1.139816 7.239300 2.483775 H 0.777477 6.225635 2.357643 C -1.029650 8.321852 3.510396 C -1.765501 9.006875 2.335195 H -1.418541 10.036902 2.197273 H -2.846209 9.032543 2.525905 H -1.596803 8.464969 1.397546 C -1.609559 6.909411 3.668843 H -1.519182 6.334796 2.739703 H -2.677097 6.972443 3.912184 H -1.110203 6.352285 4.466690 C -1.298382 9.138970 4.781422 H -0.805313 8.708235 5.657133 H -2.375696 9.174946 4.985322 H -0.947810 10.170330 4.674933 C 3.413248 10.143059 1.674907 C 3.979090 11.115522 2.718374 H 3.189674 11.598290 3.301861 H 4.562488 11.902538 2.224047 H 4.639571 10.605467 3.428204 C 2.610398 10.952718 0.631913 H 2.181441 10.294015 -0.132139 H 3.261707 11.680252 0.130984 H 1.788431 11.502414 1.103569 C 4.580779 9.458098 0.951734 H 5.189148 8.862583 1.641491 H 5.236107 10.214290 0.503874 H 4.234424 8.802876 0.144112 C 5.361926 6.292841 4.691377 C 4.557665 5.412601 5.469813 H 4.711089 5.200580 6.519877 C 3.609938 4.753102 4.628057 C 3.784893 5.292082 3.333660	

	H	3.232185	5.007151	2.446664	
	C	4.840115	6.238660	3.370531	
	H	5.234687	6.766865	2.510682	
	C	6.696162	6.913931	5.088437	
	C	7.789370	5.869691	4.766233	
	H	7.622154	4.941464	5.324390	
	H	8.779307	6.258023	5.038447	
	H	7.800387	5.624569	3.697895	
	C	6.993541	8.185153	4.281323	
	H	7.014682	7.988503	3.203247	
	H	7.977746	8.581753	4.557483	
	H	6.251388	8.966788	4.479531	
	C	6.760202	7.236012	6.585849	
	H	5.969183	7.930460	6.889470	
	H	7.727649	7.690955	6.830607	
	H	6.669102	6.325848	7.186983	
	C	2.800648	3.500539	4.946464	
	C	2.511988	3.363088	6.445703	
	H	3.436791	3.259446	7.022874	
	H	1.909839	2.465258	6.631266	
	H	1.964593	4.228009	6.831038	
	C	1.475513	3.463777	4.169825	
	H	0.827908	4.300042	4.450840	
	H	0.941368	2.529057	4.381836	
	H	1.639350	3.504503	3.086840	
	C	3.656377	2.289870	4.508724	
	H	3.857714	2.318199	3.431967	
	H	3.135209	1.350473	4.734799	
	H	4.619391	2.280419	5.031847	
	C	0.579480	6.809840	6.880280	
	C	-0.365874	6.706227	7.968577	
	C	-0.982969	5.450524	8.128032	
	H	-0.700692	4.625712	7.481354	
	C	-1.944992	5.280339	9.115890	
	H	-2.414680	4.309462	9.245919	
	C	-2.306513	6.352951	9.933801	
	H	-3.060163	6.215458	10.704550	
	C	-1.704187	7.599539	9.762445	
	H	-1.989388	8.434668	10.395666	
	C	-0.730377	7.783073	8.785340	
	H	-0.231412	8.737113	8.645079	
	C	3.405006	8.708603	9.307334	
	C	3.586193	9.873100	10.111618	
	C	4.425002	9.824405	11.230995	
	H	4.570210	10.727005	11.819989	
	C	5.070711	8.660982	11.638748	
	C	4.808463	7.505210	10.908365	
	H	5.253024	6.569685	11.237587	
	C	3.986700	7.498030	9.774891	
	C	2.794815	11.160297	9.897997	
	H	2.556176	11.238288	8.834665	
	C	3.525944	12.447476	10.293609	
	H	3.647739	12.544308	11.379749	
	H	2.943703	13.313023	9.957665	
	H	4.515270	12.511064	9.830522	
	C	1.468987	11.058562	10.669962	
	H	0.891205	10.186856	10.344276	
	H	0.856808	11.956421	10.516701	
	H	1.656424	10.955708	11.746432	
	C	5.985238	8.654720	12.850293	
	H	6.020765	9.684961	13.232071	
	C	7.419157	8.250204	12.480546	
	H	7.455224	7.221608	12.101634	
	H	8.077154	8.306173	13.356666	
	H	7.827333	8.906042	11.703635	
	C	5.438157	7.765790	13.976460	
	H	4.428043	8.073698	14.269018	
	H	6.082819	7.820661	14.862452	
	H	5.390006	6.715279	13.664966	

	C	3.653887	6.140920	9.176287	
	H	3.398195	6.300168	8.121115	
	C	4.795378	5.119494	9.255565	
	H	5.747515	5.542249	8.921201	
	H	4.569338	4.244406	8.636279	
	H	4.937752	4.745992	10.276637	
	C	2.416881	5.566942	9.886944	
	H	2.644369	5.380251	10.944248	
	H	2.105940	4.616286	9.435592	
	H	1.572650	6.260250	9.847822	
	C	3.608610	11.664797	6.337482	
	C	2.507019	12.562998	6.274288	
	C	2.720509	13.928823	6.480365	
	H	1.864067	14.599155	6.439812	
	C	3.985345	14.464566	6.725957	
	C	5.058040	13.577998	6.749191	
	H	6.056025	13.975329	6.928900	
	C	4.905408	12.199160	6.560083	
	C	1.084134	12.121508	5.962963	
	H	1.130444	11.053102	5.723615	
	C	0.516771	12.867789	4.744874	
	H	0.369807	13.934033	4.954921	
	H	-0.461830	12.458831	4.463884	
	H	1.180934	12.795236	3.876195	
	C	0.145067	12.285702	7.164751	
	H	0.487855	11.685787	8.012099	
	H	-0.869669	11.957952	6.905198	
	H	0.084840	13.333887	7.484291	
	C	4.194678	15.951941	6.948258	
	H	5.272339	16.105829	7.100168	
	C	3.779630	16.777124	5.721979	
	H	4.315636	16.450291	4.824003	
	H	3.994670	17.840934	5.880869	
	H	2.705257	16.681214	5.523650	
	C	3.475834	16.446851	8.211104	
	H	2.389157	16.329681	8.120561	
	H	3.683101	17.510162	8.383572	
	H	3.799960	15.887903	9.095718	
	C	6.167334	11.347934	6.606301	
	H	5.874333	10.327608	6.336693	
	C	7.215216	11.818502	5.588317	
	H	6.802019	11.851635	4.573822	
	H	8.073279	11.135456	5.583858	
	H	7.596788	12.819358	5.824575	
	C	6.762234	11.288490	8.018930	
	H	7.042398	12.286738	8.379045	
	H	7.665232	10.665092	8.028977	
	H	6.046948	10.857636	8.727199	
	N	0.924211	6.450678	5.801831	
	P	2.284849	8.881123	7.779893	
	P	3.407079	9.820146	6.157683	
	Th	2.796190	7.585586	4.692563	
9	C	-0.124590	7.780690	3.368094	
	C	0.675540	8.864661	2.917087	
	H	0.576627	9.891403	3.247382	
	C	1.539528	8.423431	1.868695	
	C	1.312226	7.037642	1.719609	
	H	1.795430	6.389337	0.999852	
	C	0.316538	6.636353	2.649757	
	H	-0.098327	5.637910	2.726684	
	C	-1.403035	7.885062	4.190797	
	C	-2.536442	8.261508	3.209476	
	H	-2.333890	9.222311	2.722369	
	H	-3.492063	8.343955	3.743542	
	H	-2.647861	7.502885	2.426069	
	C	-1.760539	6.549704	4.855659	
	H	-1.910153	5.755938	4.114315	
	H	-2.695296	6.650166	5.420275	
	H	-0.978289	6.232005	5.551412	

	H	4.627374	6.792095	11.753138	
	C	3.537910	7.630491	10.112873	
	C	1.494678	10.923806	10.271594	
	H	1.136478	10.793156	9.245850	
	C	2.301673	12.228569	10.313667	
	H	2.681016	12.433174	11.322677	
	H	1.671674	13.075508	10.016220	
	H	3.157180	12.187039	9.631938	
	C	0.256089	11.013763	11.173997	
	H	-0.340071	10.095118	11.132465	
	H	-0.383723	11.845785	10.855821	
	H	0.525571	11.187695	12.222731	
	C	4.189346	8.573991	13.782342	
	H	3.821887	9.480780	14.282834	
	C	5.722767	8.600722	13.845712	
	H	6.156376	7.708987	13.377530	
	H	6.064029	8.628665	14.887586	
	H	6.126002	9.478828	13.329530	
	C	3.627147	7.365408	14.544537	
	H	2.531549	7.365676	14.536457	
	H	3.961711	7.378092	15.588976	
	H	3.964285	6.422461	14.097580	
	C	3.984332	6.473966	9.229062	
	H	3.624666	6.657365	8.212490	
	C	5.514325	6.372060	9.154306	
	H	5.960005	7.307623	8.804573	
	H	5.805295	5.575665	8.459486	
	H	5.955017	6.131505	10.129246	
	C	3.395094	5.142146	9.719905	
	H	3.767264	4.892749	10.721187	
	H	3.682748	4.325184	9.047612	
	H	2.302894	5.175384	9.767409	
	C	3.806949	10.921837	6.553833	
	C	2.937741	11.989133	6.181421	
	C	3.348822	13.312967	6.363838	
	H	2.665013	14.111110	6.081064	
	C	4.593664	13.652148	6.892147	
	C	5.434709	12.604188	7.250133	
	H	6.410361	12.841989	7.671551	
	C	5.074441	11.258759	7.103356	
	C	1.548185	11.791225	5.590148	
	H	1.412647	10.715462	5.434255	
	C	1.396687	12.498100	4.234776	
	H	1.440722	13.588988	4.338057	
	H	0.425182	12.258791	3.783742	
	H	2.183565	12.205365	3.532212	
	C	0.446744	12.270007	6.546072	
	H	0.485649	11.729838	7.495439	
	H	-0.543967	12.104436	6.105119	
	H	0.541110	13.342282	6.758862	
	C	5.021787	15.097321	7.072569	
	H	6.029521	15.082075	7.511206	
	C	5.114689	15.834440	5.728955	
	H	5.797376	15.322058	5.041968	
	H	5.479893	16.858604	5.873608	
	H	4.133916	15.895922	5.242012	
	C	4.105445	15.848204	8.048665	
	H	3.081711	15.914432	7.661073	
	H	4.467240	16.871127	8.209735	
	H	4.062923	15.343539	9.020035	
	C	6.093675	10.231412	7.575711	
	H	5.667183	9.242881	7.372862	
	C	7.416016	10.339993	6.804835	
	H	7.257831	10.242431	5.725338	
	H	8.107623	9.548922	7.119592	
	H	7.913894	11.301356	6.982918	
	C	6.334954	10.334511	9.088281	
	H	6.760859	11.307888	9.362516	
	H	7.040509	9.561575	9.417501	

	H	5.403102	10.203065	9.647958	
	N	1.678247	6.759127	6.285247	
	P	1.922033	8.815346	7.984196	
	P	3.349230	9.114795	6.340907	
	Th	2.526099	7.127709	4.293706	

Table S7. Frequencies of the stationary points optimized for 4+PhCN.

Species	Frequencies (cm ⁻¹)												
4	13	16	17	26	31	32	37	39	43	48	49	50	54
	57	60	64	66	70	77	81	84	85	86	86	86	91
	94	98	103	106	110	117	131	134	134	139	141	141	143
	157	170	172	180	185	187	191	205	206	210	216	216	222
	225	231	236	236	237	244	245	245	249	252	253	253	254
	256	256	258	261	264	268	272	273	275	278	287	287	287
	292	293	294	297	300	302	303	317	318	319	330	330	338
	340	342	346	349	353	356	362	365	366	369	372	372	380
	384	387	390	404	413	419	426	430	441	448	448	448	451
	462	472	481	484	494	501	502	510	526	529	557	557	562
	578	582	607	614	617	619	621	642	642	651	654	654	660
	666	669	685	686	766	770	775	789	826	831	832	832	833
	835	836	838	845	855	858	886	893	895	900	902	902	903
	903	914	933	933	935	936	938	939	939	940	942	942	946
	948	950	953	954	954	956	959	959	960	962	964	964	965
	966	971	973	973	974	975	975	975	975	977	985	1040	1040
	1044	1049	1050	1052	1054	1055	1057	1057	1078	1081	1082	1082	1082
	1084	1086	1098	1100	1114	1122	1131	1132	1134	1138	1140	1140	1140
	1140	1142	1143	1167	1168	1191	1192	1199	1200	1201	1207	1207	1207
	1214	1218	1228	1230	1231	1239	1240	1244	1244	1251	1272	1272	1272
	1272	1275	1279	1285	1286	1287	1288	1296	1302	1336	1336	1336	1336
	1344	1346	1347	1349	1352	1358	1358	1360	1372	1373	1390	1390	1390
	1393	1396	1399	1402	1404	1412	1413	1413	1414	1414	1415	1415	1415
	1415	1416	1417	1418	1419	1422	1424	1430	1431	1433	1434	1434	1434
	1435	1436	1436	1445	1448	1448	1459	1463	1471	1474	1475	1475	1475
	1480	1486	1499	1501	1502	1502	1503	1503	1505	1506	1506	1506	1506
	1507	1508	1508	1508	1509	1510	1510	1511	1511	1511	1511	1511	1511
	1512	1512	1513	1516	1521	1522	1522	1522	1523	1523	1524	1524	1524
	1524	1525	1525	1526	1527	1528	1529	1530	1531	1534	1535	1535	1535
	1536	1537	1538	1543	1546	1550	1551	1607	1610	1610	1661	1661	1661
	1662	3041	3042	3044	3046	3046	3046	3046	3047	3048	3048	3048	3048
	3048	3049	3049	3050	3050	3051	3052	3052	3053	3053	3053	3053	3053
	3055	3056	3058	3060	3063	3064	3067	3082	3098	3117	3118	3118	3118
	3118	3118	3119	3120	3121	3122	3122	3123	3123	3123	3124	3124	3124
	3124	3124	3125	3125	3126	3127	3127	3128	3128	3129	3130	3130	3130
	3130	3131	3131	3132	3132	3133	3134	3134	3135	3135	3135	3135	3135
	3136	3136	3137	3139	3139	3140	3140	3140	3141	3143	3146	3146	3146
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	3277												
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	463	481	482	484	485	498	503	507	523	527	536	558	

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	971	972	973	974	974	977	993	1014	1017	1033	1044		
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	265	265	268	269	269	274	280	283	296	299	312	313	
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	361	364	367	368	368	380	381	385	386	398	402	414	
	418	423	424	429	441	446	446	449	454	466	478	481	
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	597	614	615	620	620	627	630	634	646	653	653	661	
	662	668	674	693	694	702	738	772	774	779	782	786	
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	860	902	903	906	906	918	918	923	935	936	937	938	
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	974	974	975	975	978	979	1002	1016	1044	1044	1051		
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	1245	1250	1270	1275	1276	1277	1283	1288	1288	1290	1290		
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	1412	1414	1414	1415	1415	1416	1417	1417	1418	1419	1422		

	1424	1424	1433	1434	1435	1436	1436	1437	1442	1444	1450
	1451	1469	1469	1475	1478	1484	1485	1488	1500	1501	1502
	1503	1504	1504	1506	1506	1507	1507	1508	1508	1509	1509
	1510	1511	1511	1511	1512	1512	1513	1513	1514	1520	1520
	1521	1521	1522	1522	1523	1523	1524	1525	1525	1526	1526
	1527	1528	1529	1530	1531	1531	1534	1535	1538	1540	1542
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	3057	3059	3059	3060	3072	3080	3087	3104	3114	3114	3119
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	3124	3126	3126	3126	3127	3127	3128	3128	3129	3130	3131
	3132	3132	3133	3133	3134	3134	3134	3134	3136	3136	3136
	3136	3140	3141	3141	3145	3145	3147	3148	3151	3154	3156
	3162	3178	3184	3185	3194	3197	3206	3219	3229	3231	3248
	3249	3256	3261	3265	3268						

Table S8. The energies (with ZPE correction), enthalpies and free energies (in au at 298K) and corresponding relative values (in kcal/mol) for 4+PhCN, obtained with B3PW91-PCM method

Species	E	H	G
4	-3275.383200	-3275.309967	-3275.464220
PhCN	-324.260020	-324.252976	-324.278440
4+PhCN	-3599.643220	-3599.562943	-3599.742660
TS9	-3599.628032(9.5)	-3599.547804(9.5)	-3599.714990(17.4)
9	-3599.679216(-22.6)	-3599.599086(-22.7)	-3599.766590(-15.0)

^a : The relative energies in parentheses are with respect to the corresponding energy of 4+PhCN.

4. NMR Spectra

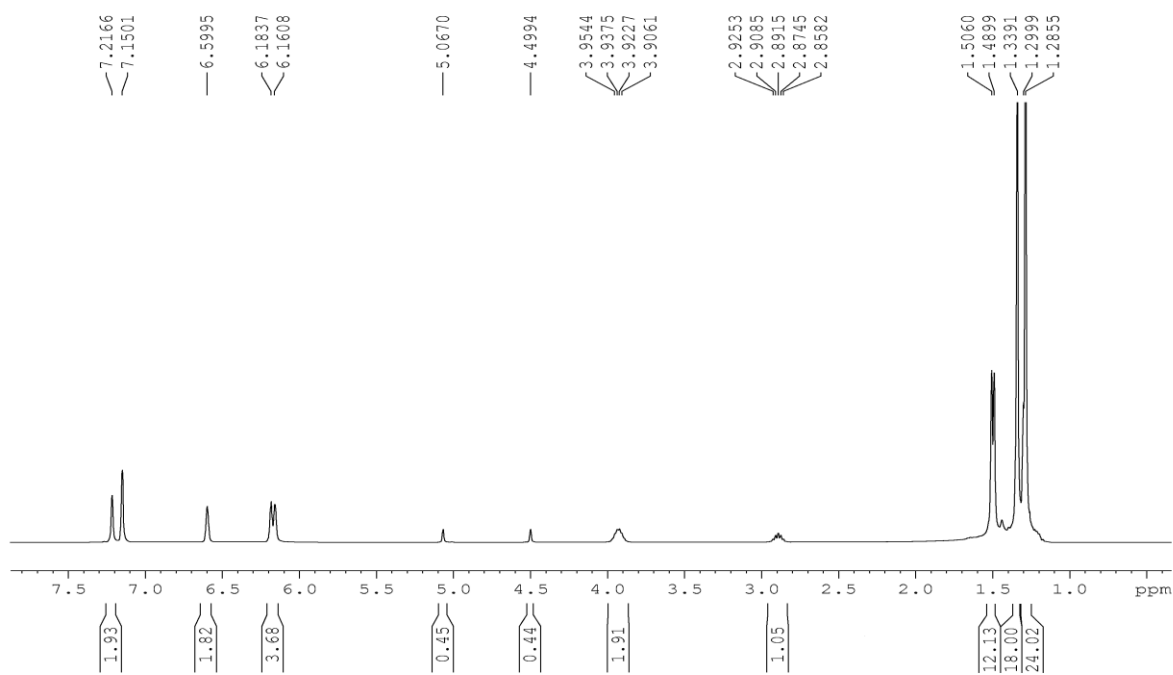


Figure S2. ^1H NMR spectrum for **2**.

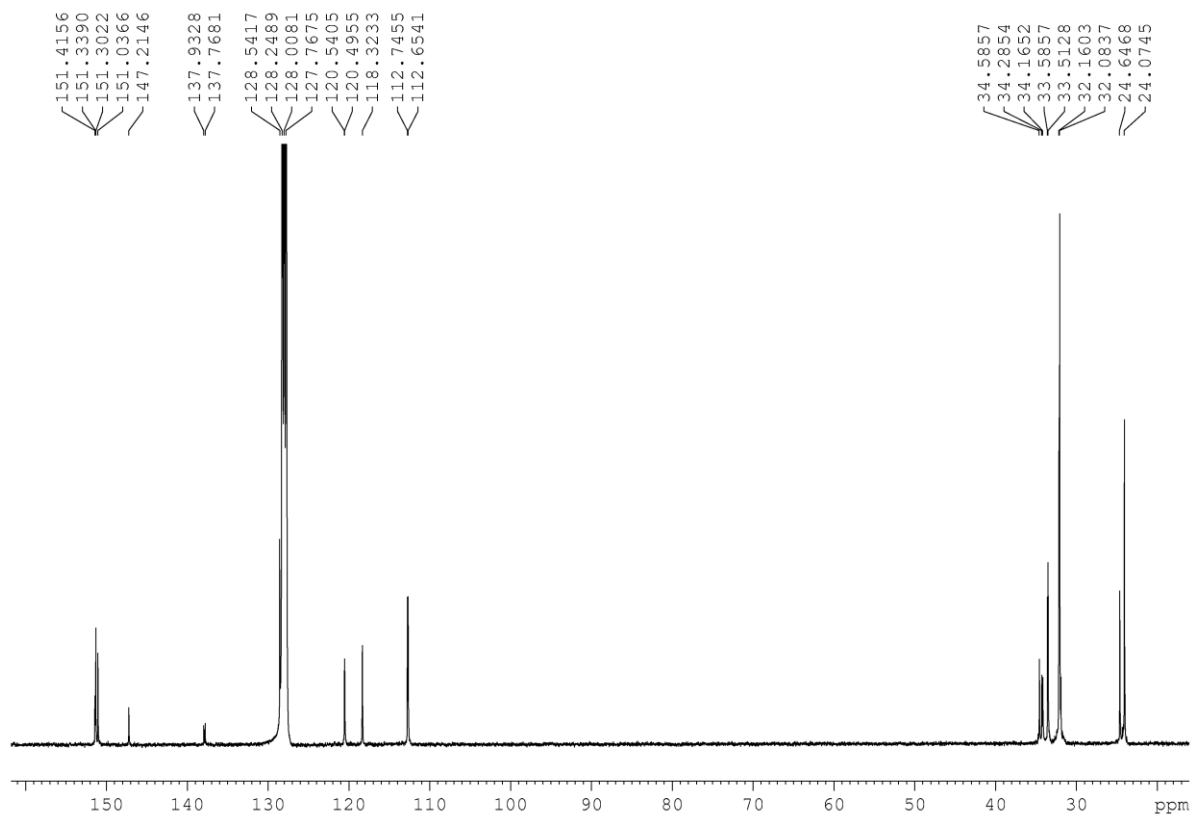


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum for **2**.

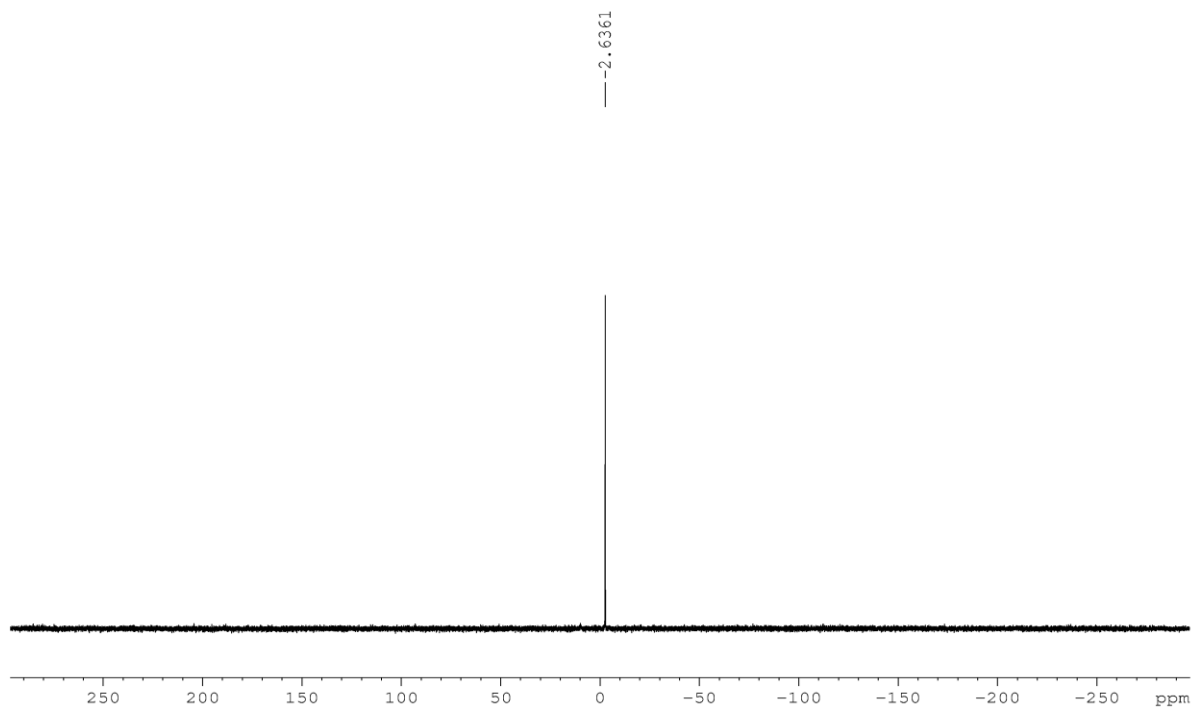


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **2**.

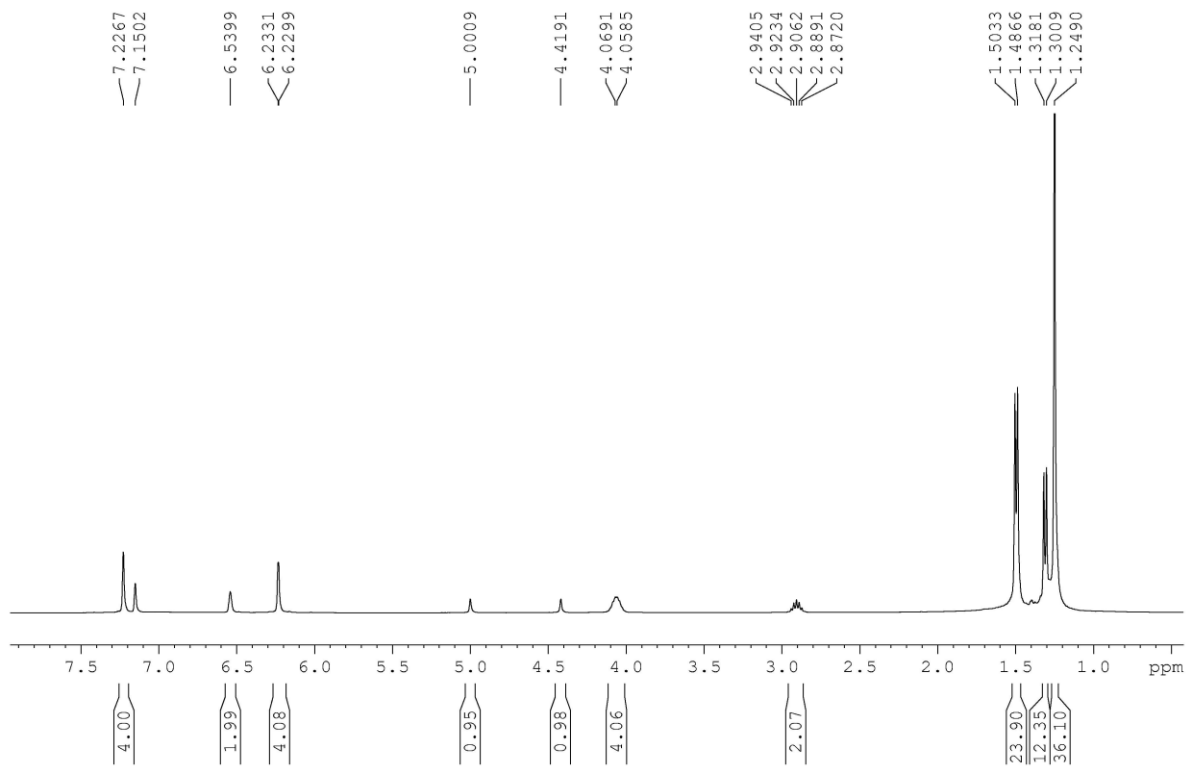


Figure S5. ^1H NMR spectrum for **3**.

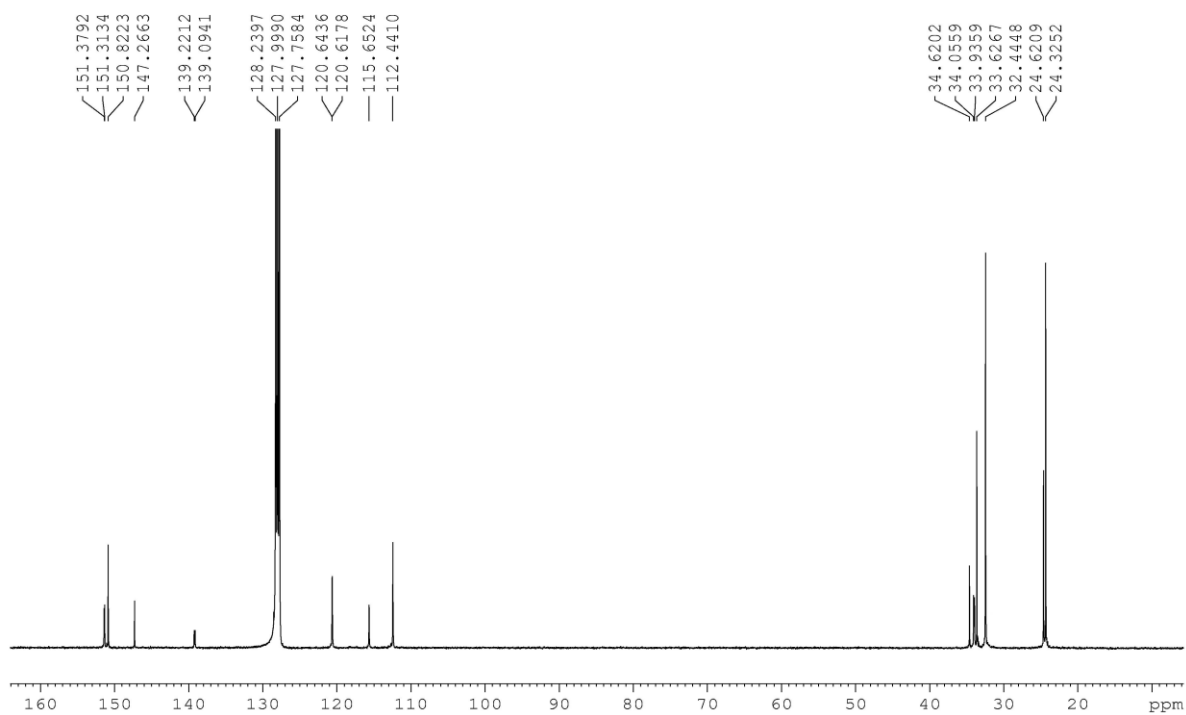


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum for **3**.

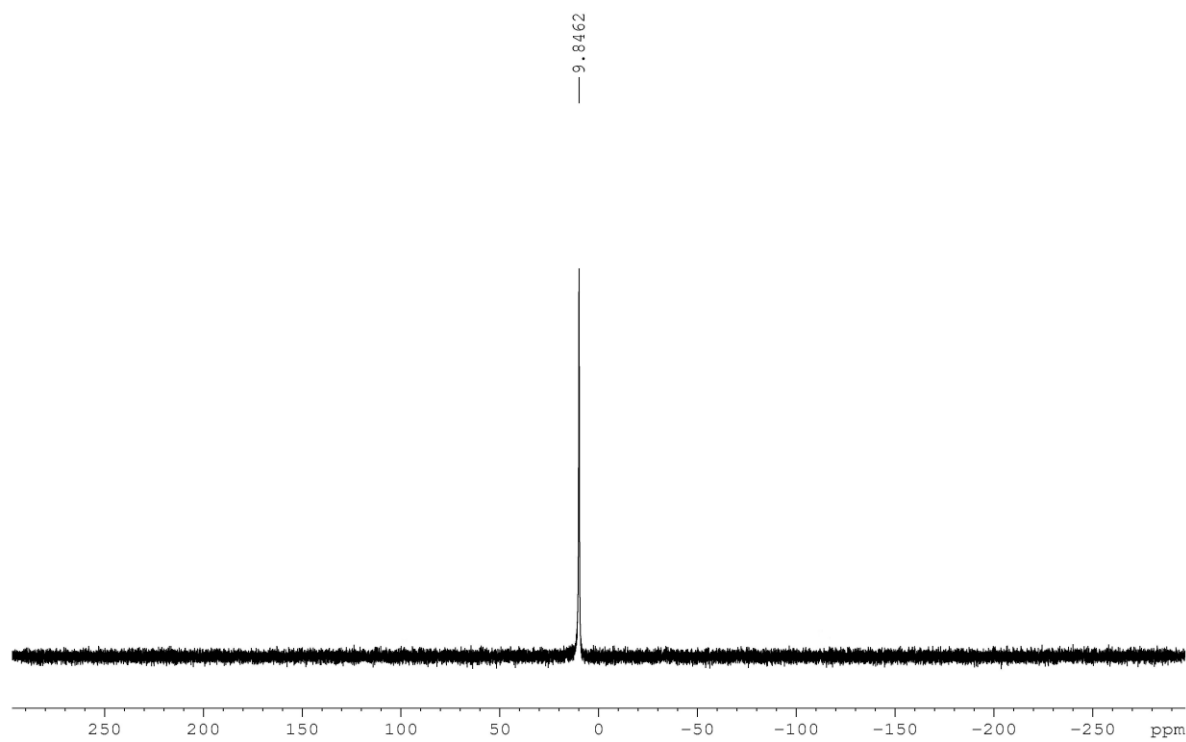


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **3**.

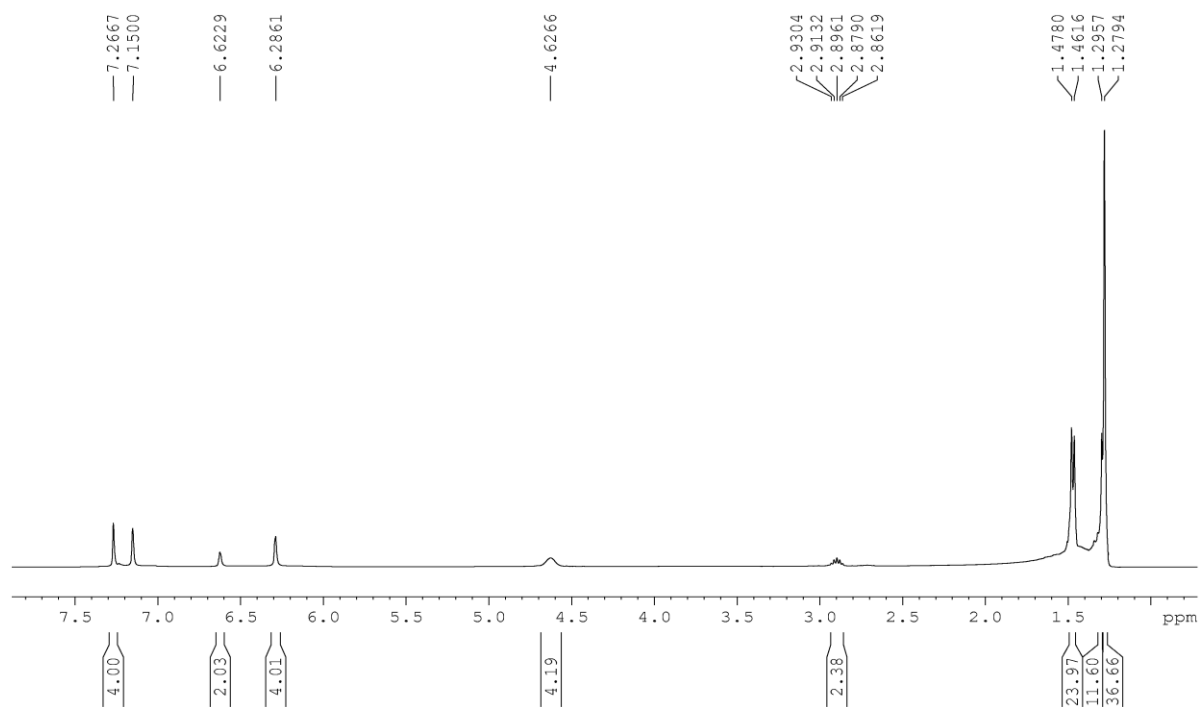


Figure S8. ¹H NMR spectrum for **4**.

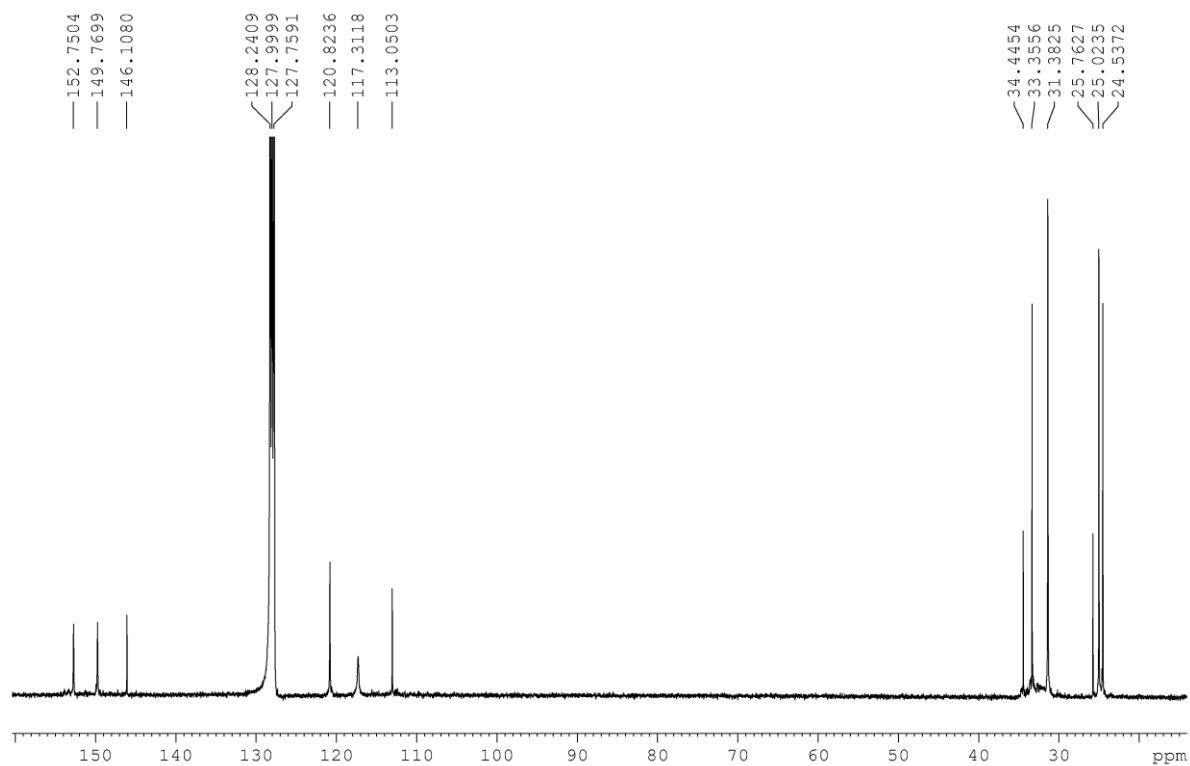


Figure S9. ¹³C{¹H} NMR spectrum for **4**.

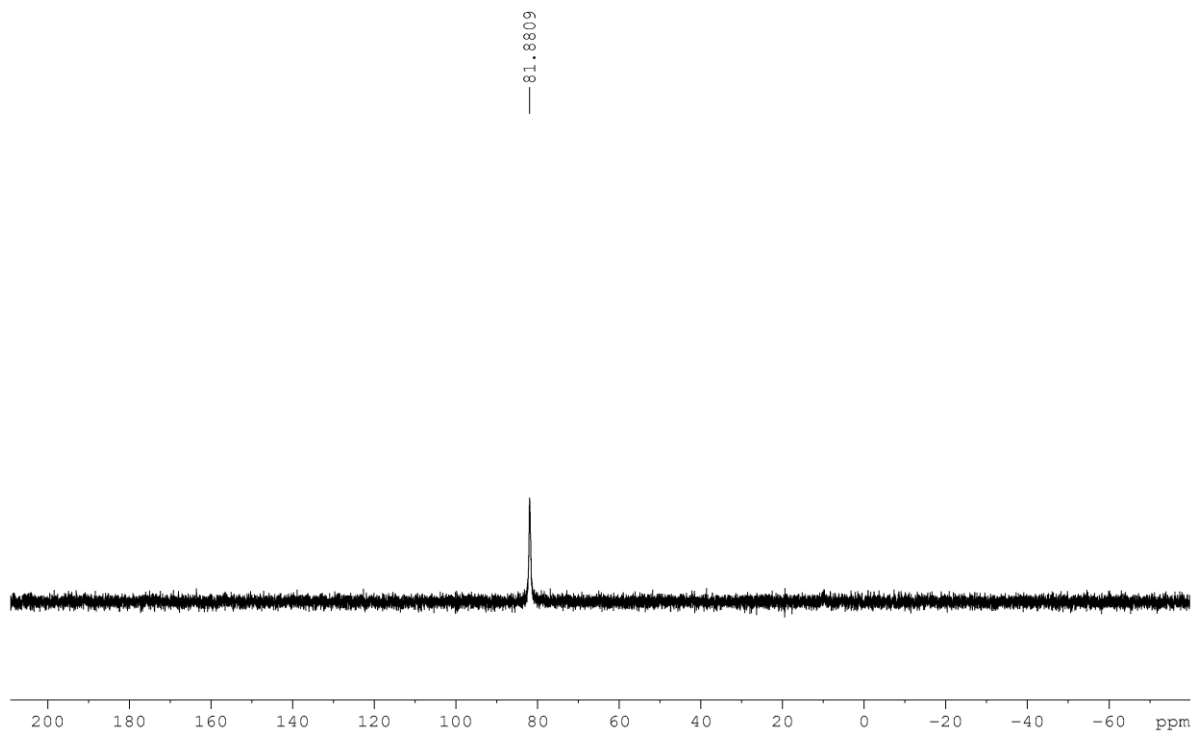


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **4**.

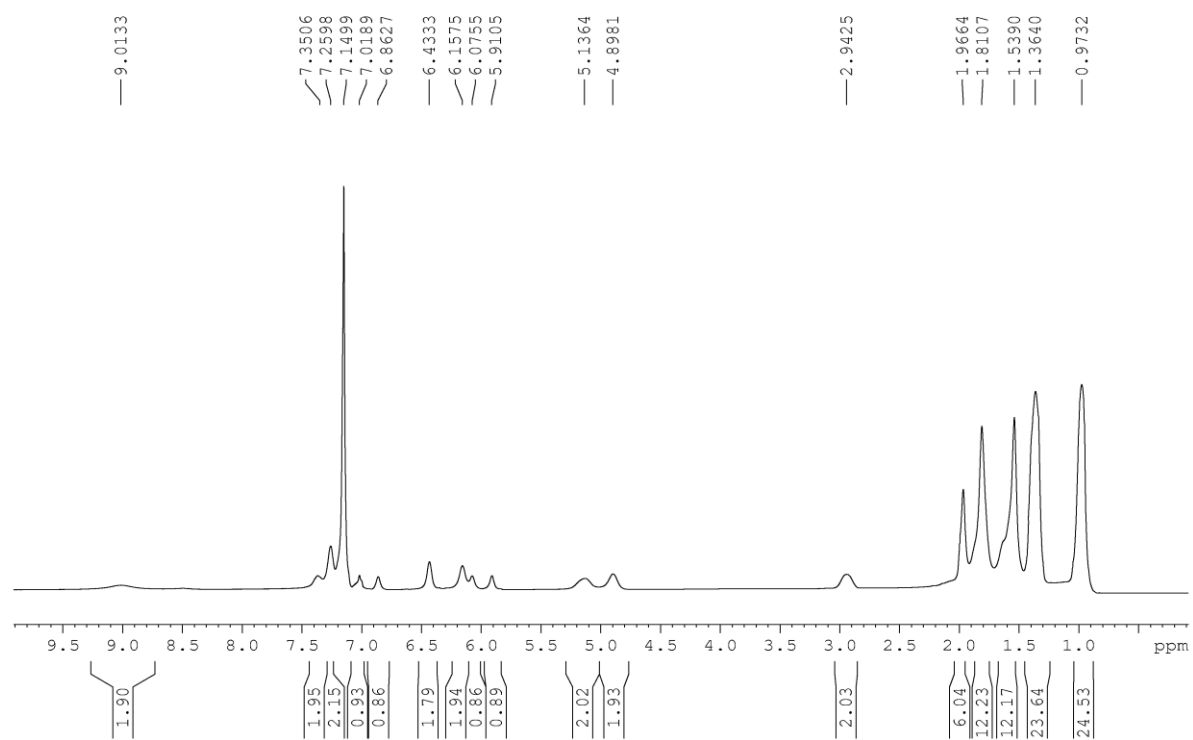


Figure S11. ^1H NMR spectrum for **5**.

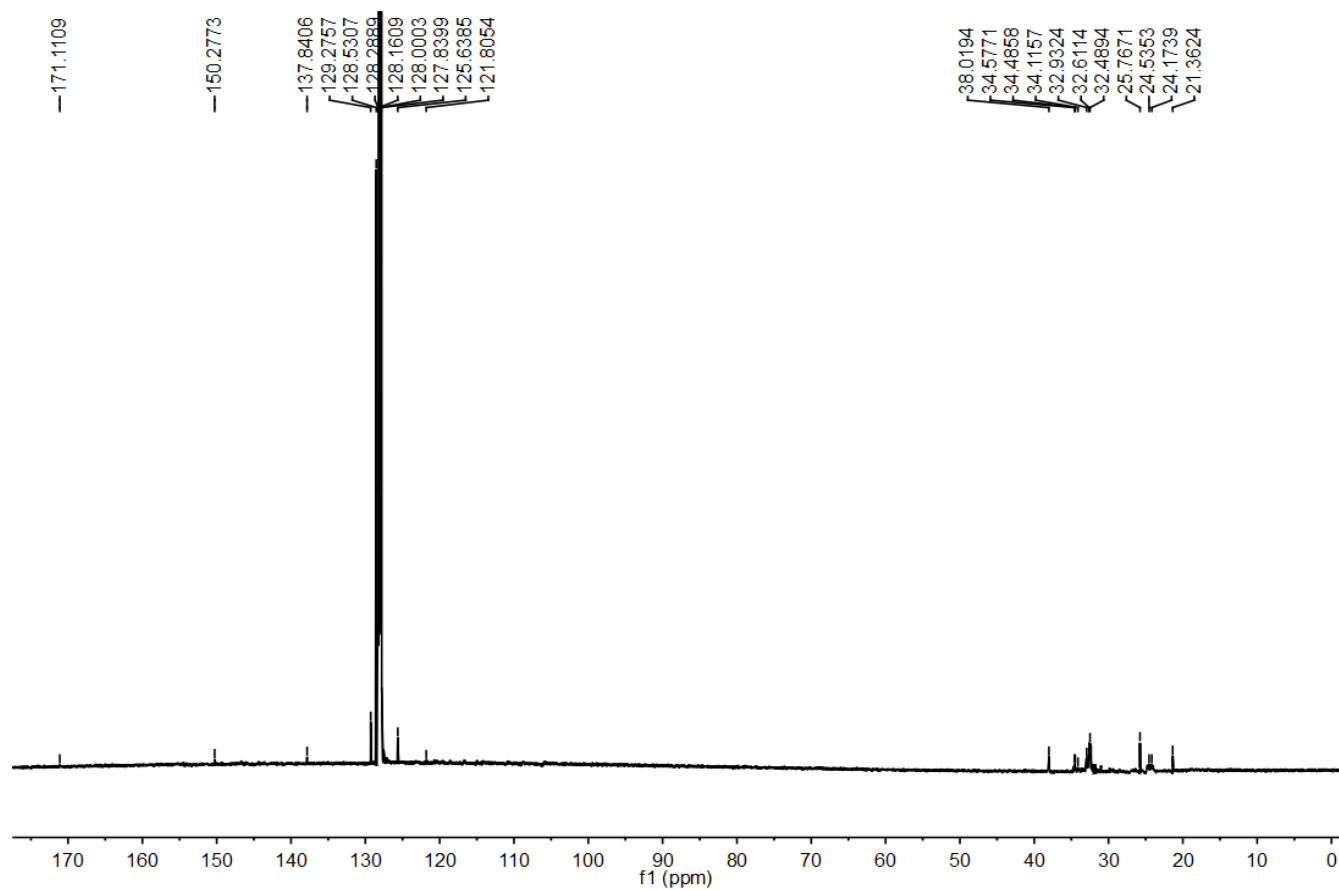


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum for **5**.

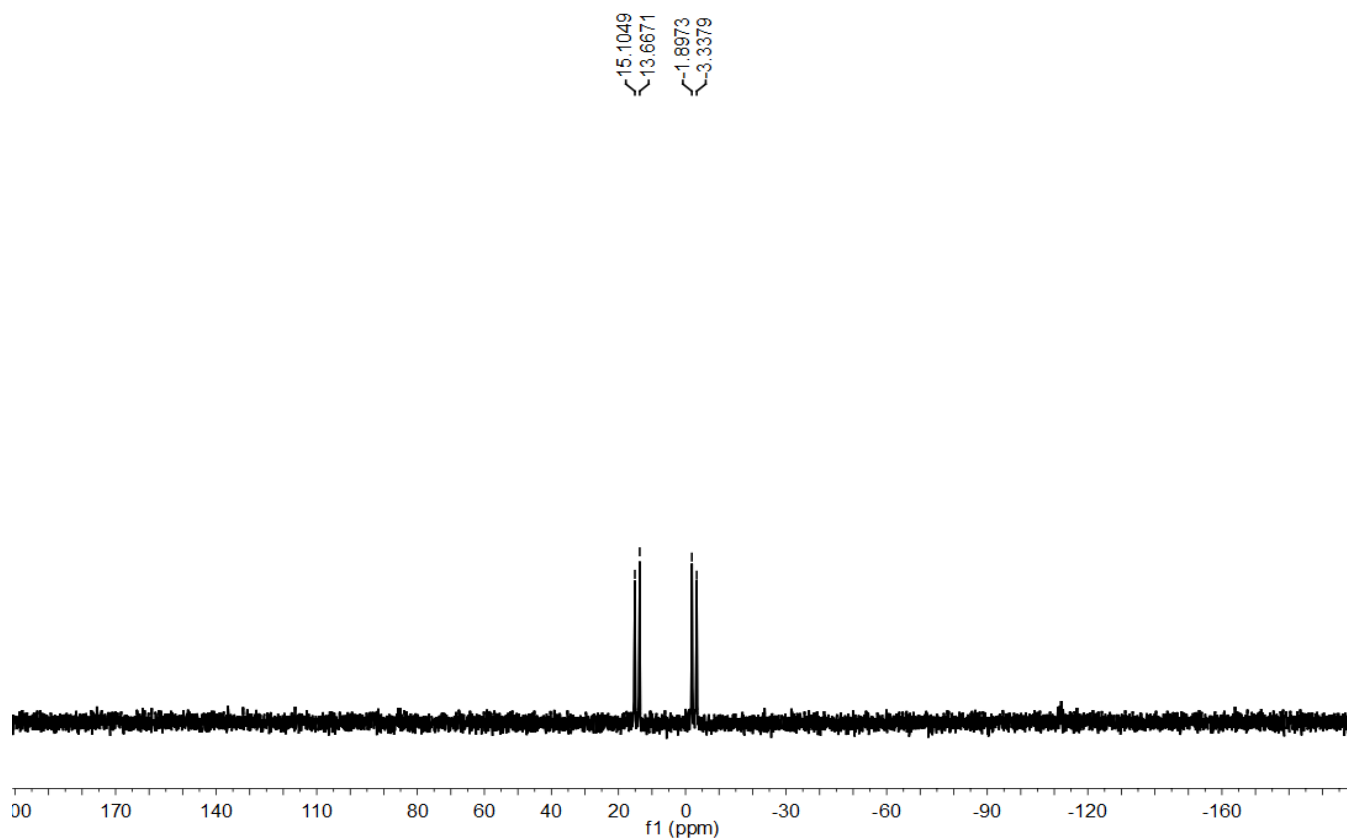


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **5**.

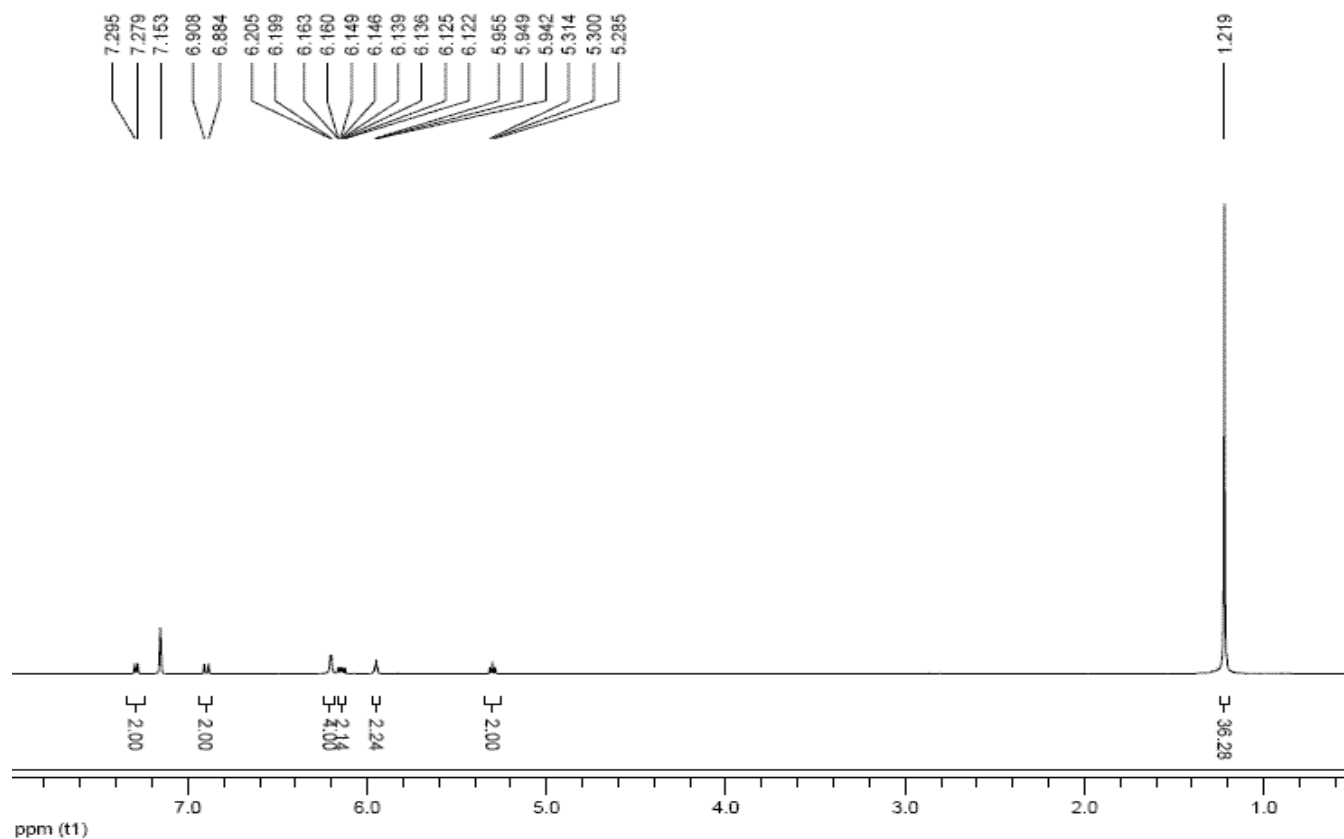


Figure S14. ^1H NMR spectrum for **6**.

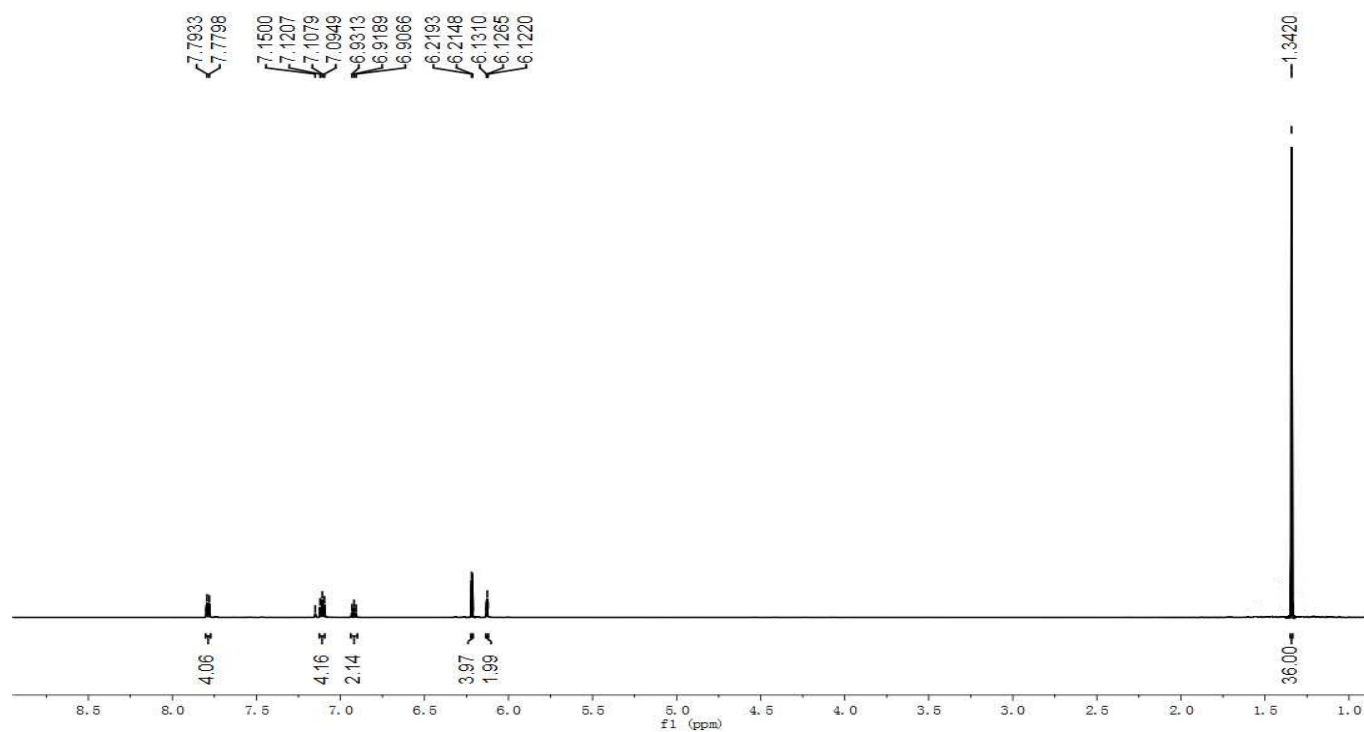


Figure S15. ^1H NMR spectrum for **7**.

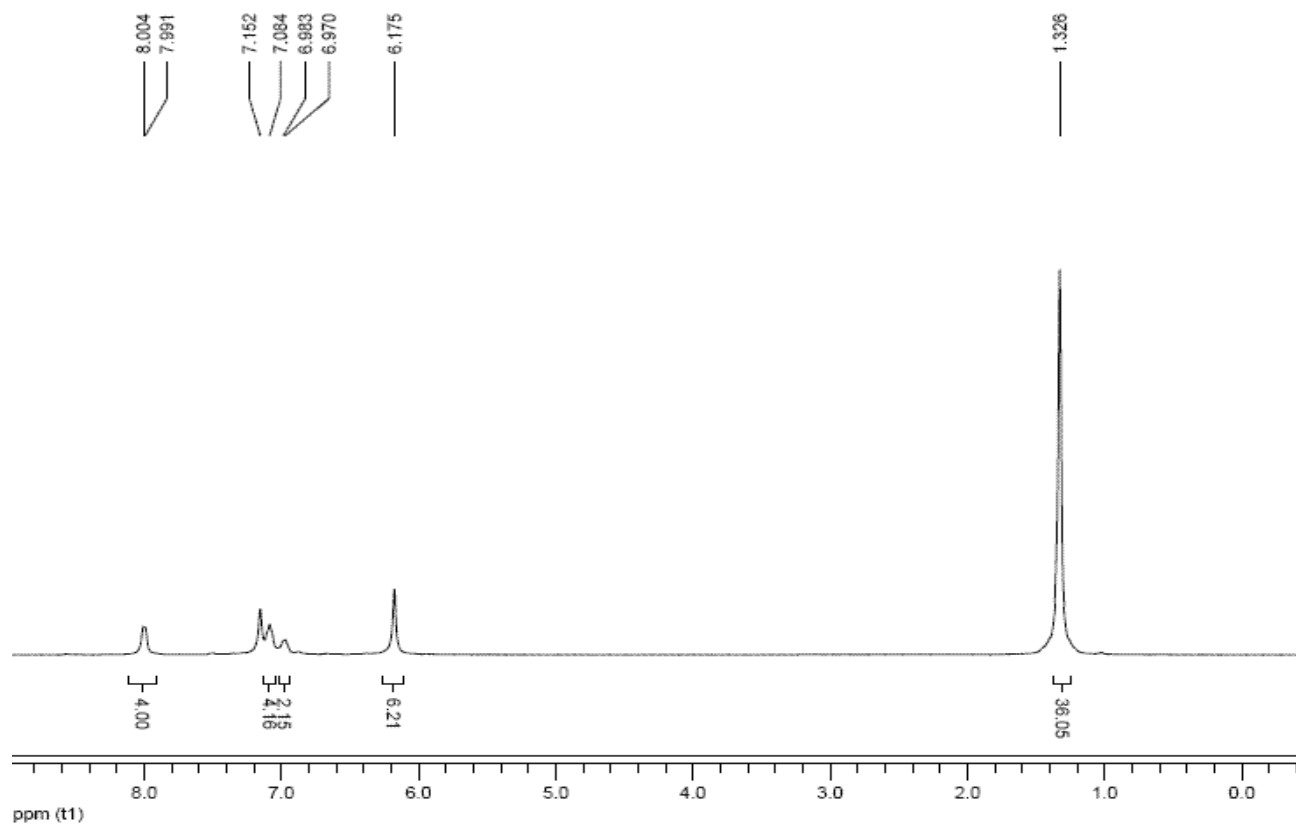


Figure S16. ^1H NMR spectrum for **8**.

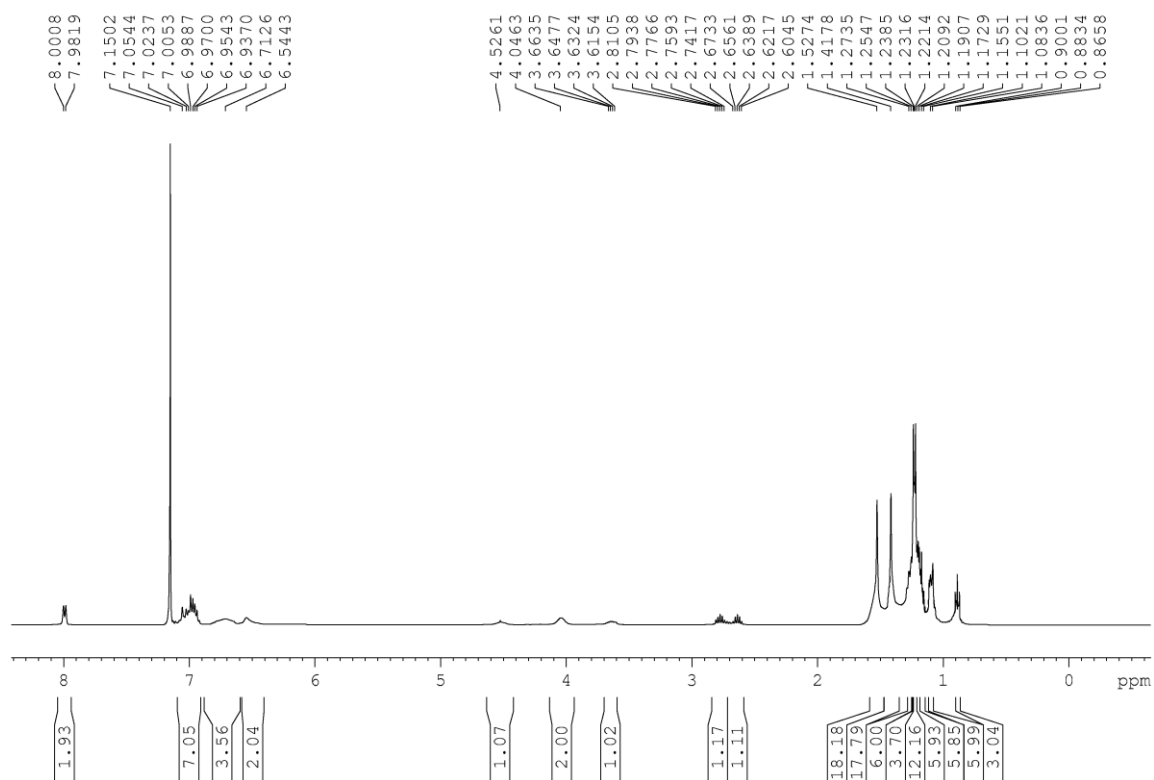


Figure S17. ^1H NMR spectrum for **9**.

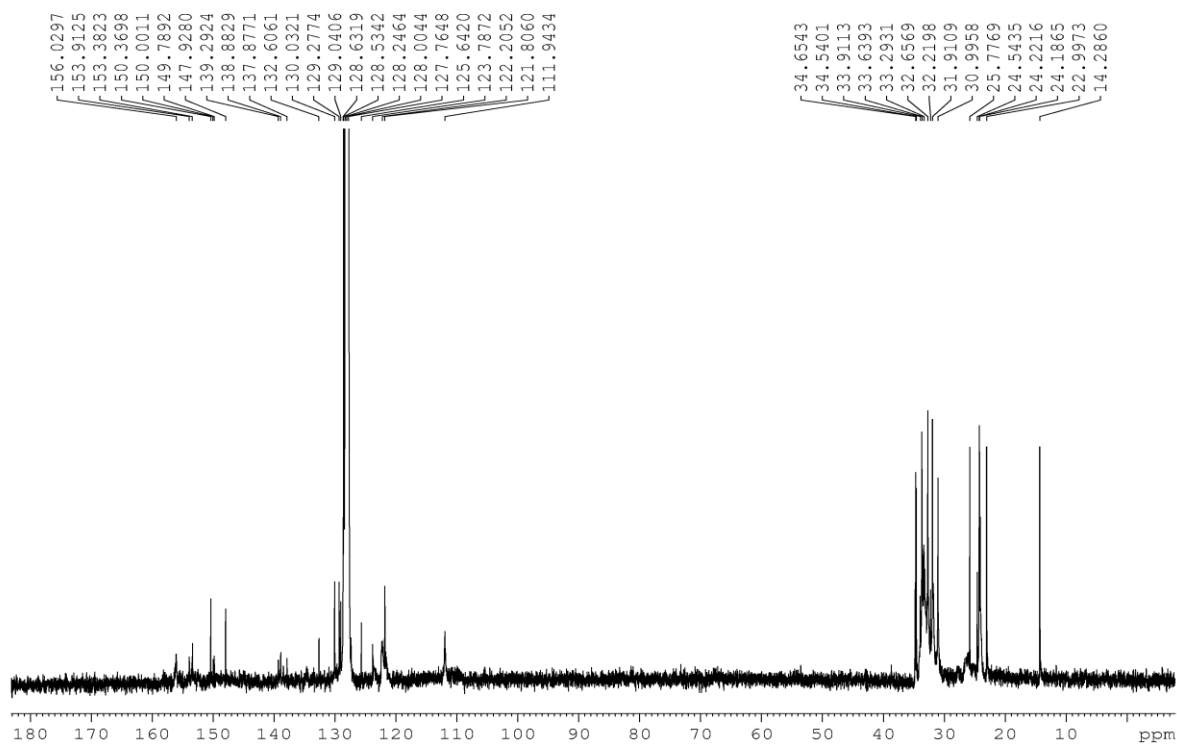


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum for **9**.

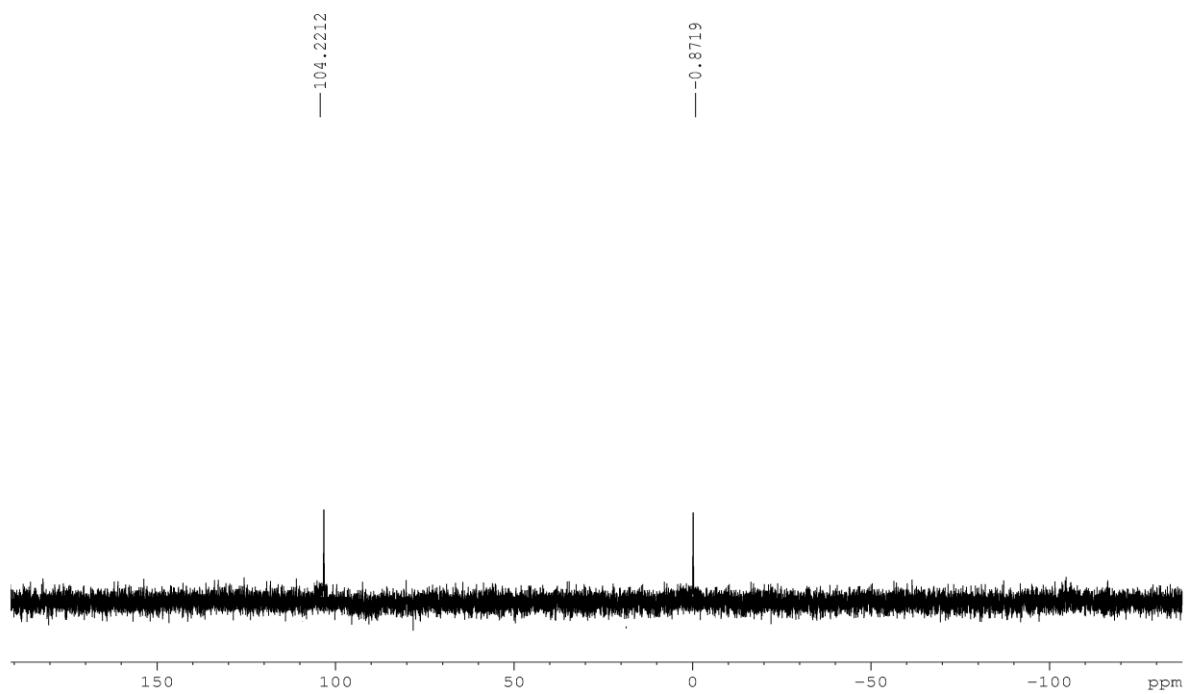


Figure S19. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **9**.

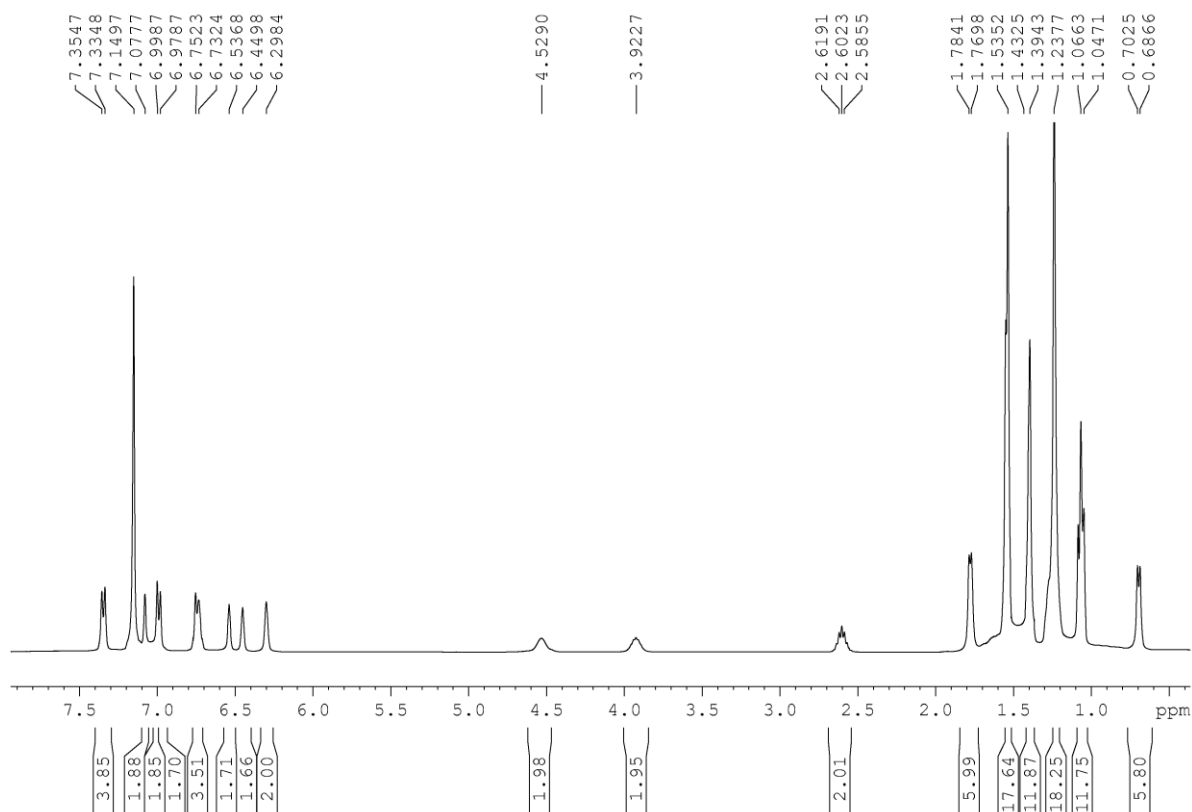


Figure S20. ¹H NMR spectrum for 10.

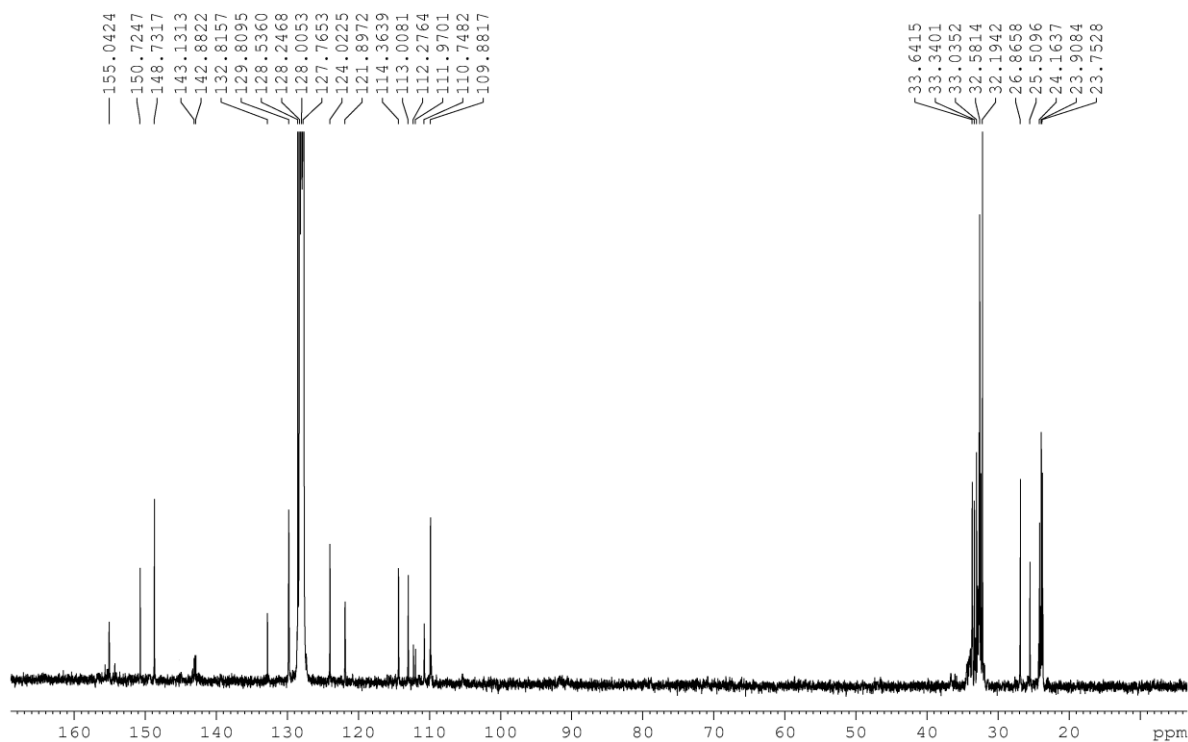


Figure S21. ¹³C{¹H} NMR spectrum for 10.

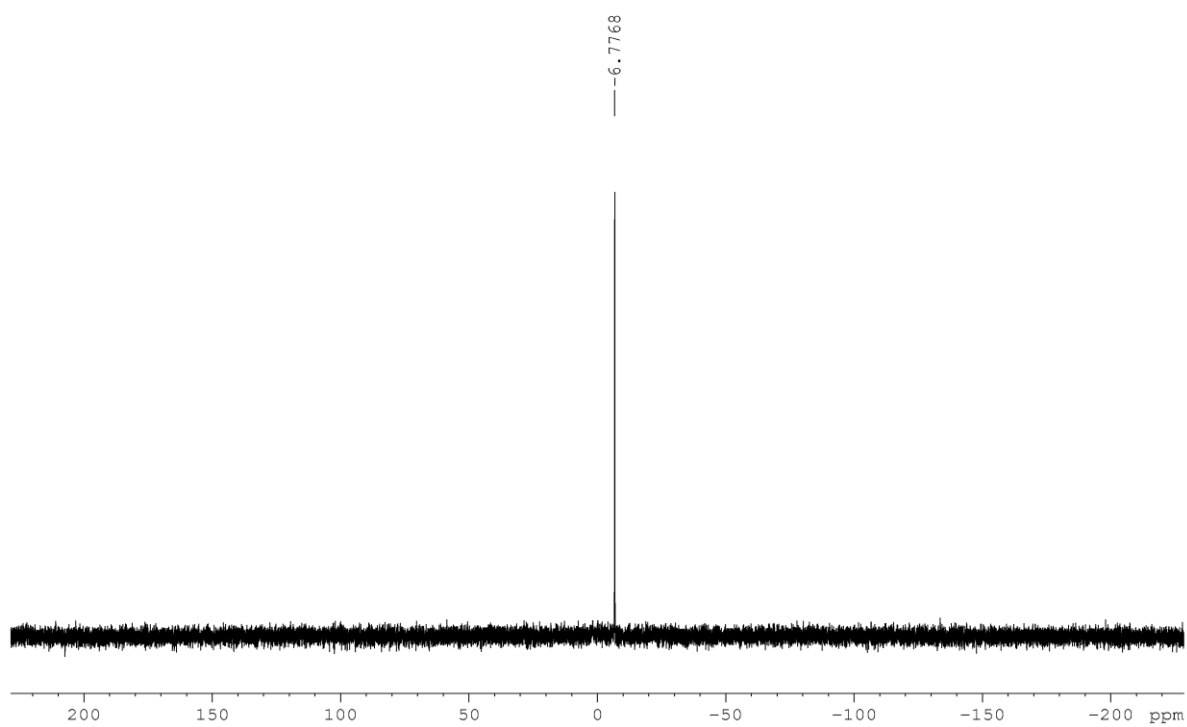


Figure S22. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum for **10**.