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Supporting Information for:

[3]Ferrocenophanes with bisphosphanotetryl bridge: Inorganic rings on the way to tetrylenes

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Content

Computational details

Calculations were performed using the Gaussian 09 suite of programs.[1] Geometry optimizations were carried out using M06-2X or B3LYP functional with 6-31+G*, 6-31G*, 6-311+G** or cc-PVDZ basis set. For the Sn and I containing systems Def2-TZVP basis was used for the Sn and I atoms. For the energy difference between the isomeric/dimeric structures further single point energy calculations were also carried out at B3LYP/Def2-TZVP level. The nature of the stationary point obtained by geometry optimization has been verified by a subsequent analysis of the second derivatives, which have been found all positive in case of minima, and exhibited a single negative value in case of transition states. The structures were visualized by the MOLDEN package.[2] The topological analysis of the electron density was carried out by the AIMAll package.[3]

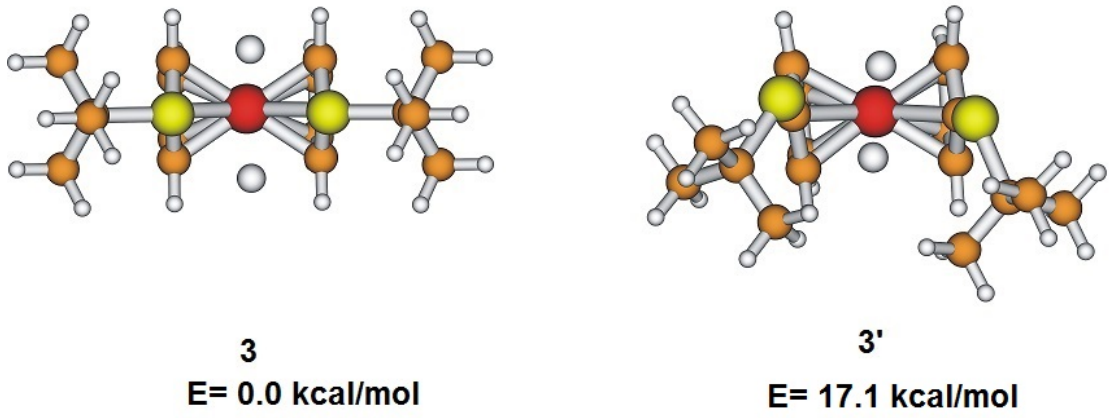

Figure S1: Optimized structures of **3** and their relative energies at B3LYP/6-311+G** level of theory

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision B.01*, Gaussian Inc., Wallingford, CT, 2010.

[2] G. Schaftenaar and J. H. Noordik, *J. Comput.-Aided Mol. Des.*, 2000, **14**, 123-134.

[3] A. Todd and T. K. Keith, *AIMAll 11.10.16*, Gristmill software (http://aim.tkgristmill.com), Overland Park, 2011.

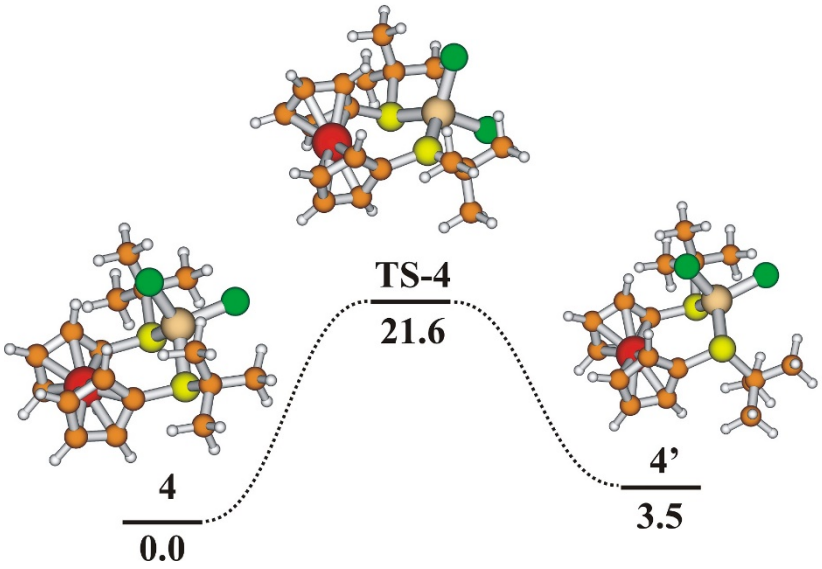

Figure S2: Phosphorus inversion of 4 at M06-2X/6-311+G** level of theory.

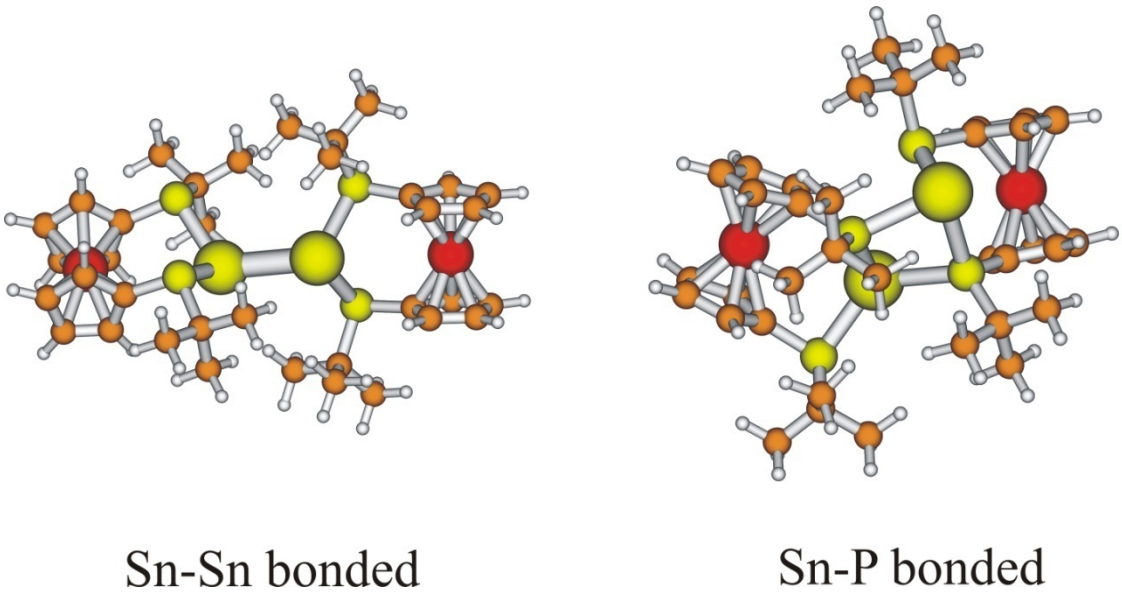

Figure S3: Sn-Sn bonded and Sn-P bonded dimeric structures

	E:Sn							E:Ge						
	B3LYP/cc-pVDZ		B3LYP/6-31G*		M06-2X/cc-pVDZ		B3LYP/Def2-TZVP// B3LYP/6-31+G*	B3LYP/cc-pVDZ		M06-2X/cc-pVDZ		B3LYP/6-31G*		B3LYP/Def2-TZVP// B3LYP/6-31+G*
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE
E-E bonded	-9.8	4.4	-10.5	4.8	-25.1	-8.8	7.7	-10.4	5.7	-27.8	-13.5	-52.4	-30.5	0.0
E-P bonded	-9.2	8.2	-10.7	7.9	-28.6	-10.7	7.2	-8.1	10.1	-29.8	-12.3	-45.9	-23.4	-4.3

Table S1: Dimerization energy (ΔE) and Gibbs free energy (ΔG) of the E-E and the E-P bonded dimers at different level of theory. There are significant differences in the calculated ΔE and ΔG between the B3LYP and the dispersion corrected M06-2X functional, due the interaction of the bulky ^{t}Bu groups. Interestingly significantly higher dimeriazation energy and Gibbs free energy were obtained in case of the Ge analogues using split valence (e. g. 6-31G*) basis sets for the energy calculations.

XYZ coordinates and total energies of the investigated systems

3

*E(B3LYP/6-311+G**)* = -2663.367628

C	-0.076596	0.029823	-0.000875
C	-0.077152	0.030452	1.425521
C	1.278018	0.032569	1.861200
C	2.143361	0.045146	0.713154
C	1.278911	0.031496	-0.435543
Fe	0.891298	-1.660495	0.713406
C	-0.212701	-3.264961	-0.001518
C	-0.215718	-3.264420	1.424874
C	1.133839	-3.378906	1.862968
C	1.997070	-3.464416	0.716457
C	1.138695	-3.379835	-0.433770
P	3.835353	-3.605578	0.720119
C	4.194599	-5.480354	0.722715
P	3.987018	0.032835	0.714194
C	4.501044	1.871210	0.712458
Li	4.350107	-1.806961	-0.788016
Li	4.346232	-1.802210	2.223517
C	3.613983	-6.153163	1.978325
C	3.979978	2.592524	1.967260
C	3.981671	2.589676	-0.544682
C	6.039706	1.890024	0.713464
C	5.726355	-5.627152	0.725668
C	3.618563	-6.155743	-0.533614
H	1.475027	-3.402779	-1.460067
H	-1.080585	-3.170839	-0.637809
H	-1.086312	-3.169850	2.057389
H	1.465829	-3.400964	2.890694
H	1.614186	0.025575	-1.462422
H	-0.950441	0.007866	-0.635590
H	-0.951461	0.009047	2.059614
H	1.612494	0.027714	2.888349
H	3.842440	-7.230491	-0.525836
H	2.532669	-6.043698	-0.585510
H	4.046448	-5.727005	-1.443751
H	6.004627	-6.687623	0.727220
H	6.175042	-5.166785	-0.160002
H	6.171783	-5.165041	1.612071
H	3.837969	-7.227907	1.973620
H	4.038460	-5.722486	2.889139
H	2.527896	-6.041113	2.025962
H	6.405269	2.923658	0.712562
H	6.446241	1.394161	1.600321
H	6.447414	1.392200	-0.171754
H	4.294312	3.642052	-0.539448
H	4.371178	2.124926	-1.454373
H	2.890153	2.568389	-0.595126
H	4.292538	3.644911	1.960011
H	2.888396	2.571249	2.016349
H	4.368353	2.129905	2.878522

3‘

*E(B3LYP/6-311+G**)* = -2663.340401

C	-0.220990	0.086601	-0.026266
C	-0.060687	-0.029930	1.401229
C	1.354921	-0.172221	1.617679
C	2.025250	-0.207200	0.358986
C	1.045869	-0.033494	-0.661037
Fe	1.088145	1.615680	0.587025
C	0.885318	3.515285	1.669087
C	2.247852	3.094962	1.493367
C	2.540789	2.987306	0.099464
C	1.348413	3.265749	-0.621399
C	0.331968	3.566800	0.336025
P	-0.113823	4.008968	3.149781
C	1.140939	4.339163	4.573797
C	0.285801	4.934288	5.710149
P	-1.512090	-0.011818	2.559892
C	-1.103113	-1.262590	3.972634
C	-0.140330	-0.709404	5.044305
C	1.856473	3.083615	5.109777
C	2.181820	5.389206	4.145709
C	-0.538587	-2.573460	3.403976
C	-2.460447	-1.545963	4.645082
Li	-1.116519	2.213305	1.795175
Li	-0.487621	1.695326	4.083859
H	3.495599	2.717904	-0.327304
H	0.827836	-0.414568	4.627713
H	-0.664931	3.914504	0.088893
H	1.229862	3.263097	-1.694486
H	2.960944	2.917380	2.282082
H	-1.172342	0.190644	-0.528711
H	1.232156	0.006375	-1.724032
H	3.088223	-0.324808	0.208029
H	1.844632	-0.260740	2.575905
H	0.915624	5.158686	6.578947
H	-0.201650	5.859417	5.394515
H	-0.497771	4.242524	6.039014
H	2.834815	5.643410	4.990750
H	2.815150	5.035806	3.330302
H	1.688795	6.303872	3.809633
H	2.582747	3.350189	5.889236
H	1.151319	2.388003	5.587001
H	2.396676	2.541254	4.331621
H	0.065015	-1.457705	5.821160
H	-0.582031	0.145079	5.582098
H	-2.328471	-2.222732	5.498044
H	-2.929415	-0.628710	5.016877
H	-3.155083	-2.010912	3.942763
H	-1.217650	-2.994317	2.659292
H	0.431606	-2.428590	2.924788
H	-0.411665	-3.311807	4.206223

4

*E(B3LYP/6-311+G**)* = -3858.335017

C	0.210844	0.089632	0.106912
C	0.292784	0.036137	1.541318
C	1.687670	-0.070814	1.873914
C	2.439172	-0.071232	0.665599
C	1.526699	0.024846	-0.426098
Fe	1.122934	-1.677756	0.701430
C	0.055790	-3.307209	-0.016341
C	0.137290	-3.365099	1.417910
C	1.534971	-3.409903	1.752982
C	2.287573	-3.390636	0.545512
C	1.373921	-3.324166	-0.547402
P	-1.373347	-3.414725	2.462671
C	-1.284051	-5.104484	3.377438
P	-1.210494	0.147313	2.591924
C	-0.970728	1.751193	3.626365
Si	-0.927455	-1.700080	3.896740
C	-1.234540	-6.167178	2.261444
C	-0.820892	2.883001	2.590112
C	0.229368	1.767862	4.582913
C	-2.274668	1.964520	4.419021
C	-2.604589	-5.254924	4.156923
C	-0.093604	-5.299573	4.326249
H	1.943472	-3.424597	2.750691
H	3.365087	-3.393518	0.471945
H	1.638015	-3.270217	-1.592999
H	-0.861931	-3.247226	-0.581987
H	2.092651	-0.165440	2.868678
H	3.512703	-0.161133	0.588754
H	1.788069	0.022785	-1.473767
H	-0.706791	0.154482	-0.458336
Cl	-2.427893	-1.684951	5.371023
Cl	0.875166	-1.823109	5.013172
H	-0.127627	-6.312812	4.744874
H	0.861755	-5.190465	3.810285
H	-0.112797	-4.597576	5.161205
H	-1.296481	-7.164085	2.712025
H	-2.071765	-6.063570	1.565402
H	-0.305494	-6.115633	1.689131
H	-2.649579	-6.255789	4.600455
H	-2.689075	-4.528772	4.967321
H	-3.473577	-5.137180	3.504210
H	-0.793324	3.846145	3.111914
H	0.101516	2.788661	2.012542
H	-1.661729	2.906759	1.891120
H	-2.229770	2.930607	4.933931
H	-3.148586	1.973947	3.762351
H	-2.427660	1.192383	5.175046
H	0.286145	2.746901	5.074144
H	0.143728	1.011715	5.364722
H	1.172563	1.610181	4.057213

*E(M06-2X/6-311+G**)* = -3857.771056

C	-0.091659	-0.081841	0.053536
C	-0.060741	-0.065009	1.467554

C	1.303142	-0.048753	1.894094
C	2.109717	-0.063431	0.713446
C	1.250680	-0.085461	-0.411572
Fe	0.903849	1.686126	0.729311
C	-0.076860	3.438541	-0.006004
C	-0.045892	3.469262	1.407780
C	1.317862	3.455972	1.834831
C	2.124373	3.423947	0.654477
C	1.265398	3.415154	-0.470769
P	1.748863	3.507141	3.613307
Si	3.127561	1.727137	3.709224
Cl	4.696135	1.696830	2.310981
P	1.733986	-0.043452	3.673325
C	2.767264	-1.616198	3.910132
C	4.169081	-1.585758	3.302604
C	1.954526	-2.756393	3.284399
C	2.869009	-1.838219	5.425445
C	2.795106	5.078428	3.797417
C	2.898529	5.350461	5.304437
C	1.991876	6.203629	3.133429
C	4.196716	5.016110	3.191852
Cl	4.102958	1.754203	5.552126
H	3.186792	-0.014986	0.681967
H	1.563931	-0.068487	-1.444645
H	-0.977168	-0.063668	-0.563310
H	-0.912840	-0.034779	2.130465
H	3.200995	3.365409	0.624805
H	1.578356	3.360632	-1.502630
H	-0.962573	3.406967	-0.622015
H	-0.898126	3.468619	2.071206
H	4.638841	-2.567202	3.432535
H	4.145798	-1.364041	2.234234
H	4.805821	-0.846069	3.793922
H	2.432771	-3.710222	3.529811
H	0.931814	-2.781711	3.671701
H	1.906832	-2.666556	2.196838
H	3.409863	-2.771064	5.615786
H	3.412208	-1.028921	5.918346
H	1.879823	-1.916195	5.882567
H	2.477893	7.161195	3.346947
H	1.943648	6.077782	2.049471
H	0.969336	6.250309	3.519197
H	3.446946	6.284749	5.463494
H	1.909968	5.451817	5.758313
H	3.435074	4.553807	5.824477
H	4.674418	5.997534	3.288794
H	4.827354	4.288287	3.708120
H	4.171797	4.758671	2.131567

4’

*E(B3LYP/6-311+G**)* = -3858.329464

C	-0.193312	-0.497929	-0.256824
C	-0.123143	-0.149688	1.137356

C	1.244432	0.197014	1.402304
C	1.991961	0.079117	0.199171
C	1.100666	-0.338863	-0.830740
Fe	1.147113	-1.758663	0.671087
C	0.718390	-3.704569	0.118723
C	0.444770	-3.517012	1.517345
C	1.685693	-3.129185	2.134599
C	2.691046	-3.082905	1.130727
C	2.094725	-3.437816	-0.114398
P	-1.241864	-3.750051	2.195446
C	-1.106756	-5.325200	3.295797
P	-1.436381	0.137627	2.407733
C	-3.104382	0.337594	1.474957
Si	-1.426886	-1.881471	3.488940
C	-0.634735	-6.438562	2.338825
C	-3.661577	-0.917418	0.785022
C	-2.903125	1.471911	0.449146
C	-4.112176	0.828391	2.536378
C	-2.526618	-5.657443	3.790323
C	-0.141346	-5.228217	4.484308
H	1.825183	-2.889764	3.176277
H	3.721623	-2.797582	1.281869
H	2.594672	-3.471394	-1.070962
H	-0.014090	-3.982309	-0.624348
H	1.631512	0.496395	2.364924
H	3.051464	0.256989	0.091064
H	1.362838	-0.535475	-1.859712
H	-1.070104	-0.828095	-0.788719
Cl	-3.198538	-2.082980	4.609782
Cl	0.075792	-1.603939	4.949498
H	-0.084802	-6.202593	4.984648
H	0.868702	-4.962797	4.166591
H	-0.469764	-4.496812	5.224252
H	-0.638817	-7.395126	2.873178
H	-1.295705	-6.537501	1.472995
H	0.380269	-6.261905	1.976175
H	-2.510893	-6.619724	4.314273
H	-2.907261	-4.907720	4.485641
H	-3.232689	-5.740129	2.959553
H	-4.596370	-0.664911	0.269660
H	-2.976961	-1.329736	0.042834
H	-3.887221	-1.708866	1.502325
H	-5.065823	1.054271	2.046468
H	-4.303377	0.078266	3.304392
H	-3.762622	1.739175	3.029155
H	-3.873124	1.728960	0.009188
H	-2.503587	2.373795	0.921279
H	-2.231484	1.191396	-0.362590

*E(M06-2X/6-311+G**)* = -3857.765478

C	-0.210189	-0.008406	0.170549
C	-0.128477	0.063288	1.580007
C	1.246533	-0.011324	1.961236
C	2.007051	-0.145213	0.757114
C	1.110040	-0.140369	-0.336540

Fe	0.942371	1.700239	0.745537
C	-0.068666	3.465911	0.157391
C	0.246847	3.537487	1.538226
C	1.669379	3.501908	1.681810
C	2.211341	3.387465	0.366311
C	1.146326	3.361596	-0.566513
P	2.766283	3.793603	3.135823
Si	3.358040	1.651981	3.571640
Cl	4.820167	1.321389	2.108744
P	1.737164	0.087741	3.715898
C	2.571037	-1.585172	4.052697
C	3.943386	-1.781309	3.409430
C	1.598371	-2.647680	3.524780
C	2.685678	-1.718002	5.576711
C	1.649987	4.363105	4.553868
C	2.597219	4.767189	5.695219
C	0.650297	3.329642	5.077229
C	0.929389	5.634223	4.078210
Cl	4.397642	1.577464	5.380119
H	3.081799	-0.191418	0.687734
H	1.386096	-0.187560	-1.379224
H	-1.112129	0.057959	-0.418736
H	-0.951379	0.193281	2.267579
H	3.264983	3.315541	0.138151
H	1.243992	3.255037	-1.636016
H	-1.063635	3.453143	-0.261156
H	-0.477369	3.590774	2.334499
H	4.283617	-2.806115	3.595926
H	3.911183	-1.630352	2.328594
H	4.689682	-1.103669	3.830681
H	1.952785	-3.636768	3.832660
H	0.591027	-2.509062	3.928199
H	1.536703	-2.628734	2.434474
H	3.107916	-2.698019	5.822021
H	3.339903	-0.954992	6.002844
H	1.706790	-1.638007	6.055589
H	-0.020498	3.805412	5.801652
H	0.040970	2.888040	4.286618
H	1.160937	2.510032	5.588824
H	2.003327	5.177908	6.518324
H	3.161905	3.918204	6.082406
H	3.306002	5.533138	5.371814
H	0.413849	6.084697	4.932628
H	1.640715	6.368658	3.691189
H	0.189965	5.440138	3.302283

TS-4

*E(B3LYP/6-311+G**)* = -3858.3043656

C	1.851102	3.411896	-0.106505
C	1.861368	2.282140	-0.969884
C	1.677969	1.097437	-0.178200
C	1.551247	1.526986	1.188976
C	1.659532	2.944432	1.226685

Fe	0.051613	2.371557	0.036438
C	-1.519257	2.115103	-1.285431
C	-1.712667	1.313456	-0.104486
C	-1.769033	2.218205	1.012202
C	-1.607643	3.541636	0.525090
C	-1.454761	3.478073	-0.892964
P	-1.832536	-0.481917	-0.029995
C	-3.567598	-1.236765	-0.237170
C	-3.784946	-1.689299	-1.692561
P	1.681142	-0.576068	-0.935972
C	3.382977	-1.309693	-0.408503
C	3.339164	-2.827352	-0.657742
Si	0.009538	-1.608478	0.222322
Cl	0.466524	-2.095344	2.241590
Cl	-0.303488	-3.501449	-0.636821
C	-4.587315	-0.147207	0.134066
C	-3.712864	-2.433359	0.718865
C	3.813842	-1.021763	1.036007
C	4.394007	-0.664610	-1.379722
H	1.386685	0.882190	2.038449
H	1.579188	3.561596	2.109399
H	1.943224	4.444095	-0.410156
H	1.961609	2.299749	-2.044915
H	-1.886268	1.920706	2.042993
H	-1.577521	4.439954	1.123915
H	-1.288368	4.320018	-1.548624
H	-1.412899	1.726280	-2.286482
H	4.803212	-1.461988	1.210293
H	3.892778	0.050014	1.228269
H	3.126403	-1.453507	1.764041
H	5.396986	-1.053737	-1.170553
H	4.154775	-0.891240	-2.422062
H	4.431566	0.422209	-1.264958
H	4.350428	-3.238915	-0.565384
H	2.706934	-3.343766	0.067542
H	2.972939	-3.066976	-1.659937
H	-4.789249	-2.117403	-1.800451
H	-3.697130	-0.850225	-2.386348
H	-3.057876	-2.448581	-1.985857
H	-4.713011	-2.866213	0.600246
H	-2.987410	-3.219878	0.503565
H	-3.590156	-2.128845	1.759975
H	-5.596921	-0.552494	0.003932
H	-4.479564	0.169825	1.173578
H	-4.497283	0.734707	-0.504262

*E(M06-2X/6-311+G**)* = -3857.736675

C	0.028233	-0.025819	-0.018609
C	0.030045	-0.014762	1.394150
C	1.388689	-0.003992	1.840727
C	2.217882	0.015848	0.673173
C	1.380027	0.004797	-0.464180
Fe	1.058724	-1.753004	0.719731
C	2.034069	-3.509457	-0.010751
C	0.653197	-3.567085	-0.341765

C	-0.085295	-3.533398	0.865633
C	0.833389	-3.450011	1.956715
C	2.148658	-3.444923	1.397937
P	0.275977	-3.338220	3.693093
Si	1.859143	-2.001182	4.598427
Cl	1.248279	-1.604932	6.555964
P	1.952273	-0.122930	3.536728
C	2.605483	1.451556	4.308460
C	3.627372	1.071725	5.385064
C	1.452509	2.250289	4.926686
C	3.285524	2.273597	3.209717
C	0.609472	-5.096354	4.335431
C	-0.638160	-5.891866	3.922988
C	0.704500	-5.052374	5.863735
C	1.847086	-5.771261	3.743695
Cl	3.748857	-2.868962	4.909539
H	3.067405	-3.362430	1.962220
H	2.854242	-3.483507	-0.712244
H	0.241049	-3.596933	-1.338897
H	-1.161542	-3.522397	0.958527
H	3.297456	-0.004051	0.680002
H	1.705628	-0.013551	-1.493259
H	-0.845605	-0.073217	-0.650458
H	-0.828967	-0.063939	2.046632
H	1.941341	-6.773770	4.175827
H	1.762918	-5.878990	2.660283
H	2.762919	-5.222924	3.967690
H	-0.526395	-6.932923	4.243616
H	-1.541662	-5.484538	4.382901
H	-0.770187	-5.888670	2.836859
H	0.674085	-6.074866	6.253963
H	1.639823	-4.597574	6.198945
H	-0.126312	-4.497113	6.308057
H	1.837146	3.182163	5.356606
H	0.704011	2.503665	4.172190
H	0.962537	1.677201	5.716399
H	4.014675	1.988328	5.842052
H	3.179126	0.470656	6.179449
H	4.464302	0.515017	4.958826
H	3.654673	3.208188	3.644864
H	4.132060	1.734587	2.778538
H	2.589880	2.526117	2.405811

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*E(B3LYP/6-311+G**)* = -8086.170332

C	0.197627	0.075636	0.133402
C	0.295992	0.027455	1.567340
C	1.695477	-0.065343	1.884633
C	2.433563	-0.064067	0.668316
C	1.508472	0.021609	-0.413526
Fe	1.128878	-1.680164	0.722723
C	0.059814	-3.307414	0.013434
C	0.150275	-3.363819	1.447589
C	1.549532	-3.411290	1.774562

C	2.294890	-3.392947	0.562626
C	1.374989	-3.326980	-0.525159
P	-1.356112	-3.407045	2.496490
C	-1.291803	-5.124859	3.361906
P	-1.196617	0.137042	2.633779
C	-0.960969	1.774361	3.616215
Si	-0.910047	-1.705719	3.959615
C	-1.199247	-6.151752	2.215223
C	-0.861248	2.871996	2.537455
C	0.266827	1.843329	4.533539
C	-2.244150	1.995040	4.438824
C	-2.637229	-5.308452	4.089304
C	-0.132407	-5.342641	4.342541
H	1.963716	-3.425936	2.769975
H	3.371987	-3.396906	0.482856
H	1.633064	-3.274625	-1.572356
H	-0.861271	-3.245408	-0.546500
H	2.113004	-0.151923	2.875002
H	3.506916	-0.145255	0.579944
H	1.758235	0.019229	-1.464064
H	-0.726361	0.129641	-0.422526
Br	-2.582172	-1.698536	5.509399
Br	1.019423	-1.836214	5.217169
H	-0.171285	-6.369323	4.726745
H	0.838821	-5.209186	3.862851
H	-0.186229	-4.668093	5.198346
H	-1.283966	-7.161350	2.632472
H	-2.006712	-6.023556	1.488614
H	-0.247345	-6.087575	1.683775
H	-2.690092	-6.323774	4.497824
H	-2.755328	-4.609751	4.919113
H	-3.483496	-5.174473	3.410428
H	-0.830847	3.852309	3.025922
H	0.043332	2.770039	1.933820
H	-1.724522	2.860595	1.866027
H	-2.205119	2.984178	4.908630
H	-3.138054	1.956632	3.810662
H	-2.356236	1.254628	5.232456
H	0.311387	2.833755	5.002759
H	0.227211	1.100895	5.331710
H	1.196872	1.701226	3.980717

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*E(B3LYP/6-311+G**)* = -8086.164418

C	-0.133915	-0.381676	-0.234721
C	-0.104851	-0.120655	1.179967
C	1.265732	0.144349	1.516469
C	2.054338	0.064689	0.336489
C	1.187853	-0.250096	-0.749320
Fe	1.113975	-1.755536	0.664274
C	0.550674	-3.656031	0.072532
C	0.368543	-3.507009	1.491167
C	1.660203	-3.200847	2.045980
C	2.607701	-3.169736	0.986331

C	1.923281	-3.449809	-0.232565
P	-1.277465	-3.722599	2.264231
C	-1.090725	-5.304839	3.347769
P	-1.461196	0.167918	2.405954
C	-3.104378	0.305834	1.416620
Si	-1.402845	-1.831563	3.545719
C	-0.638854	-6.406702	2.367995
C	-3.580340	-0.961171	0.690040
C	-2.911509	1.467305	0.418174
C	-4.174711	0.743434	2.438740
C	-2.491076	-5.656784	3.882017
C	-0.092177	-5.206627	4.507864
H	1.869710	-2.999494	3.083827
H	3.658517	-2.940795	1.085569
H	2.365173	-3.473720	-1.217594
H	-0.236452	-3.873052	-0.634064
H	1.627936	0.364550	2.509376
H	3.124042	0.200195	0.279133
H	1.481206	-0.395323	-1.778393
H	-1.001840	-0.635718	-0.819821
Br	-3.265132	-2.026208	4.850220
Br	0.291224	-1.459036	5.049951
H	-0.027511	-6.178187	5.012757
H	0.910910	-4.950340	4.161912
H	-0.396216	-4.468076	5.251069
H	-0.621597	-7.367104	2.895242
H	-1.324742	-6.504471	1.521467
H	0.363561	-6.220784	1.976933
H	-2.449229	-6.625656	4.392268
H	-2.855731	-4.919235	4.598149
H	-3.222317	-5.735351	3.073046
H	-4.499582	-0.739428	0.134156
H	-2.846843	-1.341197	-0.022110
H	-3.805991	-1.768082	1.389662
H	-5.109016	0.955434	1.907112
H	-4.382721	-0.028737	3.179461
H	-3.875984	1.651881	2.968075
H	-3.873840	1.688503	-0.056705
H	-2.575241	2.376858	0.923685
H	-2.195235	1.237273	-0.370191

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*E(B3LYP/def2-TZVP//B3LYP/6-311+G**)* == -3533.5883663

C	0.207025	0.077917	0.169094
C	0.307570	0.022257	1.603039
C	1.707408	-0.070935	1.917722
C	2.443740	-0.064635	0.700080
C	1.517230	0.026886	-0.379990
Fe	1.135285	-1.678576	0.749113
C	0.049931	-3.292690	0.041988
C	0.150333	-3.354616	1.475684
C	1.551709	-3.415743	1.791410
C	2.288413	-3.398740	0.574102
C	1.361072	-3.322345	-0.506432

P	-1.350350	-3.400750	2.534212
C	-1.285416	-5.150303	3.337635
P	-1.186226	0.127394	2.667060
C	-0.962445	1.798032	3.599573
Si	-0.920733	-1.706688	4.030573
C	-1.250420	-6.129286	2.145921
C	-0.832344	2.856365	2.484731
C	0.247180	1.890074	4.537739
C	-2.258698	2.063411	4.386838
C	-2.603215	-5.352804	4.107613
C	-0.092581	-5.424372	4.261697
H	1.974722	-3.439152	2.783128
H	3.364833	-3.410892	0.486469
H	1.611577	-3.268604	-1.555403
H	-0.874308	-3.221428	-0.511575
H	2.127239	-0.161428	2.906937
H	3.516952	-0.145892	0.609958
H	1.765486	0.029207	-1.430867
H	-0.717850	0.134575	-0.385093
I	-2.837292	-1.678438	5.646272
I	1.155769	-1.858509	5.493794
H	-0.139893	-6.461677	4.615284
H	0.860966	-5.297444	3.746204
H	-0.095361	-4.776094	5.139129
H	-1.328244	-7.154358	2.525000
H	-2.085869	-5.963852	1.459591
H	-0.320646	-6.051023	1.578716
H	-2.659980	-6.390123	4.456186
H	-2.672463	-4.704665	4.982513
H	-3.474103	-5.162572	3.474849
H	-0.816413	3.852833	2.940062
H	0.088397	2.735187	1.910379
H	-1.676838	2.821061	1.790487
H	-2.220475	3.072472	4.812383
H	-3.141092	2.002606	3.744417
H	-2.390907	1.360720	5.210898
H	0.294954	2.897778	4.968451
H	0.181034	1.180746	5.363958
H	1.186774	1.714333	4.011069

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*E(B3LYP/def2-TZVP//B3LYP/6-311+G**)* = -3533.5883663

C	-0.148025	-0.392329	-0.230372
C	-0.119172	-0.126125	1.183968
C	1.251990	0.139883	1.518533
C	2.039896	0.057900	0.338376
C	1.173108	-0.260218	-0.746338
Fe	1.098169	-1.761543	0.670209
C	0.516768	-3.655233	0.084582
C	0.351280	-3.506410	1.505332
C	1.651174	-3.211045	2.046201
C	2.587440	-3.185334	0.976397
C	1.887761	-3.459220	-0.235034
P	-1.285787	-3.724628	2.297785

C	-1.068848	-5.324519	3.356161
P	-1.478403	0.171698	2.404991
C	-3.105579	0.327957	1.389132
Si	-1.430859	-1.824555	3.585217
C	-0.575197	-6.396609	2.363437
C	-3.593510	-0.943186	0.678114
C	-2.876441	1.470952	0.376470
C	-4.183102	0.806324	2.384440
C	-2.461586	-5.730523	3.870451
C	-0.083980	-5.215847	4.526210
H	1.873771	-3.010902	3.081834
H	3.640960	-2.964311	1.064025
H	2.318645	-3.484840	-1.224882
H	-0.278382	-3.868479	-0.613936
H	1.614320	0.361058	2.511002
H	3.109571	0.193381	0.280106
H	1.466359	-0.409819	-1.774803
H	-1.014790	-0.654116	-0.813560
I	-3.488281	-2.047522	5.007517
I	0.405898	-1.339881	5.259107
H	0.007235	-6.193229	5.015507
H	0.912803	-4.921552	4.192904
H	-0.416760	-4.499869	5.279285
H	-0.543061	-7.365186	2.874772
H	-1.245974	-6.496554	1.505141
H	0.427650	-6.179774	1.990896
H	-2.391727	-6.705071	4.366672
H	-2.857967	-5.017327	4.594220
H	-3.182193	-5.820722	3.053262
H	-4.494491	-0.714691	0.095629
H	-2.850987	-1.354521	-0.006623
H	-3.852620	-1.728770	1.390507
H	-5.104263	1.026591	1.833549
H	-4.418982	0.053077	3.135851
H	-3.874552	1.718349	2.901894
H	-3.831998	1.715159	-0.100893
H	-2.514297	2.376229	0.871806
H	-2.167667	1.212450	-0.409135

8 isomer-1

*E(B3LYP/6-311+G**)* = -3398.659090

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.425758
C	1.353428	0.000000	1.864130
C	2.208841	-0.003250	0.712526
C	1.354050	-0.008889	-0.440960
Fe	0.975923	-1.689264	0.707815
C	-0.065943	-3.327337	-0.025785
C	-0.066829	-3.349103	1.399828
C	1.285263	-3.409552	1.838171
C	2.140880	-3.422630	0.686766
C	1.287669	-3.365535	-0.466515
P	3.973952	-3.576726	0.791755
C	4.294642	-4.940266	-0.456329

C	3.712620	-4.693022	-1.761173
P	4.046548	0.075631	0.819285
C	4.422204	1.444617	-0.407301
C	5.860637	1.554543	-0.553340
Si	4.601104	-1.753034	-0.419792
C	3.753699	-6.178411	0.069866
C	5.727553	-5.104998	-0.605084
C	3.930544	2.694875	0.138248
C	3.831721	1.241195	-1.715906
H	1.614965	-3.344373	-1.495237
H	-0.937538	-3.264293	-0.660348
H	-0.939302	-3.305510	2.034497
H	1.624159	-3.430942	2.863203
H	1.680272	-0.027149	-1.470075
H	-0.873462	-0.018592	-0.634858
H	-0.873514	-0.018481	2.060223
H	1.692934	-0.007725	2.889153
H	6.084761	-1.780766	-0.571253
Cl	4.016349	-1.731430	-1.797677
H	3.942116	-5.525510	-2.424662
H	2.632553	-4.593429	-1.663922
H	4.126071	-3.774440	-2.174919
H	3.930532	-6.983319	-0.642013
H	4.241540	-6.415323	1.014220
H	2.682757	-6.066479	0.232581
H	5.929115	-5.894427	-1.327646
H	6.165809	-4.171669	-0.955441
H	6.163901	-5.372618	0.356114
H	4.094692	2.074139	-2.366270
H	4.208525	0.313438	-2.143935
H	2.748475	1.183230	-1.620324
H	6.093937	2.346510	-1.263467
H	6.306599	1.789572	0.411959
H	6.261689	0.610106	-0.918191
H	4.139760	3.503199	-0.560867
H	2.855881	2.623082	0.299078
H	4.426738	2.897330	1.086259

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*E(B3LYP/6-311+G**)* = -3398.657156

C	-0.097481	-0.003010	0.143165
C	0.064721	-0.001643	1.559534
C	1.458091	-0.001318	1.840968
C	2.180957	-0.001090	0.599762
C	1.196765	-0.011571	-0.449677
Fe	0.959582	-1.689072	0.732348
C	-0.163595	-3.322392	0.117481
C	-0.002074	-3.352080	1.533617
C	1.390079	-3.412248	1.814648
C	2.112795	-3.422102	0.573394
C	1.130172	-3.356256	-0.475499
P	3.952272	-3.539796	0.524182
C	4.306425	-5.128336	-0.504293
C	3.905515	-5.069893	-1.985567

P	4.023685	0.043977	0.551773
C	4.441328	1.632786	-0.452173
C	5.966517	1.822244	-0.331204
Si	4.318508	-1.743926	-0.834401
C	3.550943	-6.274978	0.193629
C	5.822859	-5.380177	-0.387073
C	3.731674	2.797720	0.263350
C	4.039272	1.613114	-1.934155
H	1.334294	-3.318252	-1.534030
H	-1.101807	-3.254748	-0.413206
H	-0.796638	-3.312180	2.263701
H	1.844772	-3.434400	2.793668
H	1.399484	-0.041342	-1.508738
H	-1.037503	-0.025027	-0.388172
H	-0.730992	-0.021126	2.289195
H	1.913048	-0.012407	2.820053
Cl	6.321775	-1.778601	-1.515495
H	3.523123	-1.718398	-2.090936
H	4.144744	-6.025354	-2.468373
H	2.834656	-4.900844	-2.112811
H	4.446403	-4.289137	-2.525997
H	3.819428	-7.227064	-0.278381
H	3.813113	-6.343528	1.253317
H	2.467683	-6.156531	0.117962
H	6.075857	-6.321425	-0.888251
H	6.408521	-4.586458	-0.855056
H	6.134858	-5.460457	0.657482
H	4.316612	2.565606	-2.402212
H	4.548972	0.819844	-2.486552
H	2.962614	1.488797	-2.063941
H	6.257047	2.760251	-0.817895
H	6.280883	1.874019	0.714441
H	6.520398	1.013116	-0.811345
H	4.038136	3.745510	-0.193944
H	2.644600	2.723692	0.185890
H	3.995731	2.839463	1.323964

RP-Ge-PR [3]ferrocenophanes R=^{t}Bu isomer-1

E(B3LYP/cc-pVDZ)= -4725.157751
G(B3LYP/cc-pVDZ)= -4724.818665

C	0.064597	0.011551	-0.175361
C	-0.122738	-0.003249	1.241489
C	1.165417	-0.005013	1.858121
C	2.169469	0.021533	0.823708
C	1.467088	0.030289	-0.433429
Fe	0.973358	-1.668467	0.658329
C	0.082741	-3.368145	-0.154839
C	-0.104787	-3.338181	1.261747
C	1.183256	-3.315091	1.878183
C	2.187567	-3.343377	0.844069
C	1.485360	-3.374928	-0.412800
P	4.023575	-3.401047	0.975567
C	4.422088	-5.031853	1.920756
P	4.004735	0.100533	0.954443

C	4.385604	1.746842	1.879820
Ge	5.018113	-1.637621	2.163114
C	3.946023	-5.042875	3.383173
C	3.909425	1.770384	3.342051
C	3.710490	2.888031	1.096711
C	5.914127	1.928517	1.831282
C	5.952490	-5.197581	1.874391
C	3.759428	-6.189641	1.151498
H	1.960164	-3.392094	-1.391574
H	-0.706613	-3.365624	-0.903970
H	-1.061550	-3.310429	1.779933
H	1.374186	-3.266679	2.947400
H	1.941777	0.040693	-1.412355
H	-0.724608	-0.008538	-0.924383
H	-1.079199	-0.035002	1.760004
H	1.356747	-0.038403	2.927840
H	4.030810	-7.152275	1.620877
H	2.661183	-6.110766	1.159745
H	4.091200	-6.220108	0.101491
H	4.211408	-6.004927	3.859557
H	4.418908	-4.238683	3.969019
H	2.854266	-4.931072	3.458501
H	6.238185	-6.148434	2.358010
H	6.327215	-5.216363	0.838818
H	6.471858	-4.385133	2.408060
H	6.189527	2.888173	2.303347
H	6.442233	1.128232	2.374667
H	6.288645	1.938835	0.795514
H	4.164404	2.740927	3.806753
H	2.818938	1.647723	3.418847
H	4.390953	0.978474	3.937510
H	3.971452	3.859139	1.554399
H	4.041929	2.909395	0.046374
H	2.613161	2.797404	1.106037

E(B3LYP/6-31G)*= -4722.915474
G(B3LYP/6-31G)*=-4722.570040

C	0.040611	-0.021135	-0.135095
C	-0.106586	-0.040105	1.284476
C	1.196713	-0.036912	1.863127
C	2.170049	0.004424	0.801943
C	1.433209	0.008584	-0.432077
Fe	0.979233	-1.668373	0.669409
C	0.058405	-3.335255	-0.114939
C	-0.089018	-3.300641	1.304314
C	1.214228	-3.282790	1.882819
C	2.187974	-3.326528	0.822108
C	1.451248	-3.353592	-0.411691
P	4.018832	-3.387990	0.925349
C	4.424190	-4.988802	1.897768
P	4.000128	0.086835	0.904386
C	4.388155	1.703551	1.857368
Ge	4.817512	-1.638161	2.251219
C	3.898754	-5.011804	3.344265
C	3.862416	1.738362	3.303520

C	3.774981	2.871644	1.060990
C	5.923999	1.841665	1.862978
C	5.961432	-5.110287	1.904950
C	3.823689	-6.172967	1.115594
H	1.895557	-3.376935	-1.398284
H	-0.747257	-3.330815	-0.837929
H	-1.025953	-3.266566	1.845763
H	1.435787	-3.234492	2.940003
H	1.877347	0.024732	-1.418892
H	-0.764877	-0.043017	-0.857961
H	-1.043159	-0.077685	1.826320
H	1.418660	-0.069992	2.920815
H	4.095464	-7.118763	1.604323
H	2.730263	-6.119676	1.076959
H	4.198496	-6.207271	0.086512
H	4.192727	-5.950792	3.834746
H	4.306779	-4.185976	3.938725
H	2.806733	-4.955940	3.375469
H	6.255319	-6.044023	2.403031
H	6.368771	-5.128091	0.887872
H	6.439341	-4.283985	2.444993
H	6.207780	2.784460	2.349725
H	6.410748	1.027141	2.412928
H	6.331185	1.851570	0.845730
H	4.146236	2.686314	3.782605
H	2.771059	1.671127	3.335472
H	4.279271	0.924212	3.907879
H	4.036518	3.826146	1.538244
H	4.149464	2.897555	0.031545
H	2.682195	2.806114	1.023072

RP-Ge-PR [3]ferrocenophanes R=^{t}Bu isomer-2

E(B3LYP/cc-pVDZ)= -4725.160588
G(B3LYP/cc-pVDZ)= -4724.821688

C	-0.708781	1.331195	-0.707220
C	-1.101112	1.147071	0.652292
C	-0.145708	0.285099	1.273364
C	0.838848	-0.057666	0.300319
C	0.507489	0.593195	-0.941552
Fe	0.799983	1.997565	0.537589
C	0.760957	4.049061	0.774498
C	1.119776	3.438839	2.013601
C	2.310446	2.676598	1.804879
C	2.691727	2.821908	0.438292
C	1.729968	3.668881	-0.223018
P	1.597215	4.147134	-1.991171
Ge	1.978673	2.496038	-3.606913
P	1.567394	0.509870	-2.438925
C	0.686748	-0.732634	-3.620507
C	0.586479	-2.082323	-2.885975
C	-0.717843	-0.260985	-4.031274
C	1.574843	-0.893451	-4.866103
C	2.887808	5.558019	-2.236012

C	2.766097	6.047893	-3.689076
C	4.327032	5.096692	-1.953572
C	2.512814	6.703077	-1.277121
H	-1.214186	1.959148	-1.437724
H	-1.963966	1.601447	1.135527
H	-0.152453	-0.031031	2.314842
H	1.715785	-0.680089	0.466126
H	-0.111120	4.674297	0.594596
H	0.566299	3.516058	2.947623
H	2.823567	2.072634	2.550829
H	3.539935	2.339378	-0.042475
H	0.125376	-2.834352	-3.551196
H	1.579020	-2.457047	-2.589111
H	-0.037310	-2.010702	-1.981252
H	-1.199744	-1.021759	-4.673139
H	-1.368080	-0.107137	-3.156414
H	-0.676240	0.681864	-4.599190
H	1.132479	-1.647239	-5.541053
H	1.666128	0.046364	-5.433476
H	2.589178	-1.231727	-4.600557
H	3.445893	6.903186	-3.849599
H	3.041468	5.265230	-4.413743
H	1.742121	6.382197	-3.920470
H	5.025778	5.946069	-2.069020
H	4.438401	4.714570	-0.927182
H	4.640995	4.304636	-2.651582
H	3.206710	7.550750	-1.420762
H	1.490129	7.068448	-1.462382
H	2.579841	6.392559	-0.222673

RP-Sn-PR [3]ferrocenophanes R=^{t}Bu isomer-1

*E(B3LYP/Def2-TZVP//B3LYP/6-311+G**)* = -2862,7588639

C	0.043548	-0.020655	-0.062581
C	-0.105438	-0.016291	1.351985
C	1.197348	-0.002377	1.931283
C	2.149965	0.012640	0.872142
C	1.444285	-0.008087	-0.380578
Fe	0.938990	1.675502	0.742735
C	0.032235	3.397521	0.008058
C	-0.116571	3.333708	1.421209
C	1.186340	3.304501	1.999657
C	2.138925	3.339586	0.940961
C	1.432991	3.407393	-0.309951
P	2.071219	3.575805	-2.022119
Sn	3.736026	1.755507	-2.679629
P	2.083330	-0.101352	-2.098175
C	2.996205	-1.786414	-2.200331
C	2.972939	5.269638	-2.054386
C	4.227678	-1.903016	-1.286165
C	4.203718	5.356477	-1.135985
C	1.953397	6.350150	-1.647495
C	3.405036	5.501488	-3.514094
C	3.429588	-1.954870	-3.668326

C	1.983883	-2.889528	-1.838565
H	-0.754563	-0.021983	-0.789660
H	-1.039846	0.000542	1.893092
H	1.421895	0.025207	2.987396
H	3.221776	0.050428	0.989819
H	-0.765944	3.423609	-0.718481
H	-1.050789	3.288332	1.961000
H	1.411176	3.234781	3.053765
H	3.210974	3.304072	1.057159
H	3.911339	-2.930095	-3.802641
H	2.575299	-1.904048	-4.348388
H	4.149975	-1.189386	-3.972632
H	2.452431	-3.874337	-1.952834
H	1.642740	-2.799700	-0.804484
H	1.106341	-2.856264	-2.489340
H	4.686414	-2.893341	-1.400733
H	4.985894	-1.155838	-1.536530
H	3.961695	-1.786156	-0.234091
H	3.880325	6.484589	-3.607903
H	4.130425	4.754008	-3.849665
H	2.551025	5.473185	-4.195812
H	4.655896	6.353696	-1.209448
H	3.938630	5.194479	-0.089683
H	4.966819	4.625303	-1.416897
H	2.415423	7.341912	-1.720884
H	1.076022	6.338024	-2.299229
H	1.612970	6.215405	-0.618066

E(B3LYP/cc-pVDZ) = -2862.531339
G(B3LYP/cc-pVDZ) = -4724.818665

C	-0.001928	-0.000414	0.007862
C	-0.004633	-0.000221	1.447776
C	1.344447	0.001400	1.910212
C	2.201990	0.002976	0.766676
C	1.380176	-0.008268	-0.401302
Fe	0.993649	-1.683880	0.738936
C	0.085641	-3.414796	0.004662
C	0.083074	-3.417852	1.444572
C	1.430502	-3.351172	1.907020
C	2.286899	-3.306610	0.763492
C	1.465489	-3.335309	-0.404471
P	-1.446524	-3.584654	-1.005094
C	-1.261948	-5.275199	-1.916213
C	-1.066695	-6.363535	-0.844365
P	-1.540801	0.092576	-1.001698
C	-1.443140	1.792053	-1.909652
C	-2.784903	1.963638	-2.644704
Sn	-1.746573	-1.750906	-2.748352
C	-0.100428	-5.330680	-2.922432
C	-2.593199	-5.513957	-2.651626
C	-0.286023	1.908863	-2.915694
C	-1.303889	2.886967	-0.835768
H	-0.809706	-3.461063	2.064831
H	1.750592	-3.318259	2.946658
H	3.372885	-3.234904	0.779946

H	1.819845	-3.292610	-1.431576
H	-0.898447	-0.004018	2.068039
H	1.665816	-0.017025	2.949813
H	3.290224	-0.012980	0.783088
H	1.736245	-0.030797	-1.428455
H	-2.572676	-6.496641	-3.155306
H	-3.448054	-5.505931	-1.957066
H	-2.778437	-4.751543	-3.426782
H	-1.028477	-7.358626	-1.323205
H	-0.126668	-6.222591	-0.288580
H	-1.894687	-6.368578	-0.118013
H	-0.057240	-6.328859	-3.396787
H	-0.223335	-4.586133	-3.725602
H	0.870528	-5.157869	-2.435240
H	-2.814785	2.947018	-3.146553
H	-2.930847	1.194177	-3.421290
H	-3.638201	1.910517	-1.950215
H	-0.294069	2.908824	-3.388190
H	0.692530	1.785140	-2.428763
H	-0.370633	1.160489	-3.720253
H	-1.316738	3.883598	-1.312751
H	-2.131027	2.848213	-0.109460
H	-0.357855	2.793352	-0.280188

E(B3LYP/6-31G)= -2862.285120
G(B3LYP/6-31G)= -2861.942719

C	-0.007082	-0.023936	-0.009270
C	-0.004341	-0.027783	1.429697
C	1.344469	-0.029268	1.887919
C	2.197800	-0.027887	0.743087
C	1.373312	-0.035493	-0.421073
Fe	0.986131	-1.684045	0.716676
C	0.079317	-3.391527	-0.012450
C	0.081981	-3.390286	1.426522
C	1.428979	-3.320492	1.884762
C	2.281159	-3.275917	0.739941
C	1.457266	-3.308393	-0.424213
P	-1.444486	-3.577030	-1.016120
C	-1.259933	-5.267705	-1.903933
C	-1.081104	-6.349283	-0.819992
P	-1.538400	0.085091	-1.012719
C	-1.440707	1.784644	-1.897368
C	-2.775667	1.961846	-2.646570
Sn	-1.746336	-1.750877	-2.761716
C	-0.086726	-5.340785	-2.897359
C	-2.584202	-5.511766	-2.653311
C	-0.272679	1.919626	-2.890416
C	-1.317702	2.871964	-0.811400
H	-0.803707	-3.435679	2.046561
H	1.749635	-3.287217	2.918137
H	3.361313	-3.203969	0.752975
H	1.806735	-3.268212	-1.446857
H	-0.891184	-0.029060	2.049745
H	1.666421	-0.048022	2.921256
H	3.280222	-0.044360	0.756076

H	1.724371	-0.055742	-1.443763
H	-2.559720	-6.494897	-3.142685
H	-3.442708	-5.494752	-1.972877
H	-2.756807	-4.761204	-3.434610
H	-1.034185	-7.342157	-1.288682
H	-0.155519	-6.203007	-0.253233
H	-1.916776	-6.350254	-0.111604
H	-0.042468	-6.339166	-3.356411
H	-0.197616	-4.608454	-3.705726
H	0.872936	-5.165087	-2.402091
H	-2.801565	2.945819	-3.134173
H	-2.909482	1.204831	-3.429249
H	-3.632244	1.899614	-1.966339
H	-0.279598	2.919824	-3.347592
H	0.694674	1.792413	-2.395279
H	-0.345798	1.184093	-3.700172
H	-1.321705	3.866801	-1.278254
H	-2.152407	2.828772	-0.103188
H	-0.385900	2.772296	-0.244717

E(B3LYP/def2-TZVP//B3LYP/6-31+G)* = -2862.325372

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.440465
C	1.379500	0.000000	1.850349
C	2.204848	-0.008238	0.688728
C	1.351873	-0.014626	-0.457097
Fe	0.985892	1.668502	0.684067
C	0.031287	3.309463	-0.103233
C	0.032138	3.399223	1.334431
C	1.411633	3.398687	1.744331
C	2.236304	3.318920	0.584940
C	1.382926	3.270019	-0.559558
P	-1.365368	3.585264	2.509600
Sn	-3.131968	1.758401	2.317030
P	-1.400120	-0.085987	2.624165
C	-2.234221	-1.783091	2.291591
C	-3.315477	-1.956876	3.376952
C	-1.161409	-2.877898	2.462611
C	-2.881299	-1.916619	0.900111
C	-2.167408	5.273817	2.071400
C	-1.074001	6.356678	2.174597
C	-3.244595	5.535303	3.143136
C	-2.812587	5.332602	0.673887
H	1.719826	0.019327	2.878047
H	3.287457	0.019056	0.675080
H	1.674611	0.005343	-1.490934
H	-0.879147	0.030017	-0.630160
H	1.752138	3.437015	2.771437
H	3.318195	3.270365	0.573682
H	1.704580	3.179567	-1.589962
H	-0.848637	3.256854	-0.730821
H	-3.798186	-2.938233	3.267605
H	-2.889196	-1.901083	4.385242
H	-4.101418	-1.195036	3.299370
H	-1.620427	-3.870015	2.343935

H	-0.366317	-2.785521	1.714622
H	-0.699591	-2.836972	3.455843
H	-3.328027	-2.915907	0.787400
H	-3.679131	-1.178512	0.753892
H	-2.146597	-1.794302	0.098056
H	-3.708731	6.516884	2.972537
H	-4.044835	4.785096	3.112682
H	-2.818895	5.534410	4.153212
H	-3.240417	6.331188	0.498855
H	-2.080754	5.146701	-0.118516
H	-3.624299	4.602023	0.573416
H	-1.514246	7.347976	1.994062
H	-0.612513	6.368972	3.168750
H	-0.281187	6.202873	1.434342

RP-Sn-PR [3]ferrocenophanes R=^{t}Bu isomer-2

*E(B3LYP/Def2-TZVP//B3LYP/6-311+G**)* = -2862.640722

C	-0.091768	0.022245	0.190558
C	-0.030941	-0.109105	1.609134
C	1.338529	-0.110677	1.993913
C	2.148386	0.017948	0.812868
C	1.241133	0.101234	-0.300466
Fe	0.990456	-1.686841	0.705887
C	0.825566	-3.286670	-0.621185
C	-0.113910	-3.438421	0.440742
C	0.609922	-3.478201	1.664850
C	2.013160	-3.349653	1.375143
C	2.128712	-3.233413	-0.053299
P	3.310283	-3.275034	2.665022
C	4.048691	-5.046809	2.726171
P	3.970456	0.003252	0.634800
C	4.520148	1.800050	1.031595
Sn	5.185948	-1.605852	2.200895
C	2.919963	-6.014053	3.130471
C	4.121403	2.251424	2.446470
C	3.868641	2.732476	-0.007234
C	6.049351	1.855594	0.874199
C	5.135105	-5.051953	3.815204
C	4.649679	-5.493644	1.383133
H	3.049719	-3.084531	-0.596103
H	0.587194	-3.195969	-1.670738
H	-1.187790	-3.485101	0.335694
H	0.185995	-3.557551	2.654643
H	1.536233	0.177200	-1.336249
H	-0.990935	0.030518	-0.407656
H	-0.875989	-0.220052	2.272607
H	1.713101	-0.233751	2.998706
H	5.012105	-6.526708	1.459001
H	3.909889	-5.460736	0.580254
H	5.495253	-4.863481	1.094291
H	3.319859	-7.031127	3.220679
H	2.481720	-5.738291	4.093222
H	2.120620	-6.035651	2.385979
H	5.543449	-6.062969	3.924267

H	5.967769	-4.387452	3.566986
H	4.733996	-4.745968	4.785327
H	6.399808	2.881324	1.034970
H	6.559917	1.217335	1.601143
H	6.362354	1.547476	-0.127172
H	4.200481	3.763735	0.162700
H	4.147176	2.453156	-1.026738
H	2.778525	2.717685	0.064279
H	4.414632	3.297195	2.603666
H	3.042357	2.183539	2.601514
H	4.615075	1.647409	3.212615

Ge Ge bonded dimeric structure of the germylene

E(M06-2X/cc-pVDZ)) = -9449.3555357
G*(M06-2X/cc-pVDZ*) = -9448.640943

C	-5.459706	-1.283964	-2.311842
C	-5.630981	-2.327057	-1.359959
C	-4.374851	-2.562927	-0.742015
C	-3.410516	-1.667322	-1.301672
C	-4.101669	-0.871214	-2.271687
Fe	-4.979294	-0.545018	-0.374670
C	-4.842700	1.515904	0.096513
C	-4.179392	0.760143	1.116208
C	-5.166086	-0.093391	1.702894
C	-6.410287	0.134343	1.058801
C	-6.210498	1.134215	0.066578
P	-2.411172	0.727589	1.643544
C	-2.158547	2.502123	2.305701
C	-2.688801	3.624699	1.414793
P	-1.653170	-1.617691	-0.742233
C	-0.713386	-2.048949	-2.357026
C	-0.872819	-3.562641	-2.547340
Ge	-1.427638	0.797205	-0.575435
Ge	0.966009	0.425494	0.293165
P	2.551220	2.082813	-0.192248
C	1.926367	3.115034	-1.664370
C	0.791834	4.001312	-1.139379
C	4.034560	1.265694	-0.883516
C	4.159207	0.286035	-1.920402
C	5.537977	0.012282	-2.113852
C	6.280447	0.817523	-1.206079
C	5.359871	1.591003	-0.453719
Fe	4.959146	-0.468055	-0.119779
C	5.392666	-2.509915	0.295702
C	3.991556	-2.288438	0.330544
C	3.711009	-1.330785	1.358381
C	4.964829	-0.972904	1.949086
C	5.994995	-1.692963	1.293047
P	2.114501	-0.692264	1.990810
C	1.225923	-2.246214	2.615528
C	2.093726	-2.749560	3.777788
C	1.045253	-3.365105	1.591242

C	-0.140485	-1.798603	3.133184
C	3.108539	3.998237	-2.084088
C	1.447961	2.300428	-2.866357
C	-0.653056	2.689837	2.517556
C	-2.874159	2.549164	3.661319
C	-1.187373	-1.325964	-3.616980
C	0.767552	-1.722969	-2.130518
H	3.261419	-2.732221	-0.341261
H	-4.168542	-3.280701	0.048624
H	-6.563865	-2.835739	-1.130747
H	5.600701	2.293562	0.340652
H	-4.368682	2.236036	-0.567313
H	5.916696	-3.163108	-0.397427
H	-6.239467	-0.852028	-2.934229
H	-7.344088	-0.381739	1.266707
H	-3.665081	-0.062027	-2.852756
H	-6.963229	1.513284	-0.620228
H	3.334807	-0.203447	-2.433708
H	7.361122	0.817811	-1.090721
H	5.951488	-0.713944	-2.809009
H	5.090018	-0.246140	2.748041
H	7.059522	-1.615899	1.497732
H	-4.970429	-0.815564	2.492185
H	0.466219	4.688217	-1.937916
H	-0.085048	3.404908	-0.843729
H	1.118502	4.604175	-0.278087
H	2.771205	4.702956	-2.861721
H	3.496190	4.585027	-1.236673
H	3.933205	3.399663	-2.499475
H	1.155215	2.985233	-3.680759
H	2.244577	1.648239	-3.253380
H	0.565359	1.693058	-2.614039
H	-0.517780	-1.571507	-4.460020
H	-2.202982	-1.637785	-3.896374
H	-1.180819	-0.232210	-3.483051
H	-0.357008	-3.889245	-3.466893
H	-0.451783	-4.118321	-1.695327
H	-1.936450	-3.833235	-2.638434
H	1.388365	-2.184315	-2.918401
H	0.942665	-0.632460	-2.190932
H	1.130018	-2.102380	-1.158709
H	-2.764030	3.549694	4.113605
H	-3.950026	2.344186	3.544740
H	-2.456928	1.806150	4.357453
H	-2.407385	4.602544	1.843829
H	-2.272418	3.567860	0.396147
H	-3.785199	3.593792	1.344319
H	-0.462145	3.592150	3.122557
H	-0.198419	1.831830	3.042476
H	-0.131863	2.833548	1.555693
H	0.530842	-4.210816	2.078864
H	0.411871	-3.040980	0.752220
H	2.008438	-3.738198	1.216487
H	1.603865	-3.623856	4.236963
H	3.091629	-3.061399	3.432161

H	2.217123	-1.979269	4.553832
H	-0.626599	-2.641154	3.651909
H	-0.056498	-0.963582	3.846989
H	-0.802789	-1.486374	2.312971

E(B3LYP/6-31+G)* = -9450.3320065
G(B3LYP/6-31+G)* = -9449.628288

C	-6.306710	1.121596	0.329742
C	-6.474433	-0.027957	1.162642
C	-5.200168	-0.360435	1.711640
C	-4.222528	0.581254	1.229096
C	-4.927706	1.492550	0.362456
Fe	-5.116916	-0.430490	-0.363218
C	-4.596200	-2.342271	-0.988360
C	-3.622388	-1.391200	-1.460435
C	-4.339917	-0.442005	-2.274720
C	-5.717912	-0.817135	-2.310385
C	-5.876822	-1.991403	-1.510693
P	-1.825829	-1.519917	-1.025641
C	-1.016458	-1.820167	-2.764947
C	0.503056	-1.902639	-2.539107
P	-2.442573	0.505841	1.740706
C	-2.223322	2.177051	2.703647
C	-3.109116	2.073065	3.960767
Ge	-1.419517	0.875532	-0.479379
Ge	1.036411	0.358361	0.264365
P	2.244478	-0.798302	1.957943
C	1.351283	-2.407432	2.534874
C	0.135653	-1.963738	3.365041
C	3.820353	-1.404602	1.223984
C	5.102631	-1.157876	1.833801
C	6.103121	-1.843752	1.084554
C	5.458263	-2.521928	0.003948
C	4.058910	-2.251237	0.082109
Fe	5.093093	-0.480160	-0.123978
C	5.853853	0.158090	-1.951103
C	4.449191	0.397967	-1.871983
C	4.198346	1.274127	-0.754365
C	5.475542	1.556775	-0.151201
C	6.486715	0.870185	-0.885341
P	2.624948	2.032989	-0.185228
C	2.101308	3.200815	-1.629252
C	1.660561	2.474449	-2.908593
C	0.953825	4.077471	-1.096857
C	3.323549	4.090709	-1.927964
C	2.354707	-3.136894	3.451497
C	0.903151	-3.343825	1.403792
C	-1.517916	-3.195836	-3.248605
C	-1.315051	-0.764191	-3.839175
C	-2.586624	3.451736	1.928305
C	-0.748953	2.245190	3.136695
H	3.302213	-2.609770	-0.611389
H	-4.376409	-3.181329	-0.331568
H	-6.812579	-2.513427	-1.319768
H	5.627537	2.182865	0.725454

H	-4.481189	2.314907	-0.191268
H	5.950930	-3.119059	-0.761109
H	-6.511373	-0.286348	-2.833509
H	-7.406100	-0.564263	1.333071
H	-3.907996	0.426625	-2.765659
H	-7.087347	1.612889	-0.248406
H	3.693173	-0.021932	-2.531105
H	7.551648	0.870929	-0.661427
H	6.353031	-0.477985	-2.679661
H	5.265761	-0.541721	2.715546
H	7.172366	-1.835133	1.286769
H	-4.983802	-1.191061	2.380174
H	0.671509	4.818436	-1.865285
H	0.056208	3.481685	-0.868431
H	1.251034	4.626540	-0.189319
H	3.043145	4.848528	-2.680398
H	3.670512	4.624057	-1.028312
H	4.168156	3.512509	-2.332280
H	1.406544	3.216398	-3.687645
H	2.458740	1.834648	-3.313775
H	0.765225	1.859062	-2.733864
H	-0.755370	-0.997148	-4.764557
H	-2.382796	-0.743518	-4.100667
H	-1.022765	0.247452	-3.515524
H	-1.040899	-3.457162	-4.211019
H	-1.280387	-3.991283	-2.524075
H	-2.607910	-3.194533	-3.404828
H	1.014058	-2.209474	-3.469617
H	0.926922	-0.922244	-2.253789
H	0.760811	-2.633958	-1.755822
H	-2.977102	2.970906	4.592032
H	-4.176568	2.001494	3.699352
H	-2.847888	1.190648	4.566775
H	-2.371989	4.342545	2.547965
H	-2.006896	3.546702	0.996242
H	-3.655691	3.482933	1.672487
H	-0.589805	3.104438	3.812666
H	-0.435004	1.334665	3.671774
H	-0.073339	2.385840	2.276069
H	0.451057	-4.253254	1.840578
H	0.140310	-2.877309	0.761829
H	1.749417	-3.670145	0.780303
H	1.853544	-4.007525	3.909392
H	3.230574	-3.506994	2.897290
H	2.711932	-2.488775	4.268109
H	-0.363051	-2.854936	3.785145
H	0.434833	-1.318711	4.207271
H	-0.614287	-1.424581	2.765613

E(B3LYP/6-31G)* = -9445.914466
G(B3LYP/6-31G)* = -9445.188622

C	-5.603934	-2.180203	0.184360
C	-6.152636	-1.435101	1.271938
C	-5.074996	-0.823822	1.975833
C	-3.842009	-1.184238	1.331841

C	-4.188296	-2.017945	0.210381
Fe	-5.078806	-0.206443	0.013079
C	-5.242841	1.845811	-0.122087
C	-4.057210	1.397739	-0.799891
C	-4.491893	0.464664	-1.808151
C	-5.914240	0.372949	-1.763822
C	-6.377451	1.219145	-0.711817
P	-2.377832	2.059071	-0.429197
C	-1.737719	2.655348	-2.150507
C	-0.283516	3.096791	-1.922963
P	-2.176646	-0.678601	1.911157
C	-1.431410	-2.361153	2.473038
C	-1.371763	-3.398975	1.341885
Ge	-1.235548	-0.029317	-0.172099
Ge	1.234120	-0.031760	0.174922
P	2.375071	2.058712	0.421481
C	1.734389	2.664214	2.139498
C	2.592728	3.878311	2.538971
C	4.053636	1.398878	0.798116
C	4.484804	0.464730	1.806929
C	5.907357	0.373784	1.768070
C	6.374280	1.221913	0.719225
C	5.241680	1.848733	0.125784
Fe	5.079318	-0.203318	-0.012978
C	5.613992	-2.174061	-0.188952
C	4.197506	-2.018706	-0.211287
C	3.844388	-1.185060	-1.330643
C	5.074148	-0.817376	-1.976847
C	6.156482	-1.424383	-1.276466
P	2.175562	-0.687408	-1.907017
C	1.435520	-2.373795	-2.463337
C	0.020205	-2.145939	-3.030958
C	2.335849	-2.877184	-3.612101
C	1.392439	-3.414424	-1.333850
C	1.747216	1.621638	3.270543
C	0.280436	3.105107	1.909773
C	-2.595454	3.867926	-2.555843
C	-1.751237	1.607176	-3.276458
C	-0.021996	-2.126039	3.052360
C	-2.338366	-2.871571	3.613287
H	-3.843403	-0.093671	-2.467212
H	5.152638	-0.178865	-2.847264
H	7.207228	-1.321980	-1.516042
H	-5.158743	-0.187147	2.847112
H	3.833698	-0.095121	2.462217
H	-6.531420	-0.254389	-2.394609
H	6.182206	-2.733442	0.543466
H	7.406191	1.354721	0.420183
H	3.493461	-2.419183	0.505093
H	6.522416	-0.254148	2.400332
H	-3.480059	-2.413033	-0.504949
H	-7.204439	-1.338366	1.509242
H	-6.167730	-2.741058	-0.550331
H	-5.254778	2.546891	0.702386
H	-7.408207	1.350840	-0.408342

H	5.256508	2.551025	-0.697606
H	0.317188	-3.038422	3.561592
H	0.718570	-1.886343	2.280202
H	-0.019140	-1.314038	3.788580
H	-1.954253	-3.830059	3.987991
H	-2.361351	-2.169446	4.454674
H	-3.366867	-3.033010	3.275893
H	-0.791621	-4.279498	1.651442
H	-2.370855	-3.742320	1.060680
H	-0.901834	-2.968344	0.453511
H	0.811288	-4.295905	-1.638712
H	2.396023	-3.755561	-1.066187
H	0.932648	-2.988001	-0.438181
H	1.955417	-3.838342	-3.983740
H	2.346164	-2.174580	-4.453313
H	3.368510	-3.031310	-3.284007
H	-0.320143	-3.061405	-3.533848
H	-0.714805	-1.905074	-2.253868
H	0.008605	-1.336768	-3.770235
H	2.225197	4.301319	3.484538
H	3.643103	3.601858	2.684050
H	2.550842	4.667167	1.779566
H	1.243837	2.032203	4.157066
H	1.212785	0.712642	2.973637
H	2.763071	1.352451	3.569101
H	-0.134776	3.530990	2.832925
H	0.205547	3.867332	1.127112
H	-0.357415	2.265139	1.622893
H	-1.243902	2.011545	-4.163566
H	-1.221230	0.697464	-2.973739
H	-2.767262	1.340509	-3.576667
H	-2.228084	4.285909	-3.503712
H	-3.646067	3.591402	-2.699053
H	-2.552710	4.660608	-1.800488
H	0.131429	3.518861	-2.847980
H	-0.208355	3.862262	-1.143496
H	0.354420	2.258034	-1.632779

E(B3LYP/6-31+G)* = -9446.021611

C	6.407671	1.270574	0.630784
C	5.961696	0.471048	1.727157
C	4.537064	0.544107	1.774762
C	4.083374	1.413967	0.718485
C	5.259305	1.848620	0.016449
Fe	5.131883	-0.223228	-0.029224
C	4.336486	-2.110658	-0.152526
C	3.883418	-1.313142	-1.262265
C	5.059243	-0.899157	-1.982126
C	6.207268	-1.433866	-1.329494
C	5.760354	-2.184917	-0.199305
P	2.190705	-0.851191	-1.790344
C	1.442875	-2.535995	-2.332312
C	2.230461	-2.942873	-3.599930
P	2.400927	2.072333	0.336375

C	1.863649	2.833174	2.035748
C	1.510927	1.813338	3.135358
Ge	1.237234	-0.022482	0.241159
Ge	-1.205760	0.006758	-0.184562
P	-2.387797	2.083186	-0.323287
C	-1.826131	2.840186	-2.015460
C	-2.971054	3.741034	-2.521263
C	-4.067680	1.432338	-0.722615
C	-4.514220	0.571447	-1.789179
C	-5.939802	0.508621	-1.759666
C	-6.393553	1.305758	-0.664766
C	-5.249085	1.872323	-0.032981
Fe	-5.135306	-0.200474	0.002137
C	-6.233602	-1.411622	1.282280
C	-5.090058	-0.887707	1.951224
C	-3.909039	-1.304071	1.240968
C	-4.354217	-2.093863	0.122639
C	-5.778769	-2.158892	0.152574
P	-2.217909	-0.866524	1.788959
C	-1.492824	-2.560841	2.330934
C	-0.022097	-2.362893	2.744381
C	-2.298639	-2.963088	3.588665
C	-1.602680	-3.688292	1.290579
C	-1.454820	1.817051	-3.106236
C	-0.599091	3.726745	-1.727660
C	1.547690	-3.669091	-1.297920
C	-0.029295	-2.316836	-2.729798
C	0.630371	3.715745	1.762252
C	3.013236	3.738290	2.521969
H	-3.878419	0.046791	-2.488796
H	5.058004	-0.263680	-2.858986
H	7.238416	-1.271679	-1.618430
H	-5.095012	-0.258100	2.832259
H	3.906347	0.019824	2.479240
H	-6.563821	-0.076897	-2.423929
H	6.394091	-2.690560	0.519231
H	7.434306	1.392263	0.307872
H	3.703874	-2.549890	0.607468
H	6.589575	-0.122545	2.380572
H	-3.714371	-2.533289	-0.631135
H	-7.266973	-1.244635	1.560240
H	-6.407463	-2.656237	-0.576044
H	-5.252006	2.518918	0.835736
H	-7.423186	1.432994	-0.353804
H	5.255860	2.499251	-0.849264
H	0.338896	-3.260441	3.265928
H	0.628321	-2.192737	1.881266
H	0.095615	-1.507192	3.420033
H	-1.920078	-3.920428	3.973584
H	-2.203470	-2.217883	4.386912
H	-3.363915	-3.091541	3.367613
H	-1.116714	-4.595759	1.678529
H	-2.645515	-3.940372	1.076070
H	-1.112230	-3.427433	0.347287
H	1.048769	-4.570082	-1.684843

H	2.589307	-3.933252	-1.092273
H	1.068040	-3.405829	-0.349712
H	1.836502	-3.893466	-3.986398
H	2.137777	-2.192303	-4.393492
H	3.296002	-3.085615	-3.389353
H	-0.408831	-3.205866	-3.252847
H	-0.668056	-2.144544	-1.857800
H	-0.142138	-1.455206	-3.398681
H	2.697723	4.274681	3.428354
H	3.912725	3.165139	2.767278
H	3.282638	4.487994	1.768010
H	1.201519	2.344865	4.047402
H	0.680792	1.162782	2.840351
H	2.364181	1.180962	3.398230
H	0.335990	4.227056	2.689852
H	0.844830	4.483566	1.010578
H	-0.238120	3.142408	1.423265
H	-1.142922	2.346826	-4.018350
H	-0.620043	1.177105	-2.801239
H	-2.299423	1.174719	-3.372827
H	-2.641750	4.276126	-3.423347
H	-3.865115	3.165607	-2.780255
H	-3.254401	4.492017	-1.773718
H	-0.295576	4.237551	-2.652508
H	-0.825166	4.494740	-0.979573
H	0.266962	3.156253	-1.378198

Ge-P bonded dimeric structure of the germylene

E(M06-2X/cc-pvdz) = -9449.3586961
G*(M06-2X/cc-pVDZ*) = -9448.638957

C	-5.771191	0.026401	-0.196580
C	-4.583395	-0.380274	0.467957
C	-3.815615	-1.197337	-0.420747
C	-4.564321	-1.293875	-1.637435
C	-5.761903	-0.543358	-1.499453
Fe	-4.050589	0.720195	-1.264405
C	-3.525495	2.751640	-0.941817
C	-2.339549	1.943979	-0.917816
C	-2.239908	1.323144	-2.203890
C	-3.336089	1.746628	-2.998492
C	-4.128102	2.631868	-2.221409
P	-1.152681	1.636563	0.456522
Ge	0.868490	0.892332	-0.676155
P	2.833699	2.070938	-1.295396
C	3.687923	3.167079	0.001889
C	3.793623	2.604610	1.414943
P	-2.094644	-1.844326	-0.263419
C	-2.415969	-3.535563	0.569895
C	-1.053298	-4.099889	0.982335
C	3.835985	0.512047	-1.456550
C	3.927853	-0.179752	-2.705162
C	4.905944	-1.202557	-2.601617
C	5.428359	-1.168591	-1.280550
C	4.758174	-0.134404	-0.572051

Fe	3.357149	-1.638053	-1.212521
C	2.127440	-3.274549	-1.880061
C	1.311030	-2.276255	-1.297426
C	1.701346	-2.102578	0.072660
C	2.764342	-3.033395	0.311975
C	3.028486	-3.740259	-0.887969
P	1.059521	-0.738307	1.127604
Ge	-1.371867	-0.559200	1.654771
C	1.935903	-0.946283	2.813140
C	1.508532	-2.299603	3.397597
C	1.454167	0.152593	3.761898
C	3.460126	-0.825603	2.717758
C	5.083034	3.507814	-0.534718
C	2.828934	4.436722	0.036644
C	-3.032710	-4.438939	-0.503852
C	-3.352037	-3.475035	1.776287
C	-1.417615	3.059601	1.681725
C	-1.339905	4.407159	0.957848
C	-2.750011	2.878605	2.421561
C	-0.291873	2.989999	2.712867
H	-4.232300	-1.816109	-2.532416
H	-4.286924	-0.087684	1.474435
H	4.926308	0.114259	0.470496
H	6.180933	-1.836707	-0.869265
H	-1.471161	0.611733	-2.496299
H	0.531507	-1.715540	-1.801534
H	-6.538781	0.679847	0.210507
H	5.188173	-1.899177	-3.386907
H	3.804000	-4.490144	-1.021522
H	3.340400	0.061908	-3.588315
H	2.084080	-3.602595	-2.915122
H	-3.923512	3.350430	-0.130561
H	-3.543318	1.423561	-4.015133
H	-5.048910	3.116850	-2.534478
H	-6.522323	-0.403439	-2.263347
H	3.306383	-3.181173	1.238695
H	-1.178360	-5.115823	1.393487
H	-0.362564	-4.156989	0.125931
H	-0.576578	-3.481752	1.761193
H	-3.180557	-5.454431	-0.097978
H	-4.013744	-4.058805	-0.828942
H	-2.378034	-4.511415	-1.385697
H	-3.514222	-4.492482	2.173013
H	-2.933409	-2.860457	2.588714
H	-4.332684	-3.058992	1.499148
H	2.004256	-2.443273	4.372432
H	0.420856	-2.318192	3.569645
H	1.766560	-3.149980	2.752789
H	3.894139	-1.044615	3.707895
H	3.920590	-1.497822	1.986087
H	3.737415	0.201684	2.452168
H	1.953421	0.017625	4.735316
H	1.714611	1.151795	3.385217
H	0.368458	0.101686	3.928970
H	5.579167	4.221434	0.145286

H	5.714708	2.609375	-0.607928
H	5.024024	3.968009	-1.532346
H	3.301014	5.188381	0.690423
H	2.709485	4.873553	-0.966024
H	1.825894	4.221289	0.438804
H	4.079673	3.405691	2.118969
H	2.834364	2.176407	1.745914
H	4.566583	1.827427	1.481451
H	-0.407340	3.819085	3.429964
H	-0.333074	2.049118	3.277271
H	0.699287	3.078677	2.241199
H	-1.420179	5.217915	1.700786
H	-0.375338	4.516784	0.439447
H	-2.135195	4.543780	0.215498
H	-2.900167	3.725865	3.111847
H	-3.617120	2.830760	1.750248
H	-2.734716	1.953037	3.016958

E(B3LYP/6-311G)* = -9445.904158
G(B3LYP/6-311G)* = -9445.177420

C	-3.615621	-1.216348	-0.613785
C	-4.274064	-1.288140	-1.891000
C	-5.514044	-0.590032	-1.810721
C	-5.642935	-0.075967	-0.485359
C	-4.483608	-0.462037	0.248692
Fe	-3.929118	0.655191	-1.363395
C	-2.169474	1.341714	-2.147515
C	-2.366738	1.853118	-0.814029
C	-3.604201	2.593858	-0.844593
C	-4.137149	2.543093	-2.165279
C	-3.252683	1.767006	-2.966460
P	-1.213350	1.553185	0.585153
Ge	-1.306036	-0.681544	1.683586
P	-1.935351	-1.894790	-0.303874
C	-2.365944	-3.595198	0.500621
C	-3.469200	-3.528575	1.569174
Ge	0.788755	0.800504	-0.569834
P	1.162750	-0.754798	1.209162
C	2.019647	-0.967458	2.930282
C	3.537615	-0.717698	2.895397
C	1.942156	-1.985836	0.084117
C	3.112418	-2.804927	0.260935
C	3.392835	-3.478615	-0.961877
C	2.401583	-3.100705	-1.910412
C	1.513112	-2.190714	-1.280337
Fe	3.441513	-1.441346	-1.252393
C	4.830929	-1.008402	-2.694241
C	3.765898	-0.066326	-2.766538
C	3.693576	0.663730	-1.531277
C	4.700769	0.097506	-0.675328
C	5.414432	-0.904858	-1.397614
P	2.594124	2.147359	-1.374323
C	3.337886	3.337956	-0.072823
C	2.389874	4.553536	-0.133200
C	3.351362	2.785816	1.355920

C	4.751094	3.760487	-0.511354
C	1.681031	-2.388529	3.425972
C	1.412489	0.035018	3.923870
C	-1.631225	2.868782	1.919033
C	-0.543674	2.776063	2.997322
C	-1.628881	4.286106	1.320350
C	-2.980480	2.530427	2.590797
C	-1.071753	-4.133616	1.134938
C	-2.806243	-4.524221	-0.645683
H	-3.867206	-1.765899	-2.773064
H	-4.262575	-0.211796	1.278626
H	4.908006	0.393783	0.342618
H	6.238496	-1.495618	-1.017591
H	-1.343510	0.715567	-2.456214
H	0.660902	-1.713111	-1.736440
H	-6.465571	0.519937	-0.110284
H	5.128902	-1.694900	-3.476788
H	4.225308	-4.149209	-1.133816
H	3.129501	0.110168	-3.624220
H	2.341137	-3.426284	-2.940703
H	-4.073320	3.102123	-0.016839
H	-3.386609	1.520108	-4.011641
H	-5.063662	2.999226	-2.489909
H	-6.223097	-0.453038	-2.617500
H	3.700257	-2.910898	1.158526
H	-1.226052	-5.155159	1.508935
H	-0.246314	-4.159285	0.414364
H	-0.763752	-3.512478	1.983274
H	-3.029992	-5.528455	-0.258179
H	-3.711693	-4.152224	-1.138758
H	-2.022087	-4.622188	-1.404897
H	-3.645878	-4.528556	1.991558
H	-3.191641	-2.862413	2.395051
H	-4.415954	-3.172512	1.150668
H	2.143240	-2.554984	4.408943
H	0.597494	-2.497347	3.542438
H	2.032292	-3.173941	2.751586
H	3.958721	-0.945029	3.884242
H	4.069665	-1.320136	2.160721
H	3.750719	0.331865	2.680605
H	1.880194	-0.114237	4.906090
H	1.601573	1.067701	3.621159
H	0.334868	-0.111977	4.042929
H	5.146828	4.523919	0.173617
H	5.447155	2.915007	-0.507598
H	4.745999	4.187130	-1.520554
H	2.693430	5.311045	0.601456
H	2.391759	5.018183	-1.125106
H	1.359762	4.252783	0.092146
H	3.568897	3.581173	2.083000
H	2.381711	2.339786	1.596362
H	4.117388	2.015156	1.477761
H	-0.752616	3.503038	3.793014
H	-0.529305	1.781923	3.445396
H	0.451292	2.995160	2.597491

H	-1.868814	5.012781	2.108518
H	-0.642713	4.546833	0.922043
H	-2.355777	4.413689	0.515665
H	-3.182799	3.258318	3.388514
H	-3.825892	2.555077	1.899692
H	-2.945268	1.533089	3.043781

E(B3LYP/cc-pVDZ) = -9450.328368
G(B3LYP/cc-pVDZ) = -9449.621182

C	-3.844583	-1.060501	-0.607550
C	-4.446165	-1.073258	-1.917007
C	-5.639433	-0.291488	-1.886208
C	-5.795192	0.218944	-0.560788
C	-4.699806	-0.253604	0.223860
Fe	-3.983456	0.864328	-1.364271
C	-2.161702	1.471065	-2.144261
C	-2.321174	1.989722	-0.808492
C	-3.515676	2.800680	-0.827798
C	-4.055057	2.791689	-2.149303
C	-3.219935	1.968127	-2.960335
P	-1.153836	1.636537	0.583590
Ge	-1.419144	-0.628183	1.701820
P	-2.226150	-1.889488	-0.259499
C	-2.810771	-3.533692	0.594257
C	-3.807085	-3.340537	1.746589
Ge	0.910132	0.861872	-0.574720
P	1.088229	-0.830135	1.203943
C	1.947061	-1.084453	2.932786
C	3.469427	-0.870925	2.881686
C	1.809510	-2.112251	0.086700
C	2.943739	-2.983458	0.268318
C	3.167528	-3.704180	-0.942222
C	2.181791	-3.295132	-1.887860
C	1.352512	-2.320916	-1.266571
Fe	3.350555	-1.665429	-1.293562
C	4.690163	-1.283807	-2.824534
C	3.730980	-0.229967	-2.789980
C	3.814667	0.450646	-1.524033
C	4.808826	-0.257537	-0.758994
C	5.366223	-1.296731	-1.566116
P	2.909009	2.052676	-1.230166
C	3.946045	3.127173	-0.003080
C	3.172956	4.459036	0.059441
C	4.120733	2.585740	1.418810
C	5.321818	3.369493	-0.652271
C	1.597521	-2.498800	3.435607
C	1.373494	-0.058636	3.921195
C	-1.400931	3.074859	1.852298
C	-0.271154	2.980624	2.887908
C	-1.290134	4.429788	1.129975
C	-2.743960	2.934065	2.594251
C	-1.544488	-4.242156	1.105945
C	-3.460366	-4.394970	-0.504817
H	-4.030694	-1.575871	-2.788081

H	-4.526821	-0.022867	1.273113
H	5.112178	-0.028008	0.257974
H	6.151441	-1.987302	-1.263944
H	-1.371335	0.797428	-2.464413
H	0.503819	-1.821955	-1.722271
H	-6.595359	0.871417	-0.215714
H	4.864454	-1.964741	-3.655343
H	3.962660	-4.428212	-1.110039
H	3.058941	0.049652	-3.598935
H	2.085094	-3.648427	-2.912321
H	-3.952887	3.331937	0.010510
H	-3.373091	1.734444	-4.011882
H	-4.959827	3.305469	-2.467810
H	-6.299888	-0.095827	-2.728825
H	3.545193	-3.092355	1.163221
H	-1.801448	-5.244685	1.492936
H	-0.797047	-4.370214	0.306352
H	-1.066585	-3.685853	1.928948
H	-3.757388	-5.375667	-0.089645
H	-4.366121	-3.919467	-0.913468
H	-2.764082	-4.577150	-1.339082
H	-4.085381	-4.321776	2.174322
H	-3.381752	-2.732335	2.561269
H	-4.733860	-2.854142	1.405298
H	2.065325	-2.659490	4.423842
H	0.510045	-2.619554	3.561372
H	1.951135	-3.293656	2.764507
H	3.885287	-1.026082	3.893404
H	3.991318	-1.552904	2.201252
H	3.710036	0.155632	2.577276
H	1.816076	-0.236961	4.916585
H	1.623929	0.969533	3.625055
H	0.281079	-0.143018	4.020315
H	5.903676	4.085638	-0.043351
H	5.908803	2.441293	-0.730361
H	5.220949	3.791636	-1.664683
H	3.726618	5.188350	0.676682
H	3.033152	4.895660	-0.942016
H	2.176674	4.325964	0.512794
H	4.625962	3.339327	2.051356
H	3.150427	2.351398	1.882973
H	4.740132	1.678174	1.443061
H	-0.354747	3.825792	3.593032
H	-0.335923	2.054158	3.473444
H	0.723323	3.029866	2.418139
H	-1.365257	5.243640	1.872967
H	-0.318331	4.530852	0.621190
H	-2.077478	4.585340	0.380954
H	-2.842586	3.750620	3.332142
H	-3.615714	2.984266	1.928354
H	-2.793417	1.979836	3.141551

*E(B3LYP/6-311+G**)* = -9446.027649

C	-5.126757	-0.490658	-2.432580
C	-5.669395	-0.223621	-1.138605

C	-4.710921	-0.631142	-0.161874
C	-3.560042	-1.162630	-0.842571
C	-3.835437	-1.065667	-2.252454
Fe	-3.892003	0.805663	-1.383324
C	-3.759462	2.525474	-0.293968
C	-2.435578	2.015677	-0.542078
C	-2.273747	1.962649	-1.971983
C	-3.467768	2.446965	-2.581595
C	-4.384155	2.801712	-1.546534
P	-1.156763	1.598259	0.697364
Ge	0.772084	0.777461	-0.514097
P	2.608967	2.082241	-1.344185
C	3.720205	3.182119	-0.226953
C	5.060899	3.410051	-0.954843
P	-1.984719	-1.901495	-0.259398
C	-2.565598	-3.543857	0.565762
C	-2.937538	-4.512767	-0.573926
C	3.550279	0.530420	-1.718094
C	4.706286	-0.087408	-1.124954
C	5.155986	-1.143216	-1.976490
C	4.255841	-1.228130	-3.080846
C	3.262641	-0.221901	-2.907880
Fe	3.258710	-1.578695	-1.315568
C	3.369833	-3.564199	-0.760867
C	3.138573	-2.750929	0.386524
C	1.885193	-2.055508	0.223056
C	1.382038	-2.439365	-1.073840
C	2.280828	-3.373043	-1.659203
P	1.106763	-0.785500	1.301987
Ge	-1.380144	-0.658907	1.736760
C	1.921334	-1.024955	3.051694
C	1.195924	-0.173192	4.110115
C	3.403660	-0.611006	3.076291
C	1.742111	-2.507303	3.450588
C	2.974838	4.531706	-0.142795
C	3.969323	2.650889	1.191231
C	-1.249453	3.005343	2.007205
C	-2.304039	2.646767	3.072904
C	0.132728	3.110867	2.671543
C	-1.563323	4.360907	1.347185
C	-3.755806	-3.414245	1.530635
C	-1.353253	-4.107133	1.332804
H	-3.150405	-1.363403	-3.036455
H	-4.821424	-0.536181	0.910665
H	5.183175	0.209545	-0.201407
H	6.011767	-1.782699	-1.796660
H	-1.393038	1.603430	-2.487984
H	0.461205	-2.090322	-1.514055
H	-6.624944	0.245122	-0.935298
H	4.300368	-1.946649	-3.889947
H	4.240269	-4.187225	-0.926776
H	2.432764	-0.021768	-3.574540
H	2.169896	-3.824227	-2.637387
H	-4.218375	2.665050	0.675211
H	-3.655839	2.500191	-3.646726

H	-5.392494	3.172144	-1.683622
H	-5.599331	-0.262654	-3.380185
H	3.811240	-2.685247	1.226763
H	-1.579135	-5.119629	1.697016
H	-0.459015	-4.170219	0.701583
H	-1.110535	-3.493871	2.208869
H	-3.236047	-5.487090	-0.159290
H	-3.777529	-4.132766	-1.167422
H	-2.091508	-4.678961	-1.250992
H	-3.967754	-4.389145	1.994789
H	-3.546043	-2.700485	2.336096
H	-4.664930	-3.092421	1.012521
H	2.201986	-2.667737	4.436317
H	0.682730	-2.771735	3.537911
H	2.205670	-3.204161	2.749893
H	3.819010	-0.821126	4.072111
H	4.016775	-1.137939	2.343442
H	3.511061	0.460580	2.890709
H	1.525423	-0.500243	5.105737
H	1.450659	0.885437	4.023247
H	0.107938	-0.282864	4.066470
H	5.662914	4.142162	-0.396868
H	5.647542	2.491017	-1.044192
H	4.903644	3.805740	-1.965144
H	3.544824	5.235937	0.479056
H	2.845595	4.980606	-1.134240
H	1.980172	4.420428	0.304848
H	4.639803	3.331509	1.738516
H	3.036808	2.574177	1.759575
H	4.437110	1.662677	1.182991
H	0.071457	3.775707	3.544145
H	0.495211	2.141007	3.009437
H	0.879211	3.520696	1.985349
H	-1.457068	5.154386	2.100105
H	-0.868105	4.582275	0.529266
H	-2.578028	4.414536	0.947358
H	-2.379270	3.458910	3.809955
H	-3.297507	2.493845	2.638354
H	-2.035567	1.728158	3.604716

10

E(M06-2X/cc-pVDZ) = -5723,8944075
G(M06-2X/cc-pVDZ) = -5723,181157

C	-5.594766	-0.705153	-2.016150
C	-5.875033	-0.387084	-0.658560
C	-4.745998	-0.758194	0.119475
C	-3.749744	-1.307884	-0.748222
C	-4.293294	-1.269421	-2.070860
Fe	-4.160028	0.706018	-1.301568
C	-3.926628	2.632327	-0.452939
C	-2.625946	2.077178	-0.686108
C	-2.527740	1.841952	-2.093839
C	-3.737118	2.255322	-2.710563

C	-4.598700	2.752289	-1.697734
P	-1.294496	1.755023	0.543818
Sn	-1.520205	-0.640558	1.828214
P	-2.036518	-1.886699	-0.401439
C	-2.370870	-3.652485	0.262143
C	-1.050252	-4.179934	0.833767
Sn	0.818219	0.875684	-0.909963
P	1.131035	-0.766715	1.209883
C	2.047381	-0.871160	2.879733
C	3.565605	-0.712473	2.751009
C	1.812002	-2.142764	0.189322
C	1.430002	-2.382356	-1.174627
C	2.258430	-3.398695	-1.710946
C	3.162098	-3.807105	-0.698686
C	2.886857	-3.047421	0.467719
Fe	3.475942	-1.726416	-1.124766
C	5.045428	-1.386109	-2.515084
C	4.082229	-0.360903	-2.700848
C	3.985271	0.419125	-1.504046
C	4.879999	-0.184669	-0.563266
C	5.548056	-1.271532	-1.191174
P	3.052736	2.030038	-1.479955
C	3.881045	3.167080	-0.204149
C	5.305044	3.456491	-0.693743
C	3.051197	4.456280	-0.264965
C	3.923413	2.674480	1.239655
C	1.671118	-2.203230	3.543402
C	1.556258	0.266728	3.776820
C	-1.301992	3.271674	1.687474
C	-1.317676	4.548544	0.843950
C	-2.480295	3.249181	2.667636
C	-0.011955	3.209158	2.505218
C	-2.775830	-4.505527	-0.945473
C	-3.467282	-3.736014	1.323751
H	5.328245	-2.139132	-3.246448
H	2.032337	0.168424	4.766108
H	-0.728166	-3.607296	1.721281
H	-3.448015	3.367673	2.166115
H	-3.762529	-1.585900	-2.966166
H	-4.642500	-0.617970	1.194826
H	5.038482	0.133305	0.461845
H	6.287296	-1.919185	-0.726229
H	-1.682927	1.380473	-2.599690
H	0.628927	-1.880266	-1.707190
H	-6.779935	0.087088	-0.286539
H	3.948861	-4.550782	-0.796649
H	3.517689	-0.167846	-3.610700
H	2.216525	-3.774450	-2.729559
H	-4.356070	2.889158	0.509477
H	-3.968182	2.176467	-3.769445
H	-5.610327	3.123790	-1.838421
H	-6.248682	-0.515618	-2.863660
H	3.433330	-3.143559	1.398607
H	-1.173521	-5.230226	1.147912
H	-0.238210	-4.135725	0.091497

H	-2.944201	-5.550022	-0.630771
H	-3.708592	-4.133257	-1.397518
H	-1.990006	-4.498442	-1.715856
H	-3.601169	-4.785799	1.638219
H	-3.214329	-3.151292	2.223170
H	-4.430902	-3.374490	0.935793
H	2.208162	-2.297016	4.502432
H	0.591434	-2.235631	3.759273
H	1.918015	-3.075708	2.924255
H	1.836144	1.246523	3.364325
H	0.466106	0.236720	3.928893
H	4.024438	-0.841080	3.745804
H	4.032131	-1.426005	2.063853
H	3.805258	0.298516	2.399038
H	-2.375875	4.086251	3.378672
H	-2.499647	2.312994	3.246382
H	0.060829	4.103565	3.145406
H	-0.011386	2.327608	3.160642
H	0.881330	3.169822	1.862713
H	-1.263145	5.425939	1.509785
H	-0.453902	4.582442	0.161956
H	-2.232518	4.630793	0.240464
H	4.213871	3.503161	1.909224
H	2.944516	2.290869	1.567930
H	4.670909	1.880738	1.368455
H	3.522068	5.231975	0.361104
H	2.976443	4.840412	-1.293362
H	2.029337	4.290925	0.114300
H	5.795313	4.174539	-0.013865
H	5.913804	2.539810	-0.720032
H	5.295206	3.889856	-1.704692

E(B3LYP/cc-pVDZ) = -5725.077358
G*(B3LYP/cc-pVDZ) = -5724.375158*

C	-4.529315	2.829758	-1.746170
C	-3.629020	2.335010	-2.736230
C	-2.457319	1.866292	-2.071633
C	-2.610967	2.072037	-0.653957
C	-3.917468	2.654856	-0.467802
Fe	-4.127180	0.825326	-1.391086
C	-4.837125	-0.583437	-0.050353
C	-3.798257	-1.167155	-0.859405
C	-4.245286	-1.071575	-2.224848
C	-5.529569	-0.450999	-2.250522
C	-5.896771	-0.148158	-0.902925
P	-2.170219	-1.923642	-0.411513
C	-2.713455	-3.670307	0.247726
C	-3.820156	-3.641819	1.311740
P	-1.307544	1.748172	0.621101
Sn	0.881920	0.866789	-0.799365
P	3.146466	2.004264	-1.452219
C	4.155663	3.134764	-0.258689
C	4.256894	2.684927	1.202714
C	3.984668	0.344496	-1.575104
C	4.954116	-0.321517	-0.743505

C	5.496791	-1.435252	-1.456461
C	4.828985	-1.515760	-2.716568
C	3.889689	-0.445338	-2.776853
Fe	3.478449	-1.757029	-1.172333
C	2.324436	-3.432598	-1.650665
C	1.480027	-2.430635	-1.094998
C	1.929394	-2.127816	0.243735
C	3.076639	-2.966399	0.480846
C	3.313136	-3.763747	-0.679004
P	1.171242	-0.806532	1.289155
Sn	-1.545001	-0.690199	1.844419
C	2.057829	-0.906926	3.013314
C	1.467545	0.179774	3.924664
C	3.573256	-0.658127	2.925887
C	1.755007	-2.286541	3.630251
C	5.565125	3.308957	-0.855870
C	3.409226	4.482466	-0.317834
C	-1.380527	3.278744	1.804011
C	-0.097357	3.262996	2.648281
C	-1.414135	4.570255	0.968176
C	-2.585919	3.214696	2.761057
C	-1.451267	-4.335372	0.824752
C	-3.198749	-4.478096	-0.970793
H	4.993530	-2.267908	-3.485705
H	1.916556	0.090049	4.929043
H	-1.091316	-3.819785	1.731442
H	-3.548872	3.280758	2.237263
H	-3.674227	-1.404332	-3.089159
H	-4.814582	-0.478869	1.032757
H	5.260395	-0.011937	0.251407
H	6.267291	-2.111683	-1.091037
H	-1.594278	1.412150	-2.552598
H	0.611581	-1.997221	-1.581980
H	-6.810510	0.350771	-0.584796
H	4.118612	-4.486091	-0.797174
H	3.233619	-0.219186	-3.615105
H	2.231618	-3.855952	-2.648490
H	-4.377235	2.912914	0.480804
H	-3.809651	2.297711	-3.808546
H	-5.521572	3.239095	-1.925412
H	-6.114525	-0.222197	-3.139440
H	3.678194	-3.006867	1.381439
H	-1.670313	-5.380367	1.108729
H	-0.625494	-4.349354	0.095608
H	-3.466052	-5.505756	-0.662513
H	-4.092380	-4.025375	-1.429081
H	-2.418204	-4.548437	-1.744950
H	-4.065727	-4.671762	1.631318
H	-3.512044	-3.083608	2.211436
H	-4.744939	-3.185901	0.926970
H	2.236472	-2.357453	4.622320
H	0.672408	-2.428793	3.775459
H	2.125625	-3.119867	3.017310
H	1.695275	1.186474	3.547246
H	0.376713	0.084020	4.041019

H	4.011278	-0.741671	3.936820
H	4.098150	-1.366556	2.275582
H	3.782565	0.353422	2.555126
H	-2.540365	4.063446	3.467290
H	-2.582596	2.286019	3.353127
H	-0.063785	4.166803	3.281189
H	-0.066528	2.392392	3.317092
H	0.808593	3.252275	2.022590
H	-1.393753	5.443067	1.644991
H	-0.538560	4.641584	0.303213
H	-2.317716	4.646949	0.347382
H	4.755087	3.466738	1.806042
H	3.263255	2.502462	1.640186
H	4.851802	1.767166	1.310155
H	3.953713	5.241428	0.271075
H	3.320245	4.853045	-1.351345
H	2.392200	4.400198	0.100921
H	6.139298	4.042665	-0.260500
H	6.129074	2.363256	-0.856816
H	5.519413	3.676179	-1.893150

E(B3LYP/def2-TZVP//B3LYP/6-31+G)* = -5725,5299545

C	-4.524071	2.816399	-1.758255
C	-3.617780	2.325836	-2.743506
C	-2.448161	1.863257	-2.073674
C	-2.608175	2.067776	-0.657257
C	-3.917334	2.644462	-0.478473
Fe	-4.112609	0.823113	-1.402009
C	-4.837133	-0.577506	-0.071461
C	-3.789387	-1.162827	-0.865851
C	-4.218324	-1.066317	-2.235801
C	-5.499696	-0.443725	-2.278661
C	-5.883917	-0.140476	-0.936859
P	-2.177917	-1.923839	-0.398717
C	-2.731322	-3.657404	0.258679
C	-3.844106	-3.623898	1.319783
P	-1.315723	1.750867	0.620370
Sn	0.886098	0.872955	-0.786357
P	3.158632	1.993217	-1.443202
C	4.177902	3.116142	-0.266454
C	4.290772	2.669778	1.197185
C	3.982105	0.335733	-1.575317
C	4.959235	-0.338714	-0.761876
C	5.480091	-1.455966	-1.483417
C	4.790005	-1.530691	-2.730480
C	3.859793	-0.453538	-2.773687
Fe	3.470946	-1.757623	-1.168060
C	2.323633	-3.425579	-1.646244
C	1.480147	-2.424113	-1.092002
C	1.927725	-2.119453	0.246325
C	3.073056	-2.959107	0.483838
C	3.310427	-3.756517	-0.673978
P	1.172783	-0.805889	1.290561
Sn	-1.544536	-0.679704	1.847510
C	2.057540	-0.903882	3.005467

C	1.468483	0.181352	3.923070
C	3.574626	-0.648701	2.922528
C	1.760176	-2.285219	3.627774
C	5.586937	3.285903	-0.871761
C	3.439692	4.471270	-0.317407
C	-1.400535	3.268410	1.804031
C	-0.126413	3.251395	2.666285
C	-1.424472	4.567362	0.975144
C	-2.614747	3.209461	2.754510
C	-1.476812	-4.333606	0.845042
C	-3.217846	-4.470884	-0.958556
H	4.929392	-2.284366	-3.495819
H	1.925085	0.094960	4.918694
H	-1.118423	-3.820059	1.746681
H	-3.568551	3.291445	2.228276
H	-3.635436	-1.388890	-3.089593
H	-4.825075	-0.468757	1.006132
H	5.280494	-0.038016	0.225325
H	6.242777	-2.139508	-1.130283
H	-1.589087	1.408360	-2.549124
H	0.621611	-1.988839	-1.582382
H	-6.792103	0.366499	-0.633377
H	4.117423	-4.469204	-0.793340
H	3.188875	-0.228226	-3.593619
H	2.238749	-3.840505	-2.642822
H	-4.384418	2.891865	0.463124
H	-3.796800	2.278608	-3.810481
H	-5.516627	3.209720	-1.940499
H	-6.065085	-0.205879	-3.171519
H	3.674147	-2.998346	1.378318
H	-1.708339	-5.369854	1.130592
H	-0.651856	-4.359773	0.123805
H	-3.492083	-5.489326	-0.644942
H	-4.101721	-4.017091	-1.421497
H	-2.437966	-4.552691	-1.724787
H	-4.096298	-4.648190	1.633874
H	-3.537217	-3.071909	2.216938
H	-4.758754	-3.162356	0.933096
H	2.246567	-2.353259	4.611642
H	0.684134	-2.427336	3.779610
H	2.124752	-3.114952	3.016338
H	1.686869	1.183990	3.545156
H	0.385024	0.080486	4.048760
H	4.011886	-0.757814	3.925599
H	4.099036	-1.331384	2.254511
H	3.777682	0.368492	2.581794
H	-2.562914	4.047666	3.464565
H	-2.625805	2.280155	3.335183
H	-0.095967	4.155931	3.289154
H	-0.111009	2.390623	3.339602
H	0.783782	3.231164	2.056841
H	-1.419439	5.431614	1.654567
H	-0.542657	4.646072	0.328665
H	-2.313424	4.643009	0.342859
H	4.795544	3.447759	1.790172

H	3.304668	2.495160	1.641173
H	4.878506	1.753659	1.300069
H	3.990493	5.218964	0.270242
H	3.350725	4.846800	-1.343364
H	2.429184	4.395650	0.103591
H	6.165842	4.007801	-0.276490
H	6.141281	2.341011	-0.883428
H	5.538354	3.659975	-1.900733

E(B3LYP/6-31G)*= -5724.587229
G*(B3LYP/6-31G*)* = -5723.872802

C	-4.506066	2.804397	-1.771196
C	-3.607010	2.284128	-2.746534
C	-2.443570	1.819222	-2.068789
C	-2.599051	2.053208	-0.656605
C	-3.901822	2.647447	-0.488432
Fe	-4.108515	0.829071	-1.379394
C	-4.807599	-0.539805	-0.026280
C	-3.786280	-1.139016	-0.844303
C	-4.250586	-1.043483	-2.202992
C	-5.526033	-0.408269	-2.214990
C	-5.871162	-0.094562	-0.865715
P	-2.172844	-1.912516	-0.411283
C	-2.724229	-3.651769	0.226593
C	-3.821147	-3.627102	1.302762
P	-1.307635	1.736727	0.619301
Sn	0.887593	0.855128	-0.787343
P	3.134649	2.001265	-1.447257
C	4.153264	3.120429	-0.267630
C	4.258380	2.677992	1.197131
C	3.951829	0.340894	-1.573459
C	4.922302	-0.331098	-0.751045
C	5.451303	-1.446924	-1.467088
C	4.772448	-1.524652	-2.718964
C	3.839469	-0.450766	-2.771100
Fe	3.448430	-1.734811	-1.174802
C	2.325075	-3.406011	-1.654573
C	1.477876	-2.416384	-1.087060
C	1.941046	-2.107709	0.245168
C	3.097960	-2.935150	0.465419
C	3.328133	-3.726663	-0.697640
P	1.177686	-0.807058	1.297261
Sn	-1.535930	-0.692629	1.844623
C	2.062238	-0.913045	3.010657
C	1.462433	0.154541	3.941284
C	3.576322	-0.642256	2.931934
C	1.778893	-2.305199	3.613475
C	5.564409	3.279678	-0.869232
C	3.421105	4.477825	-0.326115
C	-1.381308	3.257286	1.796307
C	-0.101100	3.241632	2.648271
C	-1.409751	4.552536	0.963098
C	-2.589581	3.199713	2.753246
C	-1.464121	-4.340927	0.783133
C	-3.231336	-4.441533	-0.996837

H	4.923565	-2.274783	-3.484844
H	1.910834	0.053123	4.938505
H	-1.089446	-3.840442	1.685231
H	-3.545931	3.269083	2.229886
H	-3.698175	-1.383804	-3.069225
H	-4.769975	-0.430433	1.050241
H	5.238903	-0.024914	0.235388
H	6.215233	-2.125247	-1.108522
H	-1.588352	1.350104	-2.536086
H	0.600155	-2.000637	-1.559149
H	-6.769649	0.414167	-0.539485
H	4.136772	-4.435016	-0.825802
H	3.182238	-0.222351	-3.600315
H	2.225184	-3.826302	-2.646809
H	-4.360686	2.927293	0.447753
H	-3.781631	2.228241	-3.813193
H	-5.489004	3.216427	-1.960592
H	-6.115610	-0.177069	-3.093145
H	3.707985	-2.973568	1.353478
H	-1.693661	-5.379723	1.058281
H	-0.651358	-4.358807	0.048362
H	-3.506869	-5.463243	-0.697941
H	-4.118200	-3.974485	-1.439249
H	-2.462596	-4.513705	-1.774415
H	-4.083959	-4.653265	1.598944
H	-3.493248	-3.098705	2.206383
H	-4.733142	-3.142904	0.939185
H	2.267750	-2.384566	4.594535
H	0.704501	-2.458346	3.764914
H	2.148954	-3.121068	2.987335
H	1.680295	1.163925	3.581824
H	0.378361	0.048425	4.055407
H	4.012135	-0.745341	3.935493
H	4.108779	-1.322652	2.267920
H	3.770742	0.375839	2.589001
H	-2.541336	4.043955	3.455352
H	-2.591532	2.275382	3.341420
H	-0.071916	4.139341	3.279961
H	-0.072910	2.373495	3.311300
H	0.803364	3.234025	2.030145
H	-1.397264	5.419171	1.638329
H	-0.533212	4.626142	0.309249
H	-2.303402	4.626044	0.337984
H	4.759502	3.456145	1.791716
H	3.270321	2.502978	1.636484
H	4.846021	1.762463	1.304648
H	3.972931	5.226098	0.258691
H	3.335403	4.847997	-1.353663
H	2.409626	4.407876	0.093208
H	6.147320	3.998303	-0.275118
H	6.110770	2.330569	-0.876878
H	5.520256	3.651134	-1.898723

Sn-Sn bonded dimeric structure

E(M06-2X/cc-pvdz) = -5723.8887551

G*(M06-2X/cc-pVDZ*) = -5723,18

C	-4.654448	-0.588847	-3.069096
C	-5.581012	0.440890	-2.746275
C	-4.887225	1.441333	-2.018149
C	-3.521318	1.042004	-1.878856
C	-3.390605	-0.224186	-2.536340
Fe	-4.789028	-0.401753	-0.950005
C	-4.134257	-1.855909	0.443676
C	-4.328400	-0.607520	1.121168
C	-5.708984	-0.266334	0.969240
C	-6.349094	-1.282735	0.215114
C	-5.375735	-2.268487	-0.106997
P	-3.145870	0.461406	2.038475
C	-2.654100	-0.624059	3.524647
C	-1.619188	0.181122	4.316916
P	-2.246677	2.124185	-1.112046
C	-1.121297	2.528539	-2.592168
C	-2.038702	3.044023	-3.707597
Sn	-1.115800	0.494483	0.489663
Sn	1.560049	-0.526907	1.324795
P	1.626288	-1.503753	-1.102760
C	0.832050	-3.235792	-0.953730
C	0.967086	-3.901811	-2.328573
C	3.426674	-1.903768	-1.160027
C	4.287923	-2.462989	-0.160895
C	5.603374	-2.547515	-0.689251
C	5.577068	-2.033320	-2.015104
C	4.244018	-1.639115	-2.303012
Fe	4.977765	-0.511280	-0.641237
C	6.304197	1.158808	-0.753843
C	4.979132	1.592988	-1.019482
C	4.166526	1.323404	0.125841
C	5.019427	0.708097	1.098473
C	6.330192	0.613976	0.559731
P	2.357484	1.680584	0.179968
C	2.230736	3.010038	1.549062
C	2.963885	2.678535	2.848749
C	0.739948	3.209373	1.847053
C	2.805855	4.304632	0.960426
C	1.433266	-4.152747	0.111043
C	-0.650760	-3.007929	-0.641647
C	-3.924264	-0.805854	4.363734
C	-2.076882	-1.994719	3.173377
C	-0.281344	1.358979	-3.102147
C	-0.196810	3.659929	-2.128895
H	-2.479090	-0.813633	-2.599538
H	3.888657	-1.181849	-3.223657
H	6.432042	-1.935577	-2.679417
H	-6.166746	0.643052	1.351434
H	4.707397	0.352539	2.078875
H	-4.881742	-1.510072	-3.599507
H	6.482268	-2.908747	-0.161010
H	7.144735	1.206017	-1.441539
H	3.987517	-2.756167	0.843493

H	7.192773	0.171537	1.051730
H	-3.188584	-2.384783	0.344132
H	-7.393347	-1.295092	-0.086853
H	-5.545563	-3.163824	-0.699850
H	-5.310752	2.354997	-1.607870
H	-6.640622	0.444952	-2.988874
H	4.615170	2.031238	-1.945913
H	-1.381479	-0.341301	5.258165
H	-0.673397	0.284991	3.757938
H	-1.992841	1.186361	4.565964
H	-3.688171	-1.380567	5.274962
H	-4.346352	0.163957	4.667585
H	-4.694714	-1.357780	3.803145
H	-1.841174	-2.545891	4.099870
H	-2.791376	-2.600987	2.598439
H	-1.138197	-1.902403	2.602524
H	0.867702	-5.100152	0.151572
H	2.479091	-4.397989	-0.121192
H	1.395163	-3.695705	1.113487
H	0.503000	-4.903308	-2.316359
H	0.480262	-3.301464	-3.111939
H	2.027684	-4.021192	-2.600062
H	-1.217785	-3.949367	-0.743366
H	-0.789215	-2.652301	0.394951
H	-1.100949	-2.274385	-1.335393
H	2.748405	5.119876	1.702142
H	3.862672	4.170590	0.681356
H	2.250727	4.614744	0.062127
H	2.792324	3.477495	3.590966
H	2.610349	1.730737	3.286923
H	4.047898	2.602505	2.683588
H	0.594039	4.086633	2.499218
H	0.154308	3.386665	0.927437
H	0.317521	2.340984	2.384893
H	0.323215	1.688415	-3.965032
H	0.414614	0.988186	-2.334179
H	-0.910892	0.523971	-3.443118
H	-1.417510	3.409286	-4.541958
H	-2.695879	2.249553	-4.091639
H	-2.669220	3.878528	-3.362290
H	0.410877	4.006830	-2.981136
H	-0.769084	4.516691	-1.740780
H	0.504696	3.308733	-1.356590

E(B3LYP/cc-pvdz) = -5725.078252
G*(B3LYP/cc-pVDZ) = -5724.381218*

C	-6.596663	-0.332146	1.220356
C	-6.580643	0.744366	0.280225
C	-5.254806	1.274745	0.242055
C	-4.432558	0.540794	1.171666
C	-5.283012	-0.460106	1.762386
Fe	-5.233120	-0.721593	-0.300385
C	-4.517459	-0.854809	-2.235736
C	-3.678081	-1.640827	-1.365348
C	-4.533880	-2.626734	-0.757315

C	-5.860724	-2.459569	-1.254700
C	-5.850526	-1.364427	-2.173316
P	-1.860083	-1.555070	-1.018360
C	-1.088484	-2.026857	-2.735527
C	-1.484034	-3.489695	-3.017629
P	-2.652291	0.740107	1.651217
C	-2.643262	2.480360	2.508419
C	-3.174991	3.645984	1.661653
Sn	-1.619449	1.083580	-0.760857
Sn	1.184058	0.532197	0.265275
P	2.413257	-0.629163	2.183699
C	1.361752	-2.066269	2.921910
C	2.269512	-2.776968	3.945775
C	3.876757	-1.468964	1.441920
C	3.962331	-2.415259	0.358343
C	5.312318	-2.866788	0.254309
C	6.080649	-2.200101	1.258675
C	5.204758	-1.341081	1.985477
Fe	5.209059	-0.811740	-0.023054
C	6.764474	0.245248	-0.915679
C	5.888769	1.140938	-0.234343
C	4.569522	1.015270	-0.798228
C	4.654964	0.014362	-1.832461
C	6.003375	-0.447981	-1.907310
P	3.149077	2.062310	-0.271845
C	2.738595	3.156227	-1.805488
C	1.611952	4.106334	-1.361184
C	4.007069	3.974081	-2.116912
C	2.303620	2.380376	-3.058022
C	0.840440	-3.083511	1.896331
C	0.182995	-1.403914	3.655085
C	-1.505704	-1.147356	-3.922938
C	0.438054	-1.952053	-2.555964
C	-1.182513	2.759186	2.904438
C	-3.494126	2.349994	3.786891
H	3.135241	-2.727237	-0.274953
H	-4.206413	-3.368010	-0.031433
H	-6.731266	-3.048363	-0.971392
H	6.157087	1.809152	0.581196
H	-4.920911	2.094294	-0.390279
H	5.694392	-3.575369	-0.478145
H	-6.711346	-0.971317	-2.711124
H	-7.455559	-0.954269	1.465394
H	-4.193345	-0.008145	-2.836878
H	-7.423256	1.083125	-0.319878
H	3.828728	-0.334228	-2.447372
H	7.821920	0.098972	-0.704187
H	6.379614	-1.213960	-2.582721
H	5.479111	-0.690940	2.813560
H	7.150293	-2.312721	1.424537
H	-4.958012	-1.193993	2.496784
H	1.390817	4.825408	-2.169230
H	0.677014	3.563387	-1.144276
H	1.894526	4.680745	-0.464500
H	3.800741	4.675733	-2.944618

H	4.332769	4.565425	-1.246407
H	4.844215	3.328553	-2.424949
H	2.095255	3.087074	-3.882094
H	3.088089	1.693131	-3.407710
H	1.382877	1.801860	-2.881016
H	-0.984112	-1.475344	-4.841801
H	-2.585730	-1.216403	-4.118538
H	-1.254727	-0.087056	-3.757454
H	-1.006478	-3.841421	-3.950739
H	-1.168841	-4.158247	-2.200570
H	-2.573413	-3.595219	-3.138848
H	0.953513	-2.332177	-3.456237
H	0.778821	-0.910689	-2.409344
H	0.775349	-2.555281	-1.696418
H	-3.468835	3.295880	4.358686
H	-4.546908	2.130469	3.549499
H	-3.119423	1.547119	4.441716
H	-3.096009	4.592421	2.228840
H	-2.603680	3.771342	0.727280
H	-4.234816	3.509832	1.400771
H	-1.118967	3.683487	3.505965
H	-0.758356	1.938587	3.505607
H	-0.538760	2.905353	2.019786
H	0.268303	-3.872436	2.418097
H	0.161875	-2.622964	1.161288
H	1.662524	-3.580301	1.359541
H	1.687783	-3.555852	4.469740
H	3.128109	-3.268654	3.462898
H	2.655294	-2.078212	4.705351
H	-0.399799	-2.176157	4.187064
H	0.530626	-0.672276	4.402725
H	-0.512857	-0.896127	2.967775

E(B3LYP/def2-TZVP//B3LYP/6-31+G)* = -5725.5291702

C	-6.806361	-1.038596	1.273820
C	-6.500491	-1.798400	0.106702
C	-5.083807	-1.916149	0.016597
C	-4.493803	-1.237752	1.138252
C	-5.579866	-0.692703	1.905736
Fe	-5.623752	0.075226	-0.021940
C	-5.026063	0.864865	-1.829526
C	-4.415745	1.615193	-0.764781
C	-5.490882	2.150786	0.022981
C	-6.728744	1.751407	-0.553106
C	-6.441992	0.960227	-1.703948
P	-2.649633	2.031428	-0.439873
C	-2.110089	2.920560	-2.065600
C	-3.020088	4.154072	-2.224026
P	-2.745653	-1.100242	1.682935
C	-2.276453	-2.919938	2.094540
C	-0.894231	-2.881156	2.769959
Sn	-1.450438	-0.279083	-0.417839
Sn	1.454752	-0.287337	0.429179
P	2.648285	2.026614	0.445332
C	2.114865	2.911999	2.075236

C	2.189183	2.062259	3.354423
C	4.416892	1.613130	0.760994
C	5.486784	2.150464	-0.032689
C	6.728532	1.752775	0.536173
C	6.449497	0.960874	1.688419
C	5.034418	0.863371	1.822008
Fe	5.623264	0.075047	0.010899
C	6.801632	-1.037839	-1.289483
C	5.572434	-0.692771	-1.916650
C	4.489700	-1.238654	-1.145045
C	5.084530	-1.916734	-0.025747
C	6.500786	-1.797963	-0.121240
P	2.739332	-1.100964	-1.682783
C	2.268992	-2.920693	-2.093084
C	3.296156	-3.433400	-3.122504
C	2.239814	-3.870482	-0.885678
C	0.881898	-2.881874	-2.758361
C	0.664923	3.377303	1.862118
C	3.022747	4.147293	2.231450
C	-2.176512	2.072774	-3.346531
C	-0.662255	3.388765	-1.844757
C	-3.310604	-3.435005	3.115741
C	-2.237789	-3.867712	0.885790
H	-4.501975	0.307228	-2.589247
H	5.455551	-0.108219	-2.816801
H	7.788010	-0.750347	-1.622163
H	-5.466842	-0.108176	2.806392
H	4.515665	0.304588	2.584563
H	-7.169483	0.488846	-2.348254
H	7.219178	-2.186740	0.585408
H	7.709521	1.987579	0.150444
H	4.548073	-2.418466	0.764737
H	7.181319	0.490303	2.328399
H	-4.544013	-2.417386	-0.771925
H	-7.794199	-0.751832	1.602766
H	-7.215895	-2.187684	-0.602684
H	-5.363461	2.751988	0.910732
H	-7.712278	1.984687	-0.172968
H	5.353348	2.751677	-0.919545
H	-0.614944	-3.888082	3.100599
H	-0.114627	-2.528568	2.089421
H	-0.895233	-2.227502	3.646245
H	-3.025946	-4.440216	3.447959
H	-3.359149	-2.791364	3.998371
H	-4.311992	-3.494874	2.684546
H	-1.965359	-4.879443	1.211885
H	-3.209804	-3.934254	0.393760
H	-1.499325	-3.547685	0.146083
H	1.964637	-4.881625	-1.211293
H	3.215750	-3.938009	-0.401629
H	1.507519	-3.551600	-0.139332
H	3.010534	-4.438682	-3.453731
H	3.337367	-2.788704	-4.004735
H	4.300740	-3.492303	-2.698643
H	0.600635	-3.888340	-3.088714

H	0.107248	-2.530869	-2.071329
H	0.876034	-2.226608	-3.633432
H	2.703473	4.732537	3.102417
H	4.067462	3.865870	2.382874
H	2.970487	4.796725	1.353507
H	1.823819	2.648513	4.206922
H	1.569010	1.164385	3.284748
H	3.211640	1.760307	3.584372
H	0.329330	3.952216	2.732688
H	0.575940	4.018478	0.982745
H	-0.029130	2.541323	1.740983
H	-1.809318	2.661676	-4.196395
H	-1.553761	1.176788	-3.275834
H	-3.197064	1.768109	-3.581394
H	-2.697645	4.741570	-3.092284
H	-4.063389	3.870638	-2.381319
H	-2.973740	4.802071	-1.344693
H	-0.324071	3.966268	-2.712606
H	-0.578966	4.028470	-0.963728
H	0.033310	2.554294	-1.722104

E(B3LYP/6-31G)* = -5724.587046
G(B3LYP/6-31G)* = -5723.877825

C	-5.805780	-1.588913	-1.999240
C	-5.865357	-2.545960	-0.941282
C	-4.556235	-2.674229	-0.393049
C	-3.660958	-1.804448	-1.108603
C	-4.459447	-1.127279	-2.098572
Fe	-5.205056	-0.729229	-0.234517
C	-5.205142	1.300941	0.025056
C	-4.418571	0.686032	1.064511
C	-5.300184	-0.216917	1.755591
C	-6.595606	-0.145425	1.165789
C	-6.537821	0.796981	0.094916
P	-2.658541	0.935452	1.560564
C	-2.643773	2.770059	2.158956
C	-3.509707	2.832018	3.434367
P	-1.855058	-1.719119	-0.745158
C	-1.078524	-2.454651	-2.352793
C	0.448881	-2.417354	-2.159320
Sn	-1.602617	0.924695	-0.863996
Sn	1.188573	0.566430	0.215169
P	3.129846	2.022787	-0.564569
C	2.676648	2.889160	-2.215869
C	2.173172	1.950433	-3.324606
C	4.489603	0.873538	-0.996367
C	4.485888	-0.300615	-1.832357
C	5.816864	-0.804484	-1.915719
C	6.658608	0.038810	-1.128901
C	5.848497	1.064482	-0.563285
Fe	5.168503	-0.780429	0.033242
C	5.371353	-2.720740	0.673062
C	4.008446	-2.307421	0.740099
C	3.912665	-1.178153	1.629658
C	5.249972	-0.900582	2.084531

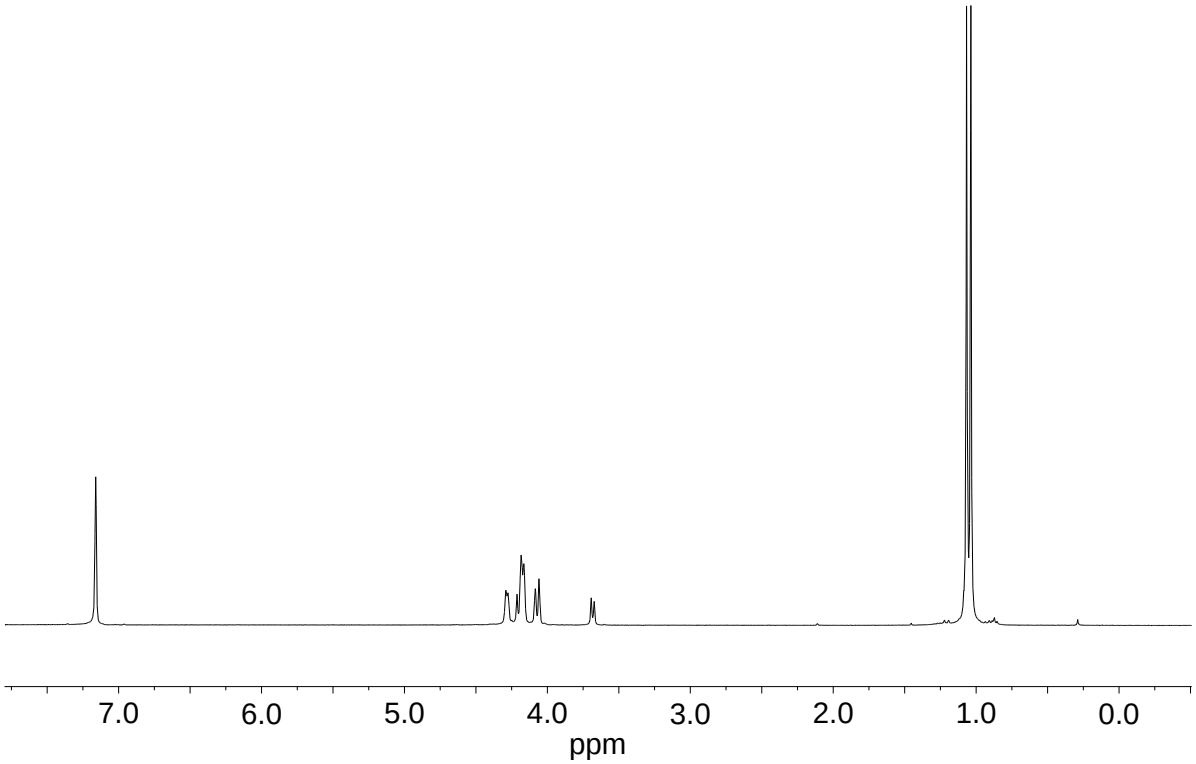
C	6.139221	-1.847963	1.501875
P	2.444517	-0.280813	2.266440
C	1.424701	-1.608096	3.203034
C	0.275844	-0.856781	3.902309
C	2.365585	-2.208784	4.268910
C	0.848017	-2.733072	2.327938
C	1.588147	3.924636	-1.873695
C	3.945956	3.621005	-2.697692
C	-3.154310	3.809487	1.148791
C	-1.184597	3.095164	2.529066
C	-1.530486	-3.928186	-2.433067
C	-1.441212	-1.740494	-3.664284
H	3.185424	-2.764918	0.208162
H	-4.266212	-3.313569	0.430400
H	-6.752333	-3.066796	-0.603635
H	6.184806	1.859431	0.089355
H	-4.846101	2.024382	-0.694662
H	5.758311	-3.538528	0.078594
H	-6.638643	-1.257553	-2.606518
H	-7.464648	-0.718796	1.462632
H	-4.099744	-0.385202	-2.798755
H	-7.355832	1.068050	-0.560628
H	3.617737	-0.732393	-2.312713
H	7.721746	-0.091574	-0.972587
H	6.129655	-1.685377	-2.461637
H	5.519994	-0.099790	2.760375
H	7.211366	-1.886832	1.645481
H	-5.010058	-0.846187	2.586759
H	1.337399	4.508840	-2.769175
H	0.663213	3.446287	-1.529401
H	1.923005	4.623880	-1.099034
H	3.714151	4.204429	-3.599186
H	4.326464	4.313559	-1.938492
H	4.747189	2.918686	-2.951258
H	1.963635	2.528051	-4.236139
H	2.918475	1.191099	-3.581270
H	1.243594	1.446998	-3.035383
H	-0.924298	-2.215886	-4.511257
H	-2.515035	-1.792968	-3.866283
H	-1.148975	-0.683779	-3.647017
H	-1.067361	-4.420193	-3.300590
H	-1.244145	-4.486537	-1.534564
H	-2.617036	-4.005585	-2.545571
H	0.953182	-2.949723	-2.977712
H	0.830028	-1.385922	-2.167762
H	0.747667	-2.892031	-1.216549
H	-3.484210	3.845609	3.859867
H	-4.555711	2.585974	3.221105
H	-3.148099	2.135606	4.199304
H	-3.069113	4.821270	1.572073
H	-2.575507	3.790070	0.217625
H	-4.207214	3.646578	0.900260
H	-1.121231	4.090879	2.989105
H	-0.774988	2.371425	3.243473
H	-0.536419	3.107286	1.642669

H	0.310402	-3.451649	2.962931
H	0.132475	-2.354126	1.589860
H	1.634954	-3.287589	1.806635
H	1.801170	-2.915172	4.892472
H	3.199460	-2.755877	3.816583
H	2.779476	-1.437712	4.928685
H	-0.285662	-1.557574	4.534397
H	0.651025	-0.052587	4.546155
H	-0.438454	-0.428855	3.189650

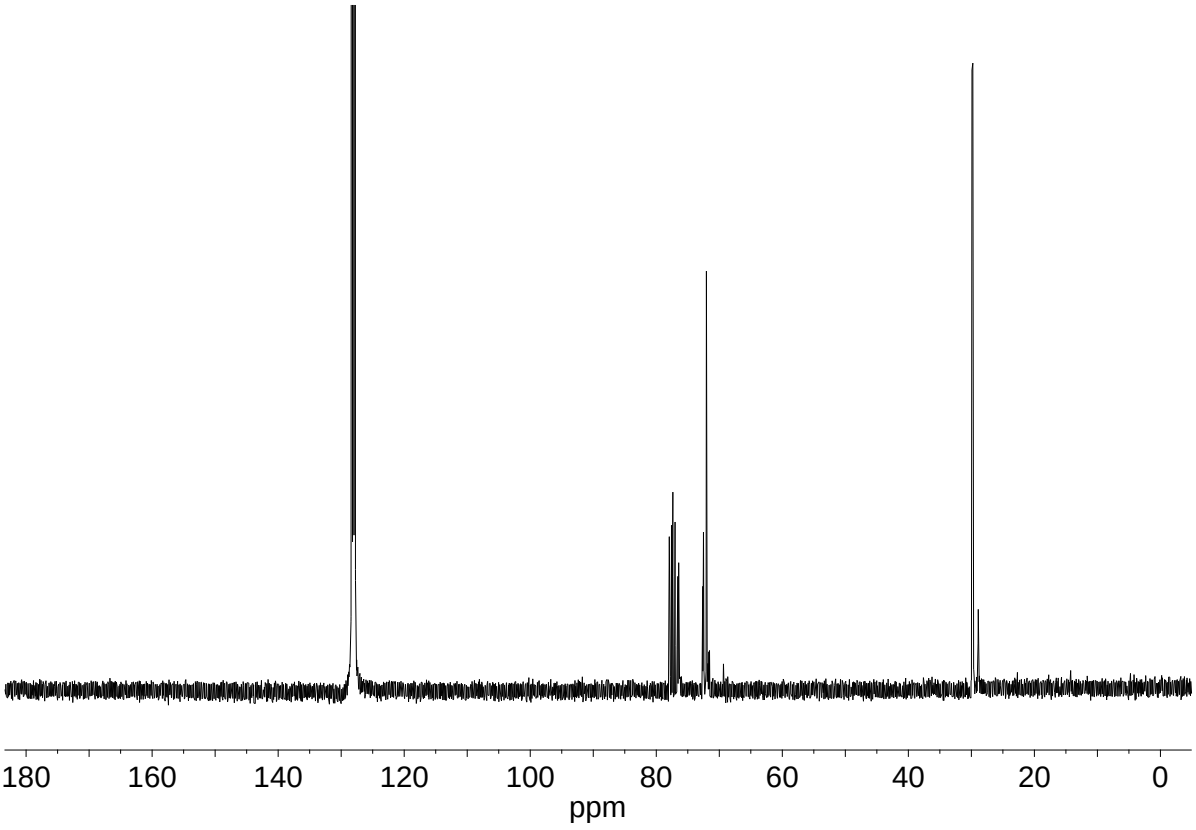
Spectral data

Figure S3: NMR spectra for compound **2**

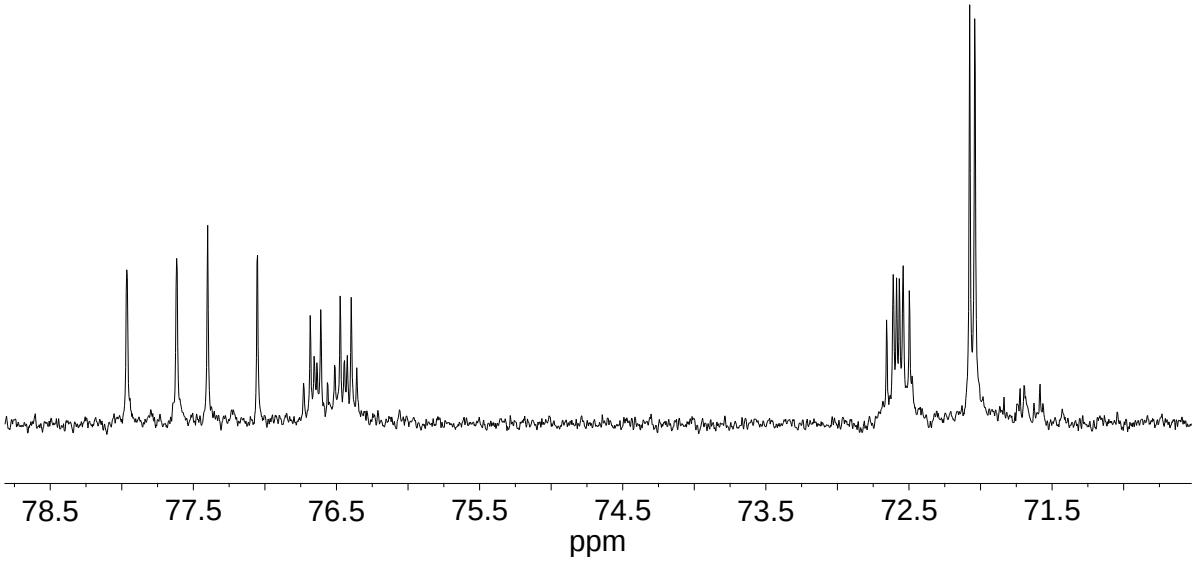
a) ^{1}H NMR (400 MHz, C_6D_6)



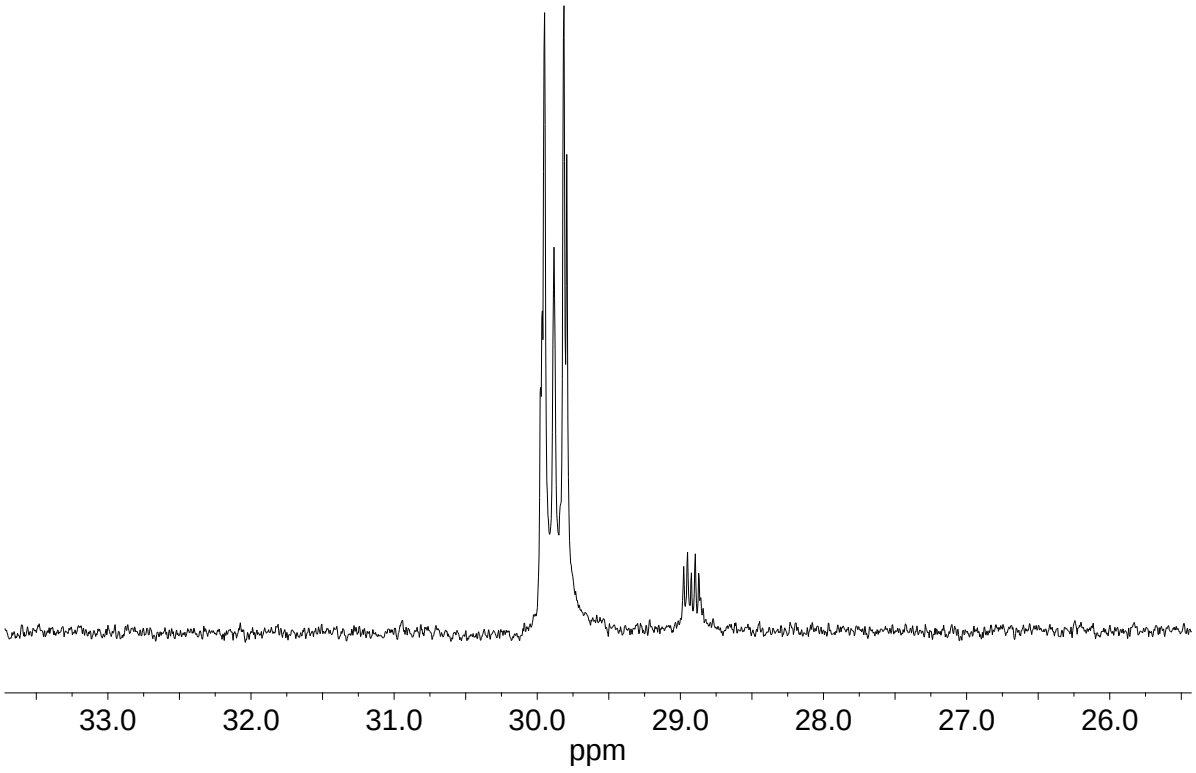
b) ^{13}C NMR (101 MHz, C_6D_6)



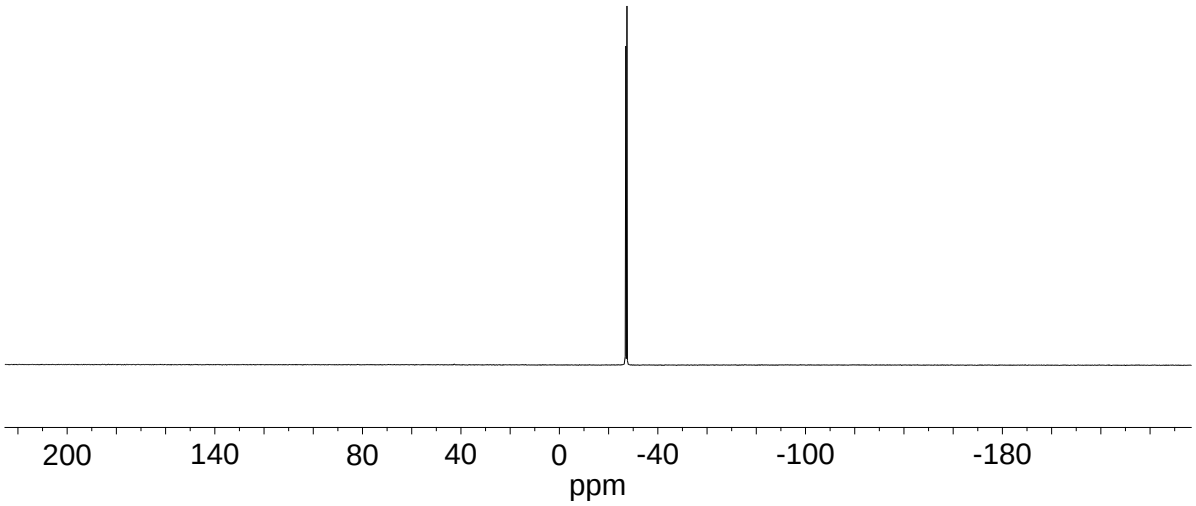
c) ^{13}C NMR (101 MHz, C_6D_6)



d) ^{13}C NMR (101 MHz, C_6D_6)



e) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



f) ^{31}P NMR (202 MHz, C_6D_6)

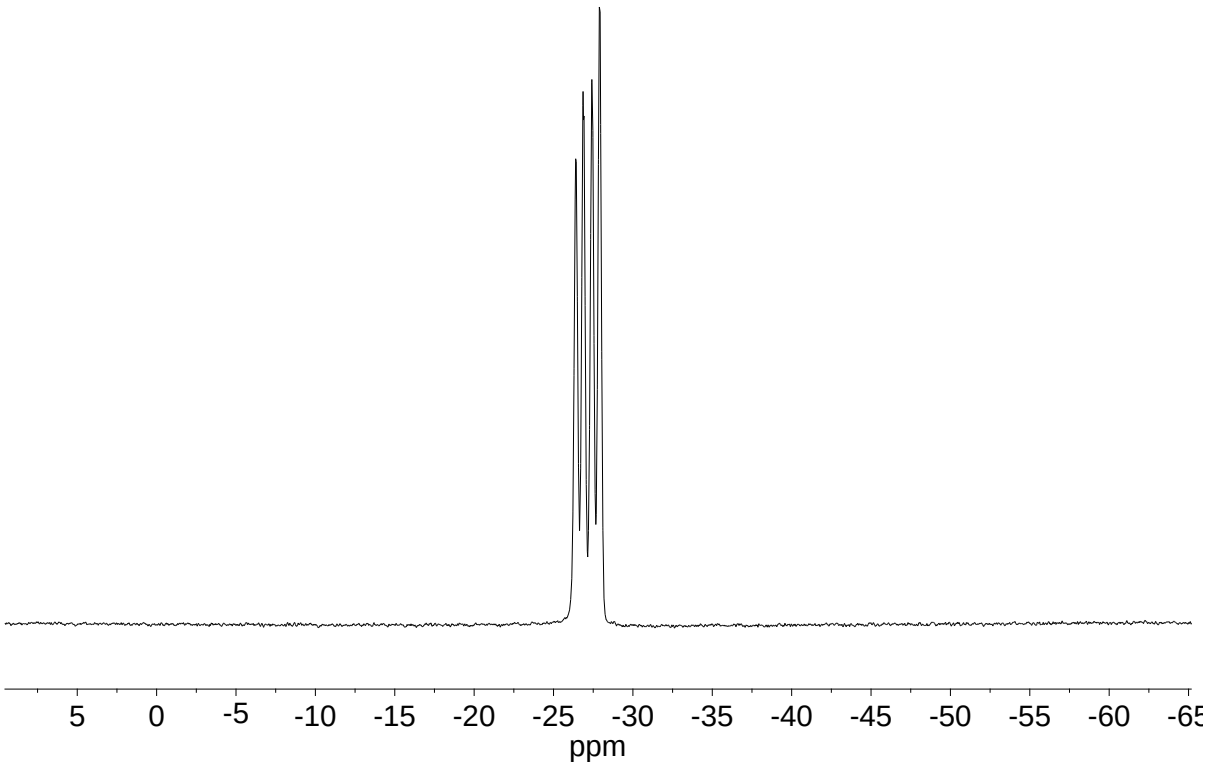
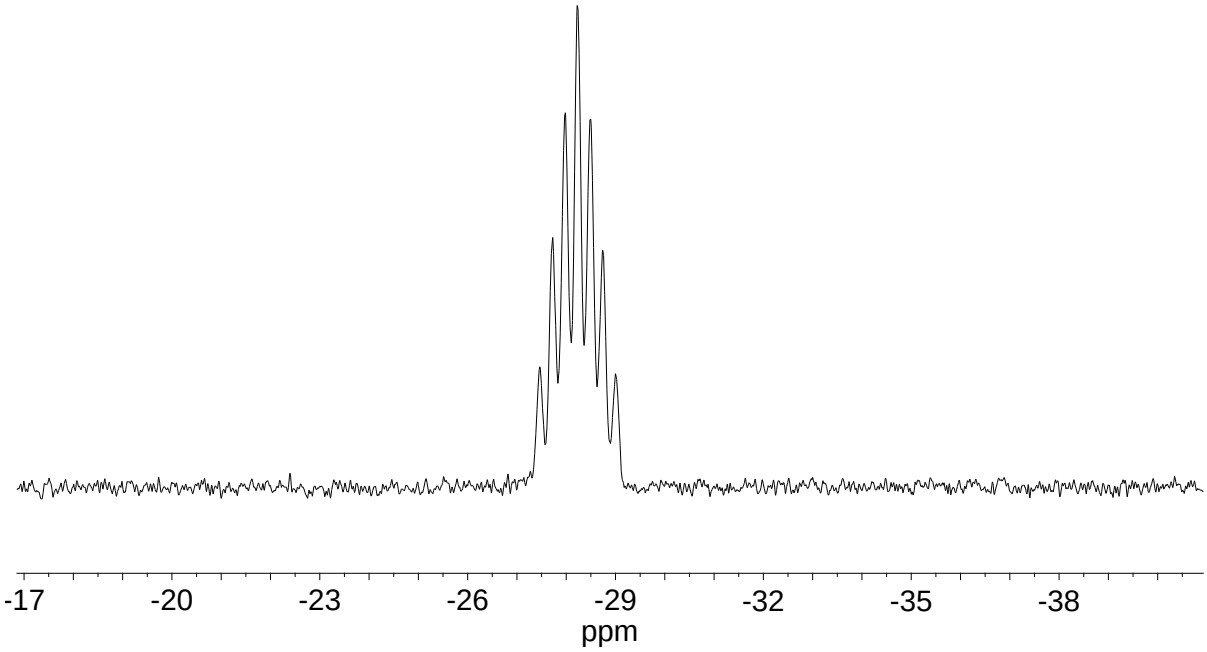


Figure S4: NMR spectra for compound **3**

a) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



b) $^{7}Li\{^{1}H\}$ NMR (194 MHz, C_6D_6)

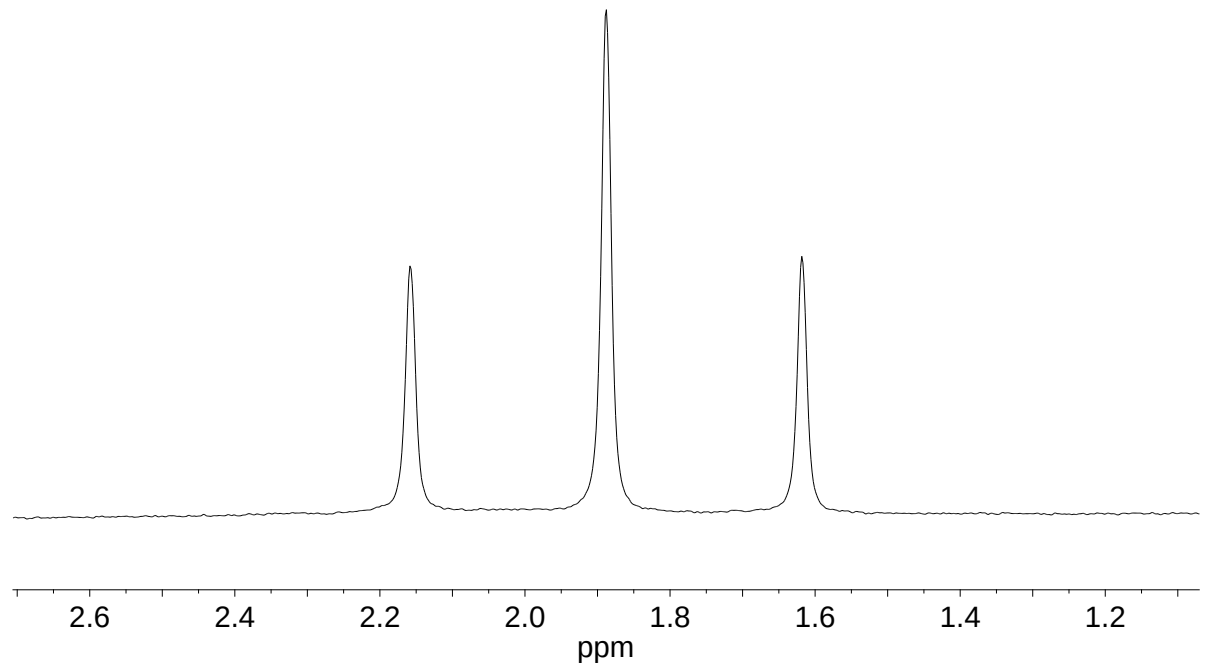
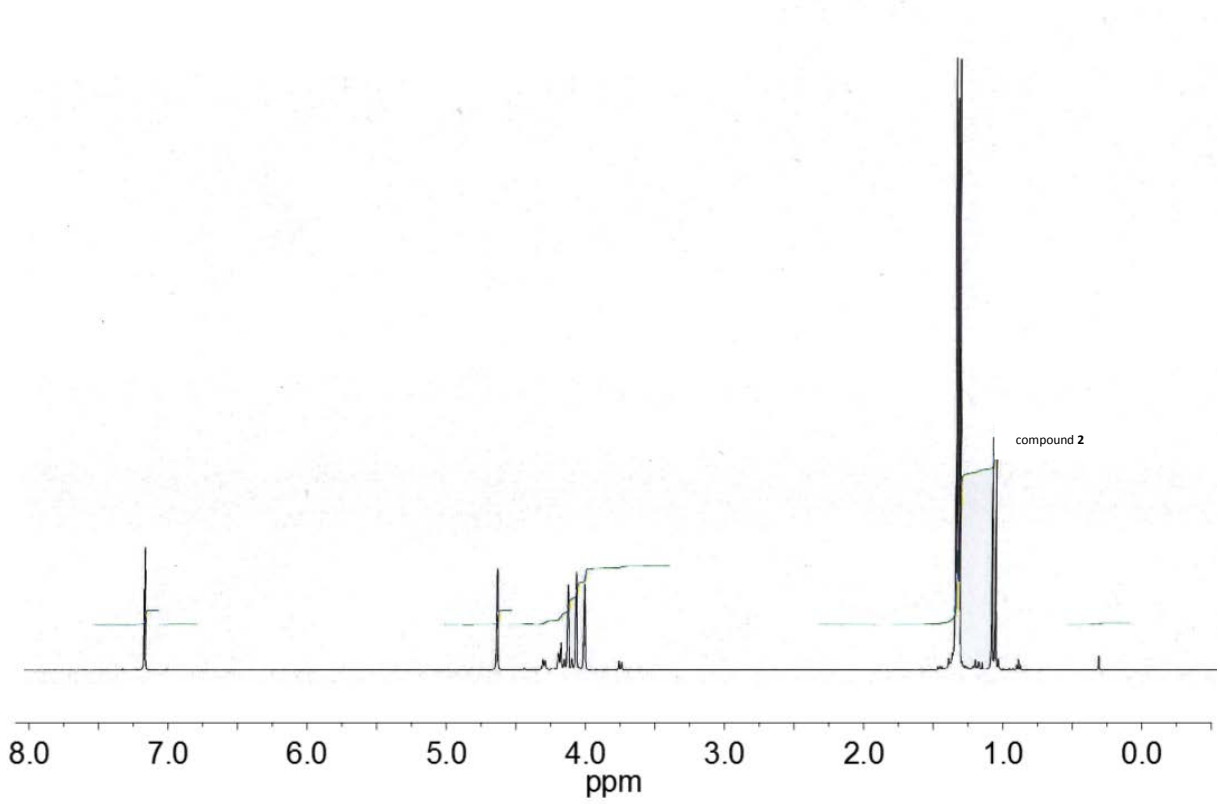
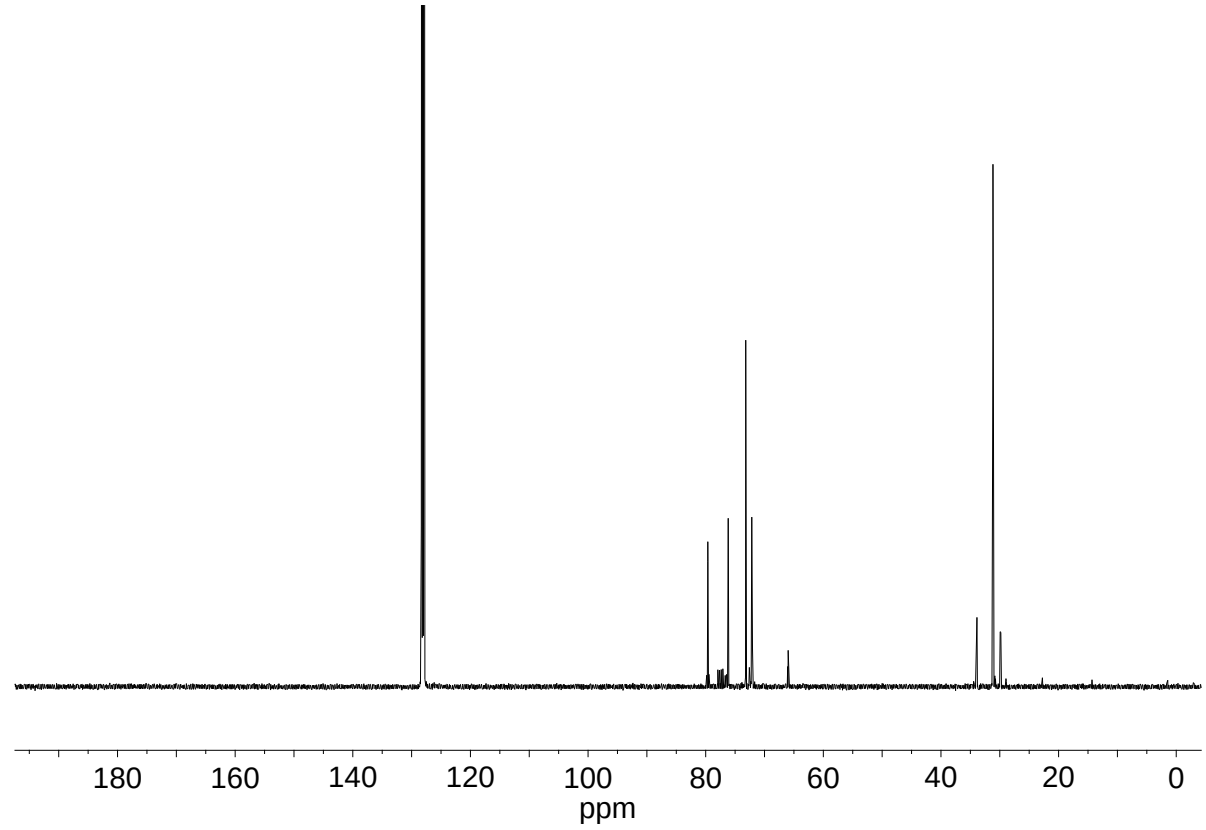


Figure S5: NMR spectra for compound **4**

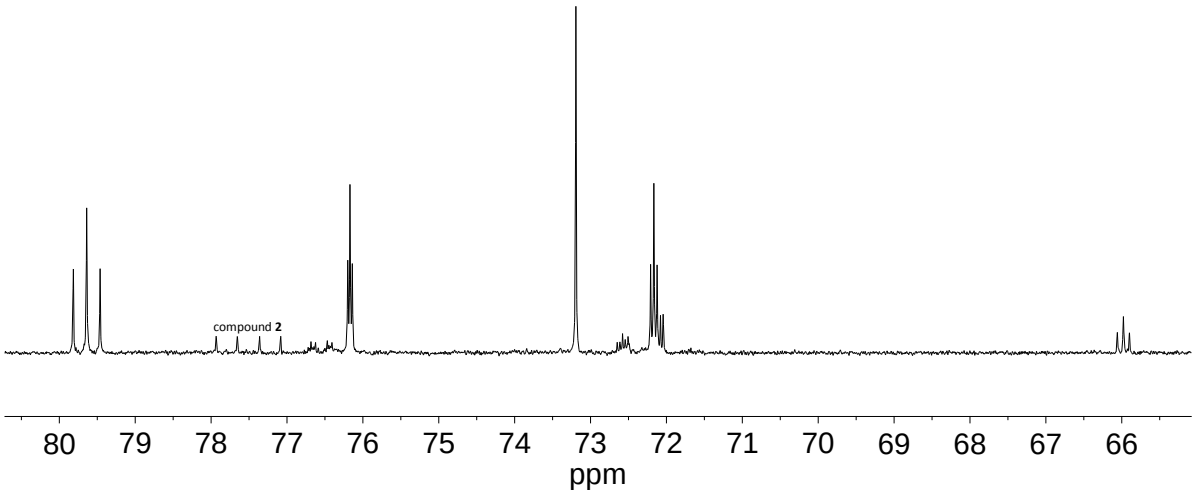
a) ^{1}H NMR (500 MHz, C_6D_6)



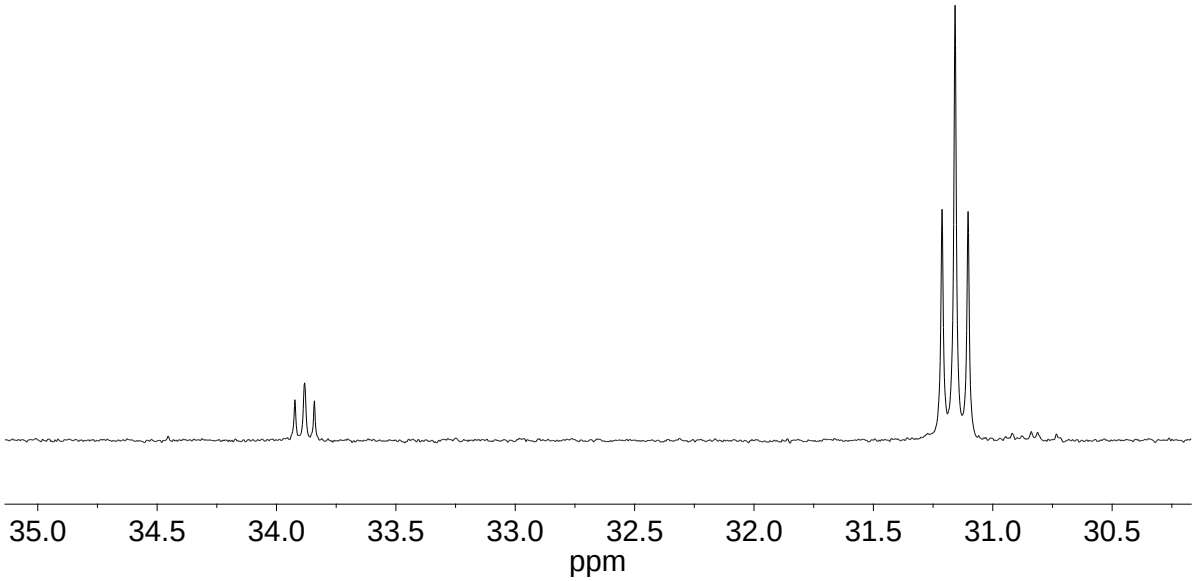
b) ^{13}C NMR (126 MHz, C_6D_6)



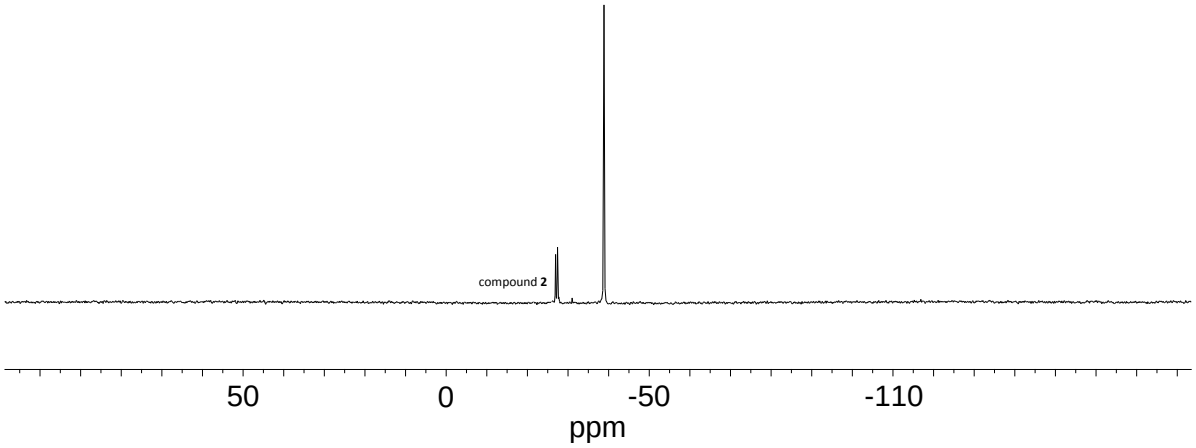
c) ^{13}C NMR (126 MHz, C_6D_6)



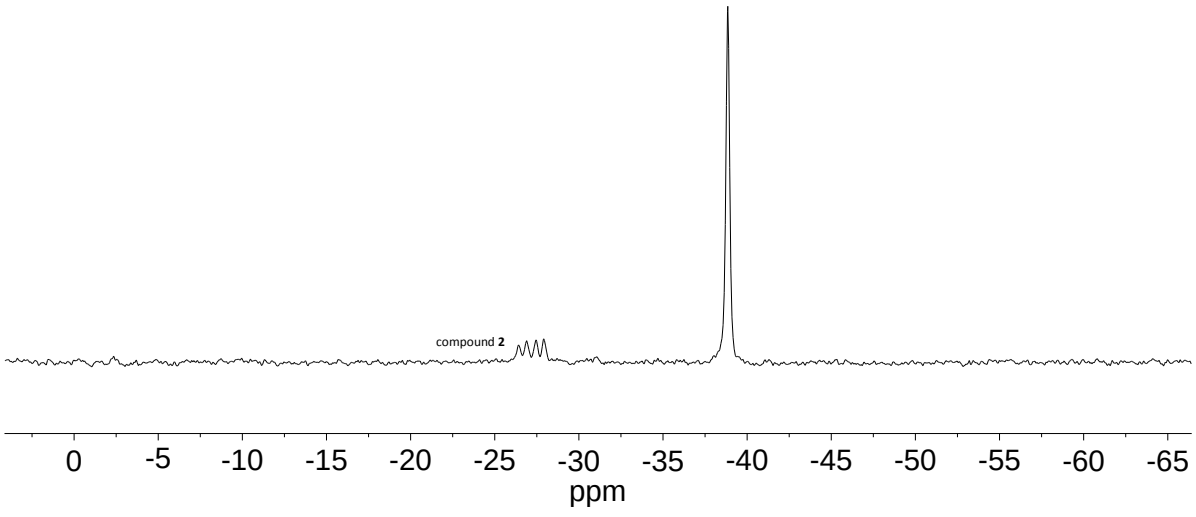
d) ^{13}C NMR (126 MHz, C_6D_6)



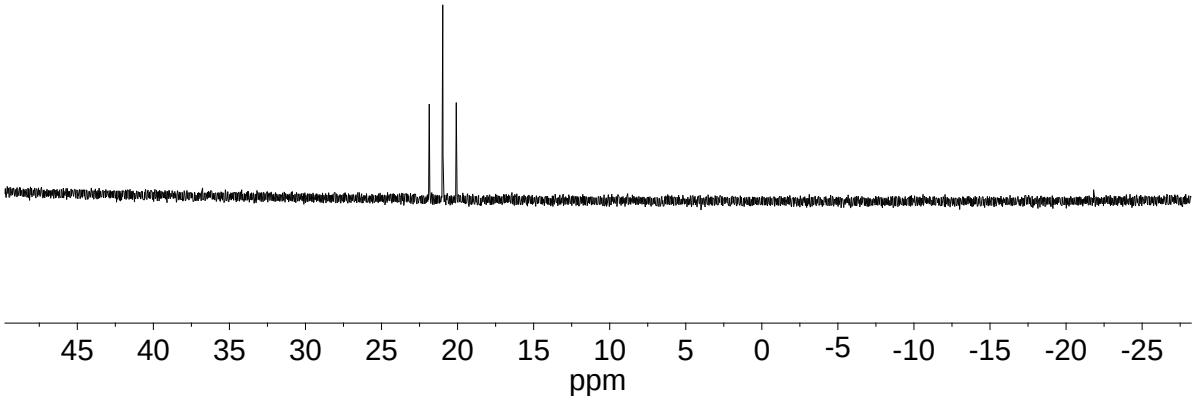
e) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



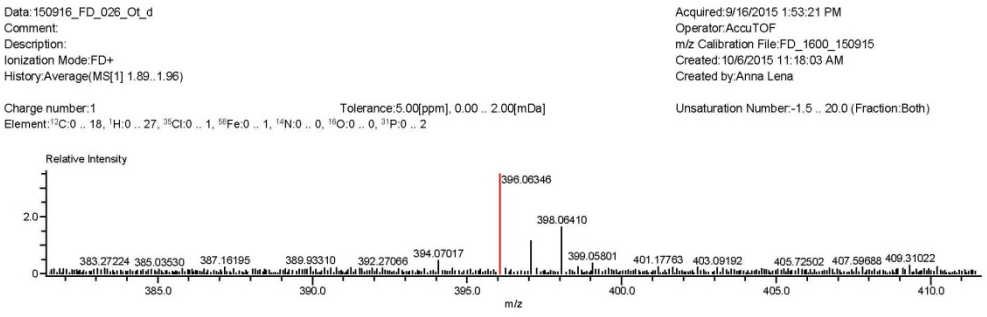
f) ^{31}P NMR (202 MHz, C_6D_6)

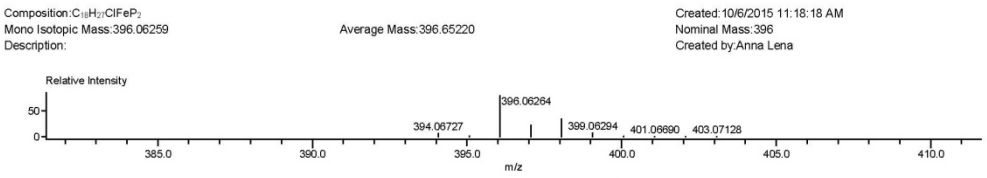


g) $^{29}Si\{^{1}H\}$ NMR (99 MHz, C_6D_6)



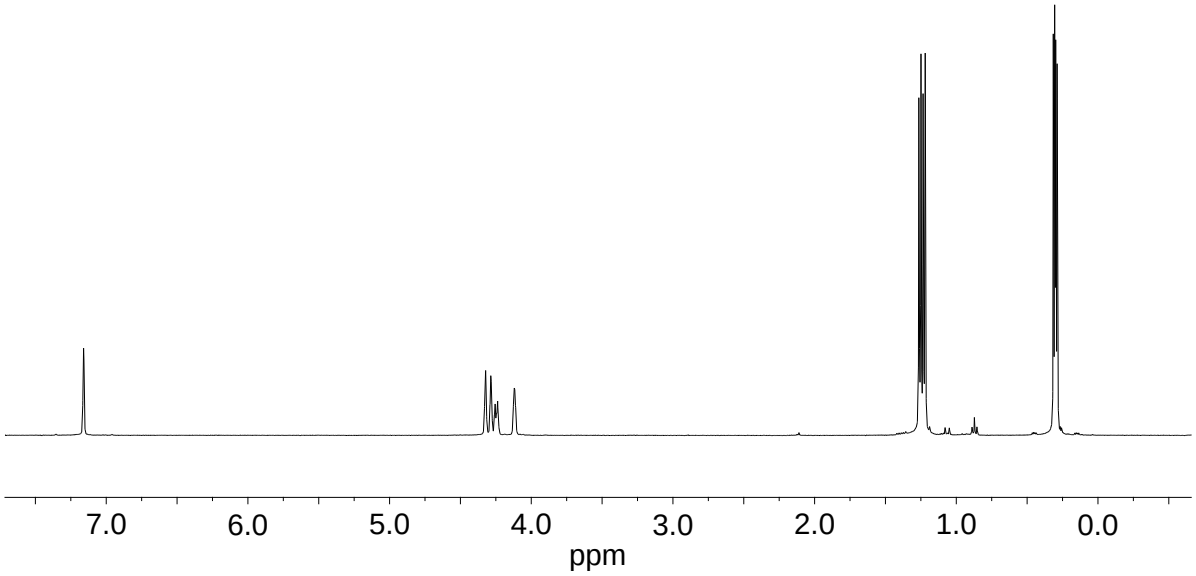
h) mass spectra (LIFDI)



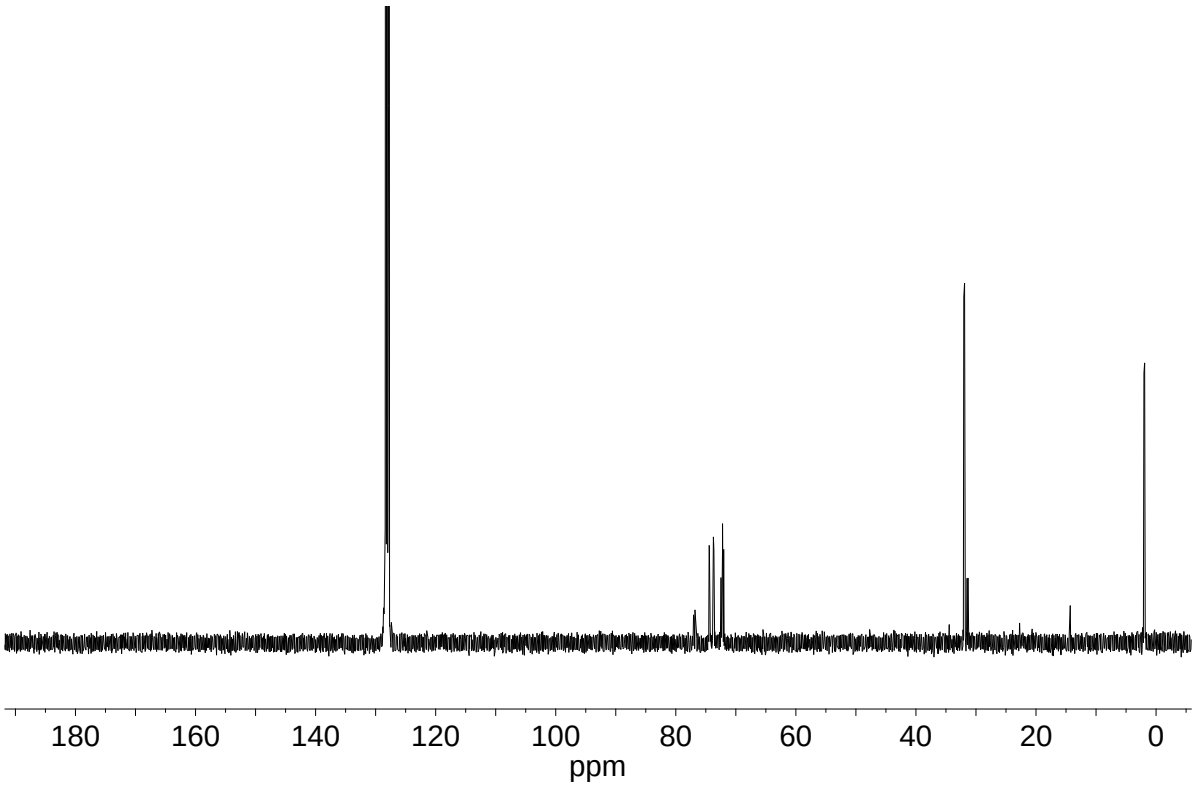


Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Possible Formula	Unsaturation Number
396.06346	12664.85	396.06259	0.87	$^{12}C_{18}{}^{1}H_{27}{}^{35}Cl_{1}{}^{56}Fe_{1}{}^{31}P_{2}$	8.5

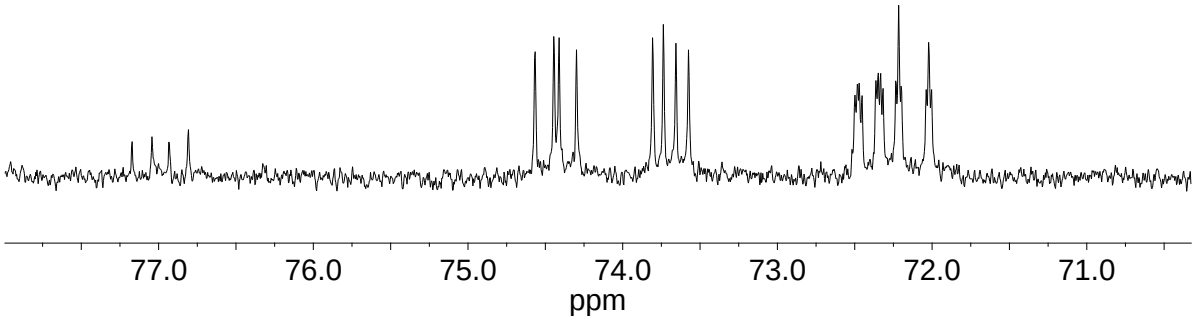
Figure S6: NMR spectra for compound **5**
a) ^{1}H NMR (500 MHz, C_6D_6)



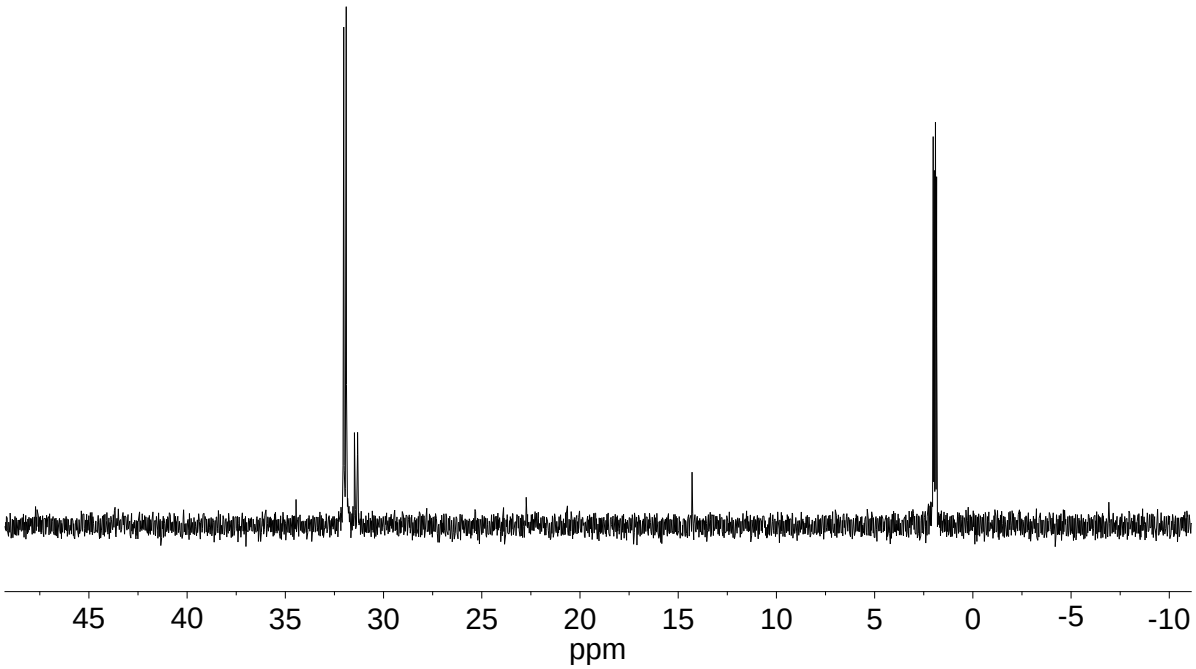
b) ^{13}C NMR (101 MHz, C_6D_6)



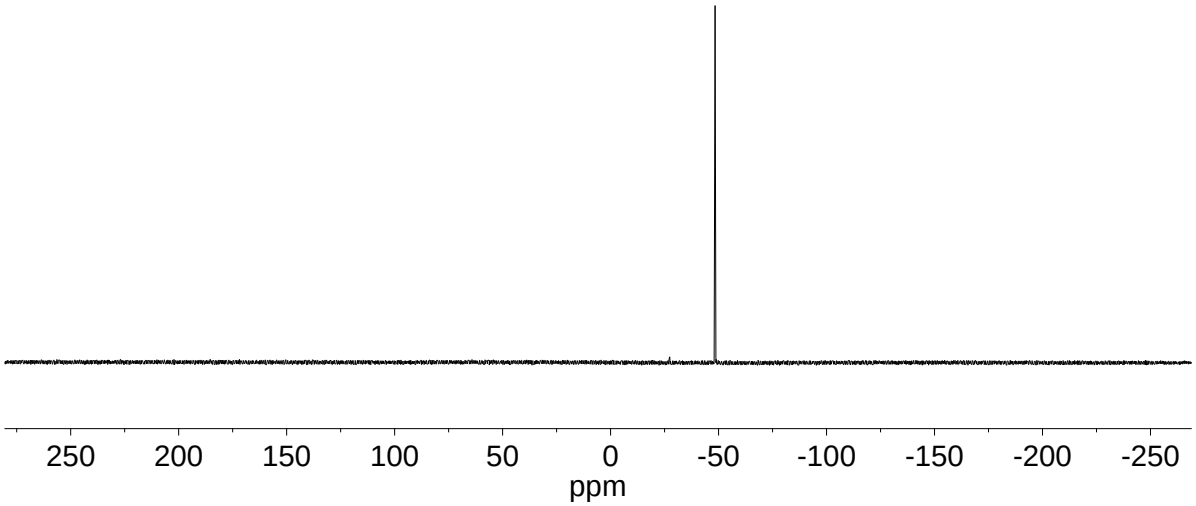
c) ^{13}C NMR (101 MHz, C_6D_6)



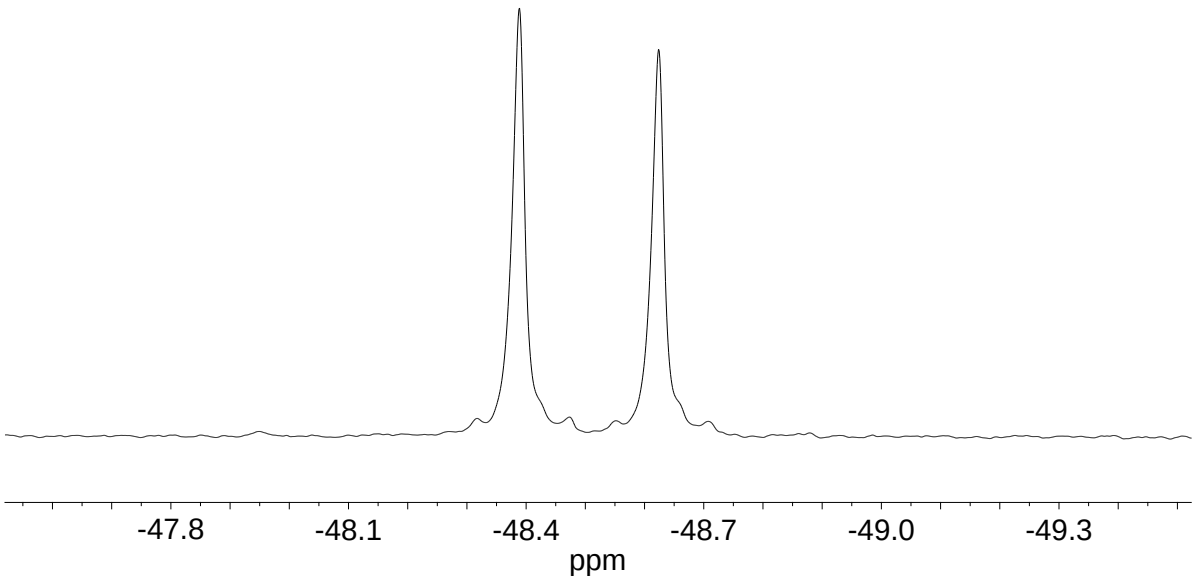
d) ^{13}C NMR (101 MHz, C_6D_6)



e) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



f) ^{31}P NMR (202 MHz, C_6D_6)



g) $^{29}Si\{^{1}H\}$ NMR (99 MHz, C_6D_6)

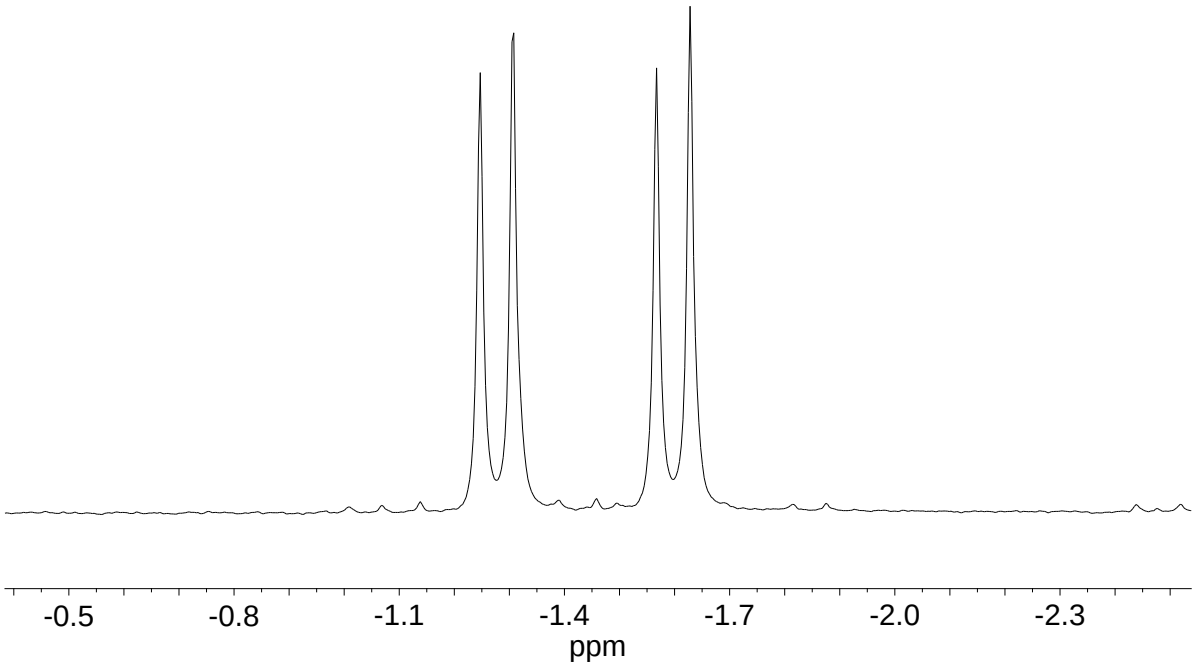
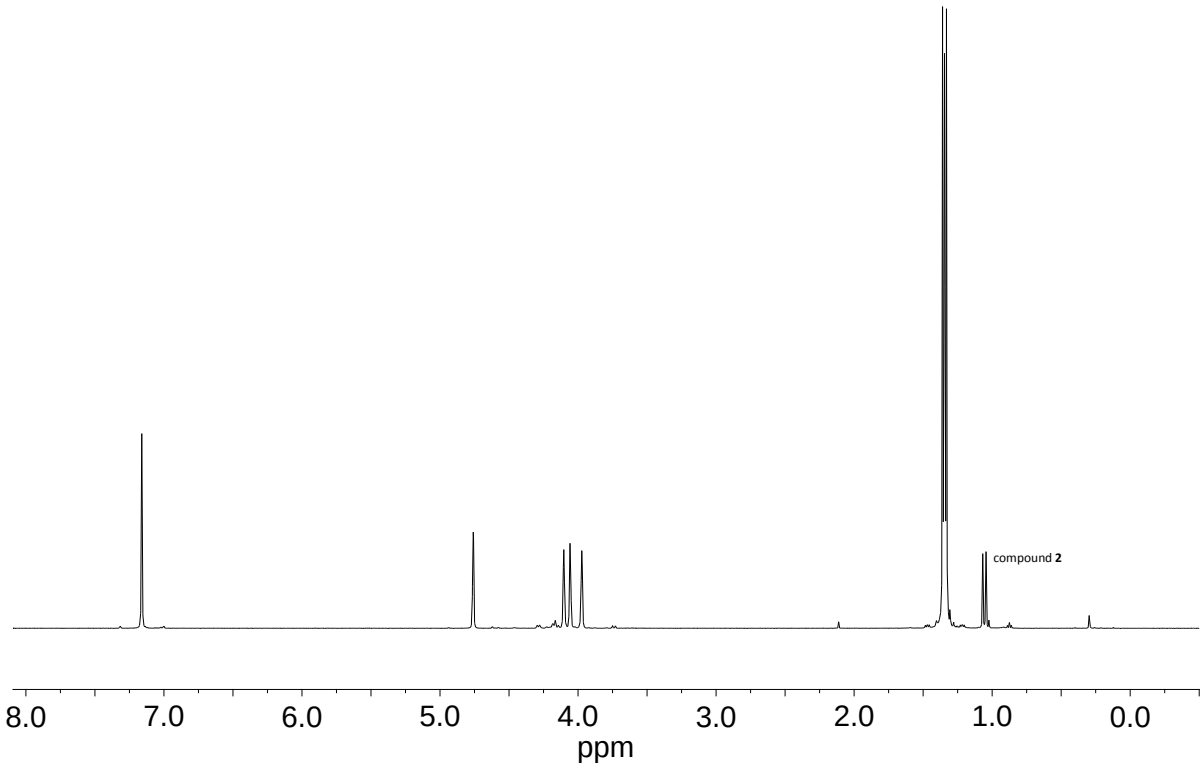
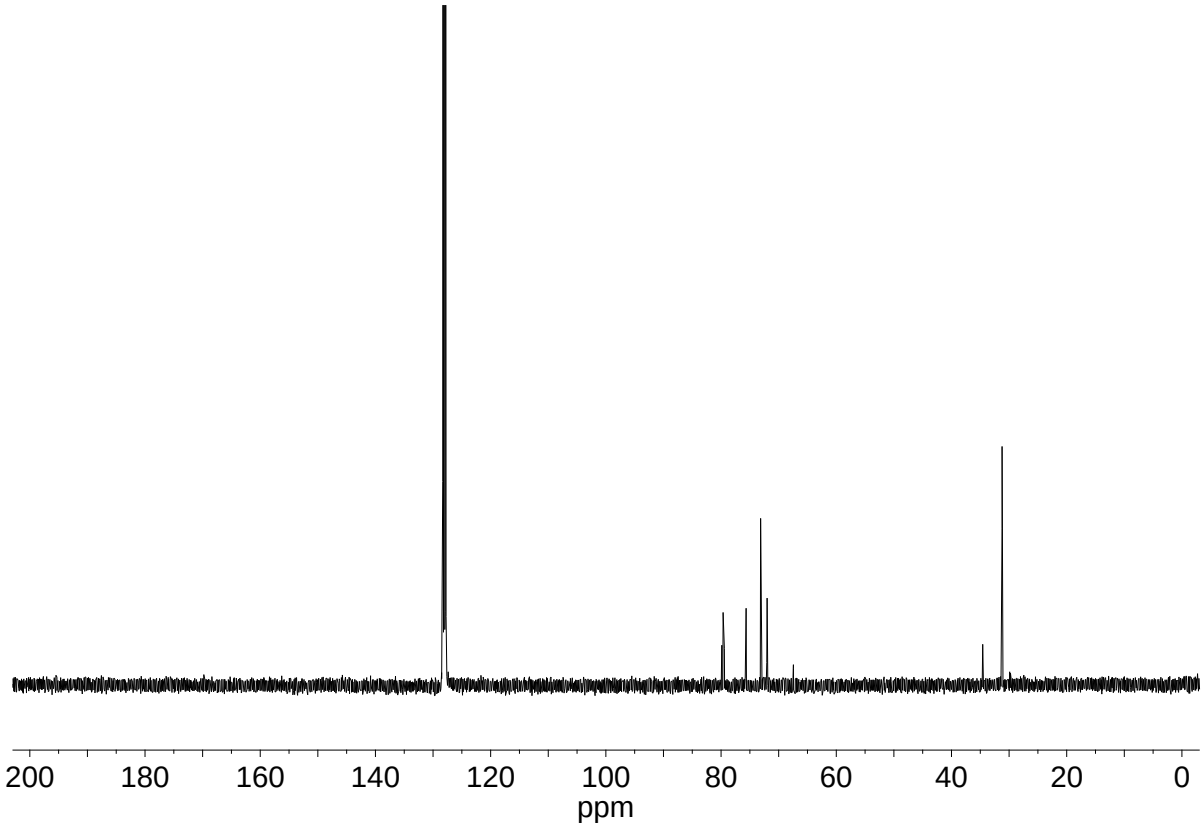


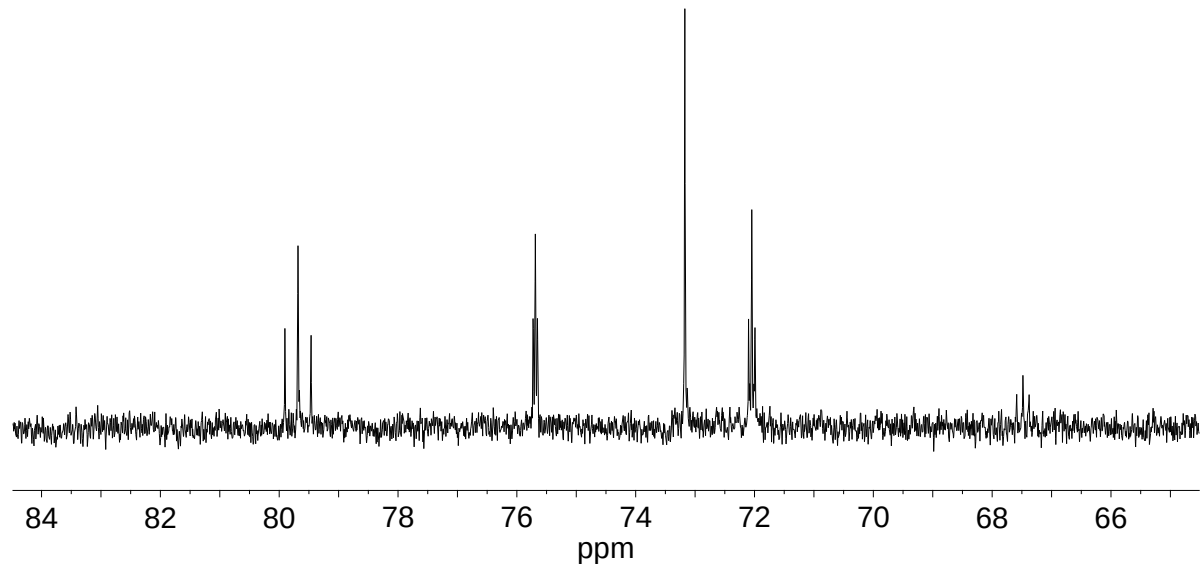
Figure S7: NMR spectra for compound **6**
a) ^{1}H NMR (500 MHz, C_6D_6)



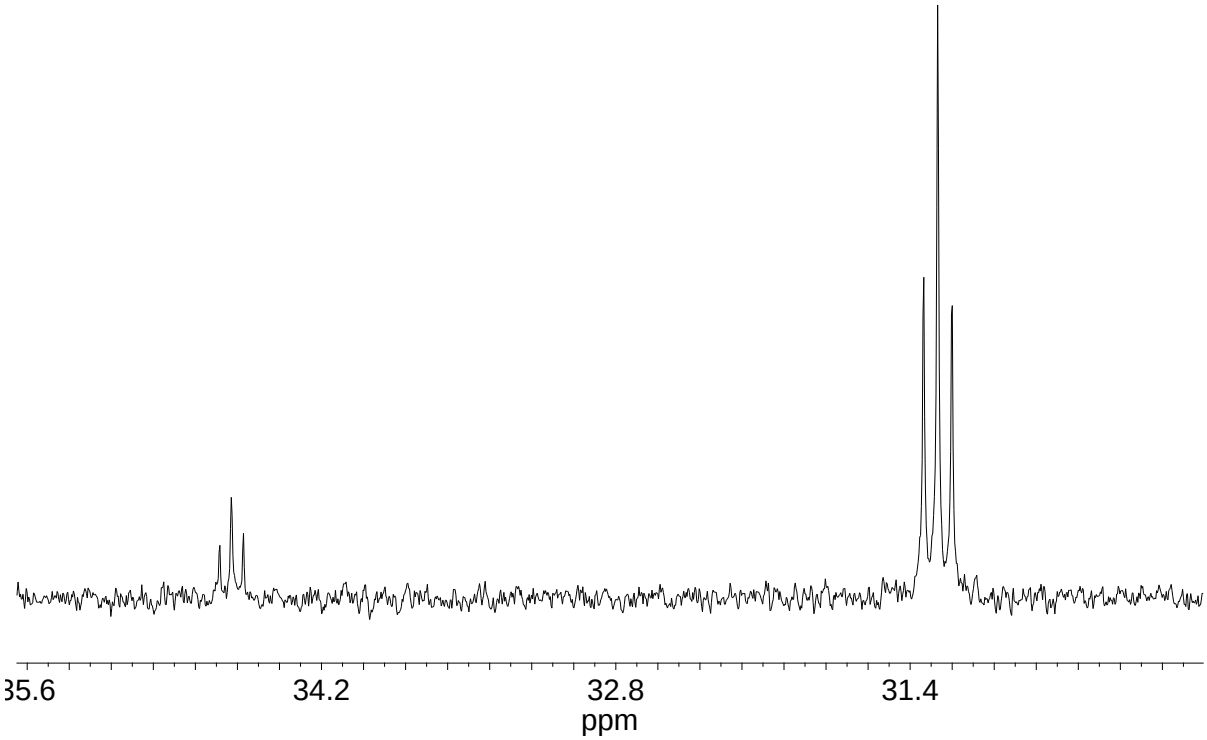
b) $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6)



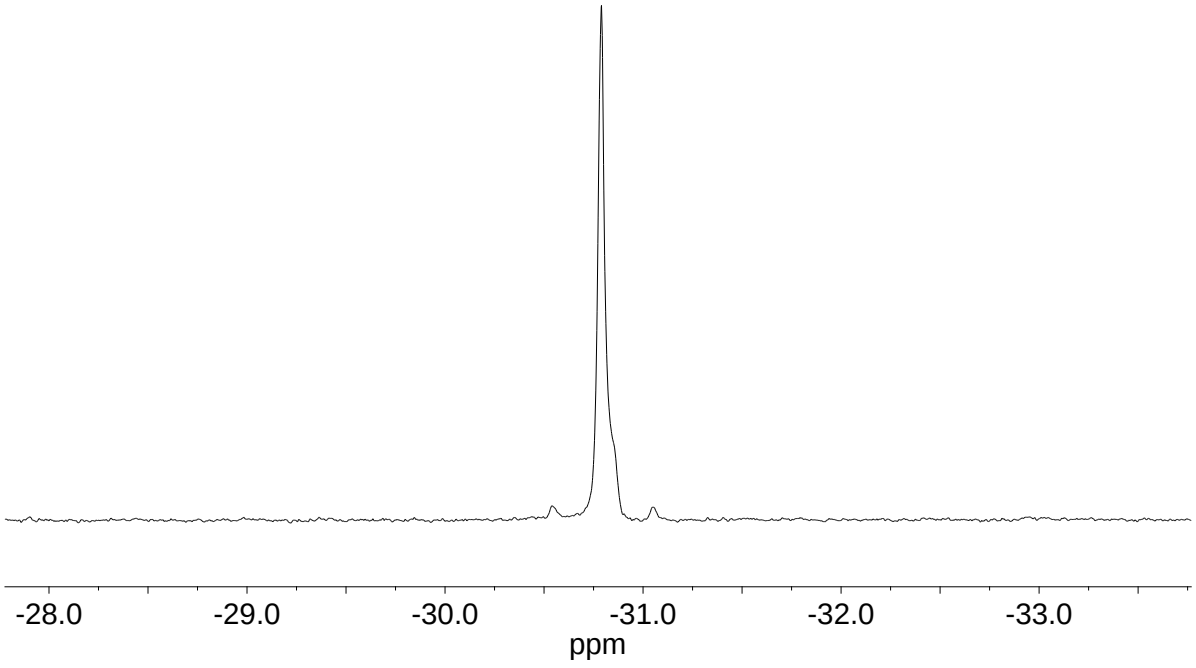
c) $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6)



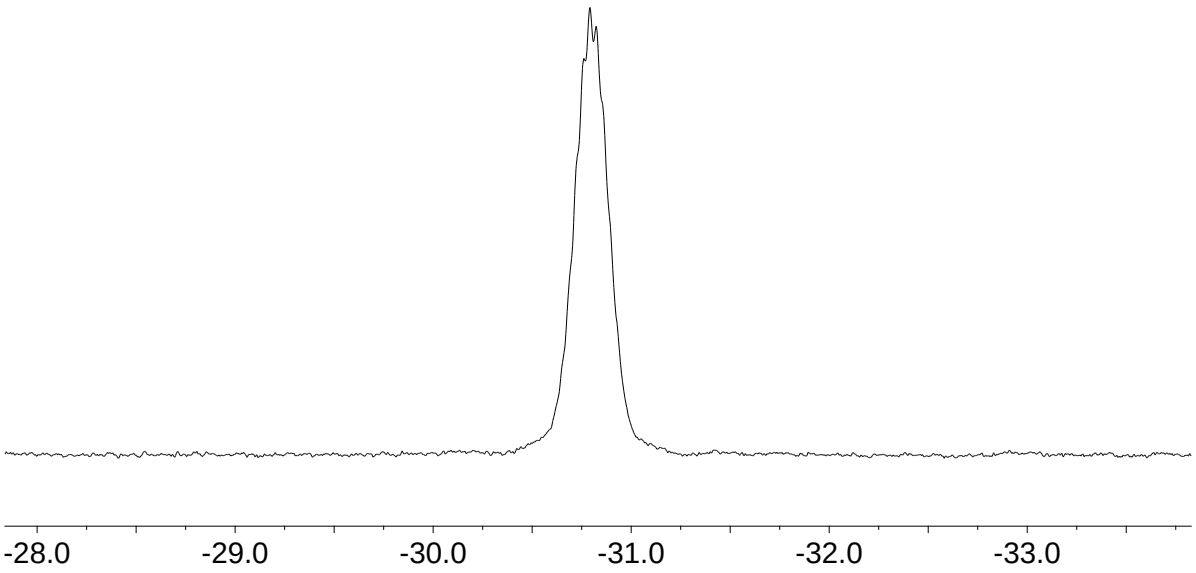
d) $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6)



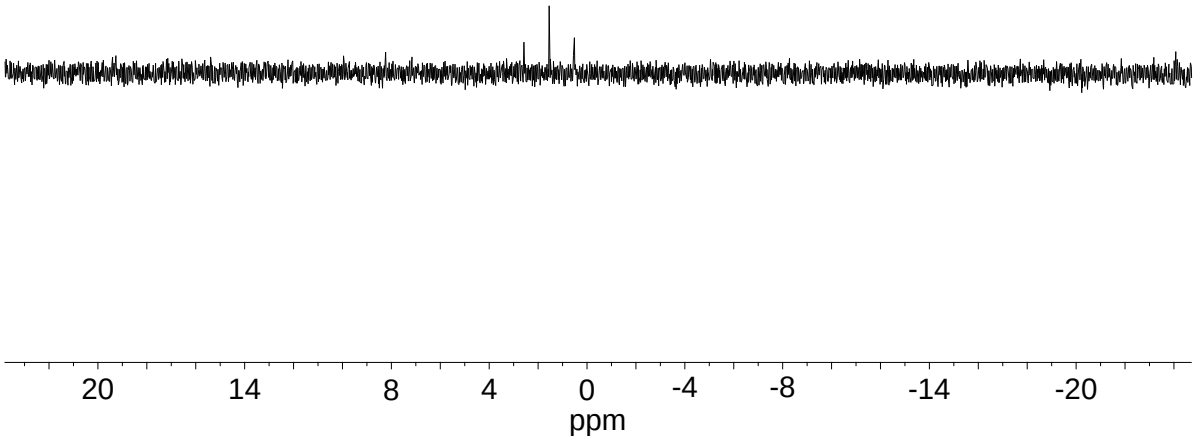
e) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



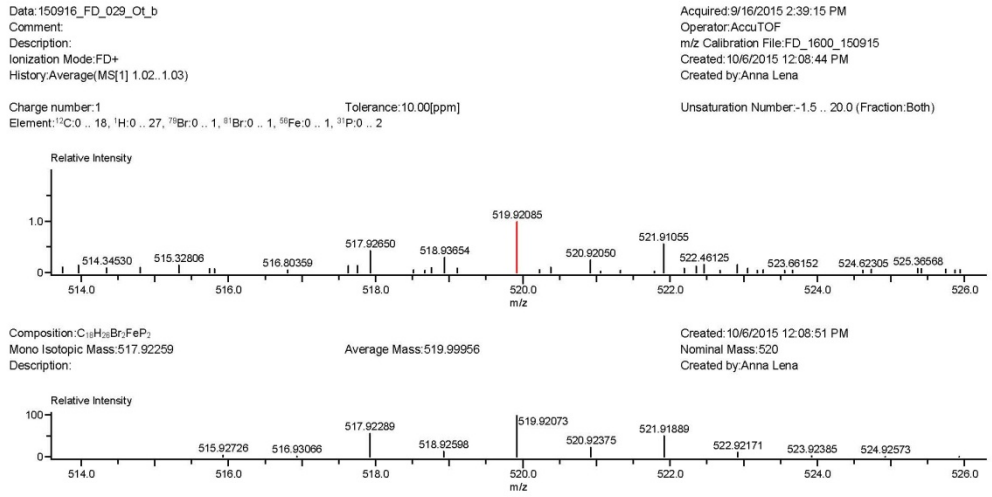
f) ^{31}P NMR (202 MHz, C_6D_6)



g) $^{29}Si(^{1}H)$ NMR (99 MHz, C_6D_6)



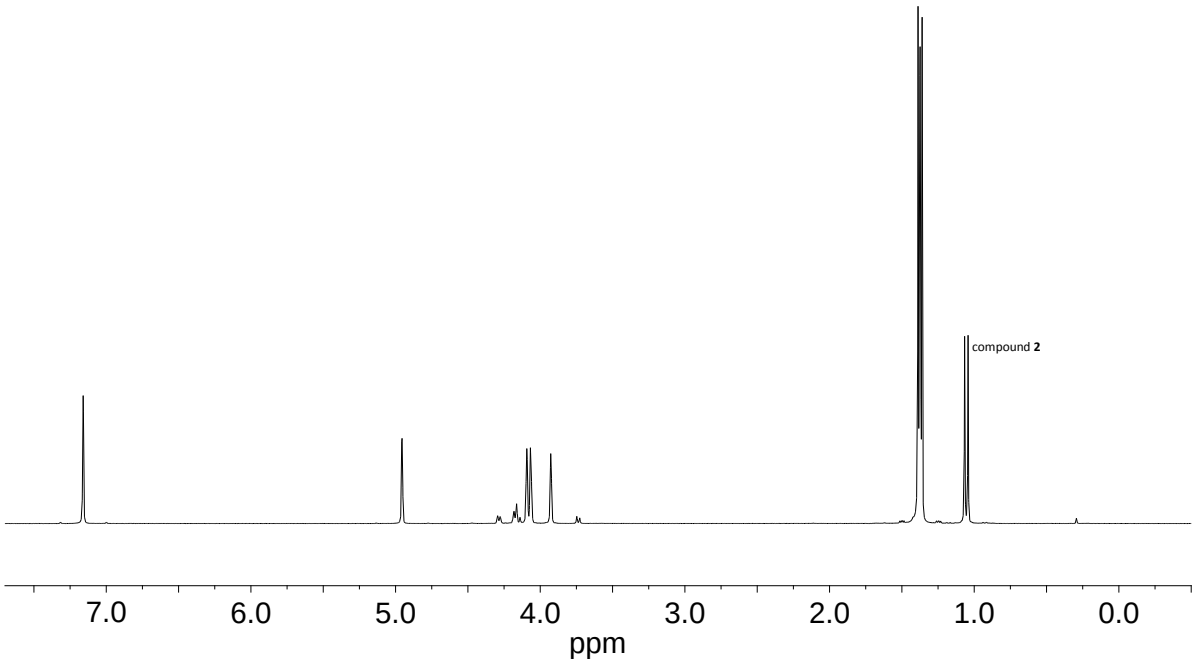
h) mass spectra (LIFDI)



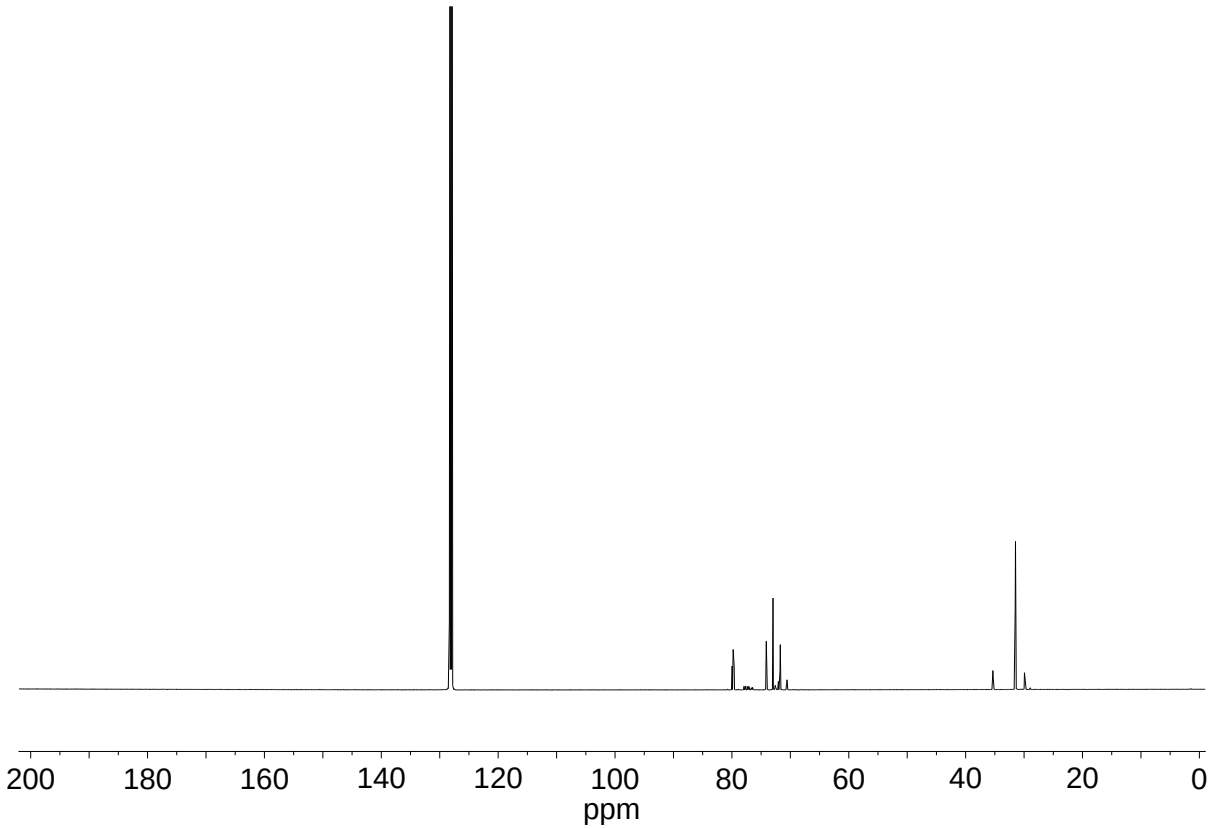
Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Possible Formula	Unsaturation Number
519.92085	8864.86	519.92054	0.31	$^{12}C_{18}{}^{1}H_{26}{}^{79}Br_{1}{}^{81}Br_{1}{}^{56}Fe_{1}{}^{31}P_{2}$	8.5

Figure S8: NMR spectra for compound **7**

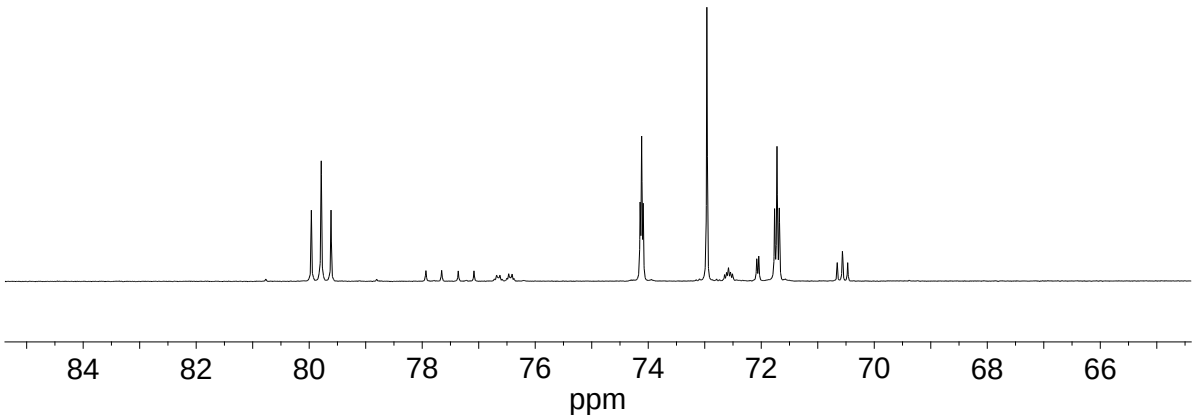
a) ^{1}H NMR (500 MHz, C_6D_6)



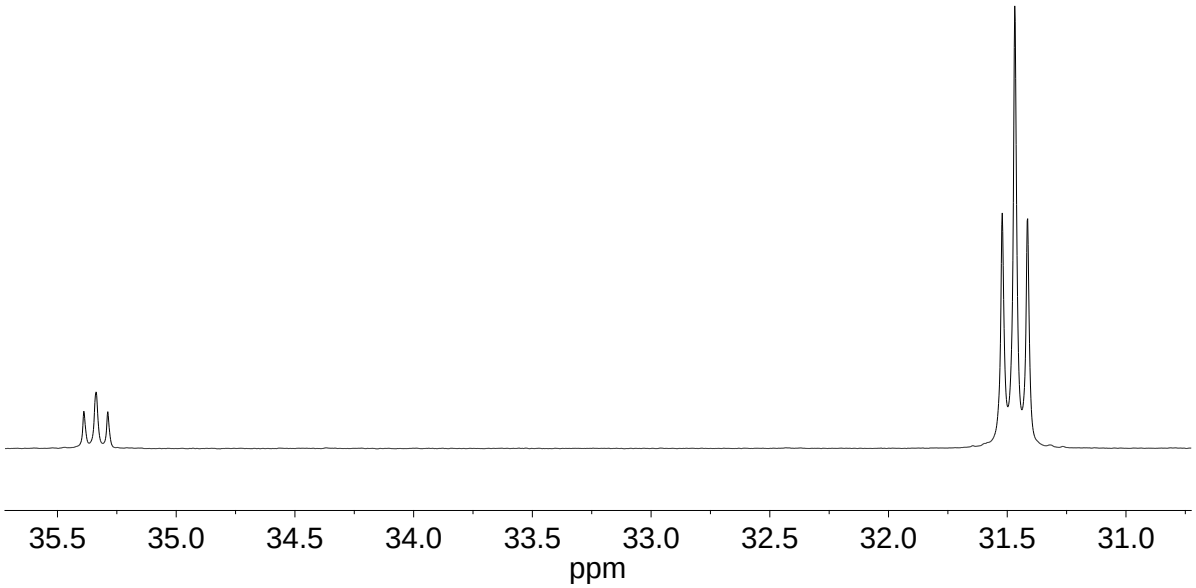
b) ^{13}C NMR (101 MHz, C_6D_6)



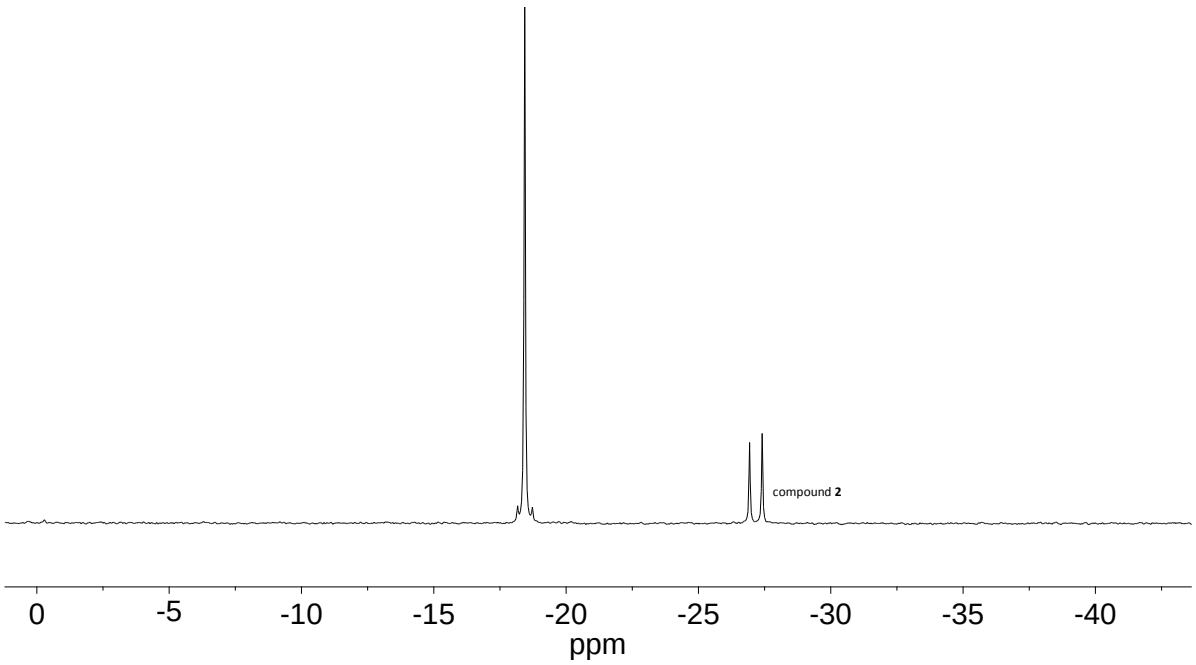
c) ^{13}C NMR (101 MHz, C_6D_6)



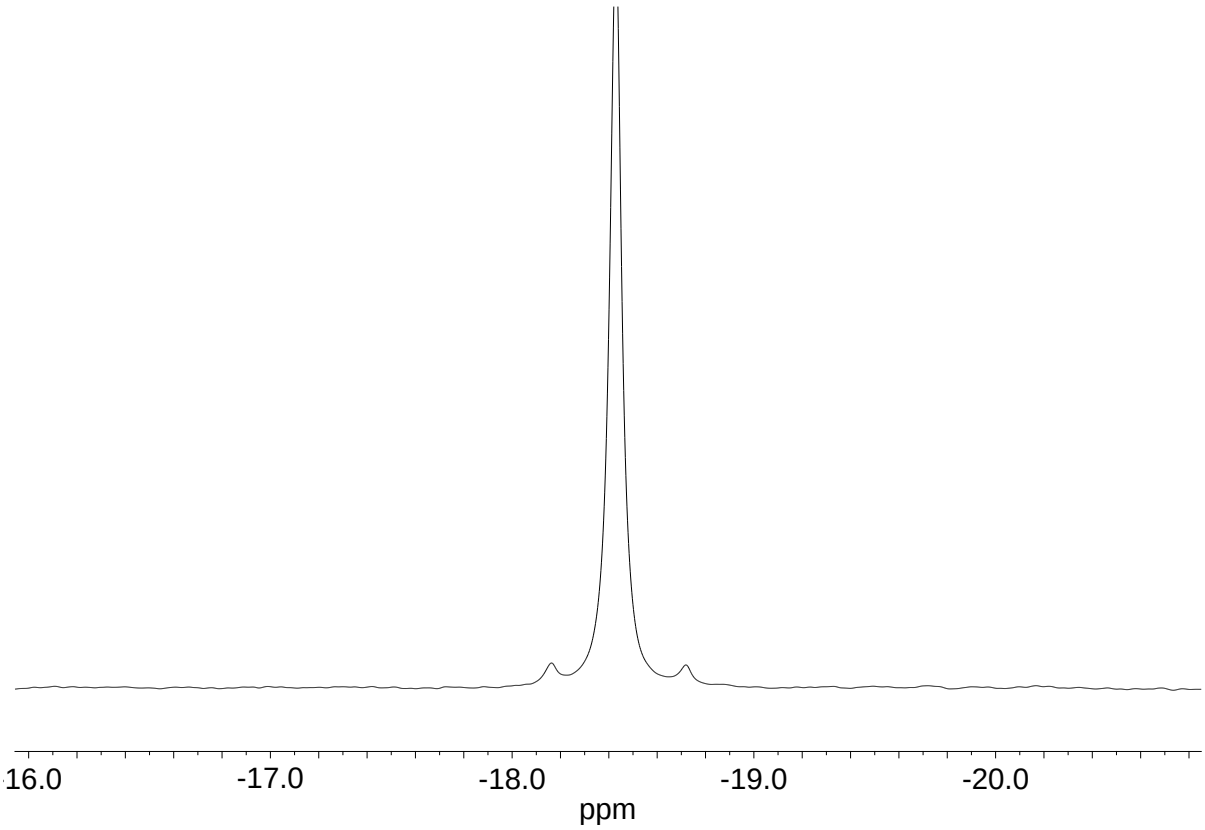
d) ^{13}C NMR (101 MHz, C_6D_6)



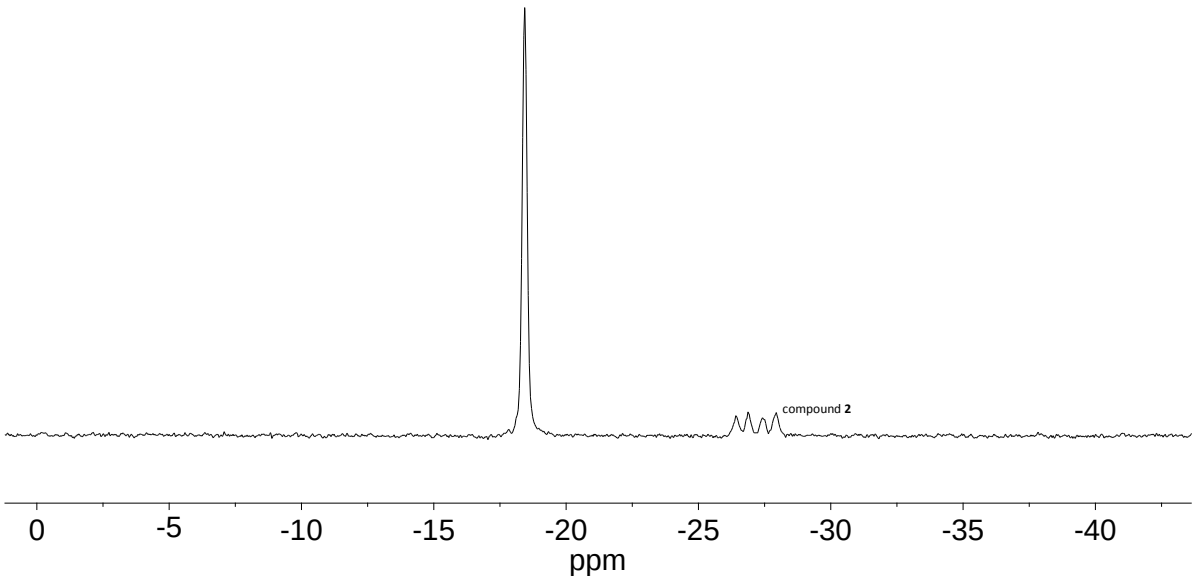
e) $^{31}P\{^1H\}$ NMR (202 MHz, C_6D_6)



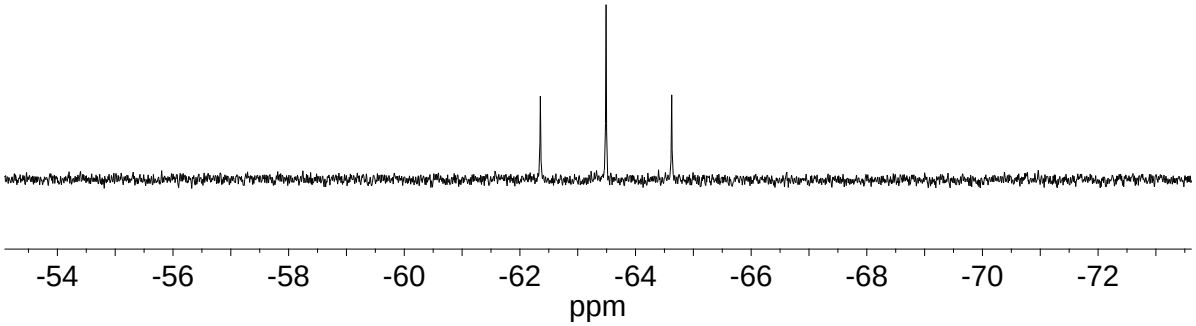
f) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



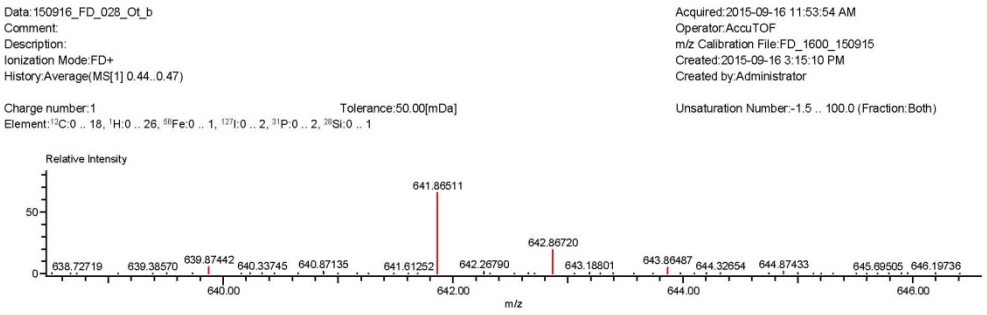
g) ^{31}P NMR (202 MHz, C_6D_6)



h) $^{29}Si(^{1}H)$ NMR (99 MHz, C_6D_6)

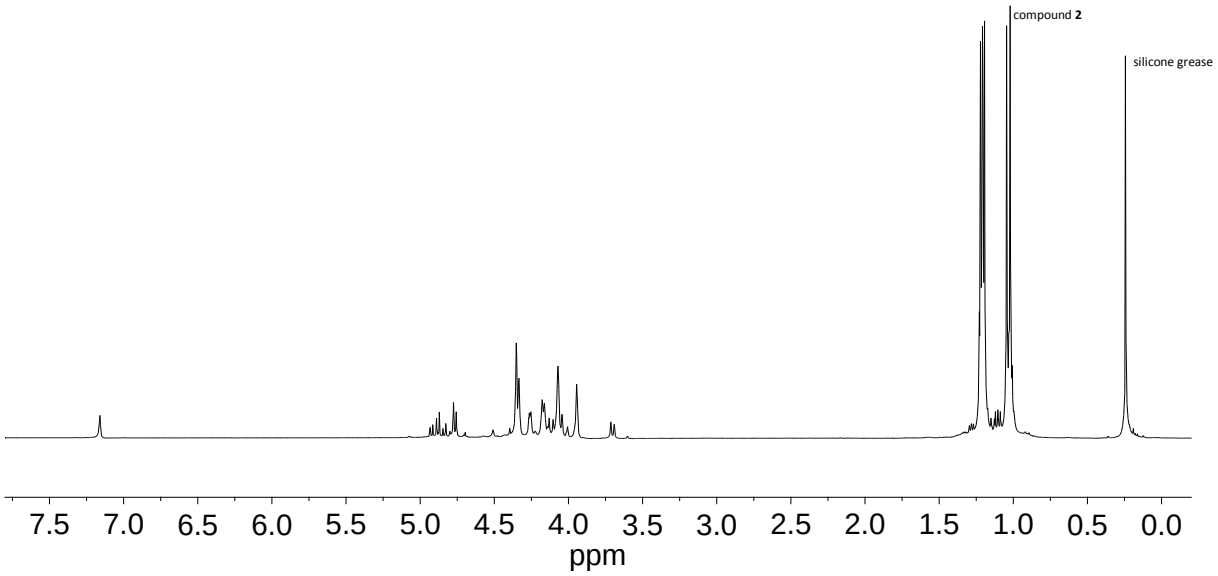


i) mass spectra (LIFDI)

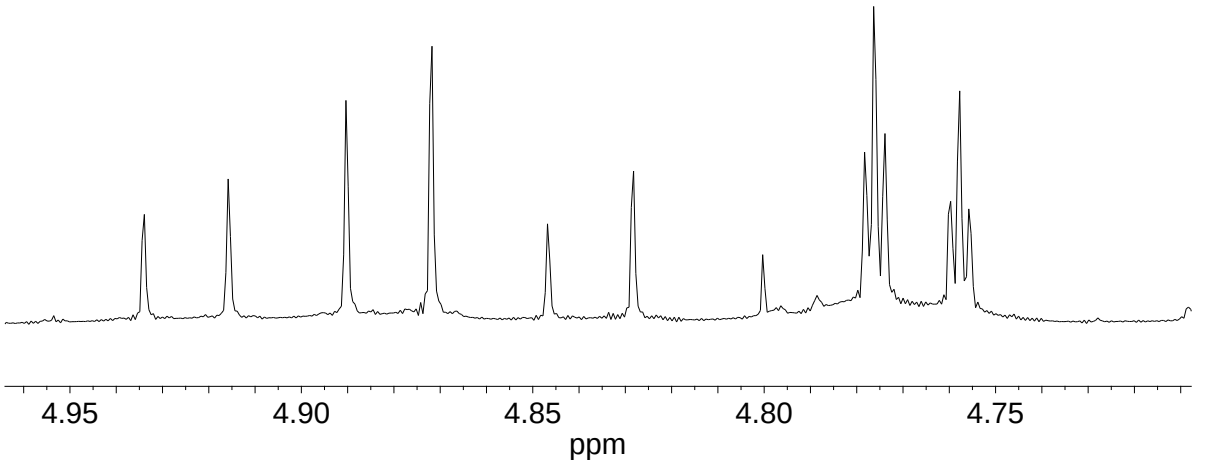


Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Possible Formula
641.86511	44901.11	641.87178	-6.67	$^{12}C_{18}{}^{1}H_{26}{}^{56}Fe_1{}^{127}I_2{}^{31}P_2{}^{28}Si_1$

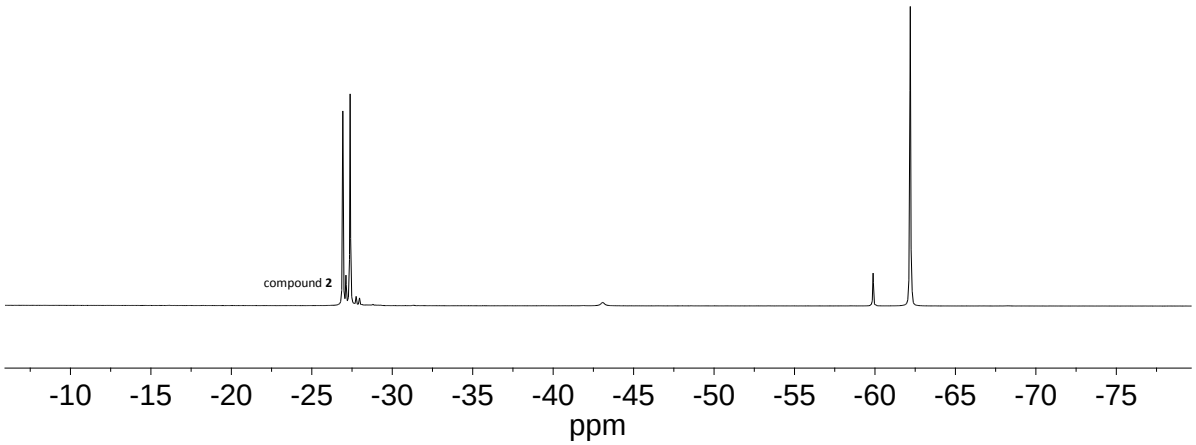
Figure S9: NMR spectra for compound 8
a) ^{1}H NMR (500 MHz, C_6D_6)



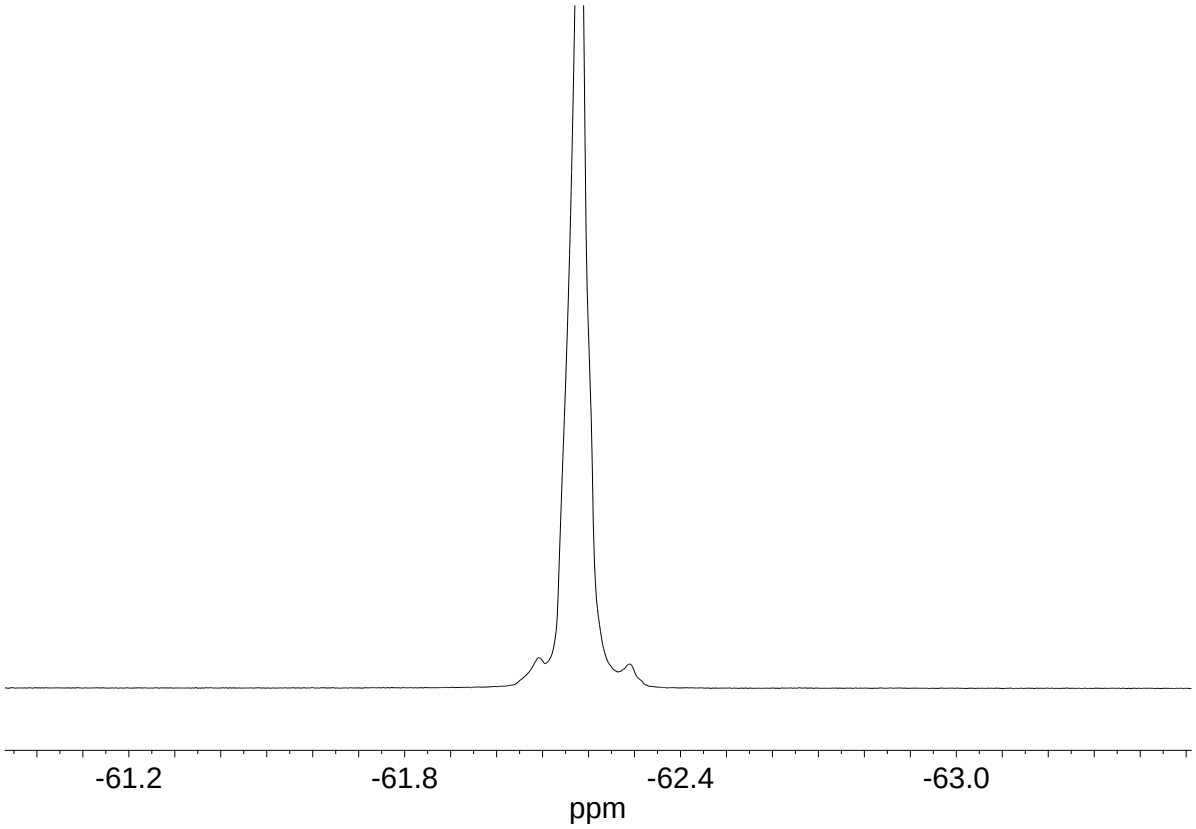
b) ^{1}H NMR (500 MHz, C_6D_6)



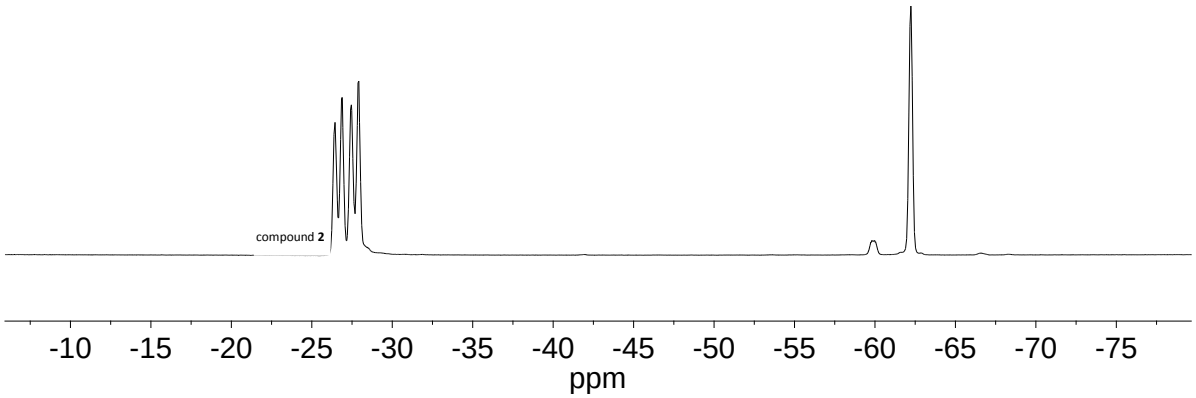
c) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



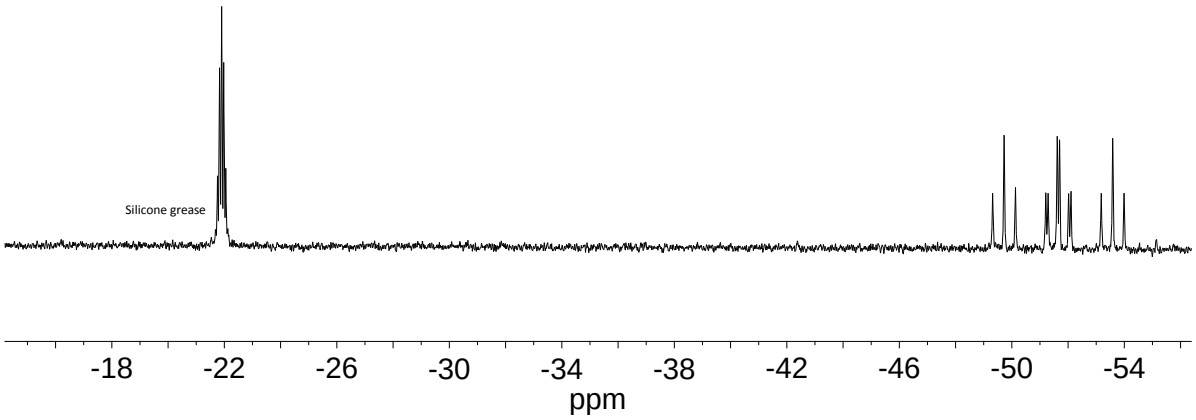
d) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



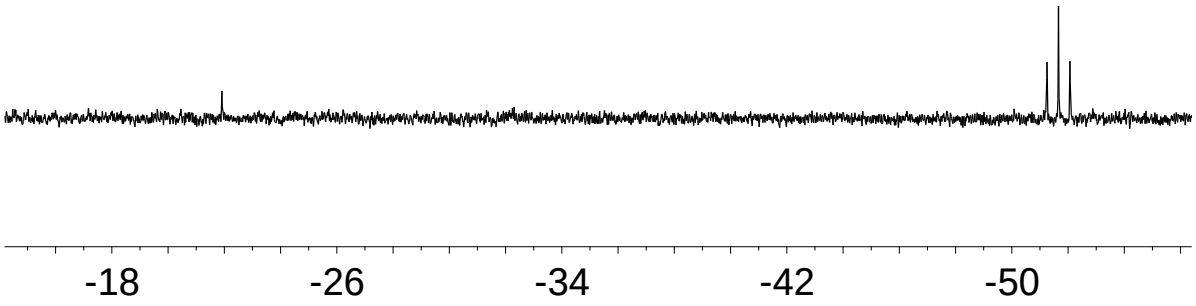
e) ^{31}P NMR (202 MHz, C_6D_6)



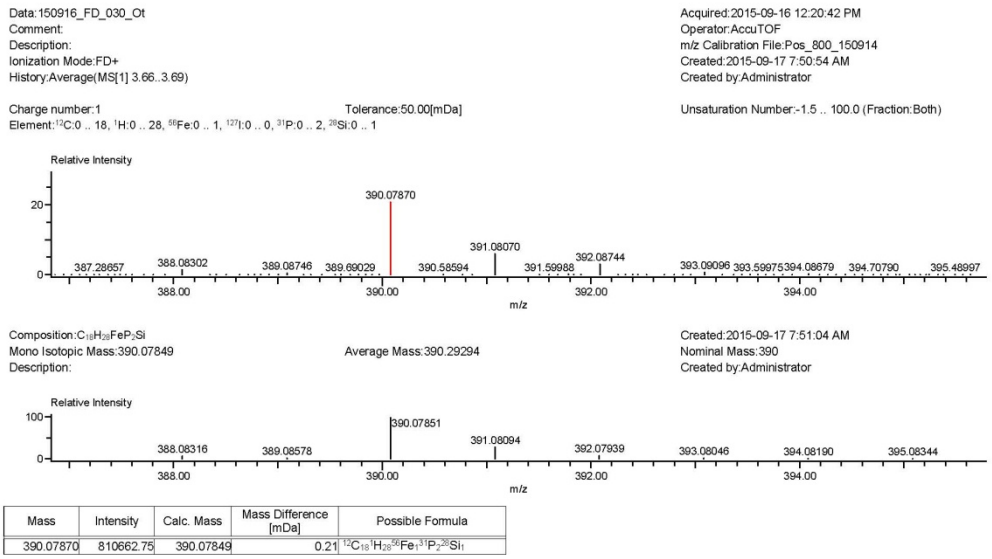
f) ^{29}Si NMR (99 MHz, C_6D_6)



g) $^{29}Si(1H)$ INEPT NMR (99 MHz, C_6D_6)



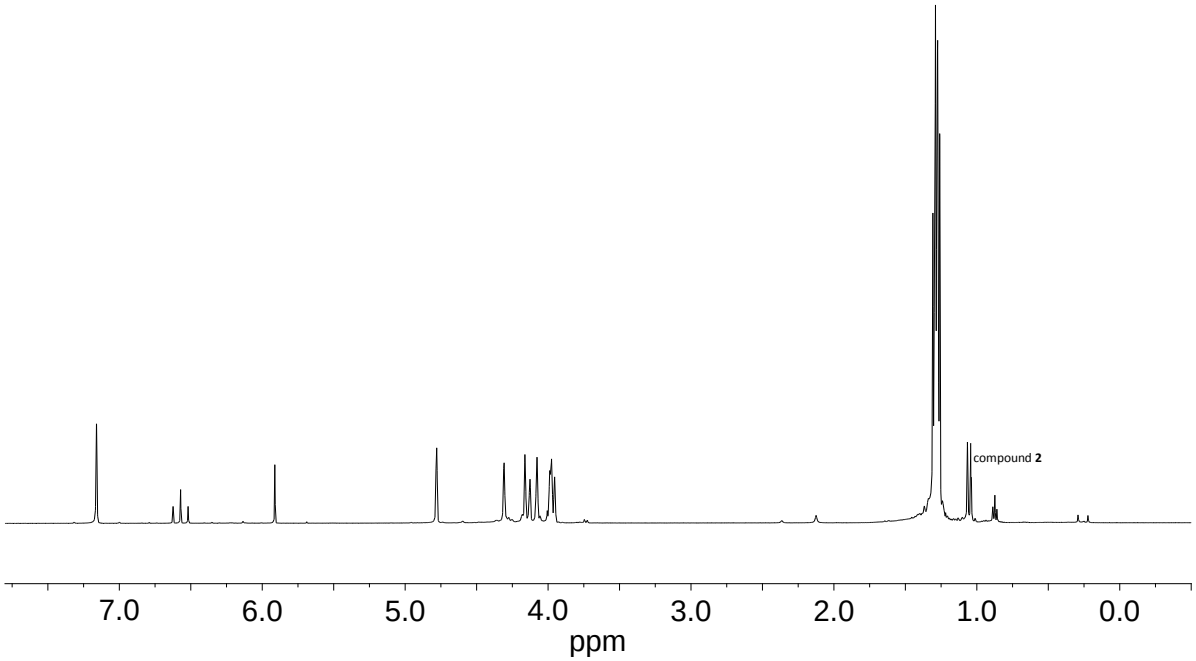
h) mass spectra (LIFDI)



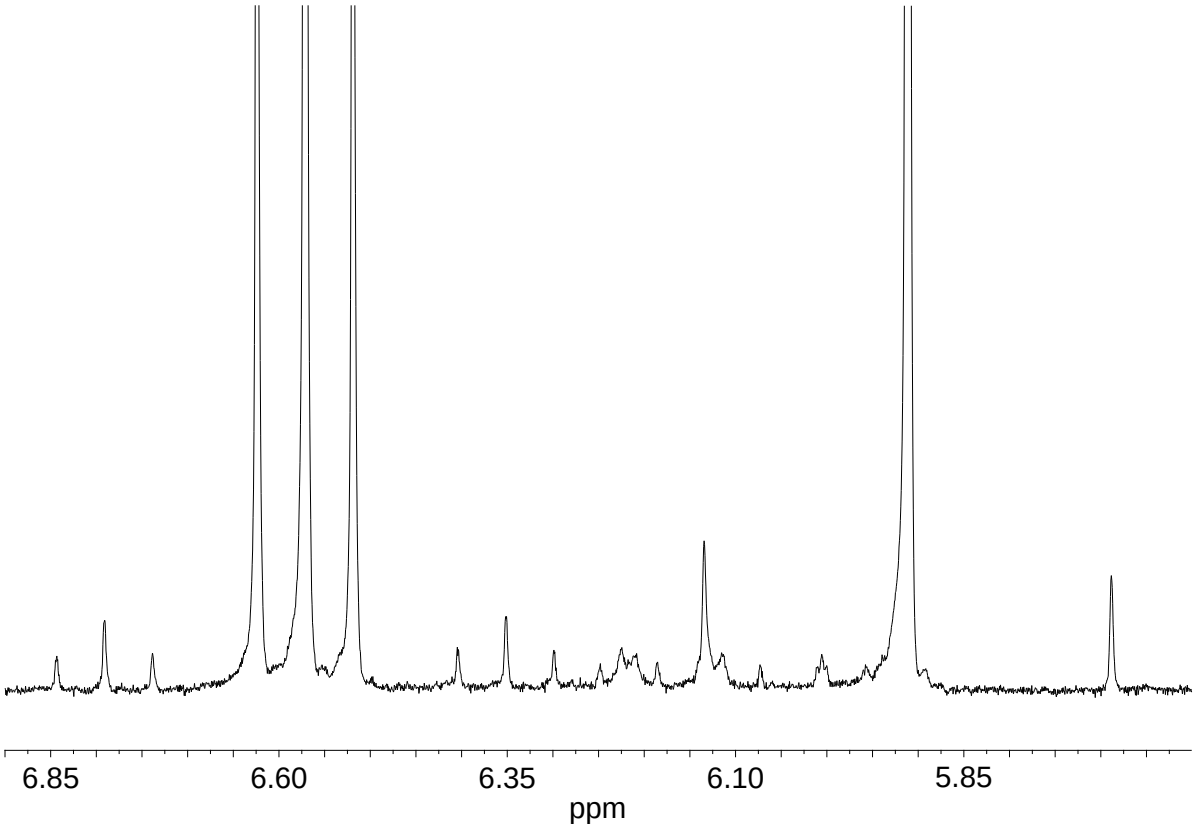
Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Possible Formula
390.07870	810662.75	390.07849	0.21	$^{12}C_{18}{}^{1}H_{28}{}^{56}Fe_{1}{}^{31}P_{2}{}^{28}Si_{1}$

Figure S10: NMR spectra for compound **9**

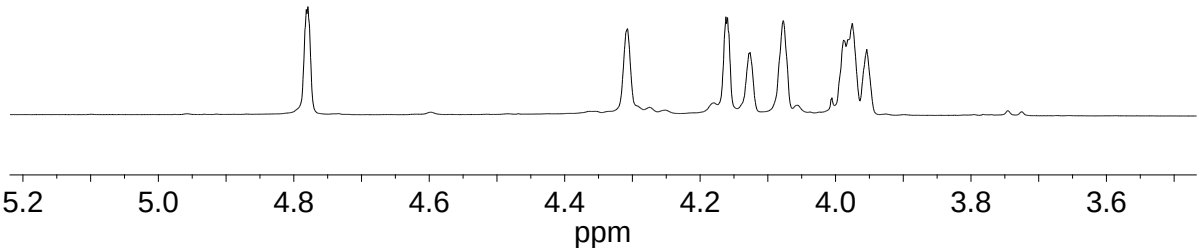
a) ^{1}H NMR (500 MHz, C_6D_6)



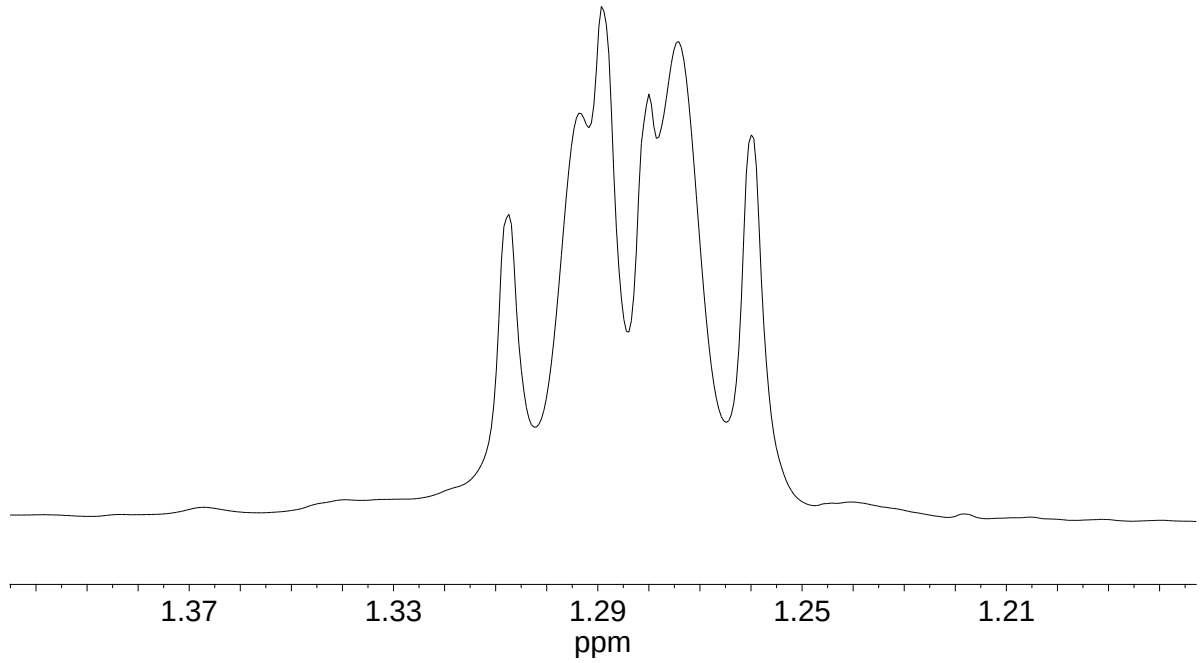
b) ^{1}H NMR (500 MHz, C_6D_6)



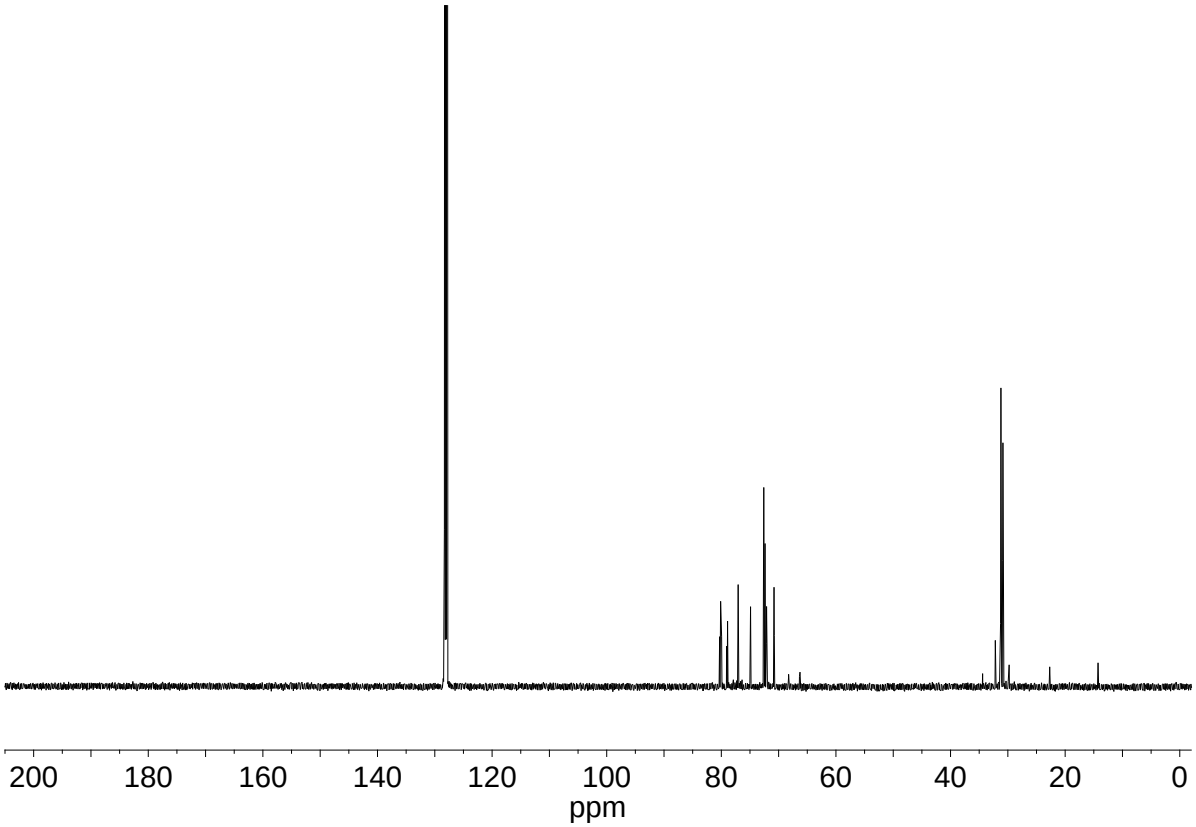
c) ^{1}H NMR (500 MHz, C_6D_6)



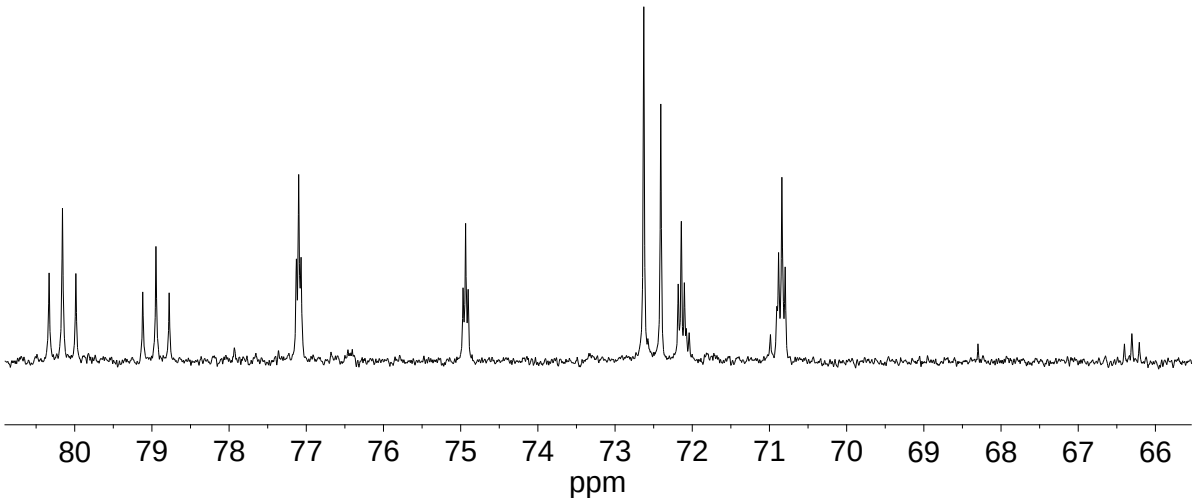
d) ^{1}H NMR (500 MHz, C_6D_6)



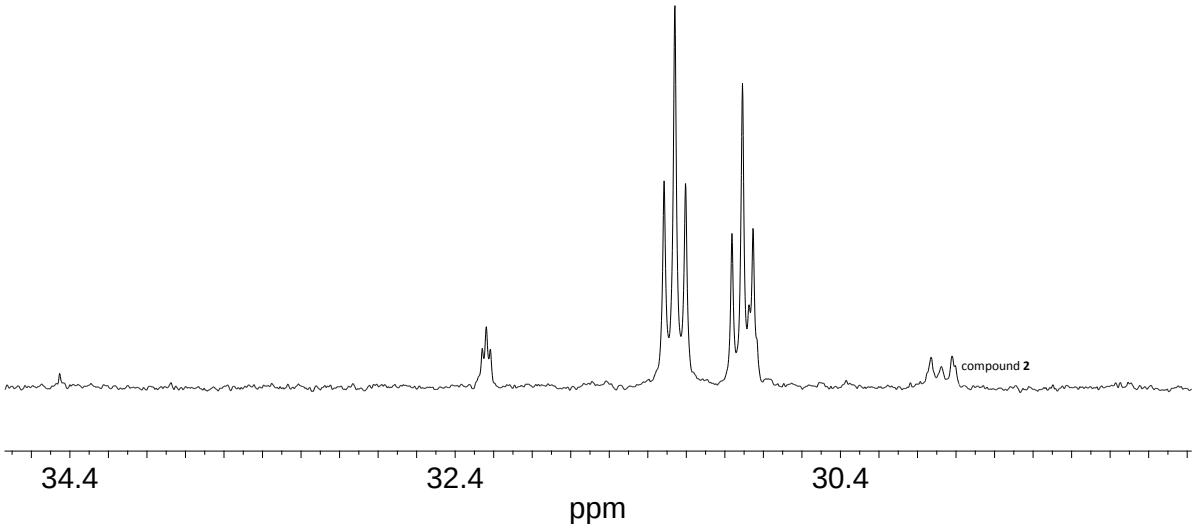
e) ^{13}C NMR (126 MHz, C_6D_6)



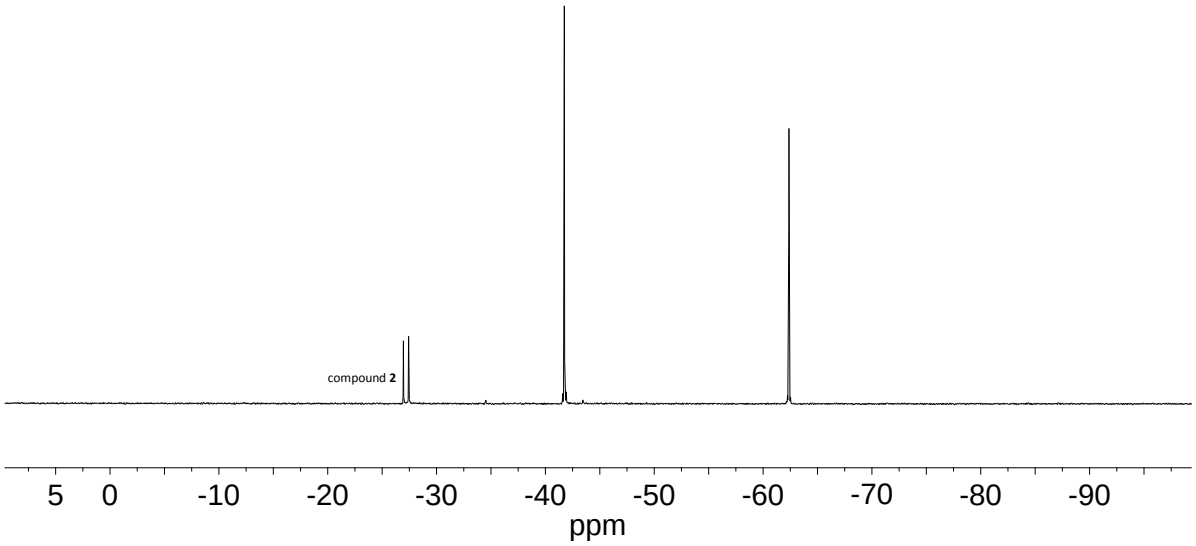
f) ^{13}C NMR (126 MHz, C_6D_6)



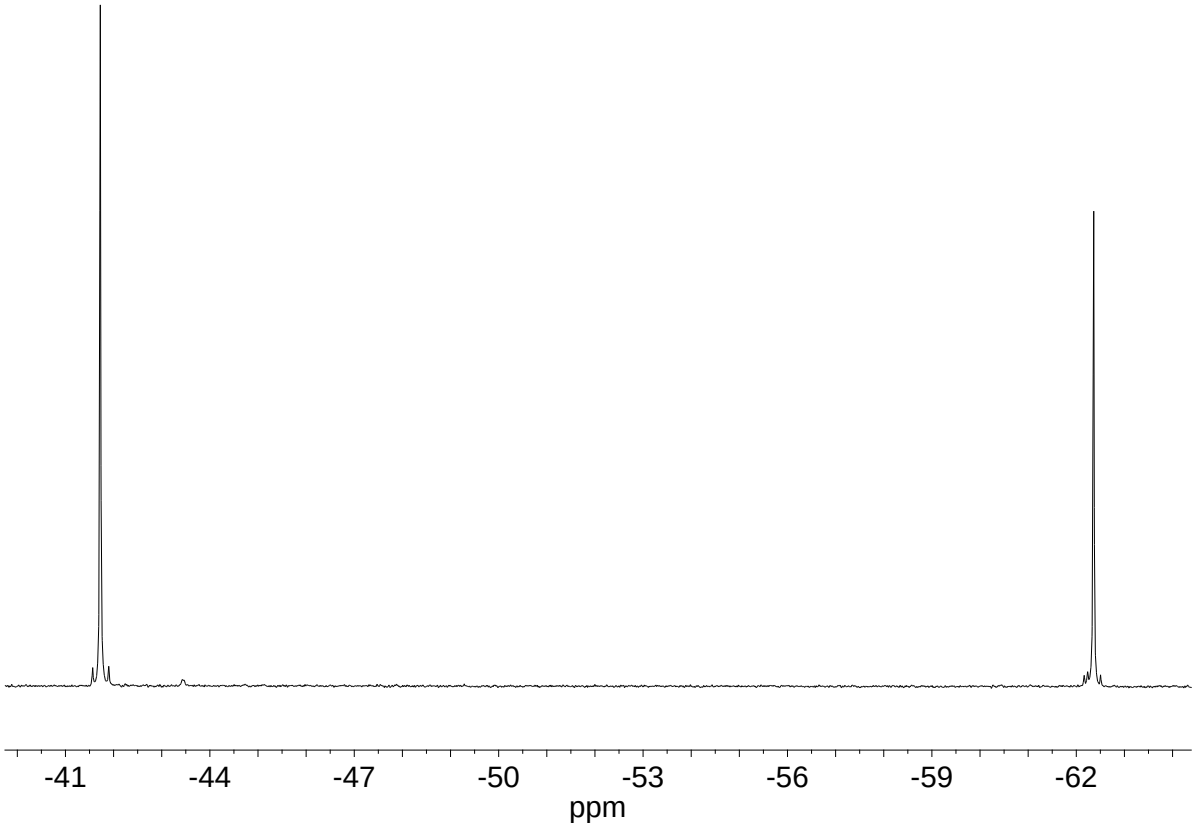
g) ^{13}C NMR (126 MHz, C_6D_6)



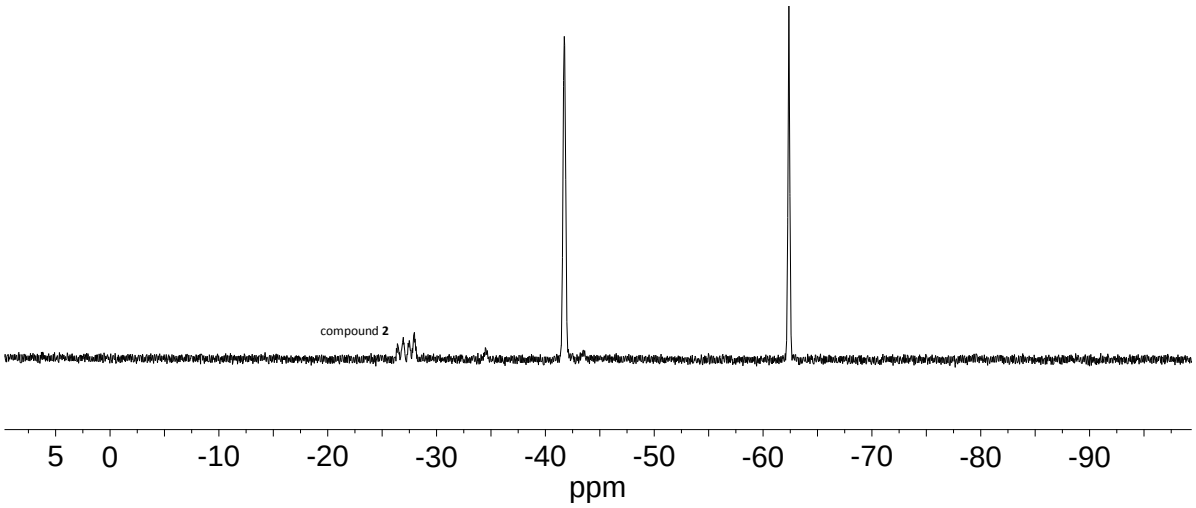
h) $^{31}P\{^1H\}$ NMR (202 MHz, C_6D_6)



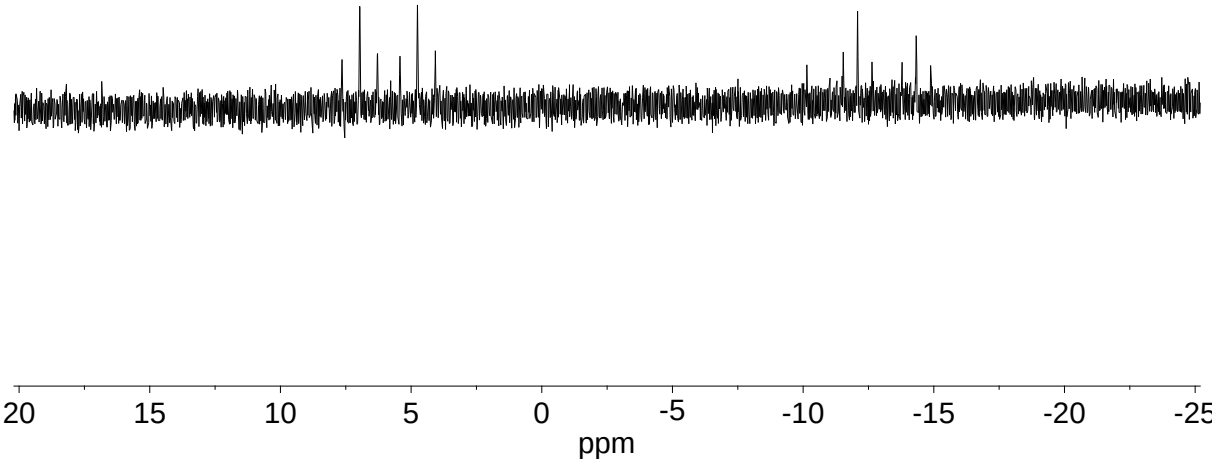
i) $^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6)



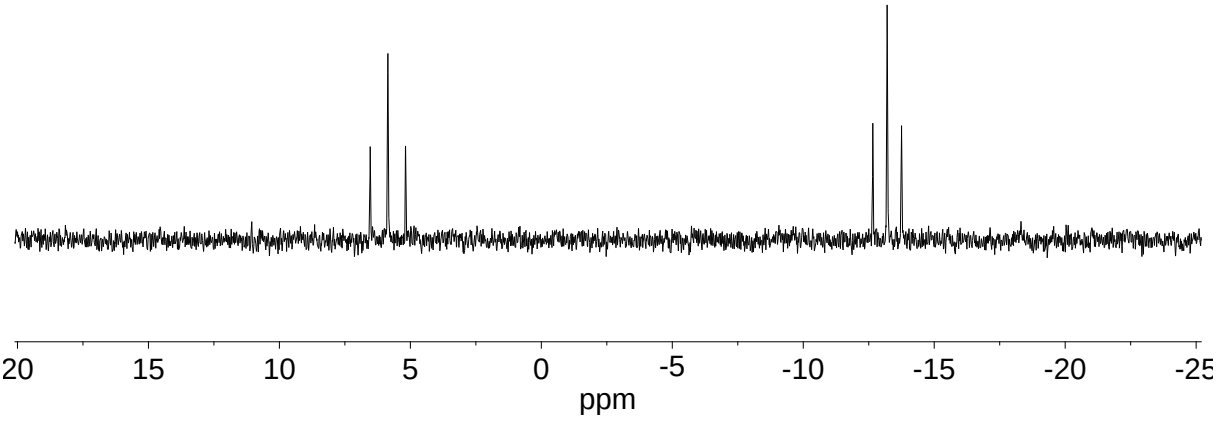
j) ^{31}P NMR (202 MHz, C_6D_6)



k) ^{29}Si NMR (99 MHz, C_6D_6)



l) ^{29}Si INEPT NMR (99 MHz, C_6D_6)



m) mass spectra (LIFDI)

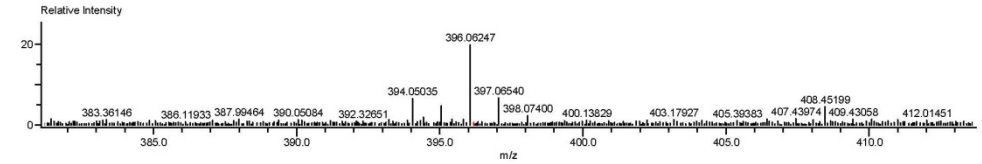
Data:150916_FD_027_Ot_d
Comment:
Description:
Ionization Mode:FD+
History:Average(MS[1] 2.43..2.54)

Acquired:9/16/2015 2:31:49 PM
Operator:AccuTOF
m/z Calibration File:FD_1600_150915
Created:10/6/2015 11:36:23 AM
Created by:Anna Lena

Charge number:1
Element:^{12}C:0 .. 18, ^{1}H:0 .. 27, ^{35}Cl:0 .. 1, ^{56}Fe:0 .. 1, ^{31}P:0 .. 2

Tolerance:2.00[mDa]

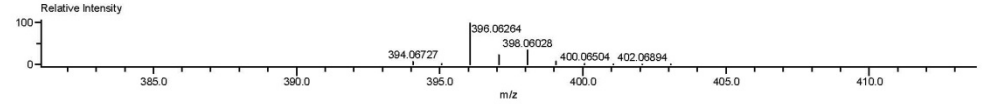
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)



Composition:$C_{18}H_{27}ClFeP_2$
Mono Isotopic Mass:396.06259
Description:

Average Mass:396.65220

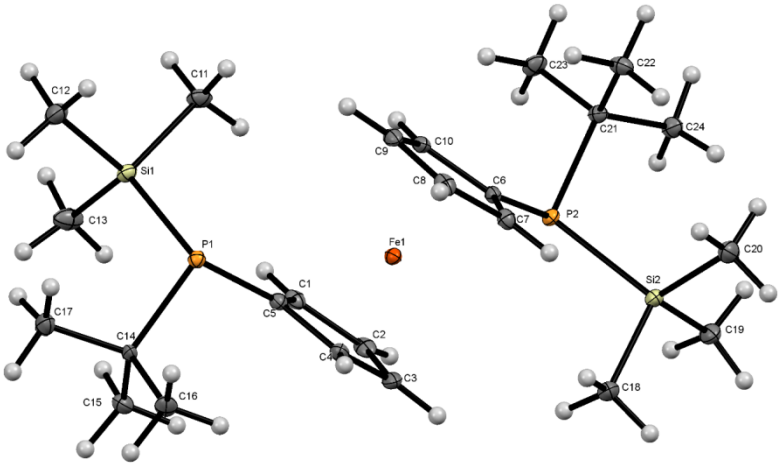
Created:10/6/2015 11:36:26 AM
Nominal Mass:396
Created by:Anna Lena



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Possible Formula	Unsaturation Number
396.06247	5365.25	396.06259	-0.12	$^{12}C_{18}{}^{1}H_{27}{}^{35}Cl_1{}^{56}Fe_1{}^{31}P_2$	8.5

X-ray crystal structure analysis of **5**

The molecular structure of the *meso* diastereomer of silyl phosphane **5** has been determined by X-ray diffraction and agrees well with the constitution established by spectroscopic methods (Figure S4). Compound **5** crystallizes in the Sohncke space group $P\,2_12_12_1$ and for the *S,R* configuration of the molecule a Flack parameter of -0.011(8) was obtained. All other structural parameters show no peculiarities and are within the normal range of comparable compounds.



Picture S4. Molecular structure of **5**. Ellipsoids are drawn at 30% probability level.

Table S2: Structure determination and refinement of **5**

	5
CCDC code	1434408
Empirical formula	$C_{24}H_{44}FeP_2Si_2$
Formula weight	506.56
Crystal description	Orange plate
Crystal size [mm]	0.340x0.150x0.075
Crystal system, space group	Orthorhombic, $P\,2_12_12_1$
Radiation and λ [Å]	Mo K_α 0.71073
Monochromator	Graded multilayer mirror
Temperature [K]	100(2)
Unit cell dimensions:	
a [Å]	8.9505(7)
b [Å]	9.6294(9)
c [Å]	31.735(3)
α [°]	90.00
β [°]	90.00
γ [°]	90.00
Volume [Å³]	2735.2(4)
Z	4
Calculated density	1.230
F(000)	1088
Linear absorption coefficient μ [mm^{-1}]	0.765
Absorption correction	Integration

Unit cell determination	STOE X-area
Diffractometer	STOE StadiVari
Radiation source	Mo Genix
Scan type	Omega scan
Θ range for data collection	2.21-31.13
Index ranges	-11<h<11 -11<k<12 -30<l<40
Refl. collected / unique	30487/5940
Significant unique refl.	5356
R(int), R(sigma)	0.0412, 0.0408
Completeness to Θ = 26.0°	0.99
Refinement method	SHELXL-2014/7
Data/parameters/restraints	5940/274/0
Goodness-of-fit on F^2	0.975
Final R indices [I > 2σ(I)]	0.0271
R indices (all data)	0.0337
Largest difference peak/hole [e/Å^3]	0.400/-0.212