Supporting Information

Direct Heteroarylation of β-Protected Dithienosilole and Dithienogermole Monomers with Thieno[3,4-*c*]Pyrrole-4,6-Dione and Furo[3,4-*c*]Pyrrole-4,6-Dione

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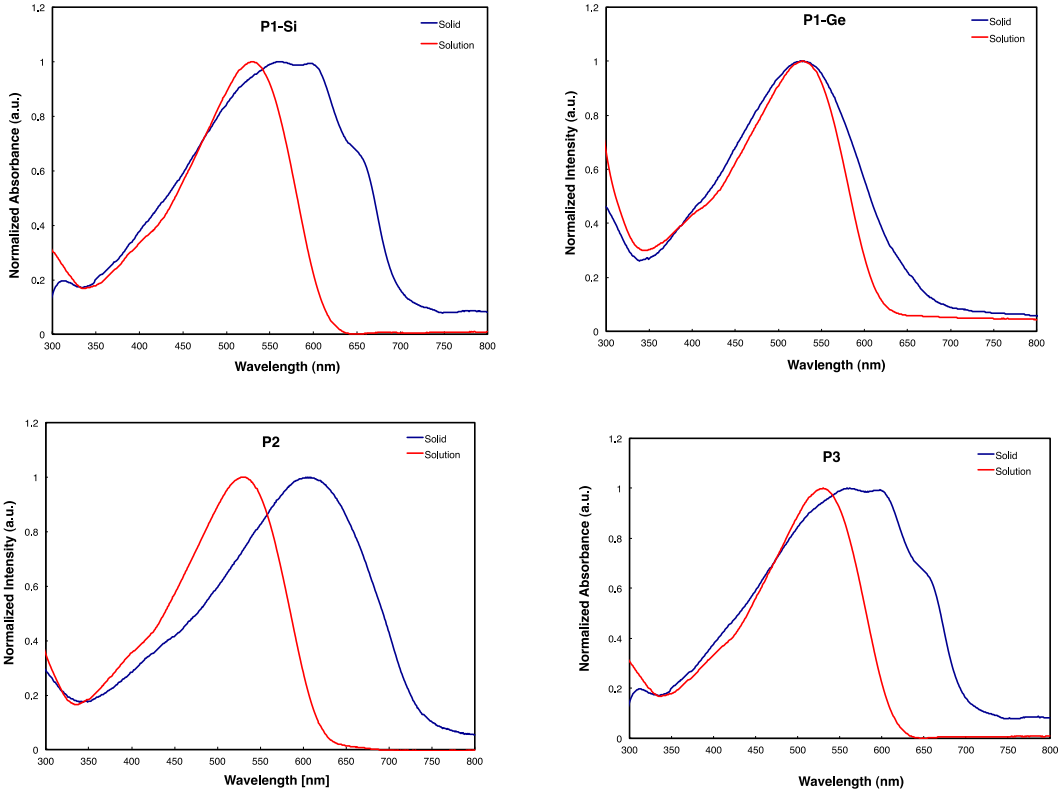
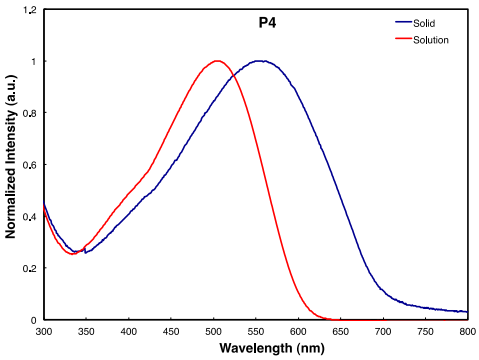
Table S1. Optimization of time for PDTSiTPD and PDTGeTPD via C-H activation.

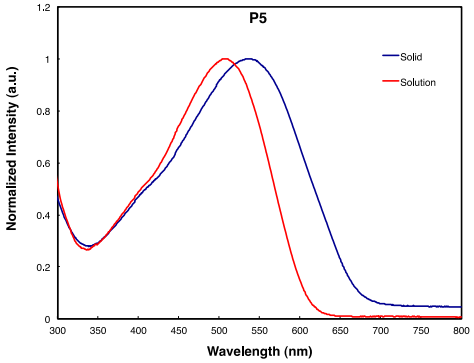
Polymer	Solvent	Time [h]	Mn [kDa] (PDI)	Yield [%]
PDTSiTPD	PhMe	16	17 (2.2)	34
PDTSiTPD	PhMe	24	20 (3.0)	39
PDTSTPD[a]	-	-	28 (1.6)[1]	38[1]
PDTGTPD	PhMe	4	15 (3.0)	94
PDTGTPD	PhMe	16	16.8 (3.4)	17
PDTGTPD	PhMe	24	10.9 (2.3) 13.8 (2.6)	60
PDTGTPD[a]	-	-	48.0 (1.7)[2]	73[2]

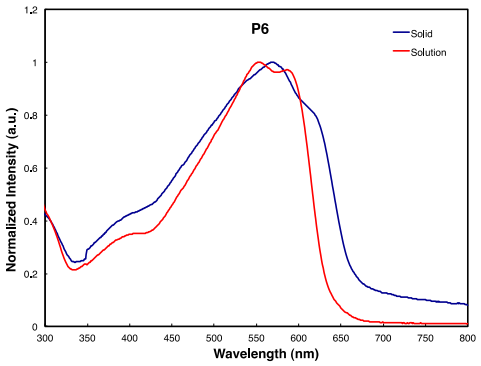
a) prepared by Stille polymerization

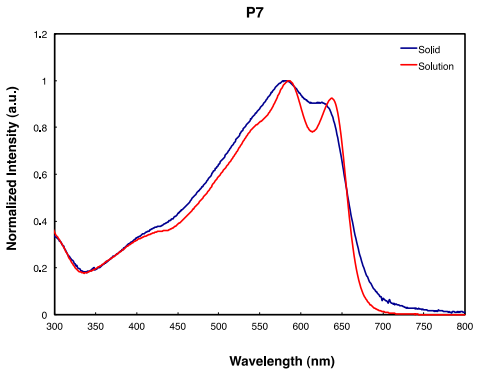
Figures S1. Solid and solution UV-vis absorption for polymers **P1**-**P9**.

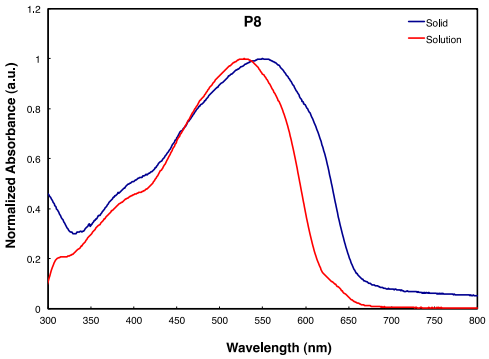


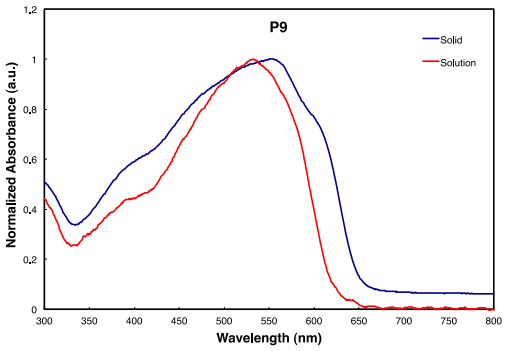




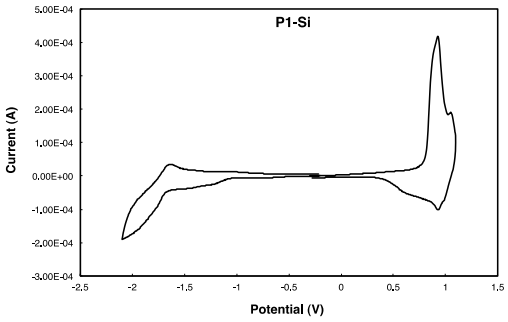


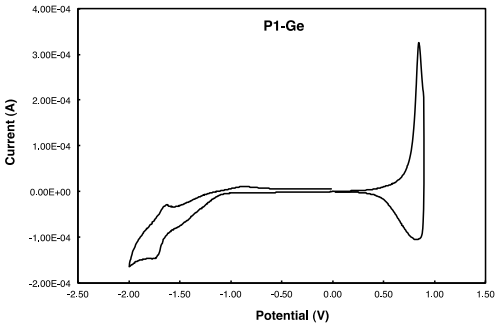


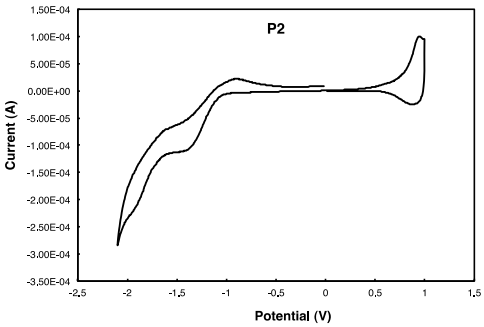


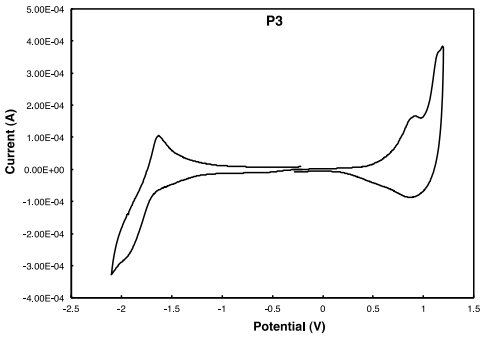


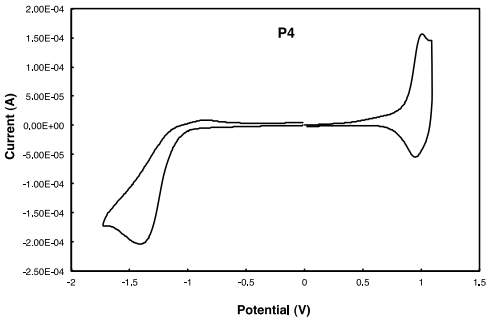
Figures S2. Cyclic voltammetry curves for thin films of **P1**-**P9** measured in $[NBu_4][BF_4]$ (0.1 M) in MeCN at a scan rate of 50 mV/s and referenced to ferrocene. -4.70 eV was used as 0.0 V vs. NHE.[3]

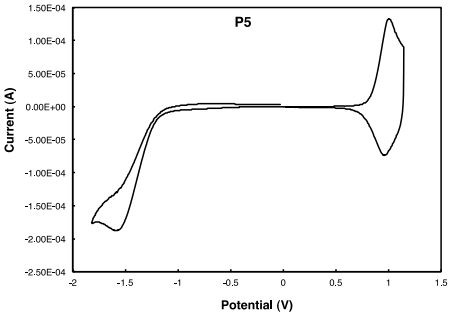












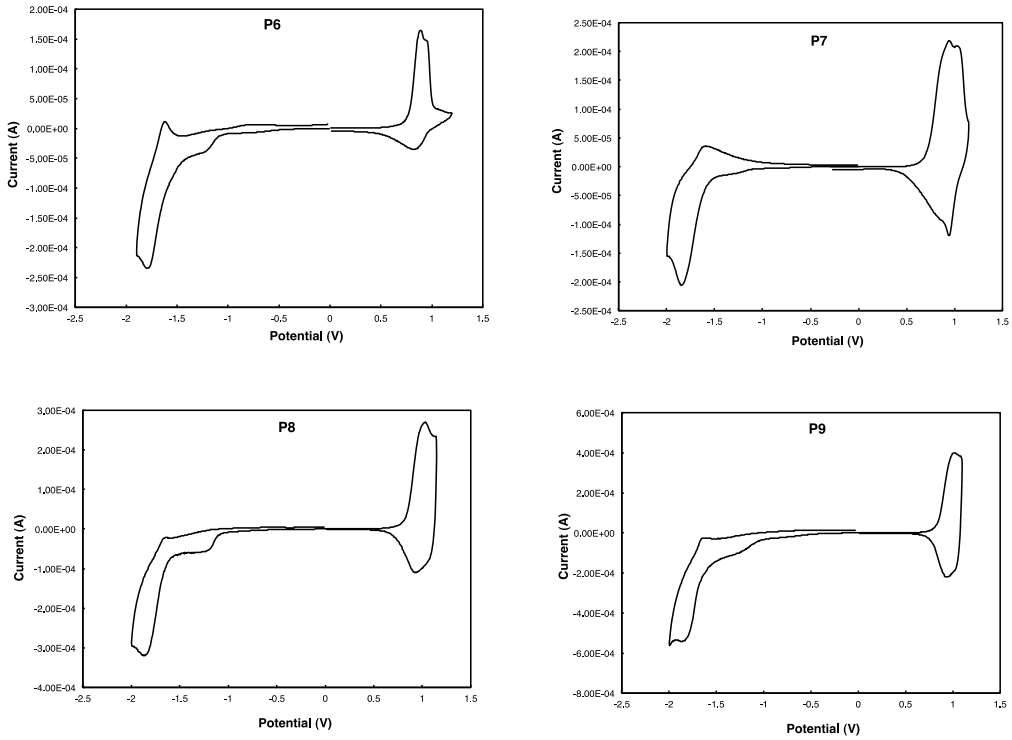


Figure S3. TGA analysis of TPD Polymers.

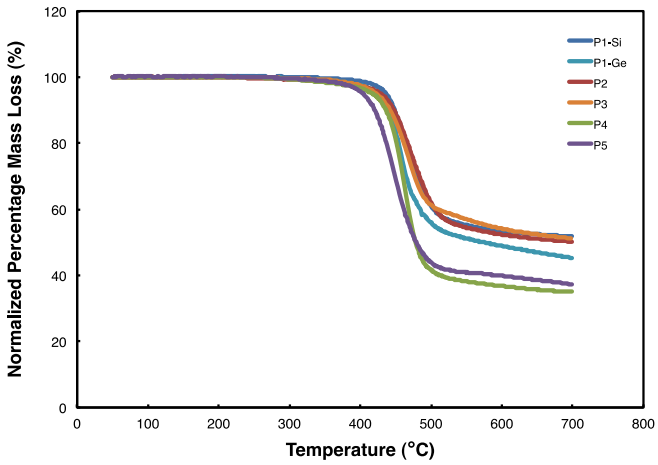


Figure S4. TGA analysis of FPD Polymers.

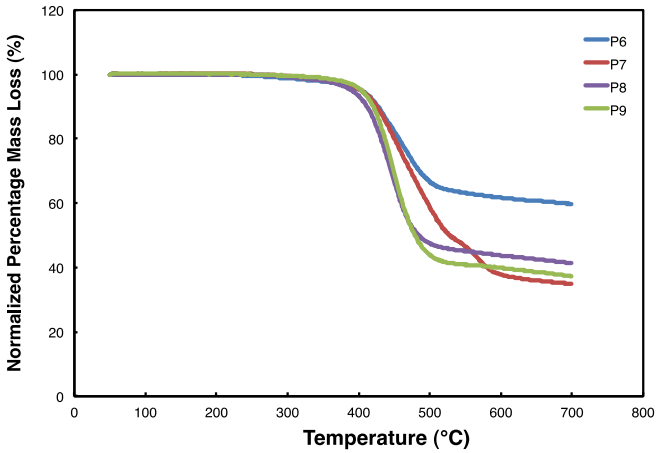


Figure S5. DSC analysis of TPD Polymers.

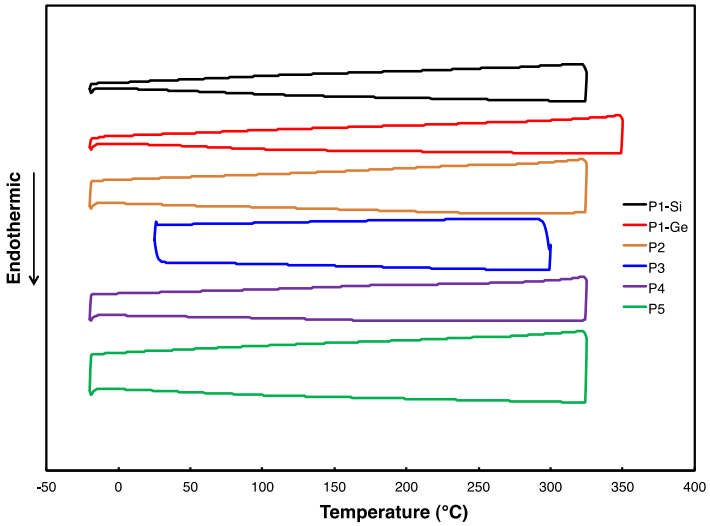


Figure S6. DSC analysis of FPD Polymers.

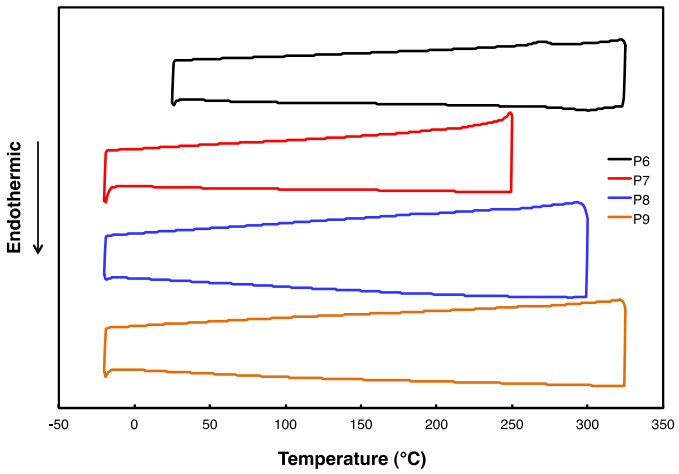


Figure S7. X-ray diffraction patterns of pristine TPD-based co-polymers.

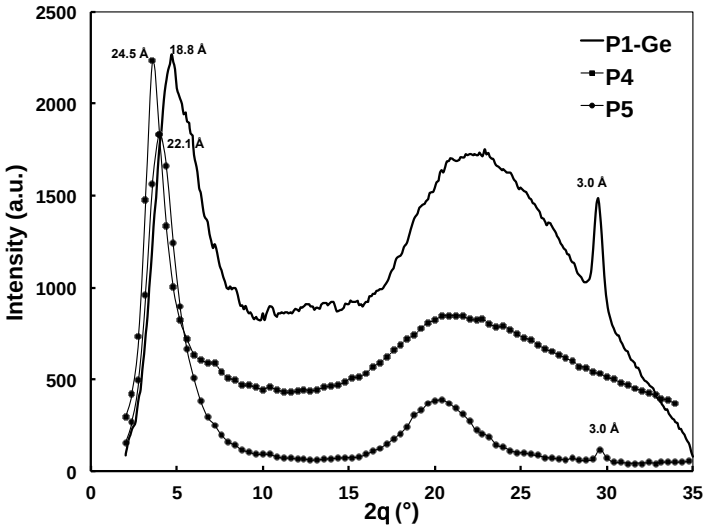


Figure S8. X-ray diffraction patterns of pristine FPD-based co-polymers.

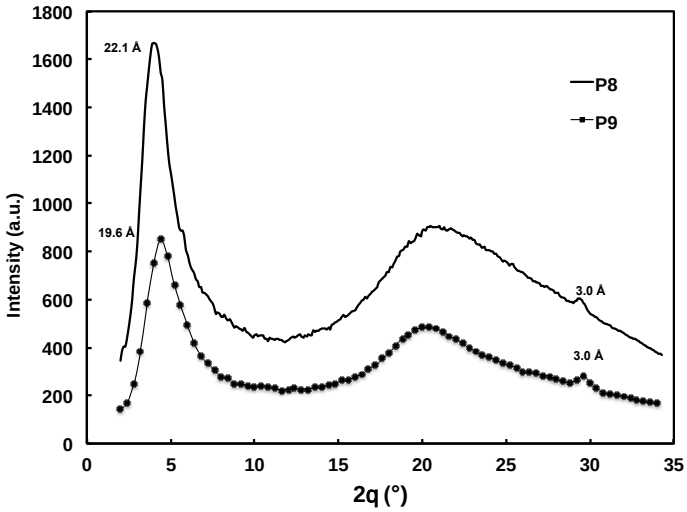
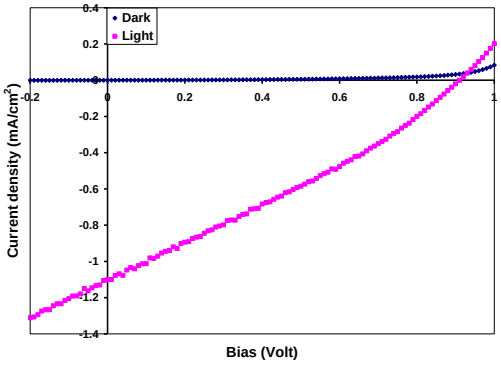


Figure S9. Current-voltage characteristics (*right*) and external quantum efficiency (EQE) as a function of wavelength (*left*) for OPVs composed of **P1-Si**:2PC$_{70}$BM (chlorobenzene + 2% DIO) blends.



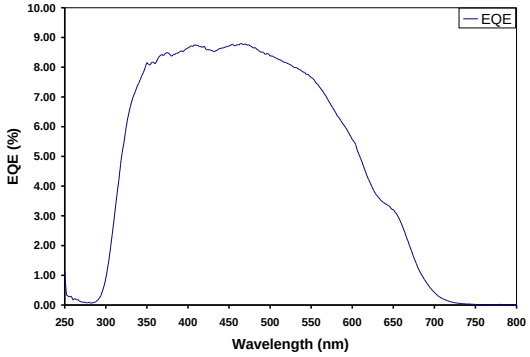


Figure S10. Current-voltage characteristics (*right*) and external quantum efficiency (EQE) as a function of wavelength (*left*) for OPVs composed of **P3**:2$PC_{70}BM$ (chlorobenzene + 2% DIO) blends.

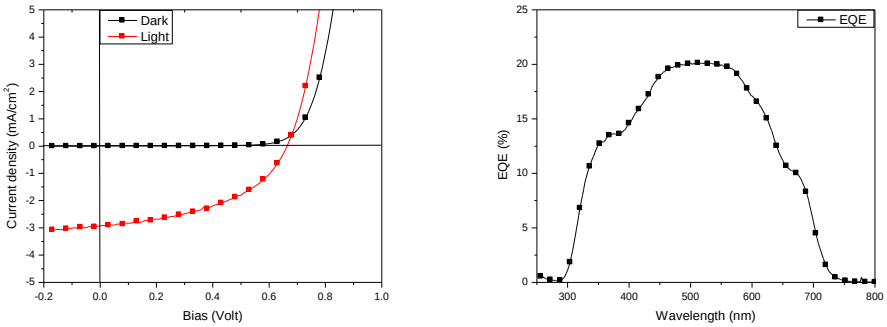


Figure S11. Current-voltage characteristics (*right*) and external quantum efficiency (EQE) as a function of wavelength (*left*) for OPVs composed of **P6**:2$PC_{70}BM$ (chlorobenzene + 2% DIO) blends.

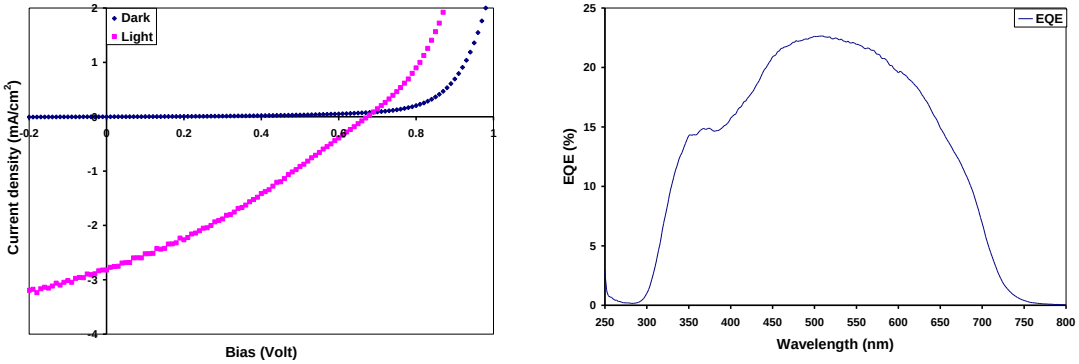
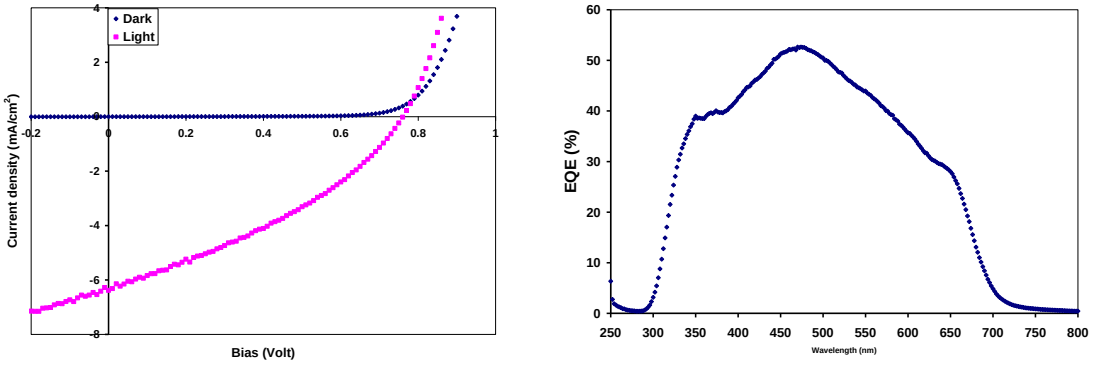
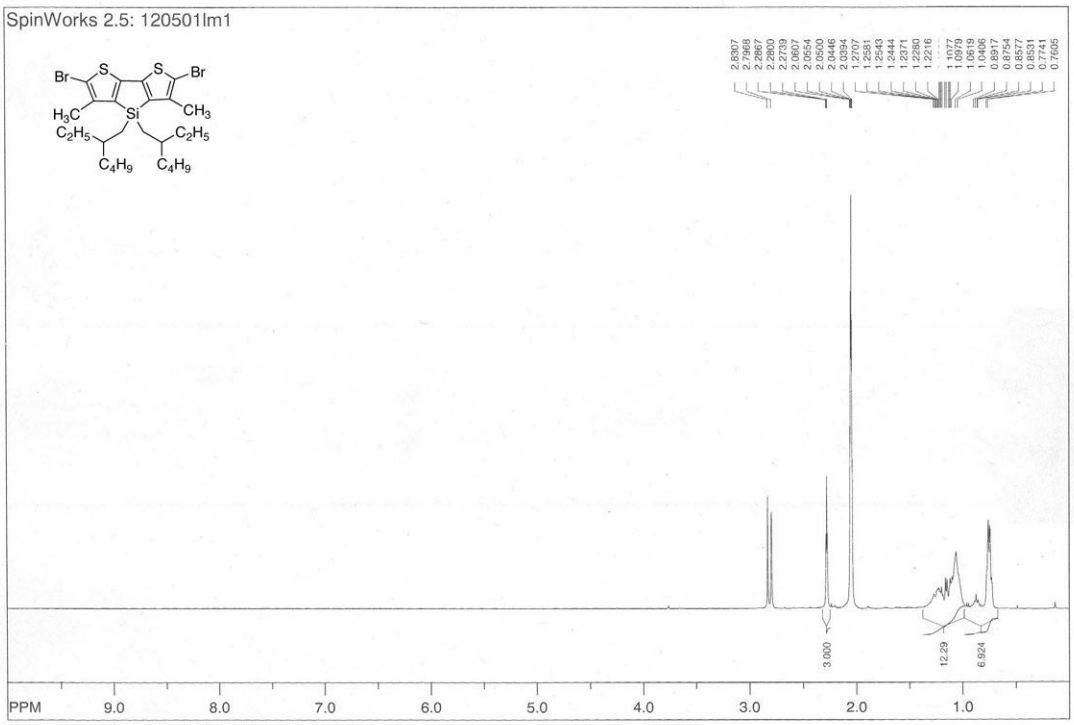


Figure S12. Current-voltage characteristics (*right*) and external quantum efficiency (EQE) as a function of wavelength (*left*) for OPVs composed of **P7**:2$PC_{70}BM$ (chlorobenzene + 2% DIO) blends.

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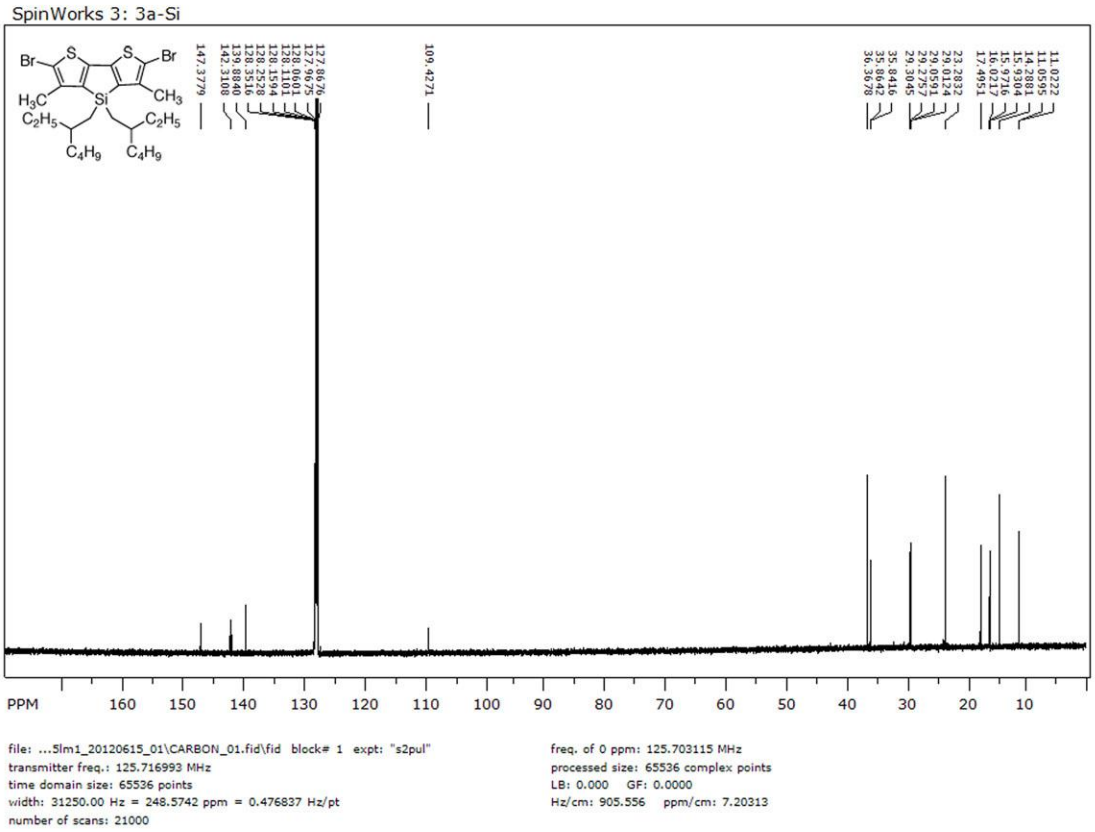

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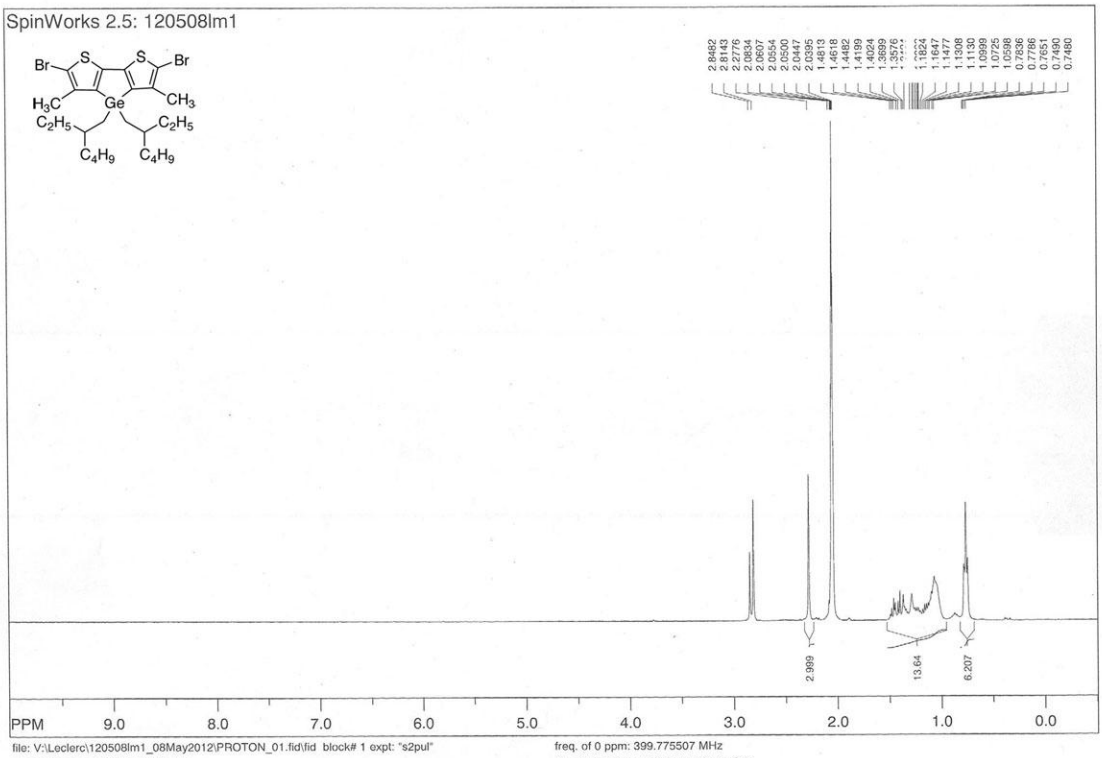

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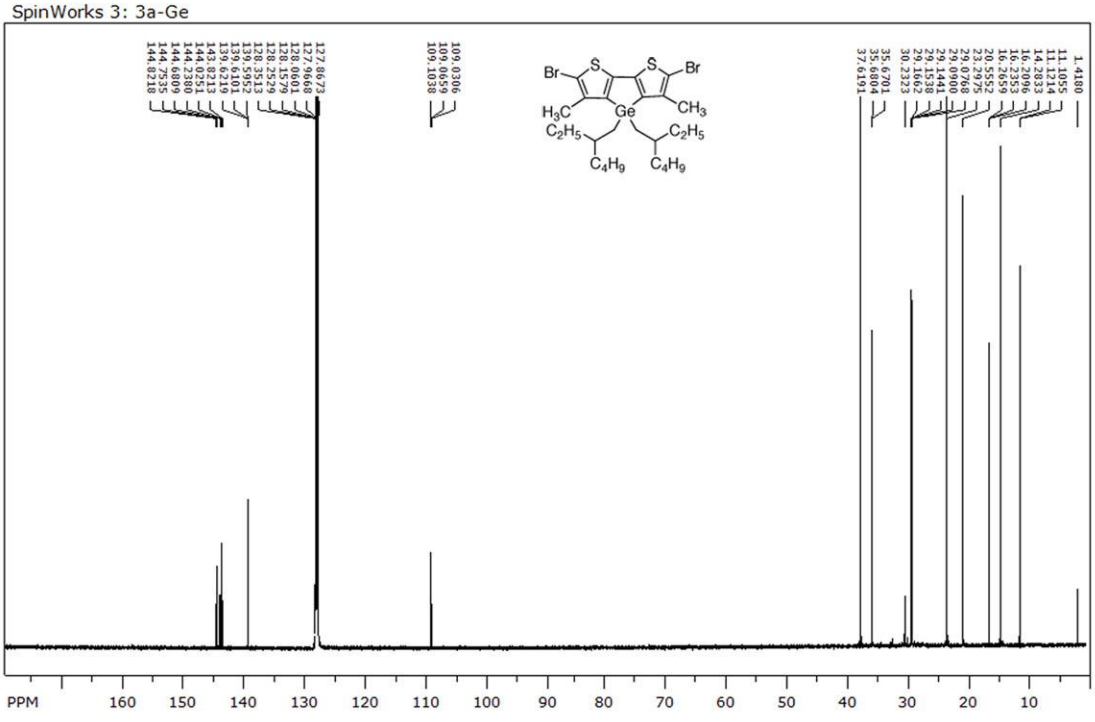

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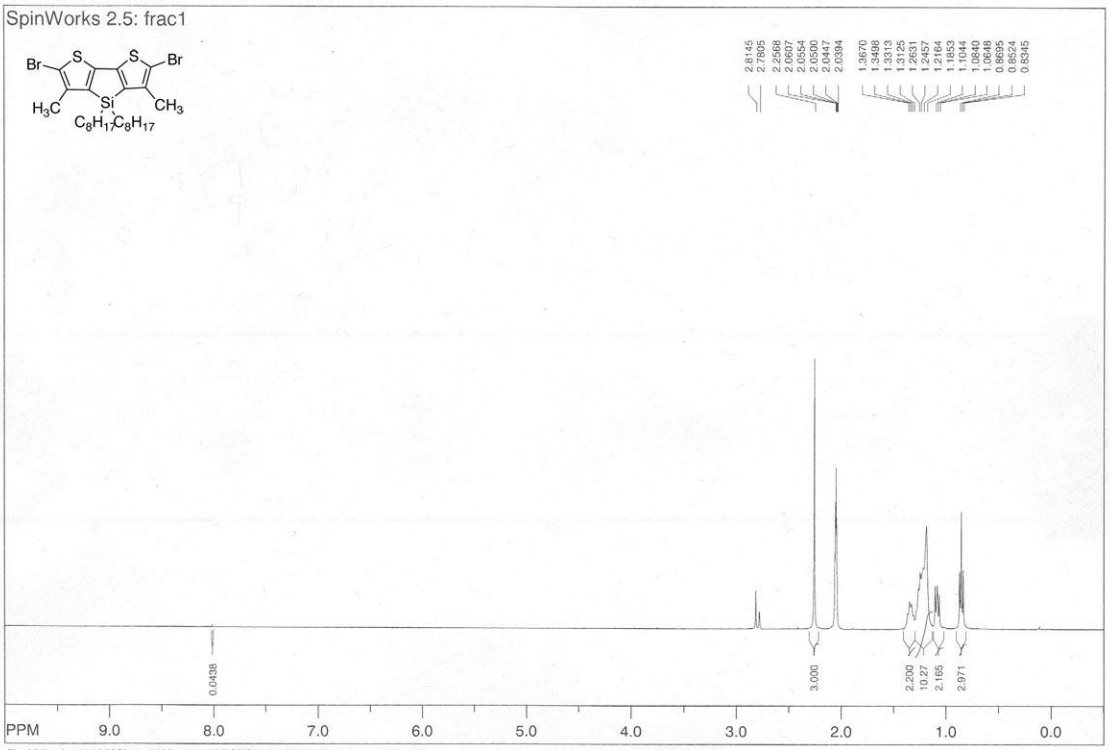

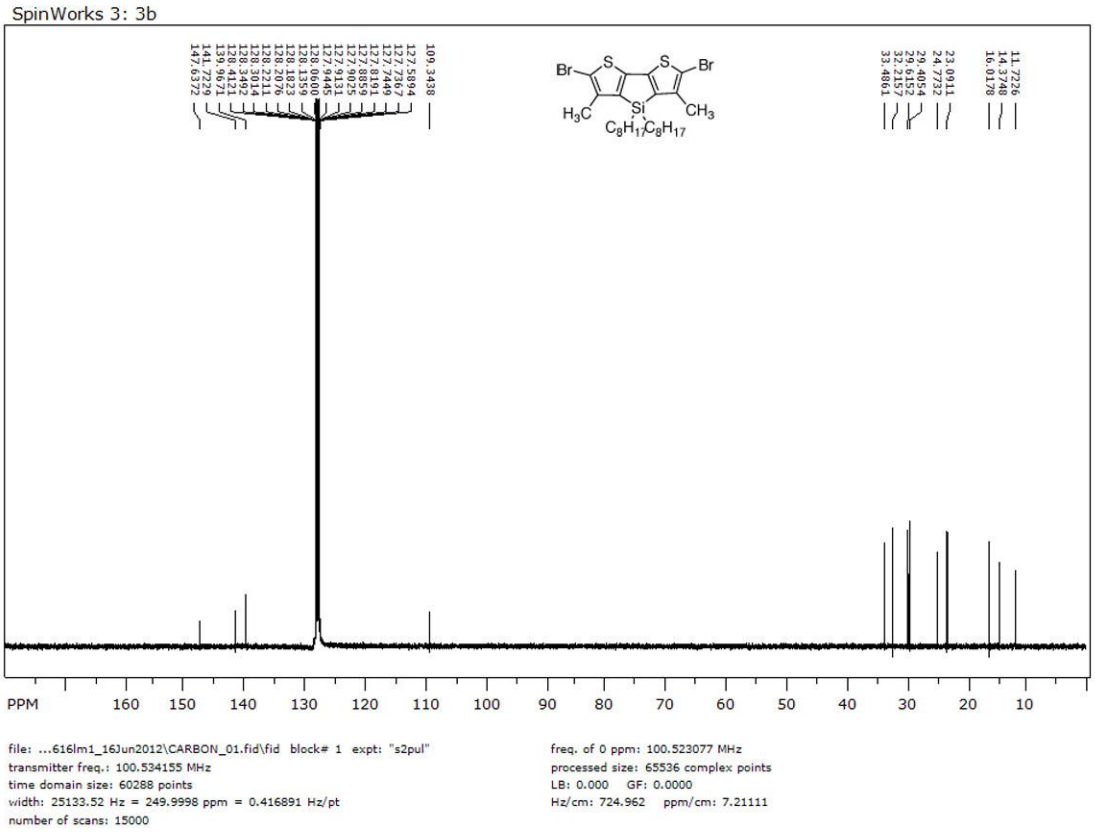

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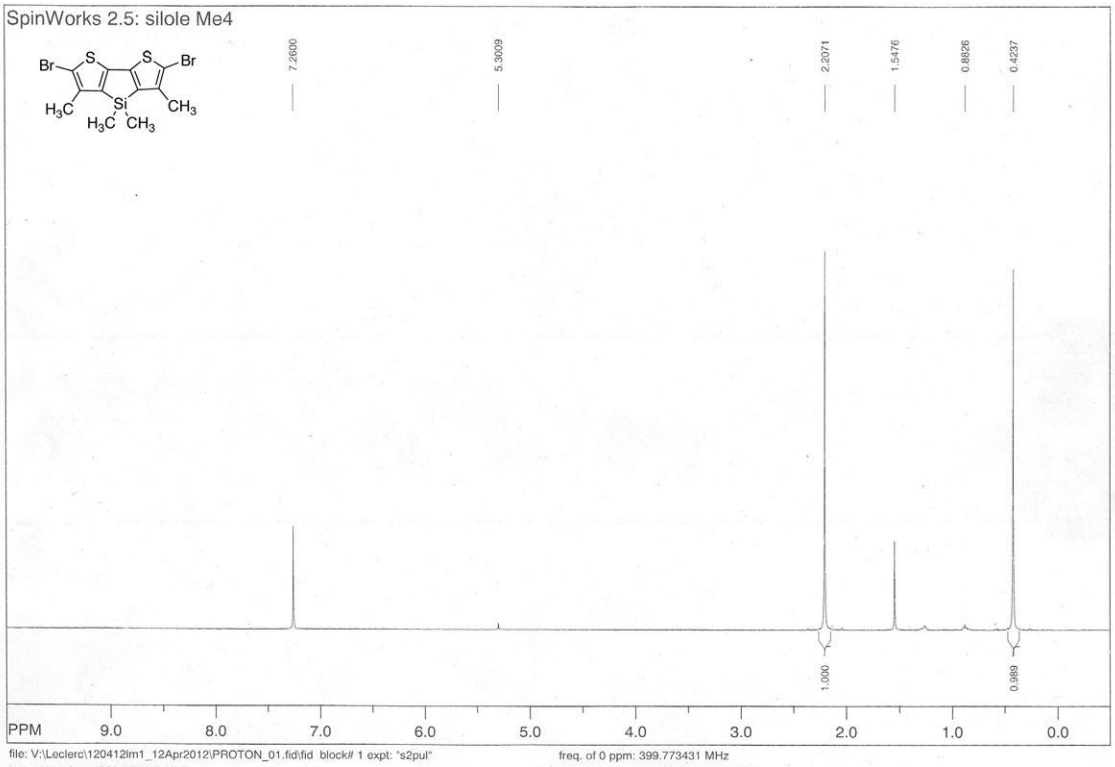

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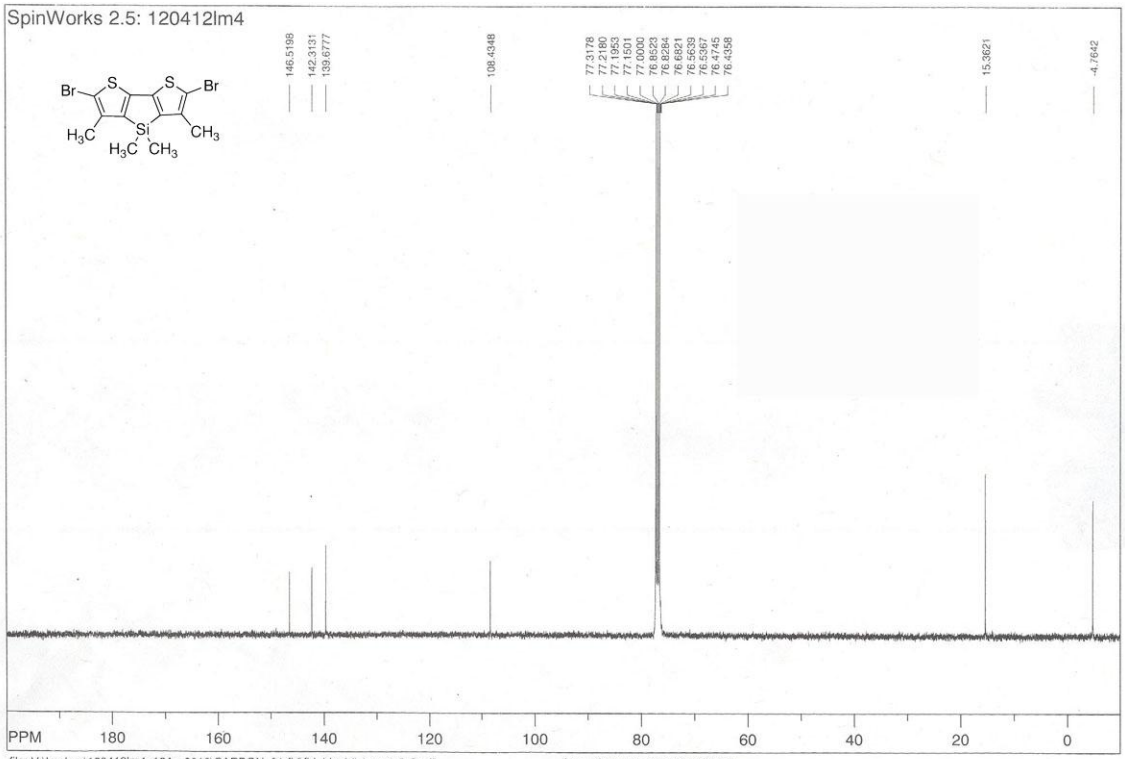

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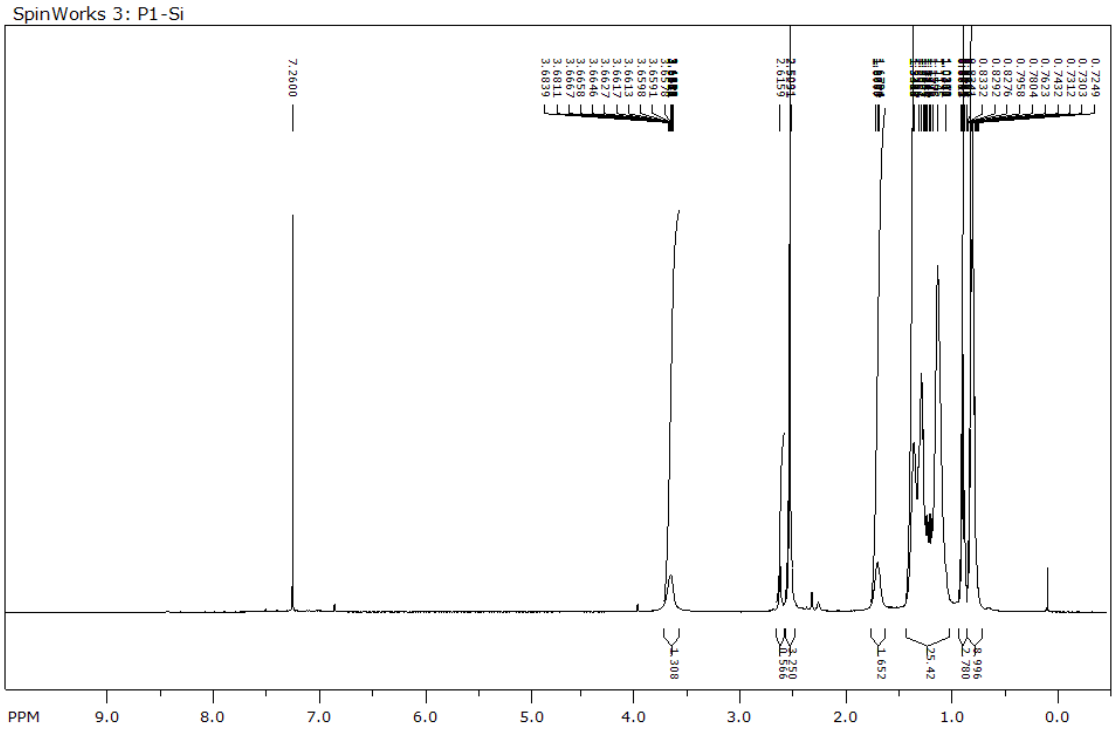

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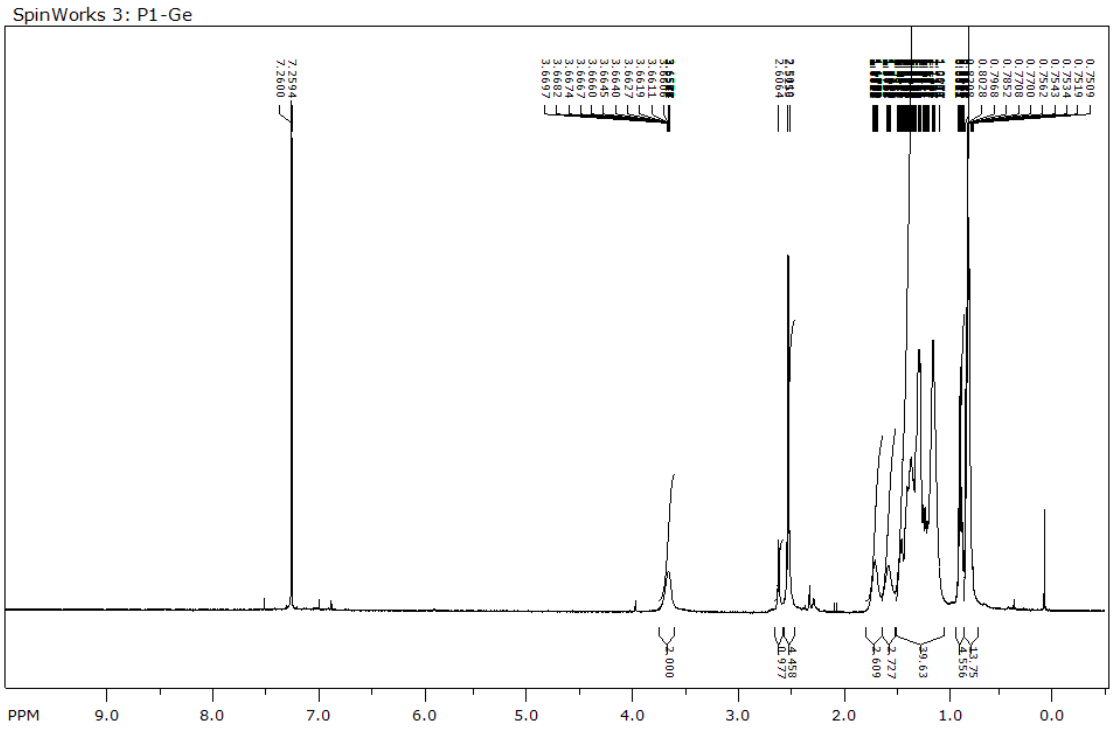

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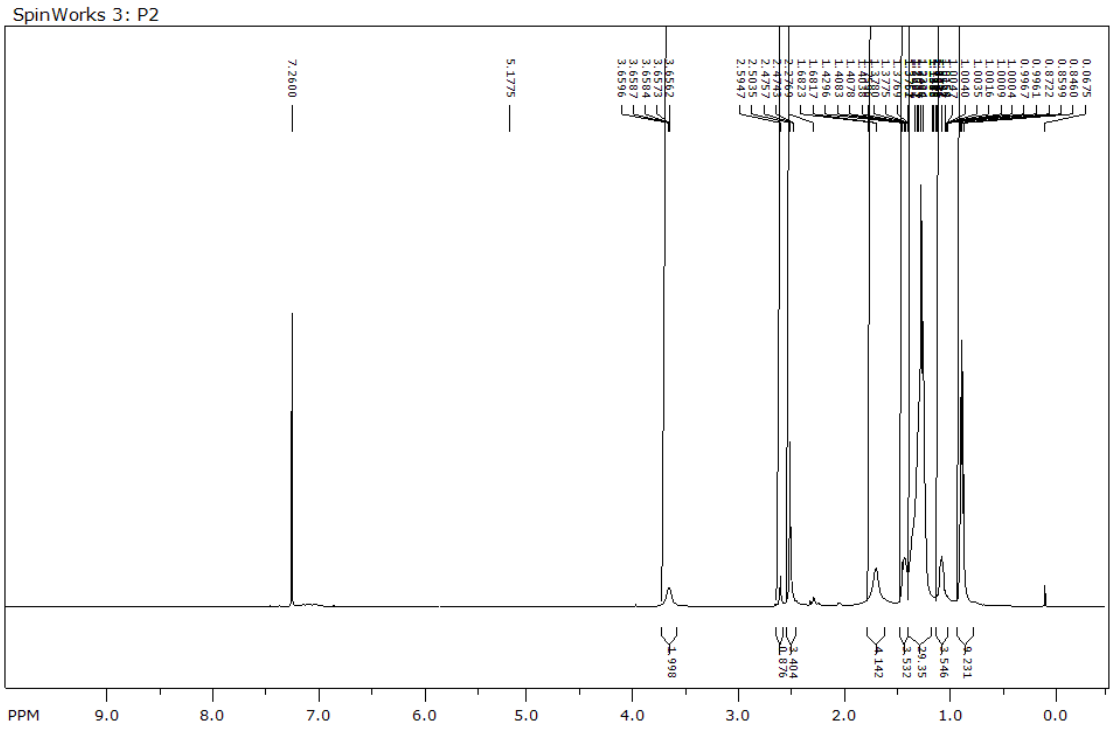

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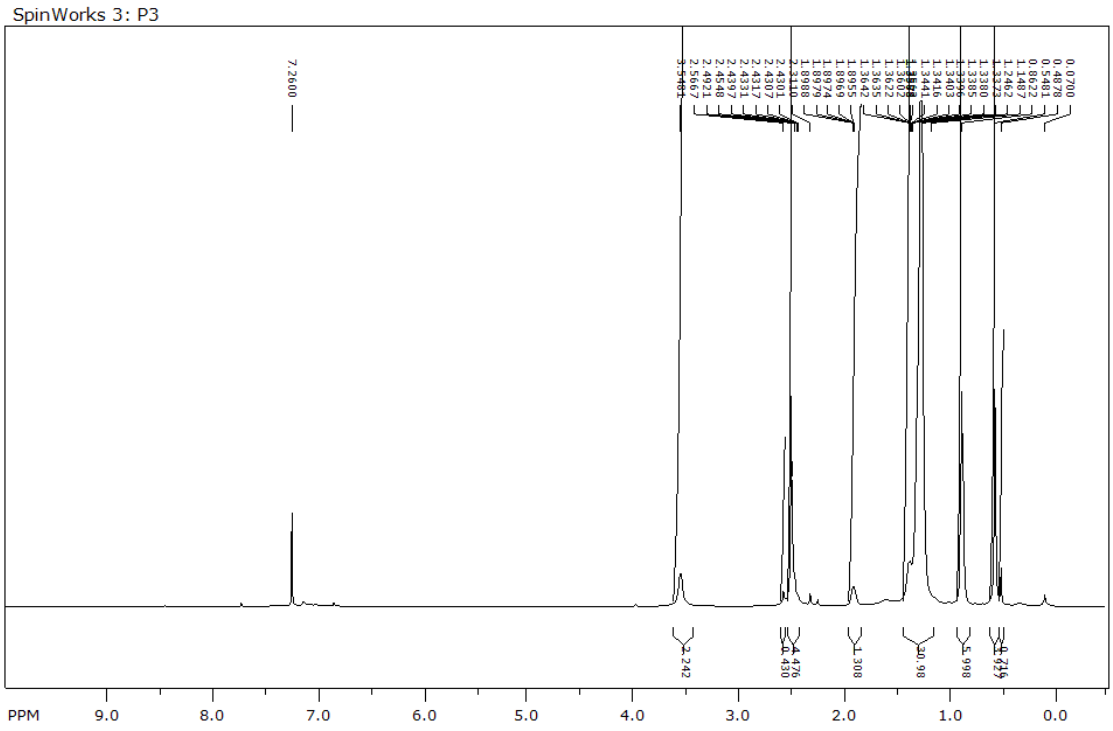

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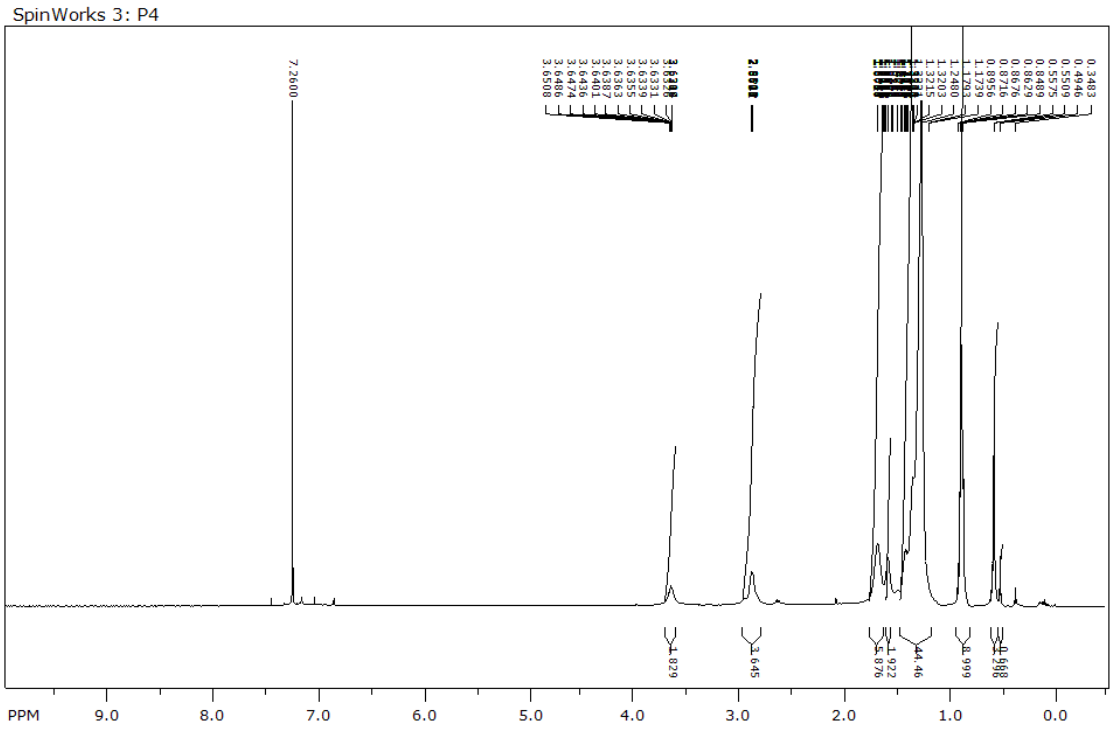

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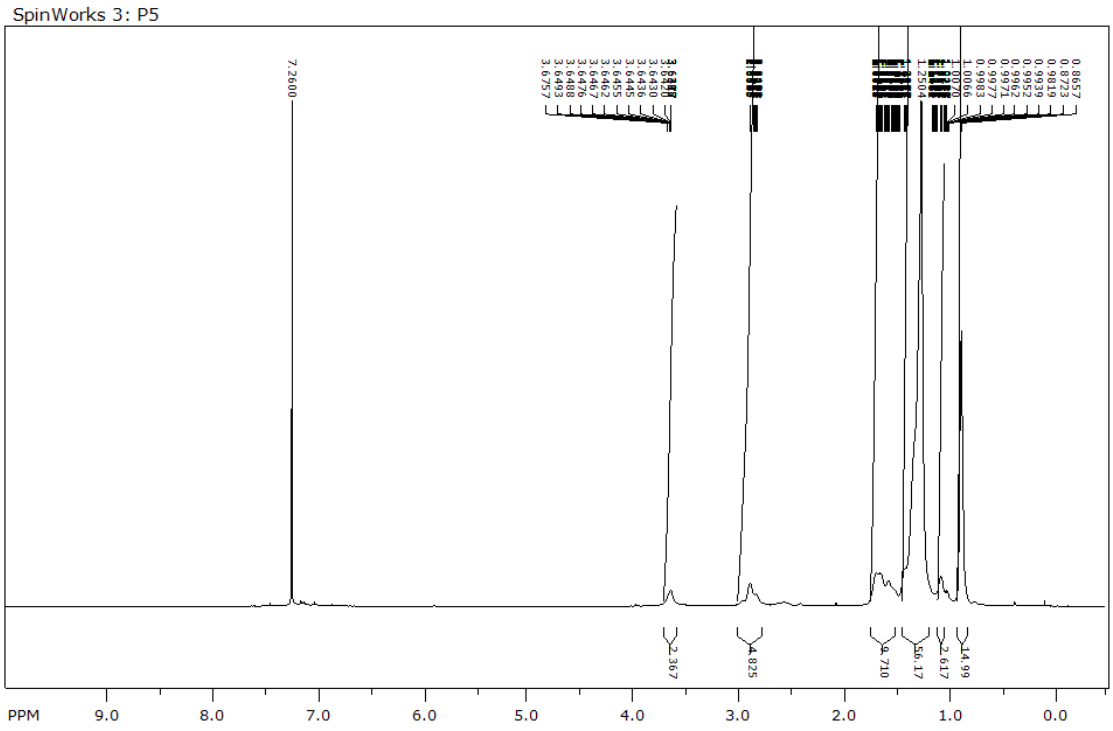

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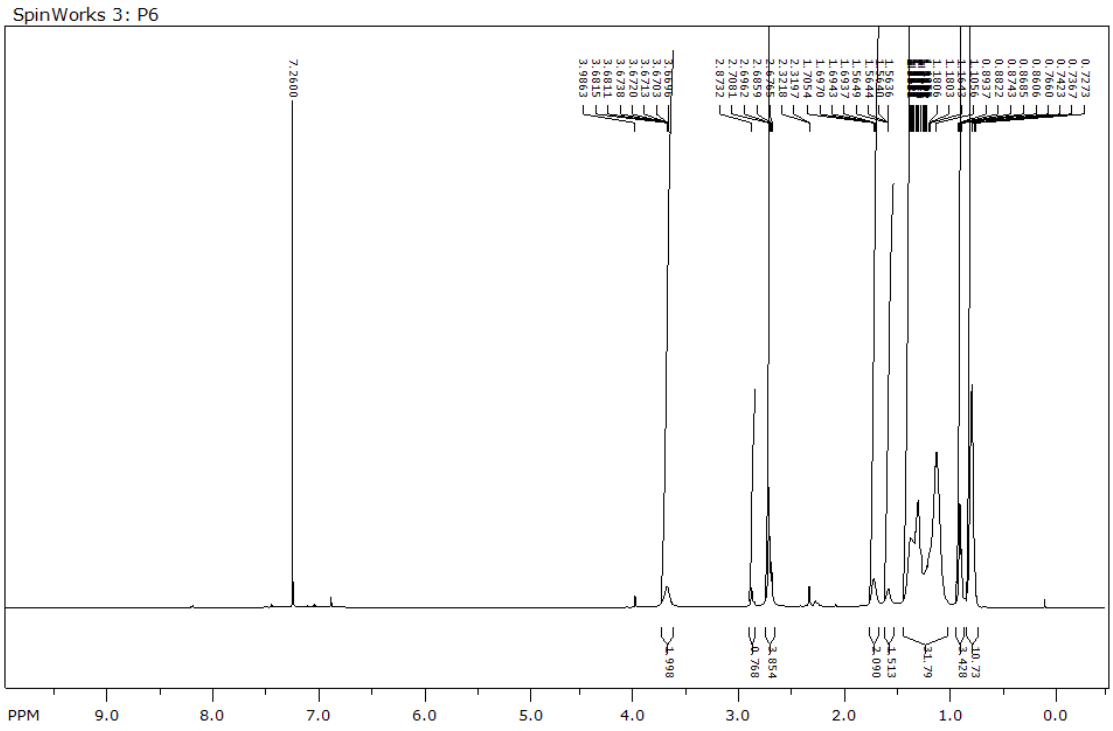
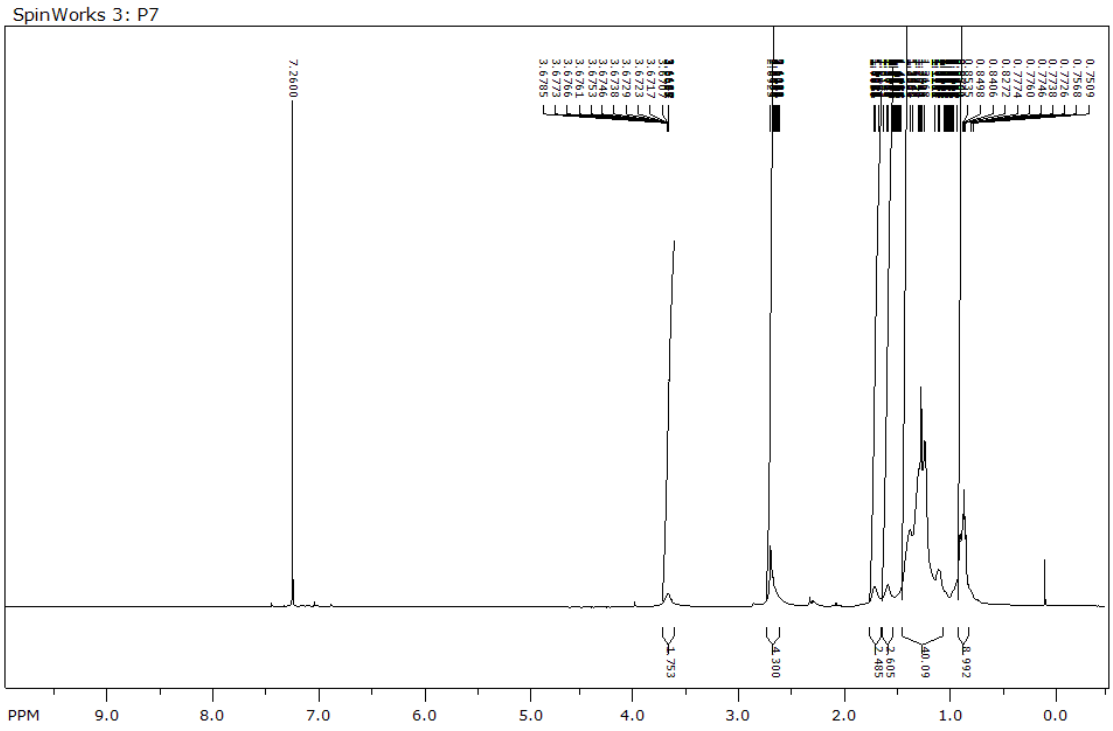
Hz/cm: 209.936 ppm/cm: 0.41994



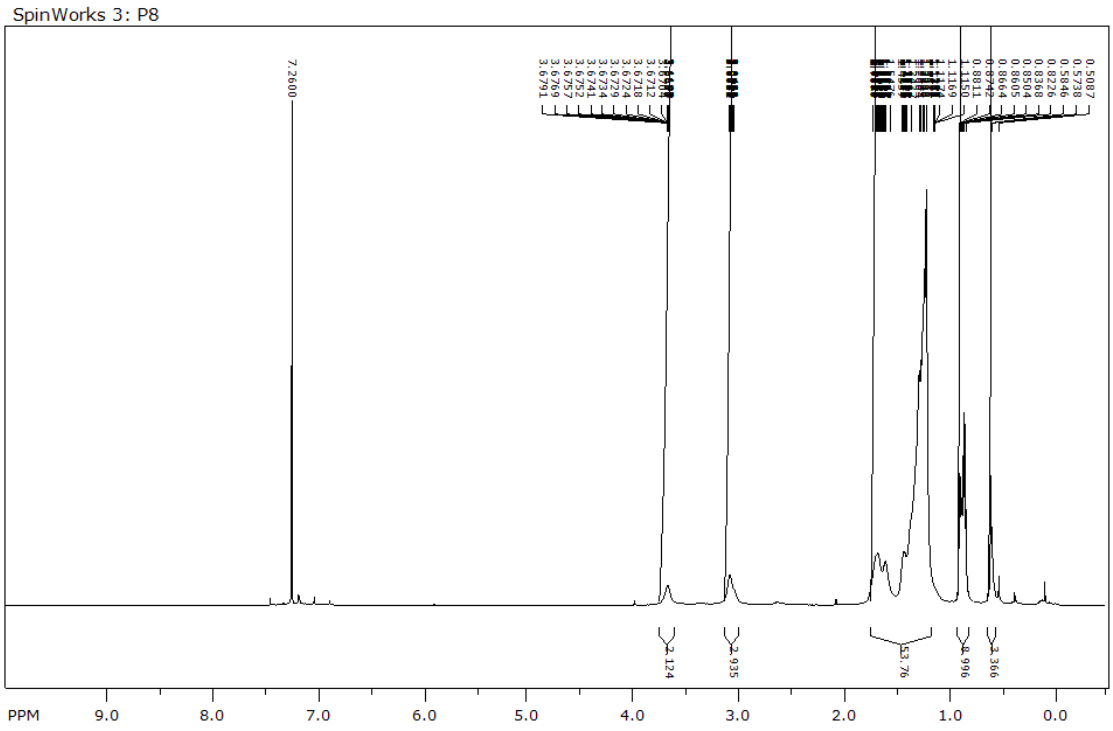
file: ..._01 LM-I-118 hex\PROTON_01.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.915722 MHz
time domain size: 65536 points
width: 8012.82 Hz = 16.0283 ppm = 0.122266 Hz/pt
number of scans: 400

freq. of 0 ppm: 499.912728 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 210.114 ppm/cm: 0.42030



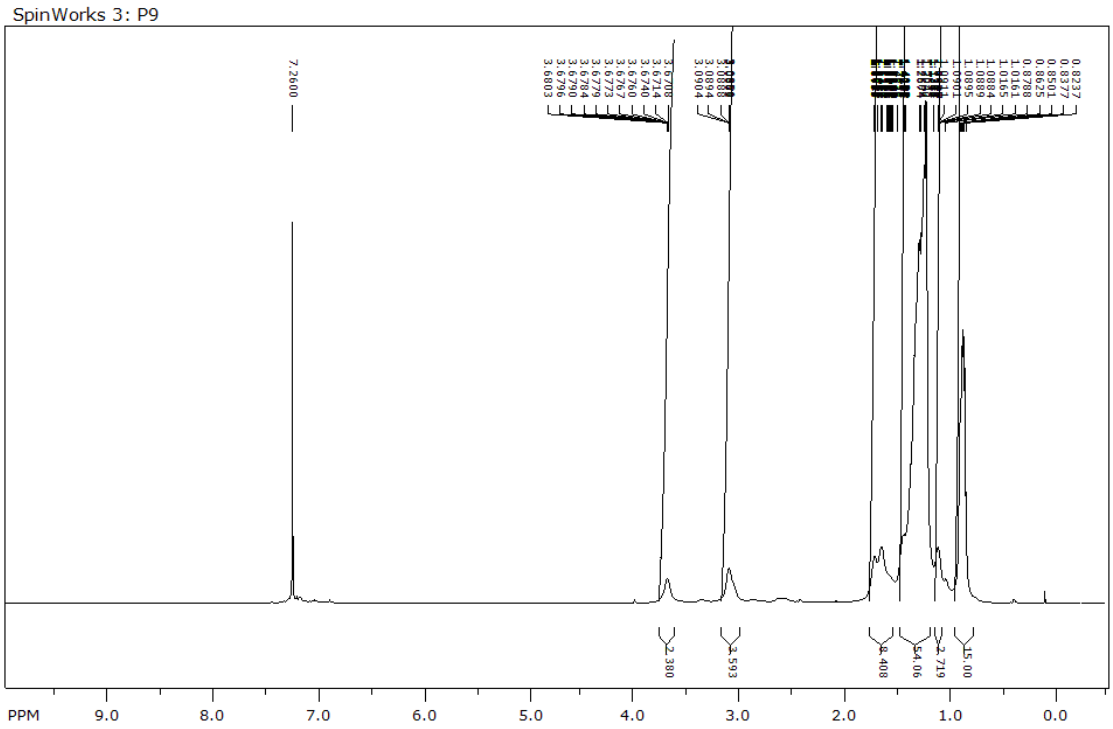
file: ...0908_01 LM-I-127\PROTON_01.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.915722 MHz
time domain size: 65536 points
width: 8012.82 Hz = 16.0283 ppm = 0.122266 Hz/pt
number of scans: 400

freq. of 0 ppm: 499.912728 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 210.114 ppm/cm: 0.42030



file: ...0906_01 LM-I-121\PROTON_01.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.915722 MHz
time domain size: 65536 points
width: 8012.82 Hz = 16.0283 ppm = 0.122266 Hz/pt
number of scans: 256

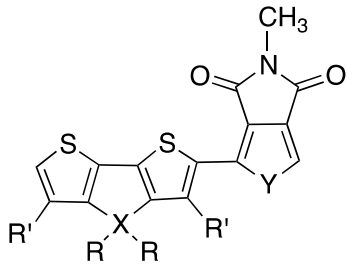
freq. of 0 ppm: 499.912728 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 209.936 ppm/cm: 0.41994



file: ...0913_01 LM-I-128\PROTON_01.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 499.915722 MHz
time domain size: 65536 points
width: 8012.82 Hz = 16.0283 ppm = 0.122266 Hz/pt
number of scans: 400

freq. of 0 ppm: 499.912728 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 210.114 ppm/cm: 0.42030

Figure S13. X,y.z coordinates of optimized structures from Gaussian 03[4] calculations carried out at the B3LYP 6-31G** level of theory.



R = *s*-Bu, R' = CH_3, X = Si, Y = S

C	2.5566981221	-0.2816191784	-0.0286647502
C	3.2012082519	0.9494148001	-0.0354166206
C	4.6266798423	0.8107848193	-0.0416827949
C	5.0144687571	-0.5078905132	-0.0429331377
S	3.670940282	-1.6157104645	-0.0345368954
C	1.106603742	-0.2661394211	-0.0179892725
C	0.4953880279	0.9844446375	0.0014870647
C	-0.9193714532	0.8927697168	0.0106262936
C	-1.380638695	-0.4342336495	0.0020051282
S	-0.0182158706	-1.5721986029	-0.0165389176
Si	1.8681210385	2.2938624895	-0.0117461212
C	-1.7873055481	2.1248590135	0.0338791791
H	-2.4486206175	2.148437047	0.9070091771
H	-1.1640140728	3.0210969182	0.0694714518
H	-2.4217859582	2.2016052662	-0.8562231765
C	5.5940295963	1.964873736	-0.0504533118
H	5.464234413	2.5992137216	0.8340094851
H	6.6305393025	1.6181631034	-0.0622457629
H	5.4437011105	2.6003653102	-0.9307209701
C	1.9803350067	3.4302072674	1.5106664
H	2.7429190873	4.1805525331	1.2524362098
C	1.7915393864	3.4396182269	-1.5293254015
H	2.7501108011	3.9756920408	-1.6006697704
H	1.0531608239	4.2139690016	-1.2712883499
H	1.0399804835	3.9972775642	1.5868075732
C	-2.7320192467	-0.9418397315	0.0018303028
C	-3.2324000649	-2.2369937362	0.0247967776
S	-4.1341495031	0.1643424585	-0.0441672698
C	-4.6544981138	-2.322215703	0.0087278821
C	-5.2962796606	-1.1272480657	-0.02805684
H	-6.3559389358	-0.9152489768	-0.0438995187
C	-2.7101181536	-3.6229067527	0.0698391463

C	-5.06215657	-3.7488935961	0.0431779604
O	-6.1707048428	-4.2476666103	0.0435465266
O	-1.5704459013	-4.0527190371	0.0964788718
N	-3.8489005716	-4.4553154936	0.0791408613
C	-3.7625280666	-5.9031039674	0.1201310386
H	-3.1740681136	-6.2228611114	0.9836827216
H	-4.7796632928	-6.288480789	0.1953934478
H	-3.2869492612	-6.2876442837	-0.7865612026
C	2.3234176071	2.8205505221	2.889593006
H	3.216015672	2.1904847302	2.7701824171
C	1.1937670219	1.9332275985	3.4317351896
H	0.2729099321	2.5152601314	3.5633308181
H	0.9683875686	1.1007418372	2.7601122352
H	1.4611268126	1.5141194306	4.4075589471
C	1.4325353802	2.8457007966	-2.9112554214
H	0.5256865743	2.2359344118	-2.7947111718
C	2.6661604957	3.9288098584	3.8979874107
H	1.8075622255	4.5932409736	4.0551100046
H	2.9419042006	3.5079718381	4.8712131332
H	3.5028525826	4.5443642489	3.5496611191
C	2.5418241324	1.9361530218	-3.4588136456
H	2.2620358925	1.5229072777	-4.4336561427
H	3.4734509768	2.5001240857	-3.5944953768
H	2.7536359007	1.0994297134	-2.7879837487
C	1.1143710372	3.9673338451	-3.9127879525
H	1.9867045172	4.6150443209	-4.0640054492
H	0.8313006717	3.5590360872	-4.8892648346
H	0.2899473955	4.5974041093	-3.561279217
H	6.0232251838	-0.8988972911	-0.0494500288

R = *s*-Bu, R’ = CH_3, X = Ge, Y = S

C	0.739759327	2.3721682906	0.014881612
C	2.1254639985	2.39928113	0.0056843661
C	2.6494030109	3.7261344539	0.0139676222
C	1.6508888775	4.6701375412	0.02549672
S	0.0548938649	3.9724601038	0.0296472268
C	0.0897678953	1.0766851124	0.0230478443
C	0.9023080803	-0.0501121301	0.0102119343
C	0.1668338648	-1.2575537544	0.0034966165

C	-1.2212203631	-1.0465105099	0.018264348
S	-1.5922194276	0.6889051092	0.0308007138
C	0.8628223348	-2.5942937955	-0.024306071
H	0.5676108105	-3.1975775801	-0.8896937389
H	1.94393888	-2.4451308502	-0.0799830841
H	0.6571128045	-3.1897746748	0.8723678224
C	4.1209458836	4.0419019789	0.0171455571
H	4.6103123091	3.6587018945	-0.885977332
H	4.3050392877	5.1179820743	0.0655449897
H	4.617484191	3.5761464172	0.8762224596
C	3.841033505	0.1094456321	-1.5706731437
H	4.8367778283	0.5007021138	-1.3222822504
C	3.7929386117	-0.0350158224	1.543220134
H	4.6657201886	0.6259209478	1.6261241747
H	4.1838722708	-1.0174267522	1.2462238157
H	3.9428771075	-0.9839235275	-1.5935923263
C	-2.2985092505	-2.0063858129	0.023346002
C	-3.6777298186	-1.8492271909	0.00186915
S	-1.9680913053	-3.7613383221	0.0713085428
C	-4.4126709295	-3.0696350295	0.0192367267
C	-3.6513588058	-4.1922759558	0.0564409996
H	-3.9547281098	-5.2294628393	0.0733730828
C	-4.6628985749	-0.7435790897	-0.0419550816
C	-5.8656560845	-2.7689854403	-0.0148254878
O	-6.8216848149	-3.5197555509	-0.0146171299
O	-4.5149133791	0.4653715184	-0.0670261517
N	-5.9287012644	-1.366507661	-0.0511702007
C	-7.1711180651	-0.618112247	-0.0909329487
H	-7.1929991034	0.0355042271	-0.9666458191
H	-7.9853268213	-1.3414035115	-0.1429369512
H	-7.278802155	-0.0016366798	0.805889913
C	3.3775397107	0.6455751946	-2.9357851818
H	3.1428047397	1.7131298413	-2.8153874998
C	2.1007422912	-0.0556699013	-3.421267319
H	2.2770653662	-1.1310835861	-3.551114518
H	1.2770164686	0.0649971617	-2.7124250936
H	1.7761070691	0.3444664479	-4.3873707328
C	3.0485445237	-0.1356057049	2.8861088576
H	2.108761034	-0.6766539876	2.7048582628
C	4.498510232	0.5199697971	-3.9783307844
H	4.7734837212	-0.5312119709	-4.1291244616
H	4.187832357	0.9239310435	-4.9481769102
H	5.4001215218	1.0571354979	-3.6639525743
C	2.6828795559	1.2476658407	3.4435422846
H	2.142439733	1.1575608973	4.3915443783
H	3.5875536444	1.8392350842	3.6333322403

H	2.0536523656	1.8128691597	2.7501873578
C	3.8710526773	-0.9353759432	3.9070653841
H	4.825202741	-0.4358463054	4.1152409882
H	3.3359429	-1.0373973247	4.8576743653
H	4.0968195546	-1.9422986814	3.5392094922
H	1.7572615407	5.7467885339	0.0337267651
Ge	2.7580554724	0.5588185219	-0.0065413669

R = *s*-Bu, R' = CH_3, X = Si, Y = O

C	-1.8645339206	1.6467595124	-0.1704210019
C	-3.0888519336	0.9912169429	-0.125765474
C	-4.1903507861	1.9024336171	-0.2144560095
C	-3.7708561122	3.2065287111	-0.3261254397
S	-2.0370885472	3.3694058586	-0.3247046248
C	-0.6740908323	0.823429875	-0.0840680311
C	-0.8692973682	-0.5494370849	0.0514160605
C	0.3535619997	-1.2668518077	0.1243317486
C	1.4653299337	-0.4218451612	0.0470326014
S	0.9945781843	1.271273213	-0.1192263247
Si	-2.7408047688	-0.8611889466	0.0603113622
C	0.4201612009	-2.7658784409	0.2731892664
H	0.9492552285	-3.057797596	1.1853620281
H	-0.5868780187	-3.1873415493	0.3131301331
H	0.9532171975	-3.2315669226	-0.5610710523
C	-5.6387588603	1.4909553459	-0.193806527
H	-5.8910917466	0.9708213143	0.7375009179
H	-6.3017510031	2.3554178323	-0.2824936849
H	-5.8675534289	0.807577113	-1.0196507556
C	-3.4755254945	-1.6000541377	1.6524002306
H	-4.5273991443	-1.8139634432	1.4092694402
C	-3.3164648078	-1.9816682323	-1.3655362746
H	-4.4106530877	-1.8949845126	-1.4469575383
H	-3.1389983852	-3.0097362211	-1.0148872833
H	-3.0164109191	-2.5867595564	1.816630832
C	2.8598544549	-0.7500770596	0.0852763292
C	4.0310856144	-0.0287841364	0.0325577927
C	5.1120502762	-0.9534276933	0.1169413898
C	4.5747551966	-2.1921927993	0.2172387983
H	4.9671587897	-3.1924535915	0.3037579549
C	4.5838295846	1.328072453	-0.0763676491
C	6.388947436	-0.2038302925	0.0633469431
O	7.5390194922	-0.5940165496	0.1031000273
O	4.0411086324	2.4142576516	-0.171276972
N	5.9874652193	1.1429866146	-0.0510722935

C	6.9235756542	2.2482418979	-0.1377067103
H	6.7903539434	2.931647188	0.7054382719
H	7.9290413033	1.8269806458	-0.1181215437
H	6.7703640068	2.8063893552	-1.0651431413
C	-3.4200445128	-0.7845384382	2.9649331427
H	-3.80372611	0.2238998127	2.7554229878
C	-1.9883315899	-0.6385773156	3.5000183145
H	-1.554328787	-1.6222327308	3.7193069488
H	-1.3321385667	-0.1376419294	2.783475614
H	-1.9762275816	-0.0582110703	4.4287158978
C	-2.6834536265	-1.8140637485	-2.7664036554
H	-1.5908704251	-1.8111700165	-2.6480346069
C	-4.3291055975	-1.4172966343	4.0306739595
H	-3.9931102144	-2.431722842	4.2784846601
H	-4.322882422	-0.830839158	4.9560974412
H	-5.3663167172	-1.4864290927	3.6846186654
C	-3.0868363798	-0.490591548	-3.4322093632
H	-2.6231867409	-0.3931515178	-4.4196105231
H	-4.1743136292	-0.4430525741	-3.5722385528
H	-2.7898640631	0.3757013769	-2.835198103
C	-3.0512714897	-3.003012886	-3.668326431
H	-4.1366947171	-3.059497687	-3.8169744994
H	-2.5857396413	-2.9110705354	-4.655863551
H	-2.7259633329	-3.9536959533	-3.2317481037
H	-4.3856584316	4.0926606569	-0.4114516298
O	3.2060311806	-2.0859871801	0.1993383058

R = *n*-Pr, R’ = CH_3, X = Si, Y = S

C	-2.0990050188	1.6424894195	-0.3261524087
C	-3.3427551988	1.0246954932	-0.2806878011
C	-4.4139346044	1.9580096595	-0.4603515614
C	-3.9536597752	3.2414454666	-0.6347562793
S	-2.2168535126	3.3568712196	-0.5867086805
C	-0.9346356399	0.7943634453	-0.155809803
C	-1.1736717251	-0.5630442154	0.0378238734
C	0.0240582733	-1.3046261597	0.1937253779
C	1.1761943699	-0.5038275455	0.1177621024
S	0.7414632725	1.1961803763	-0.1518964218
Si	-3.0513525563	-0.8231613787	0.006101497
C	0.0023391799	-2.7954490968	0.415489771
H	0.4686132655	-3.0796370809	1.3654066633
H	-1.0287537326	-3.1555824601	0.4353754611
H	0.5256816958	-3.3398009372	-0.3784950705
C	-5.87417824	1.5890238705	-0.4600502601

H	-6.1673813018	1.1287527112	0.490584574
H	-6.5085013408	2.4655560166	-0.6152569874
H	-6.1017105542	0.8674768259	-1.2532207019
C	-3.7611383518	-1.4649087487	1.6447284159
H	-4.8575838955	-1.4726708446	1.556876884
C	-3.6461131999	-1.9226620459	-1.4214881138
H	-4.7460702689	-1.9180903505	-1.4145202426
H	-3.3603421503	-2.9598925286	-1.1919305909
H	-3.4724560606	-2.5213663024	1.7485275414
C	2.5669098844	-0.8749311411	0.2248647203
C	3.7320410667	-0.1219843366	0.1612106748
C	4.9320467774	-0.8745947536	0.3153120043
C	4.7494463536	-2.2064560151	0.4995101956
H	5.4817435773	-2.9887804321	0.640229441
C	4.1236687307	1.2945027566	-0.0267266639
C	6.099455834	0.0377134682	0.2297095554
O	7.2886186372	-0.2013643649	0.3097233073
O	3.4551059521	2.2986317717	-0.1967991064
N	5.5333623343	1.3066323939	0.0261048267
C	6.3133598866	2.5216017031	-0.117621005
H	6.0636308064	3.233635571	0.6736235579
H	7.3651407621	2.2427092228	-0.0485805334
H	6.114000492	2.9919954411	-1.0841229923
C	-3.3453477417	-0.6872993005	2.9070690107
H	-3.6395483926	0.3643170792	2.80225078
C	-3.1326861299	-1.5412012047	-2.8221768527
H	-2.035761244	-1.5497945546	-2.8237540369
C	-3.9533742218	-1.2605709354	4.1916281708
H	-3.6474891095	-2.3020312637	4.3440616842
H	-3.6400614922	-0.6892799924	5.0718504392
H	-5.0486475694	-1.241292446	4.1543801485
C	-3.6508680932	-2.4713579448	-3.9243227109
H	-4.7457412865	-2.455964329	-3.9733403577
H	-3.2693944188	-2.1771920729	-4.9078256972
H	-3.343970522	-3.5081023425	-3.7442859503
H	-4.5399857491	4.1372624916	-0.7905678031
S	3.0514626062	-2.57457981	0.4872406193
H	-2.251586958	-0.6852193378	2.9907467369
H	-3.4242941722	-0.5084544007	-3.0498720489

R = *n*-Pr, R’ = CH_3, X = Si, Y = O

C	-2.0672086068	1.5529890258	-0.2959084443
C	-3.2870786544	0.8898303365	-0.2442635312
C	-4.3927561141	1.7844412717	-0.4116873692

C	-3.9810830003	3.0846079161	-0.5832953744
S	-2.2492213264	3.2630636555	-0.5473266065
C	-0.8721477378	0.7465225642	-0.1379186325
C	-1.0590753768	-0.6208303116	0.0513326156
C	0.1664690755	-1.3217057229	0.1952579009
C	1.2733420178	-0.4702029288	0.1125805337
S	0.7929241715	1.2087716389	-0.1450138933
Si	-2.9264751354	-0.9480799773	0.0318304361
C	0.2410204326	-2.8122588476	0.4114554266
H	0.7431433937	-3.059189212	1.3516641394
H	-0.7630877182	-3.2420282877	0.4372550042
H	0.8049967124	-3.3079104417	-0.3843735869
C	-5.8384129969	1.3620872215	-0.402532833
H	-6.1070833775	0.8865671215	0.5478289566
H	-6.5057346471	2.2153879825	-0.5484482149
H	-6.045101143	0.6365467054	-1.1977445151
C	-3.5978856763	-1.6223858062	1.67316275
H	-4.6932762997	-1.6805155165	1.5914708118
C	-3.4887377688	-2.0621772461	-1.3971926675
H	-4.5877126882	-2.1053851903	-1.3792988225
H	-3.1553367351	-3.0870916327	-1.1770275101
H	-3.2595909014	-2.664316013	1.7732478983
C	2.6682196436	-0.7844135855	0.2071522969
C	3.8369974108	-0.0592088701	0.1447962788
C	4.9206620584	-0.9693056461	0.3137211997
C	4.3874276861	-2.203533679	0.4715893503
H	4.7823566048	-3.1943278365	0.6275914319
C	4.3809237184	1.2934538159	-0.0296778057
C	6.1927611327	-0.2111623384	0.2503367653
O	7.3468084782	-0.5797731159	0.3442179092
O	3.8260809122	2.3638683939	-0.2027551542
N	5.7874464426	1.1205605571	0.0451025707
C	6.7298083691	2.216925592	-0.0785427069
H	6.1520663262	3.1293490821	-0.2282616747
H	7.336422787	2.3044667265	0.826966859
H	7.3968555601	2.054631539	-0.9296219111
C	-3.211003628	-0.8280059471	2.9342611683
H	-3.5553430593	0.2086856512	2.8334585451
C	-3.0064042645	-1.6499465553	-2.8002269115
H	-1.9102474318	-1.6099483342	-2.8122063464
C	-3.7828491447	-1.4315642764	4.2215569892
H	-3.4264137825	-2.4573390537	4.3703036277
H	-3.4917943733	-0.8471114713	5.100782734
H	-4.8779974078	-1.4647281845	4.1910895949
C	-3.4935322613	-2.5957346491	-3.9032289088
H	-4.5884319559	-2.6291663145	-3.9413743422

H	-3.1355960598	-2.2787883418	-4.8885017854
H	-3.1386458995	-3.6186894379	-3.7329194242
H	-4.6006058199	3.9592448813	-0.7305892294
H	-2.1180410994	-0.7745352179	3.0109322847
H	-3.3458286855	-0.6298701521	-3.0186217768
O	3.0186819957	-2.1084247756	0.4093038212

R = CH_3, R' = *n*-Pr, X = Si, Y = S

C	-2.2393283667	-1.441872408	-0.1671365376
C	-3.3910725439	-0.7416355719	0.168122301
C	-4.5580133261	-1.5722079783	0.1250930788
C	-4.2541377407	-2.8636261866	-0.2385079018
S	-2.5578933522	-3.10874181	-0.5392223757
C	-0.9871237032	-0.7090336529	-0.1376608392
C	-1.0505947481	0.6336524551	0.2230593285
C	0.2318942202	1.2482272546	0.2538383409
C	1.2613617682	0.358730997	-0.079401979
S	0.6225547358	-1.2545131395	-0.4209006465
Si	-2.8675430226	1.0261067697	0.5944854139
C	-3.6288755271	2.3372642956	-0.5320208726
H	-4.7111512311	2.4025124677	-0.3758195864
C	-3.1745713297	1.4660632724	2.4059543887
H	-4.2478614762	1.5103258475	2.6212705463
H	-2.7481037896	2.4439574273	2.6549358338
H	-3.2074880798	3.3272873844	-0.3276166388
C	2.689759901	0.5738893044	-0.188232408
C	3.7579071906	-0.2953982663	-0.0488345222
C	5.0347176516	0.2960327653	-0.2709467591
C	4.9999219097	1.6142643342	-0.5963352609
H	5.8158372934	2.2961117544	-0.7904078613
C	3.9805858947	-1.7122852694	0.3342880627
C	6.0892479311	-0.721943066	-0.0341018618
O	7.2992411748	-0.6366914839	-0.1104379811
O	3.1927920858	-2.5976353766	0.6090717889
N	5.3845523233	-1.8813879637	0.322225911
C	6.0376247633	-3.1380566925	0.6386601151
H	5.2576366521	-3.8625948117	0.8731999587
H	6.6272353482	-3.4872905098	-0.2133339964
H	6.7042276677	-3.0165967096	1.4967433144
H	-4.9362769292	-3.6968853612	-0.3444301893
H	-3.4534862518	2.1053729861	-1.5867358643
H	-2.7273424552	0.7222016537	3.0716450086
C	0.404917402	2.7006427181	0.6354990159
H	-0.2979050172	2.924899216	1.4480725623

H	1.4045882728	2.8756211203	1.0461713462
C	-5.9662322401	-1.1023882398	0.404208615
H	-6.5772097684	-1.9522371058	0.7318463529
H	-5.9558031724	-0.393263627	1.2424843795
C	-6.6462613628	-0.4390614314	-0.8099985013
H	-6.0272028758	0.3957738201	-1.1604770504
H	-6.6751851144	-1.1609228104	-1.6353843996
C	-8.0608970234	0.0572765218	-0.4996304977
H	-8.708256515	-0.7649779956	-0.1743651135
H	-8.0532999536	0.8061157414	0.3007650399
H	-8.5234952174	0.5160482962	-1.3791915068
C	0.1489420477	3.6908395873	-0.5201996597
H	0.8373160945	3.4763325445	-1.3459530341
H	-0.8585651094	3.5231918514	-0.9182671163
C	0.3033243667	5.1503620972	-0.0847725177
H	-0.3929406219	5.4004163731	0.7240145897
H	1.3170544808	5.3503976538	0.2798203172
H	0.1077612877	5.835118655	-0.9159125976
S	3.3508888438	2.160973634	-0.6508882714

R = CH_3, R’ = *n*-Pr, X = Si, Y = O

C	2.1245525263	-1.4617490075	-0.2951940311
C	3.3127598573	-0.7417201529	-0.334217709
C	4.4571630269	-1.5974183503	-0.437982362
C	4.1018951639	-2.9260811763	-0.4723709571
S	2.3828608581	-3.1779569085	-0.3792228659
C	0.8925444758	-0.7005742987	-0.2149781377
C	1.0107220834	0.6861377145	-0.1913328155
C	-0.2484971121	1.3407287836	-0.1254385757
C	-1.3120051061	0.4313436609	-0.0947019438
S	-0.7469189881	-1.2422801534	-0.1588072698
Si	2.8577142934	1.0949414383	-0.2816637078
C	3.4982089012	2.0042363809	1.2446238413
H	4.5874959274	2.1137262637	1.2099832577
C	3.344213842	2.0237534371	-1.852644234
H	4.4334969758	2.0976467328	-1.9427070218
H	2.943579341	3.0432308384	-1.8482941876
H	3.0670438171	3.0091549233	1.3093569253
C	-2.7262124722	0.6654012583	-0.0278621674
C	-3.844530066	-0.1381454999	-0.055073326
C	-4.9879620297	0.7057090416	0.0567947756
C	-4.5398388816	1.9792991276	0.1481547255
H	-5.0007773411	2.9488169531	0.2453828523
C	-4.2981734128	-1.5313527331	-0.1587568168

C	-6.2072267546	-0.1363559282	0.0246373707
O	-7.3836798112	0.1608586577	0.0889499164
O	-3.6740970238	-2.571714707	-0.2653096142
N	-5.7136945218	-1.447340175	-0.1050272834
C	-6.5802546882	-2.6090875569	-0.1746957608
H	-5.9422012544	-3.4865336365	-0.2828255957
H	-7.1803458214	-2.695344687	0.7353367382
H	-7.2557988792	-2.5313474787	-1.0308481519
H	4.7586642346	-3.7824030224	-0.5511475953
H	3.2409376898	1.4669658468	2.1622508902
H	2.9653727649	1.5150680504	-2.7438388405
C	-0.3767861032	2.8458040506	-0.0683745406
H	0.5076459981	3.2843654981	-0.5464572288
H	-1.2428960308	3.1771060562	-0.6473537991
C	5.8914538367	-1.1250972308	-0.4710539045
H	6.5149701301	-1.8852608631	-0.9571113214
H	5.9654354546	-0.2249565361	-1.0956476273
C	6.4731955286	-0.820834472	0.9238159155
H	5.8428697097	-0.0760466742	1.424906047
H	6.4134801688	-1.7286760588	1.5365727976
C	7.9199711902	-0.3232411163	0.8670136945
H	8.5768286069	-1.0642278718	0.397522736
H	8.0005883091	0.6026080083	0.2858505636
H	8.3106893571	-0.1211709887	1.8693074566
C	-0.4931103488	3.3991221022	1.3672416167
H	-1.3760453091	2.9616088238	1.8454449119
H	0.3732995163	3.0662540003	1.9521102284
C	-0.5879594268	4.9266963449	1.3996230857
H	0.2938325954	5.391675522	0.9436501684
H	-1.4676865429	5.2803862971	0.8503746472
H	-0.665246854	5.2979714	2.4264412773
O	-3.166871305	1.9715973504	0.1007770072

R = CH_3, R’ = H, X = Si, Y = S

C	-3.087635532	-1.0537230901	0.0024387342
C	-4.2327501019	-0.2684704575	0.0939456015
C	-5.4135658054	-1.0643773565	0.0646195874
C	-5.1592649445	-2.407948886	-0.0457662127
S	-3.45346627	-2.7490657529	-0.1182474014
C	-1.8131241441	-0.3608898872	0.0212913686
C	-1.8630719514	1.029909186	0.1297795729
C	-0.5672468384	1.5846441329	0.1374041849
C	0.4593566744	0.6516422439	0.0377093397
S	-0.2012079936	-0.985096906	-0.0704848335

Si	-3.6839614015	1.5364684574	0.2181077901
C	-4.2373737569	2.5911639002	-1.2448613744
H	-5.3233711062	2.7343040813	-1.2364241898
C	-4.1535814035	2.352586075	1.8528412847
H	-5.2378691951	2.4907935759	1.9247389022
H	-3.6861960665	3.3387089715	1.9481599935
H	-3.7716614311	3.582168343	-1.2131622019
C	1.8738083387	0.9213004371	0.0202184942
C	2.9837949231	0.1049049139	-0.0726964865
C	4.2298357497	0.7967254117	-0.0531133508
C	4.1231395379	2.1460507597	0.0537111795
H	4.8990157119	2.8975885153	0.0906053917
C	3.2677219302	-1.3404831887	-0.1917448178
C	5.3295244786	-0.1962851729	-0.1593791642
O	6.5345176123	-0.0419347602	-0.1801055036
O	2.5117540932	-2.2945876127	-0.2448111639
N	4.6762389815	-1.4379212971	-0.2373720443
C	5.3861211805	-2.6983443083	-0.3536770792
H	4.6401098289	-3.4921279879	-0.395796233
H	5.9956696261	-2.7108523229	-1.2612222651
H	6.0418433808	-2.8482658309	0.5082533086
H	-5.8675801556	-3.2237545289	-0.0894252885
H	-3.9658465056	2.1199736333	-2.1939309234
H	-3.833406145	1.7428592735	2.7026651147
S	2.4430928669	2.6032290963	0.134374623
H	-0.3662169161	2.6485553689	0.2139336515
H	-6.4217055803	-0.6683727095	0.1224299483

R = CH_3, R’ = H, X = Ge, Y = S

C	-2.7667132726	-1.196958616	-0.0172556143
C	-3.9338626246	-0.4502889617	0.077879693
C	-5.0916516776	-1.2736032788	0.0443382117
C	-4.8009934801	-2.6092061125	-0.073380621
S	-3.0872968212	-2.9028770197	-0.1474195373
C	-1.5030453354	-0.4866615468	0.0039628475
C	-1.5471244194	0.9010518405	0.1187534117
C	-0.2558139281	1.4579000177	0.1266291504
C	0.7712257209	0.5264521393	0.020478714
S	0.1116060277	-1.1091159493	-0.0940663733
C	-4.0107321269	2.5160216715	-1.2809649234
H	-5.0970978849	2.6347132618	-1.2479659422
C	-3.9178337829	2.255666318	1.902429371
H	-5.0037112603	2.3730044312	1.9521170256
H	-3.4580017207	3.2448408826	1.9765318728

H	-3.5512930746	3.506275054	-1.2199996904
C	2.1846750806	0.7987133879	0.0015463951
C	3.2964073393	-0.0145128596	-0.0972864895
C	4.5407656774	0.6802846397	-0.0767484446
C	4.4311151071	2.0287883592	0.0366417994
H	5.2053418084	2.7818964127	0.0756344151
C	3.5835816125	-1.4586299712	-0.2236961397
C	5.6426874179	-0.3094445989	-0.1897135537
O	6.84727281	-0.151835947	-0.2119802262
O	2.8300252068	-2.4144002411	-0.2799933383
N	4.9923887262	-1.5522495412	-0.2723520531
C	5.705221403	-2.8103120198	-0.3958191333
H	4.9610222654	-3.6053411283	-0.4458700756
H	6.3174024592	-2.8145860831	-1.3016393549
H	6.3588622064	-2.9654830938	0.4668118426
H	-5.4869009651	-3.4436695049	-0.1216087978
H	-3.7319417767	2.051865942	-2.2286223363
H	-3.5868307463	1.6451405821	2.7444000412
S	2.7501385174	2.4815715711	0.1226076775
H	-6.1088431562	-0.9025612879	0.1043746484
H	-0.0595148403	2.5220440752	0.2079561375
Ge	-3.4213191994	1.4225836458	0.2161067745

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