Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

for

Synthesis and photophysical properties of platinum-acetylide copolymers with thiophene, selenophene and tellurophene

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Experimental

General Considerations

The MSDS should be consulted before beginning work with organotellurium compounds. They should be handled with proper personal protective equipment even though the toxicity, biological solubility and accumulation of these compounds are low. All the reagents were used as received unless otherwise stated. 3-dodecylthiophene, iodine, tellurium, sodium borohydride, sodium methoxide (25 wt. % in methanol), diisopropylamine, *trans*-bis(triethylphosphine)platinum(II) dichloride, *N*,*O*-dimethylhydroxylamine hydrochloride, chloroacetyl chloride, *para*-toluenesulfonic acid monohydrate, dodecylmagnesium bromide (1.0 M in THF), ethynylmagnesium bromide (0.5 M in THF), *N*-iodosuccinimide, and *N*-bromosuccinimide were purchased from Sigma-Aldrich. Trimethylsilylacetylene, and copper iodide were purchased from Alfa Aesar. Potassium hydroxide, sodium chloride, sodium thiosulfate, sodium bicarbonate, ammonium chloride, and magnesium sulfate were purchased from Fisher Scientific. Silica gel was purchased from Silicycle. Deuterated chloroform was purchased from Cambridge Isotope Labs. Unless otherwise noted, all manipulations involving air or water-sensitive reagents were performed under an inert atmosphere of dry argon using conventional Schlenk techniques or in an Innovative Technologies glovebox. All the solvents used were purged with argon for 30 minutes and dried using an Innovative Technologies solvent purification system.

Instrumentation and Methods

NMR spectra were recorded on a Varian Mercury 400 spectrometer (400 MHz), Agilent DD2 500 spectrometer (550 MHz) or Agilent DD2 600 spectrometer (600 MHz) as noted. Chemical shifts are reported in ppm at ambient temperature. ^{1}H and ^{13}C chemical shifts are referenced to the residual protonated chloroform peak at 7.26 ppm and 77.16 ppm, respectively. ^{77}Se chemicals shifts are referenced to external standard diphenyl diselenide at 463.0 ppm. ^{125}Te chemical shifts are referenced to external standard diphenyl ditelluride at 422.0 ppm. Absorption spectra were recorded using a Varian Cary 5000 UV-Vis-NIR spectrophotometer. Emission spectra were recorded in chloroform using a Photon Technology International QuantaMaster 40-F NA spectrofluorometer with a photomultiplier detector and a xenon arc lamp source. Mass spectrometry was performed using with a Waters GCT Premier ToF mass spectrometer. Thermogravimetric analysis (TGA) was performed using SDT Q600 V8.3 Build 101 thermal analyzer with heating rate of 5 °C per minute and cooling rate of 30 °C per minute under nitrogen atmosphere. Polymer molecular weights were determined using a Waters 2695 GPC (THF, room temperature) with narrow molecular weight distribution polystyrene standards. Cyclic voltammetry was performed in the glovebox using a BASi Epsilon potentiostat. A three-electrode cell setup was used, with a gold button working electrode, a Ag/$AgNO_3$ reference electrode, and a platinum wire counter electrode. Cyclic voltammetry was performed on ~4 mg/mL solutions of the polymers in DCM with tetrabutylammonium hexafluorophosphate (0.1 M) as the electrolyte. A 100 mV/s scan rate was used. Ferrocene was added as an internal standard and the oxidation half-wave potentials were determined against ferrocene. The oxidation half-wave potentials were then referenced against NHE by the relationship Fc/Fc^+ is 0.64 V vs. NHE.[1]

Theoretical Calculations

Density Functional Theory (DFT) and time-dependent (TD-DFT) calculations were performed on three model compounds in the gas phase to provide insight into the interaction between chalcogenophenes and platinum in the polymers at a minimal computational cost. The model compounds consisted of five chalcogenophene and four *trans*-bis(trimethylphosphine)platinum subunits that are connected in a manner analogous to the polymer. Free alkyne is used as the end group and methyl groups are used in place of dodecyl side chain on the chalcogenophenes and in place of the ethyl groups on the phosphines. Geometry optimizations were performed using the Gaussian 09 program employing the Becke-three-parameter-Lee-Yang-Parr (B3LYP) hybrid functional[2] and 6-31G(d) basis set for C, H, P, S, Se atoms,[3] and SDD for Te and Pt atoms.[4] Starting geometries were created using Gaussview 5.0. Geometries were optimized to a minimum, and time-dependent DFT calculations (TD-DFT) were carried out on the optimized geometries to determine the first 60 singlet transitions.

Synthesis

2,5-diiodo-3-dodecylthiophene,[5] 2,5-bis(trimethylsilylethynyl)-3-dodecylthiophene,[6] 3-dodecylselenophene,[7] 3-dodecyltellurophene[8] and 2,5-diiodo-3-dodecyltellurophene[8] were prepared according to published procedures. The known compounds were characterized by ^1H NMR and were in agreement with literature.

2,5-Dibromo-3-dodecylselenophene

A solution of 3-dodecylselenophene (3.60 g, 12.0 mmol) in chloroform/acetic acid (240 mL/80 mL) was treated with *N*-bromosuccinimide (4.71 g, 26.5 mmol), and the mixture was refluxed for 24 hours under an inert atmosphere in the absence of light. The reaction was quenched with water (100 mL), and the organic layer was washed with sodium thiosulfate (2 x 200 mL), NaOH (2 x 200 mL), and brine (2 x 200 mL), dried over anhydrous $MgSO_4$, and concentrated. Column chromatography (silica gel, hexane) afforded 3.82 g (70%) of the title compound, a yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.98 (s, 1H), 2.48 (t, 2H, J = 7.6 Hz), 1.55-1.48 (m, 2H), 1.30-1.26 (m, 18H), 0.88 (t, 3H, J = 6.7 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.0, 134.3, 113.7, 111.2, 32.1, 30.8, 29.8, 29.8, 29.7, 29.7, 29.5, 29.5, 29.3, 22.9, 14.3. HRMS-DART: M + [H^+] calc. 456.9645, found 456.9639, Δ = -1.30 ppm.

2,5-Bis(trimethylsilylethynyl)-3-dodecylselenophene

A solution of 2,5-diiodo-3-dodecylselenophene (2.05 g, 44.8 mmol), trimethylsilylacetylene (1.30 mL, 9.42 mmol) in THF (20 mL) and NEt_3 (20 mL) was prepared and degassed by three freeze-pump-thaw cycles. The reaction mixture was treated with $PdCl_2(PPh_3)_2$ (0.157 g, 0.224 mmol), CuI (0.085 g, 0.484 mmol), and allowed to reflux for 24 hours under an argon atmosphere. The reaction was diluted with THF and filtered through Celite. The organic layer was washed with water (2 x 200 mL), and brine (2 x 200 mL), dried over anhydrous $MgSO_4$, and concentrated. Column chromatography (silica gel, hexane) afforded 1.40 g (63%) of the title compound, a pale yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.18 (s, 1H), 2.58 (t, 2H, J = 7.6 Hz), 1.59-1.54 (m, 2H), 1.29-1.26 (m, 18H), 0.88 (t, 3H, J = 6.9 Hz), 0.24 (s, 9H), 0.23 (s, 9H). ^{13}C

NMR ($CDCl_3$, 100 MHz): δ 150.6, 136.8, 127.0, 123.8, 103.6, 101.3, 99.7, 99.1, 32.1, 30.9, 30.1, 29.8, 29.8, 29.8, 29.7, 29.5, 29.5, 29.3, 22.9, 14.3, 0.1, 0.0. HRMS-DART: M + [H^+] calc. 493.2225, found 493.2234, Δ = 2.19 ppm.

2,5-Bis(trimethylsilylethynyl)-3-dodecyltellurophene

A solution of 2,5-diiodo-3-dodecyltellurophene (2.20 g, 3.67 mmol), trimethylsilylacetylene (1.10 mL, 7.70 mmol) in THF (30 mL) and NEt_3 (30 mL) was prepared and degassed by three freeze-pump-thaw cycles. The reaction mixture was treated with $PdCl_2(PPh_3)_2$ (0.129 g, 0.183 mmol), CuI (0.070 g, 0.367 mmol), and allowed to reflux for 24 hours under an argon atmosphere. The reaction was diluted with THF and filtered through Celite. The organic layer was washed with water (2 x 200 mL), and brine (2 x 200 mL), dried over anhydrous $MgSO_4$, and concentrated. Column chromatography (silica gel, 5% dichloromethane in hexane) afforded 0.798 g (40%) of the title compound, a pale yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.67 (s, 1H), 2.62 (t, 2H, *J* = 7.6 Hz), 1.59-1.54 (m, 2H), 1.29-1.26 (m, 18H), 0.88 (t, 3H, *J* = 6.9 Hz), 0.23 (s, 9H), 0.22 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.7, 145.1, 122.5, 118.9, 105.0, 104.3, 103.6, 102.8, 33.1, 32.1, 31.7, 30.2, 29.8, 29.8, 29.8, 29.5, 29.5, 29.4, 22.8, 14.3, 0.1, 0.0. HRMS-DART: M + [H^+] calc. 543.2122, found 543.2123, Δ = 0.19 ppm.

Poly[(3/4-dodecyl-5-ethynylthiophen-2-yl)ethynyl-(bis(triethylphosphine)platinum)], P-S

A solution of 2,5-bis(trimethylsilylethynyl)-3-dodecylthiophene (0.500 g, 1.12 mmol) in dichloromethane (20 mL), diisopropylamine (10 mL), methanol (10 mL) was prepared and degassed by three freeze-pump-thaw cycles. The reaction mixture was treated with sodium methoxide (0.716 g, 3.31 mmol, 25 wt. % in methanol), copper iodide (0.011 g) and *trans*-bis(triethylphosphine)platinum(II) dichloride (0.565 g, 1.12 mmol), and allowed to stir at room temperature in the absence of light under an inert atmosphere for 48 hours. The volatile compounds were removed under reduced pressure to afford an orange-yellow solid. The solid was dissolved in methanol (50 mL) and filtered through a soxhlet thimble. The solid was extracted successively with methanol, hexane, and chloroform until each solvent in the extraction chamber was colorless. The solvent was removed from the chloroform extract to yield the title polymer as a brown solid (0.554 g, 0.757 mmol, 68%). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 6.53 (s, 1H), 2.53 (br s, 2H), 2.15-2.10 (m, 12H), 1.55 (br s, 2H), 1.29-1.25 (m, 18H), 1.21-1.15 (m, 18H), 0.88 (t, 3H, J = 7.0 Hz). ^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz): δ 11.5, 11.4, 11.2. $^{1}J_{Pt\text{-}P}$ = 2378 Hz, 2371 Hz, 2366 Hz. GPC: M_n = 25 820 g mol^{-1}, M_w = 48 283 g mol^{-1}, $Đ$ = 1.87.

Poly[(3/4-dodecyl-5-ethynylselenophen-2-yl)ethynyl-(bis(triethylphosphine)platinum)], P-Se

A solution of 2,5-bis(trimethylsilylethynyl)-3-dodecylselenophene (0.405 g, 0.823 mmol) in dichloromethane (16 mL), diisopropylamine (8 mL), methanol (8 mL) was prepared and degassed by three freeze-pump-thaw cycles. The reaction mixture was treated with sodium methoxide (0.524 g, 2.42 mmol, 25 wt. % in methanol), copper iodide (0.010 g), *trans*-bis(triethylphosphine)platinum(II) dichloride (0.413 g, 0.822 mmol), and allowed to stir at room temperature in the absence of light under an inert atmosphere for 48 hours. The volatile compounds were removed under reduced pressure to afford an orange solid. The solid was dissolved in methanol (50 mL) and filtered through a soxhlet thimble. The solid was extracted successively with methanol, hexane, and chloroform until each solvent in the extraction chamber was colorless. The solvent was removed from the chloroform extract to yield the title polymer as a brown solid (0.345 g, 0.423 mmol, 54%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 6.71 (s, 1H), 2.51 (br s, 2H), 2.12-2.09 (m, 12H), 1.54 (br s, 2H), 1.28-1.25 (m, 18H), 1.21-1.14 (m, 18H), 0.88 (t, 3H, J = 6.9 Hz). ^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz): δ 11.7, 11.5, 11.3. $^{1}J_{Pt\text{-}P}$ = 2375 Hz, 2368 Hz, 2360 Hz. ^{77}Se NMR ($CDCl_3$, 95 MHz): δ 711.3 (br s). GPC: M_n = 30 983 g mol^{-1}, M_w = 64 444 g mol^{-1}, $Đ$ = 2.08.

Poly[(3/4-dodecyl-5-ethynyltellurophen-2-yl)ethynyl-(bis(triethylphosphine)platinum)], P-Te

A solution of 2,5-bis(trimethylsilylethynyl)-3-dodecylthiophene (0.384 g, 0.711 mmol) in dichloromethane (16 mL), diisopropylamine (8 mL) and methanol (8 mL) was prepared and degassed by three freeze-pump-thaw cycles. The reaction mixture was treated with sodium methoxide (0.452 g, 2.10 mmol, 25 wt. % in methanol), copper iodide (0.008 g), *trans*-bis(triethylphosphine)platinum(II) dichloride (0.357 g, 0.711 mmol), and allowed to stir at room temperature in the absence of light under an inert atmosphere for 48 hours. The volatile compounds were removed under reduced pressure to afford a brown solid. The solid was dissolved in methanol (50 mL) and filtered through a soxhlet thimble. The solid was extracted successively with methanol, hexane, and chloroform until each solvent in the extraction chamber was colorless. The solvent was removed from the chloroform extract to yield the title polymer as a brown solid (0.437 g, 0.528 mmol, 47%). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.11 (s, 1H), 2.53 (br s, 2H), 2.08-2.07 (m, 12H), 1.54 (br s, 2H), 1.31-1.25 (m, 18H), 1.18-1.16 (m, 18H), 0.88 (t, 3H, J = 7.0 Hz). ^{31}P{^{1}H}

NMR ($CDCl_3$, 242 MHz): δ 12.4, 11.9, 11.5. $^{1}J_{Pt-P}$ = 2371 Hz, 2367 Hz, 2361 Hz. ^{125}Te NMR ($CDCl_3$, 158 MHz): δ 1005.0 (br s). GPC: M_n = 13 924 g mol^{-1}, M_w = 51 379 g mol^{-1}, $Đ$ = 3.69.

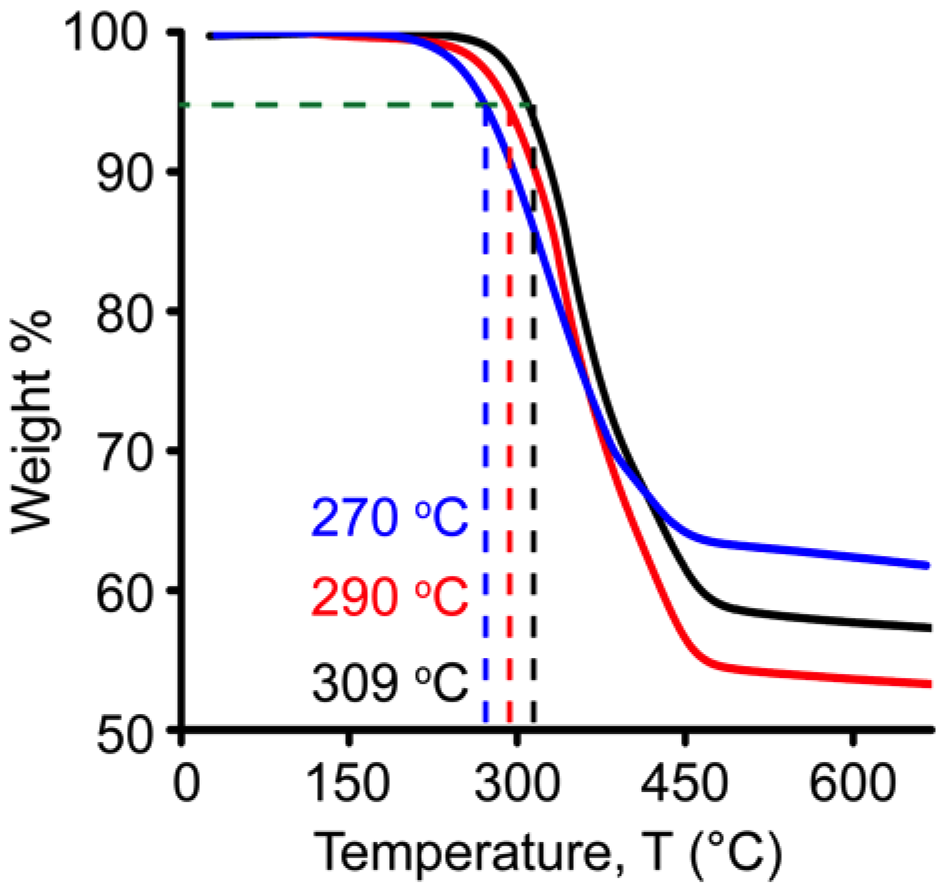

Figure S1. Thermogravimetric analysis traces of **P-S** (black), **P-Se** (red) and **P-Te** (blue). The dotted lines show 5% weight loss in the polymers.

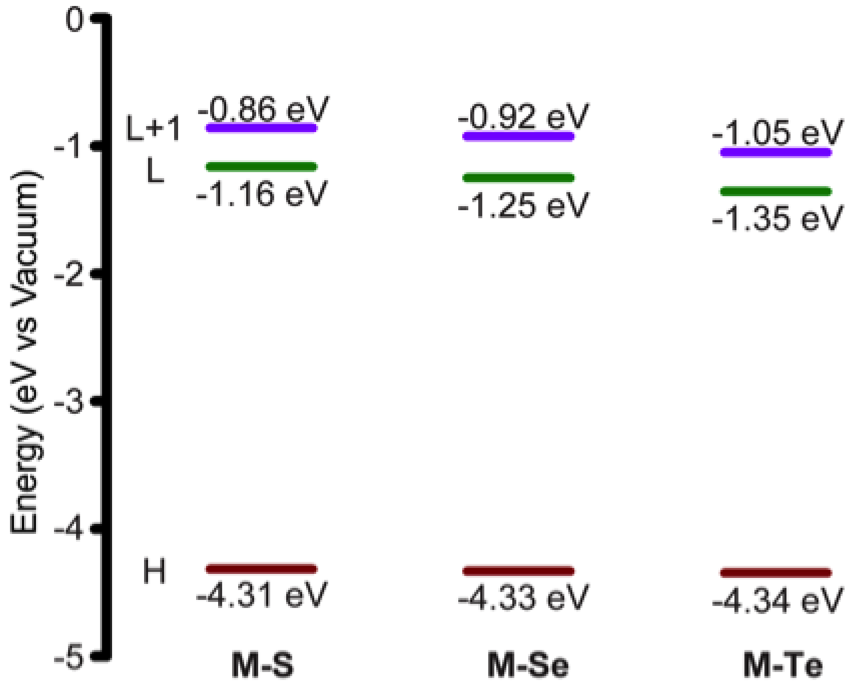

Figure S2. Calculated energies of HOMO (H), LUMO (L) and LUMO+1 (L+1) orbitals in eV vs. vacuum for model oligomers **M-S**, **M-Se** and **M-Te**.

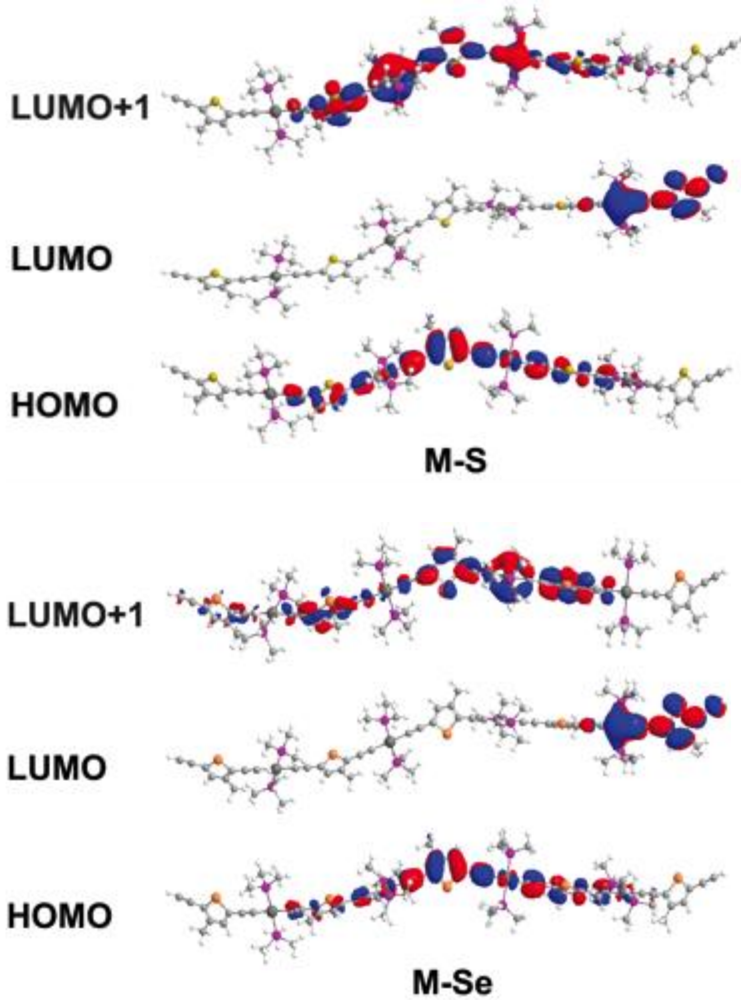

Figure S3. HOMO, LUMO and LUMO+1 molecular orbital diagrams for model oligomers **M-S**, and **M-Se** (B3LYP; 6-31G(d)/SDD; isocontour value 0.02).

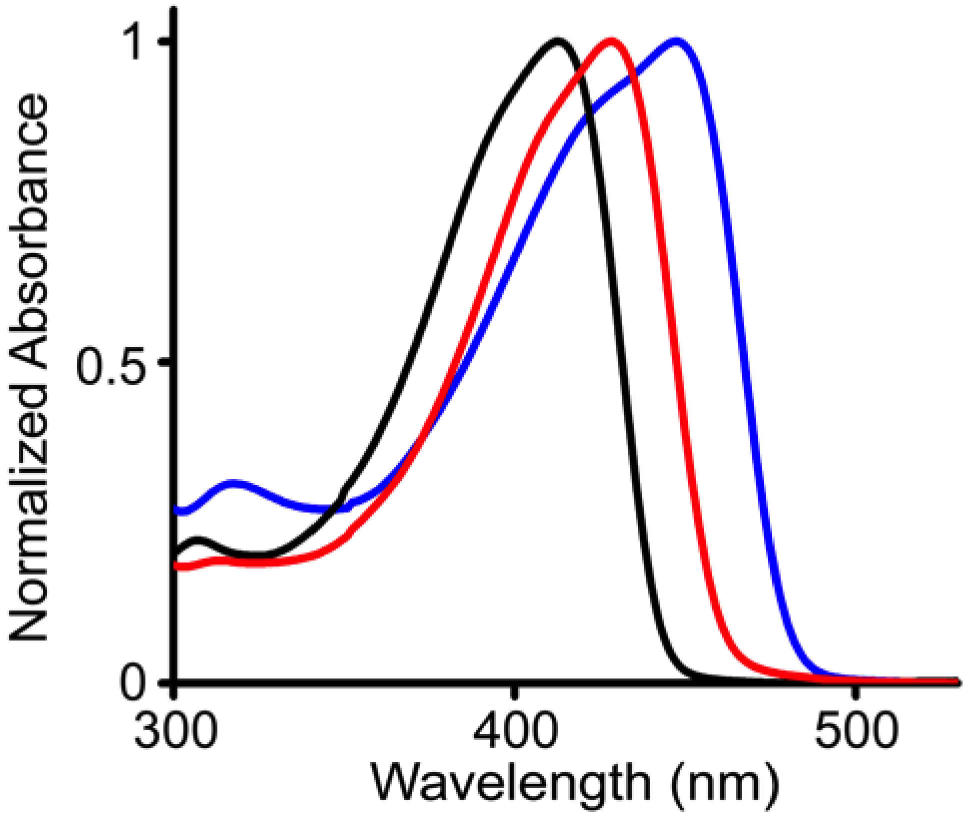

Figure S4. Solid-state absorption spectra of polymers **P-S** (black), **P-Se** (red) and **P-Te** (blue).

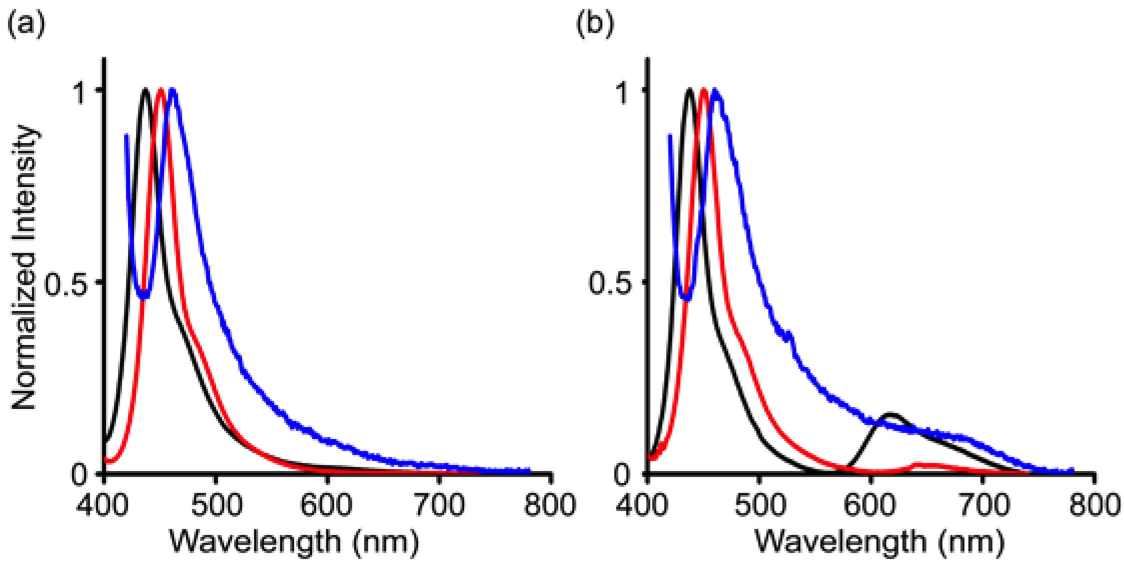

Figure S5. (a) Normalized emission spectra of **P-S** (black), **P-Se** (red) and **P-Te** (blue) in chloroform at room temperature. (b) Normalized emission spectra of **P-S** (black), **P-Se** (red) and **P-Te** (blue) in degassed chloroform at room temperature. An excitation wavelength of 380 nm was used for **P-S** and **P-Se**, and 400 nm was used for **P-Te**.

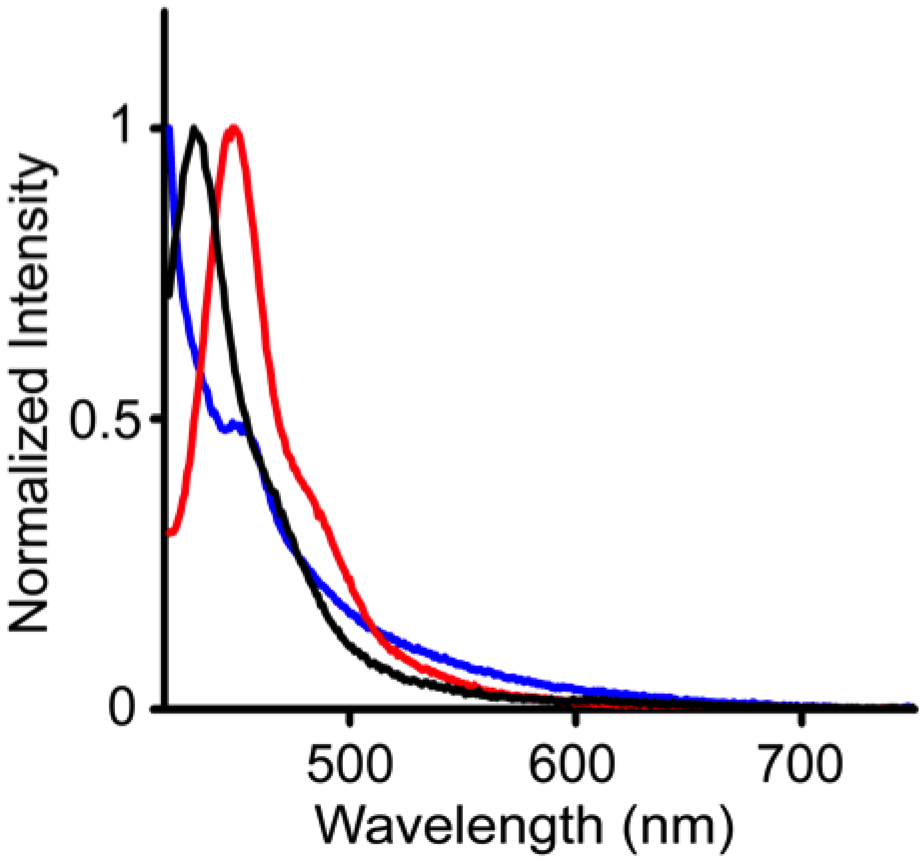

Figure S6. Normalized emission spectra of **P-S** (black), **P-Se** (red) and **P-Te** (blue) in degassed 2-methyltetrahydrofuran at room temperature. An excitation wavelength of 400 nm was used.

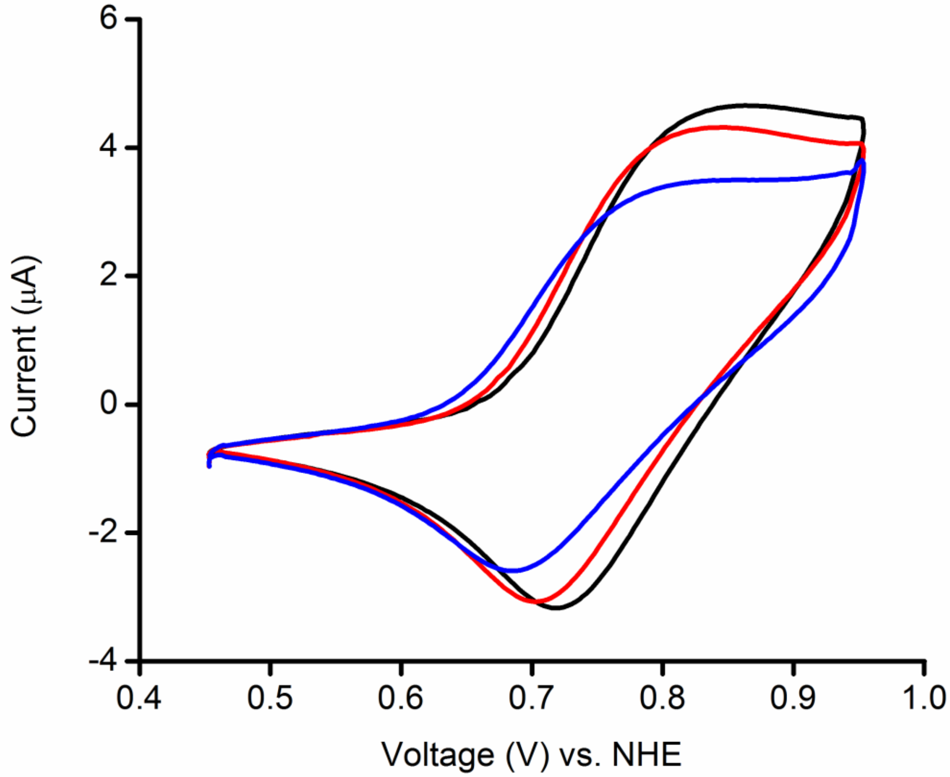

Figure S7. Cyclic voltammograms of **P-S** (black), **P-Se** (red), **P-Te** (blue) in dichloromethane with 0.1 M tetrabutylammonium hexafluorophosphate as the electrolyte, referenced to the normal hydrogen electrode (NHE).

Table S1. Electrochemical data obtained by cyclic voltammetry.

Polymer	$E_{1/2ox}$ (V vs. Fc/Fc^+)[a]	$E_{1/2ox}$ (V vs. NHE)[b]
P-S	0.141	0.781
P-Se	0.126	0.766
P-Te	0.104	0.744

[a]Experimental $E_{1/2ox}$ of Fc/Fc^+ was 0.188 V.
[b]Fc/Fc^+ is 0.64 V vs. NHE.[1]

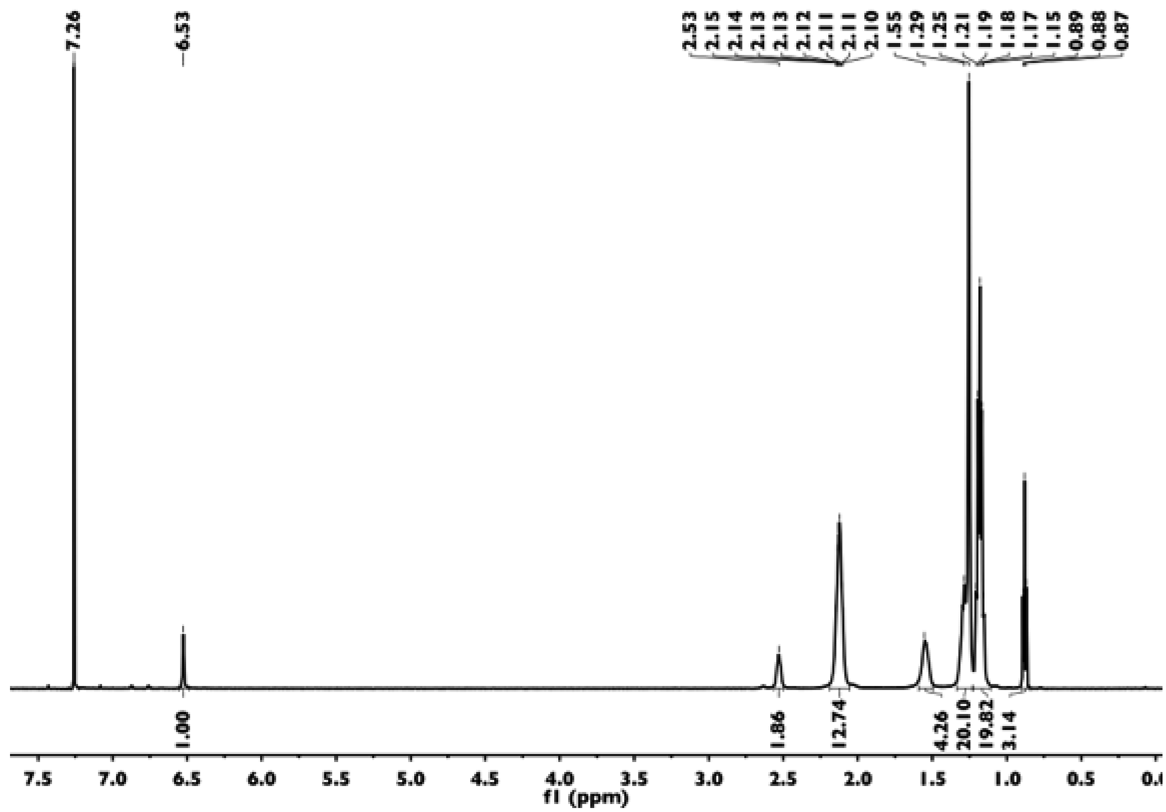

Figure S8. ^{1}H NMR spectrum of **P-S** (600 MHz, $CDCl_3$).

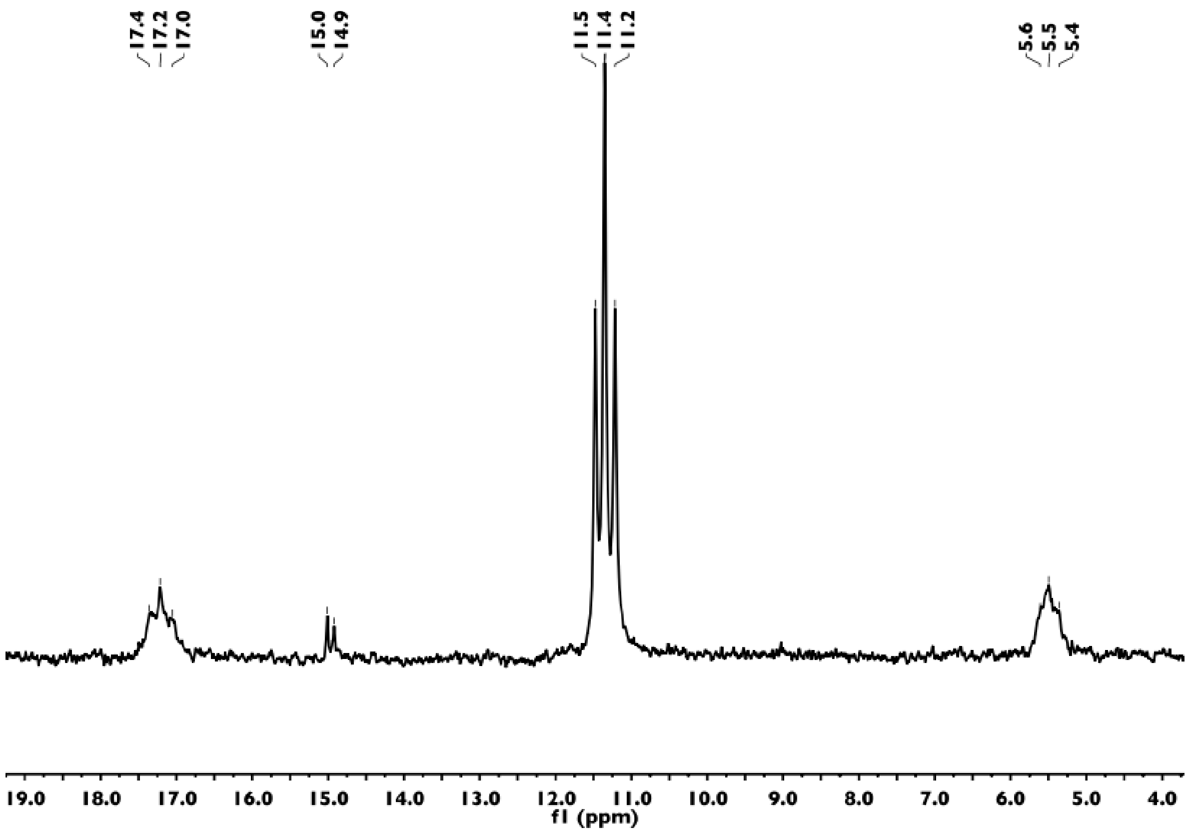

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of **P-S** (202 MHz, $CDCl_3$).

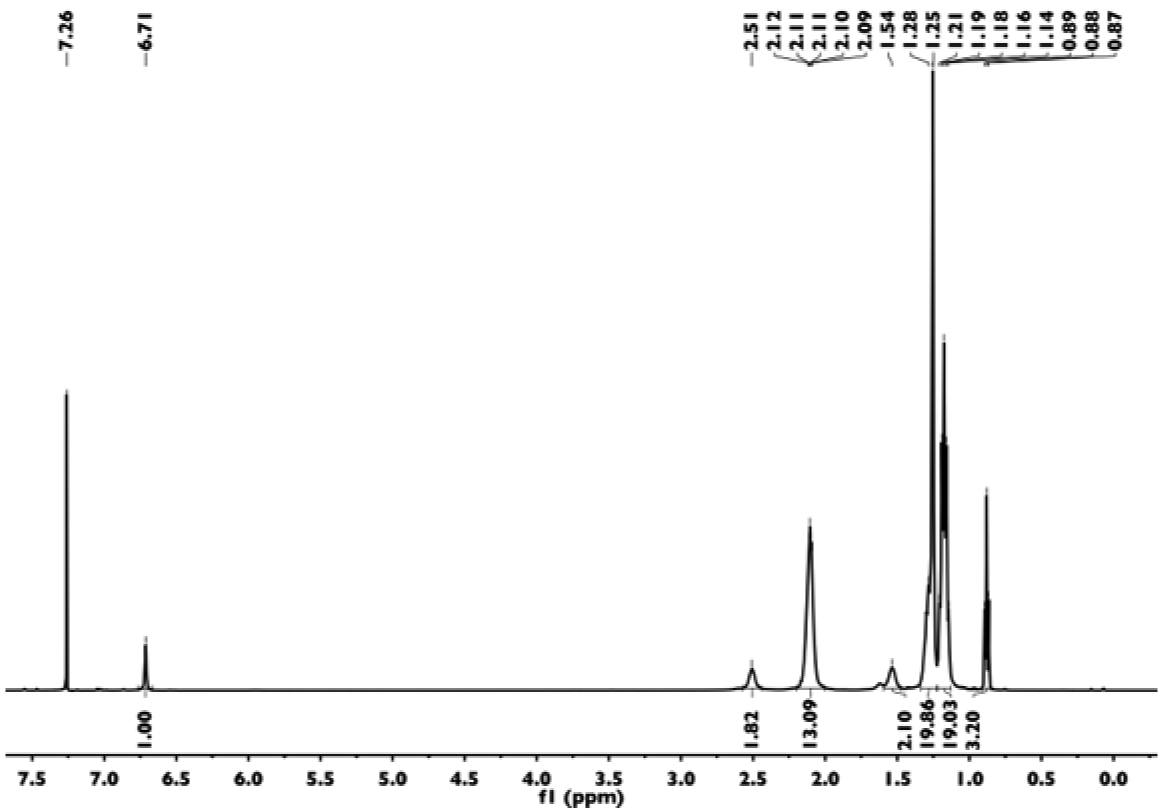

Figure S10. ^{1}H NMR spectrum of **P-Se** (500 MHz, $CDCl_3$).

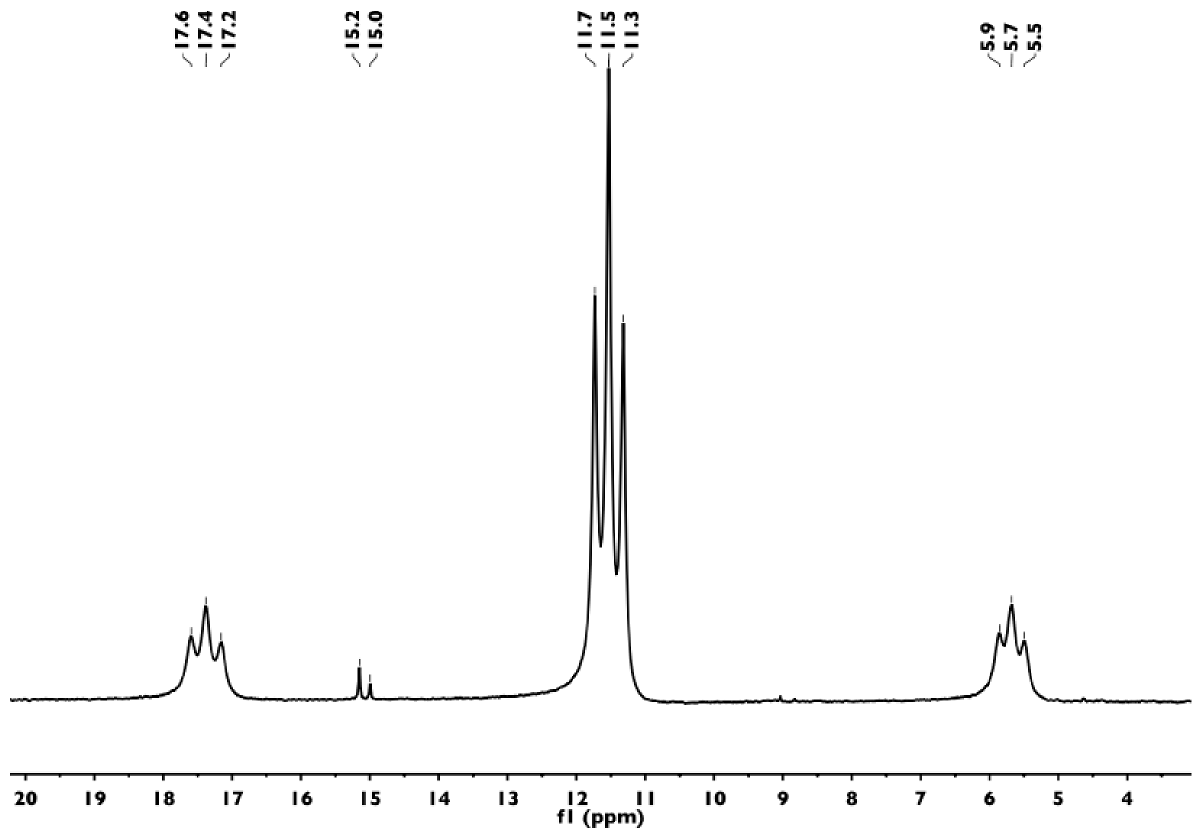

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **P-Se** (202 MHz, $CDCl_3$).

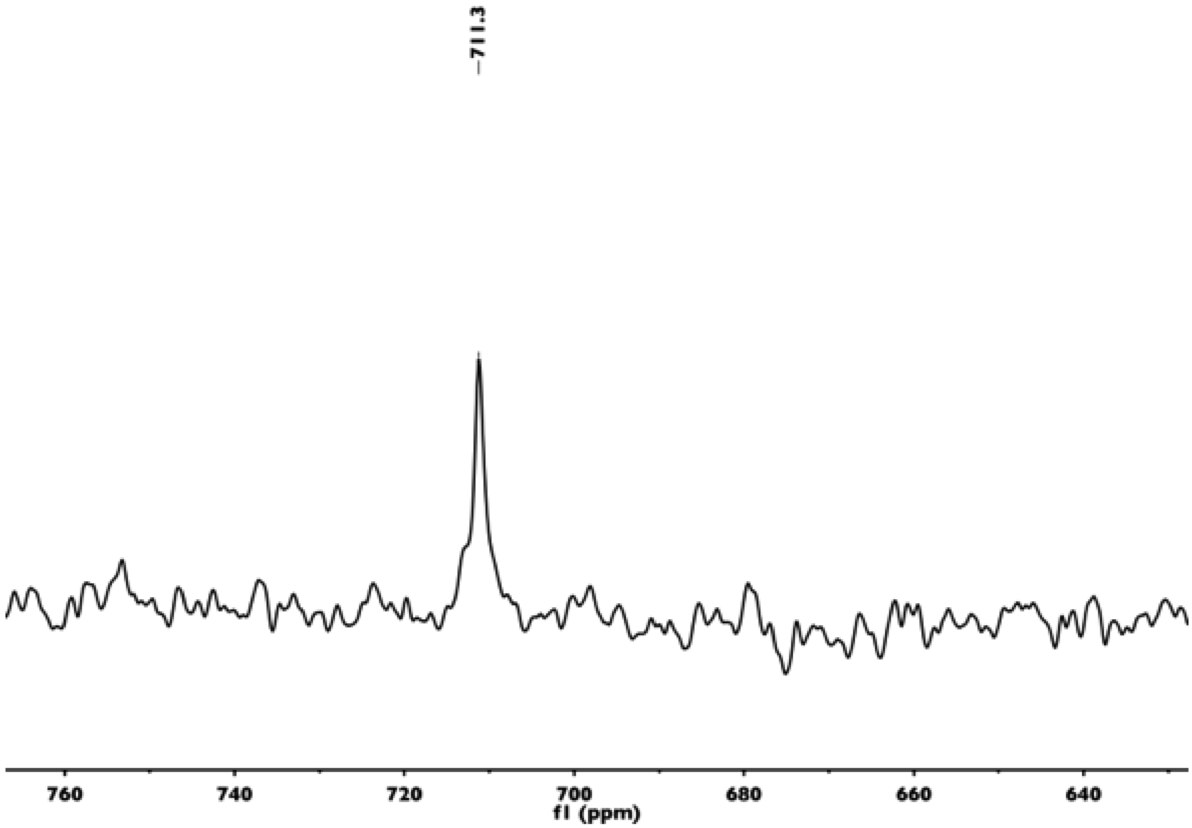

Figure S12. ^{77}Se NMR spectrum of **P-Se** (95 MHz, $CDCl_3$).

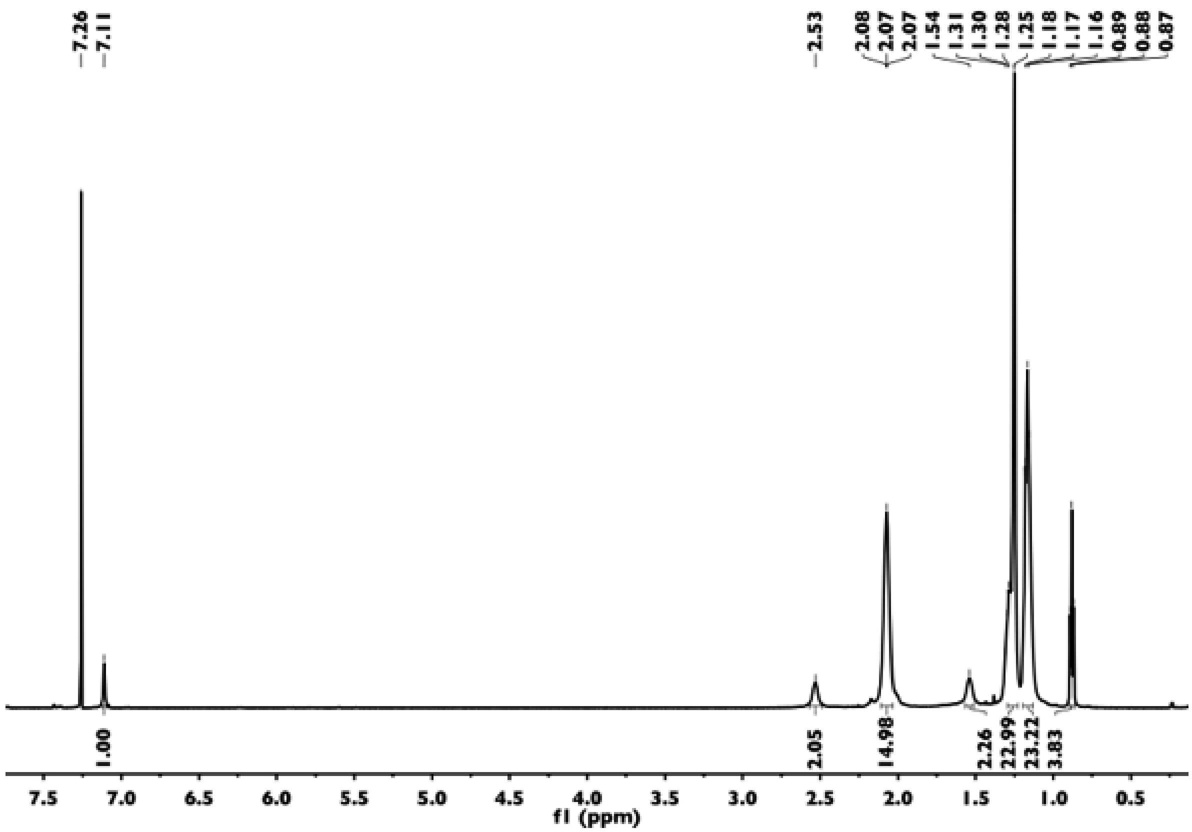

Figure S13. ^{1}H NMR spectrum of **P-Te** (600 MHz, $CDCl_3$).

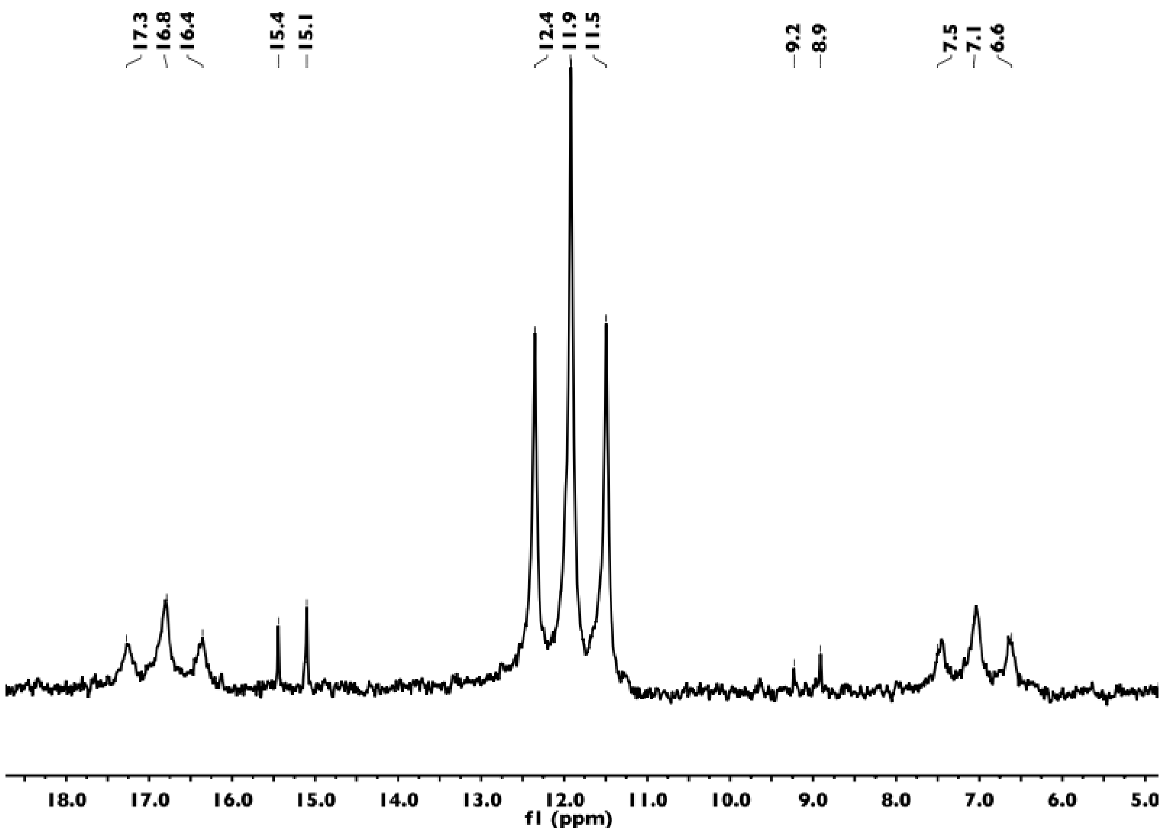

Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of **P-Te** (242 MHz, $CDCl_3$).

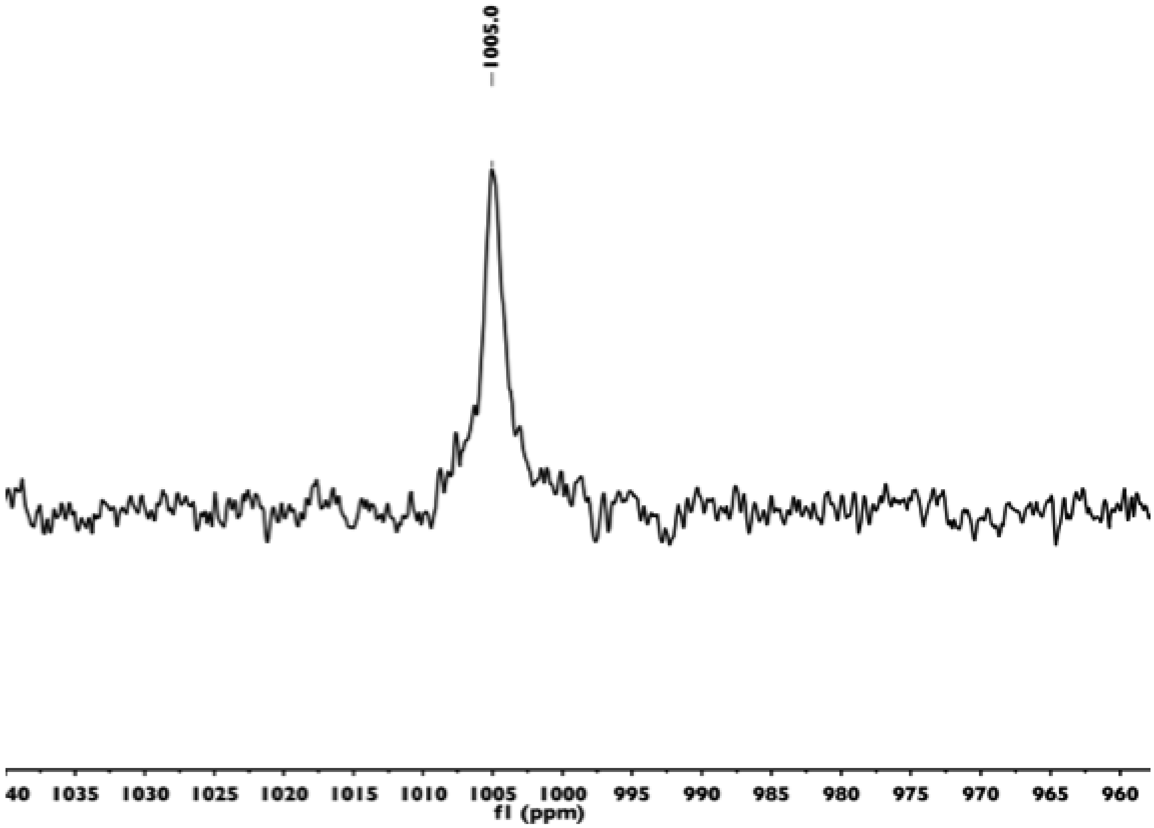

Figure S15. ^{125}Te NMR spectrum of **P-Te** (158 MHz, $CDCl_3$).

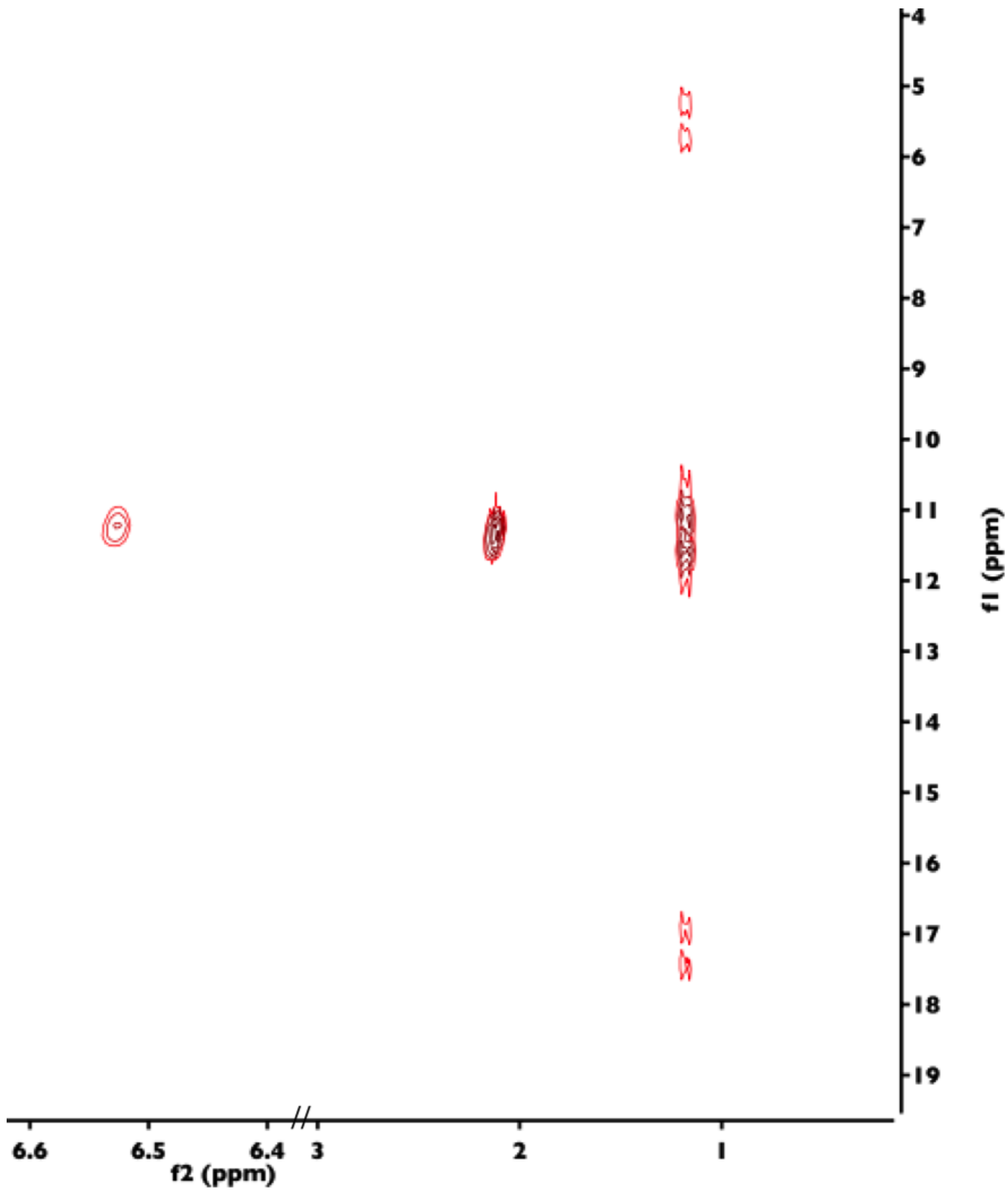

Figure S16. ^{1}H-^{31}P-CIGAR NMR spectrum of **P-S** (500 MHz, $CDCl_3$).

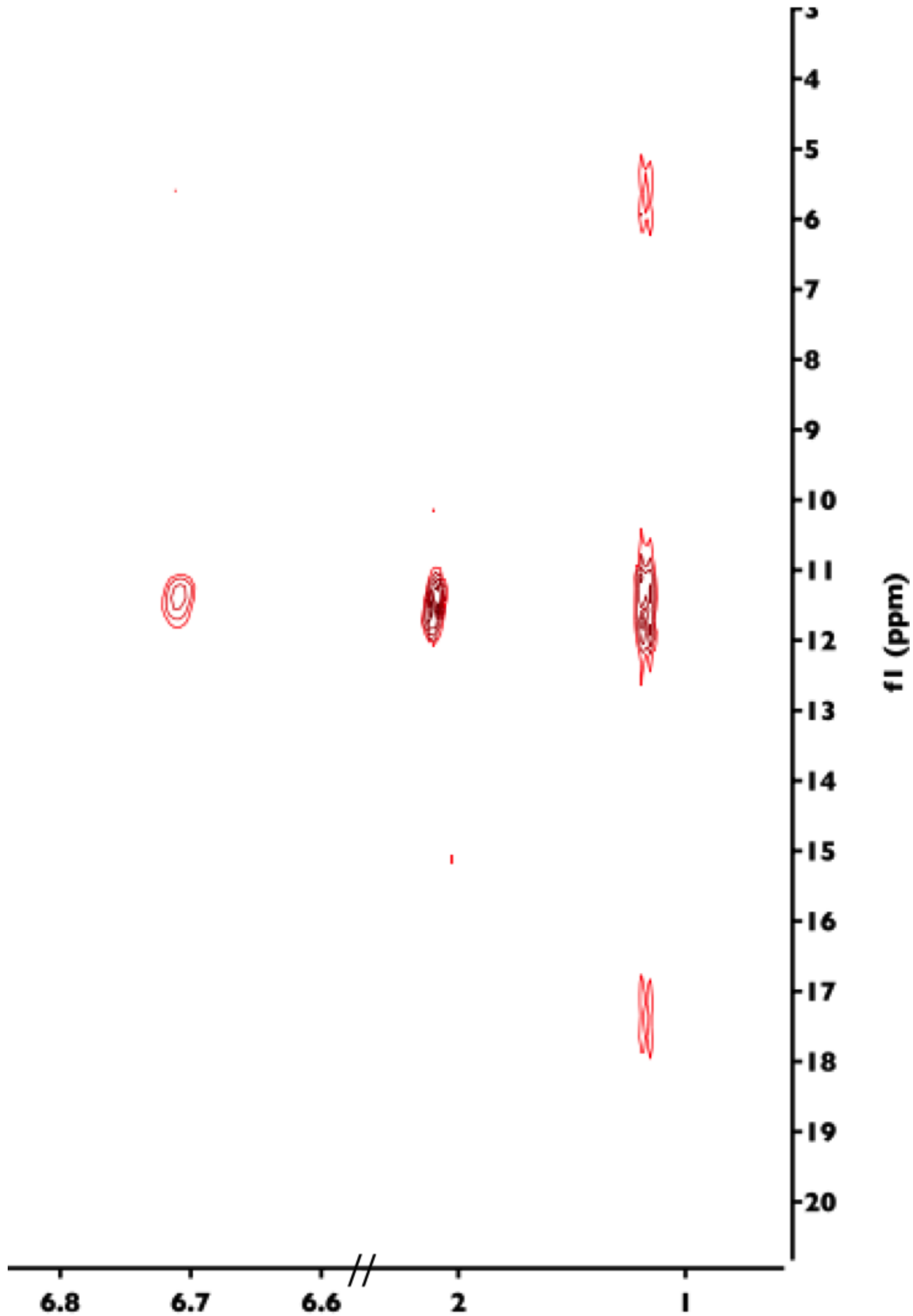

Figure S17. ^{1}H-^{31}P-CIGAR NMR spectrum of **P-Se** (500 MHz, $CDCl_3$).

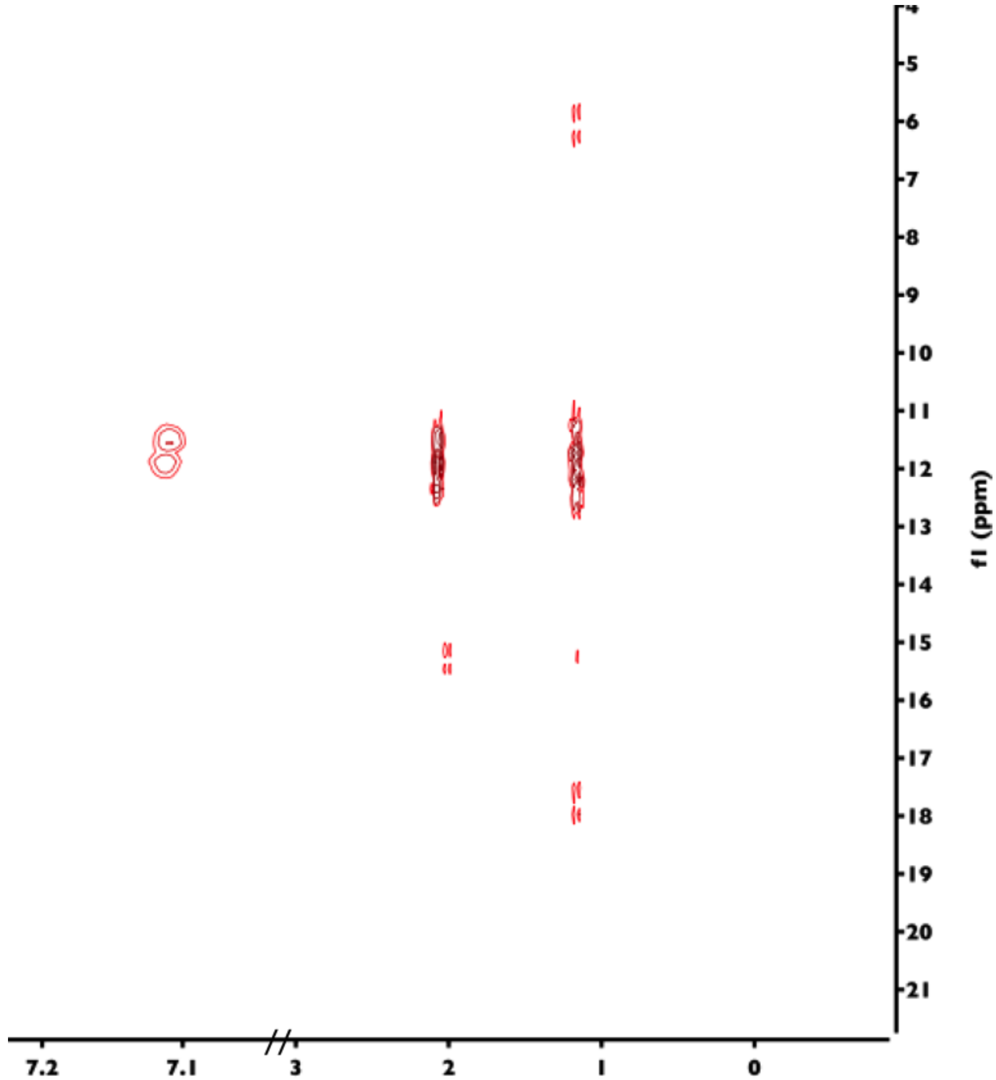

Figure S18. ^{1}H-^{31}P-CIGAR NMR spectrum of **P-Te** (500 MHz, $CDCl_3$).

Optimized geometry coordinates

P-S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.990623	-0.764822	0.562489
2	6	0	-0.339634	-0.065090	-0.444208
3	6	0	0.372718	1.064857	0.046332
4	6	0	0.289363	1.259854	1.411117
5	16	0	-0.710472	-0.003518	2.127981
6	1	0	0.941712	1.731460	-0.594252
7	6	0	-1.781396	-1.929164	0.468899
8	6	0	-2.469239	-2.947863	0.410591
9	78	0	-3.590973	-4.618479	0.328446
10	15	0	-5.488616	-3.401039	-0.286706
11	15	0	-1.773384	-5.949231	0.960085
12	6	0	-4.711886	-6.300018	0.251369
13	6	0	-5.390628	-7.327181	0.209576
14	6	0	-6.133779	-8.522445	0.166654
15	6	0	-7.501222	-8.703838	0.068373
16	16	0	-5.326742	-10.084535	0.246275
17	6	0	-7.923449	-10.060722	0.055750
18	1	0	-8.188375	-7.866289	0.008832
19	6	0	-6.856752	-10.942836	0.145866
20	6	0	-0.382901	-0.462365	-1.894879
21	1	0	0.625031	-0.640509	-2.292049
22	1	0	-0.966224	-1.378138	-2.027729
23	1	0	-0.836804	0.323630	-2.513063
24	6	0	-9.361269	-10.490833	-0.044731
25	1	0	-9.954863	-10.083507	0.783333
26	1	0	-9.817200	-10.132954	-0.976554
27	1	0	-9.447991	-11.580249	-0.021387
28	6	0	-5.310146	-1.582116	-0.484001
29	1	0	-4.956958	-1.146950	0.454214
30	1	0	-4.556636	-1.371314	-1.247053
31	1	0	-6.264949	-1.126637	-0.769671
32	6	0	-6.870314	-3.587384	0.916373
33	1	0	-7.768804	-3.061366	0.574575
34	1	0	-7.086813	-4.651917	1.038787
35	1	0	-6.563067	-3.184536	1.886164
36	6	0	-6.213350	-3.955776	-1.886036
37	1	0	-6.410938	-5.029273	-1.826936
38	1	0	-7.140702	-3.417007	-2.110869
39	1	0	-5.491730	-3.782782	-2.690178
40	6	0	-0.175116	-5.105925	1.297426
41	1	0	0.140725	-4.552894	0.409420
42	1	0	-0.308654	-4.382000	2.105228
43	1	0	0.594731	-5.834278	1.575883
44	6	0	-1.348411	-7.228769	-0.294103
45	1	0	-0.546122	-7.883015	0.064992
46	1	0	-2.241430	-7.821655	-0.508178
47	1	0	-1.028642	-6.739941	-1.219343
48	6	0	-2.098125	-6.917659	2.491752

49	1	0	-3.006039	-7.509097	2.347859
50	1	0	-1.257025	-7.578923	2.728301
51	1	0	-2.263111	-6.230375	3.327056
52	6	0	-6.891420	-12.352660	0.161291
53	6	0	-6.913864	-13.565073	0.175469
54	1	0	-6.934743	-14.630581	0.187301
55	6	0	0.863867	2.265381	2.213772
56	6	0	1.350258	3.123772	2.951591
57	78	0	2.136801	4.519782	4.186971
58	6	0	2.912722	5.906548	5.425230
59	15	0	3.484005	5.232722	2.417235
60	15	0	0.727976	3.696949	5.860274
61	6	0	3.386233	6.755585	6.180265
62	6	0	4.671422	6.599248	2.739507
63	6	0	2.511487	5.821158	0.968332
64	6	0	4.534397	3.885733	1.730120
65	6	0	0.806166	4.497175	7.513950
66	6	0	1.004164	1.911942	6.217486
67	6	0	-1.053315	3.791338	5.403923
68	1	0	4.126973	7.482193	3.083671
69	1	0	5.357003	6.304613	3.538214
70	1	0	5.239306	6.841622	1.834196
71	1	0	3.166898	6.081463	0.129513
72	1	0	1.818556	5.030747	0.668270
73	1	0	1.927884	6.700512	1.257124
74	1	0	3.890127	3.048627	1.449192
75	1	0	5.102704	4.230660	0.858925
76	1	0	5.229288	3.541432	2.502028
77	1	0	1.820978	4.412899	7.910793
78	1	0	0.579170	5.561727	7.415614
79	1	0	0.097464	4.028145	8.205598
80	1	0	0.278150	1.536320	6.947266
81	1	0	0.917041	1.350057	5.283839
82	1	0	2.016188	1.774132	6.610276
83	1	0	-1.198653	3.274100	4.451968
84	1	0	-1.684778	3.336685	6.175615
85	1	0	-1.338136	4.840016	5.275175
86	6	0	3.918434	7.739272	7.039207
87	16	0	3.434463	9.427271	6.873003
88	6	0	4.831746	7.593822	8.074828
89	6	0	4.470921	9.927356	8.208777
90	6	0	5.130430	8.826301	8.719325
91	6	0	5.439767	6.275114	8.468921
92	6	0	4.536823	11.276202	8.610941
93	1	0	5.823655	8.908437	9.550775
94	1	0	6.535537	6.304781	8.406877
95	1	0	5.184280	6.007643	9.503014
96	1	0	5.085196	5.474704	7.813106
97	6	0	4.574331	12.461958	8.943069
98	78	0	4.639929	14.410185	9.486096
99	6	0	4.708564	16.350866	10.023198
100	15	0	5.992549	13.782635	11.284135
101	15	0	3.281085	14.881594	7.645123
102	6	0	4.755893	17.536002	10.352522
103	6	0	6.555428	15.100771	12.435965
104	6	0	7.551920	12.958719	10.755053

105	6	0	5.187815	12.544402	12.384045
106	6	0	2.820224	16.637521	7.350150
107	6	0	1.664908	14.001333	7.703091
108	6	0	4.023243	14.344015	6.048169
109	6	0	4.831150	18.894942	10.721551
110	1	0	7.122073	15.852730	11.881016
111	1	0	5.685496	15.599432	12.870943
112	1	0	7.178554	14.679763	13.233032
113	1	0	8.130525	12.612516	11.618884
114	1	0	7.297609	12.112231	10.112059
115	1	0	8.155116	13.663699	10.175050
116	1	0	4.874014	11.691952	11.776070
117	1	0	5.870681	12.211251	13.173730
118	1	0	4.297782	12.989052	12.839483
119	1	0	2.294331	17.028587	8.224784
120	1	0	3.725960	17.234822	7.217758
121	1	0	2.183218	16.727489	6.463096
122	1	0	1.075313	14.193160	6.799458
123	1	0	1.852812	12.929029	7.802080
124	1	0	1.101855	14.335704	8.579747
125	1	0	4.273137	13.282174	6.118017
126	1	0	3.331982	14.510615	5.214354
127	1	0	4.945521	14.905485	5.870680
128	6	0	3.914839	19.662595	11.427953
129	16	0	6.240969	19.860008	10.284542
130	6	0	4.349290	21.005099	11.610207
131	6	0	2.606176	19.129026	11.944407
132	6	0	5.582104	21.299159	11.061445
133	1	0	3.764805	21.751412	12.139387
134	1	0	1.752949	19.661274	11.503093
135	1	0	2.502305	18.066109	11.708054
136	1	0	2.527717	19.244760	13.033415
137	6	0	6.298306	22.512685	11.057844
138	6	0	6.952466	23.556048	11.027778
139	78	0	8.048061	25.254994	10.966772
140	6	0	9.139232	26.945718	10.890346
141	15	0	6.347349	26.304846	12.175221
142	15	0	9.666278	24.051062	9.782600
143	6	0	9.798299	27.983957	10.836773
144	6	0	6.584700	28.072259	12.623849
145	6	0	6.000503	25.478793	13.783732
146	6	0	4.725703	26.277887	11.303337
147	6	0	11.205599	24.933879	9.299577
148	6	0	9.027620	23.362553	8.198954
149	6	0	10.271309	22.574266	10.699824
150	6	0	10.556574	29.170846	10.786347
151	1	0	7.493928	28.176532	13.221641
152	1	0	6.719070	28.663914	11.714787
153	1	0	5.724870	28.449420	13.188612
154	1	0	5.148808	25.943292	14.293535
155	1	0	5.791957	24.422591	13.594329
156	1	0	6.885019	25.546572	14.424209
157	1	0	4.481520	25.242124	11.052994
158	1	0	3.933239	26.708590	11.925743
159	1	0	4.804400	26.848612	10.373101
160	1	0	10.953212	25.794531	8.675202

161	1	0	11.705322	25.310842	10.195688
162	1	0	11.880771	24.265440	8.753973
163	1	0	9.783825	22.745998	7.700123
164	1	0	8.140576	22.760526	8.412837
165	1	0	8.737060	24.184093	7.537121
166	1	0	9.411910	21.956561	10.972583
167	1	0	10.972169	21.991089	10.091940
168	1	0	10.770905	22.897332	11.618177
169	6	0	10.605990	30.131551	9.782812
170	16	0	11.621811	29.600574	12.121094
171	6	0	11.494069	31.196311	10.094652
172	6	0	9.807135	30.049419	8.510623
173	6	0	12.127871	31.075958	11.314460
174	1	0	11.668815	32.041424	9.436671
175	1	0	10.460007	30.006576	7.628954
176	1	0	9.175969	29.156185	8.509423
177	1	0	9.158202	30.926181	8.387974
178	6	0	13.057484	31.954009	11.908678
179	6	0	13.857359	32.701299	12.429733
180	1	0	14.560155	33.363471	12.880560

P-Se

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.043220	-1.146061	0.682320
2	6	0	-0.292456	-0.479620	-0.271190
3	6	0	0.398726	0.672638	0.206216
4	6	0	0.250617	0.996132	1.537157
5	1	0	1.020295	1.277707	-0.448271
6	6	0	-1.829606	-2.304255	0.541301
7	6	0	-2.518062	-3.321298	0.455003
8	78	0	-3.646269	-4.983601	0.331745
9	15	0	-5.532835	-3.744648	-0.276325
10	15	0	-1.841735	-6.335371	0.954040
11	6	0	-4.777828	-6.655551	0.218276
12	6	0	-5.467558	-7.675099	0.155072
13	6	0	-6.216643	-8.861590	0.091974
14	6	0	-7.571010	-9.027363	-0.110286
15	6	0	-8.068823	-10.361371	-0.125215
16	1	0	-8.223322	-8.170431	-0.250397
17	6	0	-7.104863	-11.335121	0.069347
18	6	0	-0.206711	-0.932210	-1.705618
19	1	0	0.829366	-1.154733	-1.993508
20	1	0	-0.804369	-1.834161	-1.865065
21	1	0	-0.570381	-0.156106	-2.392143
22	6	0	-9.526671	-10.674873	-0.335650
23	1	0	-10.145334	-10.217484	0.446953
24	1	0	-9.879615	-10.282181	-1.297670
25	1	0	-9.704691	-11.753103	-0.322630
26	6	0	-5.340745	-1.924872	-0.450840
27	1	0	-4.989963	-1.502878	0.494231
28	1	0	-4.581767	-1.710230	-1.207417
29	1	0	-6.290922	-1.459703	-0.736270

30	6	0	-6.920540	-3.936711	0.918776
31	1	0	-7.813732	-3.399481	0.580568
32	1	0	-7.145486	-5.001127	1.026180
33	1	0	-6.614132	-3.549030	1.894989
34	6	0	-6.253926	-4.274683	-1.885535
35	1	0	-6.454907	-5.348234	-1.841657
36	1	0	-7.178715	-3.729650	-2.105671
37	1	0	-5.529187	-4.092872	-2.684905
38	6	0	-0.236327	-5.510488	1.302979
39	1	0	0.086596	-4.952065	0.420872
40	1	0	-0.364440	-4.793009	2.117357
41	1	0	0.526215	-6.248605	1.575716
42	6	0	-1.424579	-7.607207	-0.310776
43	1	0	-0.631286	-8.274085	0.045128
44	1	0	-2.323011	-8.187541	-0.536305
45	1	0	-1.094721	-7.112418	-1.229302
46	6	0	-2.179948	-7.314023	2.476379
47	1	0	-3.094947	-7.892908	2.326397
48	1	0	-1.347372	-7.987507	2.708641
49	1	0	-2.338118	-6.632280	3.317522
50	6	0	-7.281070	-12.731021	0.106470
51	6	0	-7.418382	-13.936016	0.140890
52	1	0	-7.540676	-14.994287	0.170658
53	6	0	0.808031	2.061234	2.265471
54	6	0	1.275368	2.974899	2.948279
55	78	0	2.028827	4.463231	4.092214
56	6	0	2.780661	5.935851	5.241104
57	15	0	3.316535	5.126047	2.260150
58	15	0	0.684526	3.676902	5.835089
59	6	0	3.249537	6.830014	5.946284
60	6	0	4.364442	6.625436	2.445113
61	6	0	2.312938	5.465312	0.754207
62	6	0	4.497184	3.819316	1.721754
63	6	0	0.773601	4.552551	7.449357
64	6	0	1.023460	1.918965	6.265913
65	6	0	-1.109073	3.696802	5.418425
66	1	0	3.732695	7.483728	2.688301
67	1	0	5.058831	6.483521	3.276902
68	1	0	4.922363	6.825199	1.523469
69	1	0	2.952034	5.685589	-0.108369
70	1	0	1.692034	4.589904	0.546626
71	1	0	1.653734	6.318236	0.942448
72	1	0	3.936759	2.900905	1.527711
73	1	0	5.041398	4.122273	0.820099
74	1	0	5.211722	3.623350	2.526919
75	1	0	1.799669	4.520869	7.824249
76	1	0	0.506830	5.603192	7.310230
77	1	0	0.098126	4.091279	8.178433
78	1	0	0.323318	1.554570	7.026026
79	1	0	0.937665	1.313086	5.360163
80	1	0	2.046364	1.830029	6.644438
81	1	0	-1.262175	3.132526	4.494766
82	1	0	-1.707872	3.259821	6.225591
83	1	0	-1.429195	4.729451	5.249364
84	6	0	3.767461	7.867485	6.742648
85	6	0	4.759849	7.809735	7.707010

86	6	0	4.339298	10.157818	7.935711
87	6	0	5.055272	9.052224	8.339996
88	6	0	5.478295	6.534742	8.064604
89	6	0	4.431199	11.486543	8.385252
90	1	0	5.816798	9.133616	9.110985
91	1	0	6.563364	6.637154	7.931547
92	1	0	5.308719	6.260127	9.114494
93	1	0	5.135852	5.706863	7.437360
94	6	0	4.487895	12.659426	8.759817
95	78	0	4.606234	14.584884	9.369642
96	6	0	4.740324	16.503322	9.966062
97	15	0	5.939021	13.858370	11.145079
98	15	0	3.260866	15.158604	7.548287
99	6	0	4.835142	17.677850	10.324222
100	6	0	6.523791	15.115420	12.353251
101	6	0	7.485172	13.028938	10.586317
102	6	0	5.108660	12.590506	12.190999
103	6	0	2.845456	16.935344	7.319441
104	6	0	1.621557	14.320461	7.579152
105	6	0	3.986982	14.658862	5.931875
106	6	0	4.987344	19.020743	10.713935
107	1	0	7.102593	15.881972	11.831935
108	1	0	5.662745	15.608341	12.811899
109	1	0	7.140049	14.647677	13.129310
110	1	0	8.054875	12.638203	11.437015
111	1	0	7.218214	12.213385	9.909271
112	1	0	8.102636	13.745900	10.036822
113	1	0	4.783291	11.768392	11.548319
114	1	0	5.782155	12.214359	12.969396
115	1	0	4.224259	13.031500	12.660814
116	1	0	2.334419	17.306958	8.211196
117	1	0	3.765712	17.513607	7.203928
118	1	0	2.206614	17.074396	6.440083
119	1	0	1.036454	14.558020	6.683529
120	1	0	1.780461	13.240891	7.642939
121	1	0	1.068642	14.640569	8.467501
122	1	0	4.204607	13.588002	5.961361
123	1	0	3.302159	14.877867	5.104896
124	1	0	4.926366	15.197787	5.775617
125	6	0	4.147395	19.809396	11.482273
126	6	0	4.602955	21.143864	11.694331
127	6	0	2.848873	19.303068	12.054373
128	6	0	5.804907	21.502698	11.125007
129	1	0	4.030158	21.856344	12.281908
130	1	0	1.993691	19.880144	11.677813
131	1	0	2.691911	18.252983	11.792203
132	1	0	2.834796	19.386807	13.149143
133	6	0	6.484170	22.732635	11.169411
134	6	0	7.120150	23.788341	11.170109
135	78	0	8.194411	25.501616	11.154648
136	6	0	9.267302	27.203938	11.123254
137	15	0	6.461340	26.513928	12.349183
138	15	0	9.845386	24.334701	9.978596
139	6	0	9.917247	28.249753	11.097217
140	6	0	6.667332	28.279919	12.818433
141	6	0	6.104731	25.666959	13.944684

142	6	0	4.852710	26.473197	11.454396
143	6	0	11.380356	25.243241	9.530603
144	6	0	9.239674	23.661790	8.375419
145	6	0	10.455632	22.852960	10.884522
146	6	0	10.668866	29.437688	11.095539
147	1	0	7.564154	28.390335	13.433564
148	1	0	6.810189	28.882065	11.917558
149	1	0	5.792709	28.640466	13.371186
150	1	0	5.239165	26.113511	14.447117
151	1	0	5.914657	24.609598	13.742615
152	1	0	6.979215	25.741822	14.598033
153	1	0	4.625825	25.436726	11.191177
154	1	0	4.046141	26.887813	12.069555
155	1	0	4.936862	27.053597	10.530645
156	1	0	11.125893	26.108969	8.914139
157	1	0	11.862106	25.614510	10.438840
158	1	0	12.071952	24.590953	8.985959
159	1	0	10.010823	23.061306	7.879861
160	1	0	8.355887	23.047173	8.565665
161	1	0	8.950374	24.489661	7.720976
162	1	0	9.600448	22.221207	11.137805
163	1	0	11.172117	22.286581	10.278987
164	1	0	10.938633	23.169989	11.813798
165	6	0	10.760584	30.406349	10.107727
166	6	0	11.618286	31.498084	10.424607
167	6	0	10.015801	30.317531	8.801439
168	6	0	12.244199	31.465882	11.650221
169	1	0	11.777753	32.323787	9.737078
170	1	0	10.706746	30.271056	7.949264
171	1	0	9.384152	29.425237	8.775546
172	1	0	9.374401	31.194928	8.647342
173	6	0	13.130837	32.412628	12.195752
174	6	0	13.896365	33.218773	12.680771
175	1	0	14.568429	33.932204	13.098961
176	34	0	-5.392109	-10.558943	0.298469
177	34	0	-0.898585	-0.273014	2.365338
178	34	0	3.109366	9.644502	6.579471
179	34	0	6.518924	20.014894	10.180462
180	34	0	11.747601	29.898932	12.589193

P-Te

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.454317	-1.766468	1.285075
2	6	0	-0.648109	-1.098722	0.384529
3	6	0	0.001605	0.097574	0.830599
4	6	0	-0.176026	0.559116	2.112582
5	1	0	0.644873	0.651186	0.149002
6	6	0	-2.184330	-2.949079	1.082749
7	6	0	-2.830508	-3.987022	0.928000
8	78	0	-3.860526	-5.689499	0.625686
9	15	0	-5.679508	-4.516023	-0.258756
10	15	0	-2.107528	-6.978891	1.483475

11	6	0	-4.883288	-7.402213	0.295087
12	6	0	-5.515215	-8.439841	0.080756
13	6	0	-6.198248	-9.640878	-0.157450
14	6	0	-7.541905	-9.819322	-0.390747
15	6	0	-8.071443	-11.130574	-0.612647
16	1	0	-8.202851	-8.955373	-0.402588
17	6	0	-7.181689	-12.184855	-0.580639
18	6	0	-0.442214	-1.595829	-1.026864
19	1	0	0.618842	-1.797291	-1.226116
20	1	0	-1.002729	-2.517805	-1.201814
21	1	0	-0.770417	-0.849648	-1.762858
22	6	0	-9.546039	-11.326375	-0.869239
23	1	0	-10.143353	-10.953308	-0.027454
24	1	0	-9.865207	-10.774206	-1.762500
25	1	0	-9.785687	-12.381900	-1.016793
26	6	0	-5.576026	-2.681109	-0.295698
27	1	0	-5.454543	-2.303715	0.722965
28	1	0	-4.695119	-2.376132	-0.865752
29	1	0	-6.478095	-2.250476	-0.744458
30	6	0	-7.253232	-4.854518	0.635394
31	1	0	-8.099953	-4.355820	0.150602
32	1	0	-7.417813	-5.934921	0.654896
33	1	0	-7.168152	-4.499707	1.667035
34	6	0	-6.048632	-4.981672	-2.001569
35	1	0	-6.185024	-6.065089	-2.053461
36	1	0	-6.949670	-4.474527	-2.364640
37	1	0	-5.200703	-4.709436	-2.637364
38	6	0	-0.661184	-6.092381	2.191568
39	1	0	-0.233689	-5.429028	1.435886
40	1	0	-0.990857	-5.469339	3.027118
41	1	0	0.097942	-6.802270	2.538353
42	6	0	-1.371667	-8.095290	0.216978
43	1	0	-0.606626	-8.745879	0.655393
44	1	0	-2.167478	-8.702712	-0.222151
45	1	0	-0.921120	-7.493676	-0.578281
46	6	0	-2.635681	-8.115186	2.832488
47	1	0	-3.466524	-8.727886	2.473259
48	1	0	-1.809594	-8.757977	3.156503
49	1	0	-2.988678	-7.525451	3.684049
50	6	0	-7.474637	-13.547073	-0.771341
51	6	0	-7.702503	-14.729128	-0.931944
52	1	0	-7.917535	-15.763000	-1.075482
53	6	0	0.381532	1.703601	2.702581
54	6	0	0.854544	2.706915	3.242736
55	78	0	1.653802	4.356626	4.100642
56	6	0	2.461969	5.988218	4.959423
57	15	0	2.822637	4.719000	2.110719
58	15	0	0.417285	3.861867	6.020226
59	6	0	2.970776	6.974210	5.496546
60	6	0	3.885778	6.214816	1.998141
61	6	0	1.716821	4.850624	0.644408
62	6	0	3.956099	3.329797	1.690129
63	6	0	0.550066	5.012723	7.448129
64	6	0	0.838069	2.216630	6.732861
65	6	0	-1.393016	3.758238	5.699652
66	1	0	3.271520	7.108213	2.137642

67	1	0	4.627371	6.197740	2.800556
68	1	0	4.389817	6.261315	1.026307
69	1	0	2.295012	4.939171	-0.282335
70	1	0	1.082259	3.961481	0.606490
71	1	0	1.073404	5.728942	0.754125
72	1	0	3.379906	2.400769	1.683522
73	1	0	4.428827	3.483661	0.713476
74	1	0	4.731514	3.249587	2.457979
75	1	0	1.593703	5.081765	7.764956
76	1	0	0.233847	6.012915	7.140758
77	1	0	-0.070595	4.668907	8.283114
78	1	0	0.189285	1.973731	7.581944
79	1	0	0.729735	1.458656	5.952456
80	1	0	1.880852	2.221103	7.064556
81	1	0	-1.564466	3.048372	4.886230
82	1	0	-1.937495	3.439454	6.595574
83	1	0	-1.762030	4.738405	5.382606
84	6	0	3.521191	8.115028	6.102372
85	6	0	4.734766	8.238421	6.749090
86	6	0	4.212728	10.583891	7.177489
87	6	0	5.072807	9.519295	7.295854
88	6	0	5.688847	7.075647	6.887565
89	6	0	4.392312	11.894955	7.646674
90	1	0	6.023691	9.656923	7.807569
91	1	0	6.650131	7.290092	6.401402
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93	1	0	5.271151	6.172374	6.435295
94	6	0	4.525771	13.053641	8.047815
95	78	0	4.784029	14.948340	8.711946
96	6	0	5.060496	16.830987	9.367238
97	15	0	5.741506	14.048129	10.645029
98	15	0	3.809046	15.692486	6.723791
99	6	0	5.241800	17.982458	9.768440
100	6	0	6.295608	15.215581	11.953563
101	6	0	7.239651	13.038089	10.290561
102	6	0	4.620035	12.885171	11.527742
103	6	0	3.677025	17.507832	6.460449
104	6	0	2.083897	15.085728	6.504133
105	6	0	4.686464	15.085985	5.223150
106	6	0	5.493455	19.292926	10.204378
107	1	0	7.036607	15.903098	11.537953
108	1	0	5.446376	15.813733	12.293615
109	1	0	6.728350	14.671469	12.800627
110	1	0	7.625833	12.568241	11.202074
111	1	0	6.975836	12.270723	9.558252
112	1	0	8.014741	13.677825	9.857804
113	1	0	4.292773	12.116542	10.822853
114	1	0	5.123855	12.420100	12.382599
115	1	0	3.738251	13.428787	11.880471
116	1	0	3.097655	17.953341	7.273052
117	1	0	4.674806	17.953354	6.486464
118	1	0	3.198691	17.726863	5.499285
119	1	0	1.674770	15.392562	5.534905
120	1	0	2.085218	13.994908	6.576450
121	1	0	1.453274	15.483431	7.305039
122	1	0	4.758907	13.996552	5.278223

123	1	0	4.159327	15.380646	4.308773
124	1	0	5.699930	15.498490	5.204193
125	6	0	4.688599	20.114349	10.968620
126	6	0	5.180871	21.421764	11.287565
127	6	0	3.332440	19.668140	11.461853
128	6	0	6.413222	21.837459	10.844595
129	1	0	4.574034	22.097655	11.887508
130	1	0	2.536502	20.324453	11.085077
131	1	0	3.116028	18.647663	11.135305
132	1	0	3.279221	19.695933	12.558446
133	6	0	7.038676	23.075082	11.060941
134	6	0	7.618498	24.150858	11.228701
135	78	0	8.560263	25.919728	11.506146
136	6	0	9.503364	27.674631	11.784044
137	15	0	6.771413	26.563126	12.864813
138	15	0	10.272058	25.119066	10.130315
139	6	0	10.083795	28.748757	11.954872
140	6	0	6.816659	28.248494	13.599146
141	6	0	6.543577	25.450825	14.314315
142	6	0	5.150881	26.498272	11.994041
143	6	0	11.689636	26.237439	9.781203
144	6	0	9.679491	24.620639	8.459897
145	6	0	11.063839	23.595270	10.795503
146	6	0	10.762458	29.953903	12.189591
147	1	0	7.711742	28.353484	14.217675
148	1	0	6.879112	28.992812	12.801148
149	1	0	5.923793	28.431535	14.207251
150	1	0	5.654402	25.728820	14.891317
151	1	0	6.448268	24.423348	13.953475
152	1	0	7.425598	25.510245	14.959130
153	1	0	5.024403	25.498475	11.570729
154	1	0	4.324023	26.723848	12.676948
155	1	0	5.150229	27.223043	11.174318
156	1	0	11.324426	27.153308	9.309537
157	1	0	12.172300	26.519685	10.720358
158	1	0	12.416439	25.747418	9.123885
159	1	0	10.488451	24.175957	7.869379
160	1	0	8.864477	23.901717	8.577140
161	1	0	9.289875	25.498632	7.935697
162	1	0	10.287748	22.847768	10.979775
163	1	0	11.806781	23.196490	10.095565
164	1	0	11.552236	23.825574	11.747288
165	6	0	10.769596	31.098486	11.414608
166	6	0	11.552284	32.203715	11.879076
167	6	0	9.989436	31.199656	10.125503
168	6	0	12.259117	32.106217	13.051552
169	1	0	11.590141	33.126643	11.304053
170	1	0	10.654052	31.391141	9.272605
171	1	0	9.440458	30.274999	9.929808
172	1	0	9.267079	32.025717	10.162124
173	6	0	13.067361	33.098183	13.633931
174	6	0	13.771364	33.937005	14.158052
175	1	0	14.384259	34.688175	14.600433
176	52	0	-5.224107	-11.515611	-0.199091
177	52	0	-1.475895	-0.754064	3.143316
178	52	0	2.484964	9.961528	6.127898

179	52	0	7.301102	20.282468	9.718631
180	52	0	11.972306	30.207515	13.906521

Gaussian Citation

Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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