

Supporting Information

Direct Arylation Polymerization of Electron-Rich Arenes with Polar Groups Enabled by Ligand-Coordination Tuning

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1 General Information

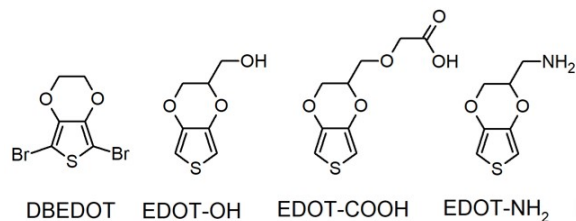
Unless otherwise stated, all solvents and chemical reagents were purchased from commercial sources (Macklin, Greagent-reagent, Adamas Chemical Co., Alfa Aesar, Sigma-Aldrich, TRC and TCI) and used without further purifications.

^1H (600 MHz) and ^{31}P (243 MHz) nuclear magnetic resonance (NMR) spectra were recorded at room temperature on an Avance III HD NMR spectrometer (Bruker Co., Switzerland), respectively. The NMR spectra of Rh-phosphine complexes were registered in its CDCl_3 solution (32 scans for ^1H and 128 scans for ^{31}P). The NMR spectra of PEE-OH, PEE-NH₂ and PPE-NH₂ were registered in its $\text{DMSO-d}_6/\text{N}_2\text{D}_4 \cdot \text{D}_2\text{O-d}_6$ (v/v = 100:1) solution (512 scans). The NMR spectra of PPE-OH were registered in its DMSO-d_6 solution (512 scans). The NMR spectra of PEE-COOH and PPE-COOH were registered in its $\text{DMSO-d}_6/\text{D}_2\text{O}/\text{N}_2\text{D}_4 \cdot \text{D}_2\text{O-d}_6$ (v/v/v = 100:5:1) solution (512 scans). Before measurement, these functionalized EDOT polymers were heated at 40 °C for more than 24 h to ensure their thorough dissolution in the specified deuterated solvents.

Ultraviolet-visible (UV-Vis) absorption spectra were recorded on a Shimadzu UV-3600 Plus spectrometer. All UV-Vis spectral data had been normalized by maximal intensity.

2. Preparation and Characterization of Substrates

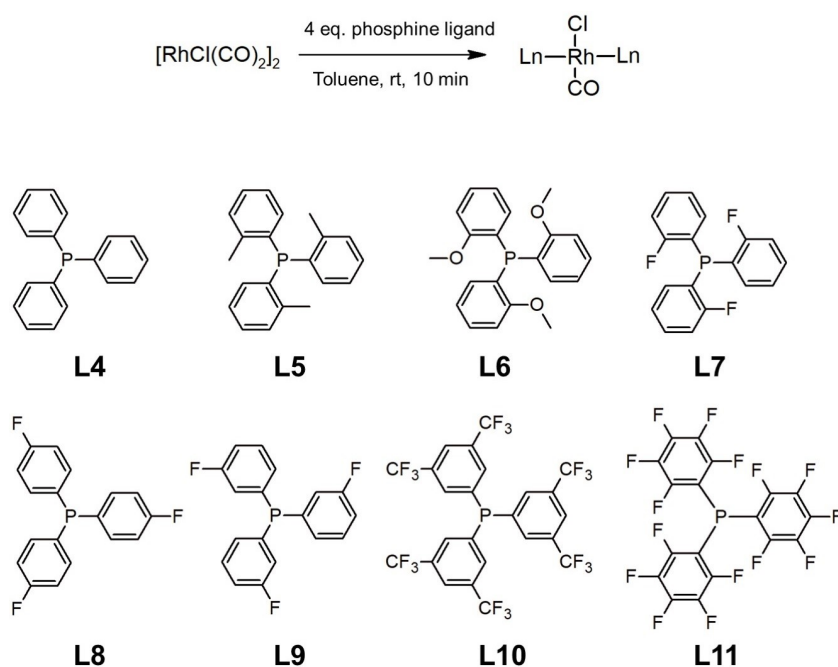
2.1 Preparation of monomer repeating units.



Scheme S1 Structures of EDOT monomers used for direct arylation polymerization.

2,5-Dibromo-3,4-ethylenedioxythiophene (DBEDOT) was synthesized following procedures previously reported¹. Hydroxyl-functionalized EDOT (EDOT-OH) was custom-synthesized by following the previously reported method². Carboxyl-functionalized EDOT (EDOT-COOH) was also synthesized following the previous approach³. Amine-functionalized EDOT (EDOT-NH₂) was synthesized following previously reported procedures⁴.

2.2 General procedure to prepare Rh-phosphine complexes.



Scheme S2 Synthesis of Rh-phosphine complexes.

A general method was employed in this study for the preparation of Rh-phosphine complexes $[\text{RhClCO}(\text{Ln})_2]$ ($\text{Ln}=\text{L4-L11}$). The reaction vial was charged with $[\text{RhCl}(\text{CO})_2]_2$ (3.9 mg, 0.01 mmol), phosphine ligand (4 eq. vs. Rh source), and toluene (1 mL). The reaction mixture was stirred at room temperature under an air atmosphere for 10 min. At the end of the reaction, the precipitate was filtered and dried in a vacuum without further purification unless otherwise stated.

2.3 Synthesis of $\text{RhClCO}(\text{L4})_2$.

$\text{RhClCO}(\text{L4})_2$ was synthesized following the abovementioned general procedure. Light yellow powder (11.0 mg, 80 % yield). ^1H NMR (600 MHz, CDCl_3): δ 7.77 – 7.72 (m, 12H), 7.47 – 7.37 (m, 18H). ^{31}P NMR (243 MHz, CDCl_3): δ 28.95 (d, $J_{\text{Rh-P}} = 126.23$ Hz).

2.4 Synthesis of $\text{RhClCO}(\text{L5})_2$.

$\text{RhClCO}(\text{L5})_2$ was synthesized following the abovementioned general procedure. Light yellow powder (8.5 mg, 55 % yield). ^1H NMR (600 MHz, CDCl_3): δ 7.35 (t, $J = 7.5$ Hz, 3H), 7.20 (p, $J = 7.5$ Hz, 9H), 2.38 (s, 9H). ^{31}P NMR (243 MHz, CDCl_3): δ 25.96 (m).

2.5 Synthesis of $\text{RhClCO}(\text{L6})_2$.

$\text{RhClCO}(\text{L6})_2$ was synthesized following the abovementioned general procedure. Light yellow powder (11.0 mg, 63 % yield). ^1H NMR (600 MHz, CDCl_3): δ 7.74 (s, 3H), 7.34 (td, $J = 7.8, 1.7$ Hz, 3H), 6.90 (t, $J = 7.5$ Hz, 3H), 6.81 (d, $J = 8.3$ Hz, 3H), 3.53 (s, 9H). ^{31}P NMR (243 MHz, CDCl_3): δ 17.98 (d, $J_{\text{Rh-P}} = 133.41$ Hz).

2.6 Synthesis of $\text{RhClCO}(\text{L7})_2$.

$\text{RhClCO}(\text{L7})_2$ was synthesized following the abovementioned general procedure. Light yellow powder (13.4 mg, 84 % yield). ^1H NMR (600 MHz, CDCl_3): δ 7.79 (p, $J = 7.0$ Hz, 3H), 7.48 (tdd, $J = 7.4, 5.1, 1.7$ Hz, 3H), 7.20 (d, $J = 7.6$ Hz, 3H), 7.08 (t, $J = 8.9$ Hz, 3H). ^{31}P NMR (243 MHz, CDCl_3): δ 10.38 (dm, $J_{\text{Rh-P}} = 136.03$ Hz).

2.7 Synthesis of RhCICO(L8)₂.

RhCICO(L8)₂ was synthesized following the abovementioned general procedure and precipitated in ethanol after being concentrated. The precipitate was filtered and dried over a vacuum. Light yellow powder (11.3 mg, 71% yield). ¹H NMR (600 MHz, CDCl₃): δ 7.68 (dq, *J* = 7.3, 5.2 Hz, 6H), 7.13 (t, *J* = 8.5 Hz, 6H). ³¹P NMR (243 MHz, CDCl₃): δ 26.82 (d, *J*_{Rh-P} = 127.93 Hz).

2.8 Synthesis of RhCICO(L9)₂.

RhCICO(L9)₂ was synthesized following the abovementioned general procedure and precipitated in ethanol after being concentrated. The precipitate was filtered and dried over a vacuum. Light yellow powder (13.2 mg, 83 % yield). ¹H NMR (600 MHz, CDCl₃): δ 7.53 (d, *J* = 7.6 Hz, 3H), 7.50 – 7.37 (m, 6H), 7.19 (td, *J* = 8.3, 2.6 Hz, 3H). ³¹P NMR (243 MHz, CDCl₃): δ 30.11 (d, *J*_{Rh-P} = 130.34 Hz).

2.9 Synthesis of RhCICO(L10)₂.

RhCICO(L10)₂ was synthesized following the abovementioned general procedure. Orange powder (23.49 mg, 79 % yield). ¹H NMR (600 MHz, CDCl₃): δ 8.23 – 8.00 (m, 9H). ³¹P NMR (243 MHz, CDCl₃): δ 32.73 (dm, *J*_{Rh-P} = 133.99 Hz).

2.10 Synthesis of RhCICO(L11)₂.

RhCICO(L11)₂ was synthesized following the abovementioned general procedure. Yellow powder (20.4 mg, 83 % yield). ³¹P NMR (243 MHz, CDCl₃): δ -23.88 (d, *J*_{Rh-P} = 150.95 Hz).

2.11 Electronic properties of phosphine ligands

Table S1 Data of ^{31}P NMR spectra and Tolman cone angle ^a of aryl-phosphine ligands.

Ligand	δ P/ppm (P ligands)	δ P/ppm (Rh-P complexes)	$J_{\text{Rh-P}}/\text{Hz}$	Tolman Cone Angle $\theta/^\circ$
L4	-5.45	29.22 / 28.70	126.23	124.44
L5	-29.58	25.96	-	149.33
L6	-39.68	18.28 / 17.73	133.41	145.67
L7	-42.45	10.66 / 10.10	136.03	134.41
L8	-9.10	27.07 / 26.64	127.93	124.83
L9	-4.81	30.38 / 29.85	130.34	125.58
L10	-4.18	33.02 / 32.47	133.99	134.37
L11	-74.30	23.56 / 24.18	150.95	141.64

^a Tolman cone angle θ of phosphine ligands was calculated by Solid-G software, and more details can be found in Section 4 of Supplementary materials.

The coupling constant ($J_{\text{Rh-P}}$) can serve as an indicator of the electron-donating strength (EDS) of phosphine ligands in binding with electrophilic transition metals. $J_{\text{Rh-P}}$ is dominated by the Fermi-contact term⁵ and can be expressed by the equation 1, where A and B are constants. a_M and a_P denote the percentages of s-character on metal M and phosphorus, respectively. S_{M-P} is the overlap integral for the Rh-P bond.

$$J_{M-P} = \frac{Aa_M^2 a_P^2}{1 + S_{M-P}^2} + B \quad (1)$$

In the case of L1-L3, no evidence had been found to indicate the formation of Rh-P(L1-L3) complexes. For other ligands, their phosphorus chemical shifts presented a downfield shift, indicating the depletion of electron density and the formation of complexes with Rh. The $J_{\text{Rh-P}}$ values for the complexes with aryl-phosphine ligands (L7–L11) increased with the introduction of the electron-withdrawing substituents onto aryls of ligands, compared to that of the complex with L4. It indicates that the incorporation of electron-withdrawing substituents onto aryls of phosphine ligands

results in a reduction in the overlap integral value of S_{M-P} , which corresponds to the hybridization between atoms Rh and P, and thus a higher J_{Rh-P} . As shown in Table S1, the J_{Rh-P} values of most ligands increase reasonably with the number of electron-withdrawing substituents. However, the J_{Rh-P} value of the L7 ligand deviate a lot from this dependence. The steric hindrance of the ligand might play a critical role in the interaction of ligands with transition metal. For evaluating this effect, the Tolman cone angles of phosphine ligands were calculated using Solid-G software (More calculation details are in Supplementary information Section 4). Reasonably, the ortho-site aryl substitution for the L7 ligand led to a larger Tolman cone angle of phosphine ligands. Similarly, due to the ortho-site aryl substitution for aryl phosphine ligands, the J_{Rh-P} values $RhClCO(L11)_2$ should be also higher than expected. That is, the coordination strength of phosphine ligands is decided by both the electronic properties and steric hindrance of substituents. On the other hand, we also included the aryl-phosphine ligands with electron-donating groups on aryls, which should have a smaller J_{Rh-P} value than the L4 ligand. Unfortunately, for the aryl-phosphine ligand with the methyl substituent(L5), the ^{31}P signal of $RhClCO(L5)_2$ is significantly broadening, leading to the indeterminate coupling unobservable. Interestingly, for the aryl-phosphine ligand with the methoxyl substituents on aryl, the J_{Rh-P} is not smaller but higher than that of the L4 ligand without aryl substituents. We considered that the methoxyl group of the L6 ligand competes with the phosphorus atom in interacting with the transition metal, leading to a smaller contribution of phosphorus and a higher J_{Rh-P} value for the L6 ligand. It thus explains why the J_{Rh-P} value for the complexes with the L6 ligand is not as low as expected based on the electronic property of substituents (i.e., EDS). In addition, the steric hindrance of the L6 ligand should have an impact on its interaction with transition metal because of its ortho-site aryl substitution.

3. Preparation and Characterization of Functionalized EDOT Polymers

3.1 General procedure for preparation of functionalized EDOT polymers.

A general method was applied to synthesize all the polymers described in this publication. A Schlenk tube was charged with functionalized EDOT monomer (1 eq.), arene dibromide (1 eq.), palladium acetate (10 mol %), potassium pivalate (2 eq.), phosphine ligand (20 mol %), N,N-dimethylacetamide (DMAc) (0.125 M) and a magnetic stir bar in glovebox at a 0.25 mmol scale. The mixture was heated in an oil bath at the desired temperature with vigorous stirring. After the polymerization was completed, the tube was extracted from the oil bath and cooled to ambient temperature in the air. The mixture was added drop by drop to 200 mL methanol, causing solid precipitation. The precipitate was filtered off and purified in a Soxhlet extraction thimble using acetone and methanol to wash it thoroughly. Finally, it was dried under a vacuum overnight to give the final product.

3.2 The molecular weight measurement of functionalized EDOT polymers.

The copolymers of EDOT derivatives with EDOT are typically insoluble in both organic solvents, such as dichloromethane (DCM), chloroform, tetrahydrofuran (THF), toluene, chlorobenzene, 1,2,4-trichlorobenzene (TCB), N,N-dimethylformamide (DMF), N,N-dimethylacetamide (DMAc), and dimethylsulfoxide (DMSO), and deionized water due to their susceptibility to doping, posing a challenge for analyzing the molecular weight of these polymers. However, adding a reductant (85% hydrazine hydrate, $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$) can significantly facilitate the dissolution of these functionalized polymers in solvents (DMAc and DMSO) for analyzing their characteristics. The copolymer of EDOT-OH with EDOT (PEE-OH) and that of EDOT-NH₂ with EDOT (PEE-NH₂) were found to be well soluble in DMSO containing 1% v/v hydrazine, while the copolymer of EDOT-COOH with EDOT (PEE-COOH) well soluble in $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$ (85%).

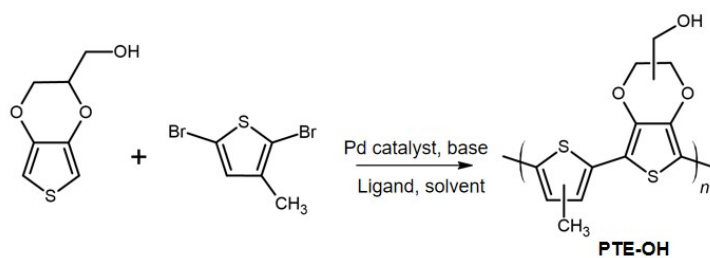
In contrast, the copolymers of EDOT derivatives with benzene present better solubility than those of EDOT derivatives with EDOT. The copolymer of EDOT-OH with benzene (PPE-OH) is soluble in DMSO, while the copolymer of EDOT-COOH with benzene (PPE-COOH) and the copolymer of EDOT-NH₂ with benzene (PPE-NH₂) are slightly soluble in deionized water and DMSO, respectively. Moreover, the addition of hydrazine to the solvent significantly enhances their solubility. Specifically, PPE-COOH dissolves well in N₂H₄·H₂O (85%), while PPE-OH and PPE-NH₂ exhibit excellent solubility in DMSO with 1% v/v N₂H₄·H₂O.

The gel permeation chromatography (GPC) measurements were performed on the Agilent 1260 Infinity II system equipped with the PLgel 300 × 7.5 mm column and the PL aqua gel-OH 20 (8μm 300 × 7.5 mm) column (Agilent, USA) to the molecular weight of functional EDOT polymers in the presence of hydrazine. However, since the dissolution of these EDOT polymers requires the addition of hydrazine hydrate (~1%), we were unable to obtain stable molecular weight results. One of most plausible explanations is that the GPC column may absorb the hydrazine hydrate, destabilizing the solution and affecting the measurements. Additionally, the Ubbelohd viscometer measurement was carried out to determine the average molecular weight of these functional EDOT polymers. However, the adsorption of free polar groups on these polymers onto the walls of the capillary prevented the acquisition of a linear intrinsic viscosity curve. Finally, we have to use the liquid ¹H NMR spectroscopy to measure the degree of polymerization (DP) and number-average molecular weight (M_n) of functionalized EDOT polymers⁶.

To clarify the quantification of brominated chain ends of polymers synthesized by direct arylation polymerization, we carried out copolymerization studies of EDOT-OH with a series of thiophene-based dibromides. Unfortunately, dibromo-EDOT (DBEDOT) is structurally unsuitable for this purpose because it lacks protons adjacent to the terminal bromine atoms, preventing observation of diagnostic end-group signals. 1,4-dibromobenzene produced aromatic resonances in the δ 7.2–8.0 ppm region after reaction, overlapping end-group signals and precluding reliable integration.

These limitations motivated the use of 2,5-dibromo-3-methylthiophene instead, whose position-4 proton provides a distinct and isolated resonance suitable for end-group analysis. Copolymerizations of EDOT-OH with 2,5-dibromo-3-methylthiophene were therefore carried out under the general polymerization conditions for L11. At reaction times of 10, 30, and 60 min (Table S2), two well-resolved end-group signals were observed: (1) the proton of terminal EDOT-OH appeared as a doublet at δ 6.59 ppm, and (2) the position-4 proton of the terminal bromothiophene appeared as a well-isolated doublet at δ 6.71 ppm. Quantitative analysis across five independent batches yielded an average integration ratio of terminal EDOT-OH C-H to terminal thiophene C-Br (1.00 ± 0.01) (Figure S1). Time-dependent measurements (10–60 min) showed nearly constant ratios (0.99–1.01), indicating that H-terminated ends consistently account for $50 \pm 1\%$ of all chain ends.

Table S2 Summary of yield molecular weight and degree of polymerization for synthesis of PTE-OH .



Entry	Ligand	Temp. (°C)	Time (min)	Yield (%)	M_n by ^1H NMR (C-H) (kg/mol)	M_n by ^1H NMR (C-Br) (kg/mol)
1	L11	120	10	61	3.63	3.66
2	L11	120	30	90	4.00	4.00
3	L11	120	60	91	5.39	5.36

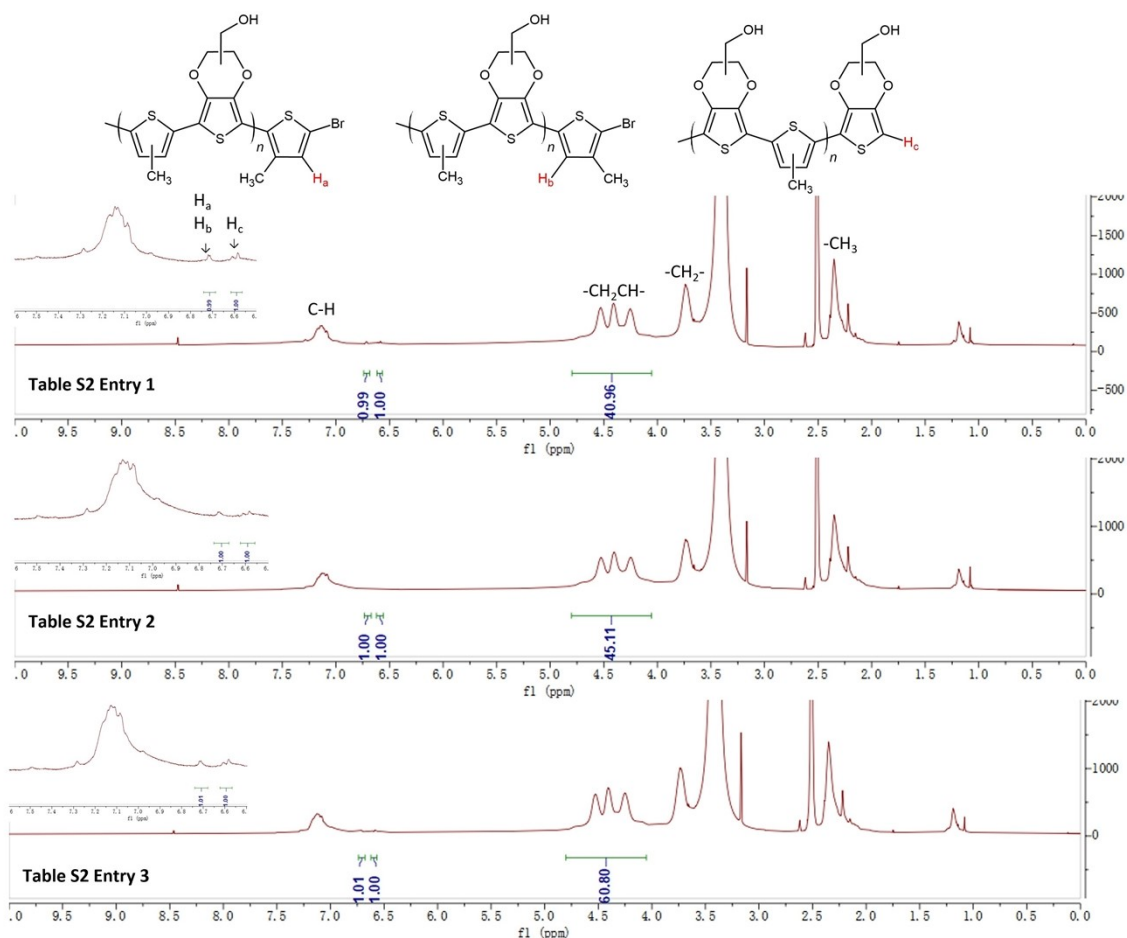


Figure S1 ^1H NMR of PTE-OH with entry 1-3 of Table S2 [600MHz, dimethyl sulfoxide- d_6 323K]

Therefore, the DP of PEEs was calculated according to the following equation:

$$DP_{PEE} = \frac{I_{\text{ethylenedioxiide}}}{I_{\text{end-groups}}} \cdot p_{PEE} \quad \#(2)$$

Where I represents the integration of NMR signals assigned to the EDOT copolymer backbone or end-groups, and p_{PEE} denotes the average proton number for one repeating unit without considering the proton of side groups. The copolymer of functionalized EDOT with EDOT (PEE) consists two alternative repeating units, i.e., EDOT (four protons) and functionalized EDOT substrates (three protons). Therefore, the value of p_{PEE} was determined to be 3.5.

The DP of PPEs was calculated according to the following equation:

$$DP_{PPE} = \frac{I_{ethylene\ dioxide}}{I_{end\ groups}} \cdot p_{PPE} \quad \#(3)$$

Where I represents the integration of NMR signals from the EDOT copolymer backbone, and p_{PPE} denotes the average proton number for one repeating unit without considering the proton of side groups. As shown in equation (3), the copolymer of functionalized EDOT with benzene (PPE) consists of two alternative repeating units, i.e., functionalized EDOT substrates (three protons) and benzene (no protons). Therefore, the value of p_{PPE} was determined to be 1.5.

In this way, the DP and M_n of the copolymers of EDOT-OH and EDOT-NH₂ with EDOT and benzene were determined by ¹H NMR end-group analysis. However, frustratingly, this end-group analysis method could not work for the copolymers of EDOT-COOH with EDOT and benzene, as the signal of the end-group could not be observed when they were dissolved in D₂O/N₂D₄·D₂O, plausibly due to the deuterium exchange. In contrast, the end group signal can be observed in DMSO-d₆/D₂O/N₂D₄·D₂O (v/v/v = 100:5:1). However, only the EDOT-COOH copolymer of small molecular weight could be dissolved well in it, and no conclusive DP of carboxyl-functionalized EDOT polymers could be obtained. Instead, UV-vis spectra of the EDOT-COOH copolymers in N₂H₄·H₂O were collected only to assess polymer formation and relative conjugation-length trends qualitatively.

3.3 Synthesis of PEE-OH.

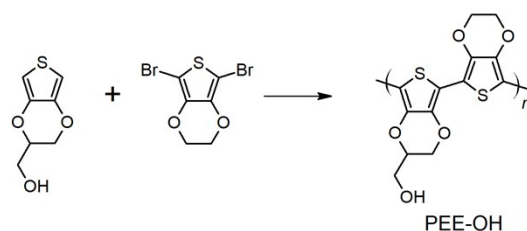


Table S3 Summary of yield, optical property, molecular weight, and degree of polymerization for synthesis of PEE-OH with different phosphine ligands.

Entry	Pd Source	Solvent	Ligand	Temp. (°C)	Time	Yield (%)	λ_{\max} (nm)	M_n (Kg / mol)	DP
1 ^a	Pd(OAc) ₂	DMAc	L1	120	1 h	-	-	-	-
2 ^a	Pd(OAc) ₂	DMAc	L2	120	1 h	-	-	-	-
3 ^a	Pd(OAc) ₂	DMAc	L3	120	1 h	-	-	-	-
4 ^a	Pd(OAc) ₂	DMAc	L4	120	1 h	55	557	2.3	15
5 ^a	Pd(OAc) ₂	DMAc	L5	120	1 h	-	-	-	-
6 ^a	Pd(OAc) ₂	DMAc	L6	120	1 h	39	555	3.1	20
7 ^a	Pd(OAc) ₂	DMAc	L7	120	1 h	85	574	3.1	20
8 ^a	Pd(OAc) ₂	DMAc	L8	120	1 h	71	548	1.8	11
9 ^a	Pd(OAc) ₂	DMAc	L9	120	1 h	75	557	2.1	13
10 ^a	Pd(OAc) ₂	DMAc	L10	120	1 h	70	566	3.4	22
11 ^a	Pd(OAc) ₂	DMAc	L11	120	1 h	88	578	4.6	30
12 ^a	Pd(OAc) ₂	DMAc	L7	120	24 h	86	566	4.2	27
13 ^a	Pd(OAc) ₂	DMAc	L11	120	24 h	91	577	13.4	86
14 ^a	Pd(OAc) ₂	DMAc	N/A	60	1 h	89	562	3.5	22
15 ^a	Pd(OAc) ₂	DMAc	N/A	120	1 h	95	564	5.0	32
16 ^a	Pd(OAc) ₂	DMAc	N/A	120	24 h	96	578	12.0	77
17 ^b	Pd ₂ (dba) ₃	Toluene	L6	110	1 h	31	-	3.7	23
18 ^b	Pd ₂ (dba) ₃	Toluene	L6	110	48 h	32	-	4.4	29
19 ^c	Pd ₂ (dba) ₃	Toluene	L6	110	24 h	78	-	-	-

^a Reactions were performed on a 0.25 mmol scale in DMAc (0.125 M) using EDOT-OH (1 eq.), dibromo-EDOT (1 eq.), Pd source (10 mol %), phosphine ligand (20 mol %) and KPivO (2 eq.). ^b Performing in toluene (0.125 M) at 0.25 mmol scale using Pd source (2 mol%), phosphine ligand (4 mol %) and Cs₂CO₃ (2 eq.). ^c Performed in toluene (0.125 M) at 0.25 mmol scale using Pd source (10 mol%), phosphine ligand (20 mol %) and KPivO (2 eq.).



3.4 Synthesis of PPE-OH.

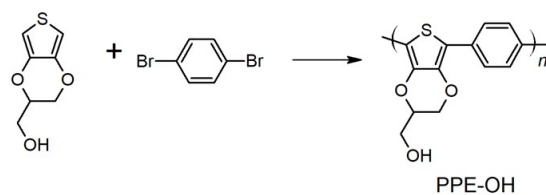


Table S4 Summary of yield, optical property, molecular weight, and degree of polymerization for synthesis of PPE-OH with different phosphine ligands.

entry	Pd Source	Solvent	ligand	Temp. (°C)	Time	Yield (%)	λ_{\max} (nm)	M_n (Kg / mol)	DP
1 ^a	Pd(OAc) ₂	DMAc	L1	120	1 h	-	-	-	-
2 ^a	Pd(OAc) ₂	DMAc	L2	120	1 h	-	-	-	-
3 ^a	Pd(OAc) ₂	DMAc	L3	120	1 h	53	461	6.8	55
4 ^a	Pd(OAc) ₂	DMAc	L4	120	1 h	-	-	-	-
5 ^a	Pd(OAc) ₂	DMAc	L5	120	1 h	23	464	8.5	68
6 ^a	Pd(OAc) ₂	DMAc	L6	120	1 h	30	458	2.7	22
7 ^a	Pd(OAc) ₂	DMAc	L7	120	30 min	79	461	15.0	121
8 ^a	Pd(OAc) ₂	DMAc	L7	120	1 h	88	465	48.9	396
9 ^a	Pd(OAc) ₂	DMAc	L8	120	1 h	73	450	2.5	20
10 ^a	Pd(OAc) ₂	DMAc	L9	120	1 h	78	453	3.2	26
11 ^a	Pd(OAc) ₂	DMAc	L10	120	1 h	68	459	3.8	31
12 ^a	Pd(OAc) ₂	DMAc	L11	120	30 min	83	462	21.8	176
13 ^a	Pd(OAc) ₂	DMAc	L11	120	1 h	92	467	120.0	972
14 ^a	Pd(OAc) ₂	DMAc	N/A	60	1 h	84	459	4.9	40
15 ^a	Pd(OAc) ₂	DMAc	N/A	120	30 min	81	461	11.2	90
16 ^a	Pd(OAc) ₂	DMAc	N/A	120	1 h	89	461	13.3	108
17 ^a	Pd(OAc) ₂	DMAc	pyridine	120	1 h	81	451	1.07	9
18 ^a	Pd(OAc) ₂	DMAc	2,2-dipyridyl	120	1 h	-	-	-	-
19 ^b	Pd ₂ (dba) ₃	Toluene	L6	110	1 h	83	-	1.7	14
20 ^b	Pd ₂ (dba) ₃	Toluene	L6	110	48 h	86	-	2.1	17
21 ^c	Pd ₂ (dba) ₃	Toluene	L6	110	24 h	98	-	-	-

^a Reactions were performed on a 0.25 mmol scale in DMAc (0.125 M) using EDOT-OH (1 eq.), dibromo-EDOT (1 eq.), Pd source (10 mol %), phosphine ligand (20 mol %) and KPivO (2 eq.). ^b Performing in toluene (0.125 M) at 0.25 mmol scale using Pd source (2 mol%), phosphine ligand (4 mol %) and Cs₂CO₃

(2 eq.). ^c Performed in toluene (0.125 M) at 0.25 mmol scale using Pd source (10 mol%), phosphine ligand (20 mol %) and KPivO (2 eq.).

3.5 Synthesis of PEE-COOH.

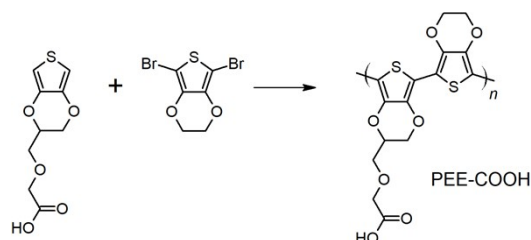


Table S5 Summary of yield and optical property for synthesis of PEE-COOH with different phosphine ligands ^a.

entry	ligand	Yield (%)	λ_{\max} (nm)
1	L1	-	-
2	L2	-	-
3	L3	-	-
4	L4	23	593
5	L5	-	-
6	L6	-	-
7	L7	-	-
8	L8	44	592
9	L9	49	597
10	L10	48	601
11	L11	-	-

^a Reaction conditions were performed on a 0.25 mmol scale in DMAc (0.125 M) using EDOT-COOH (1 eq.), dibromo-EDOT (1 eq.), Pd(OAc)₂ (10 mol %), phosphine ligand (20 mol %) and KPivO (2 eq.) at 120 °C for 1 hr.

3.6 Synthesis of PPE-COOH.

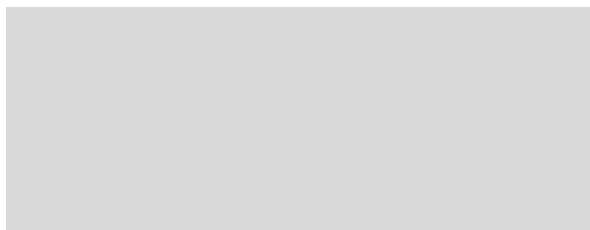


Table S6 Summary of yield and optical property for synthesis of PPE-COOH with different phosphine ligands ^a.

entry	ligand	Yield (%)	λ_{max} (nm)
1	L1	-	-
2	L2	-	-
3	L3	-	-
4	L4	20	386
5	L5	-	-
6	L6	-	-
7	L7	-	-
8	L8	52	415
9	L9	44	421
10	L10	31	412
11	L11	-	-

^a Reactions were performed on a 0.25 mmol scale in DMAc (0.125 M) using EDOT-COOH (1 eq.), dibromobenzene (1 eq.), Pd(OAc)₂ (10 mol %), phosphine ligand (20 mol %) and KPivO (2 eq.) at 120 °C for 1 hr.

3.7 Synthesis of PEE-NH₂.



Table S7 Summary of yield, optical property, molecular weight, and degree of polymerization for synthesis of PEE-NH₂ with different phosphine ligands ^a.

entry	ligand	Temp. (°C)	Time (h)	Yield (%)	λ_{\max} (nm)	M_n (Kg / mol)	DP
1	L1	120	6	-	-	-	-
2	L2	120	6	-	-	-	-
3	L3	120	6	-	-	-	-
4	L4	120	6	61	536	0.9	6
5	L5	120	6	41	536	1.0	6
6	L6	120	6	27	532	0.8	5
7	L7	120	6	-	-	-	-
8	L8	120	6	52	534	0.9	6
9	L9	120	6	82	546	1.9	12
10	L10	120	6	49	543	1.6	10
11	L11	120	6	-	-	-	-
12	N/A	60	6	-	-	-	-
13	N/A	120	6	23	533	0.5	3

^a Reactions were performed on a 0.25 mmol scale in DMAc (0.125 M) using EDOT-NH₂ (1 eq.), dibromo-EDOT (1 eq.), Pd(OAc)₂ (10 mol %), phosphine ligand (20 mol %), and KPivO (2 eq.) at 120 °C for 6 hr.

3.8 Synthesis of PPE-NH₂.

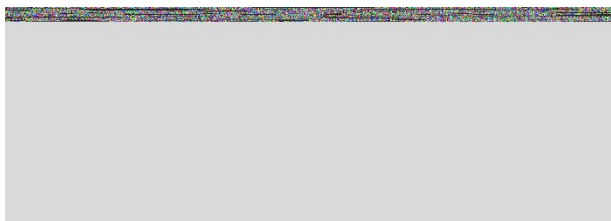


Table S8 Summary of yield, optical property, molecular weight, and degree of polymerization for synthesis of PPE-NH₂ with different phosphine ligands ^a

entry	ligand	Temp. (°C)	Time (h)	Yield (%)	λ_{\max} (nm)	M _n (Kg / mol)	DP
1	L1	120	6	-	-	-	-
2	L2	120	6	-	-	-	-
3	L3	120	1	-	-	-	-
4	L3	120	3	23	440	3.2	26
5	L3	120	6	66	452	6.7	53
6	L4	120	3	-	-	-	-
7	L4	120	6	46	450	6.8	55
8	L5	120	1	23	443	2.1	17
9	L5	120	3	44	449	2.4	19
10	L5	120	6	67	451	4.6	37
11	L6	120	1	-	-	-	-
12	L6	120	3	24	453	3.8	31
13	L6	120	6	43	456	4.4	53
14	L7	120	6	-	-	-	-
15	L8	120	1	34	451	3.0	23
16	L8	120	3	61	460	16.1	130
17	L8	120	6	73	465	87.9	711
18	L9	120	1	29	451	3.8	31
19	L9	120	3	48	458	5.2	42
20	L9	120	6	67	464	31.2	253
21	L10	120	1	-	-	-	-
22	L10	120	3	29	444	4.6	37

23	L10	120	6	37	445	4.8	39
24	L11	120	1	-	-	-	-
25	L11	120	3	26	441	1.1	8
26	L11	120	6	55	452	5.6	67
27	N/A	60	6	-	-	-	-
28	N/A	120	1	-	-	-	-
29	N/A	120	3	28	441	1.2	10
30	N/A	120	6	41	443	2.4	20

^a Reactions were performed on a 0.25 mmol scale using EDOT-NH₂ (1 eq.), dibromobenzene (1 eq.), Pd(OAc)₂ (10 mol %), phosphine ligand (20 mol %), and KPivO (2 eq.) in DMAc (0.125 M) at 120 °C.

4. Small Molecule Model Reaction

4.1 General Methods of Direct Arylation of EDOT-NH₂ with bromoarenes

The small molecule model for the direct arylation of EDOT-NH₂ with bromoarene was conducted under conditions similar to those used in the polymerization conditions. In a typical procedure, a Schlenk tube was charged with EDOT-NH₂ (1 eq.), bromoarene (2.1 eq.), palladium acetate (10 mol %), potassium pivalate (2 eq.), phosphine ligand (20 mol %) or performed ligandless, N,N-dimethylacetamide (DMAc) (0.125 M) and a magnetic stir bar. All reagents were introduced in a glovebox at a 0.25 mmol scale. The mixture was heated in an oil bath at the desired temperature with vigorous stirring, and the monomer conversion was monitored by ¹H NMR. For NMR analysis, 10 μL aliquot from reaction mixture was taken and immediately diluted into 0.5 mL DMSO-d₆. These samples were stored at -20 °C until prior to the NMR measurement.

4.2 Small Molecular Model for Direct Arylation of EDOT-NH₂

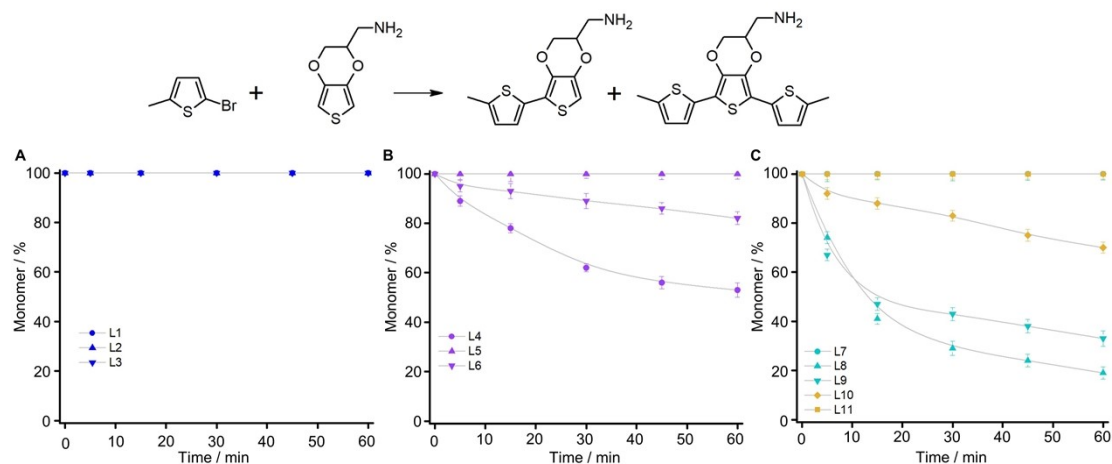


Figure S2 Consumption of EDOT-NH₂ monitored by ¹H NMR for the direct arylation of 2-bromo-5-methylthiophene (0.2625 M) with EDOT-NH₂ (0.125 M), KPivO (0.2625 M) and Pd(OAc)₂ (10 mol %) under various ligand conditions. (A) Phosphine ligands P1-P3 (20 mol %) at 120 °C, (B) Phosphine ligands P4-P6 (20 mol %) at 120 °C, (C) Phosphine ligands P7-P11 (20 mol %) at 120 °C.

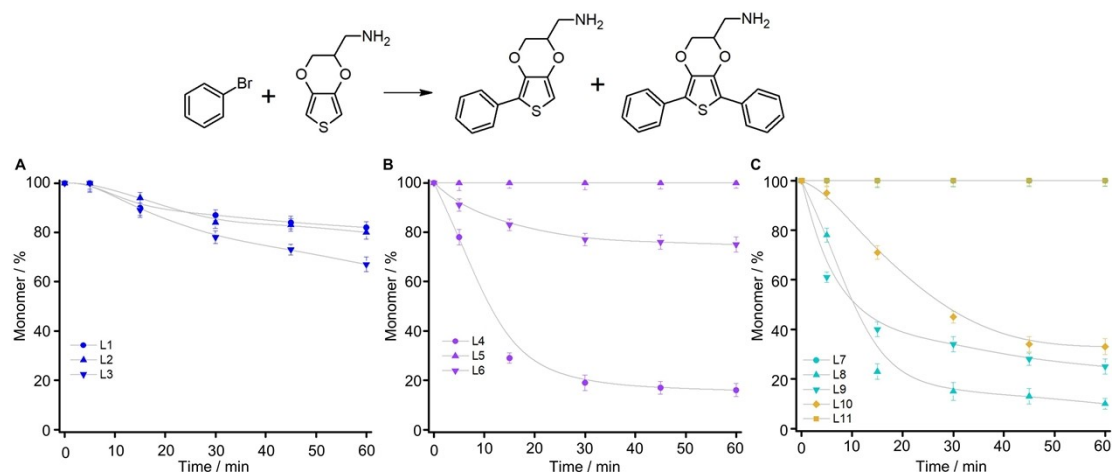


Figure S3 Consumption of EDOT-NH₂ monitored by ¹H NMR for the direct arylation of bromobenzene (0.2625 M) with EDOT-NH₂ (0.125 M), KPivO (0.2625 M) and Pd(OAc)₂ (10 mol %) under various ligand conditions. (A) Phosphine ligands P1-P3 (20 mol %) at 120 °C, (B) Phosphine ligands P4-P6 (20 mol %) at 120 °C, (C) Phosphine ligands P7-P11 (20 mol %) at 120 °C.

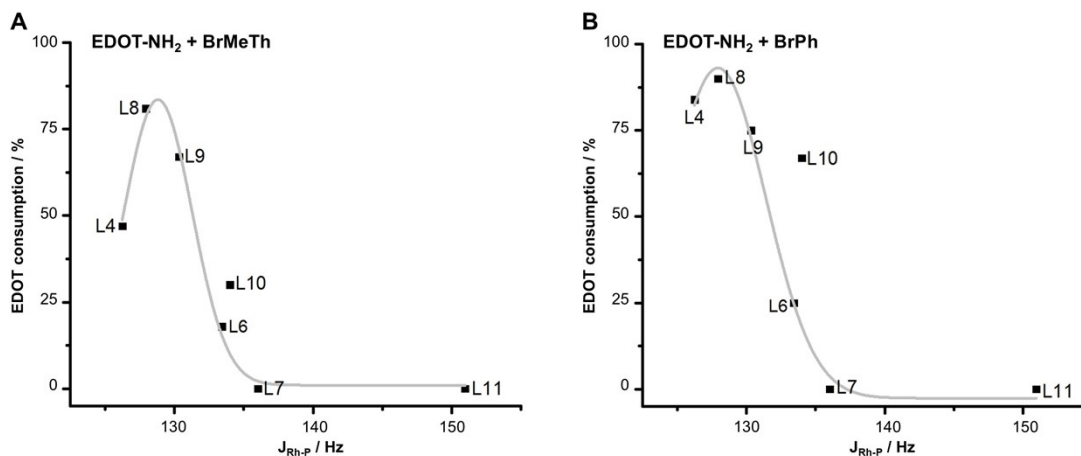


Figure S4 The plot for the consumption of EDOT as a function of aryl-phosphine ligands' EDS (L4-L11).

5. Computational Studies

5.1 Computational methods.

All calculations were performed with the Gaussian 09 package⁷. Geometry optimizations and frequency calculations were carried out via density functional theory (DFT) at the M06L/ (SDD basis-set for Pd and 6-31G(d) for all other atoms)^{8,9}. Single point energy calculations were performed by M06-L/(SDD basis-set for Pd and 6-311++G(d,p) for all other atoms) and corrected by Gibbs free energy corrections to simulate the whole concerted metalation-deprotonation process. PCM solvent compensation (DMAc, $\epsilon=37.781$) was assessed throughout the study. The intrinsic reaction coordinates (IRC) were followed to verify the connections between reactants and products for all transition states, and subsequently, the geometry optimization was carried out until the corresponding minima were reached.

The electrostatic potential (ESP) characteristic parameter of pristine EDOT was calculated using Multiwfn 3.7(dev) programs with the electronic wave function information. The corresponding ESP distribution was plotted by VMD¹⁰. The geometry optimization of selected phosphine ligands was calculated using the DFT at M06L/6-31G(d) level.

Moreover, the Tolman cone angle θ of those ligands was calculated by Solid-G

software with a metal-P distance of 2.28 Å^{11, 12}. The Tolman cone angle θ of the metal-L1 complex was visualized in the schematic presentation using VMD and Multiwfn 3.7(dev) programs, as embedded in Figure 3C. The frontier orbitals were calculated using Gaussian 09 programs with electronic wave function information and visualized through the VMD and Multiwfn 3.7(dev) programs.

The Wiberg bond order (WBO) was calculated for the optimized structure of reaction intermediates using the natural bond order (NBO). The atomic orbital pair contributions for the optimized structure of reaction intermediates were further calculated using the natural atomic orbital (NAO) analysis. Both were calculated by using the Gaussian input file of a single point task with *pop=full*, *NBORead* keyword in the route section, and *DMNAO NAOMO* keyword added between \$NBO ... \$END field after the molecular geometry section. The functional and basis sets employed in the optimization were identical to those previously utilized. The contributions from NAO pairs were obtained from Multiwfn 3.7(dev) program.

5.2 Computational results.

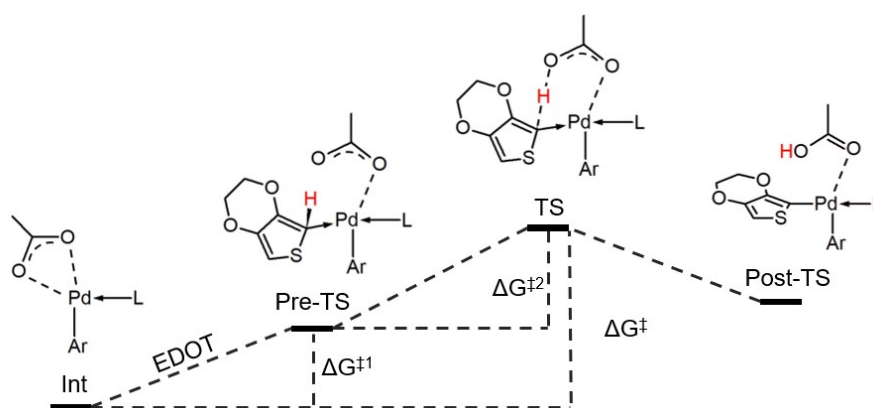


Figure S5 The typical concerted metalation-deprotonation (CMD) pathway for EDOT activation, where a prior intermediate (Pre-TS) occurs ahead of the transition state (TS).

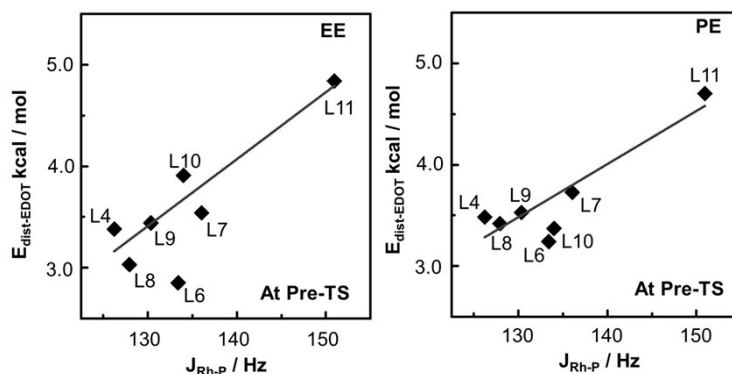


Figure S6 The plots of the distortion energies (kcal/mol) of EDOT at Pre-TS as a function of J_{Rh-P} for the Pre-TS involving **(Left)** EDOT/**(Right)** benzene (oxidative addition substrate) and EDOT (arylation substrate). EE/PE indicates the CMD processes of coupling between EDOT/benzene (oxidative addition substrate) and EDOT (arylation substrate).

Table S9 Summary of the energies (ΔE) and free energies (ΔG) of the potential energy surface 1 from (Int + EDOT) to Pre-TS_{EE} and the potential energy surface 2 from Pre-TS_{EE} to TS_{EE} shown in Figure S1 with different phosphine ligands, and the distortion energies (E_{dist}) of PdL and ArH at Pre-TS_{EE} with different phosphine ligands. All values are given in Kcal/mol.

Ligand	$\Delta E^{\ddagger 1}$	$\Delta G^{\ddagger 1}$	$\Delta E^{\ddagger 2}$	$\Delta G^{\ddagger 2}$	$E_{dist}(PdL)$	$E_{dist}(ArH)$
L1	-5.59	9.03	17.89	17.05	10.93	3.47
L2	-8.27	11.09	18.15	13.71	8.63	2.98
L3	-10.25	3.94	20.81	17.69	8.32	2.97
L4	-7.01	4.63	19.72	17.01	7.49	3.39
L5	-9.15	9.35	17.33	14.01	11.87	3.71
L6	-9.47	6.97	17.32	12.48	9.41	2.85
L7	-9.17	7.22	17.56	14.32	9.80	3.54
L8	-9.67	5.23	15.91	15.89	8.29	3.44
L9	-11.71	5.67	16.72	14.80	7.79	3.04
L10	-12.03	3.91	15.86	13.20	7.98	3.91
L11	-12.03	5.16	14.41	10.34	7.50	4.85
DMAc	-14.69	2.66	14.51	8.88	16.80	8.68

Table S10 Summary of the energies (ΔE) and free energies (ΔG) of the potential energy surface from (Int + EDOT) to TS_{EE} shown in Figure S1 with different phosphine ligands and the distortion-interaction energies for TS_{EE} with different phosphine ligands. All values are given in Kcal/mol.

Ligand	ΔE^\ddagger	ΔG^\ddagger	$E_{\text{dist}}(\text{PdL})$	$E_{\text{dist}}(\text{ArH})$	$E_{\text{dist}}(\text{total})$	E_{int}
L1	12.30	26.08	19.77	45.95	65.73	53.43
L2	9.88	24.80	15.29	50.11	65.40	55.52
L3	11.43	21.63	16.19	50.64	66.83	55.40
L4	9.47	21.63	15.22	49.63	64.85	55.38
L5	10.32	23.36	18.04	47.86	65.90	55.58
L6	8.17	19.45	16.23	45.95	62.18	54.01
L7	8.09	21.54	15.34	48.63	63.98	55.89
L8	6.73	20.03	14.51	38.77	53.27	46.54
L9	7.05	21.56	15.50	39.27	54.77	47.72
L10	4.15	17.10	15.06	35.52	54.58	50.43
L11	2.38	15.50	14.26	38.00	52.25	49.87
DMAc	-0.18	7.79	19.47	36.45	55.92	58.00

Table S11 Summary of the energies (ΔE) and free energies (ΔG) of the potential energy surface 1 from (Int + EDOT) to Pre- TS_{PE} and the potential energy surface 2 from Pre- TS_{PE} to TS_{PE} shown in Figure S1 with different phosphine ligands, and the distortion energies (E_{dist}) of PdL and ArH at Pre- TS_{PE} with different phosphine ligands. All values are given in Kcal/mol.

Ligand	$\Delta E^{\ddagger 1}$	$\Delta G^{\ddagger 1}$	$\Delta E^{\ddagger 2}$	$\Delta G^{\ddagger 2}$	$E_{\text{dist}}(\text{PdL})$	$E_{\text{dist}}(\text{ArH})$
L1	-4.07	8.28	15.47	15.47	12.86	2.79
L2	-5.36	6.36	17.52	17.52	11.84	2.66
L3	-8.13	7.33	15.70	15.70	9.05	2.77
L4	-9.21	5.36	18.35	14.08	8.55	3.48
L5	-9.65	9.25	14.42	14.42	9.71	3.50
L6	-9.09	10.86	14.43	14.43	9.96	3.24
L7	-9.40	7.26	17.63	11.22	9.42	3.73
L8	-9.81	6.33	18.13	12.45	8.30	3.42
L9	-10.33	6.07	18.10	13.41	7.94	3.53
L10	-10.52	-1.82	16.52	13.47	8.39	3.37
L11	-20.21	-3.81	17.34	15.36	9.38	4.70
DMAc	-12.71	2.66	13.69	11.01	15.69	7.24

Table S12 Summary of the energies (ΔE) and free energies (ΔG) of the potential energy surface from (Int + EDOT) to TS_{PE} shown in Figure S1 with different phosphine ligands and the distortion-interaction energies for TS_{PE} with different phosphine ligands. All values are given in Kcal/mol.

Ligand	ΔE^\ddagger	ΔG^\ddagger	$E_{dist}(PdL)$	$E_{dist}(ArH)$	$E_{dist}(total)$	E_{int}
L1	13.00	23.75	19.36	45.52	64.88	51.88
L2	12.09	23.88	17.32	47.20	64.52	52.43
L3	9.71	23.04	14.88	43.89	58.77	49.06
L4	9.14	19.43	14.82	41.20	56.02	46.88
L5	7.31	23.67	13.97	39.12	53.08	45.77
L6	8.81	25.59	14.77	37.42	52.12	43.37
L7	8.22	18.47	15.19	39.34	54.53	46.31
L8	8.42	18.78	14.92	43.05	57.97	49.65
L9	7.78	19.47	14.80	42.98	57.77	50.00
L10	6.00	11.65	15.54	40.33	55.87	49.87
L11	-2.87	11.55	15.67	37.63	53.30	46.64
DMAc	0.98	13.67	18.79	34.90	53.69	52.71

Table S13 WBOs of Pd-L, Pd-C, and C-H bonds of different intermediates in the CMD process for coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

Ligand	Pre-TS			TS			Post-Ts		
	WBO (Pd-L)	WBO (Pd-C)	WBO (C-H)	WBO (Pd -L)	WBO (Pd -C)	WBO (C-H)	WBO (Pd-L)	WBO (Pd-C)	WBO (C-H)
L1	0.611	0.220	0.844	0.528	0.430	0.302	0.494	0.539	0.079
L2	0.637	0.205	0.853	0.560	0.415	0.281	0.528	0.521	0.081
L3	0.618	0.208	0.843	0.555	0.418	0.281	0.497	0.529	0.048
L4	0.619	0.235	0.854	0.550	0.428	0.284	0.517	0.582	0.036
L5	0.581	0.250	0.829	0.522	0.445	0.293	0.483	0.573	0.063
L6	0.575	0.219	0.838	0.495	0.431	0.318	0.451	0.552	0.069
L7	0.594	0.250	0.834	0.535	0.442	0.291	0.479	0.566	0.043
L8	0.615	0.236	0.856	0.551	0.410	0.362	0.513	0.590	0.034
L9	0.616	0.220	0.859	0.543	0.417	0.369	0.518	0.585	0.033
L10	0.610	0.245	0.860	0.539	0.428	0.364	0.507	0.541	0.087
L11	0.574	0.286	0.851	0.507	0.454	0.380	0.467	0.617	0.032
DMAc	0.283	0.448	0.847	0.264	0.550	0.394	0.248	0.688	0.044

Table S14 WBOs of Pd-L, Pd-C, and C-H bonds of different intermediates in the CMD process for coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

Ligand	Pre-TS			TS			Post-Ts		
	WBO (Pd-L)	WBO (Pd-C)	WBO (C-H)	WBO (Pd-L)	WBO (Pd-C)	WBO (C-H)	WBO (Pd-L)	WBO (Pd-C)	WBO (C-H)
L1	0.589	0.203	0.840	0.521	0.404	0.305	0.476	0.525	0.052
L2	0.613	0.202	0.846	0.554	0.392	0.296	0.523	0.510	0.075
L3	0.595	0.208	0.834	0.539	0.386	0.323	0.500	0.514	0.054
L4	0.602	0.231	0.858	0.550	0.392	0.339	0.527	0.556	0.036
L5	0.583	0.231	0.854	0.536	0.399	0.360	0.507	0.569	0.039
L6	0.567	0.219	0.858	0.511	0.373	0.374	0.477	0.554	0.045
L7	0.589	0.240	0.858	0.532	0.399	0.291	0.505	0.572	0.036
L8	0.603	0.229	0.857	0.548	0.399	0.362	0.526	0.557	0.036
L9	0.598	0.233	0.858	0.545	0.398	0.369	0.520	0.561	0.037
L10	0.594	0.227	0.856	0.544	0.404	0.364	0.514	0.524	0.082
L11	0.572	0.274	0.855	0.524	0.419	0.380	0.488	0.585	0.033
DMAc	0.266	0.392	0.852	0.245	0.506	0.405	0.234	0.656	0.048

5.3 Atomic orbital pair contributions (AOPC) for reaction intermediates by NAO analysis.

Table S15 The AOPC for WBOs of Pd-C bond between palladium and arylation substrate in Pre-TS for coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

State	5s-2p	4d-2p	Total
Pre-TS_{EE}(L1)	-	0.0986	0.2195
Pre-TS_{EE}(L2)	-	0.0867	0.2051
Pre-TS_{EE}(L3)	-	0.0904	0.2079
Pre-TS_{EE}(L4)	-	0.0974	0.2350
Pre-TS_{EE}(L5)	-	0.1069	0.2496
Pre-TS_{EE}(L6)	-	0.0952	0.2187
Pre-TS_{EE}(L7)	-	0.1058	0.2497
Pre-TS_{EE}(L8)	-	0.0919	0.2196
Pre-TS_{EE}(L9)	-	0.1004	0.2366
Pre-TS_{EE}(L10)	-	0.1019	0.2445
Pre-TS_{EE}(L11)	0.0535	0.1256	0.2863
Pre-TS_{EE}(DMAc)	0.0727	0.2434	0.4481

Table S16 The AOPC for WBOs of Pd-C bond between palladium and arylation substrate in Pre-TS for coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

State	5s-2p	4d-2p	Total
Pre-TS_{PE}(L1)	-	0.0889	0.2033
Pre-TS_{PE}(L2)	-	0.0858	0.2027
Pre-TS_{PE}(L3)	-	0.0885	0.2078
Pre-TS_{PE}(L4)	-	0.0893	0.2306
Pre-TS_{PE}(L5)	-	0.0876	0.2314
Pre-TS_{PE}(L6)	-	0.0862	0.2189
Pre-TS_{PE}(L7)	-	0.0920	0.2400
Pre-TS_{PE}(L8)	-	0.0882	0.2289
Pre-TS_{PE}(L9)	-	0.0903	0.2325
Pre-TS_{PE}(L10)	-	0.0911	0.2268
Pre-TS_{PE}(L11)	0.0557	0.1088	0.2740
Pre-TS_{PE}(DMAc)	0.0609	0.2068	0.3921

Table S17 The AOPC for WBOs of Pd-L bond between palladium and phosphine ligand in Pre-TS for coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

State	5s-3s	5s-3p	5p-3s	4d-3s	4d-3p	Total
Pre-TS_{EE}(L1)	0.0673	0.1315	0.0682	0.0513	0.2300	0.6111
Pre-TS_{EE}(L2)	0.0678	0.1355	0.0577	0.0634	0.2505	0.6368
Pre-TS_{EE}(L3)	0.0654	0.1342	0.0550	0.0593	0.2481	0.6181
Pre-TS_{EE}(L4)	0.0676	0.1268	0.0596	0.0644	0.2303	0.6185
Pre-TS_{EE}(L5)	0.0670	0.1110	0.0683	0.0577	0.2074	0.5809
Pre-TS_{EE}(L6)	0.0661	0.1106	0.0570	0.0646	0.2166	0.5748
Pre-TS_{EE}(L7)	0.0674	0.1150	0.0617	0.0633	0.2175	0.5943
Pre-TS_{EE}(L8)	0.0672	0.1235	0.0582	0.0668	0.2325	0.6159
Pre-TS_{EE}(L9)	0.0679	0.1211	0.0630	0.0646	0.2275	0.6154
Pre-TS_{EE}(L10)	0.0667	0.1153	0.0626	0.0651	0.2288	0.6100
Pre-TS_{EE}(L11)	0.0662	0.1034	0.0681	0.0594	0.2033	0.5738

Pre-TS_{EE}(DMAc)	5s-2p (0.0520)/4d-2p (0.0786)	0.2826
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Table S18 The AOPC for WBOs of Pd-L bond between palladium and phosphine ligand in Pre-TS for coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

State	6p-3s	5s-3s	5s-3p	5p-3s	4d-3s	4d-3p	Total
Pre-TS_{PE}(L1)	-	0.0704	0.1335	0.0719	-	0.2024	0.5893
Pre-TS_{PE}(L2)	-	0.0727	0.1428	0.0605	0.0551	0.2177	0.6129
Pre-TS_{PE}(L3)	-	0.0688	0.1390	0.0592	0.0519	0.2166	0.5952
Pre-TS_{PE}(L4)	-	0.0715	0.1310	0.0605	0.0576	0.2114	0.6019
Pre-TS_{PE}(L5)	-	0.0705	0.1085	0.720	0.0556	0.2047	0.5843
Pre-TS_{PE}(L6)	-	0.0695	0.1099	0.0599	0.0594	0.2057	0.5667
Pre-TS_{PE}(L7)	-	0.0705	0.1157	0.0652	0.0580	0.2067	0.5888
Pre-TS_{PE}(L8)	-	0.0720	0.1305	0.0603	0.0581	0.2118	0.6027
Pre-TS_{PE}(L9)	-	0.0714	0.1283	0.0610	0.0573	0.2102	0.5984
Pre-TS_{PE}(L10)	-	0.0710	0.1202	0.0638	0.0570	0.2104	0.5938
Pre-TS_{PE}(L11)	0.0667	0.0679	0.1050	-	0.0531	0.1978	0.5715
Pre-TS_{PE}(DMAc)		5s-2p (0.0508)/4d-2p(0.0626)					0.2826

Table S19 The AOPC for WBOs of Pd-C bond between palladium and arylation substrate in TS for coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

TS	6s-2p	5p-2s	5s-2p	4d-2s	4d-2p	Total
TS_{EE}(L1)	-	-	0.0619	0.0543	0.1755	0.4179
TS_{EE}(L2)	-	-	0.0665	-	0.1550	0.4148
TS_{EE}(L3)	-	-	0.0656	-	0.1542	0.4179
TS_{EE}(L4)	0.0749	0.0501	-	-	0.1532	0.4276
TS_{EE}(L5)	-	-	0.0688	0.0548	0.1649	0.4450
TS_{EE}(L6)	-	-	0.0703	0.0519	0.1700	0.4307
TS_{EE}(L7)	-	-	0.0767	0.0520	0.1602	0.4421
TS_{EE}(L8)	0.0735	-	-	-	0.1527	0.4100
TS_{EE}(L9)	-	-	0.0758	-	0.1582	0.4174
TS_{EE}(L10)	-	-	0.0765	-	0.1649	0.4283
TS_{EE}(L11)	-	-	0.0819	0.0501	0.1817	0.4542
TS_{EE}(DMAc)	-	-	0.0950	0.0751	0.2644	0.5534

Table S20 The AOPC for WBOs of Pd-C bond between palladium and arylation substrate in TS for coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

TS	5s-2p	4d-2s	4d-2p	Total
TS_{PE}(L1)	0.0693	-	0.1502	0.4039
TS_{PE}(L2)	0.0715	-	0.1376	0.3925
TS_{PE}(L3)	0.0720	-	0.1341	0.3864
TS_{PE}(L4)	0.0788	-	0.1309	0.3916
TS_{PE}(L5)	0.0686	0.0526	0.1378	0.3985
TS_{PE}(L6)	0.0718	-	0.1306	0.3733
TS_{PE}(L7)	0.0798	-	0.1370	0.3991
TS_{PE}(L8)	0.0802	-	0.1335	0.3990
TS_{PE}(L9)	0.0800	-	0.1344	0.3983
TS_{PE}(L10)	0.0804	-	0.1403	0.4041
TS_{PE}(L11)	0.0853	-	0.1477	0.4192
TS_{PE}(DMAc)	0.0980	0.0631	0.2240	0.5057

Table S21 The AOPC for WBOs of Pd-P bond between palladium and phosphine ligand in TS for coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

TS	6s-3s	6s-3p	5s-3s	5s-3p	5p-3s	5p-3p	4d-3s	4d-3p	Total
TS_{EE}(L1)	-	-	0.0586	0.1181	0.0728	0.0505	-	0.1668	0.5282
TS_{EE}(L2)	-	-	0.0614	0.1236	0.0638	-	-	0.1888	0.5595
TS_{EE}(L3)	-	-	0.0581	0.1212	0.0657	-	-	0.1903	0.5551
TS_{EE}(L4)	0.0591	0.1151			0.0636	0.0512	0.0512	0.1818	0.5499
TS_{EE}(L5)	-	-	0.0575	0.1001	0.0754	0.0575	-	0.1616	0.5222
TS_{EE}(L6)	-	-	0.0585	0.1025	0.0616	-	-	0.1577	0.4949
TS_{EE}(L7)	-	-	0.0582	0.1034	0.0682	0.0514	0.0501	0.1750	0.5351
TS_{EE}(L8)	0.0602	0.1134			0.0645	0.0505	0.0516	0.1817	0.5507
TS_{EE}(L9)	-	-	0.0599	0.1119	0.0645	0.0503	0.0501	0.1780	0.5429
TS_{EE}(L10)	-	-	0.0593	0.1079	0.0670	0.0504	-	0.1768	0.5393
TS_{EE}(L11)	-	-	0.0568	0.0948	0.0703	0.0508	-	0.1614	0.5067
TS_{EE}(DMAc)			5s-2p (0.0509) / 4d-2p (0.0596)						0.2543

Table S22 The AOPC for WBOs of Pd-P bond between palladium and phosphine ligand in TS for coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

TS	6s-3s	6s-3p	5s-3s	5s-3p	5p-3s	5p-3p	4d-3s	4d-3p	Total	
TS_{PE}(L1)	-	-	0.0630	0.1278	0.0724	-	-	0.1506	0.5206	
TS_{PE}(L2)	-	-	0.0668	0.1342	0.0647	-	-	0.1721	0.5544	
TS_{PE}(L3)	-	-	0.0609	0.1290	0.0646	-	-	0.1724	0.5386	
TS_{PE}(L4)	-	-	0.0656	0.1252	0.0636	-	-	0.1724	0.5497	
TS_{PE}(L5)	-	-	0.0652	0.1073	0.0781	-	-	0.1602	0.5359	
TS_{PE}(L6)	-	-	0.0632	0.1086	0.0620	-	-	0.1626	0.5107	
TS_{PE}(L7)	-	-	0.0636	0.1112	0.0665	-	-	0.1671	0.5315	
TS_{PE}(L8)	-	-	0.0657	0.1242	0.0639	-	-	0.1701	0.5476	
TS_{PE}(L9)	-	-	0.0653	0.1230	0.0640	-	-	0.1709	0.5449	
TS_{PE}(L10)	-	-	0.0646	0.1167	0.0675	-	-	0.1719	0.5440	
TS_{PE}(L11)	-	-	0.0618	0.1034	0.0708	-	-	0.1666	0.5240	
TS_{PE}(DMAc)			5s-2p (0.0517) / 4d-2p (0.0523)							0.2449

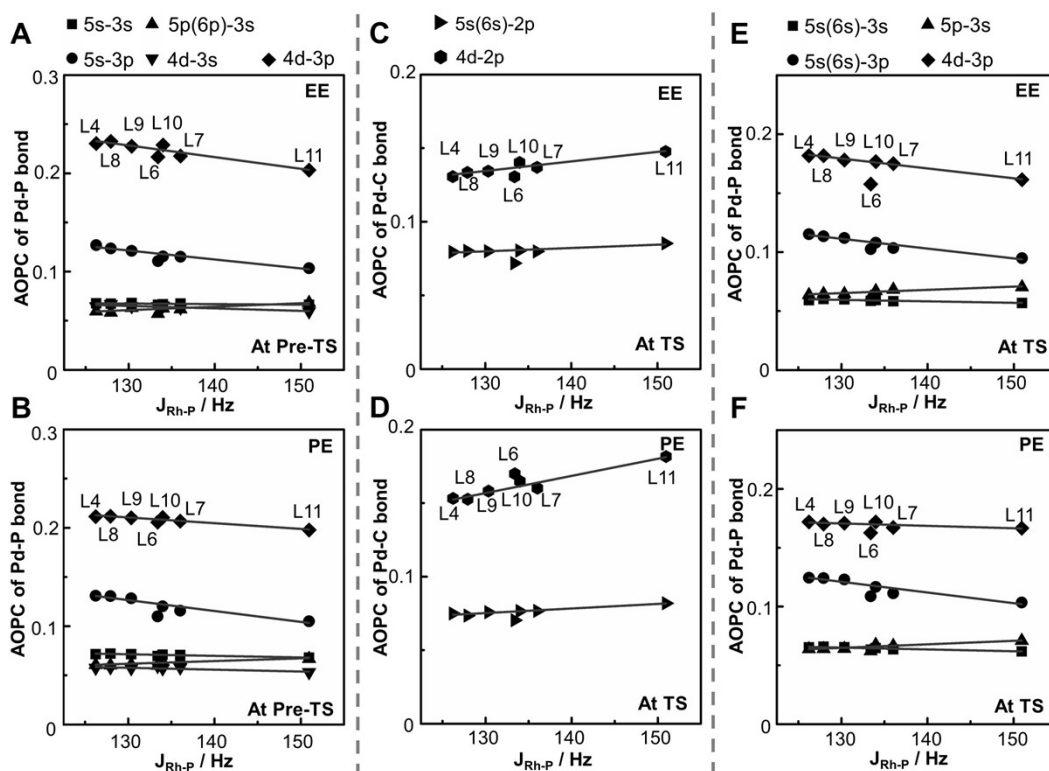


Figure S7 (A and B) The atomic orbital pair contribution of Pd(5s)-P(3s), Pd(5s)-P(3p), Pd(5p/6p)-P(3s), Pd(4d)-P(3s) and Pd(4d)-P(3p) to WBOs of the Pd-P bonds as a function of J_{Rh-P} for the pre-TS of the coupling between (A) EDOT/(B) benzene (oxidative addition substrate) and EDOT (arylation substrate). **(C and D)** The atomic orbital pair contribution of Pd(5s/6s)-C(2p) and Pd(4d)-C(2p) to WBOs of the Pd-C bonds as a function of J_{Rh-P} for the TS of the coupling between (C) EDOT/(D) benzene (oxidative addition substrate) and EDOT (arylation substrate). **(E and F)** The atomic orbital pair contribution of Pd(5s/6s)-P(3s), Pd(5s/6s)-P(3p), Pd(5p)-P(3s) and Pd(4d)-P(3p) to WBOs of the Pd-P bonds as a function of J_{Rh-P} for the pre-TS of coupling between (E) EDOT/(F) benzene (oxidative addition substrate) and EDOT (arylation substrate).

Table S23 The AOPC for WBOs of EDOT C_α-C_β bond in Pre-TS for the coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

State	2px-2px	2px-2py	2py-2px	2pz-2pz	2p-2p	Total
EDOT	0.2017	0.0894	0.0588	0.5414	0.8969	1.5443
Pre-TS_{EE}(L1)	0.2042	0.0910	0.0664	0.4980	0.8730	1.5098
Pre-TS_{EE}(L2)	0.2016	0.0901	0.0639	0.5010	0.8771	1.5153
Pre-TS_{EE}(L3)	0.2003	0.0898	0.0632	0.4991	0.8766	1.5149
Pre-TS_{EE}(L4)	0.2009	0.0900	0.0637	0.4946	0.8738	1.5112
Pre-TS_{EE}(L5)	0.2023	0.0910	0.0650	0.4936	0.8709	1.5082
Pre-TS_{EE}(L6)	0.2008	0.0906	0.0643	0.5018	0.8769	1.5148
Pre-TS_{EE}(L7)	0.2016	0.0906	0.0644	0.4943	0.8724	1.5096
Pre-TS_{EE}(L8)	0.2055	0.0902	0.0601	0.4913	0.8707	1.5071
Pre-TS_{EE}(L9)	0.2050	0.0902	0.0600	0.4959	0.8728	1.5101
Pre-TS_{EE}(L10)	0.2086	0.0902	0.0630	0.4886	0.8662	1.5024
Pre-TS_{EE}(L11)	0.2057	0.0903	0.0624	0.4751	0.8614	1.4959
Pre-TS_{EE}(DMAc)	0.2063	0.0749	0.0903	0.4418	0.8426	1.4693

Table S24 The AOPC for WBOs of EDOT C_α-C_β bond in Pre-TS for the coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

State	2px-2px	2px-2py	2py-2px	2pz-2pz	2p-2p	Total
EDOT	0.2017	0.0894	0.0588	0.5414	0.8969	1.5443
Pre-TS_{PE}(L1)	0.2027	0.0910	0.0657	0.5048	0.8768	1.5145
Pre-TS_{PE}(L2)	0.2015	0.0907	0.0646	0.5047	0.8776	1.5155
Pre-TS_{PE}(L3)	0.2002	0.0907	0.0638	0.5021	0.8765	1.5151
Pre-TS_{PE}(L4)	0.2069	0.0906	0.0641	0.4983	0.8700	1.5086
Pre-TS_{PE}(L5)	0.2068	0.0907	0.0643	0.4986	0.8697	1.5092
Pre-TS_{PE}(L6)	0.2059	0.0907	0.0641	0.5004	0.8717	1.5113
Pre-TS_{PE}(L7)	0.2069	0.0907	0.0647	0.4956	0.8684	1.5072
Pre-TS_{PE}(L8)	0.2066	0.0906	0.0638	0.4984	0.8703	1.5093
Pre-TS_{PE}(L9)	0.2068	0.0905	0.0641	0.4970	0.8696	1.5080
Pre-TS_{PE}(L10)	0.2089	0.0896	0.0592	0.4983	0.8736	1.5111
Pre-TS_{PE}(L11)	0.2081	0.0911	0.0666	0.4859	0.8628	1.4992
Pre-TS_{PE}(DMAc)	0.2029	0.0728	0.0936	0.4552	0.8494	1.4798

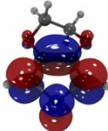

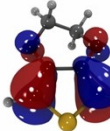


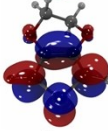
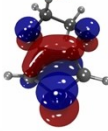
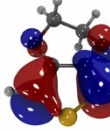
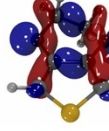
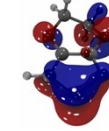
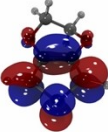
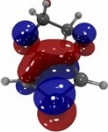
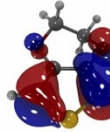
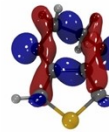
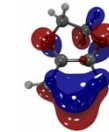
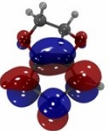
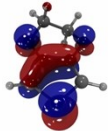
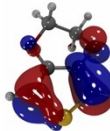
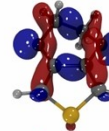
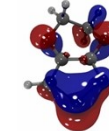
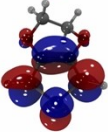
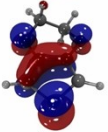
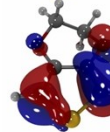
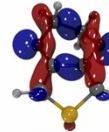
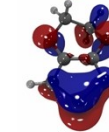
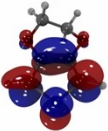
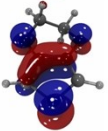
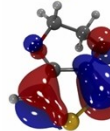
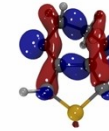
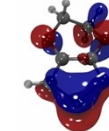
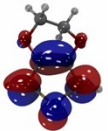
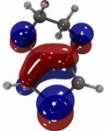
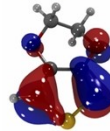
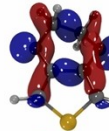
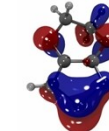
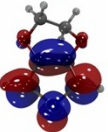
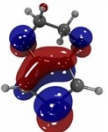
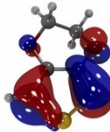
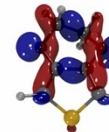
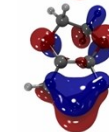
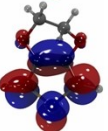
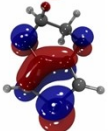
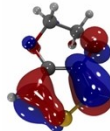

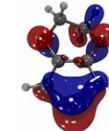
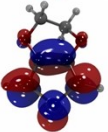
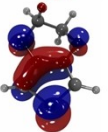
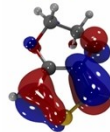
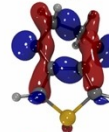
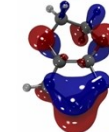
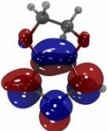
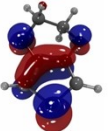
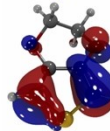
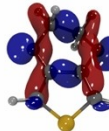

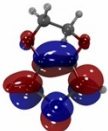
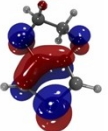
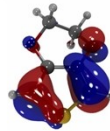
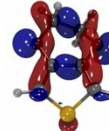

Table S25 The energy levels for the frontier orbitals of EDOT and those of Pre-TS EDOT for the coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

	LUMO (eV)	HOMO (eV)	HOMO-1 (eV)	HOMO-2 (eV)	HOMO-3 (eV)
EDOT	-1.05	-5.46	-5.54	-7.67	-8.23
EDOT_{EE}(L1)	-1.29	-5.39	-5.49	-7.84	-8.23
EDOT_{EE}(L2)	-1.24	-5.38	-5.49	-7.83	-8.24
EDOT_{EE}(L3)	-1.24	-5.38	-5.49	-7.81	-8.25
EDOT_{EE}(L4)	-1.26	-5.38	-5.49	-7.82	-8.25
EDOT_{EE}(L5)	-1.28	-5.38	-5.49	-7.84	-8.24
EDOT_{EE}(L6)	-1.24	-5.39	-5.49	-7.83	-8.98
EDOT_{EE}(L7)	-1.27	-5.38	-5.49	-7.83	-8.25
EDOT_{EE}(L8)	-1.26	-5.37	-5.51	-7.84	-8.25
EDOT_{EE}(L9)	-1.24	-5.37	-5.51	-7.82	-8.26
EDOT_{EE}(L10)	-1.31	-5.39	-5.50	-7.85	-8.23
EDOT_{EE}(L11)	-1.33	-5.37	-5.51	-7.85	-8.26
EDOT_{EE}(DMAc)	-1.30	-5.22	-5.33	-7.70	-8.05

Table S26 The energy levels for the frontier orbitals of Pre-TS EDOT for the coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

	LUMO (eV)	HOMO (eV)	HOMO-1 (eV)	HOMO-2 (eV)	HOMO-3 (eV)
EDOT_{PE}(L1)	-1.25	-5.40	-5.48	-7.82	-8.24
EDOT_{PE}(L2)	-1.24	-5.40	-5.48	-7.81	-8.25
EDOT_{PE}(L3)	-1.23	-5.39	-5.49	-7.79	-8.26
EDOT_{PE}(L4)	-1.30	-5.41	-5.49	-7.85	-8.22
EDOT_{PE}(L5)	-1.31	-5.41	-5.49	-7.85	-8.22
EDOT_{PE}(L6)	-1.29	-5.42	-5.50	-7.84	-8.22
EDOT_{PE}(L7)	-1.32	-5.41	-5.49	-7.85	-8.21
EDOT_{PE}(L8)	-1.30	-5.41	-5.49	-7.84	-8.22
EDOT_{PE}(L9)	-1.30	-5.40	-5.49	-7.85	-8.22
EDOT_{PE}(L10)	-1.27	-5.38	-5.50	-7.87	-8.22
EDOT_{PE}(L11)	-1.37	-5.41	-5.49	-7.87	-8.20
EDOT_{PE}(DMAc)	-1.25	-5.24	-5.31	-7.67	-8.07

Table S27 The frontier orbitals diagrams of EDOT and those of Pre-TS EDOT for the coupling between EDOT (oxidative addition substrate) and EDOT (arylation substrate).

	LUMO	HOMO	HOMO-1	HOMO-2	HOMO-3
EDOT					
EDOT _{EE} (L1)					
EDOT _{EE} (L2)					
EDOT _{EE} (L3)					
EDOT _{EE} (L4)					
EDOT _{EE} (L5)					
EDOT _{EE} (L6)					
EDOT _{EE} (L7)					
EDOT _{EE} (L8)					
EDOT _{EE} (L9)					
EDOT _{EE} (L10)					
EDOT _{EE} (L11)					

EDOT_{EE}(DMAc)

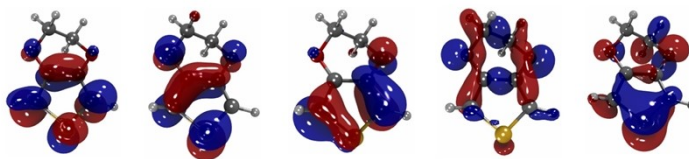
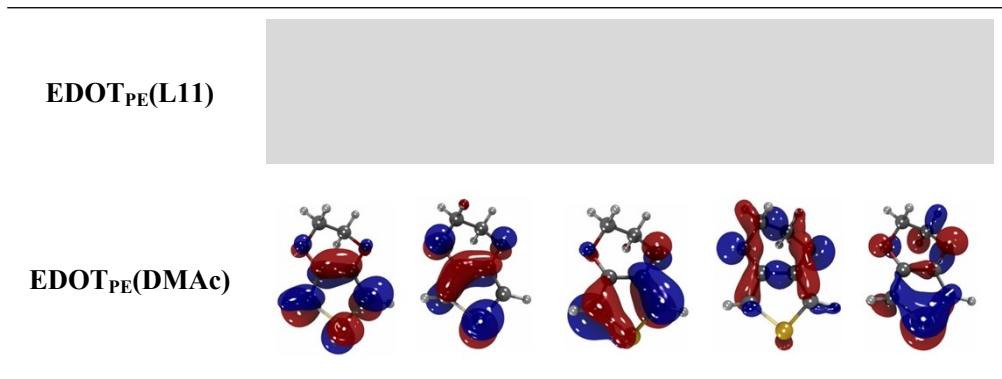


Table S28 The frontier orbitals diagrams of Pre-TS EDOTs for the coupling between benzene (oxidative addition substrate) and EDOT (arylation substrate).

	LUMO	HOMO	HOMO-1	HOMO-2	HOMO-3
EDOT _{PE} (L1)					
EDOT _{PE} (L2)					
EDOT _{PE} (L3)					
EDOT _{PE} (L4)					
EDOT _{PE} (L5)					
EDOT _{PE} (L6)					
EDOT _{PE} (L7)					
EDOT _{PE} (L8)					
EDOT _{PE} (L9)					
EDOT _{PE} (L10)					



6. Cartesian Coordinates

EDOT

M06-L electronic energy (Hartree): -780.905491

M06-L thermal correction to free energy (Hartree): 0.079796

Three lowest frequencies (cm⁻¹): 116.61, 202.45, 311.65

C	0.00896600	0.71275100	-0.04215700
C	0.00896100	-0.71275000	0.04210900
C	-1.25025100	1.24181100	-0.07593800
C	-1.25026200	-1.24179200	0.07599900
S	-2.44153100	-0.00000200	0.00000900
O	1.15660300	1.44440600	-0.09698700
C	2.29874400	0.68170400	0.32061000
O	1.15658300	-1.44440800	0.09696500
C	2.29876300	-0.68170700	-0.32058500
H	-1.53452900	2.28111300	-0.13349700
H	3.17501200	1.25413500	0.01740000
H	2.29420700	0.59264600	1.41376400
H	3.17501200	-1.25413300	-0.01731700
H	-1.53448700	-2.28113500	0.13318100
H	2.29427300	-0.59266400	-1.41373700

Int_{EE}(L1)

M06-L electronic energy (Hartree): -1951.834633

M06-L thermal correction to free energy (Hartree): 0.465889

Three lowest frequencies (cm⁻¹): 9.58, 26.96, 44.20

Pd	0.06706600	1.09030800	-0.08291400
O	-0.86628400	3.07988500	-0.12771700

O	1.30341200	2.91856900	-0.50274500
C	0.25929600	3.63130500	-0.36825600
C	0.34555500	5.12307700	-0.46207600
C	-1.55957800	0.13641500	0.52227700
C	-2.65892400	-0.25320400	-0.19994800
S	-1.99932300	0.22402500	2.20804300
C	-3.82040300	-0.52704000	0.59112300
C	-3.62462900	-0.31412100	1.92747700
H	-4.32587600	-0.45894300	2.73975600
O	-2.67630400	-0.36479400	-1.57149300
C	-3.73824500	-1.21921200	-2.00810300
H	-3.49742800	-2.26357400	-1.75530900
O	-4.99290500	-0.97462000	0.05302500
C	-5.04183800	-0.81168600	-1.36957500
H	-5.86624400	-1.44039000	-1.71537300
H	-5.26923400	0.23720300	-1.60982300
H	-3.78448300	-1.11815300	-3.09495000
H	0.47351200	5.54241000	0.54283700
H	1.20292600	5.43110500	-1.06564500
H	-0.57485900	5.54235500	-0.87754200
C	2.51976000	-0.40375700	1.55128100
C	2.62847800	-0.63211100	-1.56915700
C	0.77513600	-2.51330800	0.03791400
P	1.48923400	-0.73369600	-0.02863100
C	1.90830100	-1.25987700	-2.76798800
H	0.88521600	-0.87770700	-2.87821100
H	2.46069600	-0.98920700	-3.67761700
H	1.87183500	-2.35163900	-2.73002300
C	2.86080900	0.83392600	-1.95014200
H	1.92915200	1.31791100	-2.26095200
H	3.29369600	1.44165200	-1.15368900
H	3.55229000	0.85476500	-2.80391000
C	3.98839700	-1.31137100	-1.38315500
H	3.92006300	-2.35786500	-1.07342800
H	4.51531000	-1.29095400	-2.34715600
H	4.62321100	-0.78536000	-0.66328300
C	1.81770000	-3.61239500	-0.19770600
H	1.31617100	-4.58169500	-0.07184800
H	2.22671000	-3.59887800	-1.21170000
H	2.65082500	-3.58495900	0.51059100
C	-0.33403600	-2.67298700	-1.01622400
H	0.05898400	-2.92533900	-2.00404800
H	-0.98498400	-3.50392200	-0.71193600
H	-0.95891300	-1.78327800	-1.11620000

C	0.14056700	-2.75824200	1.41140200
H	0.87473900	-2.78884600	2.22206800
H	-0.62370300	-2.01387100	1.65455300
H	-0.34749600	-3.74160400	1.38747800
C	1.55803900	-0.04946400	2.69595100
H	0.82374600	-0.82747500	2.91942700
H	2.15032300	0.11941000	3.60587700
H	1.00850700	0.87602100	2.47854300
C	3.41747400	-1.56281800	1.98946500
H	4.03134600	-1.22384400	2.83529700
H	2.85020000	-2.43153900	2.33790900
H	4.10334700	-1.89389700	1.20365500
C	3.38871200	0.83996200	1.33024300
H	4.21899700	0.66926100	0.63812000
H	2.80155300	1.69283600	0.96814700
H	3.82870600	1.12401100	2.29585000

Pre-TS_{EE}(L1)

M06-L electronic energy (Hartree): -2732.749040

M06-L thermal correction to free energy (Hartree): 0.568997

Three lowest frequencies (cm⁻¹): 21.60, 29.17, 36.05

Pd	-0.35058100	0.73934500	-0.10926200
O	-0.92536000	3.47453600	-1.44136600
O	-1.35129000	2.55663200	0.57006300
C	-1.38913100	3.52224700	-0.28709900
C	-2.08518500	4.77057400	0.21331600
C	0.89550400	-0.70723800	-0.64868800
C	1.69451600	-1.49560700	0.13815600
S	1.31339900	-0.97384900	-2.31422000
C	2.61192800	-2.31642100	-0.58571400
C	2.51998000	-2.16252000	-1.94500500
H	3.10892700	-2.64317800	-2.71603000
O	1.60287800	-1.53620100	1.51201400
C	2.27750400	-2.66879200	2.06086300
H	1.66893300	-3.57494700	1.90888400
O	3.50018600	-3.15310700	0.03043500
C	3.63301000	-2.84480600	1.42383600
H	4.17721700	-3.68189300	1.86782000
H	4.22813800	-1.92528500	1.53916100
H	2.36660700	-2.47943100	3.13416800
C	3.54233100	1.24455500	0.79785500

C	2.76256700	1.75988400	-0.26619700
C	2.92689800	1.39593600	2.01708500
C	1.50151000	2.20772600	0.12609900
S	1.38798500	2.13039400	1.88074300
O	4.76194800	0.67477300	0.61353600
C	4.98095800	0.34647800	-0.76960300
O	3.19773600	1.81369000	-1.53543200
C	4.60032300	1.49768300	-1.66231000
H	3.28286600	1.02144800	2.96985600
H	6.04534800	0.11999100	-0.85982200
H	4.39393400	-0.54714300	-1.02626900
H	4.75198600	1.24779500	-2.71441000
H	0.94147200	2.95850200	-0.42626100
H	-3.16731500	4.59199100	0.25496200
H	-1.76615400	5.01972200	1.23062100
H	-1.90243000	5.62134700	-0.44815600
H	5.17944300	2.39702600	-1.41669400
C	-3.71769700	0.27441400	-0.85109600
C	-2.65735700	-0.90826100	1.84910600
C	-2.20285300	-2.43134700	-0.82037000
P	-2.26304000	-0.67876300	-0.01384400
C	-1.73128600	-1.97259500	2.44686400
H	-0.67486000	-1.76312600	2.23676000
H	-1.86185400	-1.96254300	3.53780700
H	-1.96457900	-2.98638900	2.10604000
C	-2.33537400	0.40070200	2.58078000
H	-1.27683500	0.66987000	2.47240600
H	-2.92493900	1.25248900	2.23631400
H	-2.54200800	0.25565400	3.65047500
C	-4.10778300	-1.29938200	2.15180300
H	-4.41083500	-2.23999000	1.68546200
H	-4.20425600	-1.43263100	3.23837300
H	-4.82836200	-0.52957400	1.86298000
C	-3.37595300	-3.32392000	-0.38609300
H	-3.37124100	-4.21693600	-1.02593000
H	-3.26079200	-3.67572500	0.64424300
H	-4.36077800	-2.86408900	-0.48096400
C	-0.91299400	-3.20705600	-0.48368500
H	-1.12643500	-4.27755000	-0.60923000
H	-0.10185800	-2.95455700	-1.16892100
H	-0.54427500	-3.06045800	0.53197900
C	-2.21634400	-2.29213200	-2.34694200
H	-3.17208200	-1.95175800	-2.75350300
H	-1.42382700	-1.62003400	-2.69710200

H	-2.01645400	-3.28199900	-2.77971700
C	-3.16023900	0.89348600	-2.14090500
H	-2.79487800	0.15213000	-2.85708400
H	-3.96456300	1.45719300	-2.63454700
H	-2.34144500	1.59196500	-1.92662900
C	-4.95918200	-0.56150300	-1.17980500
H	-5.70949000	0.11514000	-1.61192700
H	-4.78562800	-1.35093500	-1.91499000
H	-5.41129100	-1.01154100	-0.28907900
C	-4.20156900	1.43707000	0.02550100
H	-4.78293000	1.10466600	0.89056000
H	-3.38349200	2.06747800	0.37418200
H	-4.87204700	2.05653900	-0.58691600

TS_{EE}(L1)

M06-L electronic energy (Hartree): -2732.720523

M06-L thermal correction to free energy (Hartree): 0.567653

Three lowest frequencies (cm⁻¹): -483.15, 24.62, 31.33

Pd	-0.35407100	0.65521500	-0.02827800
O	0.49548100	3.73818300	-0.78174000
O	-1.28469600	2.70039900	0.11723200
C	-0.75250000	3.68323100	-0.44399900
C	-1.58319900	4.87959900	-0.79262200
C	0.73570900	-0.90309900	-0.63124800
C	1.67606600	-1.63310700	0.04819100
S	0.96709500	-1.16788900	-2.33909600
C	2.53868600	-2.41733900	-0.77636500
C	2.28050900	-2.27696200	-2.11339600
H	2.74476300	-2.79383200	-2.94428900
O	1.81117100	-1.60192100	1.41773000
C	2.53633200	-2.73370500	1.89768400
H	1.90667100	-3.63532900	1.83344600
O	3.52004800	-3.22506200	-0.26478000
C	3.80497800	-2.92780600	1.10672500
H	4.38573800	-3.77333300	1.48410500
H	4.42367200	-2.01824200	1.16646400
H	2.75953600	-2.53137600	2.94871500
C	3.81829400	1.25073600	0.89320400
C	2.80863500	1.28533700	-0.10948200
C	3.33636500	1.56815300	2.13668700
C	1.52731500	1.60248100	0.32927900
S	1.64555700	1.88144600	2.06716800

O	5.12049900	0.93237300	0.62878700
C	5.25675500	0.30184100	-0.65098100
O	3.08987700	1.05873500	-1.41727200
C	4.49372800	1.06146800	-1.70315000
H	3.89999600	1.64162800	3.05976500
H	6.32706100	0.28641700	-0.86915400
H	4.88665400	-0.73407400	-0.59485600
H	4.60115400	0.59268400	-2.68477400
H	0.97429900	2.78342600	-0.36980800
H	-1.94073100	4.77059300	-1.82385800
H	-2.45750800	4.94395600	-0.14089000
H	-0.99864100	5.80103100	-0.74080700
H	4.84886200	2.10015800	-1.76089700
C	-3.50663700	-0.01047600	-1.45845200
C	-3.44348500	0.02045300	1.66325100
C	-2.41904200	-2.45113000	0.15736000
P	-2.49702500	-0.52612700	0.08331100
C	-2.85546500	-0.71630300	2.87299700
H	-1.75824300	-0.66814200	2.88894000
H	-3.21948700	-0.22514900	3.78559600
H	-3.15792900	-1.76449900	2.93331800
C	-3.20238100	1.50789300	1.94027500
H	-2.14470400	1.71236700	2.13944000
H	-3.51675200	2.16677700	1.12941600
H	-3.77285500	1.78052300	2.83962100
C	-4.95729100	-0.21425200	1.61543000
H	-5.23907200	-1.24029000	1.36607800
H	-5.37248000	0.00626800	2.60912300
H	-5.45920700	0.45446000	0.90844400
C	-3.73189600	-3.14229200	0.54722400
H	-3.56708900	-4.22814900	0.49854800
H	-4.04602000	-2.91969400	1.57101900
H	-4.56381100	-2.91301700	-0.12636300
C	-1.33851500	-2.88327800	1.16801200
H	-1.73472000	-2.98231700	2.18170600
H	-0.96004000	-3.87297600	0.87659300
H	-0.48261600	-2.20450700	1.20044200
C	-2.00751400	-3.00169000	-1.21279700
H	-2.76278900	-2.83723600	-1.98711800
H	-1.05642300	-2.58825300	-1.55803000
H	-1.88296800	-4.08890300	-1.11722700
C	-2.54395200	-0.03638400	-2.65525200
H	-2.10553500	-1.02011100	-2.84579000
H	-3.09107900	0.26688600	-3.55912300

H	-1.71714900	0.67269100	-2.50724600
C	-4.73509200	-0.86816300	-1.76772600
H	-5.25259300	-0.43576000	-2.63563900
H	-4.48535300	-1.90097300	-2.02792200
H	-5.45230000	-0.88870200	-0.94059700
C	-3.96470400	1.44507200	-1.30994800
H	-4.75927400	1.56856600	-0.56750900
H	-3.13737600	2.11255500	-1.04666800
H	-4.37268200	1.77563000	-2.27530100

Post-TS_{EE}(L1)

M06-L electronic energy (Hartree): -2732.725075

M06-L thermal correction to free energy (Hartree): 0.565592

Three lowest frequencies (cm⁻¹): 17.35, 23.61, 28.32

Pd	-0.25510500	0.60635000	0.00168200
O	0.62818000	3.54259200	-1.19936900
O	-1.06054300	2.77272200	0.07577600
C	-0.56769700	3.64284200	-0.65170600
C	-1.30148300	4.88963000	-1.01075900
C	0.72696200	-1.01599300	-0.60235700
C	1.56575000	-1.87456000	0.05834000
S	0.88807400	-1.29416000	-2.31502300
C	2.27593500	-2.78176600	-0.78721700
C	2.01573400	-2.59588300	-2.11787100
H	2.37950400	-3.17213800	-2.95944700
O	1.73056600	-1.88037300	1.42706000
C	2.24154000	-3.13592500	1.87766000
H	1.45899600	-3.90688200	1.79426200
O	3.10887400	-3.75217000	-0.30064600
C	3.45229400	-3.53489100	1.07169700
H	3.87648600	-4.47682700	1.42936000
H	4.22155400	-2.75058000	1.13916100
H	2.49808500	-3.00355800	2.93180400
C	3.94051100	1.55141400	0.88829400
C	2.93031300	1.15052800	-0.04118100
C	3.42988800	2.08609900	2.03984600
C	1.63035700	1.37009300	0.37093900
S	1.70377100	2.09506600	1.96836900
O	5.27693600	1.41558000	0.63628800
C	5.51967200	0.48949700	-0.42826400

O	3.25081200	0.60522000	-1.25252900
C	4.62340300	0.78806800	-1.60138500
H	3.97621700	2.49444800	2.88148600
H	6.57445700	0.59894800	-0.69151000
H	5.34388200	-0.53692500	-0.07063800
H	4.81585400	0.10220300	-2.43131700
H	1.04477800	2.69931000	-0.82947600
H	-1.66500600	4.80329600	-2.04160400
H	-2.15856000	5.03033000	-0.35046900
H	-0.64161400	5.76002000	-0.97199800
H	4.78483700	1.82054100	-1.94714300
C	-3.51327000	0.18458100	-1.42024400
C	-3.41432300	0.22480800	1.69692400
C	-2.60242800	-2.32668400	0.18741300
P	-2.52991900	-0.40414400	0.11344800
C	-2.88143900	-0.54919900	2.90874900
H	-1.78397400	-0.59095500	2.92240000
H	-3.20190400	-0.02612100	3.82001700
H	-3.26940500	-1.56889000	2.97459700
C	-3.03680800	1.68772400	1.95266000
H	-1.95862600	1.79730700	2.11819800
H	-3.31506100	2.36762900	1.14558600
H	-3.55169000	2.01897300	2.86565300
C	-4.94161400	0.11306900	1.67013900
H	-5.30229800	-0.89842900	1.46482700
H	-5.32927200	0.40294300	2.65723100
H	-5.39941900	0.78788400	0.94015300
C	-3.95975300	-2.92062300	0.57892500
H	-3.88165000	-4.01553300	0.51790800
H	-4.24667300	-2.68400200	1.60780900
H	-4.77685500	-2.61785600	-0.08289500
C	-1.55230900	-2.83650600	1.19267700
H	-1.93579400	-2.87587800	2.21510100
H	-1.27277100	-3.86344800	0.91811800
H	-0.63802500	-2.23755400	1.19244900
C	-2.22364900	-2.89790600	-1.18363800
H	-2.95989900	-2.67527800	-1.96173400
H	-1.24368000	-2.54723900	-1.51937600
H	-2.17457200	-3.99197700	-1.09571300
C	-2.55763000	0.09871600	-2.62033800
H	-2.18171400	-0.90986700	-2.81416500
H	-3.08533500	0.43840000	-3.52285000
H	-1.68528100	0.75196600	-2.47373500
C	-4.80008300	-0.58296400	-1.72984300

H	-5.29538800	-0.10484800	-2.58687600
H	-4.62356100	-1.62640700	-2.00725900
H	-5.51029500	-0.56769700	-0.89605700
C	-3.87248200	1.66752400	-1.27132400
H	-4.65753400	1.84766700	-0.53066900
H	-3.00331200	2.27733500	-1.00797600
H	-4.25429000	2.02651300	-2.23727600

Int_{EE}(L2)

M06-L electronic energy (Hartree): -2184.157387

M06-L thermal correction to free energy (Hartree): 0.571343

Three lowest frequencies (cm⁻¹): 8.78, 26.35, 32.26

Pd	0.12456500	1.51093400	-0.14048800
O	-0.03190100	3.70936300	-0.31633200
O	1.88569100	2.70316000	-0.76152700
C	1.19400000	3.76805600	-0.66371100
C	1.81982700	5.10095400	-0.93600600
C	-1.69772100	1.01130200	0.45501600
C	-2.82113100	0.78901900	-0.30089800
S	-2.13164300	0.94085000	2.14054200
C	-4.01241800	0.57008100	0.46170900
C	-3.80202100	0.61087400	1.81282400
H	-4.52987300	0.50467000	2.60715800
O	-2.82715200	0.78190200	-1.67792500
C	-3.99573600	0.13706500	-2.19366800
H	-3.90894200	-0.95210100	-2.05097800
O	-5.22504400	0.32230900	-0.11512200
C	-5.23701000	0.65059000	-1.50959900
H	-6.13635000	0.18526600	-1.92057800
H	-5.31373100	1.74135000	-1.62846700
H	-4.01599400	0.35342100	-3.26445500
H	1.97644600	5.63151600	0.01013700
H	2.78475100	4.99292600	-1.43660000
H	1.15388100	5.72016500	-1.54436200
C	3.44520200	0.29291500	3.75552200
H	3.13303900	1.34926000	3.78074600
H	4.13921900	0.15393600	4.59462500
C	4.14546500	0.01169300	2.43171500
H	5.00335600	0.68324700	2.29758300
H	4.55103700	-1.01292100	2.44327000
C	2.21701200	-0.59275000	3.92659200
H	2.53161300	-1.64574000	4.00817500

H	1.69212400	-0.35215000	4.86012100
C	1.26390000	-0.44996700	2.74540500
H	0.38044100	-1.08906600	2.88552200
H	0.88740200	0.58639600	2.69566500
C	3.18871300	0.15391600	1.25236300
H	3.71462700	-0.06086300	0.31219700
H	2.83760600	1.19533000	1.17579600
C	1.97526000	-0.76585100	1.42379800
H	2.33082200	-1.81074000	1.45375500
P	0.78721600	-0.65354900	0.01272000
C	3.90170300	-1.73620800	-3.36800800
H	4.75893300	-1.34792900	-2.79454000
H	4.30619200	-2.10946000	-4.31781400
C	2.91088300	-0.60568000	-3.61633700
H	3.39102000	0.21923700	-4.15863500
H	2.09828500	-0.97283200	-4.26385300
C	3.24925500	-2.86873400	-2.58580300
H	2.44587900	-3.31668900	-3.19212500
H	3.97150200	-3.67053100	-2.38448800
C	2.65991000	-2.36699500	-1.27081600
H	2.18312800	-3.19443800	-0.72944200
H	3.47641300	-2.00495300	-0.62660100
C	2.31253900	-0.08759300	-2.31297100
H	1.57174400	0.69846200	-2.51047000
H	3.09880000	0.38900000	-1.70869900
C	1.66242600	-1.22787000	-1.52161500
H	0.84722100	-1.62502800	-2.14926200
C	-2.24429500	-4.29102600	0.28115100
H	-1.74614000	-4.96285600	-0.43601600
H	-3.14339300	-4.81830500	0.62562100
C	-2.62368200	-2.99967200	-0.43615100
H	-3.24606200	-3.21959500	-1.31438700
H	-3.23295800	-2.36515500	0.22988200
C	-1.30245300	-4.03018800	1.45152300
H	-1.83255300	-3.45406900	2.22762600
H	-0.99914300	-4.97609400	1.91876900
C	-0.06644400	-3.24152400	1.02066700
H	0.58556000	-3.06963100	1.88707200
H	0.51449700	-3.83903700	0.30168100
C	-1.37974500	-2.22177300	-0.85341600
H	-1.65043900	-1.29430200	-1.37572900
H	-0.80128700	-2.83153600	-1.56638000
C	-0.51303800	-1.92492700	0.37460200
H	-1.15579300	-1.40961500	1.10537400

Pre-TS_{EE}(L2)

M06-L electronic energy (Hartree): -2965.076060

M06-L thermal correction to free energy (Hartree): 0.681996

Three lowest frequencies (cm⁻¹): 11.62, 26.42, 30.08

Pd	-0.09626300	-0.99495100	-0.01393100
O	0.76924300	-3.51724300	-1.38847200
O	1.16365900	-2.63261400	0.64295600
C	1.30148500	-3.54234900	-0.26356300
C	2.21679700	-4.68272000	0.13222900
C	-1.39185900	0.40811400	-0.59843600
C	-2.14239300	1.30684400	0.11639000
S	-1.76953400	0.59593800	-2.29010800
C	-3.00796300	2.12515500	-0.67769700
C	-2.91269600	1.87139900	-2.02004200
H	-3.47320600	2.32383400	-2.82857400
O	-2.06800100	1.43529300	1.48755100
C	-2.71290800	2.62260400	1.95375300
H	-2.06548300	3.49491800	1.76808700
O	-3.85167500	3.05144800	-0.13216700
C	-4.04137500	2.81989900	1.26897600
H	-4.56069600	3.70077900	1.65377400
H	-4.67973400	1.93358300	1.41178200
H	-2.83592200	2.49829200	3.03267200
C	-3.81501100	-1.58131000	0.94013000
C	-3.05061200	-2.17561900	-0.09841600
C	-3.20613400	-1.68720900	2.16492500
C	-1.79781900	-2.61844000	0.31804700
S	-1.67802000	-2.45546900	2.06426600
O	-5.01135900	-0.97721500	0.71709900
C	-5.18997200	-0.69277500	-0.68159300
O	-3.49079300	-2.29179300	-1.36142700
C	-4.87230500	-1.90250500	-1.51822700
H	-3.55374100	-1.26255200	3.09926100
H	-6.23596800	-0.40148400	-0.79820100
H	-4.54157200	0.14966200	-0.96523000
H	-4.99928600	-1.69254800	-2.58234700
H	-1.21398400	-3.37434400	-0.20013200
H	3.25918300	-4.33657700	0.11588800
H	2.01170100	-5.01935800	1.15364100
H	2.12572700	-5.52484800	-0.55878600
H	-5.50395400	-2.75561400	-1.23925100

C	4.52448500	-2.13263400	-2.60617900
H	3.89322900	-3.02058300	-2.43457700
H	5.35156400	-2.45655900	-3.25161000
C	5.05541400	-1.62878700	-1.27044800
H	5.63994700	-2.40959500	-0.76530700
H	5.74723400	-0.78983300	-1.45005800
C	3.69249200	-1.05783700	-3.29423000
H	4.33705400	-0.19838400	-3.54185200
H	3.28784400	-1.42780400	-4.24540800
C	2.55443100	-0.59589800	-2.39323800
H	1.95888000	0.18321000	-2.89340800
H	1.86630700	-1.43640000	-2.20461400
C	3.92839900	-1.16426900	-0.35300600
H	4.35141500	-0.77780200	0.58294700
H	3.29725800	-2.01610100	-0.07462300
C	3.07308000	-0.09391800	-1.03743300
H	3.72215700	0.78204000	-1.20631800
P	1.62593400	0.53489900	-0.06369600
C	3.87653400	0.92366500	4.05944800
H	4.70224400	0.26575000	3.74295400
H	4.10246300	1.23257300	5.08847300
C	2.56774400	0.14438600	4.01048000
H	2.61692400	-0.73763600	4.66243000
H	1.75602600	0.77767500	4.40410500
C	3.82408200	2.13724600	3.14017900
H	3.04995600	2.83424500	3.50034700
H	4.77399800	2.68720000	3.16468500
C	3.49662600	1.73361700	1.70575400
H	3.43029500	2.62594500	1.06845500
H	4.32056000	1.12737200	1.30008200
C	2.22274200	-0.28179200	2.58748900
H	1.25124300	-0.79482200	2.55585100
H	2.96109300	-1.01511800	2.23256000
C	2.18779500	0.93481700	1.65573900
H	1.38559300	1.59026700	2.03541200
C	1.10717200	5.07419600	-1.40351400
H	1.87834500	5.49578400	-0.73853800
H	0.67250500	5.92167200	-1.94964300
C	0.04800100	4.38036300	-0.55649200
H	-0.38220700	5.07857100	0.17450200
H	-0.78428400	4.04389900	-1.19725700
C	1.76089700	4.09927500	-2.37449400
H	1.01075700	3.76108700	-3.10783000
H	2.55286100	4.59773500	-2.94862000

C	2.33277500	2.87132300	-1.66656200
H	2.75929900	2.19306400	-2.41638800
H	3.16370100	3.17487700	-1.00996500
C	0.63582400	3.17052500	0.15954400
H	-0.12462700	2.67918600	0.77777000
H	1.42832700	3.51123800	0.84608600
C	1.22998300	2.18237200	-0.85253600
H	0.42609600	1.93084000	-1.55968400

TS_{EE}(L2)

M06-L electronic energy (Hartree): -2965.047137

M06-L thermal correction to free energy (Hartree): 0.674923

Three lowest frequencies (cm⁻¹): -596.18, 2.31, 27.41

Pd	0.12031700	-0.79837500	-0.13251400
O	0.58911400	-3.91363200	0.43503500
O	-0.92021700	-2.67663800	-0.68341400
C	-0.55659500	-3.74724100	-0.14945300
C	-1.47847400	-4.92492200	-0.12629500
C	1.18473500	0.78238800	0.47045600
C	2.13062100	1.46114100	-0.25392200
S	1.29670000	1.29700400	2.13016500
C	2.93308000	2.36702700	0.50450600
C	2.60260000	2.39724500	1.83268800
H	3.02021200	3.01863200	2.61518500
O	2.31927300	1.27696000	-1.60529100
C	3.06108000	2.35049900	-2.18082400
H	2.42510300	3.24782000	-2.25007100
O	3.93002200	3.12147600	-0.05553600
C	4.28926700	2.65092900	-1.35923800
H	4.88966300	3.44397400	-1.81222700
H	4.90850100	1.74409300	-1.26758800
H	3.33278400	2.03007900	-3.19050400
C	4.32711400	-1.47020200	-0.69125100
C	3.21214300	-1.49366900	0.19352300
C	3.99080900	-1.82430600	-1.97228900
C	1.99025300	-1.82685500	-0.37782800
S	2.30703100	-2.15227900	-2.08170000
O	5.58748400	-1.12041900	-0.29303200
C	5.55415300	-0.40459300	0.94754500
O	3.33887800	-1.20773500	1.51616100
C	4.69940700	-1.12638500	1.95595200
H	4.65612600	-1.91505900	-2.82342400

H	6.59025800	-0.33283700	1.28579900
H	5.16028800	0.60980600	0.77697900
H	4.67445600	-0.58755200	2.90713500
H	1.20831100	-2.99888200	0.20810200
H	-1.92653500	-5.00210000	0.87210900
H	-2.28259300	-4.80103600	-0.85441400
H	-0.93573100	-5.85556200	-0.31105900
H	5.08651900	-2.14075100	2.12873800
C	-3.14897000	-1.56320700	4.08892400
H	-2.18309900	-2.08166000	4.20155700
H	-3.75060500	-1.83325000	4.96663600
C	-3.82164800	-2.04420300	2.80853100
H	-3.94603400	-3.13540500	2.82400700
H	-4.83461100	-1.61546900	2.73940200
C	-2.90376500	-0.05954500	4.05301700
H	-3.87103900	0.46832900	4.05231800
H	-2.37325300	0.26682500	4.95714800
C	-2.11709300	0.35269500	2.81243400
H	-1.96121000	1.44075900	2.80882300
H	-1.11250300	-0.10322900	2.83969100
C	-3.01715700	-1.62997900	1.58254800
H	-3.48625700	-2.00251500	0.65998900
H	-2.01996500	-2.09807600	1.62413800
C	-2.82791600	-0.10955500	1.53749200
H	-3.82194700	0.36691900	1.50663700
P	-1.90826300	0.40204000	0.01216500
C	-5.23508100	-0.84490600	-3.15346700
H	-5.52089000	-1.77603000	-2.63789200
H	-5.86931500	-0.77722400	-4.04714800
C	-3.76392400	-0.92130700	-3.54364400
H	-3.57793700	-1.79539400	-4.18174000
H	-3.50241100	-0.03571600	-4.14544500
C	-5.49247700	0.33563700	-2.22543900
H	-5.30117600	1.27606900	-2.76737700
H	-6.54564500	0.36407700	-1.91626100
C	-4.59390900	0.28336100	-0.99424100
H	-4.79821300	1.14443900	-0.34515700
H	-4.84047800	-0.61442400	-0.40518500
C	-2.86306900	-0.97303800	-2.31494200
H	-1.80439500	-1.01018800	-2.60816000
H	-3.05030300	-1.90015300	-1.75338800
C	-3.11642800	0.23296400	-1.40579700
H	-2.91566900	1.13524800	-2.00939000
C	-1.81900700	5.11583400	-0.38156700

H	-2.50153700	5.19364100	-1.24315800
H	-1.51384500	6.14159100	-0.13584700
C	-0.61011300	4.27884500	-0.78583200
H	-0.11909400	4.71656000	-1.66549100
H	0.13651300	4.28628100	0.02559200
C	-2.57014800	4.49116300	0.78970700
H	-1.93487000	4.51872700	1.69000400
H	-3.46899000	5.07592700	1.02618200
C	-2.94890800	3.03948300	0.50262800
H	-3.48344300	2.60956900	1.36219100
H	-3.64670700	3.01054300	-0.35016600
C	-1.01037900	2.83470800	-1.06904500
H	-0.13647300	2.23830000	-1.36137900
H	-1.70885900	2.81975700	-1.92176300
C	-1.69426200	2.23147500	0.16370500
H	-0.98551000	2.33460900	1.00072700

Post-TS_{EE}(L2)

M06-L electronic energy (Hartree): -2965.051312

M06-L thermal correction to free energy (Hartree): 0.678866

Three lowest frequencies (cm⁻¹): 14.15, 20.57, 32.32

Pd	0.22348500	-0.72863300	-0.11643200
O	0.74749500	-3.83556300	0.67508200
O	-0.68071400	-2.71278100	-0.65334100
C	-0.34766800	-3.74294200	-0.05389100
C	-1.18104900	-4.97735800	-0.06993600
C	1.15807500	0.93658500	0.45154100
C	2.01877200	1.70778500	-0.28474800
S	1.20372000	1.48444500	2.10297400
C	2.68937900	2.72996400	0.45510400
C	2.35686200	2.74024500	1.78299100
H	2.68156200	3.43082500	2.55137400
O	2.24086000	1.52279700	-1.63268900
C	2.79518900	2.69351700	-2.23087000
H	2.02413000	3.47758400	-2.30424200
O	3.55523500	3.61780200	-0.12350300
C	3.96844400	3.19813900	-1.42811800
H	4.42494100	4.07429200	-1.89648100
H	4.72906400	2.40740600	-1.33702100
H	3.10408000	2.40710000	-3.23967100
C	4.48668400	-1.62801600	-0.64074100
C	3.36470100	-1.30624500	0.18360400

C	4.12587900	-2.11604700	-1.86798700
C	2.12605900	-1.53428300	-0.38313300
S	2.40482700	-2.17112700	-1.99426500
O	5.78166100	-1.46751000	-0.23102200
C	5.86986400	-0.58683700	0.89400300
O	3.52634600	-0.80412000	1.44581100
C	4.85559800	-0.96358200	1.94237400
H	4.77757000	-2.46734700	-2.65925900
H	6.89024400	-0.67962200	1.27364500
H	5.70341300	0.45046500	0.56445000
H	4.93001700	-0.31065000	2.81647300
H	1.27046200	-2.98188600	0.52977600
H	-1.62419600	-5.12210600	0.92257700
H	-1.98210800	-4.88705200	-0.80482900
H	-0.56922400	-5.85880000	-0.27997600
H	5.01130800	-2.00545900	2.26140100
C	-3.13805900	-1.72618600	4.05805600
H	-2.14216600	-2.17599500	4.20029100
H	-3.74346200	-2.03381600	4.92070900
C	-3.74037700	-2.25910700	2.76303400
H	-3.78816800	-3.35621400	2.78222200
H	-4.77873300	-1.90303200	2.66511000
C	-2.99679100	-0.20922200	4.02032400
H	-3.99780000	0.25094200	3.99154200
H	-2.51445800	0.15620000	4.93645800
C	-2.20894400	0.25176100	2.79795300
H	-2.12870600	1.34790300	2.79159000
H	-1.17575400	-0.13286300	2.85385100
C	-2.93645100	-1.79283000	1.55522200
H	-3.35669500	-2.19966400	0.62302600
H	-1.90889600	-2.18691700	1.62553200
C	-2.85428700	-0.26353100	1.50785200
H	-3.87879300	0.14011700	1.45089400
P	-1.93391300	0.31068700	0.00705200
C	-5.04835700	-1.20646200	-3.25495800
H	-5.28603400	-2.15216900	-2.74144900
H	-5.64913700	-1.19358700	-4.17391200
C	-3.56114300	-1.17801800	-3.58626600
H	-3.28622700	-2.04395800	-4.20305300
H	-3.34123300	-0.28318200	-4.19089700
C	-5.43000600	-0.04017400	-2.35237400
H	-5.28842000	0.90655500	-2.89833500
H	-6.49387700	-0.08783600	-2.08473000
C	-4.57837000	-0.01087300	-1.08627100

H	-4.87170000	0.83817500	-0.45554700
H	-4.77816200	-0.91931400	-0.49568900
C	-2.70953000	-1.14592400	-2.32193200
H	-1.63983200	-1.11041400	-2.57353100
H	-2.85340600	-2.07712400	-1.75370300
C	-3.08690600	0.04798100	-1.44129400
H	-2.93205300	0.95533300	-2.05039900
C	-2.25366500	5.02537900	-0.31638700
H	-2.95495600	5.05671200	-1.16583500
H	-2.03327200	6.06970800	-0.05870100
C	-0.98339300	4.30243300	-0.75358500
H	-0.54656100	4.79353100	-1.63381100
H	-0.22664400	4.36269900	0.04614900
C	-2.92765200	4.31906700	0.85423300
H	-2.27959000	4.38235500	1.74363500
H	-3.86688000	4.82341100	1.11767500
C	-3.18952000	2.84745400	0.54347000
H	-3.67786400	2.36166700	1.40043700
H	-3.89194600	2.77551700	-0.30283100
C	-1.26123900	2.83245700	-1.05328500
H	-0.34262000	2.31674600	-1.36286400
H	-1.96463300	2.76983700	-1.89963300
C	-1.87537500	2.15285700	0.17577000
H	-1.16833300	2.30474400	1.00708300

Int_{EE}(L3)

M06-L electronic energy (Hartree): -2416.450640

M06-L thermal correction to free energy (Hartree): 0.681931

Three lowest frequencies (cm⁻¹): 19.97, 26.91, 37.01

P	-0.41497800	0.00849600	0.34778600
C	-1.26825700	1.68456500	0.41298200
C	-2.47489100	1.72113300	-0.54345200
C	-1.72877800	2.08612200	1.82772700
C	-0.23460600	2.73264800	-0.06219500
H	-3.23939700	1.00362200	-0.21300100
H	-2.16265600	1.42456200	-1.55421500
C	-3.09258300	3.12340300	-0.56653400
H	-0.86605800	2.10780500	2.50915700
H	-2.44429800	1.35314200	2.22857200
C	-2.36964800	3.48082600	1.79793100
H	0.12352600	2.46730800	-1.06963200
H	0.64795900	2.72093200	0.59653300

C	-0.86061700	4.13060800	-0.08025400
H	-3.94890600	3.11748100	-1.25581200
C	-3.56469300	3.48672500	0.84296000
C	-2.05104000	4.13781200	-1.04180100
H	-2.70321700	3.73063100	2.81513100
C	-1.33234400	4.50179800	1.32670200
H	-0.10225800	4.84962500	-0.42134200
H	-4.32575900	2.76796200	1.18342900
H	-4.03862100	4.47957300	0.84158100
H	-1.71622500	3.88659800	-2.05990100
H	-2.49468400	5.14356100	-1.08756700
H	-1.76895400	5.51159000	1.32540200
H	-0.47785800	4.52194800	2.02009700
C	-1.59677600	-1.45101800	0.39485300
C	-0.72949700	-2.69835000	0.68176200
C	-2.70678700	-1.33875600	1.45903000
C	-2.25043100	-1.66204300	-0.98967900
H	-0.21261600	-2.60201600	1.64652800
H	0.05382400	-2.78129900	-0.08884700
C	-1.59630200	-3.96060700	0.69217400
H	-3.34837200	-0.47060600	1.24768700
H	-2.27967400	-1.18158800	2.45783700
C	-3.56023900	-2.61460500	1.45880100
H	-1.46276500	-1.75770000	-1.75348200
H	-2.85490700	-0.79174200	-1.27372100
C	-3.12372400	-2.92156600	-0.98138900
H	-0.95412200	-4.82406800	0.91624400
C	-2.67578600	-3.82580800	1.76845900
C	-2.25399600	-4.14255600	-0.67658300
H	-4.33656500	-2.51357000	2.23033200
C	-4.21219300	-2.78937400	0.08577900
H	-3.58638500	-3.03152400	-1.97242900
H	-2.21087200	-3.71213500	2.75987600
H	-3.28804200	-4.73892100	1.80431400
H	-1.48403500	-4.26388200	-1.45333100
H	-2.86639800	-5.05647200	-0.68362500
H	-4.85428100	-3.68263300	0.08299700
H	-4.85922000	-1.92744000	-0.13758400
C	0.63488000	-0.07318100	1.86193900
C	0.06621900	-0.36656800	3.25047700
H	1.15998000	0.89472200	1.86740700
H	1.41583700	-0.81072400	1.64061200
C	1.11279500	-0.08734400	4.32366000
H	-0.83540000	0.21974300	3.46616400

H	-0.23987000	-1.42060500	3.31631300
C	0.64159100	-0.46506900	5.71601700
H	2.03723700	-0.63246500	4.07658500
H	1.37860300	0.98082800	4.29320500
H	1.40475400	-0.25337100	6.47318400
H	-0.26371700	0.08998100	5.99284700
H	0.40143700	-1.53411100	5.77674000
Pd	0.68214900	-0.10210300	-1.64760400
O	1.28910700	-0.10819300	-3.77672100
O	-0.74791400	0.54225800	-3.21529400
C	0.13337100	0.31395100	-4.10803100
C	-0.20201700	0.51052700	-5.55409400
C	2.32995600	-0.69698500	-0.73049900
C	3.26216200	0.04015800	-0.04536400
S	2.86643500	-2.35205800	-0.80105700
C	4.39601700	-0.70678400	0.40274900
C	4.32822800	-2.03416500	0.07562000
H	5.06092300	-2.80879700	0.26361500
O	3.12492200	1.38403000	0.22091500
C	3.97944800	1.78891600	1.29314000
H	3.58653800	1.39988600	2.24689400
O	5.42691100	-0.14379700	1.09990200
C	5.38433800	1.28795000	1.07241500
H	6.05575900	1.62416500	1.86648500
H	5.76706700	1.64738800	0.10590700
H	3.94589000	2.88094700	1.31544100
H	-0.98163300	1.26638600	-5.67834100
H	0.68521600	0.79016800	-6.12817000
H	-0.58095900	-0.43121900	-5.96841500

Pre-TS_{EE}(L3)

M06-L electronic energy (Hartree): -3197.371079

M06-L thermal correction to free energy (Hartree): 0.782955

Three lowest frequencies (cm⁻¹): 19.44, 24.08, 35.58

P	1.22078200	0.39536000	-0.08168900
C	2.00863300	0.39319300	1.64098200
C	2.89768700	-0.84360300	1.87895700
C	2.84040200	1.66191400	1.91770400
C	0.84163800	0.36343900	2.65544800
H	3.75620200	-0.83204200	1.19250200
H	2.32334100	-1.75532400	1.67761300
C	3.42031900	-0.85227700	3.32047000

H	2.21600200	2.55821900	1.79200400
H	3.67446800	1.74196100	1.20464600
C	3.38414600	1.64145300	3.35349100
H	0.22722600	-0.53185900	2.48168100
H	0.18397800	1.23370900	2.49719800
C	1.37589100	0.35739600	4.09094600
H	4.04314600	-1.74792500	3.45881500
C	4.25800500	0.40402100	3.56399100
C	2.24249300	-0.88724000	4.29677000
H	3.98088600	2.55150200	3.51036000
C	2.21271500	1.61389700	4.33732900
H	0.52201300	0.33575200	4.78353000
H	5.11693800	0.42410900	2.87567500
H	4.66501000	0.40059700	4.58632300
H	1.64291100	-1.79599200	4.13130300
H	2.61031100	-0.92648400	5.33317500
H	2.58810100	1.62376700	5.37160500
H	1.59129200	2.51361800	4.21176000
C	2.39630900	-0.15589700	-1.43480300
C	1.73005600	0.21679000	-2.77825100
C	3.79335200	0.49207800	-1.36208100
C	2.54583000	-1.69029300	-1.41423300
H	1.56708100	1.30179700	-2.84764000
H	0.73609700	-0.25627200	-2.83208700
C	2.59973000	-0.24633600	-3.95182900
H	4.29196900	0.22282300	-0.42034100
H	3.71880200	1.58671400	-1.37936100
C	4.64994500	0.01715600	-2.54371100
H	1.55000000	-2.15018600	-1.48725300
H	2.98065400	-2.02638900	-0.46399400
C	3.42298900	-2.15879700	-2.57979300
H	2.10774200	0.04692100	-4.89021100
C	3.97569600	0.41835000	-3.85808300
C	2.76089900	-1.76690200	-3.90190200
H	5.63770800	0.49437200	-2.47206000
C	4.80318600	-1.50439100	-2.48408400
H	3.52326800	-3.25272200	-2.52265800
H	3.87282200	1.51324100	-3.91147600
H	4.60018000	0.11286100	-4.71078600
H	1.77855600	-2.25480600	-3.99195000
H	3.37122200	-2.11032700	-4.75064600
H	5.44532300	-1.85175500	-3.30728000
H	5.29763400	-1.79690900	-1.54495600
C	0.79856900	2.16433600	-0.41425600

C	1.81973300	3.22887700	-0.81513700
H	0.26714900	2.47933100	0.49816200
H	0.02225000	2.13525700	-1.18690900
C	1.18937500	4.61492700	-0.72769900
H	2.72489400	3.20419700	-0.19648200
H	2.15677200	3.05371300	-1.84753000
C	2.10694400	5.71434900	-1.23053400
H	0.24605400	4.61803200	-1.29716200
H	0.90571200	4.81070400	0.31833600
H	1.63943200	6.70190700	-1.14821500
H	3.04321100	5.74186600	-0.65861700
H	2.37170100	5.55918300	-2.28410700
Pd	-0.66509900	-0.97007900	-0.01857000
O	-0.00498100	-3.93553500	-0.80595700
O	0.40158500	-2.58173800	0.94861300
C	0.51704500	-3.68913400	0.29661600
C	1.41236500	-4.71405700	0.96290300
C	-1.77130600	0.51561500	-0.76672700
C	-2.35313400	1.56374500	-0.09720000
S	-2.03413700	0.74292900	-2.47197500
C	-3.01323200	2.51765400	-0.93291600
C	-2.91710200	2.22161500	-2.26772800
H	-3.36377700	2.74509600	-3.10368800
O	-2.27122800	1.72399000	1.26924400
C	-2.63123400	3.04552200	1.67094200
H	-1.81034500	3.74399500	1.43767100
O	-3.67238800	3.60686100	-0.43623100
C	-3.89292400	3.48870500	0.97393000
H	-4.21508300	4.47589800	1.31416400
H	-4.70056400	2.76246800	1.15851800
H	-2.76648000	3.00963200	2.75512500
C	-4.45863000	-1.10461700	0.70221800
C	-3.66341800	-1.84008600	-0.21648800
C	-3.99205100	-1.19722700	1.98855400
C	-2.51471200	-2.38418200	0.35369700
S	-2.55518300	-2.12573300	2.09152400
O	-5.55018000	-0.39231400	0.31848300
C	-5.52301000	-0.14953600	-1.09860300
O	-3.97704900	-1.98101100	-1.51308800
C	-5.26643800	-1.42673500	-1.85254900
H	-4.38640400	-0.68584500	2.85854900
H	-6.50159000	0.26261500	-1.35318300
H	-4.74347500	0.59362600	-1.32267500
H	-5.23695700	-1.25167100	-2.93008900

H	-1.95746200	-3.22451500	-0.05718600
H	1.40040500	-4.62011200	2.05330600
H	1.13639300	-5.73179500	0.67280900
H	2.44596500	-4.54382800	0.63261000
H	-6.03339100	-2.17895400	-1.62870400

TS_{EE}(L3)

M06-L electronic energy (Hartree): -3197.337914

M06-L thermal correction to free energy (Hartree): 0.777985

Three lowest frequencies (cm⁻¹): -602.68, 14.74, 19.15

P	-1.47263500	-0.22951600	0.35464000
C	-2.33300200	1.34002000	0.97439600
C	-3.03867800	2.11023300	-0.15909300
C	-3.35383500	1.07654200	2.09898900
C	-1.21290900	2.23940500	1.54978600
H	-3.86258300	1.50897600	-0.56923100
H	-2.33490500	2.30132500	-0.97756100
C	-3.60804700	3.43307600	0.36788000
H	-2.86766000	0.55905400	2.93851900
H	-4.16283600	0.42338600	1.73871500
C	-3.94100500	2.39838800	2.61270900
H	-0.46940100	2.44969700	0.76541600
H	-0.67943100	1.70864300	2.35614900
C	-1.79313000	3.55420400	2.07990200
H	-4.09693800	3.95851600	-0.46519400
C	-4.63013100	3.14270800	1.46803900
C	-2.47586100	4.29651700	0.92859100
H	-4.67054400	2.17121000	3.40330900
C	-2.81417700	3.26331500	3.18149800
H	-0.97258200	4.16491100	2.48305600
H	-5.45681200	2.53762300	1.06506200
H	-5.06932300	4.08099200	1.83891300
H	-1.74390300	4.51984300	0.13684000
H	-2.87346300	5.25982100	1.28173700
H	-3.22318000	4.20532800	3.57643200
H	-2.32763500	2.74633100	4.02252100
C	-2.50866200	-1.19088400	-0.88167400
C	-1.84443500	-2.57855900	-1.02794100
C	-3.98823400	-1.37068200	-0.49206500
C	-2.42637300	-0.51267900	-2.26746800
H	-1.82950500	-3.11154900	-0.06685700
H	-0.79299100	-2.44272800	-1.33054300

C	-2.58443300	-3.42104700	-2.07248800
H	-4.48224800	-0.39256400	-0.40468800
H	-4.07513800	-1.85689400	0.48785300
C	-4.71177300	-2.21315300	-1.55043700
H	-1.36632200	-0.41651800	-2.55223700
H	-2.83587000	0.50534500	-2.23389000
C	-3.17331500	-1.34229900	-3.31724200
H	-2.10034100	-4.40599800	-2.13672100
C	-4.04649000	-3.58821300	-1.64994000
C	-2.52188900	-2.72153100	-3.43158800
H	-5.76222100	-2.32997100	-1.24799800
C	-4.63839900	-1.50175800	-2.90342400
H	-3.11392800	-0.82061500	-4.28368500
H	-4.10458000	-4.10677900	-0.68046100
H	-4.57980100	-4.21394600	-2.38101100
H	-1.47559200	-2.62036300	-3.75745600
H	-3.03970800	-3.32508300	-4.19204600
H	-5.18432500	-2.07860300	-3.66484200
H	-5.12391600	-0.51591700	-2.83745500
C	-1.28574100	-1.27624200	1.86843700
C	-2.42813800	-2.09432800	2.46969500
H	-0.88954900	-0.57791900	2.62420600
H	-0.44516400	-1.94763600	1.65377600
C	-2.04578700	-2.63833200	3.84130200
H	-3.35248800	-1.51035900	2.56107800
H	-2.67353900	-2.93856100	1.80861600
C	-3.12507800	-3.51832800	4.44569200
H	-1.10383900	-3.20155600	3.75740700
H	-1.83040500	-1.79316800	4.51339200
H	-2.83657800	-3.89419600	5.43372500
H	-4.06693200	-2.96712000	4.56263200
H	-3.33200100	-4.38710800	3.80785000
Pd	0.62526100	0.35784900	-0.59106400
O	1.19218000	1.53146600	-3.49808000
O	-0.30458900	1.92199200	-1.86834400
C	0.07724000	2.02275000	-3.05564500
C	-0.78766800	2.70664900	-4.06543100
C	1.60064700	-1.00860800	0.48112300
C	2.51311800	-0.75518800	1.47245300
S	1.67220200	-2.70258500	0.08871100
C	3.27662000	-1.88905200	1.88654600
C	2.93387600	-3.04005400	1.22909400
H	3.32281100	-4.03967300	1.37701900
O	2.71947700	0.49881000	2.00074500

C	3.48145600	0.45453900	3.20511900
H	2.84679800	0.11103800	4.03739700
O	4.25458700	-1.81076000	2.84283500
C	4.67281100	-0.45803100	3.05747900
H	5.28175200	-0.46980200	3.96492500
H	5.29808200	-0.12544900	2.21273600
H	3.79818100	1.48265500	3.40339900
C	4.86989700	1.03458000	-0.75775900
C	3.73872400	0.33382600	-1.26310300
C	4.57402600	2.32498600	-0.39993500
C	2.54232600	1.04009300	-1.27664400
S	2.90533600	2.64970600	-0.65581800
O	6.10797100	0.46627900	-0.63847700
C	6.02623600	-0.96347100	-0.68756800
O	3.82806400	-0.94937000	-1.70335400
C	5.17705700	-1.40664100	-1.84983100
H	5.25875400	3.07356400	-0.01825700
H	7.05287900	-1.32378600	-0.78516000
H	5.59977900	-1.34176400	0.25556700
H	5.11966600	-2.49717700	-1.90345800
H	1.78460400	1.19841600	-2.59568200
H	-1.52387700	3.34608200	-3.57384600
H	-0.19047700	3.28489700	-4.77465200
H	-1.32744100	1.94212300	-4.63795300
H	5.59099200	-1.02308300	-2.79362800

Post-TS_{EE}(L3)

M06-L electronic energy (Hartree): -3196.742140

M06-L thermal correction to free energy (Hartree): 0.784155

Three lowest frequencies (cm⁻¹): 11.88, 21.45, 25.83

P	-1.37389500	0.00425400	0.19474100
C	-2.58276800	-0.07506000	-1.25722400
C	-2.77462000	-1.51120400	-1.78172000
C	-3.96921700	0.52464900	-0.95611700
C	-1.93259800	0.77190200	-2.37608000
H	-3.26187300	-2.13435100	-1.01835800
H	-1.79947000	-1.96191600	-1.99614600
C	-3.64131700	-1.50993900	-3.04576500
H	-3.86144900	1.56338900	-0.61167200
H	-4.46552200	-0.03528800	-0.14904700
C	-4.84440100	0.51122600	-2.21637800
H	-0.93328800	0.37162500	-2.60598800

H	-1.78117900	1.80482300	-2.02226700
C	-2.80445100	0.76795900	-3.63423100
H	-3.75166200	-2.54723300	-3.39460400
C	-5.01601000	-0.92350900	-2.71755000
C	-2.96581500	-0.67053900	-4.13172800
H	-5.82600400	0.93805500	-1.96458400
C	-4.17879800	1.35523400	-3.30557100
H	-2.31463600	1.37698800	-4.40768400
H	-5.51453200	-1.53629100	-1.95075900
H	-5.66019000	-0.93700300	-3.60954400
H	-1.98172000	-1.09789100	-4.38078700
H	-3.56684400	-0.68751800	-5.05338900
H	-4.80965800	1.37388400	-4.20701000
H	-4.07384100	2.39687800	-2.96551200
C	-1.63318200	-1.37667700	1.44015900
C	-0.86274700	-0.96303400	2.71602400
C	-3.10352100	-1.65766200	1.80026300
C	-0.97843200	-2.67869300	0.92787600
H	-1.25147200	-0.01845400	3.12020600
H	0.19486300	-0.78279900	2.45974100
C	-0.96623700	-2.05631700	3.78329700
H	-3.66099100	-1.97170600	0.90676000
H	-3.59037100	-0.74598400	2.17078100
C	-3.18503800	-2.75875700	2.86412800
H	0.08072000	-2.47758100	0.69353100
H	-1.45137400	-3.01307100	-0.00567000
C	-1.07806400	-3.78210200	1.98727400
H	-0.42951100	-1.72263600	4.68289800
C	-2.43911200	-2.30559900	4.12182200
C	-0.33601500	-3.34340500	3.25233300
H	-4.24225400	-2.94104700	3.10454000
C	-2.55029300	-4.04045100	2.32090100
H	-0.62159200	-4.69849700	1.58515600
H	-2.89629200	-1.38769100	4.52299600
H	-2.51949700	-3.07310500	4.90607100
H	0.72895900	-3.17687200	3.02738700
H	-0.38546700	-4.13466500	4.01523800
H	-2.63239200	-4.84779000	3.06385400
H	-3.08991200	-4.37504100	1.42151600
C	-1.78434300	1.58890000	1.05673100
C	-2.98496300	1.78391700	1.98106700
H	-1.82723400	2.32593400	0.23839600
H	-0.87598400	1.85563300	1.61154600
C	-3.14200100	3.25635500	2.34547200

H	-3.91974800	1.41964600	1.53635200
H	-2.84870800	1.20318400	2.90514200
C	-4.23390100	3.49719400	3.37208800
H	-2.17882500	3.63879100	2.72064700
H	-3.35402700	3.83092400	1.43003600
H	-4.34102800	4.56155200	3.60999400
H	-5.20560600	3.13888200	3.00873800
H	-4.02015400	2.96764000	4.30936200
Pd	0.94697300	-0.06853400	-0.51691400
O	2.32301900	-2.96224900	-1.60043100
O	0.44399100	-1.76548300	-1.89969900
C	1.09174500	-2.80669400	-2.05068400
C	0.52190200	-4.00795700	-2.72008100
C	1.37364900	1.54350000	0.55703200
C	1.10511300	2.84164100	0.20731000
S	2.08847900	1.53398800	2.14101100
C	1.43134400	3.81047000	1.20700800
C	1.96948800	3.25504400	2.33598400
H	2.31147400	3.75544500	3.23330600
O	0.52062100	3.19980000	-0.99118300
C	-0.07280700	4.49592300	-0.90958800
H	-0.99133600	4.44816500	-0.30066500
O	1.19761600	5.14874200	1.04856800
C	0.89017100	5.48893500	-0.30757800
H	0.45708000	6.49215900	-0.27547700
H	1.81801300	5.52053100	-0.89791800
H	-0.34203900	4.77587000	-1.93142400
C	5.31026600	-0.41064800	-0.80539200
C	4.02121700	-0.59973400	-0.21274100
C	5.24850400	0.21681700	-2.01964600
C	2.95545600	-0.14634700	-0.95900100
S	3.59821000	0.56256100	-2.41565600
O	6.46862800	-0.83800100	-0.22115900
C	6.28071800	-1.17865700	1.15729500
O	3.86919500	-1.23253700	1.00104900
C	5.02826500	-1.99708900	1.34329500
H	6.06829200	0.46266500	-2.68385600
H	7.17033400	-1.74047100	1.45271800
H	6.22350900	-0.25830800	1.75727500
H	4.90193900	-2.29286900	2.38763700
H	2.61538000	-2.07990700	-1.23132800
H	-0.30770100	-3.72248800	-3.37006800
H	1.28353100	-4.55062400	-3.28420000
H	0.13405900	-4.68622400	-1.94986800

H	5.07015900	-2.90311500	0.71842000
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Int_{EE}(L4)

M06-L electronic energy (Hartree): -2173.264906
M06-L thermal correction to free energy (Hartree): 0.366013
Three lowest frequencies (cm⁻¹): 10.86, 33.63, 40.18

Pd	0.50456100	1.53398700	0.26009900
O	0.69137500	3.73629800	0.41477800
O	2.42562900	2.51112700	-0.19638900
C	1.91305500	3.64906800	0.06070000
C	2.74363900	4.89063000	-0.03598300
C	-1.37219700	1.11227600	0.73688200
C	-2.42532300	0.98034300	-0.13182300
S	-1.92016700	0.76784500	2.35265300
C	-3.66253200	0.63172900	0.49166700
C	-3.55322400	0.47167400	1.84699700
H	-4.33911400	0.25980600	2.56121700
O	-2.30797900	1.14405500	-1.48935700
C	-3.41236900	0.55767200	-2.18709300
H	-3.30414800	-0.53724200	-2.18686000
O	-4.81712300	0.44940200	-0.21216100
C	-4.71981700	0.95591300	-1.55042600
H	-5.56852400	0.53241500	-2.09321900
H	-4.81900000	2.05106700	-1.53284600
H	-3.35009900	0.92189600	-3.21561200
H	2.21758400	5.65695000	-0.61381900
H	2.90610600	5.30273200	0.96627300
H	3.71445100	4.68669800	-0.49332700
C	-0.56904000	-1.68072400	-0.76757600
C	-1.65705000	-2.06608900	0.02931500
C	-0.54344900	-2.05032600	-2.11660900
C	-2.68942000	-2.82348800	-0.51207400
H	-1.69249300	-1.77657600	1.07995500
C	-1.58181600	-2.80764100	-2.65547300
H	0.29389800	-1.75894100	-2.74871600
C	-2.65263300	-3.19900400	-1.85524900
H	-3.52909700	-3.11379100	0.11691400
H	-1.54789700	-3.09616500	-3.70392300
H	-3.46074500	-3.79295600	-2.27785400
C	1.15167600	-1.52319800	1.53526600
C	1.08535700	-2.91912100	1.64868900
C	1.54443400	-0.76009900	2.64134700

C	1.41453900	-3.53701500	2.85112800
H	0.76916700	-3.52128500	0.79718300
C	1.87030900	-1.38210300	3.84288100
H	1.57853000	0.32736800	2.55449500
C	1.80504800	-2.76994800	3.94792500
H	1.36072700	-4.62042400	2.93302300
H	2.16688100	-0.78149100	4.69994400
H	2.05387400	-3.25654100	4.88901100
C	2.18902400	-0.90504400	-1.13988800
C	2.29045800	-0.04240800	-2.24023900
C	3.14719300	-1.90861100	-0.95927500
C	3.32429000	-0.19337000	-3.15770100
H	1.55573500	0.75427400	-2.36739400
C	4.18694600	-2.04898300	-1.87553900
H	3.08445000	-2.57848300	-0.10269900
C	4.27459700	-1.19668300	-2.97444300
H	3.39237600	0.47770100	-4.01129800
H	4.93125600	-2.82880600	-1.72866900
H	5.08847100	-1.31171200	-3.68752100
P	0.76434000	-0.67901100	-0.02777900

Pre-TS_{EE}(L4)

M06-L electronic energy (Hartree): -2954.186726

M06-L thermal correction to free energy (Hartree): 0.469515

Three lowest frequencies (cm⁻¹): 15.66, 27.75, 35.26

Pd	-0.01252800	-1.02127400	-0.08805300
O	-1.32573000	-3.29790200	1.32683300
O	-1.28894200	-2.60234300	-0.81055300
C	-1.70592700	-3.36503000	0.14285300
C	-2.75867500	-4.36892900	-0.27642800
C	1.23679400	0.43108900	0.49119400
C	1.96957000	1.27780700	-0.30196600
S	1.48007100	0.88066200	2.15642200
C	2.72542800	2.25879800	0.41286100
C	2.55857900	2.18376500	1.77072700
H	3.03610800	2.77957600	2.53864600
O	1.97351300	1.20510100	-1.67477400
C	2.53840700	2.37246300	-2.27471300
H	1.80915300	3.19633600	-2.24578400
O	3.52375300	3.17245900	-0.21445600
C	3.80424600	2.78097400	-1.56452100
H	4.26828800	3.64794500	-2.04101200

H	4.52256200	1.94617300	-1.55988100
H	2.73836800	2.11223400	-3.31751100
C	3.69133600	-1.72625500	-0.64469300
C	2.80491400	-2.21922100	0.34835400
C	3.22876700	-1.94789700	-1.91677700
C	1.59777600	-2.69211600	-0.16983500
S	1.68889000	-2.69714300	-1.92889000
O	4.85956800	-1.10428500	-0.33924500
C	4.85432800	-0.66032000	1.02835200
O	3.08848300	-2.21060000	1.65799300
C	4.43582300	-1.77489400	1.94867800
H	3.68749200	-1.60977800	-2.83855700
H	5.87504500	-0.33922700	1.24542400
H	4.17293100	0.19711500	1.12614000
H	4.41971500	-1.44556100	2.98956200
H	0.95321700	-3.40829200	0.33483800
H	-2.88987500	-5.15022600	0.47689900
H	-3.71741400	-3.84873800	-0.40262400
H	-2.51505800	-4.82337300	-1.24205400
H	5.10324100	-2.64011700	1.85231200
C	-1.34690700	2.21038600	-0.62385900
C	-0.56558200	3.07884900	0.15320800
C	-1.78424600	2.63398700	-1.88449200
C	-0.23696400	4.34403900	-0.31853100
H	-0.21538400	2.76378100	1.13613100
C	-1.44906900	3.90191800	-2.35508300
H	-2.39546700	1.97772200	-2.50188400
C	-0.67613700	4.75915100	-1.57533000
H	0.37266100	5.00350100	0.29705300
H	-1.80072800	4.22046200	-3.33444700
H	-0.41605600	5.74898700	-1.94580800
C	-2.25966200	0.76526000	1.71449600
C	-2.85936600	1.95475000	2.14704400
C	-2.13225900	-0.30983300	2.60435200
C	-3.31434200	2.06988700	3.45778300
H	-2.96992000	2.79207400	1.45918800
C	-2.59415900	-0.18909200	3.91182400
H	-1.67628600	-1.24188200	2.25993900
C	-3.17984700	1.00078300	4.34140300
H	-3.77510800	2.99853700	3.78878600
H	-2.49055600	-1.02572300	4.60030300
H	-3.53300000	1.09533600	5.36657700
C	-3.14389200	-0.04056200	-0.93176700
C	-2.94676000	-0.56112300	-2.21852200

C	-4.43875900	0.01970300	-0.40596800
C	-4.03084500	-0.98987800	-2.97603100
H	-1.93358200	-0.64528600	-2.61339400
C	-5.52123300	-0.42373800	-1.16360600
H	-4.60581500	0.41381300	0.59552800
C	-5.31986400	-0.92416600	-2.44751400
H	-3.86841600	-1.38998200	-3.97481800
H	-6.52524900	-0.37414900	-0.74672700
H	-6.16776800	-1.26858800	-3.03635800
P	-1.68827800	0.53045900	0.00240700

TS_{EE}(L4)

M06-L electronic energy (Hartree): -2954.155303

M06-L thermal correction to free energy (Hartree): 0.465192

Three lowest frequencies (cm⁻¹): -585.08, 21.38, 28.15

Pd	-0.01695600	0.97412300	0.00290700
O	-0.62206500	4.08577200	0.59747400
O	1.02538300	2.88531100	-0.35776200
C	0.57066300	3.95377100	0.10880800
C	1.42082300	5.18445400	0.13777700
C	-0.97433800	-0.71331200	0.45326400
C	-1.70029700	-1.51505900	-0.38615500
S	-1.03767000	-1.37665800	2.05937200
C	-2.31082600	-2.63914900	0.25185700
C	-2.04258900	-2.71107200	1.59260300
H	-2.37344400	-3.45682100	2.30464600
O	-1.82924600	-1.27637200	-1.73461300
C	-2.32849200	-2.41715200	-2.43326000
H	-1.52527700	-3.16137100	-2.55116300
O	-3.07521500	-3.54628900	-0.42938000
C	-3.49347500	-3.02906600	-1.69734200
H	-3.91303200	-3.87549200	-2.24678100
H	-4.28145900	-2.27389400	-1.54505600
H	-2.63054500	-2.06156800	-3.42222200
C	-4.24007100	1.39165800	-0.41087500
C	-3.09617500	1.48735500	0.43087600
C	-3.98326000	1.79263300	-1.69656500
C	-1.92803900	1.92680300	-0.18041500
S	-2.33455600	2.25090600	-1.86497300
O	-5.44977400	0.93524100	0.03068700
C	-5.28992900	0.16450100	1.22805800

O	-3.14379400	1.16357000	1.74928300
C	-4.47002800	0.92541800	2.23695200
H	-4.68766000	1.85144500	-2.51828700
H	-6.29714600	-0.03064400	1.60298500
H	-4.80137800	-0.79252500	0.98521700
H	-4.35081800	0.35487800	3.16208300
H	-1.19267300	3.13706900	0.37601500
H	0.88809000	6.02580000	-0.31513600
H	1.62723200	5.45978100	1.17773100
H	2.36593700	5.01652200	-0.38152000
H	-4.94844100	1.88737600	2.46895400
C	1.84071000	-1.86843500	-0.90806600
C	1.16548400	-2.95490500	-0.33081600
C	2.32782400	-1.99018500	-2.21498900
C	0.98825400	-4.13450500	-1.04507100
H	0.77511500	-2.87622000	0.68368600
C	2.14398300	-3.17266400	-2.92865300
H	2.85895900	-1.16132400	-2.68099200
C	1.47468500	-4.24672800	-2.34687800
H	0.45777800	-4.96559900	-0.58252300
H	2.53242800	-3.25337800	-3.94212400
H	1.33205800	-5.16953100	-2.90629300
C	2.47378000	-0.74970800	1.68913900
C	3.23590400	-1.89376500	1.95556600
C	2.10870400	0.09208700	2.74752300
C	3.61612600	-2.19345500	3.26098400
H	3.52436900	-2.55584200	1.13954200
C	2.49516700	-0.20617900	4.05026300
H	1.50147600	0.97628900	2.54220500
C	3.24506300	-1.35220800	4.30852200
H	4.20297500	-3.08785500	3.46046300
H	2.20044200	0.45001900	4.86674100
H	3.53804600	-1.59264500	5.32858000
C	3.37423000	0.57165500	-0.73142000
C	3.16203100	1.32751500	-1.89304100
C	4.66279900	0.49512200	-0.19055200
C	4.22372000	1.97858500	-2.51263400
H	2.15512400	1.41132700	-2.30286000
C	5.72161000	1.15700700	-0.80803500
H	4.84221100	-0.08293900	0.71514300
C	5.50489100	1.89560400	-1.96912600
H	4.04815700	2.55987100	-3.41568500
H	6.71977900	1.09204700	-0.37931600
H	6.33401800	2.41182000	-2.44904400

P	1.94649000	-0.29012100	0.00837200
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Post-TS_{EE}(L4)

M06-L electronic energy (Hartree): -2954.166929

M06-L thermal correction to free energy (Hartree): 0.471678

Three lowest frequencies (cm⁻¹): 20.23, 23.02, 26.73

Pd	-0.68586400	-0.01635800	0.25307300
O	-2.50094600	1.38326700	-1.99653500
O	-1.36416500	2.06327900	-0.17534100
C	-2.00597800	2.31656200	-1.19931800
C	-2.28698400	3.70322200	-1.65688300
C	0.04936200	-1.82066500	0.58839900
C	0.77684200	-2.57318400	-0.29371500
S	-0.04483100	-2.66080400	2.10478400
C	1.27310400	-3.80120200	0.24322000
C	0.91416800	-3.99872400	1.54884700
H	1.16117300	-4.83290400	2.19341900
O	1.04361900	-2.17489300	-1.58434700
C	2.17685600	-2.87140400	-2.11252800
H	3.09543700	-2.49198800	-1.63824300
O	2.05646400	-4.65794200	-0.47641100
C	2.04412300	-4.35547600	-1.87741600
H	2.88610000	-4.90185500	-2.31014300
H	1.11044900	-4.72980100	-2.32288300
H	2.20580600	-2.64195700	-3.18113400
C	-4.92437100	-1.15918700	0.09335200
C	-3.81069800	-0.29402100	0.32964800
C	-4.54551900	-2.40495600	-0.32713200
C	-2.56764100	-0.84795200	0.09220200
S	-2.82252300	-2.50146200	-0.41150500
O	-6.22464800	-0.76845200	0.25445200
C	-6.33785600	0.47039100	0.96268700
O	-3.99243300	1.00319500	0.75199500
C	-5.31601700	1.46525500	0.47342100
H	-5.18534000	-3.24122000	-0.58176500
H	-7.35626500	0.82661200	0.78721600
H	-6.20376800	0.29107800	2.03967500
H	-5.41951900	2.42464100	0.98680200
H	-2.35844800	0.50089000	-1.55719700
H	-1.91562800	3.83956700	-2.67805700
H	-3.36873500	3.87334500	-1.68248800
H	-1.81548100	4.42834900	-0.99335400

H	-5.42969100	1.62610300	-0.61039000
C	2.99922300	-0.09864200	0.08791800
C	3.18109700	-1.10376400	1.04929800
C	3.97259200	0.08093900	-0.90169800
C	4.31382200	-1.91129000	1.01862400
H	2.42806500	-1.26002800	1.82254300
C	5.10582400	-0.73086900	-0.92921900
H	3.84959600	0.85820300	-1.65419300
C	5.27813100	-1.72799500	0.02851500
H	4.43676500	-2.69226000	1.76709800
H	5.85642400	-0.57932000	-1.70251800
H	6.16199100	-2.36233700	0.00303500
C	1.85126000	2.02390400	1.62696100
C	3.12397400	2.57653200	1.82648900
C	0.82412300	2.32120700	2.52990800
C	3.35979600	3.41923200	2.90737000
H	3.93040200	2.34589000	1.12937500
C	1.06388000	3.16369100	3.61337500
H	-0.16450900	1.88480300	2.37976900
C	2.32976100	3.71333900	3.80118900
H	4.34965300	3.84650300	3.05451900
H	0.26115800	3.38663500	4.31347500
H	2.51768500	4.36978800	4.64863200
C	1.55210700	2.01874400	-1.26265600
C	1.32117200	1.42346800	-2.51296900
C	1.70280300	3.40632100	-1.18258900
C	1.26657500	2.20493700	-3.66251500
H	1.18444800	0.34149700	-2.57562300
C	1.63686400	4.18612900	-2.33606300
H	1.86717100	3.88293300	-0.21714800
C	1.42272200	3.58896400	-3.57545200
H	1.09560000	1.73370400	-4.62851100
H	1.75287400	5.26575100	-2.26235500
H	1.37240900	4.20040000	-4.47417600
P	1.50051800	0.93780500	0.20484400

Int_{EE}(L5)

M06-L electronic energy (Hartree): -2291.228164

M06-L thermal correction to free energy (Hartree): 0.447445

Three lowest frequencies (cm⁻¹): 24.80, 32.81, 35.43

Pd	-0.20525700	1.50631900	-0.37475400
O	-0.16112900	3.70483100	-0.52544500

O	-2.00376800	2.69574300	0.16015700
C	-1.36990700	3.76473900	-0.11928700
C	-2.04402600	5.09544500	-0.00063600
C	1.66197600	1.03626200	-0.82389300
C	2.68479100	0.69705300	0.02415800
S	2.29298800	1.22108700	-2.43428400
C	3.95942000	0.57475700	-0.61306200
C	3.91308100	0.81921200	-1.95931900
H	4.73118200	0.81902700	-2.66893600
O	2.52771700	0.52436300	1.37727700
C	3.62676600	-0.19064500	1.94874800
H	3.55913000	-1.25125900	1.66637700
O	5.09477300	0.24053800	0.06814700
C	4.93846800	0.39130200	1.48598600
H	5.78481900	-0.13145400	1.93849600
H	4.99820500	1.45821600	1.74673200
H	3.51467600	-0.10403200	3.03286600
H	-2.90035600	5.04539200	0.67616200
H	-1.33995700	5.85847000	0.34265000
H	-2.40806900	5.40691300	-0.98673200
C	0.43349800	-1.83798300	0.68461200
C	1.42779100	-2.37755600	-0.16107800
C	0.37740800	-2.23999800	2.02748000
C	2.32721100	-3.30257200	0.38344800
C	1.28583100	-3.15650000	2.54475600
H	-0.39934100	-1.84437500	2.67873000
C	2.26588200	-3.69404200	1.71547100
H	3.09010800	-3.72534800	-0.27052800
H	1.21800700	-3.45400800	3.58892900
H	2.98070500	-4.41696000	2.10385100
C	-1.64877800	-1.55618300	-1.29659600
C	-1.55284600	-2.95633300	-1.31362500
C	-2.43170900	-0.90173800	-2.27420700
C	-2.19326900	-3.71165300	-2.28832200
H	-0.97014200	-3.46666000	-0.54911000
C	-3.06204400	-1.68533400	-3.24735600
C	-2.94570800	-3.07045900	-3.26712500
H	-2.10369900	-4.79572100	-2.27765100
H	-3.66413300	-1.18374200	-4.00440700
H	-3.44983700	-3.64619300	-4.04081200
C	-2.08330400	-0.48006200	1.35661000
C	-1.83437500	0.26806100	2.53202200
C	-3.34204700	-1.06868100	1.16414800
C	-2.85971000	0.36941600	3.47737600

C	-4.34897700	-0.93879000	2.11514800
H	-3.53880900	-1.64243800	0.26098200
C	-4.10466300	-0.21825100	3.27924100
H	-2.66740400	0.93130600	4.39105900
H	-5.31629800	-1.40657000	1.94515200
H	-4.88066600	-0.11276500	4.03485600
P	-0.80354900	-0.64231000	0.05258200
C	-2.63247300	0.58101300	-2.30572800
H	-2.94293200	0.98471800	-1.33371500
H	-1.70769800	1.11067400	-2.57914800
H	-3.39622400	0.85250400	-3.04219300
C	-0.53790800	0.96839200	2.80557800
H	-0.53557200	1.96807200	2.34519900
H	-0.39302500	1.10676600	3.88312500
H	0.33761300	0.44193400	2.40891500
C	1.55018500	-2.06814800	-1.62252000
H	0.88217200	-1.27133600	-1.95554900
H	2.57405500	-1.75358300	-1.86503200
H	1.32662300	-2.95912700	-2.22502100

Pre-TS_{EE}(L5)

M06-L electronic energy (Hartree): -2291.228164

M06-L thermal correction to free energy (Hartree): 0.553314

Three lowest frequencies (cm⁻¹): 20.06, 25.33, 32.55

Pd	0.11774300	-0.95626300	0.17294300
O	-0.58869400	-3.90253700	1.35541200
O	-1.09061000	-2.63416000	-0.44636900
C	-1.21031900	-3.67904800	0.30190800
C	-2.25386700	-4.65850800	-0.20020300
C	1.36602500	0.52664200	0.64316400
C	2.03638800	1.38106900	-0.19465000
S	1.88105400	0.82546100	2.27933700
C	2.95051900	2.26109700	0.46774000
C	2.96986600	2.09728600	1.82819100
H	3.57139300	2.62377300	2.55891500
O	1.87025700	1.38950200	-1.56039900
C	2.43334100	2.55866700	-2.15728100
H	1.77515500	3.42138900	-1.97095800
O	3.72975300	3.15832000	-0.20736100
C	3.80778900	2.83529600	-1.60159600
H	4.26863300	3.69943400	-2.08663700

H	4.45996500	1.95765600	-1.73680700
H	2.47121400	2.36438700	-3.23259800
C	3.90696200	-1.55740300	-0.64808300
C	3.10242600	-2.03277100	0.41762800
C	3.32887200	-1.77161200	-1.87561300
C	1.84774900	-2.49668100	0.01296700
S	1.79026200	-2.50780300	-1.74991300
O	5.11634600	-0.97223500	-0.45244500
C	5.26654500	-0.54908700	0.91356600
O	3.50601300	-2.04058600	1.69508100
C	4.88768600	-1.65368800	1.86363500
H	3.71677900	-1.45220700	-2.83597200
H	6.31866300	-0.28203100	1.03266600
H	4.64286400	0.33949300	1.08661400
H	4.97600900	-1.32748200	2.90219200
H	1.25558800	-3.22491000	0.57073200
H	-2.18299300	-4.79156700	-1.28483900
H	-2.16861000	-5.62812600	0.29778500
H	-3.25272000	-4.25081600	0.00448700
H	5.51158600	-2.54248700	1.70863600
C	-1.43888400	2.10933600	-0.83436400
C	-0.78495500	3.19259400	-0.20179900
C	-1.87135400	2.25949800	-2.16167300
C	-0.56945900	4.36126600	-0.94298200
C	-1.64438000	3.42994300	-2.87554800
H	-2.41482700	1.45434200	-2.64732100
C	-0.98117400	4.48882500	-2.26351100
H	-0.06509100	5.19340700	-0.45101800
H	-1.99474300	3.51160400	-3.90241600
H	-0.79183700	5.41248100	-2.80755300
C	-2.61583500	0.93597900	1.54398800
C	-3.32076700	2.14756600	1.58833700
C	-2.67056000	0.05810400	2.64840800
C	-4.05109500	2.51487100	2.71229300
H	-3.30084200	2.81227800	0.72587500
C	-3.40209100	0.45582300	3.77331800
C	-4.08173200	1.66769100	3.81644000
H	-4.59424200	3.45765400	2.72099000
H	-3.44405800	-0.21775800	4.62877300
H	-4.64509700	1.94349700	4.70574200
C	-2.98721500	-0.37401300	-0.99693400
C	-2.68406500	-0.94401800	-2.25424600
C	-4.27507700	-0.53648600	-0.46339700
C	-3.69729100	-1.62967600	-2.93261700

C	-5.26187300	-1.23211700	-1.15298100
H	-4.51719000	-0.11008100	0.50712200
C	-4.97126500	-1.78129300	-2.39747600
H	-3.46624400	-2.06002200	-3.90738600
H	-6.25262400	-1.33912500	-0.71621700
H	-5.73301400	-2.32643900	-2.95184000
P	-1.71316500	0.49450900	0.00820200
C	-2.02837500	-1.29147200	2.63706400
H	-2.35583800	-1.88667400	1.77560300
H	-0.93194700	-1.23875000	2.55988200
H	-2.27295800	-1.85290300	3.54506400
C	-1.34013200	-0.85799600	-2.91577000
H	-0.90422200	-1.85877200	-3.01429900
H	-1.42701500	-0.43689700	-3.92592300
H	-0.61609500	-0.24770200	-2.36463200
C	-0.37190500	3.21189000	1.23754500
H	-0.35952500	2.22506000	1.70114400
H	0.63428900	3.63527500	1.34667400
H	-1.05767400	3.83910300	1.82416000

TS_{EE}(L5)

M06-L electronic energy (Hartree): -3072.117204

M06-L thermal correction to free energy (Hartree): 0.548017

Three lowest frequencies (cm⁻¹): -624.14, 19.93, 29.02

Pd	0.12141600	-0.81056500	0.12939300
O	0.59713100	-3.95705100	0.76459500
O	-1.01811600	-2.69193700	-0.15822900
C	-0.60973700	-3.76586600	0.33642300
C	-1.55990600	-4.91171400	0.48982300
C	1.21953800	0.76828100	0.62119200
C	2.04051700	1.54278200	-0.15394400
S	1.44198400	1.20873900	2.28949800
C	2.83604200	2.47806500	0.57931000
C	2.62121100	2.42890000	1.93126600
H	3.06373100	3.04592800	2.70345300
O	2.11924300	1.43626200	-1.52491000
C	2.69587100	2.60801100	-2.09953500
H	1.97787600	3.44221100	-2.04276600
O	3.70978100	3.34059800	-0.02512200
C	3.97225700	2.97577300	-1.38489800
H	4.45297100	3.84407200	-1.84295200

H	4.67261100	2.12619100	-1.40951600
H	2.88608500	2.37415100	-3.15026000
C	4.28246000	-1.58905000	-0.54674600
C	3.20504500	-1.58644900	0.38439600
C	3.88276300	-1.92548400	-1.81433700
C	1.95045400	-1.88477100	-0.13801300
S	2.18605700	-2.19869900	-1.85895800
O	5.56506400	-1.27631500	-0.19631300
C	5.58838100	-0.54275300	1.03445000
O	3.39624500	-1.32869600	1.70235900
C	4.77590100	-1.25305400	2.08441500
H	4.50955300	-2.03155800	-2.69252700
H	6.63795700	-0.46967000	1.32705500
H	5.18672800	0.46955300	0.86793100
H	4.79290100	-0.71011800	3.03328600
H	1.20815300	-3.03904300	0.47224000
H	-2.37656900	-4.82674400	-0.23149400
H	-1.05142200	-5.87274300	0.38262300
H	-1.99386300	-4.87559900	1.49652300
H	5.16219400	-2.26920100	2.24529000
C	-1.86724800	1.92113500	-1.13910100
C	-1.20019700	3.11816100	-0.78434900
C	-2.44996300	1.82635000	-2.41432800
C	-1.09760400	4.13181600	-1.74603500
C	-2.34183300	2.85025900	-3.34682100
H	-3.01355000	0.93803300	-2.68428000
C	-1.64278100	4.00714500	-3.01721000
H	-0.57671000	5.04897500	-1.46900500
H	-2.80440600	2.73921300	-4.32534300
H	-1.53617800	4.81454700	-3.73929300
C	-2.73392800	0.97173800	1.50050800
C	-3.44199400	2.18000200	1.53468200
C	-2.68680600	0.15656600	2.65479300
C	-4.07667400	2.60951100	2.69478000
H	-3.49678800	2.79392500	0.63689300
C	-3.32938600	0.61177300	3.81066200
C	-4.01148100	1.82377100	3.84166400
H	-4.62196100	3.55112400	2.69802100
H	-3.29781100	-0.01254200	4.70306300
H	-4.50042300	2.14775700	4.75850700
C	-3.12842900	-0.70434500	-0.81946700
C	-2.81930500	-1.41565700	-2.00096800
C	-4.33983500	-0.96488800	-0.16181300
C	-3.74792700	-2.34541100	-2.48021700

C	-5.24003100	-1.90646400	-0.64888900
H	-4.58756600	-0.42378800	0.74931000
C	-4.94184400	-2.60162300	-1.81667400
H	-3.51083400	-2.88914200	-3.39510100
H	-6.17174400	-2.08934000	-0.11719200
H	-5.63668400	-3.34031100	-2.21190700
P	-1.91134600	0.43765000	-0.04429300
C	-2.02017600	-1.18471100	2.66937200
H	-2.39632800	-1.83599000	1.86804000
H	-0.93279200	-1.10775600	2.51068400
H	-2.18515900	-1.69352500	3.62506200
C	-1.54913200	-1.24221700	-2.78285200
H	-1.01501100	-2.19734600	-2.85791200
H	-1.76041300	-0.90882200	-3.80742700
H	-0.85375900	-0.51804600	-2.34228600
C	-0.66417400	3.41632800	0.58233200
H	-0.62853400	2.54512500	1.23608000
H	0.35247400	3.82625800	0.53049200
H	-1.29345500	4.17050200	1.07613500

Post-TS_{EE}(L5)

M06-L electronic energy (Hartree): -3072.122292

M06-L thermal correction to free energy (Hartree): 0.550152

Three lowest frequencies (cm⁻¹): 20.25, 29.01, 30.79

Pd	0.28303500	-0.69328100	0.08072300
O	0.83742400	-3.74603100	1.14233800
O	-0.63336100	-2.71761200	-0.21443700
C	-0.29049500	-3.69711500	0.45657300
C	-1.13354700	-4.91904000	0.56628600
C	1.19478900	0.99248100	0.57203400
C	1.92432800	1.86178500	-0.19078500
S	1.26816800	1.49774500	2.23427500
C	2.51479700	2.93774000	0.54495100
C	2.24638200	2.88809100	1.88611200
H	2.54279400	3.58960400	2.65604100
O	2.08913400	1.73424800	-1.55373300
C	2.48385500	2.97373200	-2.14295700
H	1.62941800	3.67000700	-2.15282600
O	3.24083400	3.93131000	-0.05145900
C	3.63554500	3.58221600	-1.38282700

H	3.97624800	4.51017500	-1.84924800
H	4.47647400	2.87312100	-1.34203100
H	2.76721400	2.74771900	-3.17397500
C	4.49498000	-1.72988600	-0.55922000
C	3.43203300	-1.26978100	0.28039800
C	4.05324200	-2.31333000	-1.71527300
C	2.16001200	-1.49489300	-0.20631000
S	2.32662500	-2.28660100	-1.76496700
O	5.81422800	-1.59870300	-0.22695400
C	6.00201200	-0.61985800	0.80075900
O	3.68269100	-0.65852200	1.47797100
C	5.02636100	-0.84557800	1.92617900
H	4.64753900	-2.76906100	-2.49816500
H	7.03554900	-0.72777200	1.13833100
H	5.86547400	0.38769700	0.37757600
H	5.17690000	-0.12337900	2.73308100
H	1.35581800	-2.91651300	0.91038100
H	-2.07831300	-4.77598100	0.03800800
H	-0.60378500	-5.78190000	0.14975900
H	-1.32786800	-5.14208200	1.62040800
H	5.14498000	-1.86233200	2.33072100
C	-2.20651800	1.68758700	-1.22660900
C	-1.65357400	2.97340100	-1.01541400
C	-2.91665800	1.44728100	-2.41447300
C	-1.78736100	3.93044300	-2.02998300
C	-3.04450700	2.41721600	-3.40130900
H	-3.39511800	0.48463900	-2.56981100
C	-2.45924600	3.66557900	-3.21605500
H	-1.35615900	4.91782300	-1.86270000
H	-3.60263200	2.19295500	-4.30804200
H	-2.54082700	4.43491100	-3.98154400
C	-2.75371300	0.82523500	1.51694600
C	-3.56407700	1.96741600	1.54235000
C	-2.55885300	0.08293000	2.70523400
C	-4.15700800	2.40464300	2.72202500
H	-3.73449900	2.52464500	0.62234500
C	-3.16291300	0.54311800	3.87934200
C	-3.94696700	1.69277600	3.89848300
H	-4.78083800	3.29594300	2.71751600
H	-3.01557400	-0.02540800	4.79738600
H	-4.39946400	2.02472700	4.83101700
C	-3.07632100	-1.04040700	-0.66999100
C	-2.75622400	-1.77151000	-1.83734900
C	-4.20547900	-1.40549700	0.07713100

C	-3.58861900	-2.83228200	-2.20818200
C	-5.01267500	-2.47171100	-0.30548400
H	-4.46096300	-0.84817600	0.97644600
C	-4.70225600	-3.18968100	-1.45631700
H	-3.34138000	-3.39491300	-3.10868800
H	-5.88148900	-2.73477400	0.29435000
H	-5.32305500	-4.02777200	-1.76785100
P	-1.96420200	0.28948200	-0.04574900
C	-1.76838900	-1.18970500	2.73844800
H	-2.15702700	-1.92778000	2.02212100
H	-0.71171500	-1.02753300	2.47166600
H	-1.79721500	-1.64407800	3.73425300
C	-1.57937000	-1.46519300	-2.71694700
H	-1.05238700	-2.38687700	-2.98921700
H	-1.89404500	-0.98240100	-3.65190700
H	-0.84476100	-0.79962100	-2.24434000
C	-1.02067900	3.41546000	0.26827000
H	-0.73838500	2.58934800	0.92252600
H	-0.12031500	4.01392800	0.08382500
H	-1.71878200	4.05203900	0.83061700

Int_{EE}(L6)

M06-L electronic energy (Hartree): -2516.895545

M06-L thermal correction to free energy (Hartree): 0.456603

Three lowest frequencies (cm⁻¹): 13.35, 27.98, 28.70

C	-0.04940100	-2.06988900	-0.92477500
C	-1.34813300	-2.46355300	-0.53363400
C	0.48912700	-2.60449000	-2.09735200
C	-2.08190700	-3.35227900	-1.32149200
C	-0.24047000	-3.49094100	-2.88524600
H	1.49416700	-2.31917200	-2.40085100
C	-1.52591600	-3.85402700	-2.49515800
H	-3.08433300	-3.65013300	-1.02711000
H	0.19548500	-3.89407000	-3.79615000
H	-2.10871900	-4.54227200	-3.10450700
C	0.98814400	-1.49795600	1.71262000
C	0.79088600	-2.85902500	1.95975500
C	1.36167200	-0.66224000	2.78542500
C	0.94186800	-3.38866700	3.23741100
H	0.51646400	-3.51367800	1.13399700
C	1.50402900	-1.18785100	4.07250000
C	1.29197600	-2.54648100	4.28891800

H	0.78469200	-4.45094400	3.40802600
H	1.78544100	-0.54373800	4.90079200
H	1.40804900	-2.94661900	5.29434700
C	2.53309200	-0.76741500	-0.59842000
C	2.79950200	-0.12031000	-1.82556700
C	3.60789500	-1.26566200	0.14334600
C	4.11199700	0.01864100	-2.27939300
C	4.91745200	-1.13749600	-0.31145900
H	3.41416200	-1.75796200	1.09488700
C	5.16164200	-0.49267100	-1.51982300
H	4.31933200	0.51692400	-3.22206000
H	5.73937400	-1.53568100	0.27863200
H	6.18088100	-0.38169200	-1.88498300
P	0.82433800	-0.80094300	0.03769600
O	1.58350900	0.63480300	2.46989000
O	1.71288400	0.32567000	-2.50456900
O	-1.79570400	-1.93933400	0.63023800
C	-3.13102100	-2.22103300	1.01421400
H	-3.27980000	-3.29562500	1.17945500
H	-3.28664500	-1.68180400	1.95003400
H	-3.84080300	-1.86036800	0.25663100
C	1.92156300	1.53528400	3.51382100
H	2.03257100	2.50735800	3.03164300
H	1.12713300	1.58068300	4.26901200
H	2.86649200	1.24941900	3.99255800
C	1.93182000	1.16287600	-3.63113000
H	2.53203600	2.03942100	-3.35492500
H	2.42823400	0.61723000	-4.44287300
H	0.94181500	1.48328100	-3.95884400
Pd	0.17116300	1.36136300	-0.09088700
O	0.06825900	3.56542000	-0.12312500
O	2.01779300	2.58335900	0.22862300
C	1.32198200	3.64005100	0.11021500
C	1.96211300	4.98338300	0.28541800
C	-1.67178600	0.90070400	-0.63903300
C	-2.83580800	1.00217200	0.07815000
S	-2.05565200	0.49590600	-2.28694200
C	-4.02083800	0.78121500	-0.69055200
C	-3.76646900	0.48773100	-2.00384900
H	-4.47848000	0.31344400	-2.80079600
O	-2.88859900	1.26389700	1.42919600
C	-4.16879500	1.78179700	1.79938000
H	-4.27807500	2.80640300	1.41212400
O	-5.27843400	0.87410900	-0.16185600

C	-5.27613100	0.90474400	1.26984600
H	-6.25712700	1.28688500	1.56430600
H	-5.16781400	-0.11874800	1.65797300
H	-4.18421000	1.81154200	2.89157200
H	1.95205900	5.25092400	1.34899600
H	3.00593600	4.96473900	-0.03914300
H	1.41539800	5.75815000	-0.25828800

Pre-TS_{EE}(L6)

M06-L electronic energy (Hartree): -3297.815619

M06-L thermal correction to free energy (Hartree): 0.33667

Three lowest frequencies (cm⁻¹): 28.63, 31.52, 35.42

C	-2.01116800	1.35150000	1.59730300
C	-1.79040600	0.60592200	2.77399900
C	-2.56068700	2.63186300	1.70979600
C	-2.08284400	1.16262400	4.02361800
C	-2.86901600	3.18240300	2.94911900
H	-2.74203300	3.21139100	0.80510300
C	-2.61963700	2.44353800	4.10277000
H	-1.90207300	0.59413800	4.93139000
H	-3.29544800	4.18075400	3.01209000
H	-2.84819300	2.86231600	5.08119400
C	-3.13820500	-0.17891100	-0.55255600
C	-4.28062700	-0.18906600	0.25225300
C	-3.13587400	-0.95148000	-1.73371600
C	-5.40361800	-0.93468100	-0.10017400
H	-4.28984500	0.39474300	1.17114200
C	-4.25486900	-1.70845200	-2.08377000
C	-5.38202600	-1.69339200	-1.26658000
H	-6.28560300	-0.92277300	0.53572200
H	-4.24810700	-2.31199400	-2.98722000
H	-6.24974900	-2.28625800	-1.55012600
C	-1.42995600	2.09269400	-1.13801600
C	-0.56767600	3.17464100	-0.83402900
C	-2.16403300	2.15566500	-2.32750800
C	-0.43964100	4.24497000	-1.72625100
C	-2.03483000	3.21866600	-3.21642600
H	-2.86398000	1.36060600	-2.56329700
C	-1.16129900	4.25699700	-2.91575300
H	0.22217600	5.07352300	-1.49006500
H	-2.62244100	3.23367900	-4.13115800

H	-1.04421700	5.09528100	-3.60017300
P	-1.59554900	0.64206800	-0.02937700
O	-2.01597100	-0.86435000	-2.49160500
O	0.07135300	3.12681900	0.35476700
O	-1.31018100	-0.64874700	2.60815800
C	-0.92734200	-1.38135100	3.76402300
H	-1.79640800	-1.60082100	4.39743700
H	-0.50752400	-2.31024800	3.37632400
H	-0.18013300	-0.82882700	4.34824100
C	-1.83268200	-1.84459400	-3.50036300
H	-0.82940100	-1.68024700	-3.89679900
H	-1.90215300	-2.85054000	-3.06800900
H	-2.56678700	-1.72769500	-4.30801900
C	0.76447100	4.28665200	0.78418500
H	1.63783100	4.49103400	0.14989700
H	0.10002000	5.16158100	0.79047400
H	1.10403100	4.06558000	1.79718700
Pd	0.03700700	-1.00135200	-0.01012000
O	-0.91719100	-3.66017100	1.49204600
O	-1.33150200	-2.62093000	-0.46946000
C	-1.54896000	-3.51910600	0.42785600
C	-2.71123000	-4.44377100	0.11339900
C	1.39895600	0.39141400	0.39241400
C	2.21253300	1.10566500	-0.44797500
S	1.76806900	0.82727600	2.03455100
C	3.13846900	1.96650200	0.21931600
C	3.02316300	1.93431100	1.58388400
H	3.60037900	2.48195000	2.31873200
O	2.14113900	1.03149500	-1.82297900
C	2.82447400	2.11724000	-2.44559300
H	2.22147000	3.03701900	-2.35931200
O	4.03710700	2.74976300	-0.45253300
C	4.17809400	2.32997300	-1.81444100
H	4.73757300	3.12113200	-2.31957600
H	4.76079900	1.39586200	-1.84984600
H	2.91786900	1.85450900	-3.50285800
C	3.75065500	-1.92552700	-0.66340600
C	2.86908000	-2.35862700	0.35916300
C	3.21429100	-2.07910300	-1.91805900
C	1.61301300	-2.73433000	-0.10928800
S	1.62025900	-2.69968100	-1.86788900
O	4.98145400	-1.41062900	-0.40502200
C	5.08740500	-1.00794000	0.97170700
O	3.20682200	-2.38972400	1.65989300

C	4.60186100	-2.09949300	1.88839700
H	3.65509900	-1.75306700	-2.85286100
H	6.14567500	-0.79972400	1.14395600
H	4.50389900	-0.08782300	1.12348700
H	4.67196000	-1.79680000	2.93532600
H	0.92331800	-3.38436900	0.42732000
H	-3.63862400	-3.98450200	0.47942200
H	-2.83315800	-4.59567800	-0.96391000
H	-2.59673500	-5.40891400	0.61599600
H	5.17492400	-3.02388500	1.74045200

TS_{EE}(L6)

M06-L electronic energy (Hartree): -3297.788015

M06-L thermal correction to free energy (Hartree): 0.554368

Three lowest frequencies (cm⁻¹): -626.71, 21.04, 25.41

C	-2.15965200	1.12979900	1.70103100
C	-1.72351100	0.34047200	2.78718600
C	-2.65752300	2.40760500	1.96324100
C	-1.76947100	0.83986200	4.08998400
C	-2.70966600	2.90982800	3.26115600
H	-2.99973400	3.02291300	1.13272000
C	-2.25920700	2.12375100	4.31764900
H	-1.42815200	0.23357200	4.92426500
H	-3.09768000	3.90928400	3.44292500
H	-2.29064800	2.50545300	5.33639000
C	-3.28547200	-0.75469700	-0.15685200
C	-4.17049900	-1.06739200	0.87544600
C	-3.35628900	-1.49391600	-1.35497000
C	-5.10657000	-2.09116200	0.73575200
H	-4.12250500	-0.50380700	1.80604600
C	-4.28776500	-2.52200400	-1.50070200
C	-5.15742700	-2.81462700	-0.45181000
H	-5.78897500	-2.31931600	1.55119700
H	-4.33590500	-3.09405300	-2.42342800
H	-5.88138800	-3.61854900	-0.57222500
C	-2.49859900	1.83111800	-1.09088400
C	-1.71533600	2.99928500	-1.21012100
C	-3.66209500	1.73778900	-1.86013500
C	-2.07810200	4.01545700	-2.09807100
C	-4.03408900	2.75062100	-2.74104700
H	-4.29186500	0.85601200	-1.76854300

C	-3.23440000	3.88253100	-2.86188000
H	-1.46648200	4.90883700	-2.18688000
H	-4.94402300	2.65096800	-3.32800700
H	-3.51058500	4.67894600	-3.55044300
P	-1.94838600	0.47555400	0.01270100
O	-2.48552900	-1.11642500	-2.32420100
O	-0.63925000	3.05501000	-0.39771900
O	-1.28060000	-0.90553700	2.47325100
C	-0.60850700	-1.64519400	3.48314400
H	-1.29424200	-1.93169000	4.29040400
H	-0.22703700	-2.54058800	2.98872300
H	0.22897800	-1.06897500	3.89803900
C	-2.26326300	-2.02320200	-3.39240300
H	-1.41437300	-1.62421200	-3.95063900
H	-2.01679300	-3.02046800	-3.00589600
H	-3.13734100	-2.08618400	-4.05329300
C	0.24747900	4.15272600	-0.52693100
H	0.65286700	4.21530900	-1.54588200
H	-0.25266200	5.09776600	-0.27638500
H	1.05758900	3.95895600	0.17988900
Pd	0.14064100	-0.67650900	-0.20414700
O	0.55000200	-3.72224300	0.73507300
O	-0.95209300	-2.58995400	-0.49407000
C	-0.61887300	-3.57756300	0.19709600
C	-1.62129200	-4.65492500	0.47113800
C	1.28873100	0.89621800	0.23257500
C	2.33783100	1.39383900	-0.49703200
S	1.36981200	1.56411100	1.83613100
C	3.21290100	2.25908800	0.22613400
C	2.82455900	2.45755900	1.52539300
H	3.27287800	3.10476600	2.26902900
O	2.56969500	1.05424300	-1.81214300
C	3.50368400	1.93275900	-2.43245500
H	3.02039100	2.89701300	-2.65844200
O	4.32872400	2.82287200	-0.33693200
C	4.70438200	2.15791200	-1.54849500
H	5.44134400	2.80427100	-2.03212700
H	5.17978000	1.19253500	-1.30985000
H	3.79503200	1.45516600	-3.37269000
C	4.32011200	-1.66317100	-0.59149700
C	3.17249900	-1.50821600	0.23283600
C	4.00496700	-2.10335000	-1.85241900
C	1.95014800	-1.79342600	-0.36865200
S	2.30474300	-2.29190500	-2.02029600

O	5.58985000	-1.39606600	-0.16146800
C	5.57888100	-0.61123000	1.03853500
O	3.26567900	-1.13167700	1.53297100
C	4.60616400	-1.17839500	2.03860600
H	4.69428900	-2.32616400	-2.65887300
H	6.60090400	-0.63198800	1.42363800
H	5.30606800	0.42843100	0.79760000
H	4.59915400	-0.58941600	2.95940500
H	1.19722200	-2.84705900	0.32846600
H	-2.20861800	-4.36176500	1.35113600
H	-2.31692300	-4.74949600	-0.36670800
H	-1.14297000	-5.61290600	0.68594400
H	4.86561500	-2.21902800	2.28002100

Post-TS_{EE}(L6)

M06-L electronic energy (Hartree): -3297.793799

M06-L thermal correction to free energy (Hartree): 0.556178

Three lowest frequencies (cm⁻¹): 16.91, 26.96, 29.52

C	-2.24907600	1.02556100	1.70724300
C	-1.76951600	0.27162000	2.79996200
C	-2.82858900	2.26989600	1.96162900
C	-1.85853300	0.77153100	4.10028300
C	-2.92155700	2.77412800	3.25673400
H	-3.20548000	2.85848300	1.12680100
C	-2.43064900	2.02261800	4.31965000
H	-1.48544700	0.19291200	4.94038900
H	-3.37354100	3.74778600	3.43069400
H	-2.49342000	2.40494900	5.33670100
C	-3.21431500	-0.95293400	-0.14334800
C	-4.07246000	-1.33979100	0.88628400
C	-3.23465600	-1.68341100	-1.34884800
C	-4.93023000	-2.42930700	0.73844500
H	-4.06601200	-0.78184300	1.82153600
C	-4.08738000	-2.77646100	-1.50346600
C	-4.93072700	-3.14309100	-0.45581500
H	-5.59178300	-2.71517700	1.55292100
H	-4.09656700	-3.34015300	-2.43259300
H	-5.59373800	-3.99697400	-0.58304800
C	-2.65732400	1.68385800	-1.07856500
C	-1.95846900	2.90063200	-1.22885100

C	-3.83602900	1.50802900	-1.80831900
C	-2.41889100	3.88616500	-2.10612100
C	-4.30503000	2.48866600	-2.67969400
H	-4.40163200	0.58619800	-1.69293900
C	-3.58892500	3.67162300	-2.82989900
H	-1.87268300	4.81833700	-2.21941500
H	-5.22502400	2.32450700	-3.23574300
H	-3.94145600	4.44429100	-3.51064700
P	-1.97885100	0.38246700	0.02136600
O	-2.39687400	-1.23233600	-2.31665000
O	-0.86041300	3.03089400	-0.45391600
O	-1.24060800	-0.94395700	2.49514600
C	-0.57888300	-1.65267700	3.53319000
H	-1.28267200	-1.95819800	4.31763400
H	-0.14862100	-2.53780100	3.06215300
H	0.22190600	-1.04497100	3.97451700
C	-2.11161900	-2.10946400	-3.39459800
H	-1.29709100	-1.64282500	-3.95156300
H	-1.78987400	-3.08977600	-3.01968000
H	-2.98112200	-2.23146100	-4.05320100
C	-0.07416400	4.20166200	-0.59130600
H	0.30272800	4.30669900	-1.61761400
H	-0.64881400	5.09817100	-0.32258800
H	0.76391700	4.07360500	0.09761800
Pd	0.25048000	-0.59091300	-0.24037100
O	0.69981200	-3.64798900	0.85640100
O	-0.73127200	-2.60062800	-0.53004000
C	-0.44263300	-3.55613600	0.19700400
C	-1.38401100	-4.68466100	0.43543700
C	1.29116100	1.04739500	0.20619900
C	2.30612700	1.65164700	-0.49119300
S	1.24474700	1.72287200	1.80911400
C	3.04618300	2.62086200	0.25349700
C	2.59437900	2.77839600	1.53698700
H	2.93796000	3.47893200	2.28799200
O	2.62463500	1.34437000	-1.79787300
C	3.42723700	2.35972300	-2.39452100
H	2.81288300	3.24944300	-2.60816900
O	4.09049100	3.32842500	-0.27998600
C	4.57308200	2.73576400	-1.48944400
H	5.22353300	3.48152700	-1.95395200
H	5.16969000	1.84087100	-1.25128300
H	3.79141000	1.94757100	-3.33964300
C	4.42838300	-1.85933600	-0.56013000

C	3.29881100	-1.36272300	0.16040900
C	4.09776000	-2.36997500	-1.78685400
C	2.08854500	-1.47649300	-0.49230300
S	2.39396000	-2.23070700	-2.04146900
O	5.70044800	-1.83203900	-0.05889900
C	5.81245200	-0.92633200	1.04407400
O	3.42559000	-0.82359000	1.41247500
C	4.68152300	-1.13271100	2.01819400
H	4.75467500	-2.84107200	-2.50813100
H	6.78100200	-1.13032600	1.50707400
H	5.80477200	0.11053200	0.67312800
H	4.77459200	-0.46357300	2.87812900
H	1.25836800	-2.85608300	0.58084300
H	-1.95608600	-4.46806400	1.34688900
H	-2.09244300	-4.76539900	-0.39145700
H	-0.85519400	-5.62764100	0.59027500
H	4.67626100	-2.17394100	2.37568800

Int_{EE}(L7)

M06-L electronic energy (Hartree): -2471.027701

M06-L thermal correction to free energy (Hartree): 0.337646

Three lowest frequencies (cm⁻¹): 10.78, 24.23, 33.73

Pd	0.35219000	1.50369800	0.29189100
O	0.54355600	3.68447400	0.54397400
O	2.25534800	2.49900900	-0.19604000
C	1.75304900	3.61974900	0.14092400
C	2.57907000	4.86628100	0.08718800
C	-1.52268800	1.11745300	0.78724800
C	-2.60024500	0.92788900	-0.03966800
S	-2.04688300	1.05155400	2.44195000
C	-3.83903900	0.74842200	0.65185500
C	-3.70524000	0.78260200	2.01359600
H	-4.48230700	0.70682200	2.76394800
O	-2.51587900	0.93176500	-1.41147900
C	-3.69186700	0.38711900	-2.01820500
H	-3.67902900	-0.70897400	-1.92513500
O	-5.02426500	0.55901600	-0.00120900
C	-4.93777000	0.94646000	-1.37885000
H	-5.83779600	0.55387100	-1.85845800
H	-4.94538700	2.04399000	-1.45046400
H	-3.63862200	0.65312100	-3.07690600
H	2.02526900	5.67157200	-0.40487900

H	2.79847300	5.20452500	1.10622700
H	3.52310200	4.69466000	-0.43504600
C	-0.57232600	-1.71731500	-0.85968400
C	-1.66481200	-2.17728400	-0.11846600
C	-0.53266300	-2.06055900	-2.21788300
C	-2.67605700	-2.94714700	-0.66951700
C	-1.54015300	-2.82677900	-2.79525500
H	0.30571300	-1.73658700	-2.82946700
C	-2.61001700	-3.27146600	-2.02170300
H	-3.49475700	-3.27794400	-0.03585300
H	-1.48253500	-3.08219800	-3.85015100
H	-3.39837200	-3.87330000	-2.46790800
C	1.27664500	-1.62096500	1.35267500
C	1.04580300	-2.99758400	1.48859500
C	2.02052200	-0.99705300	2.35695500
C	1.52243800	-3.69910700	2.58927100
H	0.48998900	-3.52440300	0.71511000
C	2.50097700	-1.67296800	3.46666400
C	2.24417400	-3.03528100	3.58020000
H	1.33053500	-4.76583300	2.67206100
H	3.06899400	-1.13002100	4.21675300
H	2.61586000	-3.57943300	4.44524600
C	2.13043800	-0.74585200	-1.23357400
C	2.14005700	0.03264200	-2.39446800
C	3.27744100	-1.50344100	-0.95921200
C	3.21483500	0.07302900	-3.26467900
C	4.37122600	-1.47923700	-1.81788900
H	3.31004800	-2.11954200	-0.06306700
C	4.33981200	-0.69208500	-2.96707700
H	3.16086000	0.69451700	-4.15400700
H	5.24922400	-2.07679000	-1.58679600
H	5.19415600	-0.66938600	-3.63947600
P	0.70831300	-0.67329300	-0.09411700
F	-1.72782900	-1.89698800	1.19641400
F	2.30668900	0.31778600	2.24186900
F	1.04330800	0.76659300	-2.68988100

Pre-TS_{EE}(L7)

M06-L electronic energy (Hartree): -3251.948276

M06-L thermal correction to free energy (Hartree): 0.444031

Three lowest frequencies (cm⁻¹): 17.70, 23.03, 32.52

Pd	0.06308600	-1.00452200	0.11061200
O	-0.89237900	-3.74655600	1.40682400
O	-1.26197300	-2.58822600	-0.49644800
C	-1.50210700	-3.53924000	0.34370100
C	-2.66093900	-4.43591300	-0.04886000
C	1.33588100	0.45777500	0.59596600
C	2.06783500	1.25996000	-0.24269300
S	1.71259200	0.87194000	2.24084400
C	2.92754700	2.18466700	0.42850000
C	2.84489500	2.10593000	1.79384400
H	3.39566300	2.67390000	2.53323000
O	2.00031600	1.17613200	-1.61453200
C	2.65898300	2.26689000	-2.25916500
H	2.01068500	3.15663500	-2.23844700
O	3.75872000	3.03437400	-0.24824800
C	3.97433300	2.57628600	-1.58933200
H	4.50416800	3.38149900	-2.10375700
H	4.61192900	1.67784000	-1.56999500
H	2.80711700	1.96138600	-3.29876000
C	3.79434800	-1.72978500	-0.58221400
C	2.94180400	-2.16763800	0.46291300
C	3.26660600	-1.97567500	-1.82529900
C	1.69983100	-2.62808400	0.01795800
S	1.71355200	-2.68933100	-1.74408600
O	4.99583800	-1.14003900	-0.35096600
C	5.07884500	-0.67000700	1.00574300
O	3.28810400	-2.13601600	1.75641400
C	4.66300900	-1.74704600	1.97125000
H	3.69522500	-1.68464400	-2.77741000
H	6.12178500	-0.38814600	1.16429800
H	4.43893600	0.21679800	1.12027800
H	4.71000400	-1.39313800	3.00323200
H	1.06552900	-3.32040600	0.57328000
H	-2.44090500	-5.48159700	0.18813500
H	-3.54455900	-4.15347800	0.53710700
H	-2.91605000	-4.34144300	-1.10822000
H	5.29100700	-2.64020300	1.86500900
C	-1.27698900	2.10778500	-0.89658800
C	-0.58867400	3.14537000	-0.25885600
C	-1.62454700	2.31432900	-2.23884400
C	-0.24472800	4.32688300	-0.89615600
C	-1.28521600	3.48924200	-2.90201000
H	-2.17528400	1.54809100	-2.77563600
C	-0.59277800	4.49547800	-2.23259800

H	0.28276600	5.09496800	-0.33639700
H	-1.57114900	3.61849800	-3.94293300
H	-0.32641500	5.41671800	-2.74592600
C	-2.42553400	1.05868300	1.51969800
C	-3.09874700	2.28412200	1.63054300
C	-2.44003800	0.22057500	2.63503300
C	-3.73723800	2.64919300	2.80890500
H	-3.12155000	2.95576500	0.77358000
C	-3.06349100	0.56479500	3.82495900
C	-3.71467800	1.79075100	3.90755200
H	-4.25293700	3.60432800	2.86976700
H	-3.03623000	-0.12874300	4.66089600
H	-4.21090200	2.07181700	4.83369000
C	-3.00770900	-0.21321100	-0.96354300
C	-2.76538700	-0.82372900	-2.19584000
C	-4.30354700	-0.32051100	-0.44248700
C	-3.74227300	-1.48945400	-2.91417000
C	-5.30304500	-0.99281000	-1.14019100
H	-4.53220500	0.12814800	0.52212900
C	-5.02339600	-1.57407300	-2.37445700
H	-3.49097200	-1.93689300	-3.87211000
H	-6.30220800	-1.05921500	-0.71674800
H	-5.80180000	-2.09909500	-2.92326600
P	-1.62809700	0.53530400	-0.03304900
F	-0.27498700	3.02220400	1.04387500
F	-1.84030400	-0.98500300	2.55947500
F	-1.52210500	-0.74489700	-2.72107100

TS_{EE}(L7)

M06-L electronic energy (Hartree): -3251.920298

M06-L thermal correction to free energy (Hartree): 0.438874

Three lowest frequencies (cm⁻¹): -610.18, 16.03, 25.61

Pd	0.08785400	-0.89169700	0.18746400
O	0.54401200	-4.03676800	0.82809000
O	-1.06993700	-2.75705400	-0.07877400
C	-0.65724600	-3.84362900	0.38349500
C	-1.57583100	-5.02239300	0.45932000
C	1.14925900	0.73786700	0.60163700
C	1.93046100	1.50015800	-0.22588100
S	1.34557100	1.29361700	2.23559100
C	2.68473100	2.51168800	0.44610500

C	2.47929200	2.53045800	1.79998100
H	2.89680800	3.21112000	2.53137900
O	2.01579600	1.30430600	-1.58616000
C	2.60012500	2.42643200	-2.24562100
H	1.87087600	3.25005400	-2.29701300
O	3.52652100	3.36609400	-0.21507300
C	3.84360700	2.88699200	-1.52643100
H	4.31844100	3.72248800	-2.04744900
H	4.56529800	2.05810400	-1.45148900
H	2.83339000	2.09768800	-3.26206500
C	4.24753300	-1.59054400	-0.42858600
C	3.16269100	-1.60344000	0.49396100
C	3.87299400	-1.98020700	-1.68855300
C	1.92545200	-1.96242900	-0.02944100
S	2.18820500	-2.31938900	-1.73796600
O	5.51390300	-1.21663600	-0.07836800
C	5.49779000	-0.44845900	1.13103700
O	3.33053700	-1.29310100	1.80424400
C	4.70322400	-1.15907300	2.19445600
H	4.51176200	-2.08995600	-2.55764400
H	6.54124500	-0.32598700	1.42956500
H	5.05801700	0.54200000	0.93277400
H	4.69434200	-0.59122900	3.12869500
H	1.16012500	-3.11848200	0.57262300
H	-1.09017700	-5.91438600	0.05326200
H	-1.80971300	-5.23382000	1.50857400
H	-2.50572400	-4.82309900	-0.07717600
H	5.12405400	-2.15629200	2.38489900
C	-1.63425200	1.88732100	-1.09647300
C	-1.04793100	3.05513900	-0.59820000
C	-1.93473500	1.86932000	-2.46616400
C	-0.76060300	4.15386700	-1.39284800
C	-1.64874100	2.95658000	-3.28563200
H	-2.40808500	0.99250000	-2.89985500
C	-1.05780900	4.09874300	-2.75064300
H	-0.30919800	5.03099400	-0.93608800
H	-1.89640400	2.91055600	-4.34315300
H	-0.83095900	4.95224100	-3.38538000
C	-2.71494300	0.97759500	1.43517700
C	-3.44667500	2.17186800	1.48128900
C	-2.70538800	0.18996200	2.58774100
C	-4.11712700	2.55809200	2.63588900
H	-3.48829100	2.80123400	0.59372400
C	-3.35975400	0.55444400	3.75354500

C	-4.06867600	1.75137100	3.77220600
H	-4.68022300	3.48799900	2.64792300
H	-3.31451800	-0.09996800	4.61955400
H	-4.59102700	2.04906500	4.67851100
C	-3.11823000	-0.58436300	-0.91726200
C	-2.76775200	-1.35111300	-2.03106400
C	-4.43380300	-0.70596200	-0.45065000
C	-3.65191600	-2.19631800	-2.67752700
C	-5.34302600	-1.55170800	-1.07939900
H	-4.74808400	-0.13117200	0.41823800
C	-4.95252300	-2.29609900	-2.19006500
H	-3.31697000	-2.76275500	-3.54213400
H	-6.35866600	-1.62756100	-0.69882900
H	-5.65910900	-2.96008900	-2.68274300
P	-1.84240600	0.40121400	-0.05467400
F	-0.77556400	3.14599600	0.71670400
F	-2.05249200	-0.99357700	2.56741300
F	-1.50535100	-1.25539000	-2.51167300

Post-TS_{EE}(L7)

M06-L electronic energy (Hartree): -3251.930740

M06-L thermal correction to free energy (Hartree): 0.444550

Three lowest frequencies (cm⁻¹): 19.50, 28.34, 32.73

Pd	0.66791300	-0.31189500	-0.41563000
O	2.40492000	-3.17252900	-0.65337900
O	0.41865100	-2.35373500	-1.31775700
C	1.17290200	-3.30900600	-1.11195100
C	0.75150600	-4.71981100	-1.32574400
C	0.79895700	1.55353300	0.23861400
C	0.28325300	2.64642100	-0.40694900
S	1.55892800	2.07434800	1.71082500
C	0.44391300	3.87975500	0.29759300
C	1.11623100	3.73735700	1.48063500
H	1.36352200	4.50089200	2.20764700
O	-0.33021300	2.58017800	-1.63975900
C	-1.14111400	3.73214600	-1.87694400
H	-2.05125100	3.67278100	-1.26172600
O	-0.05220000	5.06621900	-0.16854000
C	-0.38184300	4.99727100	-1.56092000
H	-0.98537000	5.88380600	-1.77212100
H	0.54126000	5.04533500	-2.15787000
H	-1.42317900	3.69745200	-2.93261900

C	5.01001400	0.02330600	-0.38920600
C	3.72040300	-0.31579600	0.12847400
C	4.96325100	0.44908500	-1.68902800
C	2.67741900	-0.18517600	-0.76200000
S	3.32841800	0.41903600	-2.25886300
O	6.15733300	-0.08867200	0.34272700
C	5.88809700	-0.23735600	1.74231400
O	3.55091300	-0.76433300	1.41814500
C	4.78173600	-1.23499300	1.97582800
H	5.79273100	0.73274800	-2.32541800
H	6.82515500	-0.57030100	2.19524900
H	5.61166300	0.73902400	2.16735300
H	4.59834700	-1.37787100	3.04346100
H	2.59396000	-2.19495700	-0.59051500
H	1.54856000	-5.30794400	-1.78727100
H	0.53387700	-5.17147800	-0.35053700
H	-0.15342300	-4.75563400	-1.93419000
H	5.04284200	-2.20524700	1.52521200
C	-2.72097100	1.02163000	0.15587700
C	-2.56051100	2.00880800	1.13182200
C	-3.70616600	1.24361000	-0.81488300
C	-3.33224400	3.15979100	1.17597400
C	-4.49222900	2.39248100	-0.79547000
H	-3.87621100	0.49679500	-1.58742700
C	-4.30938600	3.34802200	0.20202500
H	-3.16515900	3.88198100	1.97098800
H	-5.25459000	2.53427700	-1.55735600
H	-4.92466800	4.24438400	0.22533500
C	-1.97666300	-1.18933900	1.81338600
C	-3.09049000	-0.84675200	2.59356300
C	-1.11634500	-2.15699100	2.33638400
C	-3.31191100	-1.43285100	3.83463100
H	-3.79749300	-0.11172200	2.21289200
C	-1.31084500	-2.75501400	3.57133800
C	-2.41925200	-2.38413200	4.32537900
H	-4.18398200	-1.14745500	4.41753900
H	-0.60112700	-3.49985300	3.92067200
H	-2.58503500	-2.84505100	5.29632400
C	-2.53423900	-1.62049400	-0.94791000
C	-2.34852200	-1.50392000	-2.32646900
C	-3.33387000	-2.67805100	-0.49915800
C	-2.92084900	-2.36768500	-3.24377800
C	-3.91878100	-3.56552200	-1.39895000
H	-3.49885800	-2.80680000	0.56913200

C	-3.71414700	-3.40887800	-2.76789600
H	-2.74198200	-2.21899000	-4.30523200
H	-4.53826400	-4.37849100	-1.02797200
H	-4.16993500	-4.09919000	-3.47395600
P	-1.65747000	-0.46517000	0.16494800
F	-1.65388700	1.81027000	2.10883000
F	-0.04978000	-2.55864500	1.60625200
F	-1.58077000	-0.48869900	-2.78677000

Int_{EE}(L8)

M06-L electronic energy (Hartree): -2471.036056

M06-L thermal correction to free energy (Hartree): 0.332689

Three lowest frequencies (cm⁻¹): 10.19, 17.59, 26.48

Pd	-0.44834300	1.78219700	-0.06551600
O	-0.90419800	3.93594300	0.02418300
O	-2.48065000	2.45372000	0.47677300
C	-2.10697400	3.66764300	0.35046300
C	-3.09154700	4.77476700	0.55562600
C	1.47689800	1.70302200	-0.50350400
C	2.51433200	1.17784500	0.22207000
S	2.09774700	2.34760300	-1.99556800
C	3.79319500	1.29756500	-0.40247300
C	3.73474100	1.90983700	-1.62577100
H	4.55290500	2.15744800	-2.29019200
O	2.34945500	0.55906300	1.43734800
C	3.46608100	-0.28530200	1.73801000
H	3.43579000	-1.17499300	1.08966900
O	4.94015500	0.82275000	0.16343300
C	4.76065200	0.46225700	1.53969000
H	5.62092300	-0.15866900	1.80154800
H	4.77482000	1.37063100	2.15939000
H	3.34116500	-0.59812900	2.77791000
H	-3.62603000	4.96122100	-0.38324700
H	-3.83506000	4.50061900	1.30857400
H	-2.58902400	5.70100800	0.84459200
C	0.85398900	-1.55629500	-0.32778900
C	1.68572600	-1.34222300	-1.43693200
C	1.10418500	-2.64659300	0.51360400
C	2.74946300	-2.19550700	-1.70137000
C	2.16391500	-3.51237600	0.25762600
H	0.46901200	-2.83144900	1.37787700
C	2.96795200	-3.26955800	-0.84690300

H	2.36830400	-4.36355300	0.90084400
C	-1.78546400	-0.99977800	-1.30860600
C	-1.67370900	-2.23067300	-1.96877600
C	-2.88701400	-0.17317300	-1.57905000
C	-2.64050700	-2.63295500	-2.88387500
H	-0.82869500	-2.88706900	-1.76940100
C	-3.86104800	-0.56673500	-2.48773600
C	-3.71761100	-1.79203500	-3.12607800
H	-2.56721100	-3.58317200	-3.40526700
C	-1.27084100	-0.95279900	1.54325900
C	-0.64612400	-0.48236700	2.70916800
C	-2.39604400	-1.77890900	1.64990400
C	-1.12706900	-0.84102100	3.96129400
C	-2.89116500	-2.13824000	2.89942800
H	-2.89151300	-2.15139500	0.75501600
C	-2.24560000	-1.66296000	4.03197600
H	-3.76328700	-2.77777500	3.00175000
P	-0.57227200	-0.46163500	-0.06145400
H	0.22927100	0.16221400	2.62708400
H	-2.98231500	0.78662600	-1.07069300
H	1.50484800	-0.49659400	-2.09980700
H	-0.65541200	-0.48943200	4.87462100
H	3.40551600	-2.03622200	-2.55281000
H	-4.71912600	0.06171900	-2.70910300
F	-4.65309100	-2.17522000	-4.01091100
F	3.99308400	-4.10070700	-1.09975800
F	-2.72016300	-2.00670300	5.24098400

Pre-TS_{EE}(L8)

M06-L electronic energy (Hartree): -3251.956953
M06-L thermal correction to free energy (Hartree): 0.436927
Three lowest frequencies (cm⁻¹): 11.04, 20.19, 24.98

Pd	0.53997400	-0.74256900	-0.73380000
O	-0.46182600	-1.87459800	-3.33933000
O	-0.46267600	-2.58402900	-1.20682000
C	-0.77469800	-2.69202200	-2.45501600
C	-1.57790800	-3.93200900	-2.78846500
C	1.45298700	0.92936400	-0.13159000
C	1.45506400	2.15334200	-0.74963900
S	2.27098400	1.08033300	1.39793900
C	2.12993200	3.18534200	-0.02845500

C	2.62999200	2.76102600	1.17447700
H	3.20762700	3.32483800	1.89609700
O	0.84792700	2.38491200	-1.96136700
C	0.62728700	3.78157700	-2.17437900
H	-0.20306300	4.12388400	-1.53680200
O	2.22901800	4.46705900	-0.48738400
C	1.87587000	4.57171100	-1.87264500
H	1.72750300	5.63716700	-2.06548300
H	2.71160800	4.21073200	-2.49042300
H	0.33774900	3.88950600	-3.22263600
C	4.03904500	-1.37803600	-0.15286800
C	2.92274800	-2.16100500	-0.55624500
C	4.40811100	-0.46129900	-1.10312800
C	2.37854800	-1.74968700	-1.77831700
S	3.40103700	-0.52099900	-2.48785800
O	4.64475200	-1.54111200	1.05263300
C	3.79340200	-2.26007200	1.95705600
O	2.46250200	-3.20884900	0.15389700
C	3.27058300	-3.51509200	1.31095200
H	5.18641100	0.28707600	-1.01298500
H	4.40595000	-2.49581400	2.82930700
H	2.96360000	-1.60602500	2.26666600
H	2.61623400	-4.06938200	1.98765500
H	1.77790700	-2.36452200	-2.43992800
H	-0.97660000	-4.83226700	-2.61625500
H	-2.45151800	-4.00365200	-2.12996100
H	-1.91046400	-3.92367700	-3.82986300
H	4.09577600	-4.16449500	0.99322700
C	-1.68658000	1.81793300	0.41241200
C	-0.93111700	2.65417400	1.24902100
C	-2.68588000	2.38670900	-0.38664300
C	-1.17415300	4.02030100	1.30126200
C	-2.93651800	3.75540100	-0.34962800
H	-3.29025300	1.76305800	-1.04175000
C	-2.17724800	4.54848400	0.49829100
H	-3.71452200	4.20420100	-0.96068200
C	-1.20325500	-0.48160600	2.09194400
C	-1.95441700	0.13953400	3.09913000
C	-0.36094500	-1.55089600	2.42891100
C	-1.86397300	-0.29078100	4.41790200
H	-2.61387400	0.97141300	2.85564800
C	-0.26109800	-1.99239100	3.74253300
C	-1.01570500	-1.34947500	4.71505400
H	-2.43601500	0.18295900	5.21061300

C	-2.81457500	-0.73024400	-0.32358200
C	-3.00781500	-0.69076400	-1.71209700
C	-3.76851700	-1.35983100	0.48240600
C	-4.14165300	-1.24794800	-2.28841400
C	-4.90477900	-1.93187900	-0.08270300
H	-3.63053800	-1.41160400	1.56096100
C	-5.07215700	-1.86076400	-1.45806800
H	-5.65380400	-2.42712800	0.52880600
P	-1.30787500	0.03402700	0.35150400
H	-2.24757300	-0.24367000	-2.35269000
H	0.22874000	-2.03806000	1.64932700
H	-0.14259500	2.23492300	1.87338500
H	-4.30123400	-1.22927300	-3.36312400
H	-0.59181800	4.67320200	1.94618400
H	0.39369900	-2.81463200	4.01860600
F	-0.91893500	-1.76293200	5.98926900
F	-2.41990000	5.87012200	0.54544800
F	-6.16816800	-2.41185300	-2.00836400

TS_{EE}(L8)

M06-L electronic energy (Hartree): -3251.930305

M06-L thermal correction to free energy (Hartree): 0.435596

Three lowest frequencies (cm⁻¹): -786.48, 9.11, 19.11

Pd	0.84160200	-0.28621400	-0.51697800
O	2.56807300	-2.39117200	-2.30182400
O	0.71662000	-2.42113000	-1.02658200
C	1.51756900	-2.96104300	-1.83029600
C	1.26539900	-4.37392900	-2.26367900
C	0.86101600	1.64577800	-0.08910600
C	0.06269100	2.62316900	-0.62074400
S	1.90648400	2.36211700	1.10041500
C	0.26331300	3.92431500	-0.06532700
C	1.23373900	3.95041100	0.89916300
H	1.58005900	4.79699900	1.47868600
O	-0.88372900	2.37842200	-1.59128100
C	-1.86685600	3.41744800	-1.62826100
H	-2.52579800	3.33205700	-0.75035500
O	-0.47447300	5.01032900	-0.44284300
C	-1.20637500	4.77371900	-1.65202900
H	-1.94852000	5.57367600	-1.71549000
H	-0.52554800	4.85097800	-2.51264400

H	-2.45709900	3.24722300	-2.53293000
C	4.99543500	0.44632300	-0.01027100
C	3.82469300	-0.35820300	0.00852400
C	5.00617600	1.31656700	-1.07162200
C	2.91692100	-0.13966000	-1.02696200
S	3.57908800	1.15180800	-2.01424900
O	5.98685900	0.34502200	0.92068100
C	5.53662500	-0.35456800	2.08854200
O	3.60951300	-1.30191100	0.96457500
C	4.79979500	-1.61263900	1.70829600
H	5.79119600	2.01724800	-1.33278100
H	6.43298900	-0.58445600	2.66869200
H	4.88633000	0.30672300	2.68017100
H	4.46785700	-2.16118600	2.59229500
H	2.69701400	-1.32382200	-1.76090300
H	1.71002900	-5.05721700	-1.53102800
H	0.19209000	-4.57730300	-2.29867800
H	1.72281700	-4.57857600	-3.23416500
H	5.44109100	-2.26505600	1.10001400
C	-2.38398300	0.90571700	0.74867300
C	-1.84606500	1.82809700	1.66012300
C	-3.70464600	1.07283000	0.31531700
C	-2.60701200	2.89372800	2.12602400
C	-4.47972800	2.13342400	0.77674100
H	-4.14358800	0.36783600	-0.38821100
C	-3.91443800	3.02603000	1.67616800
H	-5.50702000	2.26924900	0.44940600
C	-1.41639700	-1.60148100	1.68274500
C	-2.59677000	-1.74661000	2.42635100
C	-0.27031600	-2.30217300	2.07977700
C	-2.64089900	-2.58132200	3.53569700
H	-3.49333900	-1.19806200	2.13766500
C	-0.29882900	-3.14046200	3.18971800
C	-1.48667500	-3.26605100	3.89537200
H	-3.54818000	-2.70351000	4.12112700
C	-2.34605400	-1.34465700	-1.05843400
C	-2.48506500	-0.70240700	-2.29929600
C	-2.89926900	-2.61736200	-0.88355800
C	-3.18198500	-1.30759000	-3.33709000
C	-3.59000700	-3.24004700	-1.91951800
H	-2.79313900	-3.13675600	0.06736800
C	-3.72188100	-2.57091400	-3.12664300
H	-4.02482200	-4.22833700	-1.79778100
P	-1.35981000	-0.50831000	0.22316800

H	-2.04350600	0.28417200	-2.44812500
H	0.65456900	-2.18890900	1.51375600
H	-0.81895200	1.71842200	2.00851500
H	-3.30519000	-0.82056600	-4.30073100
H	-2.19790900	3.61801900	2.82544600
H	0.58253700	-3.68856500	3.51133100
F	-1.52237600	-4.07472000	4.96887000
F	-4.65603500	4.05248600	2.13030300
F	-4.39217800	-3.16417700	-4.13073300

Post-TS_{EE}(L8)

M06-L electronic energy (Hartree): -3251.938308

M06-L thermal correction to free energy (Hartree): 0.437029

Three lowest frequencies (cm⁻¹): 14.04, 16.17, 20.94, 25.39

Pd	0.88370500	0.17703500	0.31506100
O	2.78406800	-1.21263400	-1.89583700
O	1.58218300	-1.90179200	-0.12116400
C	2.26559800	-2.14974700	-1.11943900
C	2.59014400	-3.53598100	-1.54906100
C	0.11516100	1.96778600	0.65326400
C	-0.61718300	2.71142800	-0.23327300
S	0.17153800	2.79970400	2.17573800
C	-1.14695200	3.92457600	0.30530500
C	-0.80982600	4.11905200	1.61741700
H	-1.08032200	4.94363700	2.26467300
O	-0.86188000	2.31605900	-1.52918100
C	-2.00683900	2.98853600	-2.06276800
H	-2.91898500	2.58405900	-1.59649400
O	-1.94062400	4.76891800	-0.41680500
C	-1.91090300	4.47406100	-1.81910600
H	-2.76244000	5.00265900	-2.25505700
H	-0.98309700	4.87175100	-2.25638900
H	-2.02348500	2.76307900	-3.13245900
C	5.11606700	1.33928100	0.22459000
C	4.00306100	0.46868800	0.44063300
C	4.73689200	2.59292100	-0.17242100
C	2.76015600	1.02607300	0.21016100
S	3.01436400	2.68826900	-0.26034100
O	6.41623200	0.94715000	0.38057200
C	6.52921600	-0.30479000	1.06542600
O	4.18448900	-0.83705900	0.83674700
C	5.51056800	-1.29121300	0.55388700

H	5.37657400	3.43542400	-0.40544500
H	7.54852900	-0.65621400	0.88612600
H	6.39193300	-0.14643200	2.14531700
H	5.61373600	-2.25981800	1.04958600
H	2.61843900	-0.33250000	-1.46190700
H	3.62037700	-3.76970900	-1.25578300
H	1.91830400	-4.25018100	-1.07153000
H	2.53370700	-3.62842500	-2.63691500
H	5.62725100	-1.43150200	-0.53258900
C	-2.79925300	0.18409500	0.05850200
C	-3.02128600	1.17722700	1.02482900
C	-3.76530300	-0.02424100	-0.93362100
C	-4.17931900	1.94582100	1.00447900
C	-4.93085300	0.73684600	-0.96576700
H	-3.61496800	-0.79074000	-1.69183800
C	-5.11599100	1.70954200	0.00655600
H	-5.68886500	0.58158100	-1.72848400
C	-1.63465800	-1.99860500	1.50073100
C	-2.91402400	-2.54428900	1.67924500
C	-0.60241500	-2.38207300	2.36653200
C	-3.15970800	-3.46022200	2.69457400
H	-3.72938200	-2.25020200	1.01852500
C	-0.83256000	-3.29787700	3.38781100
C	-2.11012400	-3.82041500	3.53092000
H	-4.14505400	-3.89187000	2.84682000
C	-1.25635900	-1.79472100	-1.36870300
C	-0.96152400	-1.11766000	-2.56331800
C	-1.41135800	-3.18423500	-1.39328900
C	-0.84274600	-1.80961900	-3.76197300
C	-1.28618800	-3.89145900	-2.58634800
H	-1.62493900	-3.72867500	-0.47489100
C	-1.00568500	-3.18980000	-3.74933900
H	-1.40089000	-4.97142600	-2.62029900
P	-1.27665100	-0.81186600	0.16634400
H	-0.82087400	-0.03522800	-2.54735400
H	0.39302800	-1.95672500	2.23830200
H	-2.27744200	1.35988400	1.80044100
H	-0.61903400	-1.29917600	-4.69472000
H	-4.35579200	2.72359600	1.74287900
H	-0.04330400	-3.60208200	4.06958100
F	-2.34393400	-4.70265900	4.51789500
F	-6.23980700	2.44874600	-0.01859500
F	-0.88055900	-3.86797700	-4.90459600

Int_{EE}(L9)

M06-L electronic energy (Hartree): -2471.034477

M06-L thermal correction to free energy (Hartree): 0.334725

Three lowest frequencies (cm⁻¹): 14.40, 21.68, 27.72

Pd	-0.60532100	1.59584800	-0.10036100
O	-1.21627700	3.70818000	-0.05624700
O	-2.68871100	2.12388000	0.39836500
C	-2.39818700	3.36046700	0.27247300
C	-3.43553400	4.40261100	0.54313700
C	1.32556600	1.65656700	-0.51796400
C	2.39058500	1.19322400	0.20923200
S	1.90697900	2.31482600	-2.01993800
C	3.65949000	1.37088200	-0.42118800
C	3.56488900	1.96364600	-1.65211800
H	4.36749800	2.25204900	-2.31906700
O	2.25836600	0.56818600	1.42474600
C	3.42271100	-0.20582000	1.73664700
H	3.44508100	-1.10393300	1.09991800
O	4.83076200	0.96438500	0.14746100
C	4.67165200	0.61316800	1.52884300
H	5.56606300	0.04645600	1.79891100
H	4.63288400	1.52932200	2.13578300
H	3.31434600	-0.51181700	2.78041000
H	-3.41248600	4.66678400	1.60690700
H	-3.23707700	5.31185200	-0.02968800
H	-4.43634100	4.02642300	0.31655500
C	0.93380600	-1.64730100	-0.32477000
C	1.73982800	-1.34446800	-1.42823100
C	1.25711600	-2.73250900	0.49754900
C	2.85888200	-2.12447800	-1.67054800
C	2.38251400	-3.50694300	0.21749900
H	0.63337400	-2.97763500	1.35450300
C	3.19872400	-3.20699700	-0.86934500
H	2.62949300	-4.35101400	0.85701400
H	4.08546000	-3.79162100	-1.09799700
C	-1.76746900	-1.31979800	-1.24296100
C	-1.55129600	-2.52823200	-1.91582600
C	-2.95562300	-0.60656700	-1.45035800
C	-2.51884400	-3.01879700	-2.79085800
H	-0.63373600	-3.09009300	-1.75660600
C	-3.89642500	-1.12514500	-2.32493500
C	-3.70285800	-2.32051700	-3.00474300

H	-2.34828600	-3.95764900	-3.31241700
H	-4.46769900	-2.68554100	-3.68455200
C	-1.18789600	-1.17104900	1.59025700
C	-0.58193300	-0.61140500	2.72306200
C	-2.22556500	-2.09841800	1.73432000
C	-1.02748200	-1.00527700	3.97383500
C	-2.65193800	-2.46797600	3.00913800
H	-2.69727800	-2.53627200	0.85719900
C	-2.05593000	-1.92400800	4.14223700
H	-3.45814400	-3.18906500	3.12126400
H	-2.37642900	-2.19707600	5.14380800
P	-0.56502500	-0.65191400	-0.04204600
H	0.22681500	0.11160000	2.62945900
H	-3.14880200	0.33775100	-0.94280300
H	1.51904000	-0.50603500	-2.08634600
F	3.64507000	-1.81354600	-2.71752700
F	-5.03778400	-0.44049700	-2.52615400
F	-0.44741000	-0.47242000	5.06514000

Pre-TS_{EE}(L9)

M06-L electronic energy (Hartree): -3251.954582

M06-L thermal correction to free energy (Hartree): 0.437467

Three lowest frequencies (cm⁻¹): 7.63, 21.19, 24.52

Pd	0.74032000	-0.32894600	-0.75040600
O	0.20404600	-2.07730800	-3.06443100
O	0.79068700	-2.47872300	-0.93355200
C	0.41651600	-2.85088800	-2.11409700
C	0.21054600	-4.34167900	-2.26484900
C	0.62084700	1.64370800	-0.45746500
C	-0.33808200	2.48080600	-0.96945100
S	1.55414300	2.52948500	0.71686400
C	-0.31148500	3.81124600	-0.45263000
C	0.66534900	3.99896700	0.49005100
H	0.93276800	4.91423200	1.00304800
O	-1.28668300	2.06501500	-1.87533200
C	-2.39989000	2.96322100	-1.90920900
H	-3.00895700	2.82700300	-1.00172400
O	-1.19410500	4.77651400	-0.84197400
C	-1.93088200	4.39303000	-2.01065100
H	-2.77592900	5.08330000	-2.07262400
H	-1.29732900	4.52450800	-2.90015800

H	-2.99462500	2.68038500	-2.78143800
C	4.13692000	0.82801900	-0.52421100
C	3.48662000	-0.41489900	-0.75288400
C	3.98091900	1.70209700	-1.56917900
C	2.73196200	-0.43018500	-1.93474300
S	3.02515800	1.04600900	-2.82903100
O	4.81346400	1.09697200	0.62293500
C	4.45252000	0.16603800	1.65442800
O	3.62219400	-1.47672800	0.06397600
C	4.55016700	-1.24824100	1.14883200
H	4.32851600	2.72720500	-1.61101200
H	5.14956700	0.33704700	2.47669800
H	3.42956200	0.38672500	1.99847200
H	4.27788600	-1.96847500	1.92267700
H	2.46266300	-1.32034800	-2.49348000
H	-0.72469500	-4.62285200	-1.76312800
H	0.13641000	-4.62955100	-3.31677000
H	1.01340000	-4.90811800	-1.78236700
H	5.56248800	-1.46603600	0.78716800
C	-2.31379700	0.68874300	0.95064800
C	-1.85700500	1.82979100	1.62239000
C	-3.66926600	0.58022000	0.61722400
C	-2.76142800	2.83129700	1.93398800
C	-4.55635700	1.60245200	0.95380000
H	-4.04116200	-0.30205200	0.10256500
C	-4.11042200	2.74249700	1.61526400
H	-5.60874500	1.50798000	0.69658900
H	-4.78410000	3.55255300	1.88060000
C	-0.54299000	-1.19102500	2.20009500
C	-1.39520900	-1.17446500	3.31200500
C	0.77301100	-1.64724400	2.33699400
C	-0.93301700	-1.61402800	4.55006100
H	-2.41806400	-0.81513100	3.21071500
C	1.20268100	-2.07157200	3.58459900
C	0.37610900	-2.06501700	4.69892500
H	-1.59609900	-1.60046100	5.41176700
H	0.75905100	-2.40198900	5.65819300
C	-2.12581600	-1.96867600	-0.13174600
C	-2.51085900	-1.84554800	-1.47200300
C	-2.52529600	-3.08257700	0.61229000
C	-3.29498900	-2.84051300	-2.03236500
C	-3.31286500	-4.06748400	0.01758100
H	-2.22402100	-3.18462600	1.65275100
C	-3.70675700	-3.95506100	-1.31258900

H	-3.62209900	-4.93466500	0.59648900
H	-4.31637000	-4.71396700	-1.79517700
P	-1.10672300	-0.62586400	0.55849300
H	-2.18965000	-1.00087700	-2.07920300
H	1.45484700	-1.66971500	1.48619100
H	-0.81018900	1.95435900	1.89548300
F	-2.31115000	3.93324600	2.56260500
F	2.47554900	-2.49656600	3.71971000
F	-3.66008300	-2.72656700	-3.32297600

TS_{EE}(L9)

M06-L electronic energy (Hartree): -3251.929235

M06-L thermal correction to free energy (Hartree): 0.435705

Three lowest frequencies (cm⁻¹): -810.56, 8.47, 18.73

Pd	0.72423800	-0.36627200	-0.47157700
O	2.52976200	-2.54121900	-2.13045700
O	0.62929400	-2.51136300	-0.92971300
C	1.46873600	-3.09208800	-1.66377300
C	1.24354000	-4.53386500	-2.00904400
C	0.71366900	1.56888900	-0.04412700
C	-0.12264200	2.52834900	-0.54904600
S	1.72182200	2.29342200	1.17475300
C	0.01695200	3.81798400	0.05062700
C	0.97993400	3.85530300	1.02204500
H	1.29150600	4.69877000	1.62509100
O	-1.06099300	2.26969700	-1.52394200
C	-2.07728100	3.27743500	-1.55148400
H	-2.74794400	3.14756300	-0.68825300
O	-0.76508400	4.88256400	-0.29735900
C	-1.46469000	4.65556200	-1.52723700
H	-2.23380900	5.43004800	-1.58327700
H	-0.77036500	4.78116000	-2.37120000
H	-2.64579100	3.11170900	-2.47076800
C	4.84938300	0.71016200	-0.35974900
C	3.75714500	-0.17105000	-0.13740600
C	4.69830700	1.44104100	-1.51158600
C	2.75357700	-0.15156300	-1.10608600
S	3.21852400	1.05752000	-2.29293400
O	5.91930100	0.80382800	0.47869700
C	5.63005000	0.22686900	1.75945200
O	3.70313300	-0.99673200	0.94148800

C	4.97503200	-1.12097800	1.60283100
H	5.39615300	2.16188300	-1.92173200
H	6.58835100	0.14080900	2.27637300
H	4.97611000	0.90689900	2.32436100
H	4.76543600	-1.57647600	2.57269400
H	2.60670900	-1.41725000	-1.68731500
H	0.17850400	-4.72327300	-2.16810000
H	1.81669400	-4.82862800	-2.89028800
H	1.56459500	-5.15661000	-1.16630700
H	5.61544500	-1.79576600	1.01889200
C	-2.51828700	0.75694300	0.83855400
C	-1.97205100	1.69033700	1.72882100
C	-3.85017100	0.89098900	0.42818900
C	-2.76658100	2.73562800	2.17266800
C	-4.62643800	1.94754800	0.90188600
H	-4.28598500	0.17008300	-0.26013200
C	-4.08975200	2.88576000	1.77942400
H	-5.66154400	2.04261100	0.58154100
H	-4.67441100	3.72228400	2.15256100
C	-1.52459000	-1.74545400	1.75164800
C	-2.71238500	-1.92670100	2.47306000
C	-0.35997900	-2.40659600	2.15255800
C	-2.73526700	-2.77015600	3.57945700
H	-3.61827600	-1.40308900	2.16938900
C	-0.41382600	-3.23690600	3.26291700
C	-1.58041000	-3.43498400	3.98634400
H	-3.65903100	-2.91064200	4.13628600
H	-1.57426100	-4.09092800	4.85251800
C	-2.44428500	-1.47087400	-0.99373800
C	-2.57197500	-0.80469900	-2.22049700
C	-2.99429100	-2.74601000	-0.83368400
C	-3.26140000	-1.42796900	-3.24718500
C	-3.67519500	-3.34868200	-1.89095000
H	-2.89285800	-3.27274300	0.11294400
C	-3.81838100	-2.69362100	-3.10935500
H	-4.10167400	-4.34108600	-1.76304200
H	-4.34447500	-3.14678800	-3.94528100
P	-1.46704200	-0.63647600	0.29987300
H	-2.13866200	0.18362800	-2.37260800
H	0.57651900	-2.27833900	1.61120400
H	-0.93852300	1.62572300	2.06613000
F	-2.22705800	3.64203900	3.00988700
F	0.71119900	-3.86581400	3.65404100
F	-3.38694300	-0.78676100	-4.42495700

Post-TS_{EE}(L9)

M06-L electronic energy (Hartree): -3251.936619

M06-L thermal correction to free energy (Hartree): 0.438224

Three lowest frequencies (cm⁻¹): 14.03, 16.39, 22.88

Pd	0.78024700	-0.18084500	-0.28030400
O	2.80829800	0.94582700	1.97197900
O	1.69504100	1.79916400	0.21097100
C	2.39147100	1.95063300	1.21958000
C	2.84433700	3.28567000	1.69267900
C	-0.17674200	-1.87246700	-0.64686200
C	-1.01273800	-2.52314800	0.22083500
S	-0.20981100	-2.68562900	-2.18001100
C	-1.69482000	-3.64545800	-0.34255900
C	-1.36636100	-3.86788800	-1.65245000
H	-1.73629300	-4.64023400	-2.31475300
O	-1.22548000	-2.10777700	1.51597300
C	-2.44807100	-2.64009500	2.03718200
H	-3.30043100	-2.11390500	1.58004600
O	-2.60807400	-4.38102500	0.35709900
C	-2.54385600	-4.12057200	1.76521500
H	-3.45824700	-4.54179400	2.19049800
H	-1.67690700	-4.64428600	2.19441900
H	-2.43723600	-2.43448100	3.11090800
C	4.85601900	-1.78567900	-0.20052900
C	3.84031700	-0.80085800	-0.40434800
C	4.34740200	-2.99825600	0.17921200
C	2.54652800	-1.22972500	-0.17941400
S	2.62417700	-2.91532800	0.26682100
O	6.18987000	-1.52855500	-0.35113000
C	6.43321100	-0.28538200	-1.01828300
O	4.15596800	0.48405100	-0.78201500
C	5.52177800	0.79430500	-0.49285700
H	4.89523800	-3.90590200	0.40129500
H	7.48324500	-0.04431900	-0.83404800
H	6.28175500	-0.41358300	-2.10023700
H	5.72544700	1.75379400	-0.97488300
H	2.55603900	0.09852300	1.51494000
H	2.27624000	4.07685600	1.20224500
H	2.74426500	3.36357500	2.77877200
H	3.90713500	3.41099500	1.45551300
H	5.65054700	0.90636700	0.59545700

C	-2.89240800	0.22616400	-0.05731900
C	-3.18937600	-0.73559700	-1.03128700
C	-3.84729900	0.54123400	0.91727500
C	-4.42559700	-1.36180700	-0.99871900
C	-5.08589500	-0.09896900	0.91635200
H	-3.62766100	1.28899100	1.67655700
C	-5.38706100	-1.06234800	-0.04276500
H	-5.82508600	0.15359500	1.67311600
H	-6.34256300	-1.57943800	-0.05566900
C	-1.47864100	2.29693800	-1.43900700
C	-2.69431700	2.96650000	-1.63037000
C	-0.38489700	2.59159300	-2.25926800
C	-2.80975700	3.92854600	-2.62990800
H	-3.54941500	2.73403700	-0.99696200
C	-0.53150100	3.55487500	-3.24646600
C	-1.72515300	4.23207800	-3.44997400
H	-3.75377400	4.44823600	-2.77683000
H	-1.79620100	4.97559100	-4.23906000
C	-1.14916800	1.98391800	1.42869500
C	-0.89761600	1.23880000	2.58979100
C	-1.20424000	3.37874800	1.49497700
C	-0.72204800	1.91191000	3.78737900
C	-1.01563100	4.02583400	2.71624100
H	-1.38771000	3.96325400	0.59565900
C	-0.77251200	3.29772200	3.87639400
H	-1.05603400	5.11175700	2.76434500
H	-0.61890200	3.78320100	4.83618100
P	-1.26151200	1.04234500	-0.13132600
H	-0.83103500	0.15073000	2.55665300
H	0.56747600	2.07889400	-2.13462800
H	-2.46899500	-1.01457000	-1.79892400
F	-4.69607400	-2.30226600	-1.92375400
F	0.52108100	3.83559500	-4.03799900
F	-0.48018300	1.19737600	4.90339300

Int_{EE}(L10)

M06-L electronic energy (Hartree): -4195.889921

M06-L thermal correction to free energy (Hartree): 0.356038

Three lowest frequencies (cm⁻¹): 11.81, 12.83, 13.62

Pd	-0.17122300	-0.32830000	2.48113700
O	-0.41443700	-0.73705600	4.62607100
O	-2.18286600	-0.53922000	3.32006400

C	-1.68120400	-0.74661600	4.47471500
C	-2.56706300	-1.01965300	5.64673600
C	1.79491400	-0.24386200	2.19240100
C	2.63625200	-1.30520100	1.96525900
S	2.71783800	1.23118600	2.19230100
C	4.01111000	-0.93811200	1.82613900
C	4.21844400	0.41164300	1.92249000
H	5.15703700	0.94892900	1.87391100
O	2.21125300	-2.60478800	1.86549700
C	3.19923900	-3.44051400	1.24977000
H	3.21628700	-3.25129800	0.16631800
O	4.99806400	-1.84770900	1.59452200
C	4.56456300	-3.19257900	1.83911500
H	5.31395900	-3.83752300	1.37339500
H	4.55487900	-3.37949000	2.92255100
H	2.87686800	-4.46960800	1.42395400
H	-3.61471500	-0.82803200	5.40501700
H	-2.46123800	-2.06740100	5.94929300
H	-2.26640400	-0.40754400	6.50235200
C	0.68418400	-0.91639200	-0.84855200
C	2.04554000	-0.61487600	-1.01374600
C	0.14088700	-2.01768200	-1.50531900
C	2.83045600	-1.40667400	-1.84117700
H	2.49155700	0.23653200	-0.50006800
C	0.94303300	-2.80970000	-2.32937900
H	-0.91161000	-2.27083200	-1.38803900
C	2.28456100	-2.50788000	-2.50440300
H	2.90785600	-3.12489300	-3.14638100
C	0.05355000	1.80836900	-0.14840800
C	0.44101700	2.18429900	-1.43668900
C	-0.05184300	2.78182600	0.84745700
C	0.72287900	3.52030700	-1.71598000
H	0.52998700	1.44139700	-2.22905000
C	0.23983700	4.11103300	0.56034200
H	-0.34582600	2.49492300	1.85832100
C	0.63079600	4.48793700	-0.72079500
H	0.86425600	5.52491600	-0.94088000
C	-2.04978300	-0.19295000	-0.24706600
C	-2.75915000	-1.24103000	0.34541700
C	-2.67319600	0.59886700	-1.21383100
C	-4.07345600	-1.49773800	-0.03396700
H	-2.28925500	-1.84844900	1.11836100
C	-3.99012100	0.33486400	-1.58299800
H	-2.14116400	1.42373900	-1.68540400

C	-4.69680000	-0.71113700	-0.99695200
H	-5.72425100	-0.90844000	-1.28615200
P	-0.32871000	0.08347300	0.29368900
C	0.16997600	5.10713900	1.67827500
C	1.14080400	3.88108500	-3.11055600
C	-4.63754100	1.22448500	-2.60220400
C	-4.79427300	-2.62977900	0.63423900
C	0.31486100	-3.98711100	-3.01184200
C	4.29696700	-1.14449000	-2.01031400
F	5.02521200	-2.17902600	-1.53088200
F	4.62712600	-1.01538100	-3.31193000
F	4.70294200	-0.03503300	-1.37442900
F	1.18887800	-4.66231000	-3.77671400
F	-0.19582800	-4.85576500	-2.11340300
F	-0.70996100	-3.60627000	-3.80270300
F	0.21243600	3.49863400	-4.01182700
F	1.33458800	5.20164200	-3.26153500
F	2.28847300	3.25923500	-3.45244900
F	0.38054800	6.36548800	1.25905900
F	1.09395700	4.83412600	2.62558900
F	-1.03047500	5.07474400	2.29214100
F	-6.05956100	-2.75903400	0.20136500
F	-4.16744400	-3.80518400	0.41714700
F	-4.83681000	-2.45888300	1.97249100
F	-5.83078700	0.75569100	-3.00512800
F	-3.86190600	1.36304600	-3.69689500
F	-4.83577100	2.46613700	-2.11104000

Pre-TS_{EE}(L10)

M06-L electronic energy (Hartree): -4976.814069

M06-L thermal correction to free energy (Hartree): 0.460716

Three lowest frequencies (cm⁻¹): 8.46, 10.29, 13.47

Pd	0.96689900	-0.66040700	-1.56704500
O	-0.46248200	-0.94370300	-4.10253200
O	-0.23343300	-2.28061900	-2.31592900
C	-0.68894200	-2.00548200	-3.49489700
C	-1.53589200	-3.09587200	-4.11313800
C	2.11572400	0.78057500	-0.77919600
C	2.20459400	2.08513500	-1.19485200
S	3.17350800	0.55701000	0.58540400
C	3.15893800	2.87307800	-0.47694600
C	3.76391700	2.18433000	0.54061200

H	4.51950600	2.53626400	1.23146800
O	1.44905300	2.60945100	-2.21350500
C	1.43902200	4.03995600	-2.16412900
H	0.82138200	4.37610900	-1.31591500
O	3.42553600	4.17407400	-0.78049300
C	2.84118500	4.57602900	-2.02568300
H	2.84975900	5.66895900	-2.02233800
H	3.46783500	4.21586800	-2.85530700
H	0.97689900	4.37473500	-3.09555400
C	4.58495300	-1.28499600	-1.91777700
C	3.40544600	-2.04387600	-2.13341000
C	4.66555600	-0.19836100	-2.75439300
C	2.53542700	-1.46082700	-3.06673300
S	3.32048100	-0.07722100	-3.80441000
O	5.51248800	-1.61745200	-0.98432500
C	4.98020900	-2.56528400	-0.04583400
O	3.15583400	-3.21228700	-1.51536400
C	4.29151000	-3.69646800	-0.76060400
H	5.43304600	0.56696200	-2.74422200
H	5.82970400	-2.92907300	0.53585700
H	4.27995500	-2.04813000	0.62469800
H	3.88870200	-4.42679300	-0.05798100
H	1.83554200	-2.02643100	-3.67174900
H	-0.90029800	-3.94302300	-4.39663900
H	-2.26737500	-3.47713900	-3.39196300
H	-2.05725000	-2.73601800	-5.00369800
H	4.97577300	-4.19871000	-1.45532800
C	-0.83510600	1.65517900	0.43771200
C	0.11128200	2.39224000	1.16607600
C	-1.97700300	2.29718100	-0.03803000
C	-0.10835400	3.73917300	1.42337300
H	1.01285600	1.91375800	1.54667100
C	-2.17800800	3.65564100	0.21245700
H	-2.72907600	1.74905100	-0.60259400
C	-1.25095500	4.38193000	0.94455300
H	-1.41369100	5.43719400	1.14658800
C	0.02155500	-0.85298100	1.62110700
C	-0.33694000	-0.35085500	2.87199100
C	0.80882500	-2.00802700	1.54310400
C	0.10199900	-0.99160800	4.03125300
H	-0.95901700	0.53989700	2.95505800
C	1.22586700	-2.64815300	2.70366900
H	1.09642500	-2.40157200	0.56567800
C	0.88230800	-2.13854900	3.95485900

H	1.21441000	-2.63647300	4.86113000
C	-2.18072800	-0.79446800	-0.25511100
C	-2.70958500	-0.68064200	-1.54808800
C	-2.91844200	-1.43863100	0.73455500
C	-3.96569900	-1.19837400	-1.83158900
H	-2.12645400	-0.20439700	-2.33611700
C	-4.17859600	-1.96232600	0.43601400
H	-2.52301800	-1.54647500	1.74346500
C	-4.70655500	-1.84566400	-0.84115800
H	-5.68410000	-2.26141300	-1.07116600
P	-0.51813300	-0.10203300	0.04849600
C	2.09597300	-3.86463500	2.60620200
C	-0.29255500	-0.41030800	5.35630000
C	-4.93365000	-2.65866500	1.52785500
C	-4.55349800	-1.09681700	-3.20699600
C	-3.41988200	4.29889200	-0.32587400
C	0.90802400	4.55406700	2.16429500
F	1.58763700	5.36073000	1.31935000
F	0.32523300	5.35780600	3.07798500
F	1.80982200	3.79422800	2.80773300
F	-3.51194500	5.59685300	0.00952400
F	-3.46475400	4.22346300	-1.67315700
F	-4.53003200	3.68087000	0.12952700
F	-1.63370400	-0.31495800	5.46749000
F	0.15015400	-1.14459100	6.39045200
F	0.19598400	0.83867500	5.50490500
F	1.92599500	-4.69147600	3.65112800
F	3.40917800	-3.53431000	2.57642800
F	1.84958500	-4.56579300	1.48065100
F	-4.87626500	-2.31648600	-3.68988900
F	-5.69146700	-0.37192600	-3.20308600
F	-3.71066800	-0.52596600	-4.08422100
F	-6.13205100	-3.10725100	1.11796800
F	-5.14380900	-1.83741300	2.57809500
F	-4.24314400	-3.71751500	2.00118100

TS_{EE}(L10)

M06-L electronic energy (Hartree): -4976.788801

M06-L thermal correction to free energy (Hartree): 0.456481

Three lowest frequencies (cm⁻¹): -759.80, 10.59, 11.56

Pd	1.25332000	-0.83776700	-1.17873200
O	2.10241900	-3.57181800	-2.79519500

O	0.39052700	-2.80643800	-1.55562500
C	0.91852400	-3.66476000	-2.30800700
C	0.10967300	-4.86333600	-2.70271500
C	1.99122200	0.98253800	-0.83617700
C	1.84873300	2.09774500	-1.62084400
S	2.99516800	1.37651500	0.52752700
C	2.52185700	3.25750100	-1.12452400
C	3.19597000	3.02902800	0.04402200
H	3.74965900	3.73735700	0.64716700
O	1.12983700	2.11408000	-2.79331500
C	0.79281900	3.44828900	-3.18520500
H	-0.01631900	3.82856100	-2.54347700
O	2.45937100	4.47018600	-1.74665400
C	1.99120100	4.35994400	-3.09614000
H	1.73419500	5.37562900	-3.40829100
H	2.80464400	3.98440500	-3.73462300
H	0.42686700	3.38142000	-4.21266800
C	5.45881100	-1.22518700	-1.15298100
C	4.13536800	-1.66517100	-0.88435500
C	5.55103400	-0.56917600	-2.35576300
C	3.18970800	-1.38308300	-1.87182600
S	4.02193500	-0.48658200	-3.13306900
O	6.50708900	-1.43940400	-0.31015600
C	6.05626000	-1.78886900	1.00583000
O	3.81171000	-2.32502700	0.25983600
C	4.97332100	-2.83429400	0.94266800
H	6.44806000	-0.16293500	-2.80886300
H	6.93380500	-2.16526700	1.53615100
H	5.68820200	-0.88638300	1.51433600
H	4.63401400	-3.11574300	1.94032200
H	2.59725900	-2.55114800	-2.38935700
H	-0.58511200	-5.13792000	-1.90508800
H	-0.48977500	-4.60608200	-3.58440000
H	0.74746200	-5.71056900	-2.96312500
H	5.33032000	-3.72918400	0.41558100
C	-1.35798500	1.48797400	-0.28363700
C	-0.67769200	2.62726000	0.17734300
C	-2.53423200	1.64460400	-1.01383200
C	-1.19258100	3.89116500	-0.08426200
H	0.24868100	2.52789700	0.74196200
C	-3.03854900	2.92009900	-1.27318500
H	-3.07817800	0.77535300	-1.38057300
C	-2.37589500	4.04599200	-0.80849900
H	-2.76976400	5.03882500	-1.00955200

C	-0.19934500	-0.14101800	1.77387700
C	-0.92605400	0.57149900	2.73109100
C	0.93145600	-0.85750300	2.17281200
C	-0.52374300	0.55869200	4.06585800
H	-1.80448300	1.14856900	2.44171500
C	1.32843200	-0.85973500	3.50582800
H	1.52376000	-1.39845000	1.43126600
C	0.60563900	-0.15255300	4.46081600
H	0.92131600	-0.14849200	5.49949500
C	-2.05895800	-1.30731600	-0.12951000
C	-2.33784400	-1.83732300	-1.39670700
C	-2.82584800	-1.70836700	0.96202600
C	-3.37019600	-2.75006900	-1.55919600
H	-1.72845000	-1.55077800	-2.25030600
C	-3.86678900	-2.62290700	0.78728700
H	-2.62017700	-1.32217200	1.95936700
C	-4.14135200	-3.14934100	-0.46697500
H	-4.94339100	-3.87162300	-0.59540800
P	-0.63762700	-0.16653100	0.00121900
C	2.58294000	-1.59643800	3.85950100
C	-1.34291600	1.32176600	5.06317200
C	-4.66744300	-3.02360300	1.98916200
C	-3.64472700	-3.37073100	-2.89485600
C	-4.30707400	3.03476500	-2.06227600
C	-0.47959300	5.13373200	0.35674800
F	-0.11525700	5.88073400	-0.71076900
F	-1.27694400	5.91649500	1.11474900
F	0.62854900	4.87465800	1.06735200
F	-4.70076500	4.31005600	-2.21952100
F	-4.16700500	2.49873700	-3.29384300
F	-5.31836300	2.36720700	-1.46752600
F	-2.58624500	0.80629700	5.16965700
F	-0.79594400	1.31250600	6.29062000
F	-1.49205400	2.61043100	4.69252800
F	2.80371200	-1.63999800	5.18228600
F	3.66444100	-1.01723500	3.28613600
F	2.55251800	-2.86922500	3.40580100
F	-3.43992200	-4.70628000	-2.86068000
F	-4.92508100	-3.18763000	-3.27557400
F	-2.85598300	-2.87182800	-3.86451300
F	-5.62952800	-3.91377300	1.69231400
F	-5.26427000	-1.95497200	2.55848900
F	-3.88264300	-3.57489700	2.93914900

Post-TS_{EE}(L10)

M06-L electronic energy (Hartree): -4976.794001

M06-L thermal correction to free energy (Hartree): 0.460099

Three lowest frequencies (cm⁻¹): 10.73, 11.29, 11.94

Pd	1.38477700	-0.61431800	-1.17152400
O	2.44949600	-3.31581100	-2.90629700
O	0.74872600	-2.70992100	-1.56525000
C	1.27766200	-3.51341600	-2.34659600
C	0.59442800	-4.77418000	-2.74974700
C	1.88668600	1.27604100	-0.81794100
C	1.62554300	2.36407000	-1.60981400
S	2.81997200	1.78513900	0.55682700
C	2.14075600	3.59749400	-1.10174900
C	2.82074200	3.45154200	0.07654800
H	3.26505300	4.22305900	0.69258900
O	0.93745200	2.29220100	-2.79861200
C	0.43641600	3.57347300	-3.19206500
H	-0.42565300	3.84134900	-2.56269000
O	1.93559900	4.79465700	-1.72327700
C	1.50497800	4.63232500	-3.07989400
H	1.12263600	5.60792000	-3.39165100
H	2.36939100	4.36972800	-3.70767900
H	0.09955200	3.46559700	-4.22596600
C	5.64675500	-1.01685800	-1.15246900
C	4.28904000	-1.31291400	-0.83279400
C	5.76746900	-0.29867600	-2.31356600
C	3.35271900	-0.85820300	-1.74201100
S	4.20864200	0.01527000	-2.98658700
O	6.69734000	-1.41595600	-0.37748700
C	6.26709300	-1.76372500	0.94479300
O	3.94005400	-1.98431100	0.31080600
C	5.05885100	-2.66357000	0.89817100
H	6.68078900	0.00806400	-2.80909700
H	7.11530100	-2.26541700	1.41647000
H	6.03460200	-0.84646700	1.50669400
H	4.74343400	-2.95189700	1.90270700
H	2.81056700	-2.43255100	-2.56539900
H	-0.08740200	-5.10389400	-1.96351900
H	-0.00285000	-4.57675400	-3.64817000
H	1.31277400	-5.55995600	-2.99156800
H	5.28039000	-3.56966700	0.31573500
C	-1.54345600	1.35352900	-0.29813700

C	-1.00693600	2.56805500	0.16044300
C	-2.72345700	1.36712500	-1.03907300
C	-1.66546400	3.76102500	-0.11276700
H	-0.08109900	2.58231600	0.73422200
C	-3.37194600	2.57260600	-1.31162200
H	-3.15824100	0.43804000	-1.40481000
C	-2.85149800	3.77173100	-0.84863600
H	-3.35826400	4.70982600	-1.05937700
C	-0.19187500	-0.11525700	1.76380100
C	-0.99148300	0.51587500	2.71983700
C	1.01313400	-0.69901800	2.16376600
C	-0.58643300	0.55694900	4.05321500
H	-1.93085800	0.98779900	2.43099200
C	1.40993900	-0.65177200	3.49643300
H	1.66308600	-1.17145800	1.42323800
C	0.61528500	-0.02310000	4.44931900
H	0.92972700	0.02043700	5.48743500
C	-1.90250800	-1.50359300	-0.12529900
C	-2.13078200	-2.06300800	-1.39018200
C	-2.60481600	-1.99452500	0.97330200
C	-3.05266300	-3.08895900	-1.54421400
H	-1.56926200	-1.70597100	-2.25068000
C	-3.53142000	-3.02619900	0.80830600
H	-2.43441700	-1.58799300	1.96920800
C	-3.75842100	-3.57825100	-0.44446200
H	-4.47152700	-4.38946200	-0.56621200
P	-0.62567700	-0.19989500	-0.00951000
C	2.72816600	-1.26540600	3.85630900
C	-1.48016700	1.23763200	5.04577700
C	-4.27183100	-3.51511000	2.01638000
C	-3.27045800	-3.73541100	-2.87819200
C	-4.64158900	2.53093900	-2.10601000
C	-1.11058300	5.08013300	0.33286100
F	-0.82149300	5.86342500	-0.73158700
F	-2.00560200	5.76458300	1.07706200
F	0.01000300	4.95520800	1.06035100
F	-5.15949700	3.75399500	-2.31158100
F	-4.44375800	1.96513800	-3.31614800
F	-5.58467200	1.78922000	-1.48711200
F	-2.67981700	0.62318200	5.12464300
F	-0.95428200	1.25680200	6.28226600
F	-1.72667700	2.51539700	4.68825000
F	2.97840900	-1.21700500	5.17462900
F	3.74933300	-0.64252600	3.22575100

F	2.78369600	-2.56258000	3.47771500
F	-2.88563800	-5.03139100	-2.85768100
F	-4.57169400	-3.72664300	-3.22931800
F	-2.57843400	-3.13073700	-3.86125400
F	-5.07214800	-4.55901500	1.74050400
F	-5.04346100	-2.54158600	2.54497800
F	-3.42057100	-3.90050400	2.99022100

Int_{EE}(L11)

M06-L electronic energy (Hartree): -3661.990729

M06-L thermal correction to free energy (Hartree): 0.224226

Three lowest frequencies (cm⁻¹): 14.75, 17.10, 23.43

Pd	0.20332800	-1.43028900	-1.54818900
O	0.62079700	-2.98693000	-3.01560400
O	2.27894200	-2.06418500	-1.88662900
C	1.86847100	-2.90682000	-2.75143500
C	2.83168400	-3.82189300	-3.43336700
C	-1.77090700	-1.27686000	-1.61805700
C	-2.72298500	-1.57667400	-0.67718500
S	-2.54622100	-0.71168200	-3.06613600
C	-4.06534600	-1.36468100	-1.12176600
C	-4.13672700	-0.88650300	-2.40222100
H	-5.02197700	-0.67556500	-2.98877000
O	-2.43362600	-2.06199700	0.57257400
C	-3.54784800	-1.93927900	1.45847600
H	-3.66224400	-0.88607100	1.76051100
O	-5.14978600	-1.61138800	-0.32995700
C	-4.81509100	-2.42554900	0.80149000
H	-5.66580100	-2.35689200	1.48357000
H	-4.69919700	-3.47041300	0.47861800
H	-3.30249200	-2.53415200	2.34182700
H	2.52476000	-4.01012000	-4.46558100
H	3.84452400	-3.41304600	-3.41147100
H	2.84287600	-4.78683900	-2.91340400
C	-0.94382300	0.71671200	1.10581500
C	-2.01197000	1.35393400	0.46434900
C	-1.00606200	0.64326400	2.49883200
C	-3.11201300	1.84650400	1.15060800
C	-2.09543800	1.13539300	3.20955300
C	-3.15212200	1.73567400	2.53594700
C	0.99299700	1.76233300	-0.58308900
C	1.40915000	2.73880500	0.32644200

C	0.95472100	2.12094600	-1.93074800
C	1.78964100	4.00837400	-0.07339900
C	1.32678400	3.39056000	-2.35674900
C	1.74576300	4.33267800	-1.42641400
C	1.74743500	-0.54449700	1.05731800
C	1.45675600	-1.70476500	1.78347500
C	3.09114900	-0.16546600	1.00334000
C	2.42242800	-2.42667000	2.46265700
C	4.08001800	-0.87557100	1.67441200
C	3.74666900	-2.00512800	2.40854900
P	0.41416300	0.14354100	0.01977400
F	-1.96874800	1.55150800	-0.85799100
F	0.54001400	1.26199500	-2.86515100
F	0.19643400	-2.14967300	1.82049600
F	2.19696500	4.91160600	0.81508300
F	2.10432000	5.54546900	-1.82649500
F	1.27726400	3.70876900	-3.64839200
F	1.47207000	2.43831900	1.62922200
F	3.49656300	0.88257800	0.28117000
F	5.34950500	-0.47911700	1.60443700
F	4.68844800	-2.68620800	3.04897000
F	2.09612100	-3.51818400	3.15174200
F	-0.00322500	0.13611100	3.21826000
F	-2.11800000	1.05289100	4.53838100
F	-4.18843400	2.21310900	3.21348400
F	-4.10785900	2.43829800	0.49555300

Pre-TS_{EE}(L11)

M06-L electronic energy (Hartree): -4442.915398

M06-L thermal correction to free energy (Hartree): 0.331417

Three lowest frequencies (cm⁻¹): 19.23, 21.94, 28.13

Pd	1.24357000	-0.67901400	-0.56311100
O	0.22556500	-2.58584700	-2.72908300
O	0.42184700	-2.67540000	-0.49116100
C	0.09938400	-3.17321800	-1.64241200
C	-0.43961400	-4.58817600	-1.57984300
C	2.00994000	1.16505600	-0.39200500
C	1.63830200	2.31169800	-1.04687600
S	3.14821800	1.58892700	0.85432900
C	2.24879400	3.50663900	-0.55846500
C	3.09905700	3.28071500	0.49141600
H	3.71868000	3.99548000	1.01820200

O	0.75981800	2.32128900	-2.10315400
C	0.22760000	3.62465600	-2.32805500
H	-0.49482400	3.86939500	-1.53258100
O	1.98511000	4.74029000	-1.08453000
C	1.32803900	4.65650400	-2.35572500
H	0.93147900	5.65506000	-2.55547900
H	2.06472500	4.40317600	-3.13224500
H	-0.30329400	3.58052800	-3.28271100
C	4.88651700	-1.03886300	-0.13868200
C	3.76157000	-1.88840300	-0.29303400
C	5.12261300	-0.27558600	-1.25503000
C	3.05728700	-1.66432800	-1.49261400
S	3.97687800	-0.54799100	-2.49346200
O	5.61658800	-0.99743600	1.00482200
C	4.87586800	-1.57210400	2.09332500
O	3.42623900	-2.83161600	0.59674700
C	4.34216800	-2.92681200	1.71277900
H	5.88824200	0.48365100	-1.36323300
H	5.57244700	-1.64748000	2.92998600
H	4.05440400	-0.89295000	2.36685600
H	3.76677600	-3.37399600	2.52570200
H	2.48653000	-2.42869600	-2.01349200
H	0.38973600	-5.28863700	-1.42435300
H	-1.12641100	-4.71821900	-0.73658200
H	-0.94485100	-4.85824600	-2.51165600
H	5.15576600	-3.60433200	1.42764600
C	-1.43489900	1.65429400	0.31290500
C	-0.69254000	2.47067300	1.17299200
C	-2.54352100	2.24680600	-0.29842600
C	-0.96862900	3.81686500	1.36140000
C	-2.85427800	3.58949700	-0.10978700
C	-2.06179000	4.37993300	0.71405800
C	-1.22117900	-0.67034300	1.83998600
C	-2.51863900	-0.58170900	2.35113000
C	-0.22999100	-1.14449200	2.70107500
C	-2.83368300	-0.95796600	3.64593200
C	-0.52060400	-1.52631900	4.00549500
C	-1.82339800	-1.43244000	4.47687700
C	-2.00164800	-0.93443000	-0.96927800
C	-2.05034600	-0.49617800	-2.29446100
C	-2.64197000	-2.14478600	-0.69540600
C	-2.72854800	-1.17829400	-3.29001600
C	-3.31281100	-2.85867500	-1.68056000
C	-3.36219700	-2.37415500	-2.98058600

P	-0.84934800	-0.07615000	0.15654500
F	0.29569000	1.93489400	1.89603700
F	1.04640300	-1.23798000	2.31470400
F	-1.40160100	0.62171200	-2.63532600
F	-4.08352900	-0.87525600	4.09749200
F	-2.10679200	-1.79570900	5.72142600
F	0.44488800	-1.97253500	4.80736500
F	-3.50807600	-0.14636200	1.56158100
F	-2.60211200	-2.70587100	0.51783900
F	-3.88541800	-4.02579500	-1.38281500
F	-3.99885100	-3.05885300	-3.92423600
F	-2.74568500	-0.71389500	-4.53880400
F	-3.38321400	1.54678200	-1.06399800
F	-3.92437700	4.11661100	-0.70305200
F	-2.36013200	5.66057400	0.89610500
F	-0.21468000	4.55397100	2.17426200

TS_{EE}(L11)

M06-L electronic energy (Hartree): -4442.892435

M06-L thermal correction to free energy (Hartree): 0.324933

Three lowest frequencies (cm⁻¹): -967.72, 15.97, 18.46

Pd	1.31100700	-0.39160000	-0.38258000
O	2.67439500	-3.08418600	-1.61350900
O	0.83974400	-2.53587300	-0.43717900
C	1.53933400	-3.35815500	-1.08453000
C	1.02272700	-4.75273500	-1.28019700
C	1.69135200	1.55216000	-0.21248800
C	1.14665900	2.60558000	-0.89752800
S	2.74114800	2.17248100	1.02592400
C	1.52117200	3.89354600	-0.40317100
C	2.38499200	3.83021800	0.65623800
H	2.82353300	4.64768100	1.21442600
O	0.31827000	2.45053500	-1.98344800
C	-0.43217700	3.63333400	-2.24726100
H	-1.22727000	3.74134100	-1.49232400
O	1.02967500	5.05447400	-0.93323800
C	0.45804900	4.85190200	-2.23184800
H	-0.10860300	5.75914500	-2.45574700
H	1.26335900	4.74202900	-2.97312000
H	-0.89682000	3.49109200	-3.22682100
C	5.54249400	-0.18004200	-0.07724300
C	4.27884200	-0.77911000	0.16590400

C	5.59813200	0.42650800	-1.30830100
C	3.34628300	-0.66871700	-0.87030400
S	4.10649100	0.27809400	-2.14247100
O	6.57115300	-0.21686000	0.81384000
C	6.10913600	-0.56207700	2.12732800
O	4.00250600	-1.44650700	1.31179800
C	5.18570200	-1.75137800	2.07463700
H	6.45275200	0.92864300	-1.74718200
H	7.00285700	-0.78531800	2.71379800
H	5.59567400	0.30362500	2.56998900
H	4.83513600	-2.02789800	3.07079200
H	2.97919900	-1.93300700	-1.31339500
H	1.78450800	-5.48689300	-1.00234400
H	0.11412500	-4.91986300	-0.69749100
H	0.79920200	-4.90961000	-2.34158800
H	5.68900400	-2.61318400	1.61677700
C	-1.90506800	1.35369600	0.17945300
C	-1.38764300	2.29282800	1.07805700
C	-3.06713500	1.71844500	-0.50309800
C	-1.93390700	3.55732500	1.24100500
C	-3.64585700	2.97341600	-0.34277700
C	-3.07608700	3.89753900	0.52530200
C	-1.47485200	-0.91705900	1.71066300
C	-2.81945100	-1.12320500	2.02777800
C	-0.53893600	-1.17942100	2.71086700
C	-3.22596900	-1.58430100	3.26872700
C	-0.92034400	-1.63954400	3.96576300
C	-2.26585900	-1.84210000	4.24274900
C	-1.78793400	-1.28345600	-1.16699400
C	-1.82150200	-0.82149400	-2.48554400
C	-2.10288100	-2.63086500	-0.97646500
C	-2.17914900	-1.62545900	-3.55574400
C	-2.45125000	-3.46139500	-2.03443400
C	-2.49356500	-2.95992500	-3.32774200
P	-0.98671200	-0.22806800	0.09137000
F	-0.35916500	1.95463200	1.86447600
F	0.76760900	-0.98379000	2.50499000
F	-1.47800600	0.44495000	-2.74552800
F	-4.51527300	-1.78494100	3.53561300
F	-2.63854600	-2.28228500	5.43844100
F	-0.00529500	-1.87889900	4.90376700
F	-3.75704200	-0.89415500	1.10037400
F	-2.05250600	-3.20159300	0.23118300
F	-2.72206000	-4.74789300	-1.80899300

F	-2.82631600	-3.75094900	-4.34201700
F	-2.20718500	-1.13369000	-4.79416600
F	-3.69916300	0.86609000	-1.31305600
F	-4.75889600	3.28646200	-1.00511600
F	-3.63004400	5.09443800	0.68080200
F	-1.38836600	4.42479900	2.09125200

Post-TS_{EE}(L11)

M06-L electronic energy (Hartree): -4442.900514

M06-L thermal correction to free energy (Hartree): 0.328323

Three lowest frequencies (cm⁻¹): 6.59, 19.51, 21.54

Pd	-1.34609500	0.41608000	-0.21213000
O	-3.37155100	-1.47957900	1.56803700
O	-1.88644200	-1.75823900	-0.09978000
C	-2.67871400	-2.22523600	0.72608200
C	-2.93928400	-3.68465500	0.85009400
C	-0.76592400	2.29152100	-0.48945500
C	-0.02684700	3.09745900	0.33563000
S	-1.03525700	3.11721200	-1.99281900
C	0.37315200	4.33735100	-0.25438300
C	-0.09427300	4.49894400	-1.53002300
H	0.06424400	5.33345300	-2.20135600
O	0.30401300	2.76205100	1.62531800
C	1.41235000	3.52430600	2.09885400
H	2.33724900	3.16398700	1.62029300
O	1.17105700	5.23635600	0.39661300
C	1.21888200	4.99240400	1.80823000
H	2.05512400	5.58505100	2.18730800
H	0.28826500	5.35022100	2.27279500
H	1.47813500	3.33660000	3.17389800
C	-5.61447900	1.26255100	-0.28089200
C	-4.42033900	0.52732000	-0.55783900
C	-5.37488900	2.42570400	0.39987300
C	-3.25844200	1.10208600	-0.08125600
S	-3.68092900	2.61174000	0.67996900
O	-6.85802600	0.82939400	-0.64267700
C	-6.80517300	-0.24626700	-1.58666100
O	-4.45351400	-0.67287300	-1.22542900
C	-5.76012000	-1.25746900	-1.19038500
H	-6.09965400	3.15414400	0.74212000
H	-7.80378900	-0.68996000	-1.59449300
H	-6.58479800	0.15417900	-2.58702000

H	-5.73594700	-2.09764500	-1.88855500
H	-3.22698800	-0.52608300	1.32401100
H	-3.85473300	-3.93004200	0.29883400
H	-2.11669100	-4.25805500	0.41920100
H	-3.10141100	-3.96812300	1.89324600
H	-5.96287000	-1.63891600	-0.17731500
C	2.36753900	0.53486800	0.14655800
C	2.55514000	1.50299900	-0.84558800
C	3.34506200	0.46424900	1.14097600
C	3.60513700	2.40913500	-0.82305400
C	4.41805500	1.34887100	1.17586100
C	4.54613500	2.32731000	0.19677000
C	1.41818100	-1.53523200	-1.45462400
C	2.57958500	-2.30726700	-1.38221400
C	0.73483400	-1.52460700	-2.67034800
C	3.04210200	-3.04966900	-2.45591800
C	1.17859700	-2.25792200	-3.76432400
C	2.33430700	-3.02025700	-3.65415400
C	0.77916100	-1.62626800	1.38830000
C	0.65393600	-1.05195800	2.65672600
C	0.54632700	-3.00141100	1.31023900
C	0.34633900	-1.78695600	3.79062500
C	0.22652600	-3.76016800	2.43033800
C	0.12634700	-3.15437100	3.67543900
P	0.87144100	-0.50256900	-0.05320400
F	1.72865500	1.53498000	-1.89709800
F	-0.37426400	-0.79450900	-2.83136500
F	0.82417800	0.26665200	2.79726500
F	4.14541600	-3.78849400	-2.35343600
F	2.76556200	-3.72458500	-4.69337000
F	0.50872600	-2.22882100	-4.91505400
F	3.26287500	-2.36140700	-0.23280200
F	0.57303500	-3.65398100	0.14217700
F	-0.01300000	-5.06570700	2.30298900
F	-0.18266400	-3.87484800	4.74717800
F	0.24805000	-1.19152900	4.97794400
F	3.31350300	-0.47819000	2.08602700
F	5.33635700	1.24955400	2.13622300
F	5.57191900	3.17005000	0.22835800
F	3.72632100	3.32814000	-1.77890900

(DMAc)Pd(EDOT)(OAc)

M06-L electronic energy (Hartree): -1424.721570

M06-L thermal correction to free energy (Hartree): 0.234382

Three lowest frequencies (cm-1): 20.89, 49.32, 54.87

Pd	-1.31028800	-0.05180600	0.28860300
O	-0.20116100	1.43144300	1.30455300
O	-2.72387400	-1.35887400	-0.52363000
O	-3.42258100	0.65535800	0.03938200
C	0.57672300	2.34175000	0.90797100
C	-3.66939100	-0.48779500	-0.44557900
C	-5.02260900	-0.84607800	-0.96289800
C	1.66351700	2.77276200	1.84578600
N	0.44135000	2.95920900	-0.27246200
C	-0.63258400	2.58948100	-1.17690000
C	1.45084400	3.83987300	-0.83525200
H	-1.57645900	2.49682000	-0.63316600
H	-0.41662400	1.63674900	-1.68111200
H	-0.73480500	3.37456800	-1.92994000
H	2.24755600	4.03721700	-0.11991300
H	0.99449200	4.79121500	-1.12829300
H	1.88954100	3.37297400	-1.72592900
H	2.64411000	2.45424600	1.47444400
H	1.49663200	2.29658000	2.81268500
H	1.69493600	3.85800800	1.98124500
C	0.29083200	-1.18645700	0.22310400
C	1.58792000	-0.92558100	-0.14648700
S	0.14094500	-2.87091300	0.64028500
C	2.44414000	-2.07214100	-0.10003100
C	1.80764700	-3.20933900	0.31473200
H	2.22604300	-4.19912900	0.44691300
O	2.04302200	0.30348200	-0.56869900
C	3.47108500	0.37775600	-0.52706600
H	3.80810500	0.46335400	0.51784300
O	3.76905200	-2.01993000	-0.43008500
C	4.09201200	-0.83710000	-1.16821200
H	5.18264100	-0.76933700	-1.16976400
H	3.73900300	-0.94201700	-2.20466000
H	3.74689700	1.28875600	-1.06506900
H	-5.20756000	-1.91944600	-0.87151900
H	-5.79910800	-0.28477100	-0.43754700
H	-5.08318900	-0.58721000	-2.02647200

Pre-TS_{EE}(DMAc)

M06-L electronic energy (Hartree): -2205.650475

M06-L thermal correction to free energy (Hartree): 0.335862

Three lowest frequencies (cm-1): 19.74, 31.07,38.21

Pd	1.29418100	0.08419600	-0.26407900
O	1.61997200	2.13072400	-1.02233900
O	3.75838800	-1.43874700	-1.26398400
O	3.32619700	-0.01322800	0.42348500
C	0.80540100	3.01637700	-0.64649400
C	4.10495800	-0.77352000	-0.27254600
C	5.53563400	-0.81993500	0.22753300
C	0.06791500	3.82403200	-1.67024400
N	0.57078800	3.26338400	0.65114500
C	1.30524200	2.55336000	1.68441400
C	-0.46257000	4.17861700	1.10665200
H	2.26470700	2.21105000	1.29181800
H	0.73084900	1.68228100	2.03097000
H	1.47251600	3.23394700	2.52505100
H	-1.29574600	4.21514600	0.40095700
H	-0.06739600	5.19228000	1.24900800
H	-0.84586200	3.81865000	2.06544600
H	-0.95787400	3.44144900	-1.76374200
H	0.55731600	3.69927300	-2.63751700
H	0.00818500	4.88817200	-1.42287100
C	-0.62396900	0.30541100	-0.76456600
C	-1.70478800	0.62786200	0.02166600
S	-1.15344600	0.20472400	-2.41912400
C	-2.93582600	0.77888400	-0.69348000
C	-2.80407800	0.58315100	-2.04270400
H	-3.56626600	0.65797800	-2.80837300
O	-1.62580700	0.77696700	1.38716300
C	-2.81769700	1.32636100	1.95225000
H	-2.82879500	2.41839300	1.80987000
O	-4.11598900	1.06602800	-0.06610800
C	-4.04903100	0.72545500	1.32414000
H	-4.96004100	1.12168200	1.77860200
H	-4.03833300	-0.37025900	1.43284900
H	-2.77230300	1.11110300	3.02362700
C	-1.17327800	-2.49596100	1.01333800
C	-0.17842400	-2.49434800	0.01538300
C	-0.69619000	-2.05207000	2.22620600
C	1.05270800	-1.90459000	0.41774900
S	0.94475300	-1.58944200	2.17409200
O	-2.45416900	-2.87581300	0.77319600
C	-2.72059900	-2.88165500	-0.64109500

O	-0.35437000	-3.00213500	-1.20154800
C	-1.64688200	-3.63351900	-1.38158700
H	-1.28704700	-1.90101000	3.12322300
H	-3.68960400	-3.36896300	-0.76427300
H	-2.78591600	-1.84349800	-1.00108200
H	-1.82542500	-3.62957200	-2.45835500
H	1.99280000	-2.32630100	0.05614300
H	5.56796500	-1.25466900	1.23340300
H	6.16947100	-1.41558100	-0.43437100
H	5.94873800	0.19129900	0.30969500
H	-1.56562900	-4.66793600	-1.02859400

TS_{EE}(DMAc)

M06-L electronic energy (Hartree): -2205.630379

M06-L thermal correction to free energy (Hartree): 0.329213

Three lowest frequencies (cm-1): -1093.31, 22.24, 26.65

Pd	-1.30488300	0.48087500	-0.05559800
O	-2.97515900	-0.92260100	-0.39777600
O	-1.43542800	3.65134300	-0.49813800
O	-2.80038600	2.04000800	0.28073400
C	-2.86618400	-2.17043400	-0.27462500
C	-2.57742800	3.21894500	-0.09819700
C	-3.69621400	4.21913700	-0.09265700
C	-3.37481000	-3.05320600	-1.37731600
N	-2.34508100	-2.74125400	0.82502000
C	-1.98582400	-1.94727400	1.98669700
C	-1.93123700	-4.13040300	0.89102600
H	-2.56078700	-1.01948400	1.99324000
H	-0.91522500	-1.70369300	1.98995100
H	-2.22566400	-2.52751500	2.88449700
H	-2.17748700	-4.66279800	-0.02645700
H	-2.41457700	-4.63244200	1.73694800
H	-0.84301900	-4.17570400	1.03542700
H	-2.53816400	-3.46421600	-1.95488800
H	-3.97925200	-2.44556100	-2.05256700
H	-3.97545000	-3.89050000	-1.00953100
C	0.02864500	-0.93248500	-0.45178000
C	1.11868900	-1.37137200	0.25885900
S	0.06282900	-1.68597900	-2.02190300
C	1.96006700	-2.29249900	-0.43803100
C	1.52126600	-2.56898200	-1.70535500
H	1.93675400	-3.26817900	-2.42027000

O	1.39943400	-0.95771900	1.53968000
C	2.32968100	-1.82376700	2.18615500
H	1.82801500	-2.76355400	2.46962900
O	3.08617500	-2.83403200	0.11986900
C	3.50340200	-2.11468700	1.28553200
H	4.24311000	-2.74722100	1.78255000
H	3.98672200	-1.17077000	0.98521300
H	2.64981100	-1.30426500	3.09383600
C	2.63362500	1.90752200	0.35687800
C	1.48983400	1.67655700	-0.44884500
C	2.30800700	2.22420400	1.65252900
C	0.25561400	1.78654900	0.20738700
S	0.61175300	2.19590800	1.89600000
O	3.90891900	1.80861900	-0.11758600
C	3.94210700	1.06808600	-1.34494400
O	1.57836500	1.39537800	-1.76563800
C	2.89934100	1.58068400	-2.30261100
H	2.99640400	2.48389100	2.44894300
H	4.94822400	1.19435100	-1.74990900
H	3.76904900	0.00048200	-1.13439100
H	2.91685100	1.02654600	-3.24399100
H	-0.59665500	2.76847700	-0.26557200
H	-3.44873800	5.04915600	0.57703700
H	-3.81868000	4.64506700	-1.09359700
H	-4.63438500	3.76190400	0.22617000
H	3.05317400	2.64828400	-2.50884200

Post-TS_{EE}(DMAc)

M06-L electronic energy (Hartree): -2205.641517

M06-L thermal correction to free energy (Hartree): 0.33667

Three lowest frequencies (cm-1): 28.63, 31.52, 35.42

Pd	0.11579800	-1.21872100	-0.05457500
O	2.04235100	-2.24309100	-0.47106700
O	-2.53799900	-2.96610300	-0.76970300
O	-0.65436600	-3.25407000	0.42926500
C	3.16463500	-1.68577600	-0.37031900
C	-1.69481200	-3.70262300	-0.06469300
C	-2.11922800	-5.12061500	0.08490400
C	4.15223900	-1.82871100	-1.49222500
N	3.52841600	-0.99964200	0.72818400
C	2.68195200	-0.97013800	1.90823500
C	4.67732100	-0.11532200	0.78216500

H	2.04140300	-1.85426100	1.92315400
H	2.04892700	-0.07332500	1.92899000
H	3.32740800	-0.97613100	2.79333000
H	5.25678500	-0.15869000	-0.13902900
H	5.32518300	-0.38518700	1.62394300
H	4.33316900	0.91809400	0.92521800
H	4.23720500	-0.88963500	-2.05160200
H	3.78460500	-2.59332000	-2.17844600
H	5.15196100	-2.10652300	-1.14416200
C	0.88906900	0.54990500	-0.47751400
C	0.97754400	1.70583200	0.25657500
S	1.64068200	0.81976800	-2.02545900
C	1.65670100	2.77887600	-0.40228300
C	2.08279300	2.45594000	-1.66196500
H	2.64480200	3.06770700	-2.35670300
O	0.47255500	1.84652400	1.53125100
C	1.09706900	2.93106500	2.21855900
H	2.13330100	2.65977200	2.47903400
O	1.87750400	3.99277400	0.18697700
C	1.08698300	4.17535700	1.36708500
H	1.52670500	5.02511200	1.89555500
H	0.05451200	4.42774000	1.08186600
H	0.52809900	3.07931600	3.13995800
C	-3.41988000	1.22644700	0.36082900
C	-2.29745000	0.71276500	-0.36380600
C	-3.60031100	0.62418800	1.57589200
C	-1.61399900	-0.29820400	0.27763500
S	-2.38282900	-0.57764400	1.82769900
O	-4.23529800	2.20699000	-0.12917600
C	-3.63126300	2.90395000	-1.22441900
O	-1.95411100	1.20249600	-1.59704600
C	-3.02503200	1.93104200	-2.20242500
H	-4.39223100	0.79868200	2.29388800
H	-4.42956300	3.48882900	-1.68775500
H	-2.86000700	3.59019800	-0.84267700
H	-2.58990600	2.45146600	-3.05929200
H	-2.22268200	-2.02147200	-0.72462200
H	-3.02829800	-5.16793000	0.69365700
H	-2.36687900	-5.54666200	-0.89178500
H	-1.33372300	-5.70738900	0.56099000
H	-3.79311500	1.23025100	-2.56357400

Int_{PE}(L1)

M06-L electronic energy (Hartree): -1403.195001

M06-L thermal correction to free energy (Hartree): 0.460221

Three lowest frequencies (cm⁻¹): 21.49, 41.32, 50.36

Pd	-0.91913900	-0.65810100	0.01830000
O	-2.78090100	-1.83196000	0.00159000
O	-0.87560800	-2.95578300	-0.01770100
C	-2.14373600	-2.93809400	-0.02103100
C	-2.90792100	-4.22835600	-0.06933200
H	-2.79787400	-4.68216400	-1.06086100
H	-2.50129100	-4.94133300	0.65441400
H	-3.97169800	-4.07286700	0.12542400
C	2.02292000	-0.68215200	-1.52243900
C	2.06057200	-0.53887900	1.60642200
C	1.65231800	2.04126900	-0.07592700
P	1.24289000	0.16450000	0.01767700
C	1.72548400	0.36433300	2.79824100
H	0.64488000	0.53592900	2.88953100
H	2.05269000	-0.14440100	3.71503400
H	2.23266800	1.33318100	2.77107800
C	1.42471700	-1.89943400	1.92387400
H	0.34948500	-1.80202900	2.11760100
H	1.54704600	-2.64181500	1.13310900
H	1.89766900	-2.29614500	2.83338400
C	3.57916500	-0.71563300	1.52414100
H	4.11599200	0.20949500	1.29805900
H	3.93872000	-1.06902600	2.50053400
H	3.87464800	-1.46866900	0.78731700
C	3.11603100	2.34442100	0.26544100
H	3.30514100	3.40327400	0.04223000
H	3.33601100	2.20145900	1.32778100
H	3.83357900	1.75744900	-0.31370500
C	0.76060000	2.86210100	0.87001900
H	0.68816600	2.46521300	1.88438800
H	1.19080300	3.87051800	0.94297600
H	-0.25341900	2.96365600	0.47750100
C	1.36108200	2.57273500	-1.48356600
H	2.05392100	2.20187500	-2.24363200
H	0.33614500	2.34954400	-1.79885800
H	1.46324600	3.66630700	-1.46097800
C	1.07246800	-0.46896200	-2.71163400
H	0.91840900	0.58031600	-2.97459300
H	1.49853200	-0.96969000	-3.59218800
H	0.08825900	-0.91538300	-2.51563100

C	3.42624600	-0.20166500	-1.90168600
H	3.77757600	-0.80766600	-2.74829500
H	3.45524300	0.84225100	-2.22643100
H	4.15271600	-0.32855900	-1.09226600
C	2.08697300	-2.19864700	-1.30279400
H	2.83747300	-2.49417900	-0.56322600
H	1.11908500	-2.61782000	-1.00824600
H	2.37660300	-2.66463800	-2.25473900
C	-1.82158400	1.10293100	0.00628300
C	-2.37899400	1.57936900	1.19871800
C	-2.10714100	1.76181000	-1.19363200
C	-3.19793300	2.70976900	1.18939600
H	-2.16464600	1.07881800	2.14371100
C	-2.92528300	2.89496300	-1.19662800
H	-1.69211900	1.39795100	-2.13454400
C	-3.46615400	3.37599500	-0.00591800
H	-3.62064900	3.07387100	2.12550500
H	-3.13616700	3.40192100	-2.13798200
H	-4.09669800	4.26319500	-0.00914600

Pre-TS_{PE}(L1)

M06-L electronic energy (Hartree): -2184.106980

M06-L thermal correction to free energy (Hartree): 0.559701

Three lowest frequencies (cm⁻¹): 21.89, 28.21, 37.13

Pd	0.01631200	0.51524100	-0.06483300
O	0.06801800	3.04154900	-1.91701100
O	-0.62053800	2.62966200	0.18675500
C	-0.43523600	3.39558200	-0.83227700
C	-0.91034200	4.82263100	-0.64310900
C	3.89988200	0.41418900	0.95215800
C	3.27113700	0.87950200	-0.22894500
C	3.28242900	0.87621200	2.09103300
C	2.11942900	1.62319600	0.00653400
S	1.92263900	1.85459600	1.73626000
O	4.98731200	-0.39756700	0.93802000
C	5.16250800	-1.00734100	-0.35284500
O	3.73513300	0.61598600	-1.46470900
C	5.04642300	0.01624700	-1.45097400
H	3.53051600	0.61678800	3.11326300
H	6.15884700	-1.45413400	-0.34144800
H	4.40901300	-1.79699100	-0.48072300
H	5.17193300	-0.44306800	-2.43365600

H	1.70419300	2.33645500	-0.70199100
H	-2.00715500	4.84763600	-0.68088400
H	-0.61920800	5.20993400	0.33873000
H	-0.52603000	5.48101900	-1.42683100
H	5.79127800	0.81308100	-1.32722300
C	-3.29409600	0.50899700	-1.09795500
C	-2.71226200	-0.27443600	1.87698600
C	-2.38381500	-2.36659800	-0.39757400
P	-2.13358900	-0.50524900	0.06309800
C	-2.05402800	-1.34432800	2.75375900
H	-0.96696200	-1.38567100	2.60106400
H	-2.22823500	-1.08497600	3.80689200
H	-2.46777500	-2.34505500	2.59588800
C	-2.19462000	1.07499900	2.39115600
H	-1.09895900	1.12487400	2.35223800
H	-2.57837100	1.93345000	1.83700100
H	-2.50421500	1.18329400	3.44029300
C	-4.22813500	-0.33250200	2.08918900
H	-4.67573100	-1.27755000	1.77216600
H	-4.42905300	-0.22446200	3.16432800
H	-4.75908900	0.48001900	1.58525200
C	-3.74688100	-2.91615100	0.04900200
H	-3.88479100	-3.89934400	-0.42170200
H	-3.78242100	-3.07941600	1.13137600
H	-4.60355100	-2.30112900	-0.23027300
C	-1.32052200	-3.29987200	0.21221500
H	-1.07491100	-3.09821000	1.25516200
H	-1.71793700	-4.32319800	0.16027600
H	-0.39061400	-3.28489800	-0.35724900
C	-2.24097400	-2.53418800	-1.91528400
H	-3.05890800	-2.09475900	-2.49153200
H	-1.29333000	-2.11841400	-2.27818800
H	-2.23057400	-3.60973700	-2.13959500
C	-2.52091700	0.74488400	-2.40392900
H	-2.24442000	-0.17822900	-2.92133400
H	-3.15639100	1.32603200	-3.08744900
H	-1.60457700	1.32179500	-2.22331200
C	-4.65325300	-0.12407800	-1.41200200
H	-5.21147100	0.58104500	-2.04367300
H	-4.59244600	-1.06427600	-1.96571300
H	-5.25573800	-0.29171700	-0.51222100
C	-3.58842500	1.89318800	-0.50627700
H	-4.29174200	1.85658600	0.33129300
H	-2.68369200	2.40939800	-0.18297600

H	-4.06319500	2.49747000	-1.29246000
C	0.98059800	-1.21689600	-0.22349100
C	1.49765600	-1.85735800	0.90766900
C	1.27757500	-1.73736400	-1.48875400
C	2.24873400	-3.02700700	0.78123600
H	1.30662200	-1.44880300	1.90248400
C	2.02928200	-2.90790900	-1.61638600
H	0.91251600	-1.23435900	-2.38636800
C	2.50099600	-3.56673000	-0.48054000
H	2.63230600	-3.52124900	1.67382400
H	2.24080600	-3.30762000	-2.60806300
H	3.07644100	-4.48576800	-0.57898200

TS_{PE}(L1)

M06-L electronic energy (Hartree): -2184.079771

M06-L thermal correction to free energy (Hartree): 0.557151

Three lowest frequencies (cm⁻¹): -466.01, 18.16, 31.55

Pd	-0.02597700	-0.43959000	0.11548400
O	-1.34077400	-3.36604200	-0.66452200
O	0.59804000	-2.62113100	0.18761500
C	-0.09493300	-3.51285300	-0.34778000
C	0.52704900	-4.83177900	-0.69198600
C	-4.30658300	-0.29423400	0.57258800
C	-3.18191900	-0.55104300	-0.26071700
C	-4.07408100	-0.62688800	1.88269400
C	-2.05819600	-1.06949200	0.37308400
S	-2.47738300	-1.24346400	2.07228900
O	-5.47678000	0.22708100	0.10114400
C	-5.27173100	0.87441000	-1.16087800
O	-3.20716400	-0.32109500	-1.60011400
C	-4.51849900	-0.02874000	-2.10271000
H	-4.77171800	-0.55702300	2.70945800
H	-6.26585000	1.10692100	-1.54942500
H	-4.71528600	1.81089700	-1.00435000
H	-4.36819700	0.44950400	-3.07401700
H	-1.65766800	-2.33965600	-0.25682000
H	1.08480800	-4.71828500	-1.63031600
H	1.24538500	-5.12696700	0.07722400
H	-0.22352700	-5.61237600	-0.83094900
H	-5.06588000	-0.97068300	-2.24899400
C	3.19908700	-0.76880100	-1.32832400
C	3.08560200	0.03778100	1.69033700

C	2.65465800	2.17108300	-0.51995400
P	2.29278600	0.34169300	-0.02591800
C	2.64519100	1.14270200	2.65651700
H	1.55793300	1.29929400	2.63567800
H	2.91449600	0.83975900	3.67774900
H	3.14015000	2.10036000	2.46495000
C	2.50856000	-1.26903800	2.25179600
H	1.41669800	-1.20581200	2.35372400
H	2.72770400	-2.14653500	1.64048700
H	2.93347000	-1.43715300	3.25144200
C	4.61469000	-0.03868100	1.71233600
H	5.09538600	0.89011700	1.39297700
H	4.93895400	-0.23003900	2.74523000
H	5.01214300	-0.85222800	1.09923000
C	4.10727700	2.60166700	-0.27815000
H	4.26392600	3.57348000	-0.76722800
H	4.31017400	2.75143400	0.78800700
H	4.85668000	1.91341700	-0.67202000
C	1.76858800	3.17849400	0.23530800
H	1.73137000	3.03375300	1.31575000
H	2.18820000	4.17856000	0.05504000
H	0.74449400	3.18050000	-0.13842400
C	2.29654400	2.36195000	-1.99947600
H	2.95905100	1.83822200	-2.69302900
H	1.26434900	2.05079200	-2.20126000
H	2.36421800	3.43326200	-2.23516600
C	2.21670100	-0.95092100	-2.49612000
H	1.91019600	-0.01149000	-2.96611700
H	2.69136500	-1.56978000	-3.27105500
H	1.30775900	-1.46822200	-2.16072100
C	4.53758100	-0.23987200	-1.85387800
H	4.93336000	-0.97308100	-2.57071400
H	4.47070800	0.71468600	-2.38120400
H	5.28236500	-0.13926500	-1.05616200
C	3.48347400	-2.17711600	-0.78728400
H	4.27603300	-2.19712400	-0.03326200
H	2.59264000	-2.65637000	-0.38005600
H	3.83705600	-2.78741900	-1.63104800
C	-0.87090700	1.36625500	0.06909200
C	-1.21303400	2.01484800	1.26196500
C	-1.22123600	1.97253500	-1.14347300
C	-1.85103100	3.25591900	1.24254700
H	-0.97511300	1.55319900	2.22177500
C	-1.85809200	3.21482200	-1.16366400

H	-1.00033000	1.47379300	-2.08783100
C	-2.17031500	3.86558300	0.02958600
H	-2.09948200	3.74852200	2.18307300
H	-2.11340200	3.67325500	-2.11971400
H	-2.66658700	4.83489700	0.01425600

Post-TS_{PE}(L1)

M06-L electronic energy (Hartree): -2184.084638

M06-L thermal correction to free energy (Hartree): 0.555731

Three lowest frequencies (cm⁻¹): 11.78, 18.35, 21.82

Pd	0.12049100	0.20957900	0.20894700
O	1.81145000	2.91648800	-0.86750400
O	-0.05462700	2.53434400	0.32850700
C	0.67156600	3.29669800	-0.31536200
C	0.31166300	4.71822800	-0.58110400
C	4.51264800	0.26573500	0.55567800
C	3.28212500	0.10876900	-0.15857900
C	4.32771300	0.65138600	1.85534100
C	2.14002800	0.38967700	0.56075800
S	2.63448500	0.82486300	2.17607800
O	5.73802000	0.07227200	-0.01655600
C	5.64564400	-0.60084400	-1.27714400
O	3.26309600	-0.25329600	-1.48552300
C	4.52844000	-0.02756500	-2.11119600
H	5.08464700	0.85766300	2.60217500
H	6.61517900	-0.46512400	-1.76313000
H	5.47873700	-1.67500000	-1.10792400
H	4.47714600	-0.51351800	-3.08874000
H	1.97210400	1.97438500	-0.57035300
H	-0.22376800	4.76664600	-1.53781900
H	-0.35652200	5.09276600	0.19628800
H	1.19837300	5.35008600	-0.66412400
H	4.68090700	1.05338400	-2.25783400
C	-2.97412400	1.24156100	-1.35582600
C	-3.14409300	0.39296700	1.64141300
C	-3.07939800	-1.75244800	-0.59661700
P	-2.36214100	-0.04627300	-0.05129500
C	-2.97810500	-0.79563400	2.59430200
H	-1.94498600	-1.16863200	2.61183400
H	-3.22518700	-0.46341600	3.61206800
H	-3.64692900	-1.62900300	2.35756000
C	-2.32974400	1.54054300	2.25414100

H	-1.27128400	1.26427700	2.35933000
H	-2.37138900	2.46631200	1.67671700
H	-2.72524100	1.75311700	3.25755000
C	-4.62347800	0.78597000	1.61637200
H	-5.26933700	-0.00189900	1.21942500
H	-4.95055200	0.98418000	2.64716000
H	-4.81419600	1.69775200	1.04325300
C	-4.59453900	-1.89174500	-0.40226800
H	-4.92226000	-2.81427200	-0.90219200
H	-4.85688100	-1.99892800	0.65612100
H	-5.18446400	-1.07132800	-0.81528300
C	-2.42962400	-2.92478800	0.15963400
H	-2.41182300	-2.81435200	1.24456300
H	-3.01795900	-3.82566200	-0.06639100
H	-1.40912600	-3.10965500	-0.17541500
C	-2.72398200	-1.98999400	-2.07016700
H	-3.26079900	-1.34445700	-2.76979100
H	-1.64697900	-1.87486400	-2.24470800
H	-2.98444500	-3.02690200	-2.32468200
C	-1.94109900	1.22899000	-2.49371000
H	-1.84334100	0.25772400	-2.98760900
H	-2.23808200	1.96107600	-3.25815200
H	-0.94610800	1.51305500	-2.12397900
C	-4.37673500	1.01724100	-1.92839700
H	-4.59267400	1.83311300	-2.63280800
H	-4.49117600	0.08245500	-2.48235100
H	-5.14968600	1.05223200	-1.15201500
C	-2.97193500	2.66760400	-0.78968900
H	-3.77463800	2.84184100	-0.06738500
H	-2.02291000	2.93605200	-0.32627500
H	-3.14379000	3.35973400	-1.62658000
C	0.59178200	-1.72365300	0.10835000
C	0.73194000	-2.49114800	1.27141800
C	0.80106500	-2.34281400	-1.13038700
C	1.00768200	-3.85719200	1.19469100
H	0.60572800	-2.02617900	2.25034400
C	1.07871900	-3.70922800	-1.20625200
H	0.73248400	-1.76042800	-2.04961200
C	1.17343700	-4.47484100	-0.04468300
H	1.09416100	-4.44092500	2.11130400
H	1.21992700	-4.17588700	-2.18132300
H	1.38578800	-5.54107700	-0.10428000

Int_{PE}(L2)

M06-L electronic energy (Hartree): -1635.517323
M06-L thermal correction to free energy (Hartree): 0.567785
Three lowest frequencies (cm⁻¹): 24.55, 44.40, 45.04

Pd	-0.99636200	-1.34447400	0.02961500
O	-2.37692600	-3.07421000	-0.00656000
O	-3.23668600	-1.03525700	0.05800500
C	-3.38747900	-2.29694100	0.03479100
C	-4.76524200	-2.88790800	0.09170500
H	-5.51148500	-2.18782400	-0.29228800
H	-4.81313200	-3.82773200	-0.46511500
H	-5.02009500	-3.11127300	1.13450000
C	-3.71202000	2.93601400	1.39275900
H	-4.34345000	2.04386900	1.25285700
H	-4.37487900	3.73492300	1.75035100
C	-3.08595400	3.32203700	0.05893000
H	-3.86247700	3.51244500	-0.69340300
H	-2.53335500	4.26781500	0.18015700
C	-2.63608000	2.62596300	2.42570500
H	-2.05747300	3.53928200	2.64081900
H	-3.08709600	2.31187800	3.37602500
C	-1.69552900	1.54167100	1.91619200
H	-0.93428400	1.30516000	2.67307900
H	-2.26268400	0.61190600	1.75077900
C	-2.12501300	2.25347100	-0.45654100
H	-1.67099700	2.60044200	-1.39329000
H	-2.67634500	1.33001400	-0.69146200
C	-1.04356100	1.94594900	0.58408100
H	-0.45175000	2.86451400	0.73769600
P	0.13641900	0.61348500	0.07258200
C	1.11724500	2.25014800	-4.24194400
H	0.23612300	2.91073200	-4.28424500
H	1.64637100	2.37796900	-5.19523300
C	0.65188500	0.80741300	-4.07967200
H	-0.00749100	0.51811000	-4.90818900
H	1.52465300	0.13537200	-4.12480200
C	2.00669500	2.67674300	-3.08066900
H	2.93302800	2.08000000	-3.09269400
H	2.31094200	3.72591300	-3.18925100
C	1.31101000	2.47460200	-1.73758400
H	1.98722700	2.75326400	-0.91779000
H	0.44362700	3.14970000	-1.66554700
C	-0.06355400	0.60541000	-2.74862000

H	-0.37502600	-0.44204900	-2.62014800
H	-0.98883000	1.19892500	-2.74151000
C	0.84381800	1.02335600	-1.58461300
H	1.73426200	0.37249200	-1.63862100
C	4.14996000	1.52921400	2.48383400
H	4.54300900	2.27589200	1.77525300
H	4.89601300	1.43746600	3.28405600
C	3.97131100	0.20218100	1.75907700
H	4.91850800	-0.13142000	1.31466900
H	3.67406500	-0.57631600	2.48035900
C	2.82398900	2.02243600	3.04716000
H	2.48490500	1.33351400	3.83744300
H	2.94553600	3.00386400	3.52381000
C	1.73988600	2.10554700	1.97451500
H	0.80689500	2.45492300	2.43253200
H	2.02080800	2.86462700	1.22725400
C	2.90251000	0.30687900	0.67716300
H	2.80889000	-0.64640000	0.14463200
H	3.22179600	1.05538400	-0.06678000
C	1.56013000	0.74448100	1.28414900
H	1.30162300	0.00847600	2.06478900
C	0.78404500	-2.23082500	-0.01804000
C	1.45904800	-2.46987700	-1.22211700
C	1.33146700	-2.72442500	1.17344700
C	2.65519000	-3.19139800	-1.23238000
H	1.06267900	-2.08396000	-2.16289000
C	2.52635800	-3.44604600	1.15893100
H	0.83230500	-2.53687800	2.12527700
C	3.19528900	-3.67596400	-0.04232000
H	3.16879900	-3.36580500	-2.17757200
H	2.93938600	-3.82053700	2.09530200
H	4.13225400	-4.23019000	-0.05102800

Pre-TS_{PE}(L2)

M06-L electronic energy (Hartree): -2416.431353

M06-L thermal correction to free energy (Hartree): 0.666253

Three lowest frequencies (cm⁻¹): 14.65, 23.36, 31.06

Pd	0.54310700	-0.68779000	-0.12720800
O	0.37794700	-3.18180100	1.66644100
O	-0.22692100	-2.72412500	-0.45378700
C	-0.12436900	-3.49791400	0.56950100
C	-0.72005700	-4.87902300	0.37334700

C	4.34320500	-0.51774000	-1.06786400
C	3.71074100	-1.07313200	0.07351600
C	3.77068300	-0.94035600	-2.24346600
C	2.59330000	-1.84431400	-0.23005000
S	2.44091500	-1.98608700	-1.97364000
O	5.39099500	0.34079600	-0.98139900
C	5.48425700	0.90428600	0.33868600
O	4.13552800	-0.85841100	1.33156500
C	5.40373800	-0.17317500	1.38710500
H	4.02813600	-0.61540000	-3.24430600
H	6.44814900	1.41570200	0.38005400
H	4.67582900	1.63654200	0.47402500
H	5.46760900	0.24800500	2.39262300
H	2.17389900	-2.60343700	0.42619600
H	-0.41873700	-5.30820000	-0.58788700
H	-0.43915800	-5.55826300	1.18275800
H	-1.81523100	-4.79802900	0.35399200
H	6.20342100	-0.91317100	1.25405300
C	-2.95866200	-1.84574900	3.85769500
H	-2.09317900	-2.52791100	3.85629800
H	-3.55822900	-2.10329000	4.74072500
C	-3.76266300	-2.06449900	2.58183400
H	-4.08454500	-3.11168200	2.50340200
H	-4.68205100	-1.45768500	2.61968500
C	-2.45833800	-0.40914100	3.95073100
H	-3.31814500	0.27315800	4.05338200
H	-1.84278900	-0.27043100	4.84922900
C	-1.66101600	-0.02601500	2.70934500
H	-1.29704100	1.00934900	2.78797200
H	-0.76407600	-0.66377300	2.63240200
C	-2.95701100	-1.68000800	1.34447700
H	-3.55389400	-1.84905000	0.43860200
H	-2.07477200	-2.32680800	1.26886300
C	-2.49000000	-0.22653700	1.43314300
H	-3.38693700	0.41474200	1.48455500
P	-1.51230600	0.37264200	-0.02268000
C	-4.60104300	-1.05513900	-3.30014800
H	-5.05638700	-1.80067600	-2.62797900
H	-5.14002600	-1.12592500	-4.25406000
C	-3.12617800	-1.38603300	-3.49131400
H	-3.00567000	-2.39159100	-3.91565500
H	-2.69268800	-0.68543200	-4.22371100
C	-4.76940400	0.33242100	-2.69534600
H	-4.38448100	1.08622300	-3.40131700

H	-5.83098600	0.56546000	-2.53981600
C	-4.01443400	0.45908100	-1.37529500
H	-4.12188600	1.47763700	-0.97891900
H	-4.47052800	-0.21226400	-0.63089800
C	-2.35272500	-1.28151400	-2.18123800
H	-1.28444300	-1.47549300	-2.34000800
H	-2.69205700	-2.06450200	-1.48757600
C	-2.53315000	0.10377700	-1.55286100
H	-2.10218100	0.82281300	-2.26950900
C	-2.06180300	5.10683900	-0.05175700
H	-2.99672300	5.12603400	-0.63483000
H	-1.80243800	6.15399000	0.15261300
C	-0.97247800	4.43589500	-0.87922200
H	-0.84101700	4.95295200	-1.83919000
H	-0.00744300	4.50454900	-0.35114600
C	-2.30273900	4.35530800	1.25133200
H	-1.39954200	4.42058100	1.88040800
H	-3.11466900	4.82270900	1.82391800
C	-2.62191800	2.88052800	1.01031700
H	-2.77304200	2.38246300	1.97599400
H	-3.57402200	2.79743300	0.46391100
C	-1.29662100	2.96585500	-1.11853800
H	-0.50622400	2.49214100	-1.71714200
H	-2.22686700	2.89564200	-1.70660900
C	-1.48363000	2.22927200	0.21339200
H	-0.56441200	2.38961100	0.79644800
C	1.46831300	1.07238300	0.12602800
C	1.93527200	1.82001500	-0.96168500
C	1.72406100	1.54886900	1.41999500
C	2.61245400	3.02642300	-0.76477900
H	1.76658600	1.46312800	-1.97988300
C	2.40100200	2.75431600	1.61906000
H	1.38264600	0.97945000	2.28701300
C	2.83749100	3.50384200	0.52613500
H	2.95758100	3.59743300	-1.62683200
H	2.58478500	3.10841000	2.63339600
H	3.35681900	4.44837200	0.67975300

TS_{PE}(L2)

M06-L electronic energy (Hartree): -2416.403543

M06-L thermal correction to free energy (Hartree): 0.666359

Three lowest frequencies (cm⁻¹): -529.45, 16.48, 24.51

Pd	0.49628500	-0.53821500	-0.32848600
O	1.57649000	-3.50718200	0.44490300
O	-0.24696600	-2.65333800	-0.55495200
C	0.36443300	-3.59437400	-0.00849200
C	-0.30943400	-4.91652100	0.19504000
C	4.76515300	-0.45298500	-0.68864900
C	3.61363100	-0.66751400	0.12104900
C	4.58897700	-0.88874600	-1.97664700
C	2.52170300	-1.24626000	-0.51305500
S	3.00822200	-1.54212000	-2.17704600
O	5.90120200	0.14074800	-0.21761600
C	5.61144600	0.92168000	0.94942600
O	3.57450400	-0.30839300	1.43174900
C	4.84471800	0.10249500	1.95513700
H	5.31541200	-0.86829600	-2.78111500
H	6.57635400	1.23649000	1.35326200
H	5.03262600	1.81240000	0.65819200
H	4.62327800	0.68626000	2.85273100
H	1.98624300	-2.49839100	0.11070400
H	-1.22007500	-4.98374500	-0.40362900
H	0.36423700	-5.74407900	-0.04345400
H	-0.58161300	-5.01584700	1.25308100
H	5.42211900	-0.78791400	2.24152600
C	-2.00982600	-1.58624100	4.32254900
H	-0.95266500	-1.89681500	4.33260500
H	-2.43588300	-1.90350400	5.28337500
C	-2.71756800	-2.27983700	3.16482300
H	-2.61659100	-3.37042000	3.24751100
H	-3.79698100	-2.06149000	3.20759400
C	-2.08099700	-0.07031000	4.18295300
H	-3.12920600	0.25560200	4.27970900
H	-1.52841800	0.41900400	4.99572700
C	-1.54412000	0.39814200	2.83333100
H	-1.61649300	1.49262000	2.76173900
H	-0.47229200	0.14727400	2.75203300
C	-2.15972800	-1.80514800	1.82895100
H	-2.64190300	-2.32869400	0.99068500
H	-1.09018300	-2.06123900	1.76917300
C	-2.29048700	-0.28590300	1.68432700
H	-3.35741700	-0.01868700	1.76330900
P	-1.69347800	0.28925100	0.02123300
C	-5.02802800	-1.86096800	-2.60198400
H	-5.02704100	-2.79417400	-2.01586700
H	-5.76583500	-1.99848500	-3.40345500

C	-3.63770000	-1.63610900	-3.18427100
H	-3.33633800	-2.49056000	-3.80484400
H	-3.66175200	-0.75977100	-3.85241000
C	-5.43432000	-0.70595500	-1.69568000
H	-5.53035600	0.21375000	-2.29531500
H	-6.42089200	-0.89017000	-1.25004600
C	-4.40446600	-0.47152500	-0.59406600
H	-4.72062900	0.36429000	0.04303700
H	-4.36457300	-1.35932600	0.05721400
C	-2.60828700	-1.39909500	-2.08495500
H	-1.61004000	-1.22343900	-2.51130500
H	-2.51057200	-2.30158100	-1.46423500
C	-3.01684000	-0.21934300	-1.19899200
H	-3.10374200	0.66335800	-1.85665500
C	-2.71876600	4.87191300	-0.57974800
H	-3.48983900	4.72932100	-1.35405700
H	-2.63543300	5.95546500	-0.42239100
C	-1.39991800	4.29904600	-1.08447100
H	-1.11391900	4.76871900	-2.03523100
H	-0.59534200	4.52997700	-0.36732000
C	-3.17250500	4.18371100	0.70409500
H	-2.46570800	4.42104100	1.51574900
H	-4.15073900	4.56798300	1.02232000
C	-3.23439100	2.66650500	0.53752800
H	-3.55751500	2.19426600	1.47629700
H	-3.99540100	2.41680100	-0.21994400
C	-1.48749200	2.78596400	-1.24939500
H	-0.53764000	2.38008900	-1.61811100
H	-2.25147800	2.55323900	-2.00914500
C	-1.87448100	2.13169800	0.08154600
H	-1.12005400	2.44633200	0.82084700
C	1.34123600	1.28058900	-0.18778300
C	1.99182100	1.80538800	-1.31398800
C	1.40738700	2.01062000	1.00550200
C	2.67534400	3.01976300	-1.25347600
H	1.98655900	1.24592300	-2.25123500
C	2.09851100	3.22345800	1.07149100
H	0.93029300	1.62840800	1.90945300
C	2.73509000	3.73549500	-0.05730600
H	3.17471200	3.40075100	-2.14483200
H	2.13810900	3.76718900	2.01583000
H	3.27370700	4.68063200	-0.00589800

Post-TS_{PE}(L2)

M06-L electronic energy (Hartree): -2416.407805
M06-L thermal correction to free energy (Hartree): 0.665333
Three lowest frequencies (cm⁻¹): 14.20, 22.48, 26.95

Pd	0.59955700	-0.35671600	-0.27941900
O	1.84712700	-3.20884200	0.80477700
O	0.09615200	-2.58618100	-0.46325500
C	0.69704600	-3.43938800	0.19651200
C	0.16505500	-4.81558100	0.40678300
C	4.96952200	-0.45461000	-0.71692900
C	3.77263900	-0.29625400	0.04870400
C	4.75179700	-1.05279400	-1.92911600
C	2.61945000	-0.76828800	-0.54421300
S	3.07032900	-1.41219900	-2.10811000
O	6.19832300	-0.05203100	-0.27293700
C	6.08607900	0.87421900	0.81306000
O	3.78579800	0.30001000	1.28444100
C	5.10173900	0.37226000	1.83790400
H	5.48694900	-1.31612100	-2.68011600
H	7.08926600	0.96910800	1.23586500
H	5.76437100	1.85424500	0.42782800
H	5.03609500	1.05343500	2.69011700
H	2.14761600	-2.28722200	0.52435800
H	-0.71580500	-4.98315500	-0.21444800
H	0.93015700	-5.56656300	0.19085800
H	-0.11333800	-4.93488600	1.46045900
H	5.40730300	-0.62159400	2.19919500
C	-2.07991600	-1.65009800	4.34594200
H	-0.99442900	-1.80573700	4.45434500
H	-2.53841000	-2.00463600	5.27838400
C	-2.57906100	-2.46498000	3.15820300
H	-2.32727900	-3.52650400	3.28541600
H	-3.67861300	-2.40894900	3.10668100
C	-2.35205300	-0.16289200	4.15170000
H	-3.43986600	0.01328500	4.15995900
H	-1.93825400	0.41707100	4.98705100
C	-1.78412700	0.34853100	2.83054700
H	-2.00686300	1.41899300	2.71824600
H	-0.68433000	0.25396900	2.83850100
C	-1.98972700	-1.93970400	1.85485200
H	-2.31748700	-2.54822400	0.99932900
H	-0.89146500	-2.02927100	1.89075400
C	-2.33708000	-0.46138100	1.65394200

H	-3.43488800	-0.36212200	1.66096700
P	-1.72954100	0.16608800	0.01304800
C	-4.61171700	-2.41897500	-2.76548500
H	-4.49740700	-3.35435900	-2.19419100
H	-5.28896700	-2.64543300	-3.59960300
C	-3.24693500	-1.98257400	-3.28472200
H	-2.79890400	-2.77159100	-3.90340100
H	-3.37161900	-1.10561800	-3.94076500
C	-5.21892300	-1.35438700	-1.86036100
H	-5.42884000	-0.44843300	-2.45207600
H	-6.18306500	-1.69177000	-1.45733000
C	-4.27845600	-0.98784600	-0.71544000
H	-4.73979500	-0.21628000	-0.08595800
H	-4.13394700	-1.86879200	-0.06940300
C	-2.30980000	-1.62062200	-2.13799200
H	-1.32869700	-1.29977600	-2.51797000
H	-2.11474700	-2.51193200	-1.52385100
C	-2.92088000	-0.52551400	-1.25951400
H	-3.11343300	0.34185600	-1.91545600
C	-3.42470600	4.52961900	-0.71800300
H	-4.11683400	4.24637100	-1.52748200
H	-3.53289600	5.61406200	-0.58350700
C	-2.00116900	4.18035900	-1.13621000
H	-1.74131100	4.68014200	-2.07907600
H	-1.29237700	4.55365400	-0.37912300
C	-3.82366000	3.79334200	0.55575400
H	-3.20592800	4.15269800	1.39488800
H	-4.86613100	4.01532300	0.81996000
C	-3.62946300	2.28564400	0.41344500
H	-3.92411700	1.77827100	1.34332900
H	-4.29957100	1.90957000	-0.37715100
C	-1.81748900	2.67192900	-1.27402000
H	-0.78644900	2.43505900	-1.56535800
H	-2.47050000	2.30396600	-2.08258800
C	-2.17880800	1.96780400	0.03821600
H	-1.52561500	2.39677800	0.81501300
C	1.19480400	1.55255000	-0.13520300
C	1.87012600	2.16471600	-1.20198800
C	0.99316900	2.30312900	1.02972600
C	2.29973200	3.48969900	-1.11614900
H	2.07499200	1.59636200	-2.11049800
C	1.43370800	3.62579300	1.12206500
H	0.48561300	1.85740600	1.88648100
C	2.08497300	4.22773500	0.04768000

H	2.81598000	3.94276100	-1.96271400
H	1.26232500	4.18540000	2.04185900
H	2.42535900	5.25968100	0.11718200

Int_{PE}(L3)

M06-L electronic energy (Hartree): -1867.807841

M06-L thermal correction to free energy (Hartree): 0.667677

Three lowest frequencies (cm⁻¹): 13.96, 17.57, 28.30

P	-0.28127800	-0.09185700	0.28832000
C	-1.10821200	1.60198300	0.26610500
C	-1.32511400	2.07492900	-1.18348000
C	-2.44338900	1.66635100	1.03164500
C	-0.12837600	2.58179500	0.95453100
H	-2.03922300	1.41250200	-1.69358300
H	-0.37738800	2.02096600	-1.73981500
C	-1.87834000	3.50390500	-1.20051200
H	-2.28369600	1.38284900	2.08215400
H	-3.17272000	0.95959800	0.61040100
C	-3.01080400	3.09233200	0.98858100
H	0.84462500	2.55462000	0.43793000
H	0.05555000	2.26355500	1.99358200
C	-0.68983800	4.00722500	0.93741100
H	-2.02267200	3.81178200	-2.24583300
C	-3.21909400	3.52968700	-0.46284600
C	-0.89042300	4.44910300	-0.51407700
H	-3.97198300	3.10011300	1.52192200
C	-2.02974300	4.04467800	1.67487700
H	0.02913600	4.67377200	1.43456200
H	-3.93696800	2.86074900	-0.96187800
H	-3.64951600	4.54170100	-0.49169900
H	0.07207700	4.44221900	-1.04813900
H	-1.26954100	5.48136300	-0.54600000
H	-2.43260000	5.06840800	1.67423300
H	-1.89263500	3.75343600	2.72720600
C	-1.07405700	-1.33528700	-0.87620700
C	-0.53030700	-2.72308600	-0.46479900
C	-2.61398500	-1.35157100	-0.84548300
C	-0.60751600	-1.08055900	-2.32725000
H	-0.80143500	-2.96007900	0.57272600
H	0.57111700	-2.70605700	-0.51006300
C	-1.08008700	-3.80943400	-1.39494400
H	-3.00810900	-0.37710500	-1.16970700

H	-2.98504700	-1.52153300	0.17340600
C	-3.14488600	-2.44835500	-1.77805300
H	0.49296800	-1.07645400	-2.35947300
H	-0.92995200	-0.09054900	-2.67416600
C	-1.15761200	-2.16185000	-3.26426100
H	-0.69266300	-4.78348300	-1.06404400
C	-2.60978400	-3.80944900	-1.32580000
C	-0.63063700	-3.53042800	-2.82992100
H	-4.24305000	-2.44642400	-1.73015200
C	-2.68721500	-2.16250700	-3.20986400
H	-0.82193300	-1.94098700	-4.28749700
H	-2.94310800	-4.02506500	-0.29888400
H	-3.01492800	-4.60547300	-1.96792400
H	0.46778700	-3.55143000	-2.89327300
H	-1.00761900	-4.31419600	-3.50381200
H	-3.08898500	-2.92413300	-3.89465800
H	-3.07980100	-1.19004100	-3.54421400
C	-0.51587700	-0.72016500	2.01176500
C	-1.84555700	-1.29449200	2.50320200
H	-0.22254200	0.12930100	2.64907300
H	0.27437200	-1.46501300	2.17190500
C	-1.84431900	-1.44077600	4.02050100
H	-2.69947900	-0.67455700	2.20384800
H	-2.02159600	-2.28060500	2.04963800
C	-3.11494900	-2.08157000	4.54877100
H	-0.96809600	-2.03241500	4.32645500
H	-1.70807200	-0.44699200	4.47434100
H	-3.09998300	-2.17074300	5.64072100
H	-3.99945400	-1.49181600	4.27620500
H	-3.25324500	-3.08870200	4.13547700
Pd	1.87060400	0.22149600	-0.40609100
O	3.77753100	0.69592700	-1.42347000
O	1.88130200	1.27122700	-2.41295600
C	3.15077200	1.22255000	-2.40309100
C	3.93765400	1.76503900	-3.55954200
H	3.31038600	2.36402900	-4.22373300
H	4.77871000	2.36769400	-3.20334700
H	4.36119600	0.93458200	-4.13599500
C	2.51892000	-0.59802200	1.28171800
C	2.71351000	0.19199700	2.42212100
C	2.90290000	-1.94456100	1.31697900
C	3.28634400	-0.35396200	3.57232400
H	2.41026400	1.24015100	2.42134600
C	3.47448600	-2.48701000	2.47060900

H	2.75868100	-2.58061700	0.44289100
C	3.66354900	-1.69572800	3.60230300
H	3.43205700	0.27449300	4.45061800
H	3.76949100	-3.53602700	2.48150600
H	4.10225800	-2.12218000	4.50265700

Pre-TS_{PE}(L3)

M06-L electronic energy (Hartree): -2648.726289

M06-L thermal correction to free energy (Hartree): 0.772117

Three lowest frequencies (cm⁻¹): 13.10, 17.98, 33.39

P	1.08559400	0.25333500	0.37113600
C	1.96170100	-1.32795400	0.93260300
C	2.59358200	-2.09224700	-0.24747000
C	3.04506500	-1.07823800	2.00022100
C	0.87056900	-2.22346000	1.56506400
H	3.39726200	-1.49322700	-0.69904600
H	1.83604900	-2.26820500	-1.02120600
C	3.18353800	-3.42255200	0.23520500
H	2.60829400	-0.56750800	2.87072300
H	3.83659400	-0.42547100	1.60260800
C	3.65255900	-2.40894900	2.46637600
H	0.08163300	-2.41752100	0.82307000
H	0.39338000	-1.69546800	2.40780000
C	1.47087200	-3.54711600	2.04853800
H	3.62031500	-3.94402100	-0.62885800
C	4.26925300	-3.14711900	1.27700600
C	2.07970000	-4.28372200	0.85290900
H	4.42831900	-2.19320700	3.21510200
C	2.55593800	-3.27349300	3.09169000
H	0.67035700	-4.15576000	2.49333600
H	5.07480100	-2.54319500	0.83163800
H	4.72382100	-4.09065600	1.61470900
H	1.30144300	-4.49384700	0.10262600
H	2.48975800	-5.25313200	1.17388200
H	2.98219400	-4.22141900	3.45287100
H	2.12227700	-2.76246500	3.96471800
C	2.05888900	1.21964700	-0.90979500
C	1.39568000	2.61253500	-1.00548700
C	3.55716600	1.38629500	-0.59017200
C	1.90759100	0.55528900	-2.29314100
H	1.43826200	3.13653900	-0.04015000
H	0.32897900	2.48458400	-1.25166700

C	2.08588800	3.46036000	-2.07938900
H	4.04831600	0.40397800	-0.54161600
H	3.69964600	1.85959700	0.38930500
C	4.23098900	2.23775700	-1.67483400
H	0.83864500	0.45664400	-2.52999000
H	2.32323100	-0.46059500	-2.28468900
C	2.60428200	1.39156200	-3.37103500
H	1.60472100	4.44840400	-2.11053300
C	3.56788400	3.61658000	-1.72790500
C	1.95191100	2.77334400	-3.43990700
H	5.29533600	2.34742700	-1.42225600
C	4.08872600	1.54253100	-3.03082200
H	2.49224500	0.87764600	-4.33737100
H	3.67608400	4.12560100	-0.75756200
H	4.06798500	4.24698100	-2.47820300
H	0.88988100	2.67669200	-3.71218900
H	2.43117600	3.38354600	-4.22021400
H	4.59917400	2.12721100	-3.81083600
H	4.57347300	0.55454700	-3.00015500
C	0.99690100	1.30955100	1.88891900
C	2.18101700	2.09834000	2.44799100
H	0.60477500	0.63095100	2.66361900
H	0.17489700	2.01194200	1.70678500
C	1.84881900	2.64333100	3.83271300
H	3.09633700	1.49681900	2.50704600
H	2.41909200	2.94076300	1.78206800
C	2.94867000	3.52247200	4.39968700
H	0.90346300	3.20615900	3.78113700
H	1.65573900	1.79808500	4.51144300
H	2.69506500	3.89665100	5.39786600
H	3.89400700	2.97114100	4.48258600
H	3.13286800	4.39219000	3.75625700
Pd	-1.01116900	-0.33538800	-0.46869500
O	-0.94911200	-0.84814200	-3.61599200
O	-0.22652200	-1.92009100	-1.77003800
C	-0.33125600	-1.76758200	-3.04357900
C	0.42100800	-2.79601100	-3.86623000
C	-4.80140500	-0.84267900	0.28006600
C	-4.13311000	-0.30028900	-0.84835700
C	-4.31572500	-2.07699300	0.63493700
C	-3.06849000	-1.07991700	-1.29301800
S	-3.02185000	-2.57481500	-0.37183800
O	-5.80045800	-0.18595000	0.92382300
C	-5.75678500	1.21928400	0.62192300

O	-4.47476300	0.86817900	-1.41739800
C	-5.67757000	1.44346600	-0.86478000
H	-4.61826200	-2.67250100	1.48785300
H	-6.67649000	1.64434900	1.02914300
H	-4.89060500	1.66851100	1.12792600
H	-5.62941900	2.50893800	-1.10102500
H	-2.64000700	-1.04226000	-2.29522700
H	0.46498000	-3.76767900	-3.36395500
H	-0.01670700	-2.91044500	-4.86206800
H	1.45611600	-2.45158200	-3.99573100
H	-6.53977800	0.99847600	-1.37761200
C	-1.87137900	0.95904700	0.79430400
C	-2.25735300	0.53292600	2.07262100
C	-2.10864000	2.29434100	0.44027500
C	-2.82430100	1.42427600	2.98614500
H	-2.09972900	-0.50704700	2.36907300
C	-2.67113800	3.18907300	1.35427100
H	-1.84373500	2.64978100	-0.55680900
C	-3.01747400	2.76081700	2.63604300
H	-3.10723100	1.07321600	3.97852200
H	-2.83707500	4.22584400	1.06130600
H	-3.44707100	3.45986300	3.35165200

TS_{PE}(L3)

M06-L electronic energy (Hartree): -2648.697855

M06-L thermal correction to free energy (Hartree): 0.768706

Three lowest frequencies (cm⁻¹): -537.48, 16.53, 20.26

P	1.23773400	0.26986800	0.29331400
C	2.67352300	-0.95768300	0.37851500
C	3.00019600	-1.57011900	-0.99787100
C	3.96684300	-0.36890700	0.97366000
C	2.19082000	-2.09016800	1.31498400
H	3.37554100	-0.79178600	-1.67762400
H	2.09079100	-1.98628800	-1.44644200
C	4.06783100	-2.66129100	-0.85695000
H	3.76925000	0.04721100	1.97237400
H	4.33847000	0.45508100	0.34555400
C	5.04308700	-1.45663000	1.09769500
H	1.26158500	-2.52332000	0.91410100
H	1.94578300	-1.67609400	2.30743900
C	3.26418800	-3.17383300	1.45232100
H	4.27267800	-3.08052900	-1.85286200

C	5.34549200	-2.04991300	-0.27939300
C	3.55631500	-3.76533500	0.07112700
H	5.95262200	-1.00185900	1.51604900
C	4.54190500	-2.56151400	2.03044100
H	2.89075700	-3.96052000	2.12366900
H	5.72779300	-1.26825300	-0.95378700
H	6.13181000	-2.81522600	-0.19553600
H	2.64250800	-4.21558700	-0.34740200
H	4.30392700	-4.56864100	0.15319700
H	5.31436600	-3.33651400	2.14649200
H	4.34519500	-2.15106700	3.03257100
C	1.32246000	1.39796200	-1.20860800
C	0.30877100	2.53666600	-0.95056200
C	2.70844800	2.00567600	-1.49604200
C	0.83430600	0.64058000	-2.46427200
H	0.57775400	3.10384300	-0.04825700
H	-0.68446000	2.09634700	-0.76406300
C	0.24729500	3.48511200	-2.15198100
H	3.43866300	1.21059700	-1.70435200
H	3.08152200	2.55460000	-0.62206900
C	2.62880900	2.95151600	-2.70197200
H	-0.16669800	0.22479900	-2.26624700
H	1.48794000	-0.21340400	-2.68533200
C	0.77756300	1.58138000	-3.67218700
H	-0.46633600	4.29118300	-1.92834800
C	1.63620600	4.07824800	-2.40394100
C	-0.21335800	2.71186300	-3.38886000
H	3.62713800	3.37490300	-2.88322200
C	2.16629300	2.16985200	-3.93362200
H	0.44602800	1.00664000	-4.54932300
H	1.96824200	4.65188600	-1.52471300
H	1.59809700	4.78101500	-3.24971900
H	-1.22064500	2.29864000	-3.22204700
H	-0.28014000	3.38671100	-4.25550100
H	2.13740200	2.83120200	-4.81262200
H	2.88236000	1.36492400	-4.16022400
C	1.45063200	1.34646400	1.78412700
C	2.48382300	2.46778400	1.88840000
H	1.59761000	0.63190700	2.61054800
H	0.45850800	1.77457900	1.97413800
C	2.57185300	2.98304500	3.32056300
H	3.48019200	2.14967800	1.55699600
H	2.20164300	3.30090900	1.22781300
C	3.51202500	4.16585400	3.46608600

H	1.56290100	3.25708100	3.66724200
H	2.89862900	2.16062000	3.97581900
H	3.56802000	4.51525300	4.50318500
H	4.52977600	3.90477400	3.14887800
H	3.18425800	5.01169100	2.84836900
Pd	-0.88222200	-0.81055300	0.22131300
O	-2.16116400	-2.72459400	-2.14990400
O	-0.12754200	-2.23070700	-1.33555200
C	-0.87063000	-2.76677900	-2.18550700
C	-0.25619300	-3.47896900	-3.35274300
C	-5.13258000	-0.54407200	0.26876300
C	-3.86941700	-0.47666100	-0.37985000
C	-5.19814600	-1.57727100	1.16959900
C	-2.93218600	-1.43314500	-0.00399800
S	-3.70764900	-2.43774000	1.20705300
O	-6.15369100	0.32530300	0.01192100
C	-5.67055800	1.51120000	-0.63044800
O	-3.58569200	0.47667800	-1.31408000
C	-4.75758000	1.16347900	-1.77871100
H	-6.04982200	-1.86539800	1.77501200
H	-6.55459100	2.04918300	-0.98035400
H	-5.14031500	2.13403300	0.10611300
H	-4.39784700	2.06230400	-2.28560100
H	-2.47772300	-2.15687000	-1.18253800
H	0.67467300	-3.96847700	-3.05355300
H	-0.94218100	-4.20444600	-3.79497800
H	-0.00294500	-2.73641200	-4.11972400
H	-5.28316100	0.52858700	-2.50583600
C	-1.54051700	0.30885000	1.74142400
C	-1.27089900	-0.12266800	3.04862700
C	-2.25055800	1.50472000	1.57456100
C	-1.66934200	0.63390800	4.15228400
H	-0.72372900	-1.05333000	3.21296200
C	-2.64869300	2.26285700	2.67853600
H	-2.49935700	1.85377600	0.57171300
C	-2.35394200	1.83533200	3.97217500
H	-1.43866200	0.28189600	5.15794500
H	-3.19604800	3.19304900	2.52178700
H	-2.66096900	2.42857500	4.83202900

Post-TS_{PE}(L3)

M06-L electronic energy (Hartree): -2648.702150

M06-L thermal correction to free energy (Hartree): 0.770617

Three lowest frequencies (cm⁻¹): 15.67, 17.35, 21.96

P	1.30823400	0.26103000	0.23352500
C	2.65355800	-1.06049200	0.36197300
C	2.75951000	-1.90439900	-0.92322300
C	4.05206900	-0.51718000	0.70931900
C	2.20263800	-1.98683100	1.51609600
H	3.10512800	-1.27942500	-1.75902700
H	1.77218300	-2.29540200	-1.19455600
C	3.74666100	-3.06032600	-0.72690700
H	4.01080300	0.06183400	1.64361100
H	4.40678200	0.16382600	-0.07939700
C	5.04699900	-1.67261400	0.88840300
H	1.19927500	-2.38324900	1.29577400
H	2.11531800	-1.40563600	2.44934800
C	3.19602700	-3.13634200	1.70861100
H	3.79315700	-3.64317700	-1.65851800
C	5.12948000	-2.49402600	-0.39960300
C	3.26858700	-3.95607900	0.41795200
H	6.03448900	-1.25098200	1.12547500
C	4.57950300	-2.57017000	2.03649600
H	2.84805800	-3.77247800	2.53522300
H	5.48502300	-1.86407300	-1.22950300
H	5.85812500	-3.30998500	-0.28017400
H	2.27782700	-4.37430300	0.18002200
H	3.95543300	-4.80611400	0.54676700
H	5.29710000	-3.38992800	2.19104900
H	4.54076800	-1.99579600	2.97458700
C	1.30815500	1.14246600	-1.42774700
C	0.42358400	2.39902900	-1.25239100
C	2.69018700	1.56363400	-1.95982200
C	0.61088900	0.25354900	-2.48230500
H	0.84455100	3.07076600	-0.49119100
H	-0.56975400	2.08986200	-0.88715100
C	0.28860300	3.15180300	-2.57995800
H	3.32732700	0.68043900	-2.11110800
H	3.20714800	2.20306000	-1.23280400
C	2.53720500	2.31432000	-3.28934400
H	-0.39048400	-0.01901500	-2.10965000
H	1.16196500	-0.68490100	-2.62914900
C	0.48037600	0.99515100	-3.81619400
H	-0.32795200	4.04739100	-2.41628700
C	1.67783300	3.56321700	-3.07537700
C	-0.37786400	2.24561900	-3.61675700

H	3.53511500	2.60751200	-3.64574100
C	1.86884000	1.39931800	-4.31825100
H	0.00067800	0.32568000	-4.54541900
H	2.15812400	4.23152700	-2.34394000
H	1.59059300	4.12716700	-4.01617700
H	-1.38636300	1.96139200	-3.27725900
H	-0.49693000	2.78254100	-4.56988200
H	1.78476100	1.91587800	-5.28619000
H	2.48712400	0.50367000	-4.48452200
C	1.77506100	1.52579000	1.50304600
C	2.89449700	2.54958100	1.31805600
H	1.96526100	0.93391800	2.41346000
H	0.84648200	2.06701700	1.72527500
C	3.18889800	3.26760000	2.63028400
H	3.81815700	2.09288400	0.94093200
H	2.60160500	3.29480900	0.56382300
C	4.22727400	4.36505900	2.48327300
H	2.25148400	3.68547500	3.03032100
H	3.52622100	2.52829500	3.37342000
H	4.43114700	4.86273800	3.43804300
H	5.17786500	3.96388500	2.10898000
H	3.89495200	5.13313500	1.77326000
Pd	-0.93879000	-0.58956300	0.55688300
O	-2.44271800	-2.41783700	-1.87968900
O	-0.46035800	-2.36338500	-0.82234700
C	-1.17694400	-2.77174400	-1.73988600
C	-0.67362000	-3.67473900	-2.81307700
C	-5.30267700	-0.62541400	0.32402800
C	-3.95985300	-0.28147200	-0.02531100
C	-5.36375700	-1.59062400	1.29301100
C	-2.96923000	-0.97740700	0.63639200
S	-3.76010300	-2.05947800	1.74999200
O	-6.39696600	-0.06094100	-0.26880700
C	-6.05847400	1.11662400	-1.01049000
O	-3.68363800	0.66630400	-0.98795800
C	-4.81359300	0.89763000	-1.83308500
H	-6.24741200	-2.04874500	1.72047100
H	-6.92172600	1.33163700	-1.64540600
H	-5.90853300	1.95657300	-0.31567500
H	-4.57450100	1.78199400	-2.42918900
H	-2.68361000	-1.85189300	-1.08798000
H	0.24358800	-4.17237400	-2.49248300
H	-1.42795500	-4.41061400	-3.10158300
H	-0.44700000	-3.07210800	-3.70138600

H	-4.95089200	0.03847200	-2.50860000
C	-1.31710200	0.79843400	1.93818200
C	-0.89184000	0.54985700	3.25165500
C	-1.93995000	2.02202500	1.66170300
C	-1.04083100	1.51617700	4.24815100
H	-0.41233600	-0.39922300	3.49934500
C	-2.08083500	2.99133100	2.65805800
H	-2.31936800	2.22401100	0.65992300
C	-1.62565900	2.74704300	3.95298400
H	-0.69136200	1.30512900	5.25895400
H	-2.55584000	3.94283800	2.41789500
H	-1.73489700	3.50465900	4.72732000

Int_{PE}(L4)

M06-L electronic energy (Hartree): -1624.622600

M06-L thermal correction to free energy (Hartree): 0.352458

Three lowest frequencies (cm-1): 19.58, 21.72, 27.32

Pd	0.42953000	1.54374600	0.00989000
O	0.94700400	3.68841500	0.03919700
O	2.58189900	2.19751500	0.07359100
C	2.19235600	3.40685400	0.06809800
C	3.19223700	4.52383900	0.06515600
H	2.86504100	5.33870800	0.71739700
H	4.17981100	4.17403400	0.37478500
H	3.27520400	4.93516700	-0.94757000
C	-0.85762800	-1.45156300	-1.24106300
C	-2.24716600	-1.42707200	-1.04930400
C	-0.34128300	-1.99506000	-2.42310600
C	-3.09861700	-1.94309700	-2.01973300
H	-2.66328200	-0.99861800	-0.13763600
C	-1.19913200	-2.50621200	-3.39461800
H	0.73495100	-2.02624800	-2.58612000
C	-2.57713500	-2.48169200	-3.19556900
H	-4.17453600	-1.91914400	-1.85713100
H	-0.78506600	-2.92917500	-4.30760300
H	-3.24537200	-2.88253200	-3.95504000
C	-0.31992700	-1.36445900	1.60528200
C	-0.97035900	-2.59964500	1.71859400
C	-0.02924500	-0.63292200	2.76431500
C	-1.32515600	-3.09011800	2.97271300
H	-1.19966700	-3.17934500	0.82532300
C	-0.38181400	-1.12758000	4.01601800

H	0.46888000	0.33433100	2.67283400
C	-1.03243200	-2.35596100	4.12047500
H	-1.83175700	-4.04966200	3.05190800
H	-0.15534300	-0.54993000	4.90963100
H	-1.31458300	-2.74069200	5.09836900
C	1.86906800	-1.45174600	-0.29236100
C	2.73685200	-0.83191300	-1.20169200
C	2.25966800	-2.64510500	0.32724500
C	3.97067900	-1.40465000	-1.49618800
H	2.44264800	0.10727300	-1.67079300
C	3.49858200	-3.20943000	0.03594900
H	1.59648900	-3.13444900	1.03926900
C	4.35326500	-2.59257700	-0.87583500
H	4.63680000	-0.91784700	-2.20540000
H	3.79610700	-4.13532500	0.52386200
H	5.32111900	-3.03643600	-1.09992300
P	0.23653100	-0.69560000	0.00702900
C	-1.56267800	1.60514100	-0.04663900
C	-2.18067900	1.88758600	-1.27058200
C	-2.34730300	1.48756100	1.10508700
C	-3.56374300	2.06215500	-1.33678600
H	-1.58600800	1.96179100	-2.18185300
C	-3.73217300	1.66159300	1.03288400
H	-1.88736100	1.24922100	2.06472000
C	-4.34346400	1.94467500	-0.18692400
H	-4.03241600	2.28252100	-2.29550300
H	-4.33268400	1.56745900	1.93717300
H	-5.42317600	2.07153700	-0.24187900

Pre-TS_{PE}(L4)

M06-L electronic energy (Hartree): -2405.542761

M06-L thermal correction to free energy (Hartree): 0.455462

Three lowest frequencies (cm⁻¹): 12.85, 19.20, 28.53

Pd	0.40228000	-0.68399000	0.06960100
O	-0.03028800	-3.48740300	-1.11431600
O	-0.62681300	-2.46963500	0.80359600
C	-0.66400100	-3.44054400	-0.04370500
C	-1.60258800	-4.56808000	0.33861300
C	4.22276600	-0.59082700	-0.35524300
C	3.39218300	-1.19478300	0.62075300
C	3.87729400	-0.96336000	-1.63221500
C	2.34540200	-1.94381100	0.07888200

S	2.52346700	-2.01132800	-1.66674300
O	5.24299500	0.25088200	-0.04444800
C	5.17704100	0.68470900	1.32330600
O	3.59213400	-1.05086100	1.94480200
C	4.87888500	-0.46862700	2.24468300
H	4.30929000	-0.58290900	-2.55050200
H	6.15328900	1.11921400	1.54872000
H	4.40456600	1.46027400	1.41516300
H	4.81995700	-0.14094500	3.28406000
H	1.87079100	-2.77964000	0.58297500
H	-1.44586100	-5.45199900	-0.28570400
H	-1.49221100	-4.83959400	1.39369500
H	-2.63809000	-4.22871100	0.20388800
H	5.64260400	-1.25187900	2.15546300
C	-1.78293800	1.95352100	-0.82515500
C	-1.32174400	3.15372900	-0.26619000
C	-2.25992100	1.95275700	-2.14054400
C	-1.34507200	4.32933100	-1.00843000
H	-0.93655500	3.16584800	0.75284400
C	-2.27647600	3.13148200	-2.88274400
H	-2.62203300	1.02872700	-2.58957400
C	-1.81857400	4.32036800	-2.32010600
H	-0.98542200	5.25464700	-0.56222800
H	-2.65310200	3.11861200	-3.90360300
H	-1.83222900	5.24015700	-2.90138800
C	-2.10933700	0.81721600	1.80708600
C	-3.13347200	1.73858100	2.06812800
C	-1.47047700	0.17935600	2.87807300
C	-3.51361000	2.00973900	3.37914900
H	-3.62882500	2.24970200	1.24286600
C	-1.85439200	0.45292700	4.18830900
H	-0.66890300	-0.53180900	2.67261000
C	-2.87535100	1.36728300	4.43932600
H	-4.30861200	2.72678800	3.57301500
H	-1.35082300	-0.04501200	5.01431500
H	-3.17197200	1.58437200	5.46352600
C	-2.89046300	-0.70286000	-0.56274900
C	-2.56443500	-1.48351500	-1.68001100
C	-4.17365200	-0.79300400	-0.01369700
C	-3.51235700	-2.32831800	-2.24874100
H	-1.55109800	-1.44622700	-2.08316300
C	-5.11778800	-1.64664400	-0.58077400
H	-4.43763700	-0.20286800	0.86275900
C	-4.79093300	-2.41136400	-1.69866500

H	-3.24622700	-2.93395300	-3.11295200
H	-6.11211300	-1.71465400	-0.14390600
H	-5.53017200	-3.07924900	-2.13644600
P	-1.60088500	0.39963300	0.10982200
C	1.31535100	1.03383400	-0.42235800
C	1.51262800	1.39763900	-1.75972600
C	1.81647500	1.87185300	0.58066800
C	2.22753600	2.55138000	-2.08675400
H	1.11102200	0.77221300	-2.55950900
C	2.52797500	3.02952300	0.25389000
H	1.66546000	1.61716600	1.63283100
C	2.74203000	3.36892700	-1.08098700
H	2.37795100	2.81391900	-3.13407300
H	2.92011000	3.66384400	1.04958400
H	3.29767700	4.26986700	-1.33587500

TS_{PE}(L4)

M06-L electronic energy (Hartree): -2405.513525

M06-L thermal correction to free energy (Hartree): 0.448656

Three lowest frequencies (cm-1): -562.02, 10.54,16.58

Pd	0.43850500	-0.47267500	-0.37302400
O	1.89037100	-3.42035600	-0.65514600
O	-0.18937400	-2.62687200	-0.33159300
C	0.62437100	-3.57031600	-0.45785300
C	0.14784300	-4.98961000	-0.36682800
C	4.67330600	0.01077200	-0.24687500
C	3.46525800	-0.57473400	0.22173400
C	4.68262600	0.15899300	-1.61104400
C	2.51826400	-0.88533200	-0.74869700
S	3.20855900	-0.40993100	-2.29039500
O	5.69852300	0.37535700	0.57680300
C	5.25415800	0.48837100	1.93420600
O	3.24408700	-0.81149500	1.54551800
C	4.44234000	-0.71759400	2.33212100
H	5.48850000	0.55045900	-2.22108900
H	6.15673000	0.57321000	2.54360600
H	4.65766200	1.40643700	2.04694800
H	4.11485400	-0.65016500	3.37200600
H	2.14045700	-2.27123400	-0.70442400
H	0.52262500	-5.44025400	0.55879800
H	-0.94232700	-5.03871700	-0.36775100
H	0.54930700	-5.58119700	-1.19474100

H	5.03167100	-1.63576600	2.20069200
C	-2.29279800	1.81358200	-0.02319500
C	-1.85015900	2.74171000	0.93007100
C	-3.03203000	2.26396300	-1.12150200
C	-2.15111000	4.09138900	0.79055600
H	-1.26170500	2.40351700	1.78310600
C	-3.32573200	3.61916200	-1.26234700
H	-3.38165300	1.55571000	-1.87178700
C	-2.88701800	4.53410000	-0.30890700
H	-1.80247300	4.80171500	1.53804300
H	-3.90409800	3.95768800	-2.11985600
H	-3.11809400	5.59167800	-0.42033100
C	-2.20923300	-0.35940200	1.85243400
C	-3.30772400	0.21566800	2.50704200
C	-1.42901700	-1.30595300	2.52940000
C	-3.62301000	-0.15821700	3.81017900
H	-3.91244800	0.96554500	1.99752200
C	-1.74837100	-1.67861900	3.83266700
H	-0.56812400	-1.74672300	2.02551000
C	-2.84492000	-1.10582400	4.47365700
H	-4.47715100	0.29461300	4.30960500
H	-1.13431100	-2.41260700	4.35060700
H	-3.09083500	-1.39319200	5.49402000
C	-2.93031900	-0.83955300	-0.93197600
C	-2.53312200	-1.10995300	-2.24809400
C	-4.20180400	-1.23754200	-0.50503000
C	-3.39839900	-1.75489000	-3.12706700
H	-1.53417200	-0.81368700	-2.57540000
C	-5.06207600	-1.89188900	-1.38337300
H	-4.52119100	-1.04037200	0.51775800
C	-4.66360900	-2.14830600	-2.69406000
H	-3.08122100	-1.95814900	-4.14789600
H	-6.04771900	-2.20172900	-1.04168800
H	-5.33830900	-2.65976900	-3.37767900
P	-1.76662000	0.07575000	0.13638200
C	0.95937300	1.46180000	-0.41393700
C	0.65026500	2.25018500	-1.52919900
C	1.65024800	2.05151900	0.65075800
C	1.02208500	3.59474700	-1.57847200
H	0.10115200	1.81792300	-2.36840900
C	2.01848100	3.39845200	0.60302500
H	1.91390500	1.45555500	1.52593100
C	1.70825200	4.17474300	-0.51212600
H	0.76820800	4.19151300	-2.45494800

H	2.55713200	3.83817000	1.44315000
H	1.99739300	5.22391400	-0.54988200

Post-TS_{PE}(L4)

M06-L electronic energy (Hartree): -2405.520807

M06-L thermal correction to free energy (Hartree): 0.455107

Three lowest frequencies (cm⁻¹): 14.28, 16.30, 28.01

Pd	0.53580600	0.25788100	0.06014200
O	2.30029100	-1.81633800	-1.68603400
O	0.93512400	-1.98117900	0.09576000
C	1.60386300	-2.50790600	-0.79555300
C	1.71215700	-3.98281600	-0.96207600
C	4.91597400	0.76744800	0.07910500
C	3.66491600	0.13004700	0.34763100
C	4.76839000	1.96417900	-0.56778500
C	2.53928100	0.80068600	-0.09125700
S	3.09071400	2.28821700	-0.82546000
O	6.12494400	0.22439200	0.41529200
C	5.99661400	-0.88329300	1.31285500
O	3.61240900	-1.08603800	0.99443200
C	4.85718200	-1.78105600	0.90189700
H	5.54752900	2.64397700	-0.89072100
H	6.95300100	-1.41166800	1.27899100
H	5.83222500	-0.51060000	2.33478100
H	4.77587400	-2.64507700	1.56653700
H	2.26215700	-0.85725200	-1.41856400
H	2.62070000	-4.33327300	-0.45784600
H	0.85236200	-4.47832900	-0.50766500
H	1.79528100	-4.25454800	-2.01722700
H	5.00469700	-2.13787900	-0.13020600
C	-2.99760200	0.82239400	-0.41780400
C	-3.36910400	1.82279800	0.49178800
C	-3.51623000	0.85580900	-1.71630300
C	-4.24893800	2.82962100	0.11015600
H	-2.96316900	1.81435300	1.50336600
C	-4.39302100	1.86982200	-2.09711500
H	-3.23906500	0.08577100	-2.43516500
C	-4.76037100	2.85776300	-1.18700700
H	-4.53001400	3.59943500	0.82652900
H	-4.79320200	1.88234700	-3.10909700
H	-5.44562700	3.64836200	-1.48628600
C	-2.30811100	-0.97893200	1.71424300

C	-3.66803700	-1.12504900	2.02186400
C	-1.34841500	-1.30584100	2.68062800
C	-4.05682800	-1.59753700	3.27169600
H	-4.42317300	-0.86242300	1.28103200
C	-1.74054100	-1.78013900	3.93014200
H	-0.29017300	-1.18060600	2.44576000
C	-3.09407100	-1.92632800	4.22572400
H	-5.11445300	-1.70777600	3.50253000
H	-0.98775700	-2.02864600	4.67542400
H	-3.40121200	-2.29216100	5.20347600
C	-1.94095900	-1.80229200	-1.05523200
C	-1.27437200	-1.73800800	-2.28828300
C	-2.67069500	-2.95118000	-0.73562500
C	-1.34839600	-2.79586400	-3.18866600
H	-0.67987900	-0.85394500	-2.53192000
C	-2.73627300	-4.01373500	-1.63569600
H	-3.18270100	-3.02372700	0.22290500
C	-2.07785000	-3.93862300	-2.86074000
H	-0.82530200	-2.73325000	-4.14093700
H	-3.30277900	-4.90535600	-1.37426900
H	-2.12710400	-4.77233500	-3.55825000
P	-1.73496000	-0.39090800	0.08799500
C	0.04689600	2.19288500	0.03983700
C	-0.25136000	2.83768800	-1.16700400
C	-0.01860400	2.92900800	1.22878900
C	-0.59826300	4.18992300	-1.18483000
H	-0.21388900	2.28320300	-2.10666400
C	-0.36959300	4.28066900	1.20955000
H	0.20906400	2.44944000	2.18208500
C	-0.65543500	4.91773900	0.00292500
H	-0.82492400	4.67485700	-2.13447900
H	-0.41357000	4.83802900	2.14531400
H	-0.92434000	5.97272800	-0.01129400

Int_{PE}(L5)

M06-L electronic energy (Hartree): -1742.586723

M06-L thermal correction to free energy (Hartree): 0.434317

Three lowest frequencies (cm⁻¹): 22.25, 25.27, 32.48

Pd	-0.07104800	1.53016800	0.21989200
O	1.94972500	2.56623700	0.17851900
O	0.07055600	3.72283100	0.35869900
C	1.34575200	3.67861400	0.27713400

C	2.11758900	4.96387000	0.26814200
H	3.16247300	4.80051600	0.54278200
H	2.09433600	5.39403600	-0.74003400
H	1.66466700	5.69545500	0.94318100
C	-0.86350000	-1.71515700	-0.95584100
C	-2.12538000	-2.03369600	-0.40413200
C	-0.56112400	-2.12090300	-2.26458800
C	-3.04025700	-2.72529300	-1.20574800
C	-1.48810300	-2.80737700	-3.04011200
H	0.41909900	-1.90314300	-2.68376900
C	-2.73994200	-3.10386600	-2.50860900
H	-4.01701300	-2.96445600	-0.78495400
H	-1.22899900	-3.10879600	-4.05267500
H	-3.47972500	-3.63449300	-3.10484000
C	0.71190200	-1.66119200	1.47835300
C	0.37405400	-3.02193900	1.50935100
C	1.37602600	-1.08347900	2.58356300
C	0.65993800	-3.81052800	2.61801200
H	-0.11725700	-3.47383400	0.64957500
C	1.65094900	-1.89742100	3.68771800
C	1.29659900	-3.24197500	3.71671900
H	0.38846700	-4.86394000	2.61728200
H	2.16436200	-1.45632700	4.54150800
H	1.52614800	-3.84499600	4.59300500
C	1.90802400	-0.74768700	-0.99459900
C	2.06876200	0.00652200	-2.18232200
C	2.97985000	-1.51430300	-0.51459000
C	3.29922600	-0.05897700	-2.84348100
C	4.19816400	-1.55056600	-1.18487500
H	2.86067500	-2.09727000	0.39613100
C	4.35799300	-0.81870300	-2.35639900
H	3.42254200	0.50831500	-3.76556800
H	5.01318400	-2.15481100	-0.79245000
H	5.30318400	-0.84019600	-2.89522900
P	0.34244800	-0.69139900	-0.03419100
C	1.81738000	0.34639300	2.60900800
H	2.39776200	0.62062200	1.71873000
H	0.96135800	1.03763600	2.63580600
H	2.43558800	0.54791800	3.49014600
C	0.99523700	0.87894100	-2.76186400
H	0.95321400	1.84661900	-2.24132800
H	1.19037400	1.08172200	-3.82057100
H	-0.00556200	0.43614500	-2.68662400
C	-2.53206900	-1.71261900	1.00341800

H	-1.89670000	-0.96333400	1.48230600
H	-3.56080500	-1.33309100	1.02774800
H	-2.49871000	-2.61463600	1.62999200
C	-2.04849600	1.34302600	0.20329800
C	-2.76641100	0.98732500	-0.94171100
C	-2.74359400	1.76004500	1.34507400
C	-4.16216500	1.04632600	-0.94442800
H	-2.24578900	0.64246900	-1.83710400
C	-4.13856300	1.81125900	1.34016500
H	-2.19932600	2.04174000	2.24766600
C	-4.85153000	1.45138800	0.19673300
H	-4.70894000	0.76438300	-1.84413100
H	-4.66775300	2.13044900	2.23763200
H	-5.93951200	1.48782700	0.19553100

Pre-TS_{PE}(L5)

M06-L electronic energy (Hartree): -2523.507589

M06-L thermal correction to free energy (Hartree): 0.544222

Three lowest frequencies (cm⁻¹): 27.69, 36.44, 38.45

Pd	0.52886900	-0.61622600	0.13933600
O	0.23397300	-3.53692500	-0.82262700
O	-0.45060800	-2.38995600	0.99028300
C	-0.42907600	-3.42901000	0.22558000
C	-1.32753100	-4.56379100	0.67432400
C	4.41054700	-0.50573100	-0.19627600
C	3.55154300	-1.06384700	0.78292400
C	4.09532300	-0.93105400	-1.46511800
C	2.51748700	-1.83247000	0.24723500
S	2.74619200	-1.98420400	-1.48711600
O	5.43218100	0.33751500	0.10534500
C	5.33740800	0.82628400	1.45153400
O	3.71632500	-0.86262300	2.10517000
C	5.00320400	-0.28452400	2.41238900
H	4.55236400	-0.59215800	-2.38778000
H	6.31131400	1.26223100	1.68373300
H	4.57099100	1.61074300	1.49212700
H	4.92476900	0.08648400	3.43570000
H	2.03076500	-2.64645400	0.77451200
H	-1.05147100	-5.50613400	0.19266300
H	-1.31051300	-4.68631200	1.76204500
H	-2.36213400	-4.32706900	0.39313900
H	5.75878300	-1.07922900	2.37224600

C	-1.85217500	1.82784900	-0.90598700
C	-1.35437300	3.06340600	-0.42909900
C	-2.49848500	1.78086900	-2.14779400
C	-1.47524800	4.18682000	-1.25236500
C	-2.61476500	2.91555900	-2.94489700
H	-2.92939400	0.84447700	-2.49695600
C	-2.08601100	4.12281900	-2.50084800
H	-1.08307500	5.13746100	-0.89096100
H	-3.11884300	2.85067000	-3.90705500
H	-2.15688200	5.01635200	-3.11809800
C	-2.37826800	0.73424500	1.66044000
C	-3.63850300	1.34714000	1.56038200
C	-1.78154400	0.57260400	2.92820400
C	-4.33198800	1.77106500	2.68588700
H	-4.08130200	1.49075300	0.57424000
C	-2.50145500	1.00912500	4.04905000
C	-3.75699400	1.59485000	3.94184800
H	-5.30941700	2.23680600	2.58053300
H	-2.04666000	0.89113500	5.03214800
H	-4.28122600	1.92177100	4.83793100
C	-2.66675300	-0.99606600	-0.66793600
C	-2.34776700	-1.60207000	-1.90812400
C	-3.77906900	-1.45694000	0.05025600
C	-3.19314700	-2.60817700	-2.38968300
C	-4.59689300	-2.46671900	-0.44619800
H	-4.01642500	-1.02537600	1.01875300
C	-4.30768000	-3.04061700	-1.67874400
H	-2.95634400	-3.06424500	-3.35087400
H	-5.45686200	-2.79696600	0.13291700
H	-4.94074400	-3.82736500	-2.08504300
P	-1.57876600	0.29476000	0.06487300
C	-0.40814200	0.01290300	3.14191300
H	-0.31259100	-1.01307600	2.76869900
H	0.35538000	0.60659900	2.61493600
H	-0.15356600	0.01894700	4.20721200
C	-1.13082000	-1.24696100	-2.70549400
H	-0.23204500	-1.66818300	-2.22951800
H	-1.19768800	-1.65466400	-3.72044600
H	-0.97846800	-0.16509400	-2.79029700
C	-0.76410700	3.24607900	0.93757100
H	-0.22833900	2.36095900	1.29505400
H	-0.05843300	4.08380100	0.94708500
H	-1.54941000	3.46335000	1.67587300
C	1.41807100	1.03533500	-0.58483400

C	1.46301300	1.28424600	-1.96167600
C	2.10839500	1.90718600	0.26637500
C	2.17855200	2.36895900	-2.47419400
H	0.94272800	0.62030200	-2.65336800
C	2.82274600	2.99378600	-0.24198300
H	2.09213300	1.74416900	1.34747100
C	2.85910900	3.22954600	-1.61509200
H	2.19762700	2.54136000	-3.55045300
H	3.35280900	3.65766900	0.44223000
H	3.41403500	4.07825200	-2.01190600

TS_{PE}(L5)

M06-L electronic energy (Hartree): -2523.480565

M06-L thermal correction to free energy (Hartree): 0.540178

Three lowest frequencies (cm⁻¹): -786.42, 20.38, 27.74

Pd	-0.60900700	0.28413500	-0.19816600
O	-1.97031100	3.11228000	-1.10748800
O	-0.23176400	2.47025800	0.16090900
C	-0.88285600	3.34476700	-0.45698700
C	-0.36324100	4.75020700	-0.49977600
C	-4.86499700	-0.06775700	-0.03040600
C	-3.62416300	0.52337900	0.33369100
C	-4.89829700	-0.42817700	-1.35434500
C	-2.67679000	0.63079600	-0.68146500
S	-3.40578100	-0.06258400	-2.12240500
O	-5.89761000	-0.24203300	0.84405700
C	-5.44922800	-0.14828000	2.20174000
O	-3.37635600	0.95485400	1.60166600
C	-4.57099400	1.06153000	2.39278600
H	-5.73077500	-0.87069700	-1.88955300
H	-6.35041300	-0.08204500	2.81525500
H	-4.90121800	-1.06445700	2.46831000
H	-4.23696500	1.15018800	3.42886000
H	-2.26744900	1.95882800	-0.93228400
H	-1.16981400	5.47748200	-0.61753300
H	0.22316900	4.97181200	0.39507800
H	0.30477800	4.84392400	-1.36486100
H	-5.10976700	1.97616300	2.10930300
C	2.53411100	-1.45646800	-0.61127300
C	2.33490200	-2.74101600	-0.05483900
C	3.31216600	-1.32118000	-1.76902400
C	2.90417900	-3.83941400	-0.70646800

C	3.87007300	-2.42956200	-2.39773200
H	3.49470200	-0.33155600	-2.18412700
C	3.65702100	-3.69799500	-1.86699200
H	2.74063700	-4.83203300	-0.28632700
H	4.46886800	-2.29759900	-3.29669000
H	4.07999100	-4.57626400	-2.35151700
C	2.40464500	-0.02624500	1.84071800
C	3.75281500	-0.39218800	1.98255600
C	1.63660700	0.25638500	2.98918100
C	4.35158100	-0.48046200	3.23292800
H	4.34061400	-0.61643500	1.09230200
C	2.25990300	0.15340100	4.23938900
C	3.59546800	-0.20852700	4.37005900
H	5.39884200	-0.76362600	3.31608700
H	1.66985800	0.36460100	5.13081100
H	4.04423700	-0.28060600	5.35901900
C	2.49948200	1.46851000	-0.65425500
C	2.14926600	1.85143600	-1.97126700
C	3.36644700	2.28284700	0.08531700
C	2.71324000	3.01879900	-2.49585000
C	3.89816400	3.45179100	-0.45136700
H	3.62922400	2.00655700	1.10347400
C	3.57266300	3.82079600	-1.75139600
H	2.45540600	3.30577400	-3.51537300
H	4.56688100	4.06568000	0.14866000
H	3.98357700	4.72945800	-2.18758900
P	1.71497200	0.00378300	0.13718700
C	0.18882800	0.63949200	2.93936400
H	0.01367300	1.52144800	2.31160200
H	-0.43244700	-0.16486600	2.51763300
H	-0.18865700	0.85650700	3.94466100
C	1.17610700	1.09309800	-2.82696200
H	0.13859200	1.38833800	-2.60690900
H	1.35306700	1.29693700	-3.88919700
H	1.22630200	0.00704700	-2.68387100
C	1.57173500	-2.97670500	1.21356900
H	0.74491600	-2.26996700	1.34767100
H	1.14574700	-3.98624000	1.22535200
H	2.22422100	-2.88121500	2.09321500
C	-1.00625200	-1.65764900	-0.48185900
C	-0.50247900	-2.38493500	-1.56473300
C	-1.86364900	-2.31114100	0.41615100
C	-0.83415000	-3.73040500	-1.74142900
H	0.17303900	-1.90940500	-2.27960400

C	-2.19180100	-3.65588600	0.24312600
H	-2.28124600	-1.76579000	1.26475900
C	-1.67870100	-4.37213300	-0.83820300
H	-0.41958300	-4.27799100	-2.58840400
H	-2.85581800	-4.14388300	0.95717300
H	-1.93643000	-5.42124600	-0.97587800

Post-TS_{PE}(L5)

M06-L electronic energy (Hartree): -2523.488200

M06-L thermal correction to free energy (Hartree): 0.535882

Three lowest frequencies (cm⁻¹): 14.20, 20.20, 24.76

Pd	0.65375200	0.29789400	0.05692300
O	2.45122400	-1.92989800	-1.58650700
O	1.00345200	-1.96644700	0.13462900
C	1.69342400	-2.55754800	-0.69789100
C	1.76913800	-4.04149000	-0.78422900
C	5.02618800	0.60589000	0.05513200
C	3.74202300	0.10103300	0.42929500
C	4.94672400	1.65428500	-0.82150100
C	2.66004500	0.73150900	-0.15236400
S	3.28957500	2.00856900	-1.16195700
O	6.20182500	0.07878500	0.51169800
C	6.00727000	-0.81879800	1.60994200
O	3.61713200	-0.96183600	1.29609500
C	4.82531100	-1.72257000	1.36529700
H	5.76271700	2.21141100	-1.26540200
H	6.93434500	-1.39089100	1.69983100
H	5.85479700	-0.24091700	2.53352800
H	4.69422100	-2.43232900	2.18592300
H	2.43762200	-0.96041600	-1.35592800
H	2.65197700	-4.38452100	-0.23179300
H	0.88212300	-4.49254100	-0.33655600
H	1.88170600	-4.36938200	-1.82051400
H	4.96228900	-2.28294500	0.42652700
C	-2.95542600	0.78448300	-0.53745800
C	-3.26451200	1.92790000	0.23400800
C	-3.62108600	0.57225100	-1.75149200
C	-4.19775700	2.83681000	-0.27388300
C	-4.55031300	1.48866500	-2.23437500
H	-3.42106200	-0.33210300	-2.32408500
C	-4.83004300	2.63464700	-1.49633400
H	-4.42833300	3.72591800	0.31329100

H	-5.05244000	1.30261900	-3.18154900
H	-5.54731400	3.36550200	-1.86501900
C	-2.43857300	-0.97862300	1.61129800
C	-3.81264100	-1.26479700	1.57580500
C	-1.73670800	-1.08920600	2.82941600
C	-4.49902700	-1.66886900	2.71366000
H	-4.35151400	-1.16493900	0.63314800
C	-2.45066100	-1.49358100	3.96533400
C	-3.80949900	-1.78187000	3.91837900
H	-5.56322700	-1.88821400	2.65962400
H	-1.91639900	-1.57423700	4.91157600
H	-4.33014400	-2.08957300	4.82323000
C	-1.73841300	-1.82134800	-1.09065000
C	-1.20552800	-1.73061000	-2.40168900
C	-2.19167600	-3.06278100	-0.62540200
C	-1.17886800	-2.88664400	-3.18902400
C	-2.14982000	-4.19981600	-1.42755400
H	-2.57910700	-3.14920500	0.38681600
C	-1.64221800	-4.11152200	-2.71844600
H	-0.77364400	-2.81546900	-4.19815600
H	-2.51076900	-5.14919300	-1.03707100
H	-1.59884900	-4.99136300	-3.35748100
P	-1.66669500	-0.37960600	0.05261200
C	-0.28009000	-0.76749500	2.97652500
H	0.35006900	-1.38627800	2.32661000
H	-0.06451300	0.27827100	2.71053000
H	0.04719600	-0.92150500	4.01030000
C	-0.65534800	-0.46147500	-2.97975800
H	0.17274100	-0.06287800	-2.37013100
H	-0.27912000	-0.62439700	-3.99495400
H	-1.40665700	0.33776400	-3.02779600
C	-2.67801300	2.17511200	1.59086300
H	-1.63410200	1.84736700	1.66574800
H	-2.70710800	3.24160400	1.83998300
H	-3.24101200	1.63770300	2.36746600
C	0.30948400	2.26829300	-0.02358500
C	-0.35796300	2.84228400	-1.11137800
C	0.73788800	3.10933000	1.01380700
C	-0.60177400	4.21737500	-1.15758100
H	-0.71110800	2.21560700	-1.93230200
C	0.48210300	4.47993900	0.97407600
H	1.28194900	2.69221100	1.86193200
C	-0.18717300	5.04099800	-0.11389400
H	-1.12862000	4.64000700	-2.01343300

H	0.81784000	5.11370400	1.79492700
H	-0.37978900	6.11209500	-0.14852900

Int_{PE}(L6)

M06-L electronic energy (Hartree): -1968.255932

M06-L thermal correction to free energy (Hartree): 0.443205

Three lowest frequencies (cm⁻¹): 17.79, 22.58, 27.88

C	-0.48471300	-1.97868000	-1.17617200
C	-1.49188300	-1.66924500	-2.11464400
C	0.19513900	-3.19254000	-1.29994200
C	-1.78300900	-2.55333500	-3.15634100
C	-0.09626000	-4.08061700	-2.33174800
H	0.96650400	-3.44381500	-0.57384300
C	-1.08194400	-3.75230200	-3.25790900
H	-2.55620500	-2.31362700	-3.88064000
H	0.44471400	-5.02051400	-2.40967400
H	-1.31766500	-4.43560400	-4.07153200
C	-1.44049200	-1.11757300	1.39345700
C	-2.40806900	-2.10898000	1.21164500
C	-1.54989400	-0.26422400	2.51356500
C	-3.46364900	-2.25879800	2.10784900
H	-2.33454000	-2.77050600	0.34994500
C	-2.61128100	-0.40441700	3.40908800
C	-3.56113000	-1.40182900	3.19968000
H	-4.20518600	-3.03796700	1.94935300
H	-2.69687600	0.25377100	4.26894800
H	-4.38388600	-1.50469100	3.90448700
C	1.40293600	-1.42105300	0.93681800
C	2.59788300	-1.42405000	0.18545300
C	1.45802100	-1.78518300	2.28465300
C	3.81104500	-1.75817100	0.79106900
C	2.66472900	-2.12507300	2.89041100
H	0.54169200	-1.79679300	2.87101400
C	3.83684500	-2.10126300	2.14013800
H	4.73279900	-1.74804900	0.21648100
H	2.68623300	-2.40406700	3.94104000
H	4.78794300	-2.35741900	2.60310400
P	-0.12375900	-0.80211200	0.16909100
O	-0.56387300	0.65842100	2.64784400
O	2.46997700	-1.09758400	-1.12153600
O	-2.14058300	-0.49837100	-1.91190600
C	-3.12493600	-0.09899800	-2.85333700

H	-3.96197600	-0.80830100	-2.87498000
H	-3.47292300	0.87479300	-2.50626700
H	-2.69634100	-0.00891600	-3.85948600
C	-0.73000400	1.67135300	3.62905200
H	0.10949800	2.35486700	3.49278200
H	-1.67407500	2.21062500	3.47896000
H	-0.70244600	1.25289100	4.64276800
C	3.66040800	-0.86600500	-1.86090800
H	4.27434600	-0.09624900	-1.37577500
H	4.24033700	-1.79042400	-1.97790900
H	3.33713300	-0.51038300	-2.84011500
Pd	-0.34892800	1.39346900	-0.36327700
O	-1.05070200	3.42805500	-0.83538900
O	-2.57533200	1.92952700	-0.25559700
C	-2.27012700	3.10036500	-0.63118800
C	-3.34964300	4.11183800	-0.88594900
H	-3.74774900	3.96601600	-1.89762800
H	-4.18062700	3.97988400	-0.18742400
H	-2.96625800	5.13324100	-0.82025600
C	1.60402000	1.74095200	-0.42473000
C	2.41842500	1.66614900	0.71041300
C	2.12952600	2.28396000	-1.60423800
C	3.73239000	2.13930300	0.66834500
H	2.03446500	1.22919900	1.63363500
C	3.44428400	2.75240900	-1.64242900
H	1.51177300	2.35070200	-2.50073000
C	4.25022100	2.68248500	-0.50637700
H	4.35294100	2.07721600	1.56258800
H	3.83879800	3.17017100	-2.56866200
H	5.27571800	3.04682600	-0.53748200

Pre-TS_{PE}(L6)

M06-L electronic energy (Hartree): -2749.175905

M06-L thermal correction to free energy (Hartree): 0.554784

Three lowest frequencies (cm⁻¹): 31.91, 36.66, 38.81

C	2.34851000	-1.10474500	1.41813700
C	1.63613200	-1.39195400	2.60113500
C	3.64188700	-1.61810200	1.27570800
C	2.24140200	-2.14431600	3.61428000
C	4.24799600	-2.36334700	2.28219700
H	4.17934300	-1.43291400	0.34471000
C	3.53898700	-2.61919600	3.45219300

H	1.69684700	-2.37027700	4.52667900
H	5.25701900	-2.74605700	2.14864800
H	3.99226500	-3.20390200	4.25059600
C	2.66703900	1.16964600	-0.36083800
C	3.78147400	1.50175400	0.41588600
C	2.28091200	2.06031200	-1.38845800
C	4.51945100	2.65765900	0.16994000
H	4.07158100	0.85007900	1.23708700
C	3.01311000	3.22413300	-1.63134200
C	4.13211900	3.51310900	-0.85670300
H	5.38590800	2.88867300	0.78529000
H	2.71079000	3.90562900	-2.42139200
H	4.69775400	4.42109200	-1.05809000
C	1.85678600	-1.43856300	-1.35866400
C	1.32845100	-2.74153400	-1.22173100
C	2.50450800	-1.10216300	-2.54717000
C	1.42623800	-3.65904000	-2.26848300
C	2.60926300	-2.01625200	-3.59416200
H	2.93445200	-0.10888200	-2.65622800
C	2.06000200	-3.28669900	-3.45261200
H	1.01000500	-4.65751900	-2.16538500
H	3.11970700	-1.73431700	-4.51235400
H	2.12950000	-4.00701900	-4.26580500
P	1.57522300	-0.25210700	-0.00209600
O	1.18874000	1.70467700	-2.10890900
O	0.75670300	-3.01418100	-0.02512900
O	0.36294800	-0.93798700	2.67833100
C	-0.42142100	-1.31871100	3.79532300
H	-0.01021300	-0.92065300	4.73182700
H	-1.40863900	-0.88660100	3.61848200
H	-0.50494300	-2.41136000	3.86774200
C	0.61449300	2.69119300	-2.95551900
H	-0.31531400	2.25633200	-3.32885500
H	0.38974500	3.59817800	-2.38271300
H	1.27494600	2.92219200	-3.80117600
C	0.18487800	-4.29326900	0.17659300
H	-0.63796300	-4.47436200	-0.52754000
H	0.93849500	-5.08578100	0.08131900
H	-0.20555600	-4.28045400	1.19715900
Pd	-0.51571000	0.62463900	0.31904500
O	-0.09760000	3.66848500	0.12111500
O	0.42659800	2.09717600	1.64912400
C	0.47841400	3.28728300	1.15809100
C	1.35125600	4.25185000	1.93936400

C	-4.36783000	0.67339800	-0.18593400
C	-3.55022000	0.93530600	0.94192000
C	-4.00216500	1.42419300	-1.27797200
C	-2.49682600	1.80954200	0.67691600
S	-2.64977900	2.42576900	-0.95933900
O	-5.39639700	-0.21659500	-0.16659200
C	-5.33871200	-1.06352800	0.99035900
O	-3.77055700	0.38445700	2.15354300
C	-5.05641900	-0.26312900	2.23484400
H	-4.41987200	1.35256600	-2.27559100
H	-6.31310700	-1.55226500	1.05608500
H	-4.56134100	-1.82468800	0.83797700
H	-5.01019100	-0.90462300	3.11684000
H	-2.01944900	2.43398400	1.42511700
H	1.20412100	4.13971700	3.01875000
H	2.40531600	4.02326600	1.73532800
H	1.16315000	5.28983300	1.64987500
H	-5.82475100	0.50575600	2.38843600
C	-1.36722800	-0.75940300	-0.85433100
C	-1.35222600	-0.61654400	-2.24678000
C	-2.07266600	-1.83854100	-0.30716200
C	-2.06008100	-1.49606600	-3.06867000
H	-0.77764000	0.19278500	-2.69834100
C	-2.77519700	-2.72478900	-1.12700300
H	-2.07181500	-2.00050800	0.77459000
C	-2.77905200	-2.55195900	-2.51092000
H	-2.04060700	-1.35857200	-4.15029200
H	-3.32199600	-3.55536500	-0.67734000
H	-3.32985200	-3.24148300	-3.14909600

TS_{PE}(L6)

M06-L electronic energy (Hartree): -2749.147385

M06-L thermal correction to free energy (Hartree): 0.549264

Three lowest frequencies (cm⁻¹): -819.07, 21.50, 26.35

C	2.17563300	0.04886300	1.93117200
C	1.41433800	0.78831200	2.86092900
C	3.30998900	-0.62642100	2.38750000
C	1.78749600	0.82858000	4.20778100
C	3.68892900	-0.58682200	3.72655500
H	3.90702200	-1.19627300	1.67621600
C	2.92142800	0.14097400	4.63121100
H	1.19900800	1.39491600	4.92420300

H	4.57660400	-1.12098800	4.05731200
H	3.20322000	0.17980500	5.68179100
C	2.51700400	1.48370100	-0.52638100
C	3.34144800	2.31399200	0.23406300
C	2.18968300	1.88250800	-1.84007600
C	3.83488200	3.51138800	-0.28248400
H	3.59057800	2.02499800	1.25399400
C	2.67209100	3.08325300	-2.36055100
C	3.49277300	3.89175600	-1.57581300
H	4.47684000	4.14278600	0.32733000
H	2.41321800	3.39024300	-3.37062200
H	3.86516100	4.82770000	-1.98823000
C	2.57626100	-1.40613800	-0.51898000
C	2.33250500	-2.69638300	0.00104200
C	3.42655200	-1.28151200	-1.61969000
C	2.92943400	-3.81714700	-0.57989700
C	4.01644300	-2.39754100	-2.20871500
H	3.62935000	-0.29259700	-2.02561300
C	3.76110300	-3.66131200	-1.68586400
H	2.74034500	-4.80997400	-0.18130700
H	4.67446400	-2.27637300	-3.06614800
H	4.21490000	-4.54266300	-2.13578800
P	1.67447800	0.01867900	0.17343400
O	1.39383900	1.02464300	-2.52986100
O	1.51208400	-2.74751000	1.07573200
O	0.34162000	1.44379800	2.35757000
C	-0.44394200	2.22788100	3.23891200
H	0.15571500	3.01662600	3.71124100
H	-1.21878900	2.67564900	2.61526800
H	-0.90903300	1.60790100	4.01675900
C	0.83063000	1.47141700	-3.75240600
H	0.11650000	0.70002900	-4.04853800
H	0.30695000	2.42778100	-3.62133800
H	1.59744500	1.58047700	-4.52991800
C	1.19053900	-4.02264200	1.60648600
H	0.70445900	-4.65308700	0.85168100
H	2.08646000	-4.52562500	1.99391500
H	0.49192600	-3.83532000	2.42335800
Pd	-0.61227100	0.26308200	-0.35105100
O	-2.21762500	2.95760300	-1.40376400
O	-0.34353100	2.49307000	-0.25160100
C	-1.10370800	3.28946600	-0.84345500
C	-0.72319500	4.73869500	-0.95168300
C	-4.80378600	-0.31945100	0.05408400

C	-3.58829800	0.38382800	0.27710600
C	-4.90014900	-0.78963600	-1.23148000
C	-2.71949400	0.46911900	-0.80700700
S	-3.49541500	-0.38060200	-2.13359900
O	-5.76037200	-0.49048500	1.01268400
C	-5.23534400	-0.24031500	2.32224700
O	-3.29114600	0.94073700	1.48604600
C	-4.43799200	1.03842200	2.34450900
H	-5.73215900	-1.32911400	-1.66965500
H	-6.09873900	-0.17812400	2.98851700
H	-4.60630500	-1.08873700	2.63041400
H	-4.04865700	1.24596700	3.34423800
H	-2.41166500	1.78860900	-1.16117700
H	0.14192400	4.96272000	-0.32364300
H	-0.47250100	4.97245400	-1.99297000
H	-1.56420400	5.38118900	-0.67391600
H	-5.06063400	1.88409700	2.02050100
C	-0.89109200	-1.70227100	-0.58244300
C	-0.35752200	-2.36033400	-1.69713400
C	-1.71256600	-2.42991600	0.28939600
C	-0.64290300	-3.70624200	-1.93925700
H	0.29779800	-1.82110700	-2.38499300
C	-1.99602000	-3.77487400	0.04938000
H	-2.14774000	-1.94012000	1.16280100
C	-1.46681100	-4.41864700	-1.06987200
H	-0.21386000	-4.19849300	-2.81305400
H	-2.63637700	-4.32261300	0.74196000
H	-1.69225500	-5.46723300	-1.25973400

Post-TS_{PE}(L6)

M06-L electronic energy (Hartree): -2749.155662

M06-L thermal correction to free energy (Hartree): 0.545390

Three lowest frequencies (cm⁻¹): 15.79, 19.96, 21.41

C	-2.31831300	-1.12638200	1.61876500
C	-1.46347700	-1.64104400	2.61505600
C	-3.69460000	-1.12526900	1.85664000
C	-1.98954800	-2.13061700	3.81430900
C	-4.22565100	-1.61470400	3.04712700
H	-4.36015600	-0.73034900	1.08928200
C	-3.36629500	-2.11423900	4.02167600
H	-1.33039800	-2.52522300	4.58241400
H	-5.30077600	-1.60494700	3.21000900

H	-3.76523800	-2.49940200	4.95828200
C	-1.67344600	-1.95782400	-1.04580800
C	-2.19023400	-3.18888700	-0.63911500
C	-1.08016000	-1.87085500	-2.32461600
C	-2.13696800	-4.30843300	-1.46943600
H	-2.64131800	-3.27368100	0.34825500
C	-1.02962400	-2.98482900	-3.16354200
C	-1.55843500	-4.19946000	-2.72870300
H	-2.54858700	-5.25622200	-1.13051600
H	-0.58024000	-2.91210100	-4.15002500
H	-1.51169900	-5.06377400	-3.38845800
C	-2.91651900	0.60255500	-0.59016500
C	-3.27620800	1.74267100	0.16086900
C	-3.50192100	0.42092100	-1.84469000
C	-4.19171700	2.66591200	-0.34822900
C	-4.40909600	1.34392400	-2.36141500
H	-3.24374200	-0.45924800	-2.43018200
C	-4.74639000	2.46496500	-1.60979600
H	-4.46458400	3.54455000	0.22935900
H	-4.85076100	1.18189600	-3.34191000
H	-5.45342600	3.19455600	-2.00047700
P	-1.60992000	-0.49455000	0.05543100
O	-0.57981300	-0.65156300	-2.65841200
O	-2.69017100	1.85353500	1.37699000
O	-0.14199800	-1.63467200	2.31975700
C	0.76850200	-2.15147000	3.27564700
H	0.56816800	-3.21091200	3.48186700
H	1.75555800	-2.04104300	2.82283700
H	0.72476100	-1.58425600	4.21452800
C	0.07853200	-0.51912800	-3.90903100
H	0.46757700	0.50088500	-3.93019600
H	0.91107500	-1.22853200	-3.99764300
H	-0.62110800	-0.66698600	-4.74156800
C	-2.95467000	3.02414700	2.13315600
H	-2.66131800	3.92471200	1.57906200
H	-4.01545800	3.08416500	2.41007400
H	-2.34507800	2.93931000	3.03408000
Pd	0.65772900	0.31312000	0.04298800
O	2.70173500	-1.46520500	-1.84607600
O	1.26358300	-1.90468600	-0.16973400
C	1.99100300	-2.28915800	-1.08400700
C	2.16898900	-3.72588500	-1.43903600
C	4.98384900	0.99704700	0.20679200
C	3.73395300	0.37427000	0.51114900

C	4.84638900	2.08244800	-0.61618900
C	2.61966200	0.94698700	-0.06839900
S	3.17527000	2.32406300	-0.98988800
O	6.18462100	0.53766000	0.67330800
C	6.02994300	-0.43173900	1.71530900
O	3.66929700	-0.74166400	1.31610600
C	4.92938800	-1.40910500	1.38567900
H	5.62731900	2.72681100	-1.00130800
H	6.99636500	-0.93469300	1.80534000
H	5.80607800	0.08071100	2.66278600
H	4.83110900	-2.16983200	2.16481500
H	2.59009300	-0.55075900	-1.46369500
H	1.38535400	-4.33056700	-0.97994500
H	2.15865400	-3.85838800	-2.52488600
H	3.14449200	-4.07246600	-1.07878000
H	5.13852800	-1.90734500	0.42503400
C	0.12832400	2.23751000	-0.00639000
C	-0.48228800	2.74243100	-1.16183100
C	0.39992200	3.12453800	1.04418200
C	-0.81351900	4.09591200	-1.26350900
H	-0.72142600	2.07098500	-1.98866500
C	0.06151500	4.47427900	0.94534300
H	0.89107200	2.76317900	1.94823200
C	-0.54313000	4.96818900	-0.21121500
H	-1.29291500	4.46476200	-2.17102100
H	0.27698500	5.14517100	1.77757200
H	-0.80063700	6.02342800	-0.29022200

Int_{PE}(L7)

M06-L electronic energy (Hartree): -1922.387875

M06-L thermal correction to free energy (Hartree): 0.328528

Three lowest frequencies (cm⁻¹): 4.28, 30.86, 33.72

Pd	0.18626600	1.55210700	0.10561900
O	0.64382400	3.69854600	0.17695200
O	2.32355300	2.26209200	0.05792800
C	1.89878100	3.45620500	0.12616800
C	2.85956000	4.60550300	0.17368900
H	2.51254200	5.42565300	-0.46193700
H	2.91433200	4.99343100	1.19752700
H	3.86219300	4.29774800	-0.13237900
C	-1.11263000	-1.58653800	-0.87621400
C	-2.37439700	-1.68670400	-0.28425700

C	-0.96715200	-2.11708900	-2.16460300
C	-3.45707800	-2.27710200	-0.91251400
C	-2.04210700	-2.70807000	-2.82079300
H	0.00064000	-2.07676000	-2.65861700
C	-3.28520700	-2.78594900	-2.19678800
H	-4.41154800	-2.32701300	-0.39535500
H	-1.90404000	-3.11442400	-3.81951100
H	-4.12682500	-3.24954700	-2.70608400
C	0.43235200	-1.58690900	1.55172200
C	-0.14545200	-2.84016900	1.79782500
C	1.23521500	-1.04790900	2.55935900
C	0.06253400	-3.50142200	3.00284600
H	-0.75899300	-3.30609600	1.02946700
C	1.45698900	-1.68514700	3.76909900
C	0.85972400	-2.92260200	3.98862100
H	-0.39598400	-4.47287000	3.16911100
H	2.09426900	-1.21338500	4.51196400
H	1.02536300	-3.43632000	4.93281800
C	1.73563700	-1.11993500	-0.95376400
C	1.98966300	-0.51320600	-2.18718400
C	2.71146400	-1.99530000	-0.45870100
C	3.14056300	-0.74594300	-2.91938600
C	3.87838500	-2.24445200	-1.17399400
H	2.55039900	-2.49004400	0.49724900
C	4.09205600	-1.62085400	-2.40134900
H	3.27575900	-0.24982200	-3.87654200
H	4.61973200	-2.93009500	-0.77174600
H	5.00216800	-1.81451900	-2.96431400
P	0.22368600	-0.69313300	-0.02358700
F	-2.53805300	-1.20095900	0.96329200
F	1.84867600	0.13434300	2.33958700
F	1.05803300	0.32284500	-2.70187400
C	-1.79962900	1.61530700	0.11003200
C	-2.56061700	1.35858800	-1.03392500
C	-2.43080100	2.09328400	1.26389000
C	-3.93977500	1.58000700	-1.02275000
H	-2.08717100	0.96858600	-1.93701500
C	-3.81029100	2.30553000	1.27144900
H	-1.85042200	2.29906200	2.16413100
C	-4.56817400	2.04581100	0.13013300
H	-4.52328900	1.37578100	-1.92036300
H	-4.29247700	2.67240000	2.17735400
H	-5.64478100	2.20753900	0.13983000

Pre-TS_{PE}(L7)

M06-L electronic energy (Hartree): -2703.308347

M06-L thermal correction to free energy (Hartree): 0.434869

Three lowest frequencies (cm⁻¹): 18.60, 27.36, 32.23

Pd	0.50558800	-0.62534500	0.20090500
O	0.08921400	-3.43987300	-0.86382500
O	-0.53059000	-2.37841600	1.02221300
C	-0.53536500	-3.38134500	0.21211200
C	-1.41598500	-4.54219800	0.63228100
C	4.35614400	-0.57359400	-0.23731000
C	3.51966100	-1.13063700	0.76128300
C	3.99496300	-0.97889100	-1.50042400
C	2.45245000	-1.87258000	0.24879400
S	2.62528100	-2.00512900	-1.49529300
O	5.40044900	0.24929900	0.04304900
C	5.34667000	0.72929900	1.39487500
O	3.73204600	-0.95376200	2.07930100
C	5.03128500	-0.38791100	2.35476500
H	4.43024300	-0.63664700	-2.43233000
H	6.33009800	1.15584800	1.60304200
H	4.58672200	1.51893400	1.46205100
H	4.98469500	-0.02675900	3.38356700
H	1.97765600	-2.69116700	0.78097700
H	-1.03294700	-5.48951700	0.24127800
H	-1.52256600	-4.60641100	1.71929300
H	-2.41947700	-4.39410300	0.21217400
H	5.77931300	-1.18779800	2.28545300
C	-1.77715800	1.87737800	-0.85049200
C	-1.26290300	3.05248100	-0.29758200
C	-2.34633800	1.96541300	-2.12565300
C	-1.27795300	4.26772900	-0.95815700
C	-2.37482000	3.17607800	-2.81246100
H	-2.77437600	1.07788400	-2.58603300
C	-1.83470900	4.32243400	-2.23374700
H	-0.85298800	5.14392600	-0.47528300
H	-2.82230800	3.22230800	-3.80233700
H	-1.85015400	5.26776800	-2.77147900
C	-2.41792300	0.67343900	1.63554500
C	-3.70002500	1.24655200	1.61803400
C	-1.83328200	0.45931000	2.88432400
C	-4.36989200	1.55540700	2.79498400
H	-4.17362900	1.44818400	0.65702000

C	-2.48261900	0.76042400	4.07347400
C	-3.75918000	1.30713700	4.02429900
H	-5.36445700	1.99230700	2.75309100
H	-1.97546500	0.57221600	5.01591500
H	-4.27470100	1.54794400	4.95127300
C	-2.62478700	-0.89179800	-0.78258700
C	-2.21655900	-1.39264500	-2.02170300
C	-3.77240000	-1.46238100	-0.21569300
C	-2.89812300	-2.38802100	-2.69982400
C	-4.47687600	-2.46453800	-0.87676400
H	-4.11224500	-1.12496500	0.76095200
C	-4.04187100	-2.92577900	-2.11772600
H	-2.52560200	-2.73053300	-3.66130400
H	-5.36562900	-2.88897700	-0.41578500
H	-4.58756800	-3.71165900	-2.63472300
P	-1.55506300	0.32006400	0.06811300
F	-0.72643200	2.99809600	0.94137100
F	-0.58276500	-0.03735000	2.96922400
F	-1.10358200	-0.87754200	-2.59363000
C	1.40348900	1.03440400	-0.48512600
C	1.43990400	1.31246900	-1.85659700
C	2.07437100	1.89538700	0.39032300
C	2.15977200	2.40483600	-2.34503600
H	0.90281800	0.67000500	-2.55516500
C	2.79227000	2.98993100	-0.09699700
H	2.04230200	1.71459200	1.46761400
C	2.84280900	3.24446300	-1.46692300
H	2.18069200	2.60106900	-3.41731400
H	3.31615000	3.64459600	0.60067000
H	3.40373700	4.09756200	-1.84559200

TS_{PE}(L7)

M06-L electronic energy (Hartree): -2703.280258

M06-L thermal correction to free energy (Hartree): 0.424653

Three lowest frequencies (cm⁻¹): -683.06, 9.17, 19.68

Pd	-0.54935900	0.44030600	-0.29213500
O	-1.92204000	3.40823400	-0.76782100
O	0.02064400	2.57899700	0.00254400
C	-0.71056400	3.53355700	-0.34644900
C	-0.16383900	4.93064400	-0.31601600
C	-4.77251700	0.02896500	-0.17629200
C	-3.55186300	0.60243900	0.27239000

C	-4.79805100	-0.13430000	-1.53892100
C	-2.61016600	0.88752300	-0.71310700
S	-3.32275000	0.39742200	-2.24168900
O	-5.79435900	-0.31117200	0.66147400
C	-5.33694500	-0.41825800	2.01507900
O	-3.31116700	0.84578000	1.59045500
C	-4.50161300	0.77818800	2.39251600
H	-5.61783100	-0.51805500	-2.13531300
H	-6.23393200	-0.48263300	2.63504500
H	-4.75448100	-1.34502900	2.13014500
H	-4.16224200	0.71501300	3.42872300
H	-2.21169800	2.24946800	-0.74809900
H	-0.91144100	5.63787100	0.05315200
H	0.73968100	4.98108300	0.29572900
H	0.09405500	5.23432700	-1.33749500
H	-5.07716800	1.70464200	2.25936100
C	2.41524000	-1.50472400	-0.78109900
C	2.09414100	-2.81334400	-0.41191600
C	3.21989100	-1.34423100	-1.91693200
C	2.53088300	-3.92436300	-1.11363500
C	3.66521100	-2.44386800	-2.64429400
H	3.50854700	-0.34446500	-2.23278400
C	3.31840300	-3.73305500	-2.24490200
H	2.24197900	-4.91497200	-0.77243000
H	4.28938900	-2.29094400	-3.52116700
H	3.66327500	-4.59545100	-2.81066600
C	2.16751300	-0.41154700	1.84932400
C	3.33965100	-1.11125600	2.17388000
C	1.38740500	0.04726800	2.91141700
C	3.70151100	-1.33823500	3.49610400
H	3.97322500	-1.48080100	1.36812100
C	1.72381600	-0.16915400	4.23966700
C	2.89061200	-0.86798900	4.52886600
H	4.61527100	-1.88259700	3.72073700
H	1.07285400	0.21074400	5.02217200
H	3.16576200	-1.04382200	5.56619200
C	2.72878900	1.32459400	-0.35526900
C	2.50911400	1.94449100	-1.58688000
C	3.66213500	1.92285100	0.49936200
C	3.17019600	3.09088200	-1.98943100
C	4.34107800	3.07914000	0.12241200
H	3.85286200	1.48089600	1.47535400
C	4.09593700	3.66156300	-1.11879100
H	2.95350200	3.52162900	-2.96317900

H	5.06251500	3.52463500	0.80288600
H	4.62309500	4.56533900	-1.41544600
P	1.68324900	-0.09710700	0.11875800
F	1.33371500	-3.00918000	0.68438800
F	0.25633400	0.74019700	2.65473400
F	1.60370500	1.39461800	-2.43211700
C	-1.07123400	-1.47938600	-0.50860900
C	-0.75555300	-2.20581300	-1.66197900
C	-1.80911300	-2.11134300	0.50069000
C	-1.15896500	-3.53620200	-1.79867100
H	-0.17647400	-1.73979000	-2.46232200
C	-2.21103600	-3.44083200	0.36424000
H	-2.07616000	-1.56030300	1.40458700
C	-1.88633200	-4.15915100	-0.78645100
H	-0.89540500	-4.08763300	-2.70166600
H	-2.78352500	-3.91494200	1.16220000
H	-2.20068300	-5.19617000	-0.89400700

Post-TS_{PE}(L7)

M06-L electronic energy (Hartree): -2703.288710

M06-L thermal correction to free energy (Hartree): 0.433671

Three lowest frequencies (cm⁻¹): 14.68, 20.67, 26.02

Pd	0.64233800	0.27141800	0.17204100
O	2.32630800	-1.81982700	-1.61095900
O	0.99535800	-1.99103700	0.19532700
C	1.64577900	-2.51600900	-0.71028000
C	1.73828500	-3.98922700	-0.90271000
C	5.01574300	0.68552900	0.11070600
C	3.75592000	0.10494900	0.45807700
C	4.88442700	1.83299500	-0.62262800
C	2.64024900	0.77582200	-0.00238500
S	3.21023600	2.18479200	-0.86566400
O	6.21788700	0.13594400	0.46076100
C	6.08219600	-0.88231600	1.45681900
O	3.68697000	-1.05612300	1.19575300
C	4.91459500	-1.78549900	1.14743600
H	5.67316900	2.46422700	-1.01400900
H	7.02504100	-1.43562400	1.45410500
H	5.94657700	-0.41539100	2.44370400
H	4.82480800	-2.58380100	1.88847100
H	2.29351200	-0.86262000	-1.33607700
H	2.77286300	-4.31711700	-0.75344900

H	1.08626200	-4.50844200	-0.19948900
H	1.46185400	-4.25233100	-1.92884900
H	5.03828200	-2.23762100	0.15005000
C	-2.87282200	0.84378200	-0.43799100
C	-3.15385700	1.86584500	0.47072700
C	-3.49192500	0.91156500	-1.69058100
C	-3.99881300	2.92249200	0.18276500
C	-4.34356400	1.96701900	-2.00881100
H	-3.30785700	0.12866400	-2.42387200
C	-4.59278000	2.97139200	-1.07614000
H	-4.17465500	3.68829900	0.93354000
H	-4.81549800	2.00075500	-2.98789500
H	-5.25441100	3.79826800	-1.32423800
C	-2.44143400	-1.19081400	1.47924000
C	-3.80591700	-1.52038800	1.44228400
C	-1.75442300	-1.45567100	2.66340800
C	-4.43773700	-2.10218900	2.53390900
H	-4.37233200	-1.31217000	0.53430300
C	-2.36296600	-2.03403900	3.76875600
C	-3.71249700	-2.35979400	3.69740300
H	-5.49440200	-2.35179500	2.47940600
H	-1.77567100	-2.21558000	4.66480900
H	-4.19940300	-2.81344500	4.55775100
C	-1.71929500	-1.68498400	-1.25466800
C	-1.16951000	-1.41843500	-2.51172200
C	-2.16222400	-2.99506200	-1.02751000
C	-1.07241600	-2.36425400	-3.51804500
C	-2.07377400	-3.96791400	-2.01961300
H	-2.57297600	-3.25817600	-0.05505400
C	-1.53447900	-3.65305400	-3.26459800
H	-0.63862800	-2.08479500	-4.47443600
H	-2.42623600	-4.97606400	-1.81530600
H	-1.46155100	-4.41075800	-4.04128300
P	-1.63248100	-0.39962400	0.04550200
F	-2.57547700	1.81319000	1.69138400
F	-0.44804800	-1.13389900	2.76547500
F	-0.69882600	-0.17190500	-2.76150200
C	0.21727900	2.22310100	0.09353000
C	-0.26301300	2.79568100	-1.09073700
C	0.39407000	3.04705600	1.21197900
C	-0.56709300	4.15721400	-1.15242600
H	-0.41643200	2.17607200	-1.97436100
C	0.07962600	4.40535000	1.15166200
H	0.78003700	2.62944000	2.14232700

C	-0.39879100	4.96735500	-0.03173700
H	-0.94213200	4.58167600	-2.08410100
H	0.21882600	5.02882100	2.03502600
H	-0.63719200	6.02884600	-0.07889600

Int_{PE}(L8)

M06-L electronic energy (Hartree): -1922.393225

M06-L thermal correction to free energy (Hartree): 0.327949

Three lowest frequencies (cm⁻¹): 18.47, 29.78, 34.83

Pd	-0.09589000	1.80470800	0.10256000
O	-0.43301900	3.98032100	0.19419100
O	-2.18148000	2.62251100	0.22621300
C	-1.69520100	3.79852600	0.24847900
C	-2.60808700	4.98496100	0.30803200
H	-2.86620000	5.29499600	-0.71144700
H	-3.53902100	4.73715800	0.82458800
H	-2.12158700	5.83167000	0.79908500
C	1.23511700	-1.46041800	-0.14402300
C	2.04126000	-1.35954400	-1.28896000
C	1.66194100	-2.25783100	0.92206200
C	3.24387700	-2.04556600	-1.37387100
C	2.87049600	-2.94502800	0.85462300
H	1.05468000	-2.34423100	1.82146600
C	3.63977200	-2.82449500	-0.29219700
H	3.21554900	-3.56742800	1.67539400
C	-1.25785000	-0.92304600	-1.48096300
C	-1.09055900	-2.16174900	-2.11454500
C	-2.24542500	-0.04223600	-1.94668800
C	-1.88973700	-2.51868800	-3.19488400
H	-0.32826300	-2.85689400	-1.76596100
C	-3.05286900	-0.38929200	-3.02296400
C	-2.85760800	-1.62349000	-3.62914300
H	-1.76987600	-3.47388000	-3.69855300
C	-1.16465600	-1.07029000	1.41138400
C	-1.05716800	-0.39024800	2.63190900
C	-1.92887400	-2.24294900	1.34625500
C	-1.68857900	-0.87187600	3.77255600
C	-2.57049400	-2.73319700	2.47688400
H	-2.02850300	-2.77966700	0.40327600
C	-2.43548600	-2.03720800	3.67177900
H	-3.17043000	-3.63842000	2.44318300
P	-0.26164800	-0.43450700	-0.03687500

H	-0.47463900	0.53052500	2.68640400
H	-2.37935800	0.92535000	-1.46121800
H	1.72752300	-0.73193200	-2.12308000
H	-1.61467600	-0.35661800	4.72608000
H	3.87620900	-1.98101500	-2.25501800
H	-3.81932800	0.28312500	-3.39867000
F	-3.63076300	-1.96167000	-4.67478000
F	4.81059800	-3.48158700	-0.36350300
F	-3.05616300	-2.50583300	4.76703200
C	1.89085500	1.69937500	0.04575100
C	2.66013500	1.20598300	1.10502900
C	2.53272500	2.26693000	-1.06001700
C	4.05253700	1.29520000	1.06468500
H	2.18034300	0.73592500	1.96520400
C	3.92711000	2.34420000	-1.10060200
H	1.94932300	2.65346600	-1.89668200
C	4.68940800	1.85885900	-0.03999900
H	4.63984400	0.91222500	1.89903400
H	4.41529100	2.78746700	-1.96824700
H	5.77587400	1.91706500	-0.07486500

Pre-TS_{PE}(L8)

M06-L electronic energy (Hartree): -2703.314348

M06-L thermal correction to free energy (Hartree): 0.433463

Three lowest frequencies (cm⁻¹): 16.80, 27.26, 33.36

Pd	0.62603000	-0.77654000	0.07721400
O	0.05622500	-3.52705800	-1.12704000
O	-0.47144700	-2.52205300	0.81722500
C	-0.56801700	-3.47008500	-0.05187800
C	-1.55587900	-4.55765000	0.32184100
C	4.45687200	-0.81976400	-0.30946900
C	3.58857500	-1.40675400	0.64541400
C	4.11970900	-1.16151300	-1.59698500
C	2.52533600	-2.11008900	0.07559400
S	2.73212700	-2.16292500	-1.66742700
O	5.50255600	-0.02199000	0.03130500
C	5.41493800	0.40947500	1.39818200
O	3.77101400	-1.28694400	1.97427100
C	5.06597500	-0.73975200	2.30621800
H	4.58076900	-0.78628400	-2.50331800
H	6.39620300	0.81790400	1.64865600
H	4.66009200	1.20395600	1.47438900

H	4.99255800	-0.41682500	3.34613500
H	2.00894000	-2.93326800	0.55920500
H	-1.56309200	-5.36618400	-0.41417000
H	-1.32748900	-4.97006700	1.31098500
H	-2.56262300	-4.12620700	0.38551700
H	5.81046200	-1.54209400	2.22830100
C	-1.47249300	1.94762700	-0.76332300
C	-0.97327500	3.10206800	-0.14222000
C	-1.91933500	2.02875300	-2.08702700
C	-0.92710300	4.31235400	-0.82007000
C	-1.87591200	3.23408000	-2.78055100
H	-2.30866000	1.14443800	-2.58952200
C	-1.37680000	4.35468400	-2.13371000
H	-2.22626900	3.31135600	-3.80624500
C	-1.90631500	0.71709800	1.79590100
C	-2.93744400	1.63277800	2.05432600
C	-1.28603200	0.06637100	2.87068800
C	-3.34922400	1.88811400	3.35630900
H	-3.42144100	2.15872000	1.23197500
C	-1.68711100	0.31289200	4.17895100
C	-2.71409000	1.22093400	4.39619800
H	-4.14546000	2.59486200	3.57245100
C	-2.63508800	-0.69830800	-0.65624600
C	-2.29103400	-1.42930700	-1.80236300
C	-3.93125600	-0.80975700	-0.14051600
C	-3.22332900	-2.24109000	-2.43660500
C	-4.87300800	-1.62533500	-0.75957800
H	-4.21552800	-0.26442800	0.75769800
C	-4.50144600	-2.32353200	-1.90003000
H	-5.88127400	-1.72663500	-0.36713100
P	-1.35172000	0.35065200	0.10314000
H	-1.27105500	-1.38250000	-2.18641400
H	-0.47985600	-0.64092800	2.67417200
H	-0.61215100	3.05724300	0.88443600
H	-2.96788700	-2.81642300	-3.32239300
H	-0.54182000	5.21310300	-0.34957400
H	-1.21228000	-0.18063200	5.02245100
F	-3.10525300	1.46994600	5.65743200
F	-1.33173000	5.52455900	-2.79675700
F	-5.40771600	-3.11482700	-2.50091300
C	1.58963000	0.89746200	-0.46074500
C	2.17569100	1.71857300	0.50927200
C	1.73320700	1.24549600	-1.80903300
C	2.91888200	2.84273100	0.13848200

H	2.06473100	1.47705700	1.56977100
C	2.47727400	2.36712400	-2.18006100
H	1.26434900	0.63393200	-2.58288900
C	3.07787200	3.16631900	-1.20775900
H	3.37779500	3.46359500	0.90882400
H	2.58461800	2.61820600	-3.23560400
H	3.65765700	4.04124100	-1.49700100

TS_{PE}(L8)

M06-L electronic energy (Hartree): -2703.285450

M06-L thermal correction to free energy (Hartree): 0.424409

Three lowest frequencies (cm⁻¹): -516.68, 8.67, 17.51

Pd	0.70427600	-0.53359400	-0.39909500
O	2.06832100	-3.52857300	-0.59173800
O	0.00354800	-2.66232800	-0.38055200
C	0.79126800	-3.63412000	-0.43970400
C	0.25507400	-5.02725700	-0.30025000
C	4.95179600	-0.14284400	-0.38165200
C	3.74596900	-0.68469700	0.14397400
C	4.92599800	-0.04862800	-1.74990700
C	2.76532500	-1.01129000	-0.78657400
S	3.42299600	-0.61493100	-2.36575200
O	6.00418800	0.23611100	0.40061900
C	5.58577700	0.43827000	1.75587000
O	3.55736300	-0.86521400	1.48149600
C	4.77024700	-0.73251500	2.24050200
H	5.72295800	0.30020800	-2.39670400
H	6.49970000	0.54999000	2.34357400
H	5.00003800	1.36776800	1.82080100
H	4.46074700	-0.59803700	3.27952900
H	2.34977200	-2.40096700	-0.67931800
H	0.95110900	-5.76819700	-0.69855300
H	0.09766400	-5.24135100	0.76336100
H	-0.71499800	-5.11368900	-0.79602000
H	5.34964300	-1.66233200	2.15678700
C	-1.96488200	1.82402000	-0.02242900
C	-1.43993800	2.72502000	0.91658200
C	-2.72683300	2.31933300	-1.08515200
C	-1.67450800	4.08788300	0.80634500
C	-2.96877500	3.68492700	-1.21099500
H	-3.13911900	1.63844100	-1.82831700
C	-2.43586800	4.54436900	-0.26218500

H	-3.56283700	4.08258800	-2.02964100
C	-1.97864900	-0.38424300	1.80121200
C	-3.03768400	0.25222800	2.46458700
C	-1.28324600	-1.40924500	2.45810200
C	-3.40566300	-0.12863900	3.74959400
H	-3.57857600	1.06172200	1.97596300
C	-1.64302900	-1.80409000	3.74176000
C	-2.70073900	-1.15486700	4.36394900
H	-4.22229300	0.35854300	4.27529000
C	-2.66873600	-0.78990100	-0.99272000
C	-2.24825400	-1.11176500	-2.28998100
C	-3.97773500	-1.10034200	-0.60507600
C	-3.11420500	-1.71987500	-3.19135800
C	-4.85372100	-1.71632800	-1.49165300
H	-4.32206400	-0.86580000	0.40156100
C	-4.40480900	-2.01234300	-2.77161300
H	-5.87079000	-1.96833500	-1.20416400
P	-1.49175700	0.06977000	0.10336800
H	-1.22329200	-0.88747700	-2.59138600
H	-0.45051400	-1.90219100	1.95558300
H	-0.83208900	2.35753800	1.74280400
H	-2.80104200	-1.97669600	-4.19965600
H	-1.26817800	4.79487300	1.52458700
H	-1.11231500	-2.59593200	4.26342000
F	-3.04966400	-1.52709200	5.60770100
F	-2.66176100	5.86639400	-0.37957500
F	-5.24724200	-2.61169900	-3.63145900
C	1.27726100	1.38679100	-0.42427800
C	1.94875200	1.96373100	0.65969200
C	0.98213800	2.19093400	-1.53237800
C	2.30001900	3.31602900	0.64278700
H	2.20361300	1.35715500	1.52978300
C	1.33638800	3.54095700	-1.55006400
H	0.44723300	1.76848600	-2.38572900
C	1.99427600	4.11020600	-0.46068200
H	2.81909100	3.74697800	1.49976700
H	1.08498400	4.15110600	-2.41797800
H	2.26583200	5.16461000	-0.47186900

Post-TS_{PE}(L8)

M06-L electronic energy (Hartree): -2703.292602

M06-L thermal correction to free energy (Hartree): 0.427277

Three lowest frequencies (cm⁻¹): 12.23, 16.68, 25.65

Pd	0.78823600	0.34214200	0.05624800
O	2.64849900	-1.68428200	-1.66580800
O	1.25173100	-1.88577400	0.08754500
C	1.95534000	-2.39413900	-0.78765000
C	2.11107700	-3.86555600	-0.94713100
C	5.14669500	0.99089300	0.10086900
C	3.91473900	0.31722900	0.36905100
C	4.96547700	2.17448700	-0.56163700
C	2.77189400	0.94666500	-0.08581100
S	3.28008100	2.44196100	-0.83390300
O	6.36967500	0.49023300	0.45138600
C	6.26969900	-0.61007200	1.36167600
O	3.89546900	-0.89276900	1.02864500
C	5.16268000	-1.54875200	0.95360100
H	5.72482200	2.87464400	-0.88816600
H	7.24256100	-1.10814600	1.34119800
H	6.08584500	-0.23038600	2.37767700
H	5.10387500	-2.40684700	1.62816400
H	2.57788100	-0.72603900	-1.40203700
H	2.22130500	-4.13794500	-1.99960800
H	3.02082600	-4.18669200	-0.42589400
H	1.25931300	-4.38597700	-0.50554200
H	5.32929000	-1.91291200	-0.07297700
C	-2.74248300	0.83790700	-0.43660500
C	-3.09538400	1.86215500	0.45481100
C	-3.28048600	0.84764000	-1.72771400
C	-3.97274600	2.86833500	0.07351600
C	-4.15688300	1.85307000	-2.12656200
H	-3.02007300	0.06317100	-2.43655000
C	-4.48562900	2.84696400	-1.21707900
H	-4.58552300	1.86877600	-3.12484800
C	-2.03766800	-0.95341700	1.69340100
C	-3.39690300	-1.09192100	2.00986200
C	-1.07621700	-1.29367700	2.65462000
C	-3.79123000	-1.56671100	3.25502800
H	-4.15726000	-0.82065400	1.27817600
C	-1.45490900	-1.77287900	3.90394400
C	-2.80924100	-1.90037900	4.17941700
H	-4.83990800	-1.67807200	3.51626500
C	-1.65391800	-1.76906400	-1.07140900
C	-0.96074500	-1.71363800	-2.29038700
C	-2.40111600	-2.91223100	-0.76896800
C	-1.01937300	-2.76501600	-3.19688300

C	-2.46344300	-3.97806500	-1.66209100
H	-2.93599600	-2.98339000	0.17669500
C	-1.77160000	-3.88373000	-2.86107200
H	-3.03565800	-4.87392500	-1.43731900
P	-1.46696500	-0.35787700	0.07154500
H	-0.35434100	-0.83614900	-2.52625100
H	-0.01777500	-1.17650000	2.41882800
H	-2.67415700	1.87962200	1.45934500
H	-0.48530800	-2.73324400	-4.14259700
H	-4.25165800	3.66740500	0.75521400
H	-0.72107800	-2.03727000	4.66014000
F	-3.18594200	-2.35640200	5.38649200
F	-5.33237500	3.82306900	-1.59580400
F	-1.82436600	-4.91306600	-3.72488300
C	0.23635100	2.26037100	0.04653600
C	0.13248000	2.98203400	1.24150100
C	-0.09566500	2.89767800	-1.15544100
C	-0.29967300	4.31022100	1.23365000
H	0.38745700	2.50807500	2.19066200
C	-0.52386100	4.22622000	-1.16148400
H	-0.02830900	2.35342400	-2.09940800
C	-0.62740300	4.93760100	0.03293400
H	-0.37651600	4.85607300	2.17405800
H	-0.78056800	4.70465700	-2.10681400
H	-0.96269500	5.97352500	0.02812200

Int_{PE}(L9)

M06-L electronic energy (Hartree): -1922.391059

M06-L thermal correction to free energy (Hartree): 0.327321

Three lowest frequencies (cm⁻¹): 18.80, 26.95, 31.10

Pd	-0.40352700	1.60030300	-0.02240000
O	-1.09336500	3.68330100	-0.13727800
O	-2.59939300	2.06076500	-0.14682200
C	-2.31038900	3.29929600	-0.18237400
C	-3.40118400	4.32400400	-0.24551300
H	-3.64915900	4.65135100	0.77112300
H	-3.07818600	5.20642700	-0.80430000
H	-4.30716600	3.90824500	-0.69358400
C	1.50396300	-1.35992500	0.20083500
C	2.43895300	-1.11757500	-0.81338800
C	1.89294600	-2.04125200	1.35757700
C	3.73983500	-1.55357500	-0.63898800

C	3.21054400	-2.47649000	1.49890400
H	1.17449400	-2.22850900	2.15287400
C	4.14873600	-2.23395600	0.50202500
H	3.50944800	-3.00933800	2.39869600
H	5.18211200	-2.55628200	0.59654400
C	-0.83304600	-1.39926200	-1.49636900
C	-0.31759800	-2.58585400	-2.03078700
C	-1.93798000	-0.78265800	-2.09610800
C	-0.90513700	-3.15134100	-3.16054200
H	0.53962800	-3.06873500	-1.56560900
C	-2.50250600	-1.37532000	-3.21427300
C	-2.00537200	-2.55000800	-3.76362700
H	-0.50322800	-4.07280800	-3.57547700
H	-2.47644800	-2.97516200	-4.64579100
C	-1.13667300	-1.36077100	1.37261900
C	-1.35912500	-0.59448800	2.52115600
C	-1.62965900	-2.66911400	1.29835200
C	-2.06352700	-1.16022800	3.57374000
C	-2.33649500	-3.20654000	2.37060600
H	-1.46056600	-3.26729800	0.40428600
C	-2.56033100	-2.45474200	3.52129800
H	-2.72016200	-4.22249600	2.31194800
H	-3.11311300	-2.85505700	4.36685900
P	-0.15470300	-0.63515200	0.01578300
H	-0.99676700	0.43040300	2.59522400
H	-2.35107000	0.14615200	-1.70256400
H	2.17317900	-0.57067400	-1.71588100
F	4.64341900	-1.29593000	-1.60322700
F	-3.56585900	-0.78613900	-3.79184600
F	-2.27455900	-0.42263400	4.67898900
C	1.57239700	1.82599300	0.07872600
C	2.28667200	1.63014000	1.26479700
C	2.24383800	2.27845400	-1.06150100
C	3.65765100	1.88903800	1.30898100
H	1.78414600	1.25486300	2.15775000
C	3.61791300	2.52657400	-1.01396000
H	1.70299700	2.43006300	-1.99655200
C	4.32761000	2.32964300	0.16872300
H	4.20375800	1.73190600	2.23900300
H	4.13234100	2.87205700	-1.91040200
H	5.39941700	2.51776400	0.20158400

Pre-TS_{PE}(L9)

M06-L electronic energy (Hartree): -2703.313009

M06-L thermal correction to free energy (Hartree): 0.433247

Three lowest frequencies (cm⁻¹): 15.32, 26.30, 29.55

Pd	0.45588600	-0.78543300	0.00376600
O	-0.25086600	-3.53685600	-1.11834600
O	-0.69435500	-2.46403500	0.81013700
C	-0.83122000	-3.44046400	-0.02093500
C	-1.81012400	-4.50844800	0.42574900
C	4.26879000	-0.97989500	-0.40792400
C	3.38460500	-1.52011700	0.55935400
C	3.91287000	-1.32931700	-1.68857600
C	2.29318100	-2.19344300	0.00534000
S	2.49062400	-2.28172000	-1.73746600
O	5.34232400	-0.21299100	-0.08457500
C	5.27871000	0.24152600	1.27648800
O	3.57603500	-1.38581100	1.88487600
C	4.89103700	-0.87962600	2.20384700
H	4.38279100	-0.98520600	-2.60269300
H	6.27687600	0.61403200	1.51609200
H	4.55739800	1.06757500	1.34449600
H	4.83268800	-0.53763000	3.23856400
H	1.75572300	-2.99313400	0.50527200
H	-1.87877300	-5.32177300	-0.30198500
H	-1.51993900	-4.91939300	1.39929200
H	-2.80411100	-4.06228000	0.55744600
H	5.60555400	-1.70967400	2.13708500
C	-1.50971800	2.00849200	-0.90755800
C	-0.84517800	3.15978300	-0.46688700
C	-2.09457600	1.99072400	-2.17817300
C	-0.78321000	4.25791400	-1.30767700
C	-2.01509300	3.11297900	-3.00043400
H	-2.61228500	1.10073300	-2.53062500
C	-1.35395300	4.26012100	-2.57348700
H	-2.47448300	3.09418100	-3.98623200
H	-1.27858600	5.14511700	-3.19914600
C	-1.79632700	1.02669400	1.80191300
C	-2.60484000	2.13507600	2.08577900
C	-1.27571600	0.25753100	2.84883600
C	-2.88947300	2.46823500	3.40813300
H	-3.00933800	2.73841100	1.27500600
C	-1.58272500	0.61226800	4.15320300
C	-2.38007000	1.70744200	4.45659200
H	-3.51490600	3.33052300	3.62716800

H	-2.58901200	1.95255000	5.49435200
C	-2.87129600	-0.49158100	-0.42913800
C	-2.67565000	-1.41491600	-1.46131000
C	-4.13382600	-0.35655300	0.15680700
C	-3.74801400	-2.18508800	-1.88058000
C	-5.19386700	-1.14297400	-0.29055800
H	-4.29061000	0.35323000	0.96705000
C	-5.01070200	-2.06798200	-1.31488600
H	-6.17485000	-1.03925300	0.16754600
H	-5.82250900	-2.69856800	-1.66745600
P	-1.42698100	0.49223500	0.09922200
H	-1.69021200	-1.57042900	-1.89909900
H	-0.64215100	-0.60590000	2.64950200
H	-0.35935600	3.20391300	0.50565700
F	-0.13689600	5.36046000	-0.88196100
F	-1.08027600	-0.12680500	5.15987900
F	-3.54726600	-3.09450700	-2.85360900
C	1.48522300	0.83591300	-0.57479700
C	2.10324200	1.65276800	0.37847800
C	1.61821800	1.16251000	-1.92906800
C	2.85958000	2.76013100	-0.01524700
H	1.99971400	1.42652600	1.44307900
C	2.37640100	2.26659200	-2.32227500
H	1.12583000	0.55226300	-2.68879100
C	3.00084400	3.06786600	-1.36691200
H	3.33999400	3.38129200	0.74150300
H	2.47284200	2.50502500	-3.38175300
H	3.58778000	3.93200900	-1.67352200

TS_{PE}(L9)

M06-L electronic energy (Hartree): -2703.284159

M06-L thermal correction to free energy (Hartree): 0.425760

Three lowest frequencies (cm⁻¹): -496.34, 10.95, 19.10

Pd	0.49442800	-0.61546500	-0.39173800
O	1.78780400	-3.64674100	-0.32520200
O	-0.22231500	-2.69329600	0.00958200
C	0.53163400	-3.69144800	-0.02832100
C	-0.00672900	-5.05217100	0.29702900
C	4.71456100	-0.26639100	-0.52500800
C	3.51897600	-0.74958900	0.07400900
C	4.66765800	-0.32437700	-1.89503400
C	2.52701100	-1.17981800	-0.80085000

S	3.15705100	-0.95640500	-2.42295800
O	5.77851800	0.19551100	0.19432500
C	5.39189400	0.52440600	1.53455800
O	3.34766600	-0.77611900	1.42536000
C	4.57623000	-0.58702200	2.14422600
H	5.45531800	-0.05158700	-2.58840800
H	6.32044300	0.68038600	2.08875900
H	4.81552300	1.46191700	1.52746200
H	4.29013000	-0.35029400	3.17150900
H	2.08960800	-2.54524000	-0.54133400
H	0.31490500	-5.77983300	-0.45378200
H	0.39926300	-5.38450400	1.25897400
H	-1.09628200	-5.03646200	0.35934900
H	5.14512800	-1.52721400	2.13864500
C	-2.12784800	1.79125000	-0.49441200
C	-1.59139300	2.93213400	0.11505300
C	-2.89020500	1.92432200	-1.65964200
C	-1.82064900	4.16923700	-0.46188800
C	-3.10987300	3.18533100	-2.21144400
H	-3.31344500	1.04435800	-2.14060700
C	-2.57275800	4.32367800	-1.61868800
H	-3.70763500	3.28208300	-3.11510300
H	-2.72476900	5.31465800	-2.03719800
C	-1.87645900	0.29169800	1.94595900
C	-2.90916900	1.05566600	2.50696300
C	-0.99385700	-0.40107300	2.78220800
C	-3.06107000	1.11604800	3.88945400
H	-3.58849100	1.61074700	1.86180000
C	-1.17039200	-0.31974800	4.15533500
C	-2.18974300	0.42648500	4.72892500
H	-3.86378200	1.70910000	4.32175000
H	-2.28664500	0.46647700	5.81026200
C	-2.93601600	-0.98123200	-0.45399700
C	-2.71626800	-1.59700600	-1.69194700
C	-4.10670400	-1.25757500	0.25920500
C	-3.67715600	-2.46081400	-2.19161100
C	-5.05064000	-2.13877900	-0.26541900
H	-4.28090300	-0.79509000	1.22874300
C	-4.84576600	-2.74845500	-1.49982900
H	-5.95719000	-2.35657200	0.29492100
H	-5.56750700	-3.44222600	-1.92236100
P	-1.63444600	0.15442700	0.14269600
H	-1.79725800	-1.42404900	-2.25193900
H	-0.17363800	-0.99052200	2.37156000

H	-0.97098200	2.86796300	1.00659700
F	-1.28245600	5.26095500	0.11650900
F	-0.31519700	-0.98076700	4.95813700
F	-3.45962500	-3.05358800	-3.38116700
C	1.12635500	1.26473800	-0.67146900
C	1.72661600	1.97214300	0.37665600
C	0.95930000	1.90556200	-1.90503700
C	2.13407900	3.29668600	0.20036000
H	1.88498900	1.48780100	1.34215100
C	1.36979500	3.22807600	-2.08092800
H	0.48863700	1.37777800	-2.73662800
C	1.95429600	3.93068000	-1.02777800
H	2.59790900	3.83141800	1.02977100
H	1.22623200	3.71180600	-3.04749000
H	2.26847600	4.96448800	-1.16421200

Post-TS_{PE}(L9)

M06-L electronic energy (Hartree): -2703.291699

M06-L thermal correction to free energy (Hartree): 0.431892

Three lowest frequencies (cm⁻¹): 9.03, 15.46, 27.70

Pd	0.65324700	0.32044600	-0.02988100
O	2.67929500	-1.68539700	-1.57502300
O	1.28619500	-1.84546400	0.18492700
C	2.03588500	-2.37005900	-0.64123200
C	2.30502100	-3.83281400	-0.67393800
C	4.93294900	1.33319000	0.01486300
C	3.75513500	0.58297700	0.32159800
C	4.67388600	2.42213200	-0.77191500
C	2.57911800	1.06394000	-0.22116600
S	2.98120500	2.51394800	-1.10908300
O	6.18066500	0.98090000	0.44868500
C	6.13882800	-0.01330400	1.47823000
O	3.81523200	-0.55201100	1.10043300
C	5.13790700	-1.09083400	1.14753900
H	5.38185600	3.14766900	-1.15371700
H	7.15163300	-0.41852700	1.54782900
H	5.87906000	0.46141900	2.43595600
H	5.12456900	-1.86610700	1.91788600
H	2.52672500	-0.71699900	-1.39611100
H	2.42815700	-4.18677700	-1.70076400
H	3.24159600	-4.03594500	-0.14072200
H	1.49850400	-4.37520800	-0.17732400

H	5.38373900	-1.55493200	0.17904800
C	-2.90408700	0.48855100	-0.56974800
C	-3.29563900	1.59238300	0.19778100
C	-3.45204300	0.30113900	-1.84264100
C	-4.21434800	2.48234800	-0.33052000
C	-4.38176600	1.21145100	-2.34342900
H	-3.15769900	-0.55589700	-2.44521700
C	-4.77080900	2.31599500	-1.59217900
H	-4.81003100	1.05790400	-3.33150500
H	-5.48882500	3.04013000	-1.96737600
C	-2.08539800	-0.98380200	1.75670300
C	-3.42822500	-1.21403800	2.08485300
C	-1.10041100	-1.08846500	2.74500600
C	-3.77811600	-1.55491100	3.38851700
H	-4.19908300	-1.12017600	1.32142600
C	-1.48076400	-1.42869300	4.03468600
C	-2.80379500	-1.66602600	4.37820200
H	-4.82061200	-1.73451800	3.64139000
H	-3.05779800	-1.92319400	5.40283700
C	-1.62830700	-2.09617300	-0.89746100
C	-0.93983000	-2.10623600	-2.11788900
C	-2.27344800	-3.25589900	-0.45881200
C	-0.92493700	-3.26807800	-2.87227100
C	-2.23429400	-4.41277900	-1.23716200
H	-2.80190700	-3.26257700	0.49249100
C	-1.55845600	-4.43065700	-2.45290500
H	-2.73452700	-5.31425800	-0.89013300
H	-1.51277700	-5.32398500	-3.06952400
P	-1.54719800	-0.54762900	0.07015200
H	-0.40326400	-1.22440800	-2.47105800
H	-0.05177300	-0.89753500	2.51684900
H	-2.87603700	1.78033400	1.18411900
F	-4.57426500	3.55205400	0.40471300
F	-0.53308100	-1.51796100	4.98660900
F	-0.25815200	-3.27357200	-4.04193300
C	-0.04458500	2.18283600	-0.19450200
C	-0.20467300	2.98546000	0.94105300
C	-0.45592100	2.68252800	-1.43610800
C	-0.78423300	4.25237400	0.83866100
H	0.11599200	2.62134300	1.91842200
C	-1.03035000	3.95099400	-1.53685000
H	-0.34377700	2.07337200	-2.33508300
C	-1.20102000	4.73851200	-0.39940700
H	-0.90820900	4.86104400	1.73446000

H	-1.35158800	4.32067200	-2.51088700
H	-1.65586500	5.72471800	-0.47775500

Int_{PE}(L10)

M06-L electronic energy (Hartree): -3647.248736

M06-L thermal correction to free energy (Hartree): 0.355628

Three lowest frequencies (cm⁻¹): 7.89, 22.08, 23.60

Pd	-0.45788800	-1.05709200	-2.37866000
O	-0.98198500	-2.01047300	-4.28022800
O	-2.41623800	-2.12045500	-2.60112100
C	-2.10380900	-2.39296600	-3.80396000
C	-3.06183800	-3.13477700	-4.68253600
H	-3.72543400	-3.77006100	-4.09078300
H	-3.68461400	-2.41432300	-5.22589300
H	-2.52967400	-3.73571500	-5.42468300
C	0.51775200	1.47043600	-0.16574100
C	1.90408900	1.64590700	-0.28660700
C	-0.30568300	2.58802300	-0.05087500
C	2.44481200	2.92292400	-0.28962600
H	2.56293700	0.78559900	-0.39285900
C	0.25017000	3.86916700	-0.05550800
H	-1.38481200	2.47508000	0.04538300
C	1.62065800	4.04365400	-0.17837300
H	2.04782800	5.04329300	-0.18405000
C	0.89285700	-1.23454600	0.72893000
C	1.53598300	-0.74486100	1.86850700
C	1.07951500	-2.56837300	0.36088200
C	2.34312500	-1.58741900	2.62944700
H	1.42465300	0.29779600	2.16543100
C	1.89890600	-3.39907200	1.11949900
H	0.59398700	-2.94942800	-0.53956600
C	2.53265600	-2.91523700	2.25940300
H	3.17474100	-3.56215700	2.84919200
C	-1.78542200	-0.10197600	0.55836900
C	-2.95089100	-0.05983100	-0.20908100
C	-1.87711100	-0.03932400	1.95122400
C	-4.19326900	0.04859900	0.41124600
H	-2.88824700	-0.12730300	-1.29490600
C	-3.12428200	0.06690400	2.56060300
H	-0.98249500	-0.07074900	2.57201600
C	-4.28769400	0.11103700	1.79636500
H	-5.25653000	0.19470900	2.27908300

P	-0.18689800	-0.20576300	-0.32152300
C	2.08119500	-4.81572900	0.66550000
C	3.02877600	-1.01224000	3.83246200
C	-3.18477300	0.11242200	4.05832500
C	-5.41578600	0.09205500	-0.45486600
C	-0.67105900	5.04521400	0.06234800
C	3.92215400	3.13713100	-0.42905000
F	4.21089000	3.85117700	-1.53879800
F	4.41428100	3.83629400	0.61576200
F	4.60612900	1.98382700	-0.50407400
F	-0.00376700	6.20582900	0.18180300
F	-1.47578800	5.15074900	-1.01677300
F	-1.48227700	4.92619800	1.13396800
F	2.15346700	-0.37030800	4.63292700
F	3.64381900	-1.94927200	4.57186400
F	3.95978200	-0.10375600	3.47294300
F	3.00567900	-5.47214500	1.38599000
F	2.46129600	-4.86366200	-0.62907700
F	0.92847800	-5.51124200	0.75181000
F	-6.54860200	0.18620200	0.26175900
F	-5.37984300	1.14591000	-1.29774100
F	-5.51111900	-1.01115000	-1.22649700
F	-4.42409200	0.36816600	4.51116000
F	-2.36434400	1.06213000	4.55357100
F	-2.78962100	-1.05761300	4.60137000
C	1.34849400	-0.30383200	-2.77639300
C	2.51955600	-1.01920100	-2.50965500
C	1.42518500	0.94437300	-3.40287000
C	3.75948500	-0.48549000	-2.87320000
H	2.47881300	-1.99055600	-2.01360800
C	2.66647400	1.46969300	-3.76397900
H	0.51979300	1.52202500	-3.59271400
C	3.83504100	0.76044400	-3.49235700
H	4.66810400	-1.04541100	-2.65527500
H	2.71839000	2.44723000	-4.24276000
H	4.80375700	1.18540500	-3.75027700

Pre-TS_{PE}(L10)

M06-L electronic energy (Hartree): -4428.170998

M06-L thermal correction to free energy (Hartree): 0.449300

Three lowest frequencies (cm⁻¹): 8.43, 9.44, 11.69

Pd 1.09027000 -0.68282700 -1.52131600

O	-0.50447600	-2.50802100	-3.21508100
O	0.37159100	-2.72196100	-1.15791800
C	-0.34687900	-3.13227400	-2.14793300
C	-1.05626000	-4.44963200	-1.91722600
C	4.61481100	-0.76257100	-2.11291000
C	3.58916900	-1.73908000	-1.97216400
C	4.49643100	-0.04229600	-3.27380600
C	2.61399200	-1.65848800	-2.97514500
S	3.12614800	-0.50625600	-4.19015600
O	5.58697300	-0.57803400	-1.18150700
C	5.28048500	-1.27419800	0.03602600
O	3.60044200	-2.67807600	-1.00448100
C	4.83721600	-2.68152400	-0.25852800
H	5.11530200	0.79118400	-3.58381100
H	6.19497700	-1.26218300	0.63232000
H	4.49281500	-0.72941800	0.57941500
H	4.63092300	-3.24053400	0.65380900
H	1.95998800	-2.47015700	-3.27806100
H	-1.44244700	-4.86469700	-2.85166500
H	-0.39988900	-5.17742700	-1.42978800
H	-1.90633600	-4.28356500	-1.24180000
H	5.59647100	-3.21286700	-0.84632300
C	-0.76553400	1.80404000	0.18941900
C	0.18717600	2.67996400	0.72997400
C	-1.91600100	2.32517500	-0.39662400
C	-0.01196000	4.05059100	0.66436600
H	1.09554000	2.29312800	1.18576100
C	-2.11020200	3.70722500	-0.45072500
H	-2.66983500	1.66485300	-0.82337400
C	-1.16155900	4.57463600	0.06972400
H	-1.31077600	5.64981200	0.01524000
C	0.25571000	-0.40786700	1.73277600
C	-0.21920800	0.20480300	2.89877000
C	1.23680800	-1.39705700	1.82389600
C	0.28402300	-0.17954000	4.13685900
H	-0.97596600	0.98523000	2.84599100
C	1.73141700	-1.77519800	3.07040300
H	1.60728900	-1.87679200	0.91676100
C	1.26098100	-1.16985300	4.22933000
H	1.65116100	-1.46477100	5.20070600
C	-1.96653900	-0.81280400	-0.11086600
C	-2.44563100	-0.98529600	-1.41272900
C	-2.69705500	-1.31548600	0.96749000
C	-3.64551000	-1.65429400	-1.63077000

H	-1.86053300	-0.63239100	-2.26024300
C	-3.89901100	-1.98014600	0.73835000
H	-2.33464000	-1.20417600	1.98679200
C	-4.37727700	-2.15412900	-0.55770300
H	-5.31120300	-2.68532100	-0.72978000
P	-0.35865800	0.03110200	0.07292700
C	2.82548700	-2.79572000	3.13938100
C	-0.20970300	0.45190700	5.40441800
C	-4.71722400	-2.50631800	1.87892000
C	-4.11942300	-1.92520800	-3.02661800
C	-3.35570900	4.22153400	-1.10547900
C	0.99531100	5.00420000	1.23183500
F	1.37862700	5.91799900	0.31570300
F	0.48146500	5.69780900	2.27143800
F	2.10273700	4.38233600	1.67306400
F	-3.40346400	3.87074700	-2.40926700
F	-4.46264700	3.70596100	-0.53041800
F	-3.45374100	5.56060300	-1.04539300
F	-0.77924700	-0.46376900	6.21537200
F	0.80394400	1.00609300	6.10131900
F	-1.11975800	1.41412500	5.17739100
F	2.86519100	-3.42376100	4.32506700
F	4.04039100	-2.22433300	2.95240400
F	2.69282900	-3.73390600	2.17834400
F	-5.45217500	-1.74783500	-3.14011000
F	-3.52448200	-1.13008700	-3.93226100
F	-3.86863800	-3.20291000	-3.38573900
F	-5.07618100	-3.79074000	1.67631600
F	-5.86219600	-1.80528100	2.02357500
F	-4.06054400	-2.44792800	3.05068400
C	1.71619900	1.21410200	-1.73503800
C	2.80360200	1.71466500	-1.01208000
C	1.03108700	2.06985900	-2.60527200
C	3.21524700	3.04032000	-1.17447900
H	3.33499200	1.07436500	-0.30494400
C	1.44423500	3.39226800	-2.77006000
H	0.16152600	1.70625500	-3.15721500
C	2.53710000	3.88125300	-2.05351300
H	4.05879800	3.41718400	-0.59656600
H	0.90288500	4.04508200	-3.45463000
H	2.84802100	4.91805300	-2.16862600

TS_{PE}(L10)

M06-L electronic energy (Hartree): -4428.144673

M06-L thermal correction to free energy (Hartree): 0.444443

Three lowest frequencies (cm^{-1}): -661.84, 1.38, 7.93

Pd	1.31504100	-1.16358700	-0.93156900
O	2.31556900	-4.31287400	-1.01339500
O	0.55622600	-3.13747100	-0.25528900
C	1.13897100	-4.22077600	-0.49949000
C	0.42229300	-5.50785700	-0.21882500
C	5.52212800	-1.20630400	-1.16965100
C	4.28315100	-1.55523000	-0.56728600
C	5.47079100	-1.28419700	-2.53950700
C	3.25722000	-1.90934200	-1.44202800
S	3.90762000	-1.76500300	-3.06608400
O	6.62828700	-0.84374200	-0.46032000
C	6.29199200	-0.48934900	0.88738700
O	4.10810000	-1.53367600	0.78412300
C	5.36091100	-1.50761800	1.49235800
H	6.28302600	-1.10351800	-3.23417400
H	7.23681200	-0.44581300	1.43385300
H	5.82661600	0.50789000	0.89624400
H	5.11710900	-1.25985500	2.52620400
H	2.72734700	-3.21415200	-1.21194700
H	-0.19838000	-5.76083800	-1.08692700
H	1.12089500	-6.33049500	-0.05174900
H	-0.24687000	-5.39484200	0.63797400
H	5.81125000	-2.50895500	1.45717400
C	-1.33660500	1.25625100	-1.02843100
C	-0.69806300	2.50237300	-1.11501700
C	-2.50206700	1.03670900	-1.75969200
C	-1.23741600	3.50717000	-1.90689100
H	0.22466200	2.68790100	-0.56653100
C	-3.02862800	2.04974600	-2.56299100
H	-3.01676800	0.07797300	-1.70696100
C	-2.40417200	3.28662500	-2.63959800
H	-2.82257600	4.07627500	-3.25787200
C	-0.06704300	0.75683400	1.48354200
C	-0.82632500	1.77248200	2.07118000
C	1.13708300	0.37754200	2.08096600
C	-0.38774700	2.38519600	3.24362100
H	-1.75942400	2.10105400	1.61314400
C	1.57612900	1.00745000	3.24124900
H	1.74924000	-0.40157300	1.62142900
C	0.81723600	2.01210800	3.83227200

H	1.16254400	2.50465000	4.73606400
C	-1.92702500	-1.19542900	0.37820300
C	-2.17749700	-2.26729600	-0.48881700
C	-2.68293700	-1.06886300	1.54150100
C	-3.16596100	-3.19329100	-0.18844200
H	-1.57359500	-2.39000700	-1.38435400
C	-3.68280300	-2.00022000	1.83088600
H	-2.49814100	-0.25428600	2.24063600
C	-3.92560400	-3.06537900	0.97477400
H	-4.69203400	-3.79798900	1.21438900
P	-0.54708400	-0.08223700	-0.06700800
C	2.91344500	0.61390800	3.78687600
C	-1.24749800	3.45297600	3.85074900
C	-4.47600700	-1.82162000	3.08978900
C	-3.40139300	-4.37913300	-1.07297000
C	-4.28344700	1.76531100	-3.33040900
C	-0.56114300	4.84006800	-2.02340500
F	0.02870300	4.99064300	-3.22989100
F	-1.44767900	5.85150800	-1.90374500
F	0.38718900	5.02069400	-1.08835300
F	-4.70020100	2.82380200	-4.04625900
F	-4.10973300	0.73802400	-4.19013400
F	-5.29312500	1.40821000	-2.50830200
F	-2.44835700	2.95942200	4.22082000
F	-0.68598400	4.00793500	4.93805800
F	-1.49499600	4.44364400	2.96873900
F	3.15965300	1.14590900	4.99341000
F	3.90983400	1.01331200	2.95806600
F	3.02958400	-0.72727600	3.89569600
F	-3.18678100	-5.53378100	-0.40450100
F	-4.67305000	-4.42432000	-1.51964800
F	-2.59224400	-4.38522400	-2.14859700
F	-5.36837600	-2.80866100	3.27929300
F	-5.15714900	-0.65596000	3.07866900
F	-3.67325100	-1.78523900	4.17448300
C	1.98528000	0.62737500	-1.54543700
C	2.80534500	1.42036400	-0.73391200
C	1.61306700	1.11248800	-2.80491400
C	3.21902800	2.68473200	-1.16226900
H	3.12725200	1.05714300	0.24385300
C	2.03065800	2.37349400	-3.23293400
H	0.97215900	0.51375200	-3.45424400
C	2.82830200	3.16690900	-2.41007000
H	3.84849500	3.29259900	-0.51242800

H	1.71467600	2.74317000	-4.20811600
H	3.13444000	4.15961800	-2.73644100

Post-TS_{PE}(L10)

M06-L electronic energy (Hartree): -4428.149857

M06-L thermal correction to free energy (Hartree): 0.448099

Three lowest frequencies (cm⁻¹): 5.28, 10.08, 11.85

Pd	-1.51138300	0.73509000	-1.12217900
O	-2.93691300	3.78560300	-1.51703500
O	-1.19233600	2.87251600	-0.43153900
C	-1.82055400	3.86342800	-0.82357500
C	-1.34115700	5.25255500	-0.57511900
C	-5.80865900	0.62107100	-1.15978500
C	-4.49077300	0.87042000	-0.67398700
C	-5.85039400	0.50110300	-2.52428700
C	-3.50513400	0.96295100	-1.63766100
S	-4.26375200	0.68156600	-3.18339800
O	-6.89882900	0.52328900	-0.34288700
C	-6.51442700	0.30184700	1.01956500
O	-4.22343600	0.99602600	0.66765700
C	-5.41293300	1.24586600	1.42788100
H	-6.72344500	0.36031200	-3.15011900
H	-7.41498400	0.46113800	1.61747100
H	-6.18185300	-0.74034300	1.14212100
H	-5.13943600	1.10273300	2.47489700
H	-3.16144000	2.80593400	-1.62897700
H	-0.77232800	5.58963200	-1.44998000
H	-2.17491600	5.94434200	-0.43659500
H	-0.67492800	5.27537000	0.28920600
H	-5.72990500	2.28838200	1.27738700
C	1.63052400	-1.08820400	-0.93942400
C	1.24603700	-2.43614800	-1.00271900
C	2.79774900	-0.68371200	-1.58441600
C	2.03598100	-3.35419800	-1.68221600
H	0.32795400	-2.77095300	-0.52086000
C	3.57614200	-1.61223300	-2.27752000
H	3.11878900	0.35661800	-1.54910600
C	3.20440700	-2.94818200	-2.32744200
H	3.81924100	-3.67065100	-2.85715200
C	0.11501300	-0.71899400	1.45685000
C	1.00646900	-1.55364100	2.13674000
C	-1.16341000	-0.51858800	1.98446100

C	0.62320600	-2.16555300	3.32871300
H	2.00316900	-1.74009000	1.73627500
C	-1.54047700	-1.14175800	3.17068100
H	-1.88131600	0.11107000	1.45268800
C	-0.65140500	-1.96647400	3.85159800
H	-0.94812300	-2.45418600	4.77490400
C	1.63894800	1.49186900	0.33978400
C	1.72971500	2.55776400	-0.56516300
C	2.35210300	1.55108200	1.53499400
C	2.52330800	3.65824300	-0.27317100
H	1.15802900	2.53013100	-1.49013900
C	3.15147700	2.66044700	1.81913000
H	2.28975300	0.74228100	2.26188100
C	3.23890700	3.71685200	0.92316200
H	3.85200900	4.58390100	1.15533000
P	0.52539700	0.11489000	-0.11895700
C	-2.93348900	-0.91120900	3.67027400
C	1.61841000	-3.04142100	4.02850800
C	3.89811200	2.68187300	3.11852100
C	2.59039900	4.82844300	-1.20639700
C	4.82712400	-1.12981300	-2.94564500
C	1.63667500	-4.79660400	-1.76901300
F	1.17582800	-5.10868500	-3.00053800
F	2.68878600	-5.61111500	-1.53827000
F	0.67509500	-5.11941000	-0.88719600
F	5.46772400	-2.10896700	-3.60723600
F	4.56177600	-0.14675500	-3.83289900
F	5.69486500	-0.61144200	-2.05007900
F	2.72764000	-2.34835200	4.36317300
F	1.12416700	-3.58260000	5.15481800
F	2.02436600	-4.05429100	3.23433700
F	-3.17437900	-1.52975100	4.83703900
F	-3.85413400	-1.34915500	2.78073900
F	-3.17676000	0.40694900	3.84954900
F	2.12574200	5.95058000	-0.61311100
F	3.85686500	5.09072200	-1.58654500
F	1.86164300	4.63748100	-2.32195200
F	4.63714100	3.79434100	3.26863200
F	4.73013900	1.62410400	3.22284500
F	3.05394500	2.60986300	4.16961400
C	-1.75532800	-1.16814000	-1.69282800
C	-2.42331900	-2.09212600	-0.87949800
C	-1.20601600	-1.60643500	-2.90353700
C	-2.50385000	-3.43571900	-1.25402800

H	-2.88476300	-1.76760700	0.05525700
C	-1.29630400	-2.94791400	-3.27900100
H	-0.67999700	-0.90454600	-3.55232200
C	-1.93748000	-3.86817500	-2.45209600
H	-3.01348600	-4.14555900	-0.60285100
H	-0.84524700	-3.27657600	-4.21499500
H	-1.98562900	-4.91843400	-2.73521900

Int_{PE}(L11)

M06-L electronic energy (Hartree): -3113.340888

M06-L thermal correction to free energy (Hartree): 0.220161

Three lowest frequencies (cm⁻¹): 21.94, 26.98, 30.29

Pd	-1.26732600	1.61844900	0.64830300
O	-2.87904300	2.28933700	2.97848900
O	-2.56433600	3.25021600	0.96982200
C	-3.11078200	3.17763900	2.14516300
C	-4.11392700	4.27301600	2.43040500
H	-3.77656000	5.23768700	2.03954600
H	-5.05882000	4.03584000	1.92662700
H	-4.31078300	4.35698300	3.50216900
C	0.00266300	-1.14559800	-1.20602500
C	-1.04918900	-2.03137800	-0.95133800
C	0.63575200	-1.26752300	-2.44369800
C	-1.50909600	-2.94021600	-1.88957100
C	0.19515800	-2.17282800	-3.40219000
C	-0.88458400	-3.00338600	-3.12925500
C	0.94813300	-1.03795000	1.40177300
C	2.04992900	-1.85999400	1.15117600
C	0.29102200	-1.20389800	2.62084800
C	2.50300900	-2.78921100	2.07201500
C	0.72313100	-2.13286000	3.56028900
C	1.83137300	-2.92307300	3.28403400
C	1.72553800	1.12270800	-0.42073000
C	1.52380800	1.92457100	-1.54974600
C	2.91039300	1.33847900	0.28752900
C	2.44762000	2.85657200	-1.98746700
C	3.85319300	2.27288400	-0.12744900
C	3.62514400	3.03037900	-1.26769700
P	0.31825100	0.08482300	0.11210200
F	-1.65506200	-2.00427600	0.24303700
F	-0.79447600	-0.48690600	2.92072600
F	0.39031000	1.78967600	-2.25428600

F	3.56592200	-3.54800500	1.81317600
F	2.25134900	-3.81093600	4.17625700
F	0.07747200	-2.27455000	4.71620400
F	2.71037400	-1.73908400	-0.00663600
F	3.18545200	0.67302300	1.41277500
F	4.97199000	2.44787700	0.57337100
F	4.52226500	3.92363900	-1.66575400
F	2.21597200	3.58604900	-3.07659300
F	1.70678100	-0.53333100	-2.75654900
F	0.81807000	-2.26065300	-4.57656300
F	-1.30639700	-3.86761900	-4.04485900
F	-2.54075100	-3.73577300	-1.61512400
C	-2.74011500	0.67106800	-0.28141000
C	-3.80110700	0.23959100	0.51421000
C	-2.75717600	0.48684800	-1.66213000
C	-4.87286700	-0.42524300	-0.08414400
H	-3.78808100	0.41705700	1.58904300
C	-3.84358700	-0.17048400	-2.24886600
H	-1.93243400	0.82616800	-2.28652200
C	-4.89297700	-0.63767500	-1.46239600
H	-5.69613900	-0.77632700	0.53672600
H	-3.85331500	-0.32210800	-3.32769500
H	-5.72981000	-1.15954300	-1.92246500

Pre-TS_{PE}(L11)

M06-L electronic energy (Hartree): -3894.278578

M06-L thermal correction to free energy (Hartree): 0.321305

Three lowest frequencies (cm⁻¹): 15.01, 21.04, 26.14

Pd	1.11208800	-0.70157500	0.53679100
O	0.45751800	-3.60215400	-0.09833600
O	-0.10477700	-2.20950700	1.57672300
C	-0.16255600	-3.33596600	0.94663200
C	-1.06459500	-4.37179700	1.59089800
C	4.94738600	-0.96081200	0.22823300
C	4.04976900	-1.27167100	1.27574600
C	4.58264100	-1.55451600	-0.95831500
C	2.93185000	-2.01197800	0.86273300
S	3.13880800	-2.46132200	-0.83072500
O	6.04201900	-0.17575100	0.39525800
C	6.00526100	0.53008200	1.64635400
O	4.24575000	-0.88766700	2.54740300
C	5.57995200	-0.37720500	2.77039800

H	5.06625700	-1.41346800	-1.91820700
H	7.01828200	0.90259600	1.81164900
H	5.31654000	1.38056700	1.55597100
H	5.53485400	0.16000800	3.71911400
H	2.42309300	-2.71665400	1.51529300
H	-0.60199200	-4.74506300	2.51234300
H	-2.02651100	-3.93257600	1.87811800
H	-1.23639400	-5.22041100	0.92241400
H	6.26127700	-1.23128500	2.86950400
C	-0.97452200	1.67469800	-1.07526000
C	-0.35903300	2.81500600	-0.54803000
C	-1.45282900	1.77004300	-2.38197600
C	-0.14985000	3.96543300	-1.28944900
C	-1.25790300	2.91423200	-3.14768300
C	-0.59679800	4.00883700	-2.60526200
C	-1.98893600	0.72622500	1.35678200
C	-3.31510800	1.08743000	1.11160500
C	-1.51267200	0.88135700	2.65863600
C	-4.14935400	1.55831400	2.11159100
C	-2.32886700	1.35455700	3.67907000
C	-3.64802700	1.69089500	3.40318800
C	-1.73942500	-1.18206300	-0.85387300
C	-1.14893500	-1.65448000	-2.02853200
C	-2.72257300	-1.99799300	-0.29059400
C	-1.53374100	-2.82864400	-2.65068800
C	-3.11359100	-3.19318000	-0.88262000
C	-2.52529300	-3.60806500	-2.06910100
P	-0.90031300	0.19785100	-0.00176700
F	0.04586700	2.80813800	0.72965500
F	-0.24297700	0.60601400	2.96852600
F	-0.13637100	-0.96569200	-2.57437200
F	-5.41570600	1.87976800	1.85283800
F	-4.43327100	2.14373700	4.37308600
F	-1.85151300	1.49877300	4.91442100
F	-3.81511100	0.95387800	-0.12267900
F	-3.30446500	-1.69750100	0.87579200
F	-4.03751700	-3.95452600	-0.29536400
F	-2.89582800	-4.75149000	-2.63495000
F	-0.93531800	-3.23103400	-3.77096100
F	-2.13517500	0.77174500	-2.95034800
F	-1.72077500	2.97193200	-4.39621900
F	-0.41313400	5.10365900	-3.33513000
F	0.46312300	5.01964500	-0.75380400
C	2.17732400	0.80729400	-0.26434700

C	2.76262900	1.74149200	0.59651900
C	2.37672100	0.94250500	-1.64211100
C	3.53405800	2.78979700	0.08994600
H	2.61461300	1.66042600	1.67581000
C	3.15310700	1.98869000	-2.14763800
H	1.93297100	0.22851000	-2.33445700
C	3.73368300	2.91511900	-1.28430100
H	3.98282600	3.50791400	0.77676200
H	3.29774700	2.07819200	-3.22419600
H	4.33496900	3.73249600	-1.67852600

TS_{PE}(L11)

M06-L electronic energy (Hartree): -3894.250950

M06-L thermal correction to free energy (Hartree): 0.318161

Three lowest frequencies (cm⁻¹): -963.94, 18.41, 21.36

Pd	1.32334400	-0.15444300	-0.24103400
O	2.72501300	-3.02206500	-0.82974200
O	0.94018100	-2.28497500	0.31809200
C	1.63146800	-3.20703900	-0.18199900
C	1.18000600	-4.63066400	-0.02837500
C	5.56383500	0.22235400	-0.00039800
C	4.31016000	-0.33403100	0.36896900
C	5.62480000	0.51167300	-1.34112000
C	3.38573100	-0.49391400	-0.66440000
S	4.14837300	0.12090400	-2.12424300
O	6.58260600	0.42571000	0.88120100
C	6.11789800	0.38733400	2.23713700
O	4.03232000	-0.69957300	1.64764000
C	5.21468200	-0.79764900	2.46186100
H	6.47308300	0.91612500	-1.88180400
H	7.01159500	0.32425500	2.86161700
H	5.58723000	1.32309200	2.46635700
H	4.86375500	-0.83951400	3.49480000
H	3.00807500	-1.82949700	-0.79494700
H	1.89546600	-5.18339000	0.58971800
H	0.19164600	-4.68197600	0.43480700
H	1.15540800	-5.12459200	-1.00533900
H	5.73661700	-1.73324000	2.22023900
C	-1.89376200	1.51071200	-0.38483900
C	-1.46622700	2.67054100	0.26820900
C	-2.90785500	1.66078400	-1.33132200
C	-1.96018700	3.92759600	-0.03808400

C	-3.42418200	2.91027800	-1.65308200
C	-2.94191300	4.04614300	-1.01434900
C	-1.64480100	-0.32060600	1.71453100
C	-3.01813200	-0.47018200	1.91860200
C	-0.82205000	-0.35843700	2.84041100
C	-3.56246900	-0.66382000	3.17719000
C	-1.34408700	-0.54714900	4.11449600
C	-2.71448800	-0.70092300	4.28024300
C	-1.57844500	-1.36408800	-1.01469300
C	-1.37142600	-1.23922100	-2.39108900
C	-1.93015900	-2.63531200	-0.55727000
C	-1.53338300	-2.28895200	-3.27919800
C	-2.08471300	-3.70994000	-1.42456400
C	-1.88849000	-3.54011300	-2.78739900
P	-0.97421900	-0.00565000	0.05012300
F	-0.54190900	2.57873600	1.23284600
F	0.50188800	-0.20384800	2.73653000
F	-0.97444500	-0.05805300	-2.89055000
F	-4.87521800	-0.82054900	3.33940700
F	-3.21418800	-0.88690400	5.49585100
F	-0.54155900	-0.57984000	5.17705800
F	-3.84417200	-0.45786100	0.86548800
F	-2.09043200	-2.89776700	0.74395400
F	-2.39160100	-4.91535900	-0.94376100
F	-2.03283300	-4.56985200	-3.61374000
F	-1.33438800	-2.11390400	-4.58505700
F	-3.43499200	0.60620600	-1.95921900
F	-4.39371700	3.02291700	-2.56061400
F	-3.43461500	5.24058600	-1.32352600
F	-1.49967200	5.00983900	0.58740000
C	1.62867300	1.78985500	-0.61986400
C	2.46912000	2.51375000	0.23745400
C	0.98870100	2.47197500	-1.66098400
C	2.63295900	3.89003600	0.07868100
H	2.98612700	2.00534700	1.05254800
C	1.16025300	3.84983700	-1.82276200
H	0.32727900	1.94074800	-2.34537600
C	1.97563800	4.56518300	-0.94983800
H	3.27926700	4.43699600	0.76525300
H	0.64004800	4.36270100	-2.63214400
H	2.10269500	5.63964600	-1.07115500

Post-TS_{PE}(L11)

M06-L electronic energy (Hartree): -3894.259163

M06-L thermal correction to free energy (Hartree): 0.319026

Three lowest frequencies (cm^{-1}): 11.82, 13.72, 19.32

Pd	1.26934200	0.55986200	0.23513000
O	3.18684900	-1.65289100	-1.22409200
O	1.64820800	-1.69286600	0.41731400
C	2.42039300	-2.27926000	-0.34622700
C	2.57661100	-3.75986900	-0.35420100
C	5.59936400	1.12062200	0.43179800
C	4.33674900	0.50877900	0.70474900
C	5.48707000	2.23223700	-0.35856900
C	3.24265900	1.12146400	0.12524200
S	3.82740200	2.51566300	-0.74558200
O	6.78595700	0.62894400	0.89769500
C	6.60314000	-0.35578400	1.92110300
O	4.24346800	-0.62469300	1.47933200
C	5.49570300	-1.31159600	1.55695700
H	6.28265800	2.87323000	-0.71818800
H	7.56075800	-0.87405700	2.01547600
H	6.37294500	0.14371500	2.87370000
H	5.37294800	-2.08406400	2.32026000
H	3.09962900	-0.67412000	-1.06271400
H	3.41528200	-4.03039000	0.29838500
H	1.67676300	-4.23986900	0.03607300
H	2.80706800	-4.13032800	-1.35610600
H	5.71029100	-1.79488900	0.59053500
C	-2.27298500	0.97522600	-0.36406300
C	-2.41970200	1.99772100	0.57848700
C	-3.05707300	1.06376300	-1.51331200
C	-3.23252200	3.09898400	0.36935500
C	-3.88249900	2.15756200	-1.74797700
C	-3.96180200	3.18082600	-0.81140200
C	-1.73025100	-1.11629200	1.41304300
C	-2.96492100	-1.75169500	1.27080000
C	-1.15195100	-1.11424600	2.68166200
C	-3.59877300	-2.37655100	2.33184100
C	-1.76789100	-1.73150600	3.76370800
C	-2.99214600	-2.36320400	3.58486400
C	-0.84131900	-1.42379900	-1.35081800
C	-0.47508300	-0.92841200	-2.60547500
C	-0.80333200	-2.81237600	-1.20603100
C	-0.13645300	-1.74346700	-3.67288400
C	-0.45245700	-3.65447900	-2.25567000

C	-0.12317600	-3.12225700	-3.49466300
P	-0.95420600	-0.22509700	0.02761000
F	-1.75570000	1.91247100	1.73979500
F	0.01461100	-0.50004000	2.90383500
F	-0.42399900	0.39770600	-2.79602800
F	-4.77026600	-2.98859600	2.16726300
F	-3.58781600	-2.95655600	4.61237300
F	-1.19796800	-1.71503600	4.96758000
F	-3.55139700	-1.78585100	0.06832700
F	-1.05242100	-3.40358700	-0.03190600
F	-0.40366400	-4.97240400	-2.06237400
F	0.21506600	-3.92277800	-4.49844100
F	0.19566500	-1.21765600	-4.85022400
F	-3.06031900	0.09133100	-2.42995700
F	-4.61464500	2.21978500	-2.86030100
F	-4.75304900	4.22499500	-1.03404000
F	-3.32135200	4.06523200	1.28146400
C	0.79281700	2.50254200	0.13634900
C	0.86167800	3.28961200	1.29210800
C	0.32734000	3.08472100	-1.04812700
C	0.42935000	4.61593200	1.27365700
H	1.23446400	2.86167600	2.22309200
C	-0.09644900	4.41645600	-1.06609200
H	0.28083000	2.50236800	-1.96666600
C	-0.05499400	5.18390600	0.09533300
H	0.47546300	5.20854200	2.18709600
H	-0.46564400	4.84876200	-1.99612800
H	-0.39167100	6.21919600	0.08279100

(DMAc)Pd(Ph)(OAc)

M06-L electronic energy (Hartree): -876.082597

M06-L thermal correction to free energy (Hartree): 0.223900

Three lowest frequencies (cm-1): 26.72, 40.70, 45.71

Pd	0.12380200	-0.44432200	0.22037600
O	-0.89582100	1.37095600	0.67935700
O	0.79938500	-2.41884900	-0.02917400
O	-1.37076000	-2.17509600	0.30704100
C	-2.12037500	1.59497900	0.47242400
C	-0.37810600	-2.92677600	0.09500200
C	-0.52849700	-4.40825400	-0.04617000
C	-2.87700600	2.37154100	1.50750800
N	-2.76770800	1.18839000	-0.62955900

C	-2.06259000	0.63840500	-1.77658000
C	-4.20482400	1.33829400	-0.80068500
H	-2.12918500	-0.45589700	-1.79697900
H	-1.01173300	0.93501100	-1.74839000
H	-2.52119400	1.03995200	-2.68601200
H	-4.70961800	1.41226800	0.16225900
H	-4.58746400	0.45387600	-1.31832500
H	-4.43940700	2.22449500	-1.40332700
H	-3.50890700	3.15033000	1.07063300
H	-2.16112500	2.82640200	2.19339800
H	-3.52436300	1.70602800	2.09090900
H	0.29805600	-4.93175600	0.44260100
H	-1.48070600	-4.74644800	0.36880500
H	-0.50062500	-4.67893800	-1.10802000
C	1.83432100	0.51284800	0.00919500
C	3.00360600	-0.25646800	0.00024700
C	1.92173800	1.90150800	-0.14262600
C	4.24745500	0.35840200	-0.15264200
H	2.94370900	-1.33890500	0.10809500
C	3.17042200	2.50735100	-0.30042200
H	1.02073200	2.51202600	-0.13284600
C	4.33457600	1.74117500	-0.30387200
H	5.15080700	-0.25111700	-0.15410600
H	3.22835500	3.58916700	-0.41992300
H	5.30498800	2.21945600	-0.42521700

Pre-TS_{PE}(DMAc)

M06-L electronic energy (Hartree): -1657.008335

M06-L thermal correction to free energy (Hartree): 0.328189

Three lowest frequencies (cm-1): 27.98, 31.24, 39.63

Pd	0.49723200	-0.00734000	-0.19140100
O	1.94517600	1.61705700	-0.62742300
O	1.97334200	-1.64338700	-2.18620600
O	2.20254100	-1.35986200	0.03090100
C	3.13188800	1.47424500	-0.23514700
C	2.54966100	-1.86186700	-1.10440200
C	3.75039100	-2.78731900	-1.04608700
C	4.24632800	1.54483000	-1.23780100
N	3.43239700	1.29309800	1.06324300
C	2.36599100	1.23944300	2.04592600
C	4.72904100	0.83979900	1.53118100
H	1.94221800	0.22590400	2.11153500

H	1.57111700	1.93679400	1.77215600
H	2.77578000	1.51978300	3.02058000
H	5.49039300	0.95593700	0.76123900
H	4.67563100	-0.22004000	1.81411900
H	5.02862300	1.42001600	2.40996000
H	5.05098200	2.22112400	-0.93248500
H	3.83490700	1.88495900	-2.18913100
H	4.68940500	0.55366500	-1.39456500
C	-2.88000500	-1.20374100	1.00472700
C	-2.14194900	-1.45019900	-0.17001600
C	-2.13187500	-1.39159600	2.14711700
C	-0.76545800	-1.70420000	0.05248000
S	-0.51433700	-1.82179700	1.81590200
O	-4.17631000	-0.80429400	0.98769600
C	-4.52635400	-0.28538800	-0.30741500
O	-2.67397300	-1.43052600	-1.39565800
C	-4.10896100	-1.24162400	-1.39342800
H	-2.45738000	-1.19649100	3.16263400
H	-5.61040200	-0.15787200	-0.29936000
H	-4.04413600	0.69328600	-0.44369400
H	-4.35415100	-0.85321500	-2.38367700
H	-0.22980500	-2.42198300	-0.56934100
H	4.09367300	-3.06374900	-2.04661500
H	4.57447000	-2.31893000	-0.49584200
H	3.48989400	-3.70266000	-0.50137900
H	-4.57976700	-2.22299400	-1.26088500
C	-1.00420800	1.29257600	-0.25608600
C	-1.47300700	1.77046900	-1.48453100
C	-1.55477200	1.79970800	0.92528300
C	-2.46340100	2.75561500	-1.52781500
H	-1.07005800	1.37303700	-2.41790100
C	-2.54465800	2.78416400	0.88209600
H	-1.22176100	1.41325100	1.89255400
C	-3.00037100	3.26506800	-0.34545200
H	-2.81884500	3.12143500	-2.49103500
H	-2.96176700	3.17225200	1.81123300
H	-3.77498600	4.02937200	-0.38105500

TS_{PE}(DMAc)

M06-L electronic energy (Hartree): -1656.986525

M06-L thermal correction to free energy (Hartree): 0.323925

Three lowest frequencies (cm-1): -1154.71, 27.87, 32.95

Pd	0.58268300	0.17934800	-0.15922900
O	2.23909400	1.33505000	-1.10660200
O	0.62617900	-3.02687800	0.44000700
O	2.08178500	-1.45507700	-0.24289500
C	3.40864500	0.92101900	-0.90676700
C	1.79125900	-2.63696000	0.06797500
C	2.86791600	-3.68505500	0.04220200
C	4.24622200	0.46725100	-2.06447000
N	3.94331900	0.89041700	0.32925500
C	3.12869400	1.29897600	1.45782200
C	5.13329300	0.12115500	0.64650700
H	2.45954500	0.48603900	1.78154300
H	2.51635200	2.15812100	1.17573000
H	3.78629100	1.57371900	2.28683100
H	5.81091300	0.07722900	-0.20622500
H	4.86096100	-0.90381200	0.93625100
H	5.65858000	0.59549900	1.47996000
H	5.23950700	0.92728700	-2.07803800
H	3.72516300	0.71298900	-2.99094500
H	4.38370600	-0.62032700	-2.02395200
C	-3.35354600	-1.07654400	0.63693800
C	-2.15942600	-1.12791000	-0.12703200
C	-3.11060500	-0.85341100	1.97017300
C	-0.96857600	-0.95192100	0.58963500
S	-1.42992400	-0.68620500	2.27604000
O	-4.59396400	-1.23464900	0.09603000
C	-4.56690100	-1.03023500	-1.32286100
O	-2.16470400	-1.35239900	-1.46198200
C	-3.44014200	-1.80789900	-1.95188600
H	-3.84791600	-0.80093900	2.76332200
H	-5.53433500	-1.37125100	-1.69748400
H	-4.45851500	0.04434800	-1.53353000
H	-3.41190200	-1.66371300	-3.03388400
H	-0.14066700	-2.03535200	0.49470000
H	2.47428300	-4.64487700	-0.30246100
H	3.70310400	-3.37119500	-0.58862800
H	3.24654800	-3.83451700	1.06029700
H	-3.54032500	-2.87923700	-1.73385600
C	-0.65702300	1.72437700	-0.09691600
C	-1.63031400	1.93046200	-1.08408700
C	-0.52456700	2.68124100	0.91897800
C	-2.42605400	3.07843800	-1.07430500
H	-1.77753500	1.18676900	-1.86811400
C	-1.31981000	3.82937400	0.92721900

H	0.20511900	2.53435700	1.71756900
C	-2.27348300	4.03205100	-0.06932000
H	-3.17467000	3.22085000	-1.85417000
H	-1.19482300	4.56554800	1.72141400
H	-2.89785400	4.92397600	-0.05851100

Post-TS_{PE}(DMAc)

M06-L electronic energy (Hartree): -1656.997281

M06-L thermal correction to free energy (Hartree): 0.326706

Three lowest frequencies (cm-1): 21.93, 23.96, 34.54

Pd	0.52922300	0.30578300	-0.08351500
O	2.49946900	0.92934000	-0.93550700
O	-0.17452600	-3.05118100	0.26338200
O	1.58421400	-1.71486600	-0.16130300
C	3.53753400	0.23905600	-0.79299200
C	1.09802600	-2.84067800	-0.02713000
C	1.90063700	-4.08881300	-0.15771700
C	4.26222800	-0.26590100	-2.00572400
N	4.03448900	-0.04883500	0.42550100
C	3.33024600	0.41310600	1.60665700
C	5.03193200	-1.07664700	0.65930900
H	2.48588100	-0.24826300	1.85061100
H	2.94528200	1.42088900	1.43783700
H	4.02783700	0.42859000	2.44840300
H	5.57472300	-1.31648300	-0.25415500
H	4.55092300	-1.99179000	1.03226500
H	5.74902900	-0.73000700	1.41030600
H	5.33974600	-0.07743800	-1.97177900
H	3.84231300	0.21835100	-2.88856500
H	4.11706200	-1.34868000	-2.10817000
C	-3.51900700	-0.98054300	0.66815500
C	-2.35735000	-0.71429500	-0.12274100
C	-3.32162300	-0.74073500	2.00087000
C	-1.24908400	-0.29477000	0.58270000
S	-1.70256500	-0.18444600	2.26631800
O	-4.68567900	-1.45145600	0.13780800
C	-4.72623900	-1.31067000	-1.28753200
O	-2.35499100	-0.88395600	-1.48657700
C	-3.42168500	-1.74008000	-1.90956000
H	-4.02039800	-0.89472100	2.81405000
H	-5.55430700	-1.93705300	-1.62821400
H	-4.94119500	-0.26317000	-1.54583400

H	-3.46043800	-1.66414000	-2.99870400
H	-0.61874300	-2.16251500	0.36533700
H	1.35943500	-4.83938100	-0.74015900
H	2.86554700	-3.87422600	-0.61940700
H	2.07140700	-4.51470500	0.83739500
H	-3.18925400	-2.77959700	-1.63115200
C	-0.21586900	2.14366700	-0.13469200
C	-1.39153000	2.48952200	-0.81733500
C	0.52424200	3.16743600	0.47428800
C	-1.79562800	3.82270700	-0.91073600
H	-1.99616500	1.71319000	-1.28538900
C	0.11144300	4.49872200	0.39099200
H	1.44293300	2.93016100	1.01290600
C	-1.04993400	4.83169700	-0.30402600
H	-2.70546800	4.07130900	-1.45756800
H	0.70357100	5.27720400	0.87221600
H	-1.37227900	5.86974200	-0.36925800

(L4)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3048.881644

M06-L thermal correction to free energy (Hartree): 0.513514

Three lowest frequencies (cm⁻¹): 9.56, 14.34, 21.59

C	-2.66520500	2.14103900	0.72205200
C	-1.84261700	2.96257600	1.50658800
C	-3.93496300	2.59604000	0.35588500
C	-2.28437000	4.21614500	1.91581700
C	-4.36947600	3.85728500	0.75872800
C	-3.54799900	4.66857500	1.53761500
C	-2.00746500	-0.29840100	1.95595000
C	-3.20697500	-0.58505200	2.62453600
C	-0.79148500	-0.50273000	2.61349000
C	-3.18211400	-1.10691700	3.91253000
C	-0.76933700	-1.01693800	3.90815600
C	-1.96250700	-1.32724300	4.55444800
C	-3.27795000	-0.37128500	-0.67727200
C	-3.72546400	0.22344900	-1.86658600
C	-3.68123500	-1.67545700	-0.36870600
C	-4.60166700	-0.46188600	-2.70277300
C	-4.55160000	-2.35851500	-1.21362700
C	-5.01982500	-1.75138600	-2.37640400
P	-2.01407800	0.48333600	0.30798500
Pd	-0.01083300	0.48791400	-0.76064000

O	-1.44912300	2.62555300	-2.17437900
O	0.26280400	2.61337000	-0.71534200
C	-0.59784600	3.20536800	-1.47651200
C	-0.55234900	4.71702200	-1.43951000
C	-0.16865600	-1.51014300	-0.94734500
C	0.17420000	-2.59361800	-0.17506800
S	-0.76359200	-2.10106200	-2.47482100
C	-0.07008000	-3.86825500	-0.78268600
C	-0.58456700	-3.77123500	-2.04573400
H	-0.85545500	-4.57206700	-2.72274300
O	0.75442400	-2.50436400	1.07076800
C	0.53275600	-3.69299900	1.83033300
H	-0.53234800	-3.76218600	2.10562900
O	0.16171000	-5.05452200	-0.14393600
C	0.95427300	-4.90572300	1.03963100
H	0.81077600	-5.82468600	1.61406600
H	2.01548700	-4.82558600	0.76097600
H	1.12702100	-3.59012100	2.74245500
C	5.72065100	0.01431200	0.16664800
C	4.78419300	1.08251900	0.33407300
C	7.00846900	0.45386200	0.03153500
C	5.37691200	2.31425500	0.32986600
S	7.08327100	2.17488900	0.11777100
O	5.33994900	-1.29440100	0.12244800
C	4.02575000	-1.48195800	0.66645000
O	3.44448500	0.86998700	0.49673900
C	3.04738500	-0.46881000	0.11837900
C	2.87846800	-0.54773000	-1.38552900
H	7.90340400	-0.13866000	-0.10719100
H	3.72614500	-2.49674700	0.39172400
H	4.06731000	-1.40780700	1.76217700
H	2.07114200	-0.61150100	0.59771300
H	3.84460700	-0.41530800	-1.89324000
H	2.48497800	-1.53637900	-1.64869000
H	4.90485900	3.28146900	0.44118400
H	-1.28972600	5.06710900	-0.70512600
H	0.42670900	5.09599500	-1.13255300
H	-0.82771000	5.14199400	-2.40931800
N	1.90596200	0.46091100	-1.82745300
H	2.28426600	1.39740300	-1.68265100
H	1.74307100	0.36712200	-2.82855400
H	-4.59340200	1.96542800	-0.23800300
H	-5.35970400	4.20183800	0.46639800
H	-4.16280700	-0.40313200	2.13243100

H	-4.11667500	-1.33821400	4.41992900
H	-3.30287300	-2.16744100	0.52636100
H	-4.85919300	-3.37201400	-0.96301600
H	-1.94592900	-1.73506300	5.56340500
H	-5.70116000	-2.28693100	-3.03487900
H	-3.89264800	5.65141200	1.85352900
H	-4.95074600	0.00979800	-3.61951100
H	-1.63777500	4.84349200	2.52635600
H	0.18426000	-1.18091400	4.40714100
H	0.13794000	-0.27006600	2.09503500
H	-0.84996600	2.61498700	1.79338100
H	-3.35878900	1.21309400	-2.13993600

(L5)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3166.845634

M06-L thermal correction to free energy (Hartree): 0.599181

Three lowest frequencies (cm⁻¹): 17.94, 26.62, 37.57

C	2.84473700	-2.00742800	-0.08448300
C	2.43977100	-3.26611500	0.42171300
C	4.00801900	-1.92950300	-0.86196900
C	3.18159400	-4.39469400	0.05423300
C	4.73581700	-3.06516700	-1.20203300
C	4.30678000	-4.31081200	-0.75850000
C	1.94306400	-0.48704200	2.11361800
C	3.22529100	-0.62389600	2.67097900
C	0.81561200	-0.47781200	2.96041900
C	3.41641600	-0.71077000	4.04371600
C	1.03427500	-0.56526200	4.34199800
C	2.30820300	-0.67525500	4.88572500
C	2.94548000	0.92601200	-0.25082200
C	3.17061500	1.19404600	-1.62284900
C	3.39641900	1.84477100	0.70654600
C	3.85755900	2.36527500	-1.96414400
C	4.07214200	3.00390500	0.34003000
C	4.30466700	3.26677500	-1.00583800
P	1.88039900	-0.47811800	0.27460600
Pd	-0.14598100	-0.36396400	-0.82217500
O	0.51708300	-2.48165200	-2.77607400
O	-0.56724000	-2.47049600	-0.80474500
C	-0.07447400	-3.05665700	-1.84696100
C	-0.23311700	-4.56282900	-1.85780800
C	0.01634700	1.62935800	-0.98088900

C	0.11074400	2.63727000	-0.05666800
S	-0.11869400	2.35598700	-2.56180600
C	0.04682300	3.96084200	-0.59495900
C	-0.08163800	3.98046400	-1.95713200
H	-0.12998400	4.83948100	-2.61447900
O	0.25533600	2.40691300	1.29281300
C	0.67535700	3.57681100	1.99736000
H	1.74542200	3.75444300	1.80815500
O	0.11839000	5.07980800	0.18703500
C	-0.12708900	4.77824000	1.56526800
H	0.16058000	5.67066900	2.12641100
H	-1.20192700	4.59290800	1.71413000
H	0.53164300	3.35961800	3.05982700
C	-5.80605200	0.18811100	0.31342200
C	-4.81784900	-0.82498800	0.51824000
C	-7.07768000	-0.31252400	0.26520300
C	-5.35490200	-2.07807500	0.62378700
S	-7.07211400	-2.02433300	0.47182800
O	-5.48456200	1.50427800	0.15580100
C	-4.15995900	1.78426500	0.62922900
O	-3.48351300	-0.54514000	0.61236200
C	-3.16130900	0.77288400	0.11280800
C	-3.06509500	0.74266700	-1.39791400
H	-8.00257600	0.23013300	0.11941500
H	-3.91754200	2.78965100	0.27369700
H	-4.15534100	1.78391800	1.72807400
H	-2.16966000	0.98968700	0.52890800
H	-4.05165400	0.55349500	-1.84457600
H	-2.71456700	1.71861300	-1.75228400
H	-4.83686600	-3.01502300	0.78208600
H	0.66778000	-5.01110300	-1.41861200
H	-1.08971100	-4.89260400	-1.26265400
H	-0.32286900	-4.94171800	-2.88009300
N	-2.09699400	-0.27834400	-1.82554100
H	-2.46488600	-1.20931700	-1.62489500
H	-1.97131400	-0.23003900	-2.83573900
H	4.37033600	-0.96015200	-1.19270600
H	5.63320200	-2.97004300	-1.81005900
H	4.09120100	-0.65871000	2.00901600
H	4.42106300	-0.81063400	4.44893400
H	3.19445600	1.67098600	1.76019400
H	4.40681000	3.69934500	1.10779400
H	2.43397100	-0.74567500	5.96450300
H	4.82792100	4.17136800	-1.31033400

H	4.85481100	-5.21239200	-1.02566800
H	4.02918400	2.57126100	-3.02104000
H	2.86176900	-5.36567200	0.43373500
H	0.16721000	-0.56127300	5.00183500
C	-0.59677700	-0.42293000	2.47015600
H	-0.79388700	0.52251800	1.95504700
H	-0.82260100	-1.22601300	1.75566800
H	-1.30089400	-0.51288300	3.30494800
C	1.31507500	-3.45084500	1.39524500
H	1.66115900	-3.27794000	2.42417200
H	0.47567800	-2.77806800	1.20533800
H	0.92934000	-4.47575400	1.34883300
C	2.72470200	0.29695000	-2.74074100
H	2.34362900	0.89455700	-3.57634400
H	3.56161800	-0.29676900	-3.13303100
H	1.93718100	-0.41077600	-2.45226100

(L6)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3392.515614

M06-L thermal correction to free energy (Hartree): 0.609507

Three lowest frequencies (cm⁻¹): 15.63, 24.04, 32.01

C	2.93135400	-1.66225400	0.79080200
C	2.30113500	-2.67497500	1.54077000
C	4.21646700	-1.89072200	0.29963100
C	2.91963500	-3.91331700	1.72263700
C	4.85325700	-3.11356800	0.50432500
C	4.19299000	-4.12445100	1.19824800
C	1.84331900	0.61461500	2.11626900
C	3.02369800	1.07138400	2.71572200
C	0.63845200	0.69815700	2.84976100
C	3.02496600	1.68460900	3.96323400
C	0.63501500	1.34260900	4.09468800
C	1.81634100	1.83700600	4.63654300
C	3.04408400	0.93035000	-0.51480100
C	3.42849200	0.48663400	-1.80053400
C	3.37441200	2.23676300	-0.14641100
C	4.21392600	1.29255200	-2.62700200
C	4.12924800	3.05851900	-0.98101800
C	4.56496800	2.57346500	-2.20950700
P	1.95205400	-0.15620800	0.46540600
Pd	0.02180100	-0.53228900	-0.67686400
O	0.22340500	-2.60097900	-2.85663200

O	0.21341400	-2.67684900	-0.59844400
C	0.41661400	-3.17827700	-1.77063400
C	0.99284900	-4.58070300	-1.75324900
C	-0.07724300	1.44764200	-1.00446500
C	-0.42753700	2.58148300	-0.31361200
S	0.32279000	1.91069100	-2.63750600
C	-0.37049200	3.79330800	-1.07842200
C	0.02587300	3.59847300	-2.37217700
H	0.15460600	4.33858600	-3.15193300
O	-0.84490600	2.59387000	1.00079200
C	-0.67318800	3.88268100	1.58760300
H	0.40119000	4.08713400	1.72907000
O	-0.65371400	5.02280600	-0.55102800
C	-1.30159000	4.94579200	0.72271400
H	-1.20128700	5.93746400	1.17180200
H	-2.37099100	4.72946400	0.57868400
H	-1.15375600	3.84019600	2.56953100
C	-5.84910500	-0.04833400	-0.24167000
C	-4.94403900	-1.05933200	0.20957700
C	-7.12775200	-0.50995600	-0.39233800
C	-5.55085900	-2.26967900	0.40023000
S	-7.23162200	-2.18066500	0.02350600
O	-5.45094700	1.22733900	-0.51114900
C	-4.17682900	1.52209700	0.07890500
O	-3.61815500	-0.81492500	0.43189800
C	-3.17359800	0.42239600	-0.17916900
C	-2.88908700	0.18966500	-1.64868700
H	-8.00021200	0.04129500	-0.71744600
H	-3.84439900	2.46078100	-0.37319900
H	-4.29839200	1.67284400	1.16172100
H	-2.23422900	0.65813600	0.33803800
H	-3.80740400	-0.09977400	-2.18055500
H	-2.51880500	1.12170200	-2.09147300
H	-5.10163900	-3.19566400	0.73466000
H	2.08296400	-4.50453000	-1.63709100
H	0.62154700	-5.16773000	-0.90696100
H	0.79171000	-5.10850600	-2.69016600
N	-1.84540200	-0.83009200	-1.79053800
H	-2.19751900	-1.73679600	-1.48497800
H	-1.56655800	-0.95491800	-2.76230200
H	4.72399200	-1.10539300	-0.25783400
H	5.85535500	-3.27606900	0.11380000
H	3.96474600	0.95101200	2.17846900
H	3.95549900	2.04164400	4.39763400

H	3.03087900	2.62512600	0.80962700
H	4.37835300	4.06894800	-0.66512300
H	1.78703800	2.32977800	5.60686300
H	5.17200500	3.19755900	-2.86263700
H	4.67398500	-5.08998000	1.34531100
H	4.53542500	0.93176900	-3.59997300
H	2.41707700	-4.70266300	2.27607600
H	-0.29121400	1.44678900	4.65201400
O	1.10813600	-2.33067300	2.07595400
O	-0.45705500	0.10923300	2.32547900
O	2.96838100	-0.73737900	-2.15875500
C	0.25000500	-3.36705400	2.51521400
H	0.09905700	-4.10390600	1.71660000
H	0.64239100	-3.85984700	3.41470000
H	-0.69946500	-2.88142500	2.75183900
C	-1.68309000	0.25869200	3.02079400
H	-1.97505400	1.31530200	3.08477700
H	-2.42352000	-0.29257900	2.43691300
H	-1.62354400	-0.16868500	4.03054900
C	3.28171000	-1.21974600	-3.45469300
H	4.36253800	-1.37739200	-3.56689900
H	2.74704200	-2.16565300	-3.54970900
H	2.93117900	-0.52407900	-4.22858500

(L7)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3346.648208

M06-L thermal correction to free energy (Hartree): 0.487712

Three lowest frequencies (cm⁻¹): 12.58, 15.18, 30.34

C	2.83810200	-1.93124600	0.59070600
C	2.23563500	-2.91894300	1.37412700
C	4.07570700	-2.23726000	0.01410700
C	2.78857800	-4.17449900	1.56006500
C	4.65650400	-3.49019500	0.19135100
C	4.00837900	-4.46040600	0.95223400
C	1.89290700	0.29150800	2.06775900
C	3.07911300	0.67150400	2.71650500
C	0.71433800	0.33961500	2.81648200
C	3.06962000	1.14703200	4.02162800
C	0.68088900	0.81407900	4.11986900
C	1.86454300	1.23065800	4.71808600
C	3.08507400	0.72982100	-0.54963500
C	3.44276900	0.36619700	-1.85016200

C	3.49398800	1.99733300	-0.11551300
C	4.23643000	1.14968500	-2.66961800
C	4.27445200	2.81615100	-0.92642200
C	4.66166100	2.38619600	-2.19369000
P	1.94198100	-0.35671400	0.36319900
Pd	-0.02232600	-0.55491600	-0.73558600
O	-0.04807800	-2.64613200	-2.85769200
O	-0.03383700	-2.69386300	-0.60321300
C	0.05621800	-3.24137500	-1.77091700
C	0.35677600	-4.72571300	-1.73378700
C	0.02743300	1.43268600	-1.02339100
C	-0.16611200	2.54041500	-0.23801700
S	0.35483000	1.96633200	-2.64917700
C	-0.06303300	3.79240800	-0.92708700
C	0.21842500	3.65174200	-2.25750900
H	0.35145200	4.42689500	-3.00162200
O	-0.46807000	2.48306500	1.10390900
C	-0.18145800	3.71747600	1.76130800
H	0.90943500	3.84443700	1.85434100
O	-0.20463100	4.99763000	-0.29880100
C	-0.78559700	4.87307600	1.00425100
H	-0.59622700	5.82357800	1.50979000
H	-1.87272700	4.73229000	0.90903500
H	-0.61155900	3.63624400	2.76333500
C	-5.77001800	0.12125800	0.08708600
C	-4.83115600	-0.88864800	0.46716600
C	-7.05364100	-0.34582200	0.01859700
C	-5.41838200	-2.10392800	0.68690400
S	-7.12154900	-2.01998300	0.42722200
O	-5.39656200	1.40127600	-0.19724900
C	-4.08718900	1.69790200	0.30983100
O	-3.49574400	-0.63816000	0.60608800
C	-3.09815200	0.60379500	-0.02304400
C	-2.92104600	0.39080200	-1.51378400
H	-7.94817800	0.20326400	-0.24427500
H	-3.79451800	2.64338200	-0.15577400
H	-4.13777800	1.83836900	1.39865300
H	-2.12892600	0.83744500	0.43235300
H	-3.88545200	0.16223900	-1.98977200
H	-2.53016300	1.31266000	-1.96025200
H	-4.94314100	-3.02951700	0.98478500
H	1.44050900	-4.86026300	-1.62192300
H	-0.11632700	-5.21522100	-0.87686800
H	0.05032400	-5.21785500	-2.66100000

N	-1.95003000	-0.68297400	-1.75239500
H	-2.33693000	-1.57611000	-1.44891100
H	-1.74716500	-0.79098700	-2.74465000
H	4.60081300	-1.48471400	-0.56895200
H	5.62012800	-3.70436100	-0.26447700
H	4.02454600	0.59300500	2.18073100
H	4.00133600	1.44600700	4.49532800
H	3.18736600	2.35465500	0.86487500
H	4.58273800	3.79305900	-0.56206500
H	1.84573400	1.60363200	5.73961600
H	5.28169100	3.01929300	-2.82388300
H	4.45614400	-5.44242200	1.08649200
H	4.49155400	0.79489900	-3.66448800
H	2.26838300	-4.90204800	2.17757800
H	-0.26803700	0.83767400	4.64919900
F	-0.43866700	-0.11623500	2.29376000
F	2.96886200	-0.80244100	-2.34245100
F	1.08144600	-2.62063800	2.00564000

(L8)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3346.656508

M06-L thermal correction to free energy (Hartree): 0.485844

Three lowest frequencies (cm⁻¹): 14.75, 17.27, 25.74

C	2.99802400	-1.69198300	-0.40708300
C	2.65262500	-3.05047100	-0.31828700
C	4.23747600	-1.34266800	-0.95630800
C	3.52423500	-4.03659600	-0.75969700
C	5.11756500	-2.32153000	-1.40799500
C	4.74515300	-3.65256500	-1.30005400
C	1.42981600	-0.95687100	1.88332300
C	2.37912300	-1.61879500	2.67398300
C	0.18048900	-0.64273900	2.43526100
C	2.09225100	-1.95812600	3.99138800
C	-0.12040500	-0.97652300	3.75061300
C	0.84502900	-1.62939300	4.50492300
C	2.76013800	1.09131000	0.31534600
C	3.02892700	1.82421200	-0.85026100
C	3.21519600	1.57915700	1.54459000
C	3.74157000	3.01511400	-0.79679300
C	3.92510000	2.77526700	1.61521900
C	4.17377700	3.47180800	0.44178600
P	1.79590700	-0.44670800	0.17510300

Pd	-0.14362400	-0.43075200	-1.00871900
O	-0.38052700	-2.71058700	-2.81198700
O	-0.45087600	-2.52296100	-0.57357900
C	-0.49950300	-3.19978000	-1.67503700
C	-0.68702300	-4.69151800	-1.49801000
C	-0.03337200	1.53294800	-1.32565100
C	-0.12136000	2.53796600	-0.39947700
S	0.01251600	2.24839600	-2.91277500
C	-0.15251000	3.85956100	-0.94286300
C	-0.08491000	3.87440800	-2.30979100
H	-0.07978000	4.73048800	-2.97271300
O	-0.18073800	2.30286100	0.95657700
C	0.16196300	3.47450600	1.70141300
H	1.24674300	3.65064600	1.62634600
O	-0.22451300	4.97756300	-0.16183000
C	-0.60018300	4.67023500	1.18690500
H	-0.37669500	5.56530300	1.77254100
H	-1.68301100	4.47655900	1.23040700
H	-0.09187800	3.25883200	2.74295300
C	-5.78284800	0.24787900	0.18721800
C	-4.82089900	-0.78021500	0.43741300
C	-7.06662000	-0.22285300	0.15796000
C	-5.38942000	-2.01342500	0.59770700
S	-7.10474200	-1.92342600	0.44110100
O	-5.43010300	1.54780100	-0.02669200
C	-4.09258000	1.81563000	0.41777700
O	-3.47967200	-0.53015000	0.51707300
C	-3.12694500	0.75154000	-0.05381200
C	-3.05332200	0.64106400	-1.56428000
H	-7.97717200	0.33619000	-0.01381300
H	-3.82692700	2.79313600	0.00468300
H	-4.07529300	1.87675500	1.51478700
H	-2.12787100	0.96235200	0.34704900
H	-4.05309300	0.47092200	-1.98876600
H	-2.66834100	1.58339900	-1.97053200
H	-4.89448700	-2.95533000	0.79559300
H	0.29523600	-5.16760800	-1.38344600
H	-1.26911500	-4.92704100	-0.60233200
H	-1.16447100	-5.13201600	-2.37769400
N	-2.13151100	-0.43739700	-1.94548400
H	-2.52925200	-1.33692000	-1.67544200
H	-2.01876900	-0.47092700	-2.95694600
H	4.53401700	-0.29804500	-1.02618100
H	6.08392500	-2.06151100	-1.83118000

H	3.27125400	-5.09118200	-0.68917400
H	1.68836800	-3.33392700	0.09985700
H	3.35484200	-1.87107200	2.26052300
H	2.81768200	-2.47017800	4.61749300
H	-1.08680400	-0.74532700	4.19036800
H	-0.55898900	-0.12380700	1.82500000
H	3.00764200	1.03591700	2.46481900
H	4.27944600	3.16848000	2.56402200
H	3.95286200	3.59229600	-1.69297300
H	2.65952400	1.46841700	-1.81143000
F	5.59476400	-4.60427700	-1.72578600
F	4.85085500	4.63195000	0.50620600
F	0.56180400	-1.95910200	5.77678600

(L9)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3346.653773

M06-L thermal correction to free energy (Hartree): 0.487806

Three lowest frequencies (cm⁻¹): 15.95, 21.28, 25.48

C	-2.53406200	2.04438500	0.78310800
C	-1.65259400	2.83859800	1.52607700
C	-3.77428500	2.56029600	0.39582000
C	-2.02662100	4.13448000	1.84031500
C	-4.12327100	3.86632700	0.73470800
C	-3.24745600	4.67146600	1.45589300
C	-2.04530700	-0.48148500	1.98137700
C	-3.19575000	-0.43138900	2.78282000
C	-0.89815900	-1.12227700	2.45053900
C	-3.19779900	-1.04148800	4.03310100
C	-0.93009600	-1.71358300	3.70457100
C	-2.05945300	-1.69187900	4.50811200
C	-3.32258800	-0.34613900	-0.65165900
C	-3.49630500	0.21579400	-1.92428100
C	-4.08710600	-1.44846700	-0.26080000
C	-4.45083100	-0.33205000	-2.76298100
C	-5.03391400	-1.97973200	-1.13587800
C	-5.22685900	-1.42477000	-2.39675100
P	-1.98365700	0.35298000	0.36167300
Pd	0.01786500	0.24303400	-0.71577600
O	-1.29911500	2.60091900	-2.07113300
O	0.41348200	2.34138000	-0.63380800
C	-0.39972900	3.05345800	-1.34260300
C	-0.17393900	4.54766500	-1.23806900

C	-0.17445300	-1.75514100	-0.89993400
C	0.47731700	-2.79976900	-0.28755600
S	-1.06342800	-2.39771500	-2.25657700
C	0.25421400	-4.08294700	-0.88056100
C	-0.56608700	-4.03198500	-1.97342900
H	-0.91264700	-4.85241100	-2.58949400
O	1.32429500	-2.65336400	0.79411500
C	1.47996200	-3.88684900	1.50297300
H	0.54488600	-4.13111500	2.02966500
O	0.79012500	-5.23786000	-0.38327500
C	1.84909300	-4.99288700	0.54721100
H	2.01220900	-5.93663800	1.07391000
H	2.76621800	-4.72850000	-0.00174000
H	2.26705400	-3.71782700	2.24288100
C	5.88079400	0.30710500	-0.04922600
C	4.89790700	1.34471300	-0.01024100
C	7.12966600	0.76968200	-0.35929400
C	5.41695900	2.57907600	-0.28607400
S	7.11007300	2.47779100	-0.59855100
O	5.57121500	-1.00201200	0.17540300
C	4.31145300	-1.14007800	0.84686600
O	3.58629000	1.10698800	0.28701200
C	3.24012800	-0.29392500	0.19588900
C	2.98552800	-0.66781500	-1.25029600
H	8.04590800	0.20197400	-0.45472000
H	4.05323300	-2.19998200	0.78858900
H	4.42481000	-0.85548100	1.90208100
H	2.30481800	-0.38447400	0.76209800
H	3.90688000	-0.56480800	-1.84124200
H	2.66535000	-1.71432700	-1.30115000
H	4.89730500	3.52761600	-0.32242900
H	0.08507000	4.83802800	-0.21424300
H	0.66531700	4.84226600	-1.87986000
H	-1.06018100	5.10010100	-1.56301100
N	1.91398900	0.17168000	-1.80376300
H	2.21327500	1.14774600	-1.81280400
H	1.73883900	-0.09051900	-2.77234800
H	-4.46914700	1.94904500	-0.17495900
H	-5.08852000	4.26342100	0.42836100
H	-0.67284200	2.47300900	1.82636500
H	-4.08774600	0.08452800	2.42856400
H	-4.09219800	-1.00932900	4.65082600
H	0.00835400	-1.17150800	1.85112600
H	-3.94025500	-1.90192600	0.71700300

H	-5.62716900	-2.83951000	-0.83287000
H	-2.88391500	1.05784300	-2.24978000
H	-2.04027000	-2.16856900	5.48458500
H	-5.95891300	-1.82584800	-3.09255400
H	-3.49376600	5.69660200	1.71823100
F	0.18345100	-2.32911200	4.15224100
F	-4.62638200	0.20734400	-3.98544500
F	-1.15836000	4.91006000	2.52019200

(L10)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -5071.515794

M06-L thermal correction to free energy (Hartree): 0.504936

Three lowest frequencies (cm⁻¹): 9.71, 11.62, 14.67

C	-1.78608500	1.87911700	0.28205800
C	-1.01132400	3.00633200	0.58872600
C	-3.17016800	2.00245800	0.19965000
C	-1.61962300	4.24089600	0.76301300
C	-3.77302400	3.24754900	0.39318100
C	-3.00562300	4.37122800	0.66271800
C	-0.39212000	-0.14250200	1.69901400
C	-1.31349900	-0.52639900	2.67485000
C	0.96050600	-0.04737800	2.03194000
C	-0.87408300	-0.84317700	3.96009500
C	1.39078700	-0.36402700	3.31425200
C	0.47667000	-0.76954800	4.28428200
C	-2.10286600	-0.91362500	-0.54321100
C	-2.85074600	-0.63730800	-1.68922900
C	-2.09123200	-2.21127100	-0.02251300
C	-3.60386600	-1.64641000	-2.28679400
C	-2.82306200	-3.21480500	-0.64450300
C	-3.59028800	-2.93791400	-1.77509400
P	-0.88560800	0.31430300	0.00297600
Pd	0.87259000	0.38194300	-1.42698900
O	-1.10760800	2.10459500	-2.74534600
O	0.85963500	2.49356200	-1.72271600
C	-0.20806100	2.86849500	-2.35290000
C	-0.31726900	4.35774400	-2.59762400
C	0.87350700	-1.63513900	-1.34115500
C	1.31770200	-2.59393600	-0.46202300
S	0.10644300	-2.43852100	-2.68373900
C	1.02509100	-3.94274400	-0.84656000

C	0.35587400	-4.02634400	-2.03610300
H	0.02283300	-4.91624400	-2.55546900
O	2.02172600	-2.31983300	0.68813700
C	1.94331700	-3.39870700	1.62334300
H	0.92651400	-3.44755700	2.04705200
O	1.35881400	-5.02168500	-0.08082900
C	2.29803200	-4.70098800	0.95166500
H	2.26420400	-5.53410100	1.65804500
H	3.30877700	-4.64080000	0.52162900
H	2.65015300	-3.16025300	2.42344900
C	6.69029200	0.20959300	-1.14194500
C	5.73191200	1.24734400	-0.91975300
C	7.93406900	0.69207300	-1.44325600
C	6.26450700	2.50001200	-1.05077500
S	7.93986400	2.41614900	-1.45041100
O	6.36738100	-1.11400900	-1.08146200
C	5.13300200	-1.32529700	-0.38288300
O	4.42858400	0.99113700	-0.59761600
C	4.05488500	-0.38015200	-0.86208900
C	3.71593500	-0.54987100	-2.32965000
H	8.83290300	0.12860400	-1.65560200
H	4.85012300	-2.36385900	-0.57477100
H	5.29134000	-1.19506200	0.69677400
H	3.15159600	-0.53817200	-0.26215700
H	4.60399500	-0.38448800	-2.95575700
H	3.36362200	-1.57328400	-2.49977000
H	5.76408100	3.45232800	-0.93493000
H	0.38025600	4.93214400	-1.98146400
H	-0.10503500	4.57548400	-3.65096700
H	-1.34122000	4.69392800	-2.40107200
N	2.63443100	0.37360000	-2.70798900
H	2.97424300	1.33540200	-2.67571100
H	2.35879200	0.20182700	-3.67381800
H	-3.79508400	1.13756000	-0.01648600
H	-2.37627300	-0.59236300	2.44019500
H	-1.47943000	-2.45678200	0.84179700
H	0.81460200	-1.03330900	5.28290200
H	-4.15446300	-3.72795100	-2.26389800
H	-3.47778100	5.34170300	0.79084100
H	-2.80643200	0.35334400	-2.14338400
H	0.07063600	2.92455000	0.65482200
H	1.67804900	0.25276600	1.27027800
C	-5.26567400	3.33376000	0.29167000
C	-0.80265500	5.46627400	1.03876800

C	-1.89156000	-1.27558700	4.97243600
C	2.84620200	-0.28022200	3.65948500
C	-2.79751300	-4.61451300	-0.11015400
C	-4.33445500	-1.32961200	-3.55472600
F	-2.63425800	-5.51649900	-1.10001900
F	-3.95657700	-4.92910000	0.50947700
F	-1.80620800	-4.80429800	0.77985700
F	-3.46909700	-1.15956900	-4.58071400
F	-5.19013500	-2.30290000	-3.91314600
F	-5.03787100	-0.18394000	-3.45213500
F	-1.34110400	-1.55863800	6.16526400
F	-2.82260900	-0.31886000	5.17049400
F	-2.55510300	-2.37639700	4.55952600
F	3.24246000	-1.34920600	4.38314000
F	3.62221800	-0.23072200	2.55770700
F	3.12720900	0.81313400	4.39606900
F	0.51875900	5.23471100	0.93155900
F	-1.02991800	5.94943400	2.27771400
F	-1.10935600	6.45835800	0.17530000
F	-5.72217700	4.58434600	0.47599200
F	-5.86504900	2.54353400	1.20770800
F	-5.70020400	2.91671300	-0.91645700

(L11)Pd(EDOT)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -4537.620290

M06-L thermal correction to free energy (Hartree): 0.378402

Three lowest frequencies (cm⁻¹): 15.01 18.46, 25.02

C	-2.31782500	1.78597200	0.40960200
C	-1.65746300	2.82162100	1.07896000
C	-3.62517800	2.04026100	-0.00576800
C	-2.22952900	4.06818500	1.27540800
C	-4.22095900	3.28254500	0.17936900
C	-3.51950400	4.30002200	0.81315100
C	-1.22339800	-0.35606700	1.85520100
C	-2.34804600	-0.84584200	2.52466400
C	-0.03129200	-0.28003800	2.57942200
C	-2.28483200	-1.31705300	3.82566100
C	0.05787200	-0.76026800	3.87997000
C	-1.06902000	-1.28046800	4.50150700
C	-2.32272100	-0.88528300	-0.84178600
C	-2.69145100	-0.44318800	-2.11489800
C	-2.47950500	-2.24742800	-0.58712800

C	-3.24681600	-1.27961900	-3.06724800
C	-3.02303300	-3.11243600	-1.53022400
C	-3.41580700	-2.62702100	-2.76964900
P	-1.32585400	0.27119600	0.15059200
F	-0.44099600	2.59878200	1.58758000
F	1.06131400	0.28685300	2.06886800
F	-2.47507800	0.83790700	-2.45182700
F	-3.36798400	-1.79519600	4.43547100
F	-0.99250300	-1.73419600	5.74651400
F	1.22109800	-0.72318100	4.53098800
F	-3.53009700	-0.87542300	1.89836300
F	-2.08049300	-2.79388500	0.56671300
F	-3.15311200	-4.40883100	-1.24951200
F	-3.93866400	-3.44558200	-3.67598500
F	-3.59283200	-0.81040100	-4.26470400
F	-4.37282200	1.09488600	-0.58199200
F	-5.47161700	3.49356800	-0.23073700
F	-4.08801000	5.48627200	0.99708800
F	-1.56260100	5.03106800	1.91092900
Pd	0.62466700	0.56795300	-0.93318000
O	0.47587200	2.40875400	-3.24771500
O	0.40956200	2.69052100	-1.01283300
C	0.26955500	3.09733700	-2.23497400
C	-0.23520100	4.51883700	-2.35543400
C	0.74969200	-1.44450500	-1.02096900
C	1.04249800	-2.45505200	-0.13936600
S	0.43785500	-2.15202800	-2.58434600
C	1.00970100	-3.77204800	-0.70363700
C	0.68989600	-3.77746900	-2.03290700
H	0.60188200	-4.62813600	-2.69721500
O	1.37400600	-2.25435200	1.18062400
C	1.16933900	-3.43654200	1.96125300
H	0.08854500	-3.61280100	2.08002800
O	1.24254400	-4.89891500	0.02980300
C	1.83222400	-4.62027600	1.30540300
H	1.70436700	-5.52798300	1.90002000
H	2.90738200	-4.42692900	1.17750300
H	1.60680300	-3.23008500	2.94240100
C	6.47610500	0.25485600	-0.22161200
C	5.50773100	1.24231800	0.14309200
C	7.73421700	0.77195500	-0.36371700
C	6.04738200	2.49166900	0.27698600
S	7.74128900	2.46686000	-0.04641700
O	6.14900200	-1.05270900	-0.42843200

C	4.87703600	-1.37925300	0.14840000
O	4.19011100	0.94246800	0.34600700
C	3.82670500	-0.34812900	-0.19827300
C	3.57894300	-0.22643500	-1.68895100
H	8.64211700	0.24834300	-0.63302400
H	4.60818900	-2.35986200	-0.25475100
H	4.97704000	-1.45850600	1.23998400
H	2.89203600	-0.60132600	0.31361200
H	4.50613800	0.04062700	-2.21563000
H	3.23404100	-1.19170500	-2.07653000
H	5.54176100	3.41064700	0.54361000
H	-1.33023600	4.50796100	-2.27042800
H	0.14500100	5.15632300	-1.55130200
H	0.02087800	4.94995200	-3.32703100
N	2.53336100	0.77187000	-1.94508800
H	2.86716900	1.69827600	-1.67788200
H	2.30705700	0.83417100	-2.93663800

(L4)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2500.237302

M06-L thermal correction to free energy (Hartree): 0.505980

Three lowest frequencies (cm⁻¹): 17.72, 19.58, 28.72

C	-2.91265900	1.77716200	0.32291600
C	-2.25994500	2.82270700	0.99171100
C	-4.17236200	2.00668900	-0.23871300
C	-2.85945700	4.07278500	1.09915400
C	-4.76567400	3.26400300	-0.13697100
C	-4.11326000	4.29721600	0.53077800
C	-2.19366000	-0.32270500	2.05710700
C	-3.44207200	-0.51093200	2.66662600
C	-1.03507700	-0.38211000	2.83819300
C	-3.52335500	-0.78138500	4.02801200
C	-1.11844700	-0.64517200	4.20405700
C	-2.36142800	-0.84984800	4.79758800
C	-3.14961500	-0.97025100	-0.63823900
C	-3.38566300	-0.66127800	-1.98702600
C	-3.61081300	-2.18582800	-0.12219300
C	-4.10253400	-1.54143400	-2.79066900
C	-4.32202800	-3.06671700	-0.93455000
C	-4.57272600	-2.74531000	-2.26619600
P	-2.07055700	0.15295500	0.30075800
Pd	0.01319100	0.18181400	-0.57938500

O	-1.22108600	1.96569900	-2.53614300
O	0.17196300	2.33756800	-0.80890100
C	-0.57213800	2.72302500	-1.78822900
C	-0.67302400	4.22187000	-1.98313200
C	5.88849000	-0.37650300	0.34326500
C	5.04819700	0.77718900	0.43584500
C	7.20182500	-0.06159200	0.13069700
C	5.73845400	1.94942600	0.29726100
S	7.41830900	1.64719200	0.04855800
O	5.40151100	-1.64745800	0.43490400
C	4.10376700	-1.66933000	1.04338400
O	3.70182800	0.69309800	0.65535600
C	3.18834000	-0.63896700	0.42112200
C	2.96932100	-0.84645500	-1.06319500
H	8.03910000	-0.73826800	0.02176200
H	3.71485800	-2.67981200	0.89085000
H	4.20045800	-1.48256100	2.12177900
H	2.21563500	-0.64789200	0.93117700
H	3.92243200	-0.76715400	-1.60518100
H	2.56456300	-1.85097800	-1.23316300
H	5.35003800	2.95898200	0.32783000
H	-1.63126300	4.56208600	-1.56913800
H	0.12681500	4.76560300	-1.47229000
H	-0.67181000	4.47847600	-3.04721600
N	1.99005500	0.13097200	-1.55537000
H	2.35877700	1.07616200	-1.44571700
H	1.84513800	-0.00118800	-2.55515500
H	-4.69941400	1.20377700	-0.75070200
H	-5.74723600	3.43066500	-0.57662000
H	-4.35335800	-0.44220300	2.07168100
H	-4.49596600	-0.93107400	4.49227400
H	-3.40539000	-2.45598400	0.91242300
H	-4.67746900	-4.00952200	-0.52330200
H	-2.42770000	-1.05698100	5.86391400
H	-5.12910800	-3.43501200	-2.89810300
H	-4.58124000	5.27651000	0.61096500
H	-4.28714300	-1.29108800	-3.83372400
H	-2.34296700	4.87609800	1.62105600
H	-0.21156000	-0.68702400	4.80378700
C	-0.01810400	-1.83427000	-0.54088100
C	0.30642900	-2.64474600	0.55411600
C	-0.28230900	-2.46104300	-1.76886700
C	0.37778500	-4.03507900	0.42361500
H	0.51172000	-2.20136500	1.52958600

C	-0.21275000	-3.84780300	-1.90123500
H	-0.55263500	-1.85866700	-2.63918400
C	0.11836200	-4.64131200	-0.80283100
H	0.63791200	-4.64295700	1.29012400
H	-0.41849500	-4.30982500	-2.86692200
H	0.17149000	-5.72412800	-0.90304900
H	-2.98283900	0.26489900	-2.40091000
H	-1.27295100	2.65432000	1.42136500
H	-0.06712000	-0.20679500	2.36395000

(L5)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2618.199555

M06-L thermal correction to free energy (Hartree): 0.588504

Three lowest frequencies (cm⁻¹): 15.81, 20.84, 33.10

C	3.09741900	-1.53440000	-0.17003700
C	2.77252000	-2.85902700	0.20056400
C	4.26341500	-1.29190800	-0.90837600
C	3.61713400	-3.88985800	-0.22405900
C	5.09166400	-2.33381300	-1.31323200
C	4.75995200	-3.64251300	-0.97739100
C	2.06937400	-0.29336200	2.15716100
C	3.35920000	-0.39552100	2.70720700
C	0.94465200	-0.42519600	3.00308600
C	3.56153000	-0.58433100	4.06739400
C	1.17729800	-0.60851000	4.37402900
C	2.45680000	-0.68440200	4.90849600
C	2.93240000	1.38949200	-0.09268600
C	3.01482200	1.80307600	-1.44567600
C	3.42191900	2.23139300	0.91279400
C	3.59436500	3.04554100	-1.72093600
C	3.99285000	3.46382600	0.61148500
C	4.07437400	3.87597700	-0.71344700
P	2.00493300	-0.13966100	0.32326400
Pd	-0.05191200	-0.12311600	-0.67007300
O	-0.11804800	-1.34453800	-3.41040500
O	0.08724300	-2.19607700	-1.33061200
C	0.16527500	-2.26328300	-2.61552300
C	0.69851900	-3.57970000	-3.14475500
C	-6.01333300	0.27772300	0.24331400
C	-5.03722900	-0.69031100	0.63992600
C	-7.27255400	-0.24681500	0.14647700
C	-5.57334000	-1.93193900	0.84329400

S	-7.27235600	-1.92408900	0.54667400
O	-5.69192600	1.57519400	-0.02767300
C	-4.41519900	1.92574000	0.52426200
O	-3.71680300	-0.38109800	0.80663000
C	-3.36867900	0.88463400	0.19729900
C	-3.15370700	0.69776900	-1.29068500
H	-8.18589500	0.26257500	-0.13160900
H	-4.15103000	2.89319500	0.08795600
H	-4.50584300	2.03866700	1.61323700
H	-2.41634500	1.16100500	0.66643300
H	-4.08772700	0.37453700	-1.77324500
H	-2.86837400	1.65754500	-1.73334700
H	-5.06221400	-2.83665700	1.14568700
H	1.79425700	-3.51758300	-3.18887200
H	0.44917500	-4.41737600	-2.48554800
H	0.33632300	-3.78071900	-4.15731400
N	-2.07825100	-0.26777300	-1.52624400
H	-2.37544000	-1.18874900	-1.20396300
H	-1.86758500	-0.37961600	-2.51999600
H	4.53823000	-0.26904100	-1.15955000
H	5.99140000	-2.11779200	-1.88571000
H	4.22292500	-0.33065200	2.04463500
H	4.57208000	-0.65743400	4.46347300
H	3.33454400	1.93613500	1.95547600
H	4.35994700	4.09999400	1.41443400
H	2.59020500	-0.83362200	5.97822900
H	4.51074900	4.84066500	-0.96606400
H	5.39304900	-4.47002900	-1.29228900
H	3.65941300	3.36586400	-2.76070100
H	3.36465700	-4.91330100	0.05372500
H	0.31537100	-0.71023100	5.03265300
C	-0.16883500	1.87792700	-0.37084900
C	0.10825000	2.59585900	0.80045000
C	-0.52447800	2.61884000	-1.51036700
C	0.02127600	3.98841500	0.83884700
H	0.44184900	2.07755000	1.70221000
C	-0.61023300	4.01179500	-1.47912600
H	-0.72963400	2.10283700	-2.45200500
C	-0.33974800	4.70395400	-0.30026500
H	0.25220200	4.51485300	1.76523800
H	-0.88571800	4.55491100	-2.38305700
H	-0.40231500	5.79044800	-0.27220700
C	1.60872100	-3.20092400	1.07842200
H	1.88720400	-3.14680600	2.14075700

H	0.75955200	-2.52955200	0.91905400
H	1.26197400	-4.22134000	0.88118700
C	-0.48107100	-0.45382400	2.53802900
H	-0.76396000	0.43019900	1.95746600
H	-0.68216400	-1.31647400	1.88694900
H	-1.16045800	-0.52581300	3.39445900
C	2.47156200	0.99983800	-2.58806300
H	1.37228000	1.01063900	-2.59282700
H	2.81495500	1.40721500	-3.54530600
H	2.75673300	-0.05874500	-2.55421100

(L6)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2843.870684

M06-L thermal correction to free energy (Hartree): 0.599987

Three lowest frequencies (cm⁻¹): 18.86, 20.63, 29.77

C	2.94477300	-1.54157500	0.27212900
C	2.36438600	-2.74031800	0.73094300
C	4.19635300	-1.58923200	-0.34137900
C	3.00179400	-3.96321900	0.51327100
C	4.85129100	-2.80398500	-0.53555800
C	4.24188100	-3.98540600	-0.12167300
C	1.94368200	0.20457200	2.26405100
C	3.17459000	0.37717300	2.90847800
C	0.77994500	0.10066400	3.05600000
C	3.26887500	0.51045800	4.28925100
C	0.87016200	0.25202500	4.44550000
C	2.10516100	0.46011200	5.05070400
C	2.98220400	1.32179600	-0.21355400
C	3.24054800	1.31501700	-1.60411500
C	3.35874800	2.44823900	0.52104100
C	3.92150100	2.37405800	-2.20655900
C	4.01999400	3.51830500	-0.07940000
C	4.31057600	3.46931900	-1.43853200
P	1.94358100	-0.02743100	0.44990300
Pd	-0.02699600	-0.08357200	-0.67430200
O	0.01560400	-1.45213200	-3.38000900
O	0.14066600	-2.18575000	-1.24611500
C	0.28966000	-2.31186300	-2.51870600
C	0.90896200	-3.63006200	-2.94631100
C	-5.96117400	0.48936200	0.04104900
C	-5.15049100	-0.68343600	0.15923900
C	-7.27840800	0.20395900	-0.18954100

C	-5.86720000	-1.83976200	0.02237200
S	-7.53494600	-1.49982300	-0.25823100
O	-5.44691200	1.74927600	0.12991700
C	-4.15927800	1.74543300	0.76051500
O	-3.80574000	-0.62891300	0.39676700
C	-3.25670800	0.69163200	0.16349100
C	-2.98236100	0.87941900	-1.31449300
H	-8.09651900	0.90007800	-0.31896900
H	-3.74176200	2.74463500	0.60878600
H	-4.27895300	1.56940100	1.83958900
H	-2.29799700	0.68051800	0.69682100
H	-3.90976600	0.76806300	-1.89537700
H	-2.59690200	1.89215800	-1.48265100
H	-5.50403900	-2.85815400	0.06684800
H	1.99942800	-3.55363400	-2.83189100
H	0.58113200	-4.45970500	-2.31095100
H	0.69564800	-3.85695100	-3.99502800
N	-1.95626100	-0.07746100	-1.73719000
H	-2.30753500	-1.03001300	-1.64252800
H	-1.70986500	0.02427900	-2.72086600
H	4.65981500	-0.66451300	-0.68201600
H	5.82720200	-2.82562100	-1.01563000
H	4.08185100	0.40591200	2.30435700
H	4.23817900	0.65053500	4.76133800
H	3.11927000	2.49783300	1.58111000
H	4.30668000	4.38152900	0.51654600
H	2.15221000	0.57028100	6.13245100
H	4.83577700	4.29322200	-1.91805300
H	4.73671900	-4.94144300	-0.28416400
H	4.13874800	2.35400600	-3.27087600
H	2.54243000	-4.89095200	0.84479300
H	-0.02311100	0.19634200	5.06025700
C	-0.12674300	1.91465400	-0.43590500
C	-0.49735700	2.61753400	0.71777200
C	0.13575400	2.65626100	-1.59960500
C	-0.62850900	4.00963400	0.70056400
H	-0.69572800	2.07796700	1.64465200
C	0.00947200	4.04524100	-1.61802700
H	0.44712200	2.14009600	-2.51183500
C	-0.37827700	4.72899100	-0.46544000
H	-0.92693600	4.53229700	1.60992200
H	0.21683500	4.59491500	-2.53660800
H	-0.47868800	5.81317100	-0.47615000
O	2.76716500	0.23858200	-2.28061800

O	1.19895800	-2.59613500	1.40631400
O	-0.38780600	-0.17058100	2.42108400
C	0.37311300	-3.74020200	1.53869400
H	0.20011500	-4.19833300	0.55724200
H	0.80928300	-4.47434400	2.22876400
H	-0.57431800	-3.38055600	1.94655400
C	2.97073200	0.17893300	-3.68295200
H	4.03993300	0.11559900	-3.92409300
H	2.44969900	-0.72106600	-4.01206700
H	2.53479200	1.05380500	-4.18336700
C	-1.54708400	-0.35349200	3.21916400
H	-1.84236200	0.58081500	3.71667300
H	-2.33473600	-0.66821200	2.53057900
H	-1.39147700	-1.13497000	3.97364200

(L7)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2798.004053

M06-L thermal correction to free energy (Hartree): 0.478762

Three lowest frequencies (cm⁻¹): 13.75, 21.06, 23.71

C	-2.87489800	1.72071800	0.20977000
C	-2.32431600	2.79096700	0.91886900
C	-4.02298400	1.97416200	-0.54836500
C	-2.84981700	4.07022200	0.88056200
C	-4.57322600	3.25231500	-0.60193700
C	-3.98366400	4.29864600	0.10415200
C	-2.18090700	-0.26031200	2.08636800
C	-3.45842300	-0.39291500	2.65600700
C	-1.09273900	-0.31535400	2.95767300
C	-3.62552300	-0.61849000	4.01620100
C	-1.23258700	-0.54121100	4.31934400
C	-2.50833700	-0.70008000	4.84706200
C	-3.08918800	-1.08880300	-0.53125800
C	-3.26671600	-0.96770800	-1.91155500
C	-3.58522000	-2.25436200	0.06846000
C	-3.94099300	-1.90138300	-2.67817400
C	-4.25870200	-3.21548600	-0.67990600
C	-4.44452900	-3.03630600	-2.04880100
P	-2.00987400	0.11824900	0.30665800
Pd	0.04182600	0.14680100	-0.63330200
O	0.30508400	1.94719800	-3.03750100
O	0.10189600	2.30675700	-0.82029200
C	0.13226100	2.68843500	-2.05189600

C	-0.10905700	4.17297100	-2.24914400
C	5.89725700	-0.51668600	0.37249800
C	5.07723200	0.65157400	0.46682300
C	7.22005100	-0.22470700	0.18752000
C	5.79281800	1.81176700	0.35774000
S	7.47093500	1.48036900	0.13397500
O	5.38478800	-1.77902500	0.43810700
C	4.07780100	-1.78328600	1.02719100
O	3.72633500	0.59056400	0.66189800
C	3.19071900	-0.72923500	0.40395700
C	2.98937300	-0.91388300	-1.08645800
H	8.04548200	-0.91644300	0.08353200
H	3.67267700	-2.78473000	0.85797400
H	4.16228800	-1.61055200	2.10903200
H	2.21288600	-0.72573500	0.90271300
H	3.95030900	-0.83315500	-1.61463900
H	2.58244400	-1.91387900	-1.27588100
H	5.42389700	2.82838500	0.39547400
H	-1.18534000	4.37093400	-2.15984200
H	0.38844400	4.76858000	-1.47686200
H	0.21720300	4.50438400	-3.23900700
N	2.02353300	0.07531900	-1.57663000
H	2.40231200	1.01610900	-1.47068500
H	1.85086200	-0.03868700	-2.57343100
H	-4.49927500	1.16269900	-1.09391300
H	-5.46743200	3.42820300	-1.19502400
H	-4.33360600	-0.31639000	2.01103900
H	-4.62567800	-0.72447100	4.42850900
H	-3.42821000	-2.41895700	1.13214700
H	-4.63624200	-4.10920700	-0.18904000
H	-2.62886500	-0.87433500	5.91377400
H	-4.97296100	-3.78491800	-2.63447600
H	-4.40905000	5.29870200	0.05903300
H	-4.05037200	-1.73789100	-3.74678200
H	-2.37431300	4.86249600	1.45253300
H	-0.34450900	-0.57338100	4.94429300
F	0.15976800	-0.11437800	2.49208800
F	-2.73056200	0.10862200	-2.53497700
F	-1.24808900	2.55501400	1.69975700
C	0.01011700	-1.86868900	-0.60769900
C	0.29453400	-2.67102900	0.50442500
C	-0.22232100	-2.50086500	-1.83868600
C	0.36472900	-4.06227600	0.38498800
H	0.47687400	-2.21640200	1.47783500

C	-0.15621700	-3.88947100	-1.95768300
H	-0.45601100	-1.90395000	-2.72359700
C	0.14042800	-4.67618600	-0.84477900
H	0.59687100	-4.66529900	1.26285000
H	-0.33596300	-4.35768200	-2.92553600
H	0.19303900	-5.75974300	-0.93630500

(L8)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2798.009298

M06-L thermal correction to free energy (Hartree): 0.475173

Three lowest frequencies (cm⁻¹): 17.36, 18.16, 25.91

C	2.97812100	-1.38957300	-0.59245000
C	2.53758200	-2.69967400	-0.83963400
C	4.29738700	-1.04741100	-0.91267100
C	3.38877700	-3.64404800	-1.39785500
C	5.15929700	-1.98345900	-1.47679800
C	4.68877300	-3.26569100	-1.71110200
C	1.52265900	-0.93708000	1.82775000
C	2.55586800	-1.58066500	2.52370600
C	0.26391900	-0.82062500	2.43126000
C	2.34233900	-2.09452300	3.79650600
C	0.03470000	-1.32846500	3.70521400
C	1.08162200	-1.95714000	4.36443700
C	2.78349800	1.28711600	0.47301800
C	3.18848100	2.04851100	-0.63469300
C	3.06495700	1.75893000	1.75841300
C	3.87630200	3.24172700	-0.46844700
C	3.74012600	2.96274000	1.94229700
C	4.13424600	3.68165000	0.82462100
P	1.80266800	-0.21854000	0.17658500
Pd	-0.18659100	0.02036000	-0.89352800
O	-0.51972100	-1.87780600	-3.08115700
O	-0.62112300	-2.12763700	-0.84995900
C	-0.68008900	-2.57289000	-2.06038300
C	-0.93091400	-4.06194700	-2.18322000
C	-5.87076100	0.54985200	0.35851200
C	-4.90033200	-0.49399900	0.47162900
C	-7.14826900	0.07622400	0.24016200
C	-5.45558500	-1.74266300	0.44244300
S	-7.16954000	-1.64823600	0.27443800
O	-5.52855100	1.87001800	0.34354900
C	-4.20469900	2.08152500	0.85369700

O	-3.56395400	-0.24452000	0.61128400
C	-3.21637100	1.11035100	0.24605300
C	-3.11018100	1.23259300	-1.26178100
H	-8.06339700	0.64512100	0.14048500
H	-3.94554800	3.11323400	0.60096100
H	-4.21173800	1.97292400	1.94679400
H	-2.22562800	1.26265500	0.69214800
H	-4.10276900	1.14180100	-1.72607600
H	-2.71148600	2.22332900	-1.50988400
H	-4.95266100	-2.69813900	0.51488300
H	0.01948600	-4.59877900	-2.06454200
H	-1.60462300	-4.42534400	-1.40118900
H	-1.33508500	-4.31527300	-3.16713800
N	-2.18730800	0.21891800	-1.78522600
H	-2.58666800	-0.71045600	-1.65524200
H	-2.06650000	0.33187100	-2.78976000
H	4.67187800	-0.04542100	-0.71551900
H	6.18523000	-1.72872700	-1.72734300
H	3.05959500	-4.66191100	-1.59104900
H	1.51511900	-2.97635500	-0.58636200
H	3.53994500	-1.68273700	2.06686300
H	3.13224400	-2.59774600	4.34703200
H	-0.93762600	-1.24939900	4.18331500
H	-0.54989200	-0.33640900	1.88815300
H	2.75141800	1.19220400	2.63300700
H	3.96104700	3.34279700	2.93597300
H	4.19259800	3.83901800	-1.31925200
H	2.95088100	1.70970000	-1.64308000
F	5.51664000	-4.17482600	-2.25627100
F	4.78511900	4.84652500	0.99437100
F	0.86758600	-2.45667700	5.59345200
C	-0.01049100	2.01856800	-0.96671900
C	-0.11242300	2.84188700	0.16317900
C	0.09496300	2.62930700	-2.22390300
C	-0.12497700	4.23212100	0.03995400
H	-0.17470800	2.39987000	1.16046200
C	0.09520600	4.02057900	-2.34787900
H	0.17539400	2.01578700	-3.12375200
C	-0.01835900	4.82696900	-1.21672300
H	-0.20993400	4.85190200	0.93258000
H	0.18209500	4.47356800	-3.33544300
H	-0.02123600	5.91139800	-1.31324200

(L9)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -2798.007621
M06-L thermal correction to free energy (Hartree): 0.475748
Three lowest frequencies (cm⁻¹): 12.82, 15.62, 23.89

C	-2.48715300	1.86981700	0.47547100
C	-1.55901800	2.84118700	0.86759000
C	-3.82328500	2.23008100	0.27113100
C	-1.98381400	4.15040800	1.01481900
C	-4.21907300	3.55647200	0.43206200
C	-3.30005300	4.53475200	0.79951600
C	-1.83093000	-0.33861500	2.09497800
C	-2.99331600	-0.55541400	2.84665900
C	-0.58415600	-0.37800000	2.72438100
C	-2.89987600	-0.83761900	4.20677800
C	-0.52204700	-0.65166800	4.08216400
C	-1.65930900	-0.89138600	4.83863600
C	-3.19773600	-0.80143400	-0.45778500
C	-3.67068500	-0.34036200	-1.69412200
C	-3.61575700	-2.04587400	0.02678600
C	-4.56825800	-1.12645800	-2.39674500
C	-4.52066800	-2.81079300	-0.70622100
C	-5.00882200	-2.35682900	-1.92775900
P	-1.87041800	0.15303200	0.33552200
Pd	0.09592700	-0.10261000	-0.75696300
O	-1.37539700	1.88663500	-2.45912000
O	0.50818500	1.97213700	-1.23001000
C	-0.39911900	2.49522000	-1.98410100
C	-0.20182500	3.97097500	-2.26791700
C	5.92348700	-0.46024600	0.06053400
C	5.05076000	0.66419300	-0.07695200
C	7.22361000	-0.16349300	-0.24183000
C	5.70196500	1.79661800	-0.48072600
S	7.38639100	1.49252100	-0.69400200
O	5.47552400	-1.69475300	0.42987700
C	4.18974300	-1.61949900	1.05854700
O	3.71161500	0.59487000	0.18799000
C	3.23325000	-0.76695700	0.25432500
C	2.98447900	-1.29178700	-1.14528300
H	8.07975300	-0.82459300	-0.22319400
H	3.82807600	-2.64846900	1.13405200
H	4.29936000	-1.20460400	2.06996800
H	2.27253000	-0.68866000	0.78277600
H	3.92490100	-1.32878500	-1.71349400

H	2.58547500	-2.31085700	-1.08255900
H	5.28331300	2.77884800	-0.65657100
H	-0.06210700	4.52266700	-1.33085800
H	0.70639500	4.12553100	-2.86231100
H	-1.05308300	4.39044500	-2.81102000
N	1.98618100	-0.45257200	-1.82108500
H	2.35376400	0.48893800	-1.96311400
H	1.79357300	-0.82989500	-2.74755200
H	-4.55689100	1.47969000	-0.01528300
H	-5.25830200	3.83264700	0.26714900
H	-0.51064800	2.59504300	1.02187700
H	-3.97135000	-0.50221300	2.37046400
H	-3.80304700	-1.01514300	4.78620800
H	0.32988000	-0.19089300	2.16035300
H	-3.22451700	-2.42905700	0.96731200
H	-4.84613200	-3.77591200	-0.32421000
H	-3.32153600	0.60291500	-2.11085300
H	-1.56768800	-1.10891500	5.89918800
H	-5.71264400	-2.93992300	-2.51559500
H	-3.58804800	5.57551800	0.92035000
F	0.68395500	-0.68990100	4.67972500
F	-5.02581700	-0.68278400	-3.58424000
F	-1.07713200	5.08743100	1.35914600
C	-0.12319900	-2.09520700	-0.52804800
C	0.33235900	-2.84099400	0.56649600
C	-0.65185800	-2.78923800	-1.62671200
C	0.27331200	-4.23733400	0.55824500
H	0.74132900	-2.34091600	1.44627100
C	-0.70621900	-4.18327400	-1.63907000
H	-1.03297000	-2.23487200	-2.48756700
C	-0.24469700	-4.91292400	-0.54409100
H	0.63528500	-4.79556000	1.42156700
H	-1.11731300	-4.69980400	-2.50654600
H	-0.29028000	-6.00068900	-0.54982300

(L10)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -4522.867697

M06-L thermal correction to free energy (Hartree): 0.504393

Three lowest frequencies (cm⁻¹): 10.08, 15.31, 16.09

C	-1.17441100	1.81384100	0.49761900
C	-0.13400900	2.60717300	1.00069100
C	-2.46678700	2.32903600	0.45233100

C	-0.39333800	3.90107600	1.42912400
C	-2.71528400	3.63355400	0.88393400
C	-1.68516600	4.42655900	1.36685600
C	-0.65195600	-0.74625300	1.58894200
C	-1.76682600	-0.98688000	2.39441400
C	0.61349600	-1.12470600	2.04028400
C	-1.60943200	-1.62504200	3.62371900
C	0.76329200	-1.77057200	3.26107500
C	-0.34930400	-2.02623900	4.05801800
C	-2.20840400	-0.54222800	-0.87373900
C	-2.70223800	0.17914400	-1.96785000
C	-2.69045600	-1.82887300	-0.62917400
C	-3.67405600	-0.38003100	-2.78896200
C	-3.66637400	-2.37793100	-1.46076300
C	-4.16487600	-1.66028300	-2.54098900
P	-0.74312700	0.11467100	-0.02121200
Pd	1.13636300	-0.09842500	-1.26030800
O	-0.31933000	2.21006100	-2.45467900
O	1.64764000	2.00629100	-1.38369700
C	0.74216000	2.68279500	-2.00581400
C	1.04878200	4.15804500	-2.15147500
C	6.92825200	-0.64017200	-0.82943200
C	6.03451900	0.47186700	-0.73914600
C	8.18870300	-0.27657000	-1.21534700
C	6.63010800	1.66181600	-1.05136800
S	8.28885900	1.42766600	-1.45911600
O	6.53138400	-1.92207100	-0.58219300
C	5.29361800	-1.96568300	0.13890900
O	4.72500500	0.33563700	-0.36883900
C	4.27058300	-1.03094900	-0.46993200
C	3.94024700	-1.35763800	-1.91315600
H	9.05068000	-0.91417000	-1.36252500
H	4.95484100	-3.00461400	0.09376800
H	5.46694700	-1.69293800	1.18892400
H	3.34639100	-1.04895700	0.12556000
H	4.85376300	-1.36013700	-2.52435400
H	3.49559800	-2.35773400	-1.96501800
H	6.18442300	2.64787000	-1.06181800
H	1.16622100	4.61703400	-1.16288700
H	1.99985200	4.30115100	-2.67634900
H	0.25680300	4.68037400	-2.69386100
N	2.96330400	-0.38952500	-2.42976800
H	3.38276000	0.54082400	-2.45477700
H	2.72338000	-0.62469800	-3.39135400

H	-3.29481300	1.72465200	0.08479100
H	-2.76322400	-0.69126000	2.06770700
H	-2.28291600	-2.43133100	0.18239600
H	-0.23756700	-2.54343700	5.00791500
H	-4.90970700	-2.10187800	-3.19622500
H	-1.88235700	5.44371300	1.69586000
H	-2.28579900	1.15686200	-2.20441200
H	0.88126000	2.21826900	1.03371300
H	1.48099400	-0.91337900	1.41587400
C	-4.11765300	4.15325000	0.78944700
C	0.70649000	4.77948000	1.94132700
C	-2.80179900	-1.83638900	4.50859600
C	2.11833200	-2.20250200	3.73372700
C	-4.15880700	-3.76229300	-1.16606700
C	-4.19604000	0.42006700	-3.94346300
F	-4.89872300	-4.26615600	-2.16964500
F	-4.92245100	-3.78706900	-0.05274700
F	-3.13560200	-4.61399300	-0.94796500
F	-4.65306500	-0.36571900	-4.93646200
F	-5.21927100	1.22052500	-3.57364800
F	-3.24239300	1.22041100	-4.46151400
F	-2.64943200	-2.90723100	5.30980900
F	-3.00839400	-0.77073500	5.31172200
F	-3.92884800	-2.01435000	3.79301100
F	2.10279000	-3.47673400	4.16941100
F	3.04766000	-2.12013100	2.75535200
F	2.55285000	-1.44602700	4.76074400
F	1.89630000	4.15417200	1.96873600
F	0.44739000	5.22249100	3.18783600
F	0.85028900	5.87991700	1.16742800
F	-4.24891900	5.38330800	1.31557800
F	-4.98615300	3.34102700	1.42790200
F	-4.52779500	4.21676400	-0.49513700
C	0.75613300	-2.08386300	-1.36849100
C	1.28964000	-3.06203500	-0.51883500
C	-0.02695300	-2.50710300	-2.45253600
C	1.03930500	-4.41888500	-0.74100400
H	1.91118200	-2.78496700	0.33472600
C	-0.27723200	-3.86124500	-2.67566700
H	-0.46889500	-1.76793600	-3.12474300
C	0.25216500	-4.82246100	-1.81632100
H	1.46307300	-5.15960400	-0.06349000
H	-0.90297700	-4.16188300	-3.51594700
H	0.04917100	-5.87919900	-1.98221600

(L11)Pd(Ph)(OAc)(EDOT-NH₂)

M06-L electronic energy (Hartree): -3988.974937

M06-L thermal correction to free energy (Hartree): 0.368577

Three lowest frequencies (cm⁻¹): 14.63, 17.30, 22.17

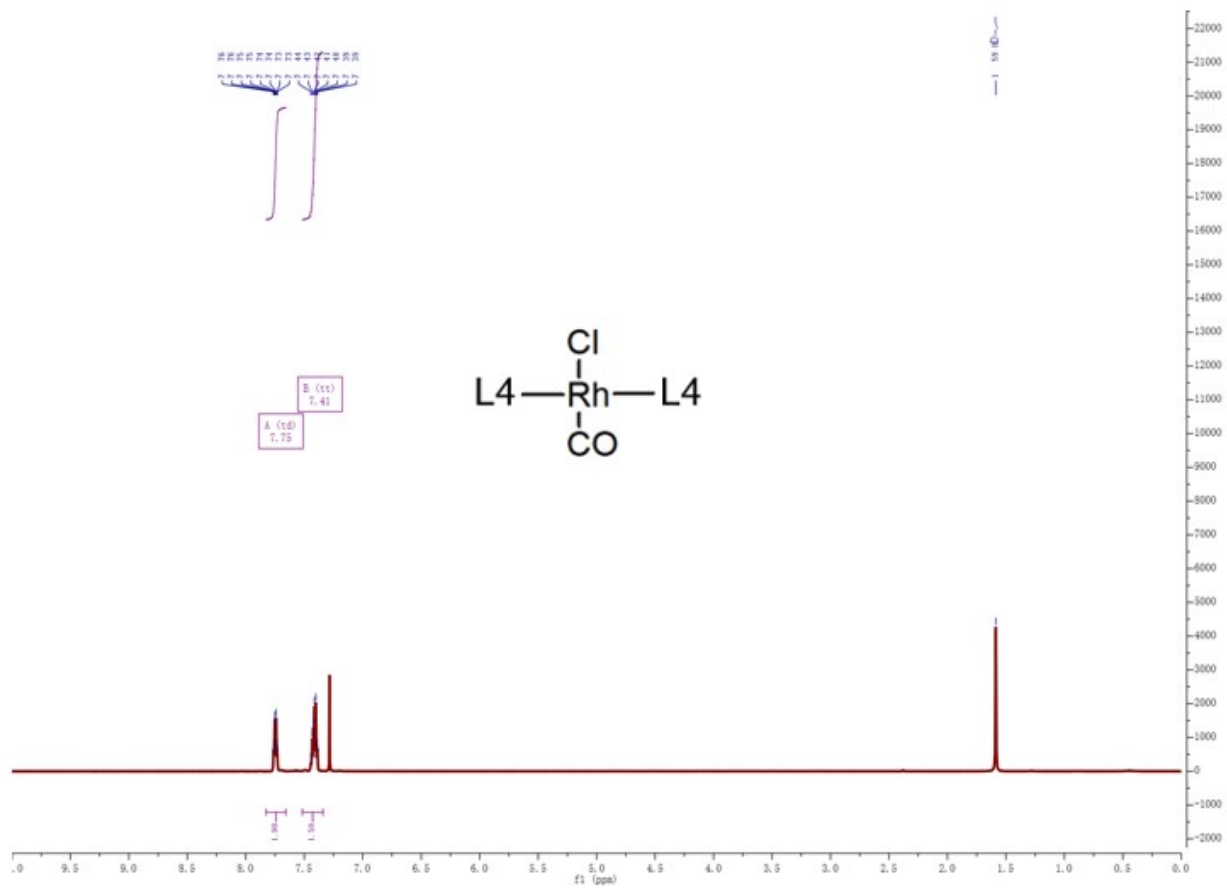
C	-2.22199100	1.65057600	-0.10801800
C	-1.61285200	2.79870200	0.40694500
C	-3.41951400	1.83014100	-0.79993300
C	-2.12182500	4.07019300	0.20107800
C	-3.95415200	3.09522700	-1.01416400
C	-3.30017700	4.21720900	-0.52113900
C	-1.48254300	-0.10606500	1.94154300
C	-2.75003300	-0.29554200	2.49824600
C	-0.41343300	0.01542800	2.83095900
C	-2.95154200	-0.41377000	3.86340700
C	-0.58879400	-0.09763700	4.20457500
C	-1.85963800	-0.31610600	4.72061000
C	-2.19283800	-1.24075900	-0.67835500
C	-2.32291100	-1.13618800	-2.06579800
C	-2.50787700	-2.47624500	-0.11371900
C	-2.78114500	-2.17466200	-2.85710100
C	-2.96497800	-3.53802700	-0.88602000
C	-3.10646400	-3.38659800	-2.25812900
P	-1.27727800	0.10559500	0.14161400
F	-0.51191100	2.67307500	1.15728900
F	0.82980100	0.25988200	2.40048000
F	-1.96231000	0.00717000	-2.66799400
F	-4.17159000	-0.61989700	4.35468600
F	-2.03294900	-0.42764700	6.03166900
F	0.45324100	0.01494400	5.02593500
F	-3.81545700	-0.38934500	1.69445200
F	-2.35305100	-2.70710800	1.19396100
F	-3.25760100	-4.70536000	-0.31406800
F	-3.54793300	-4.39739600	-2.99845100
F	-2.89699800	-2.02952500	-4.17605400
F	-4.11525800	0.79241300	-1.27377800
F	-5.10145400	3.23497000	-1.67869600
F	-3.81057500	5.42669600	-0.72802600
F	-1.49546000	5.14092500	0.68864100
Pd	0.79416800	0.17612300	-0.72934400
O	0.96716000	1.53163200	-3.39655700
O	0.65943300	2.26599100	-1.28655300

C	0.64568200	2.40554500	-2.57056900
C	0.13896000	3.75244600	-3.04548800
C	6.74348200	-0.38396800	0.19079900
C	5.91177000	0.77158200	0.32827500
C	8.05483000	-0.07079700	-0.03644900
C	6.60701300	1.94312000	0.20984000
S	8.28018500	1.63802000	-0.07704900
O	6.25055700	-1.65411200	0.25925200
C	4.96674400	-1.68298400	0.89591300
O	4.56870400	0.68961300	0.56742000
C	4.04347700	-0.63522300	0.31640900
C	3.78937500	-0.80744900	-1.16740900
H	8.88576900	-0.74932000	-0.17757500
H	4.56868600	-2.68788400	0.73116400
H	5.08835300	-1.51965400	1.97563500
H	3.08513000	-0.65197400	0.84986000
H	4.72736600	-0.69977200	-1.73054300
H	3.39376400	-1.81174700	-1.35719900
H	6.22510000	2.95357000	0.27326100
H	-0.95349800	3.69721000	-3.14536400
H	0.35779800	4.54937400	-2.32763800
H	0.54796800	4.00969300	-4.02684900
N	2.79322200	0.17453300	-1.60664400
H	3.14992000	1.11747700	-1.44841100
H	2.60669600	0.11958700	-2.60812000
C	0.87812600	-1.82723200	-0.46191500
C	1.09837900	-2.50315000	0.74286400
C	0.73319200	-2.58502000	-1.63453500
C	1.18001800	-3.89893700	0.77364900
H	1.21673400	-1.95180600	1.67515900
C	0.81266600	-3.97749300	-1.60310000
H	0.55790600	-2.08363700	-2.59013900
C	1.03629500	-4.63976500	-0.39583900
H	1.35444800	-4.40390500	1.72349300
H	0.69918200	-4.54506000	-2.52666500
H	1.09548600	-5.72627900	-0.36867400

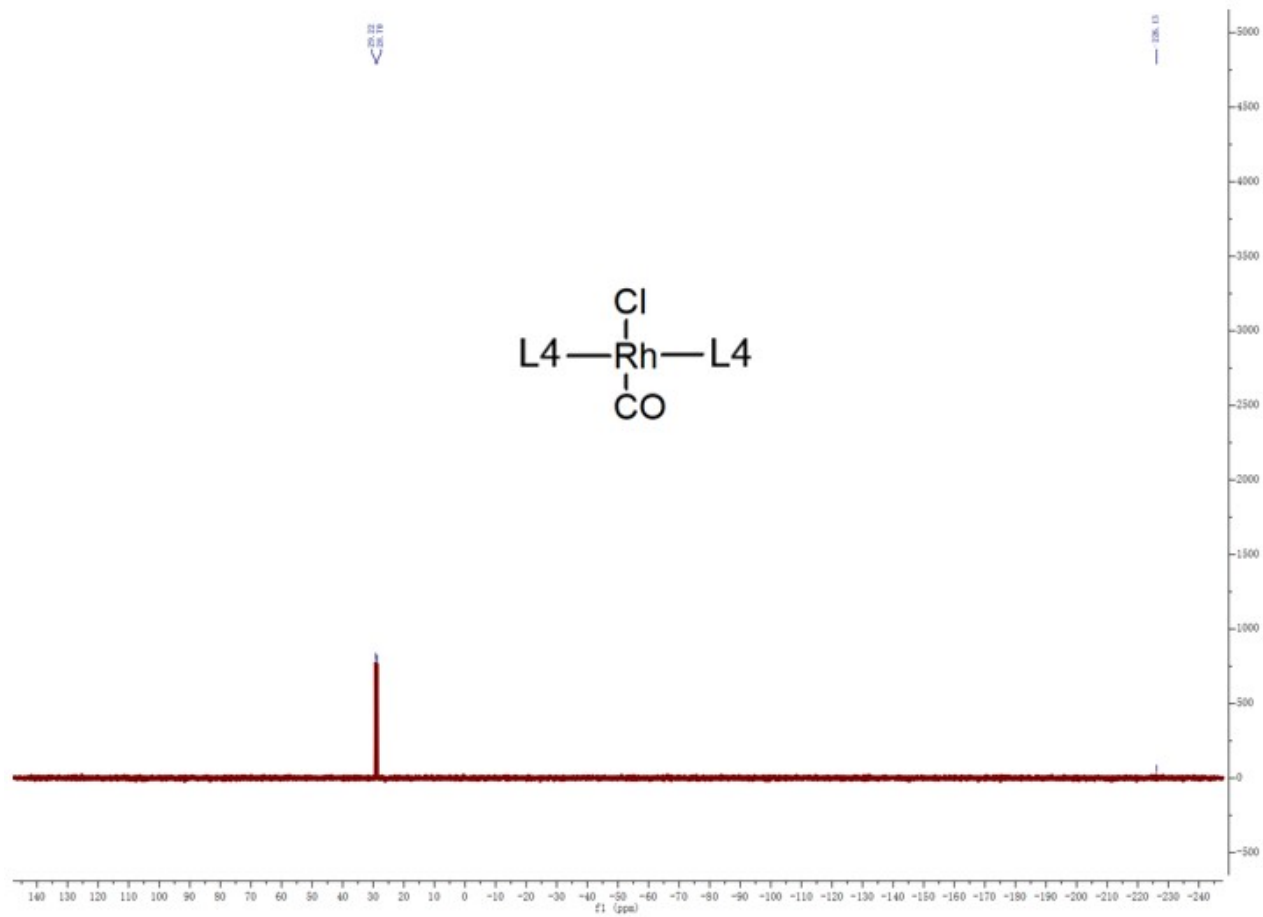
7. NMR Spectra

7.1 NMR spectra of Rh-phosphine complexes

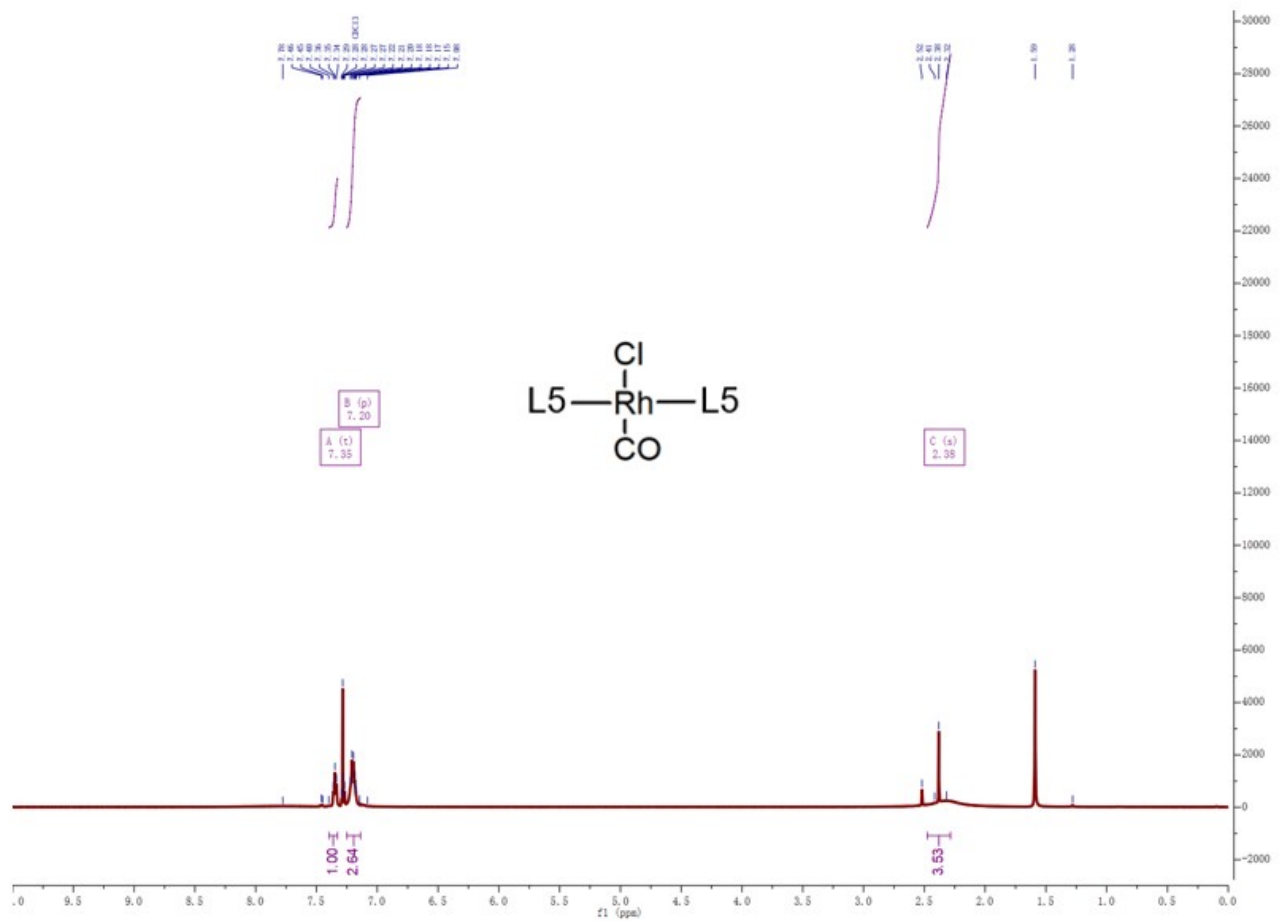
^1H NMR of $\text{RhClCO}(\text{L4})_2$ (600MHz, CDCl_3 , 323K)



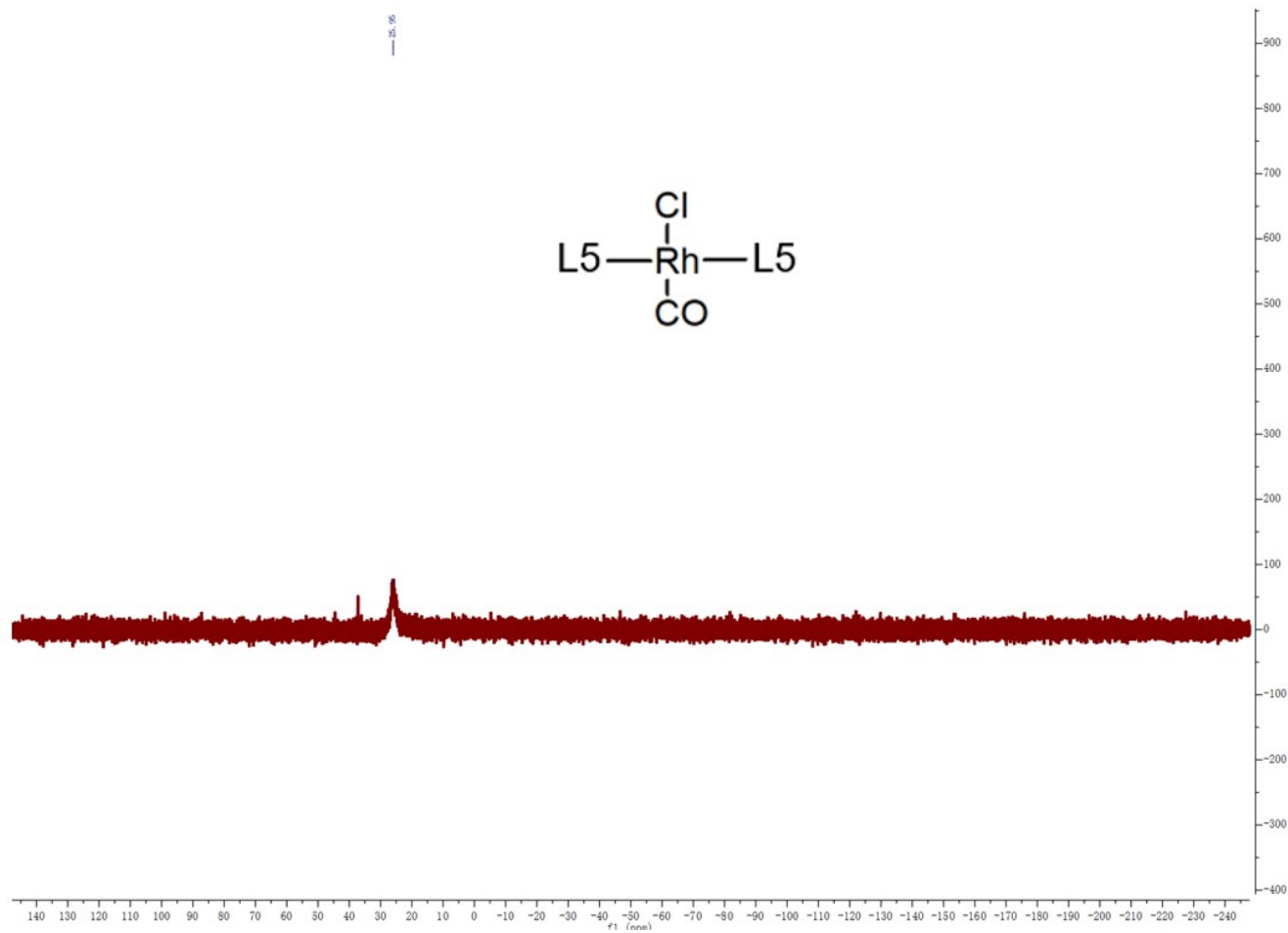
^1P NMR of $\text{RhClCO}(\text{L4})_2$ (243MHz, CDCl_3 , 323K)



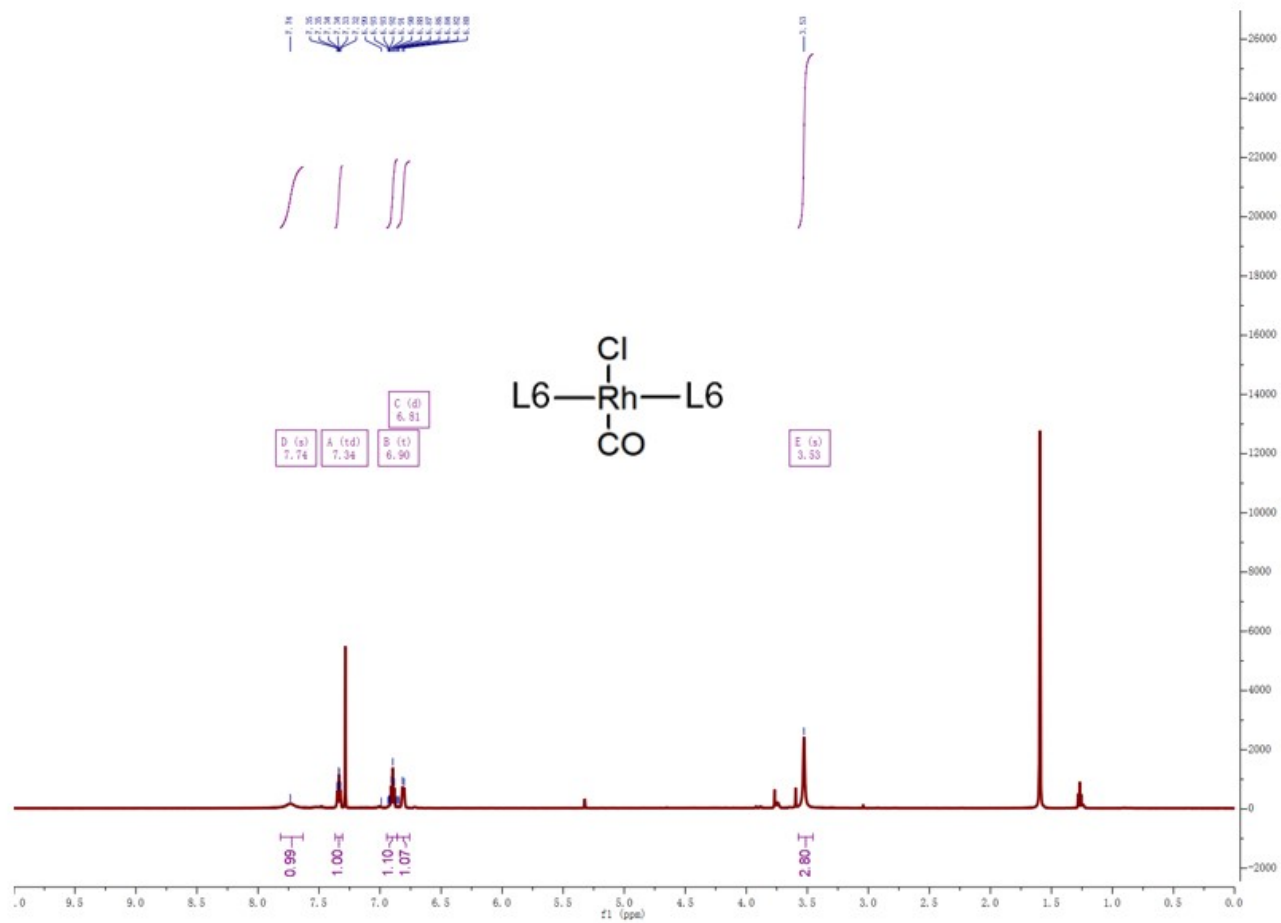
^1H NMR of $\text{RhClCO}(\text{L5})_2$ (600MHz, CDCl_3 , 323K)



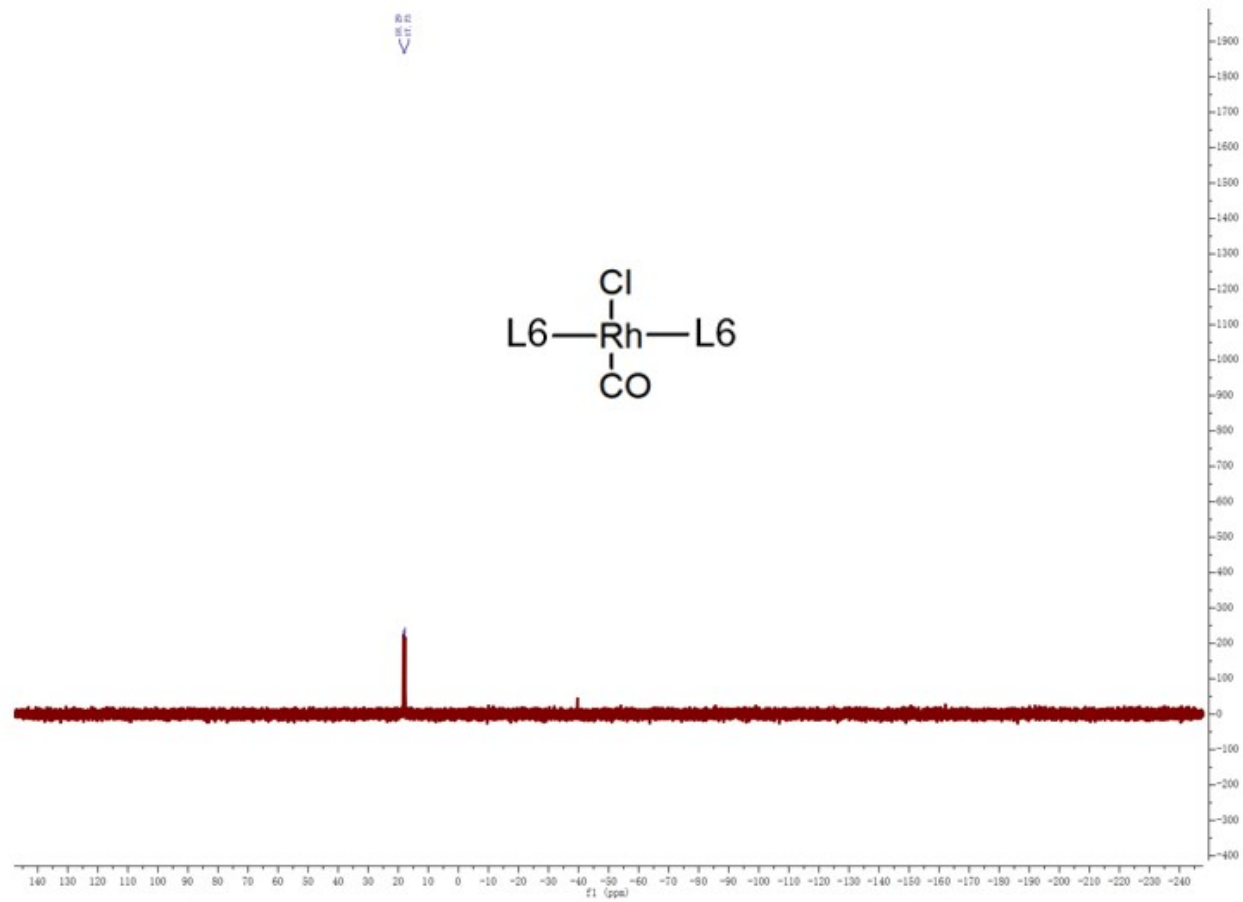
^1P NMR of $\text{RhClCO}(\text{L5})_2$ (243MHz, CDCl_3 , 323K)



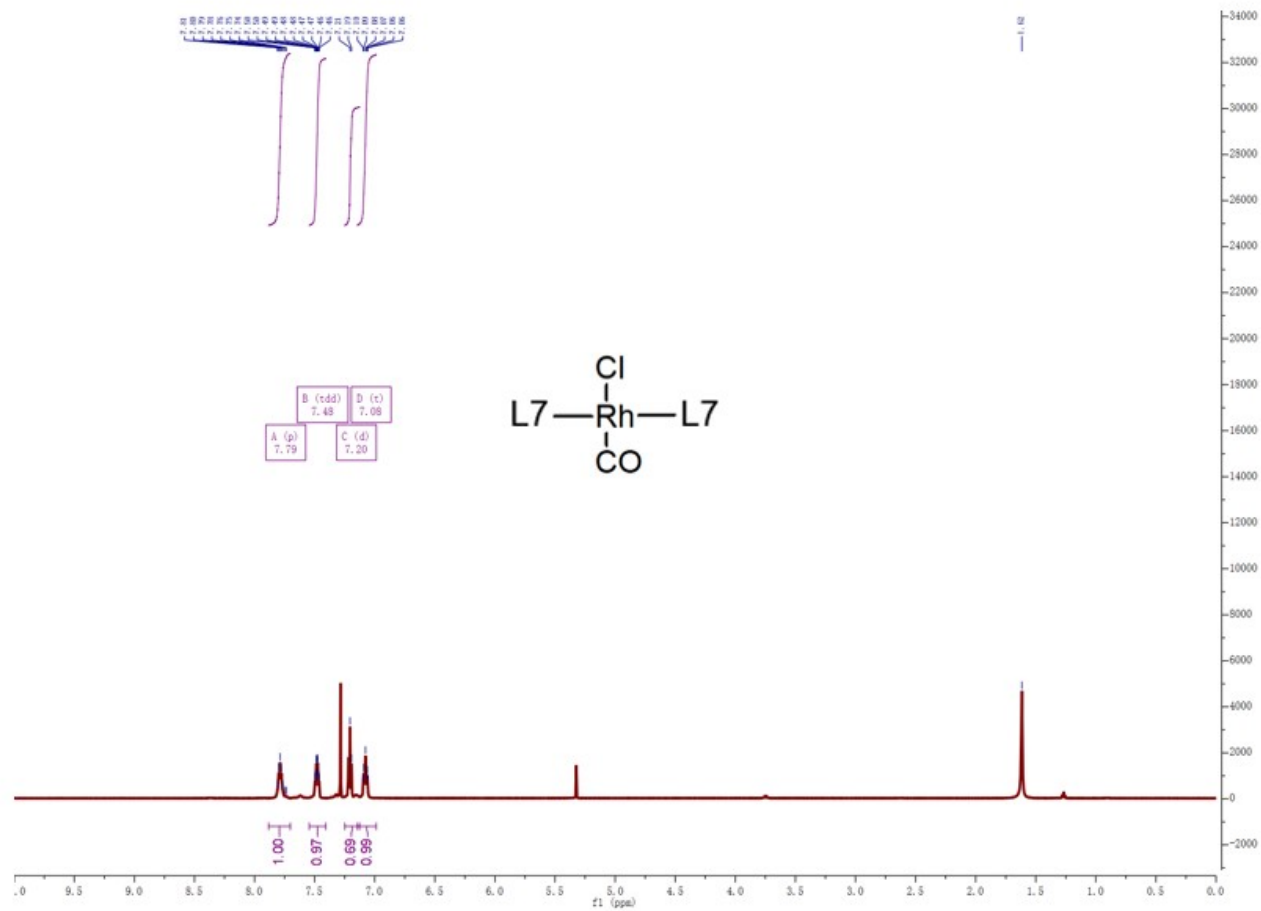
^1H NMR of $\text{RhClCO}(\text{L6})_2$ (600MHz, CDCl_3 , 323K)



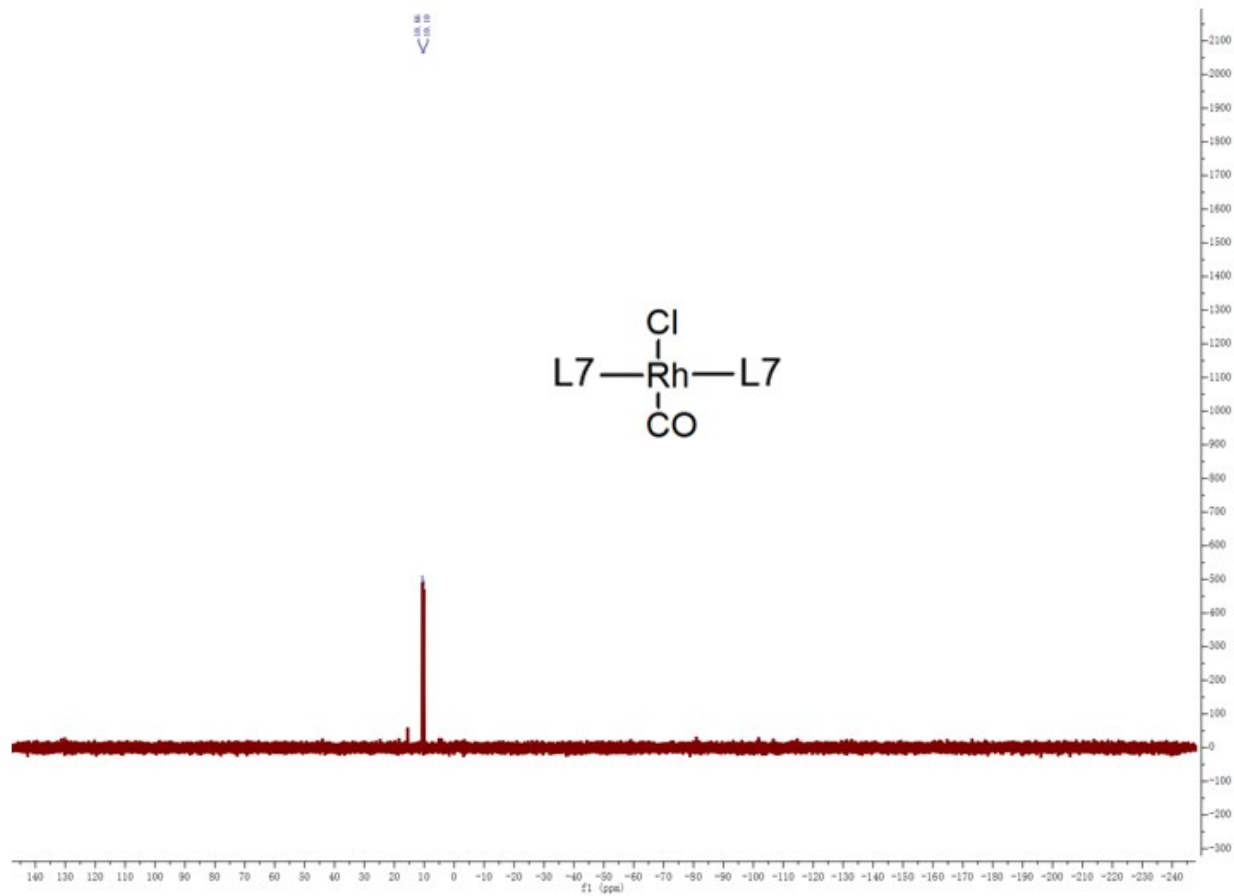
^1P NMR of $\text{RhClCO}(\text{L6})_2$ (243MHz, CDCl_3 , 323K)



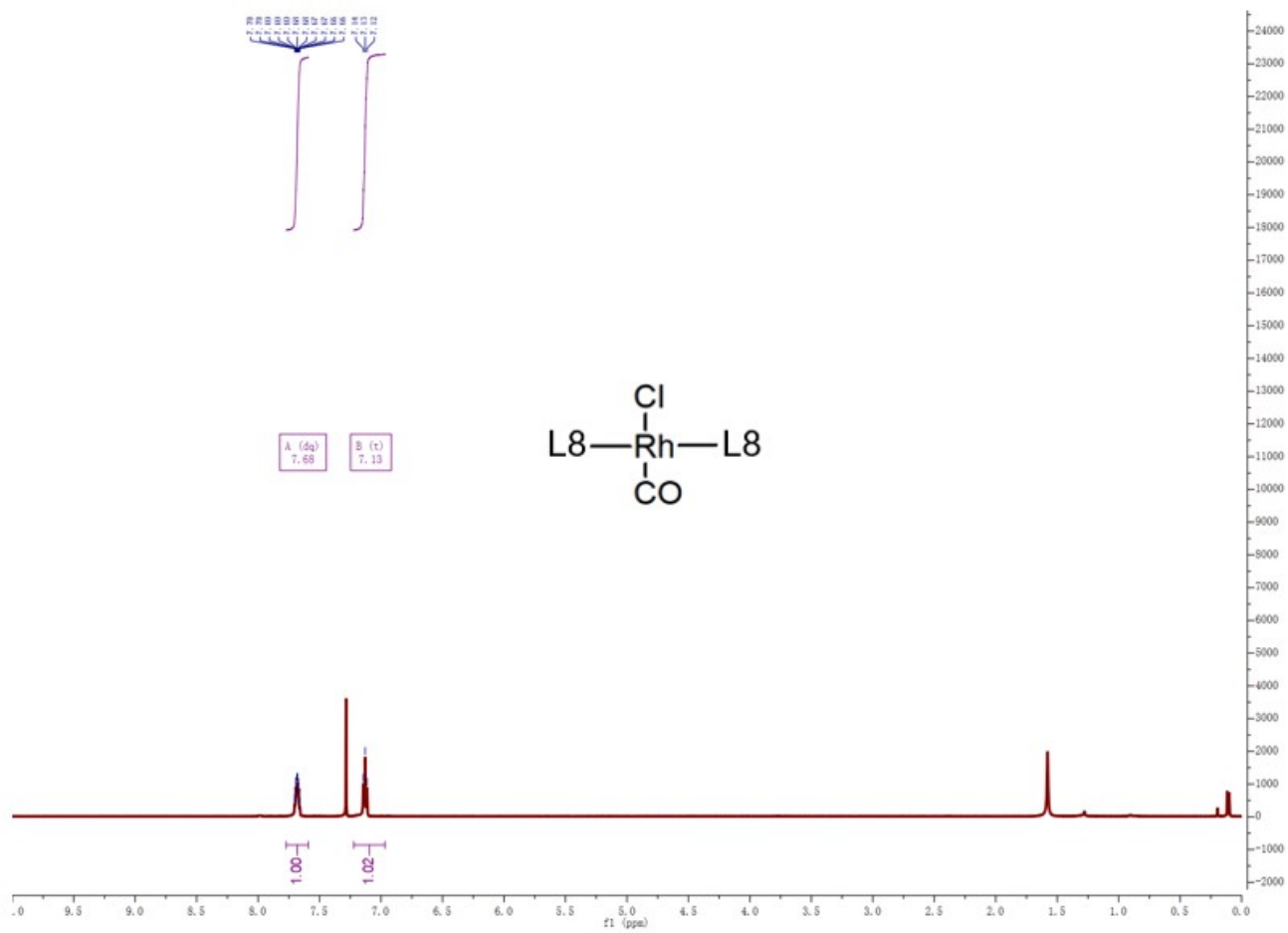
^1H NMR of $\text{RhClCO}(\text{L7})_2$ (600MHz, CDCl_3 , 323K)



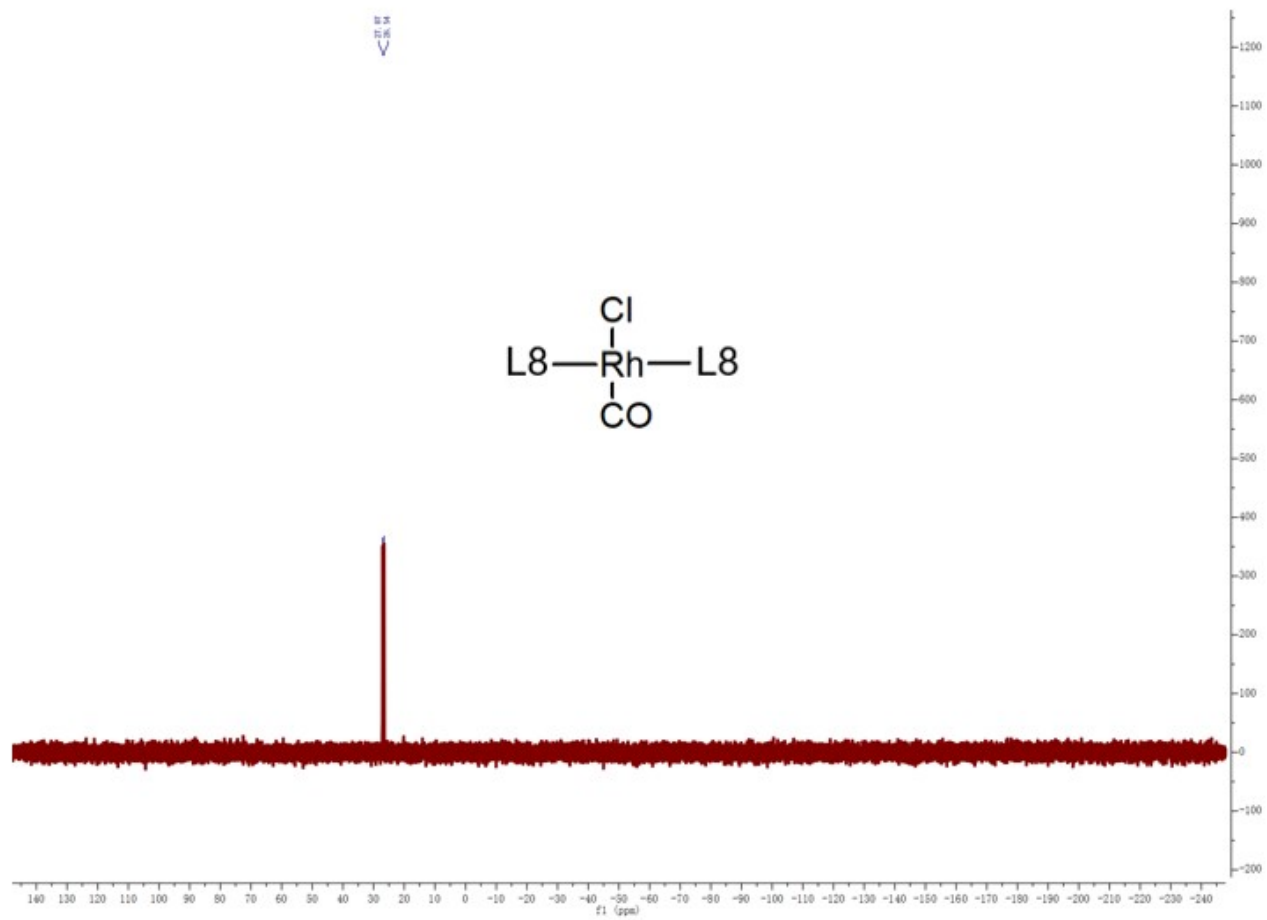
^1P NMR of $\text{RhClCO}(\text{L7})_2$ (243MHz, CDCl_3 , 323K)



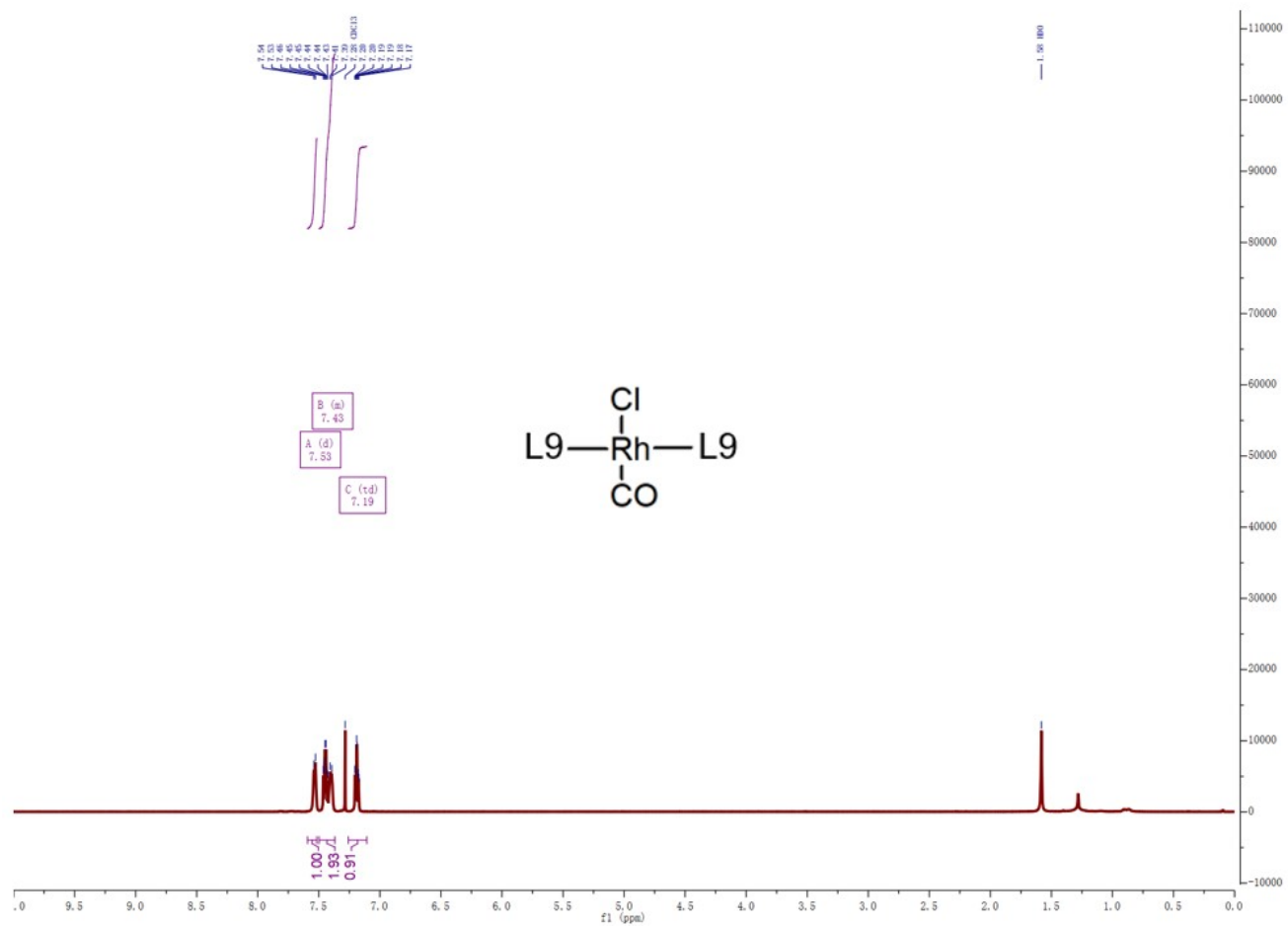
^1H NMR of $\text{RhClCO}(\text{L8})_2$ (600MHz, CDCl_3 , 323K)



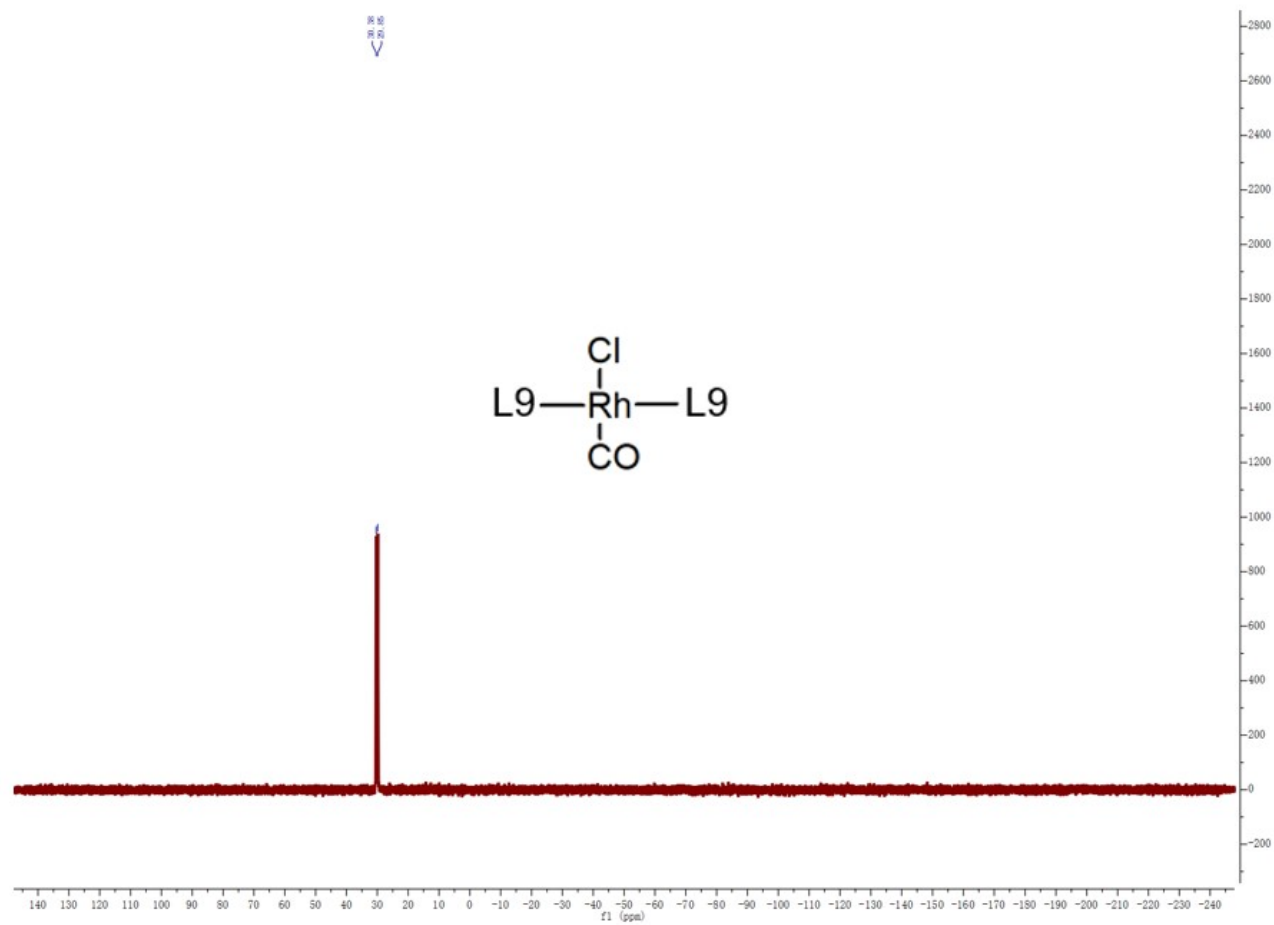
^1P NMR of $\text{RhClCO}(\text{L8})_2$ (243MHz, CDCl_3 , 323K)



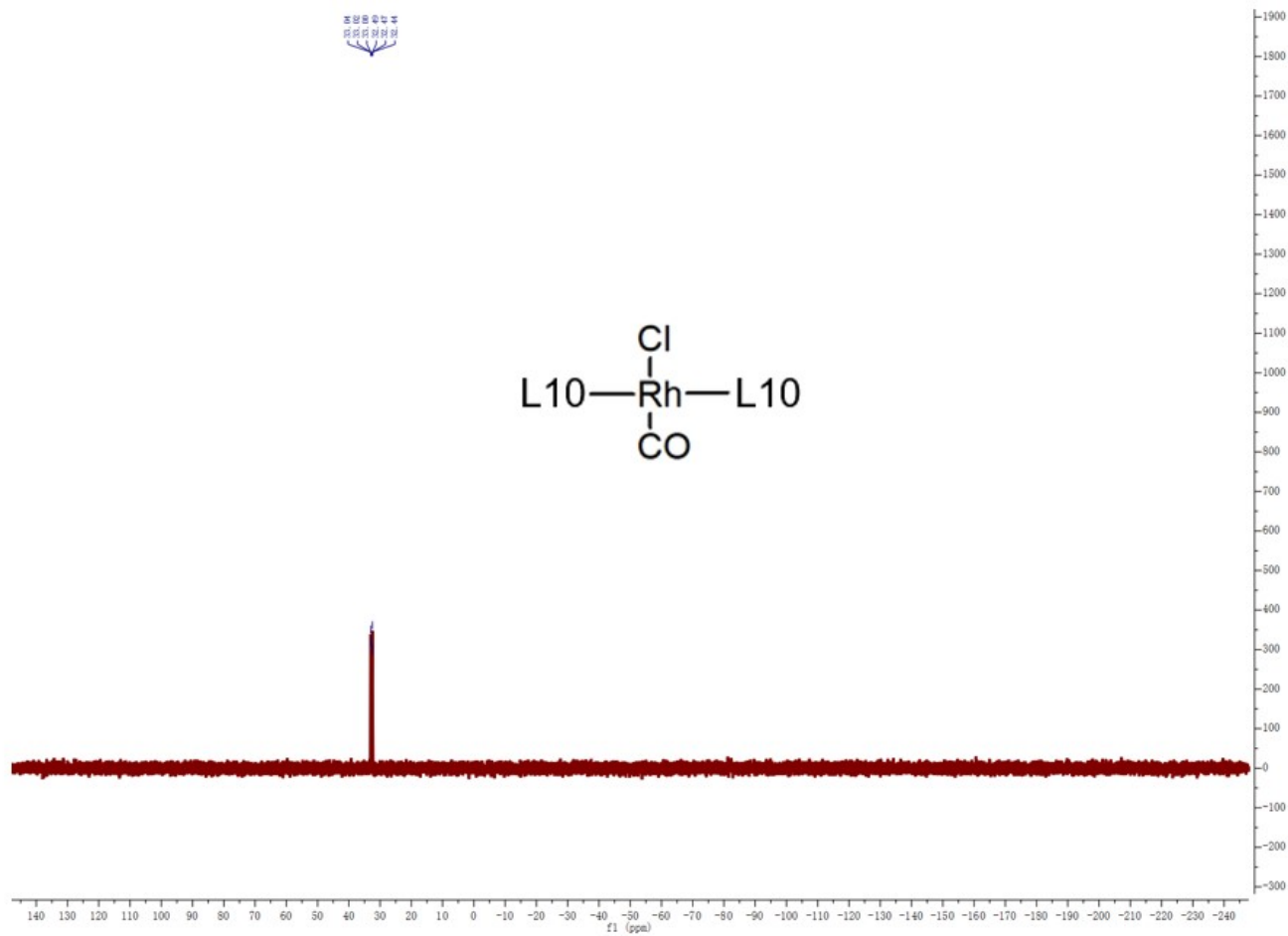
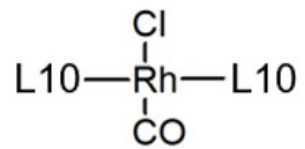
^1H NMR of $\text{RhClCO}(\text{L9})_2$ (600MHz, CDCl_3 , 323K)



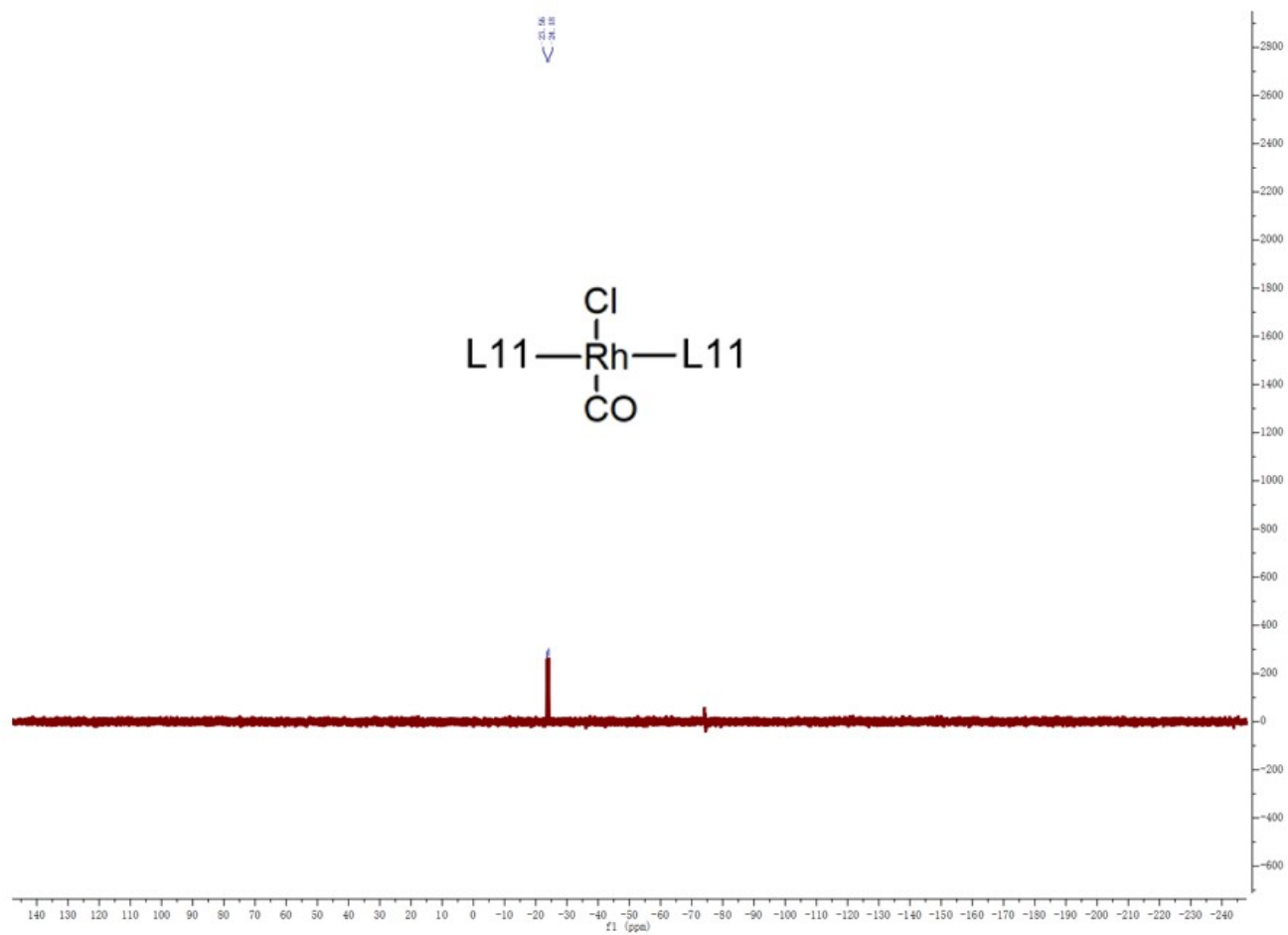
^1P NMR of $\text{RhClCO}(\text{L9})_2$ (243MHz, CDCl_3 , 323K)



^1P NMR of $\text{RhClCO}(\text{L}10)_2$ (243MHz, CDCl_3 , 323K)

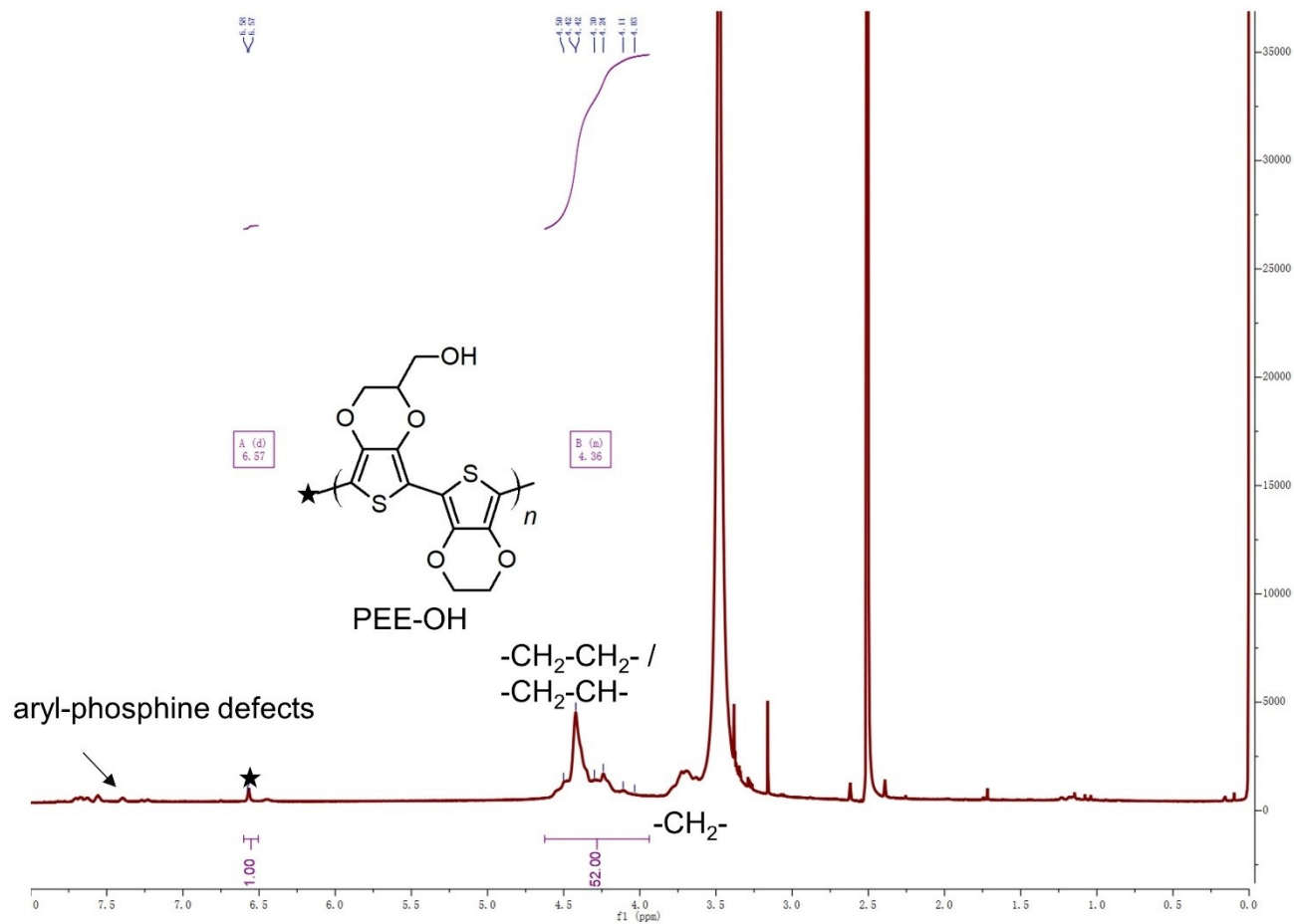


^1P NMR of $\text{RhClCO}(\text{L11})_2$ (243MHz, CDCl_3 , 323K)

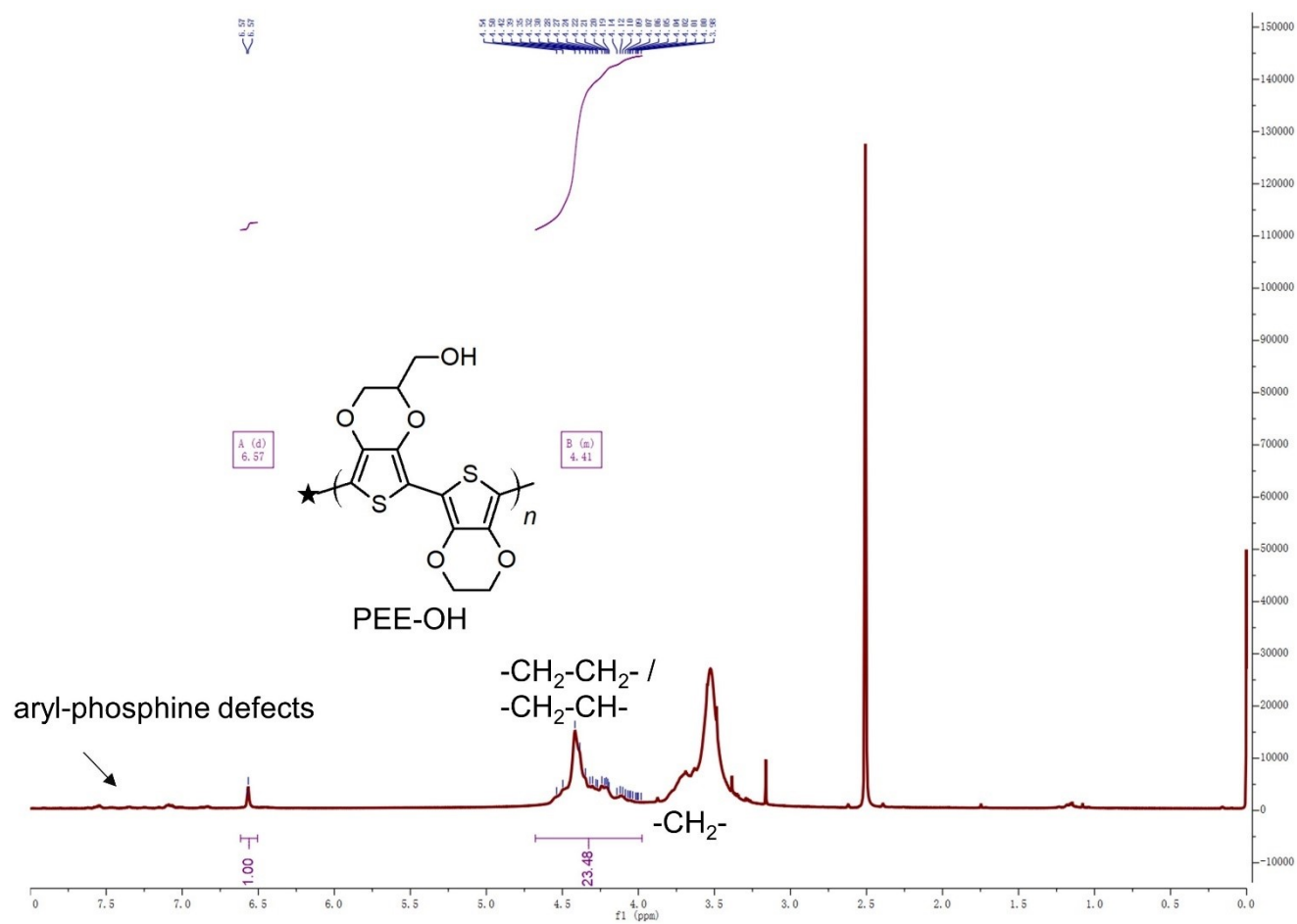


7.2 NMR spectra of functionalized EDOT polymers

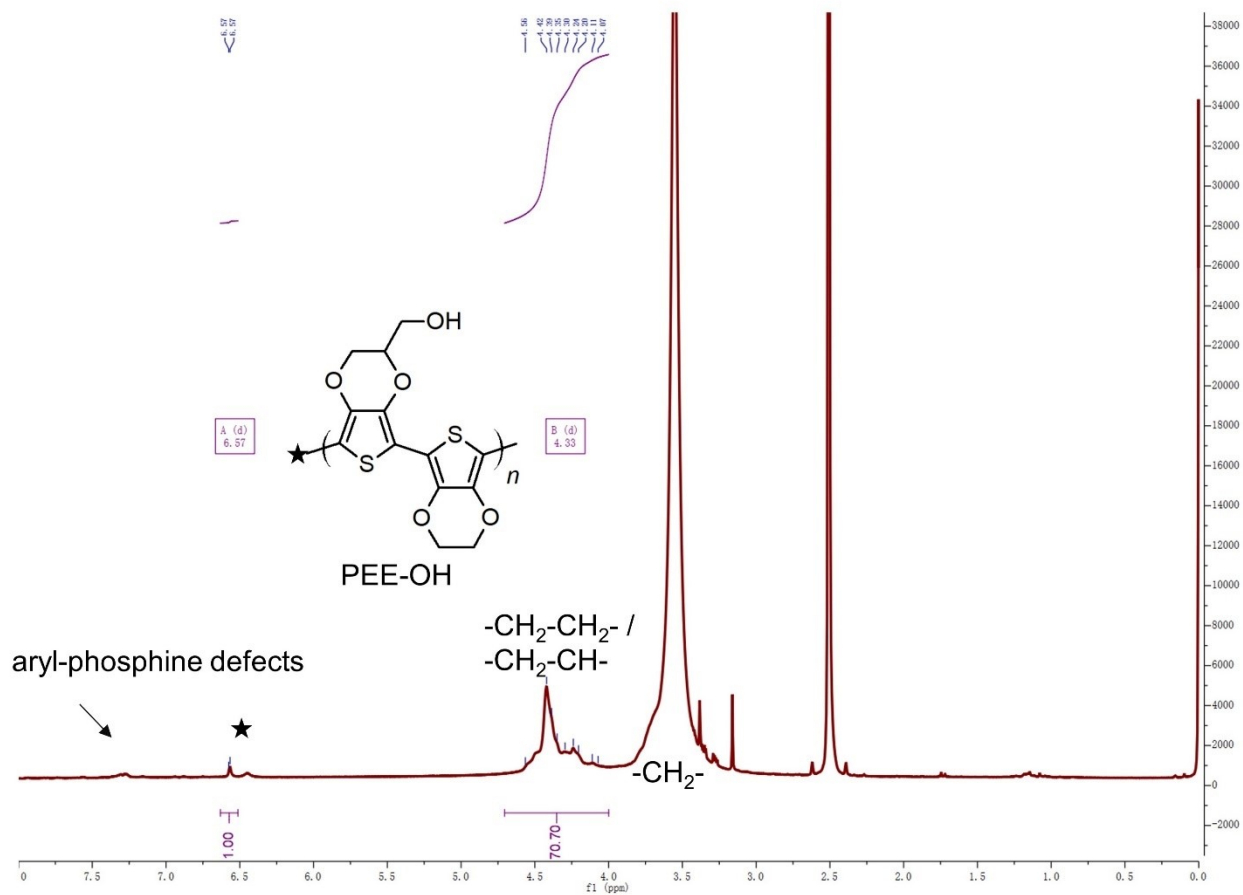
^1H NMR of PEE-OH with entry 4 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



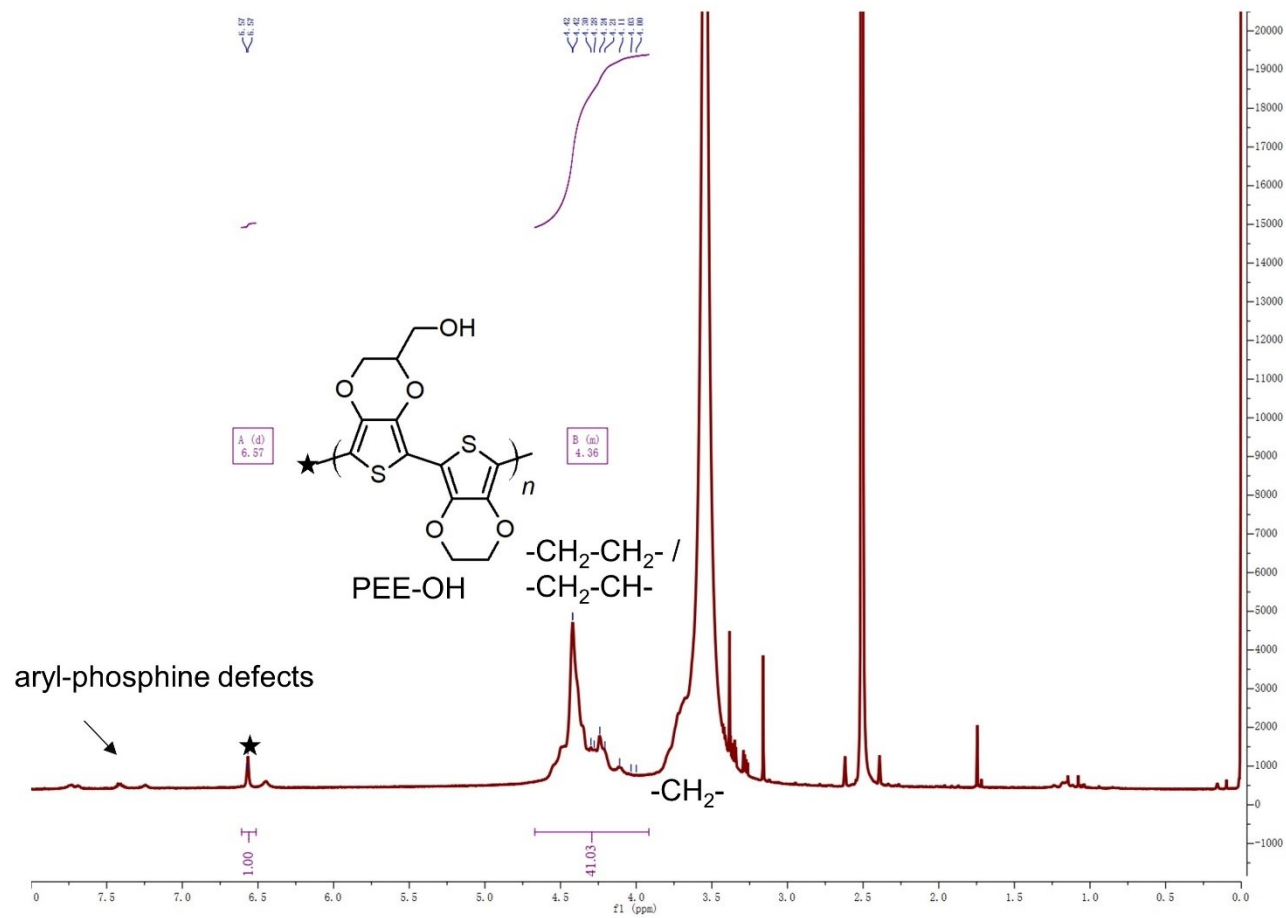
^1H NMR of PEE-OH with entry 6 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



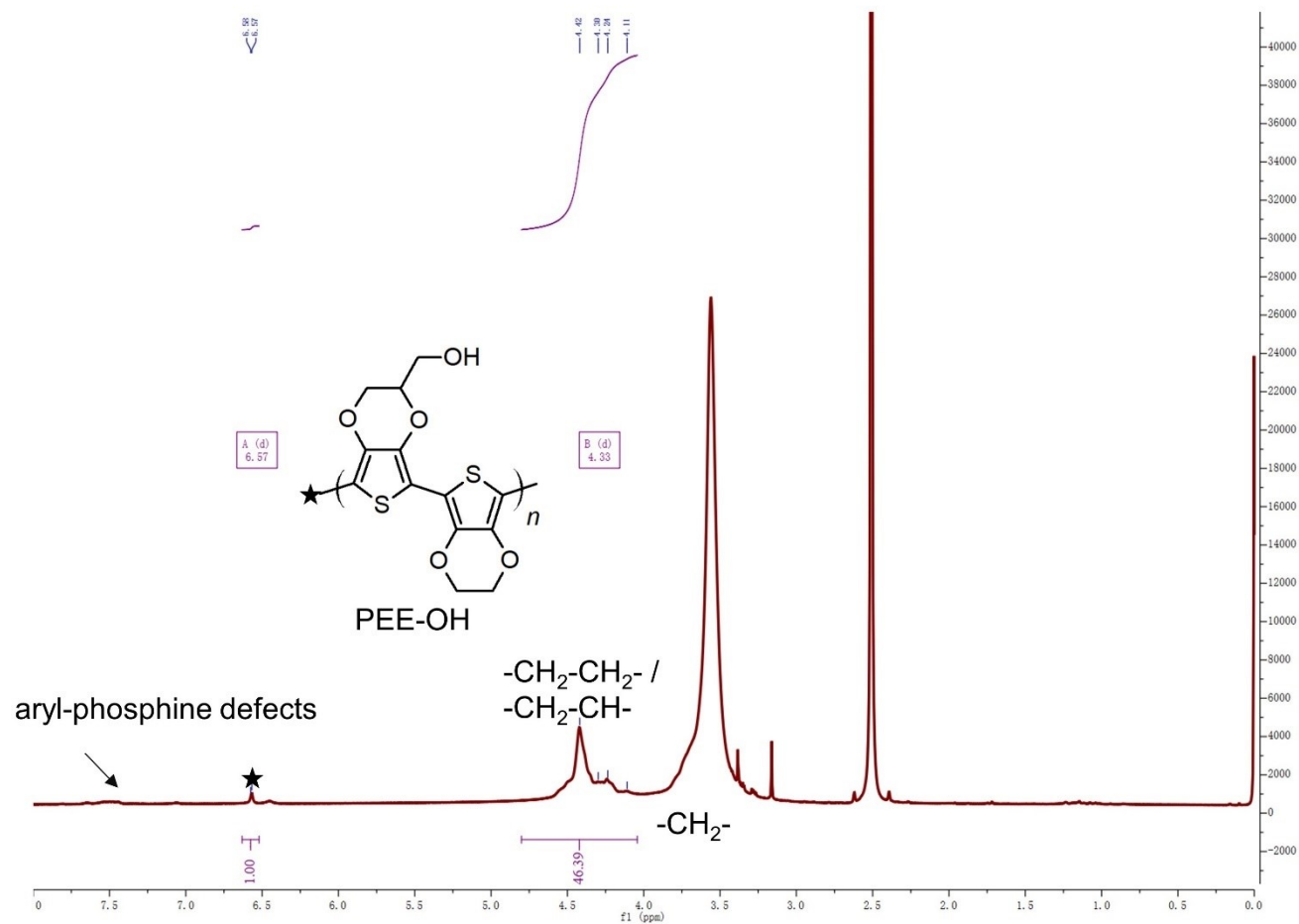
^1H NMR of PEE-OH with entry 7 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



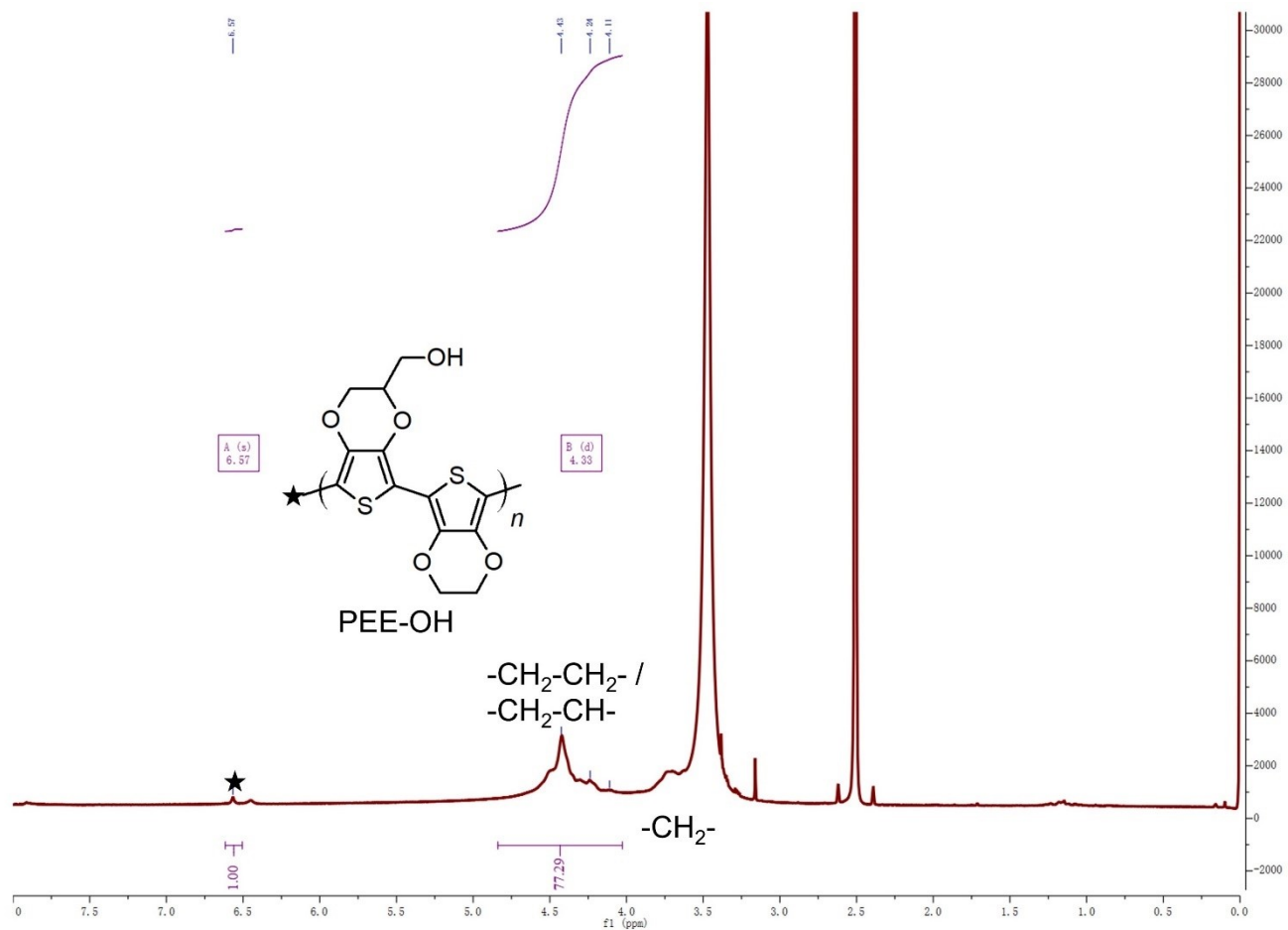
^1H NMR of PEE-OH with entry 8 of Table S3[600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



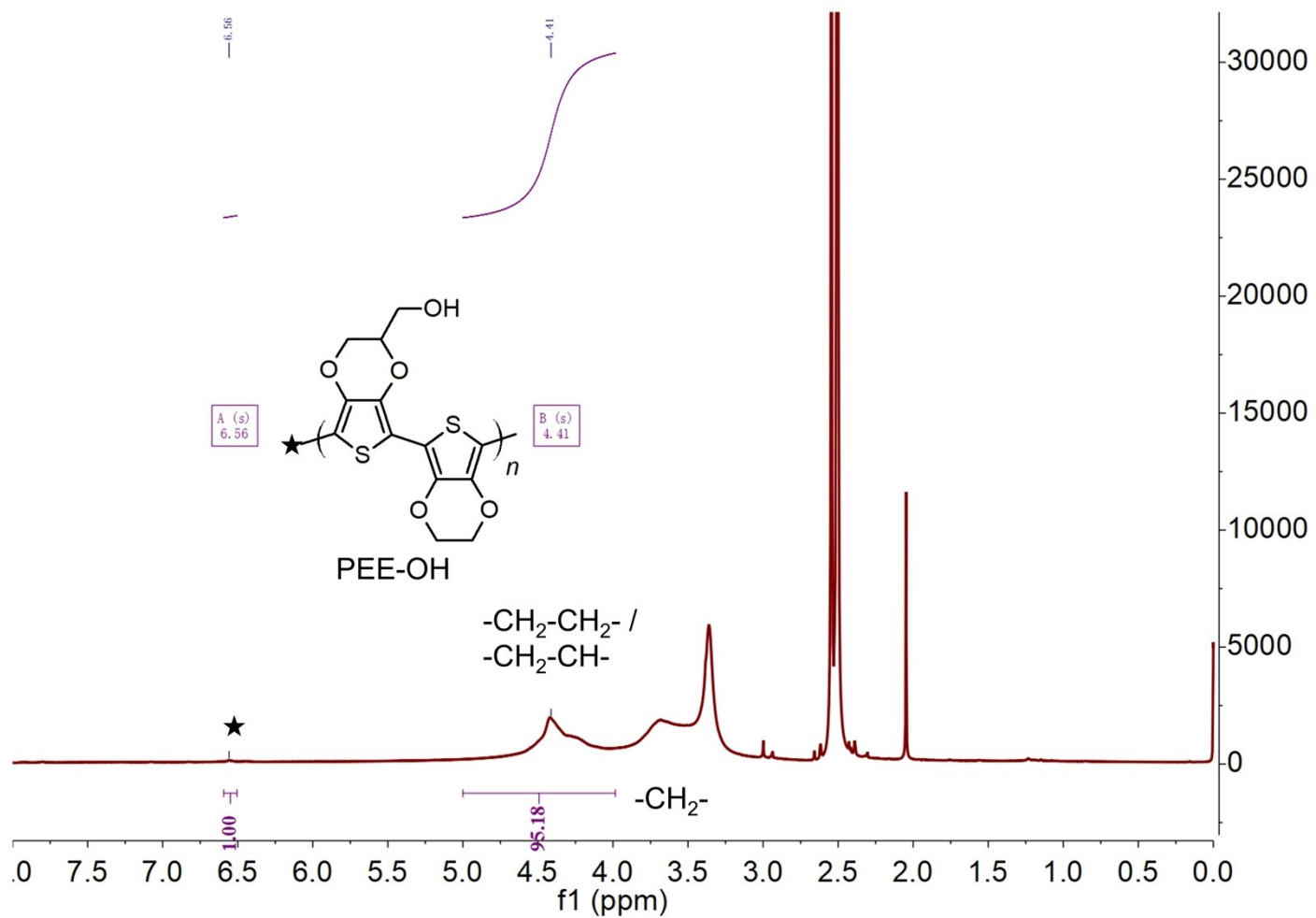
^1H NMR of PEE-OH with entry 9 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



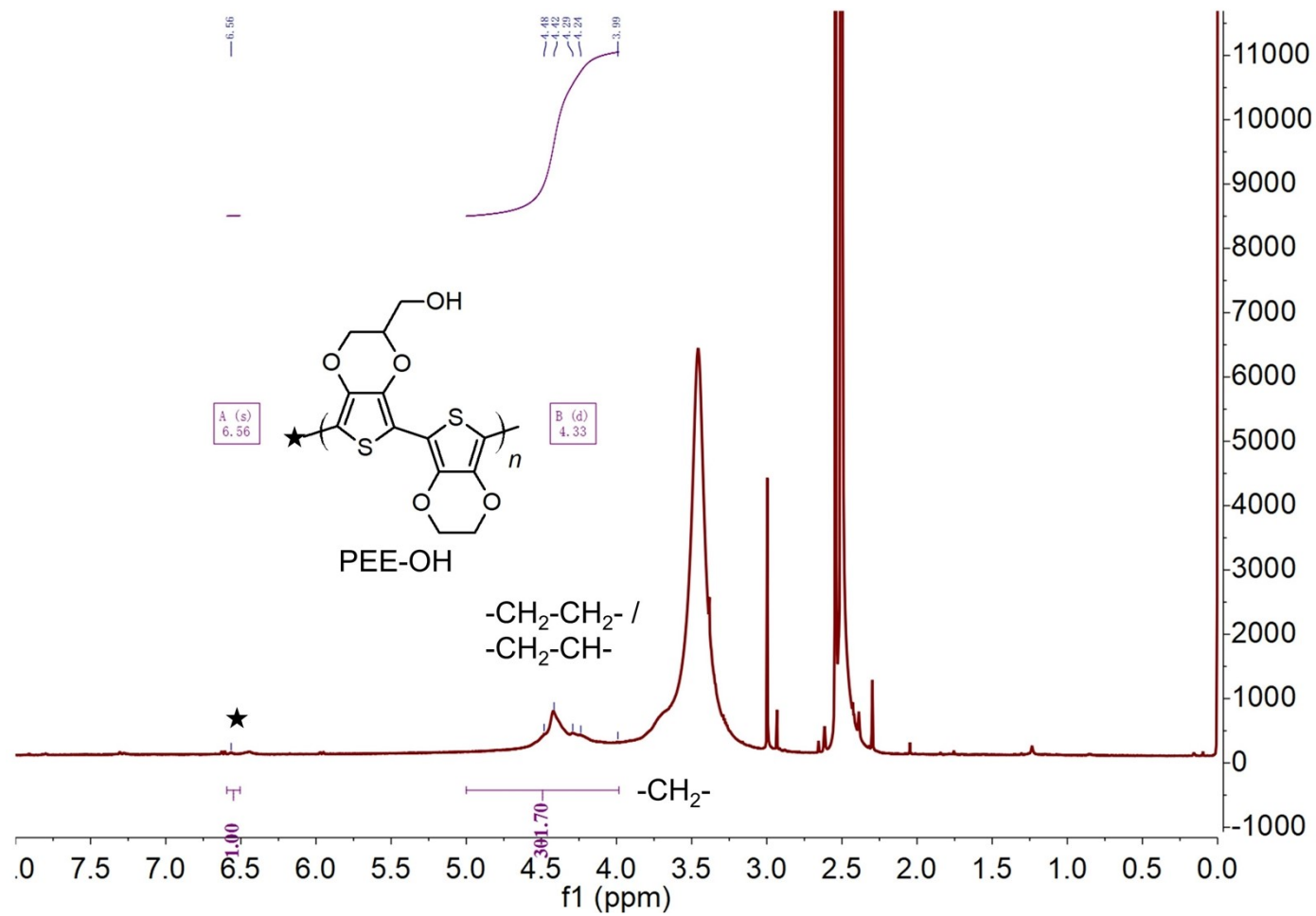
^1H NMR of PEE-OH with entry 10 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



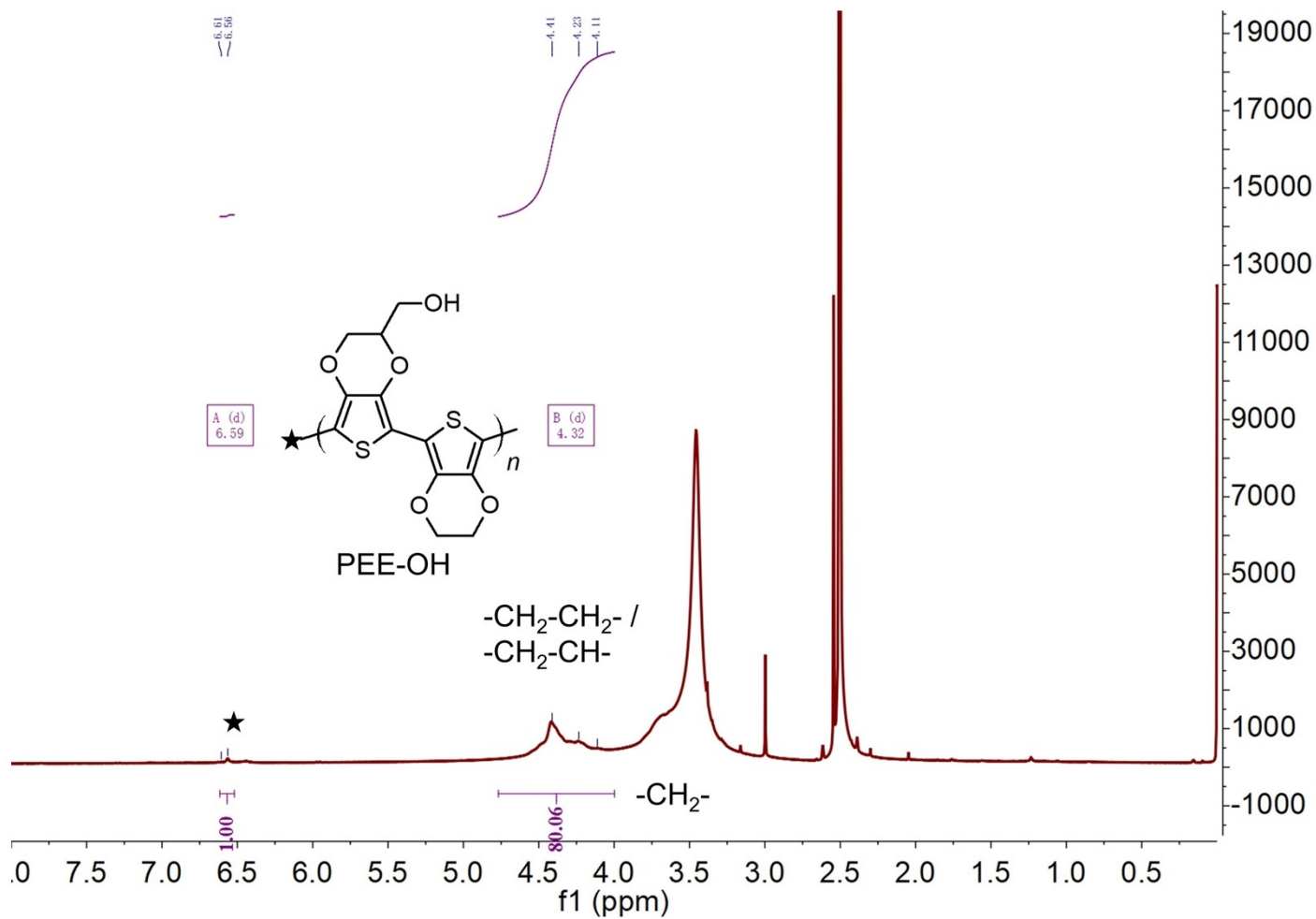
^1H NMR of PEE-OH with entry 12 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



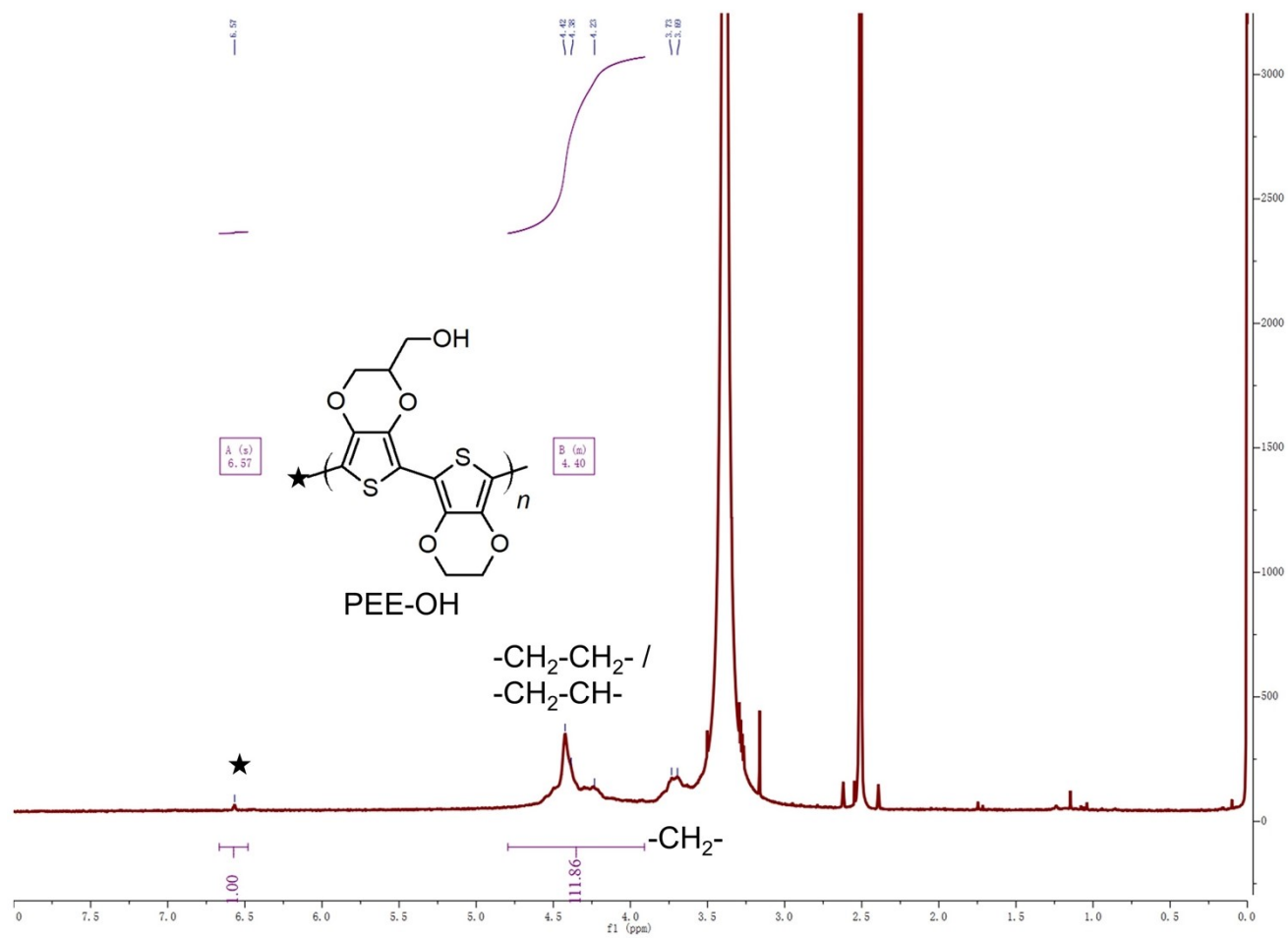
^1H NMR of PEE-OH with entry 13 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



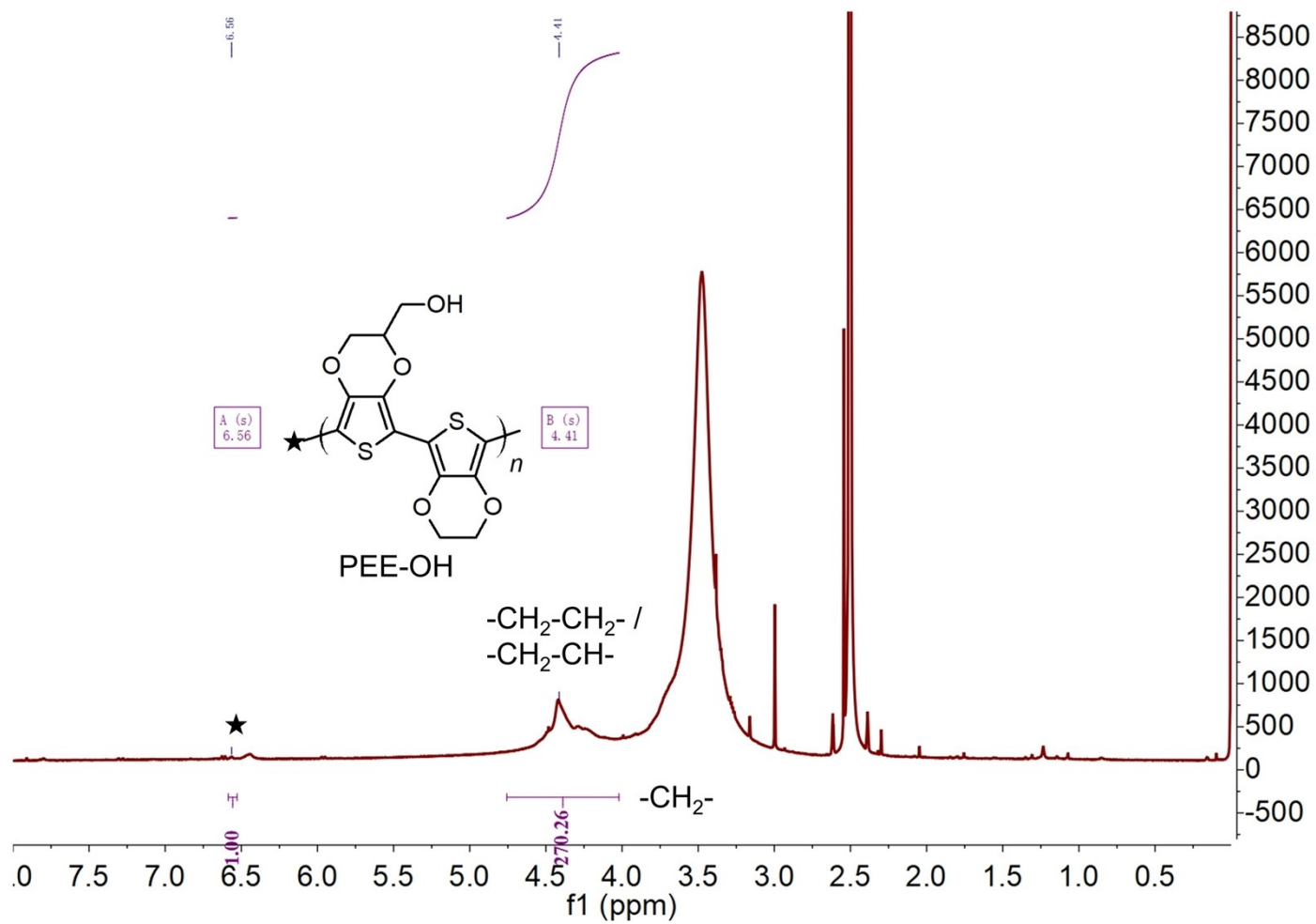
¹H NMR of PEE-OH with entry 14 of Table S3 [600MHz, dimethyl sulfoxide-d₆/ hydrazine hydrate-d₆ (v/v 100:1), 323K]



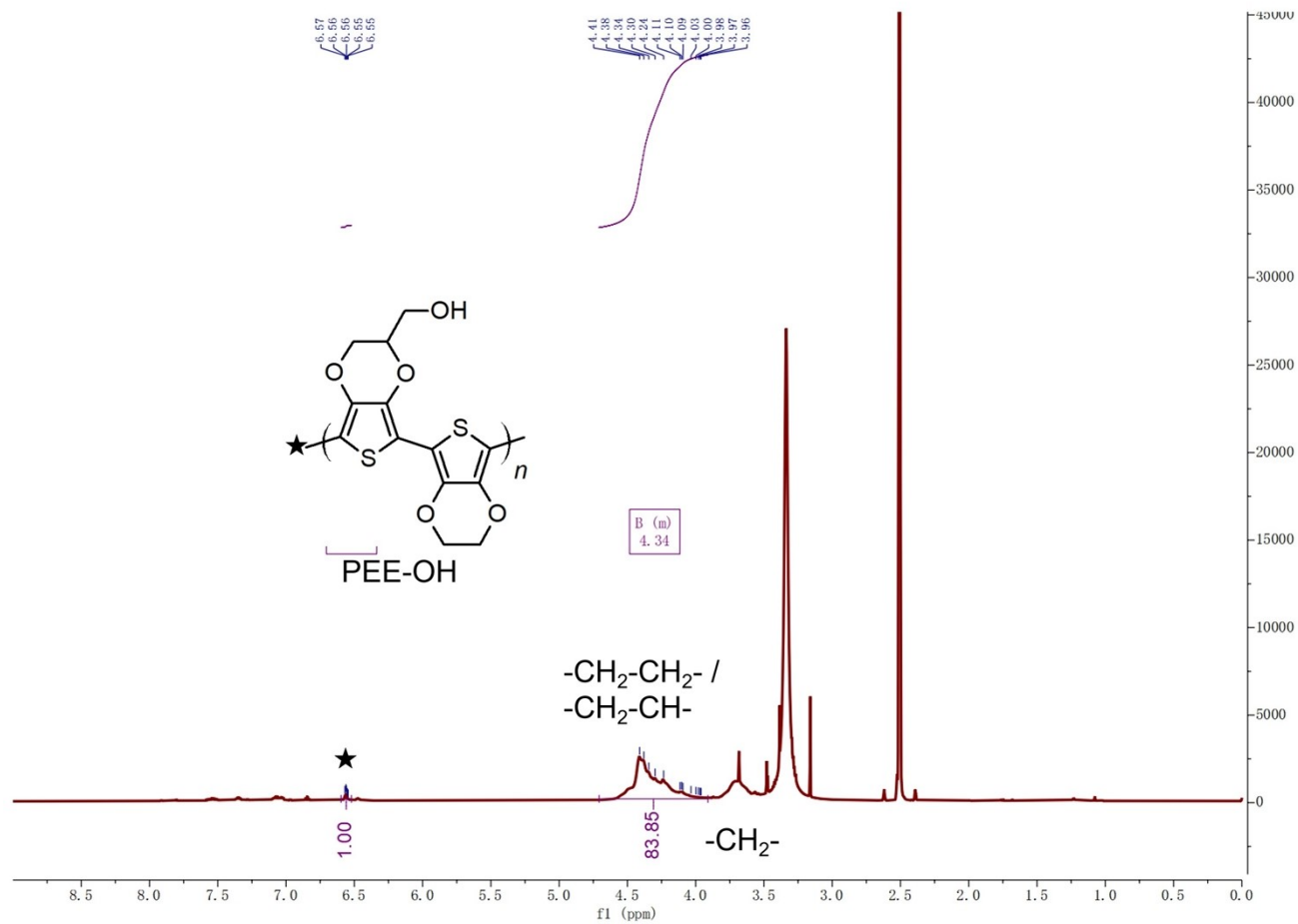
^1H NMR of PEE-OH with entry 15 of Table S3 [600MHz, dimethyl sulfoxide-d₆/ hydrazine hydrate-d₆ (v/v 100:1), 323K]



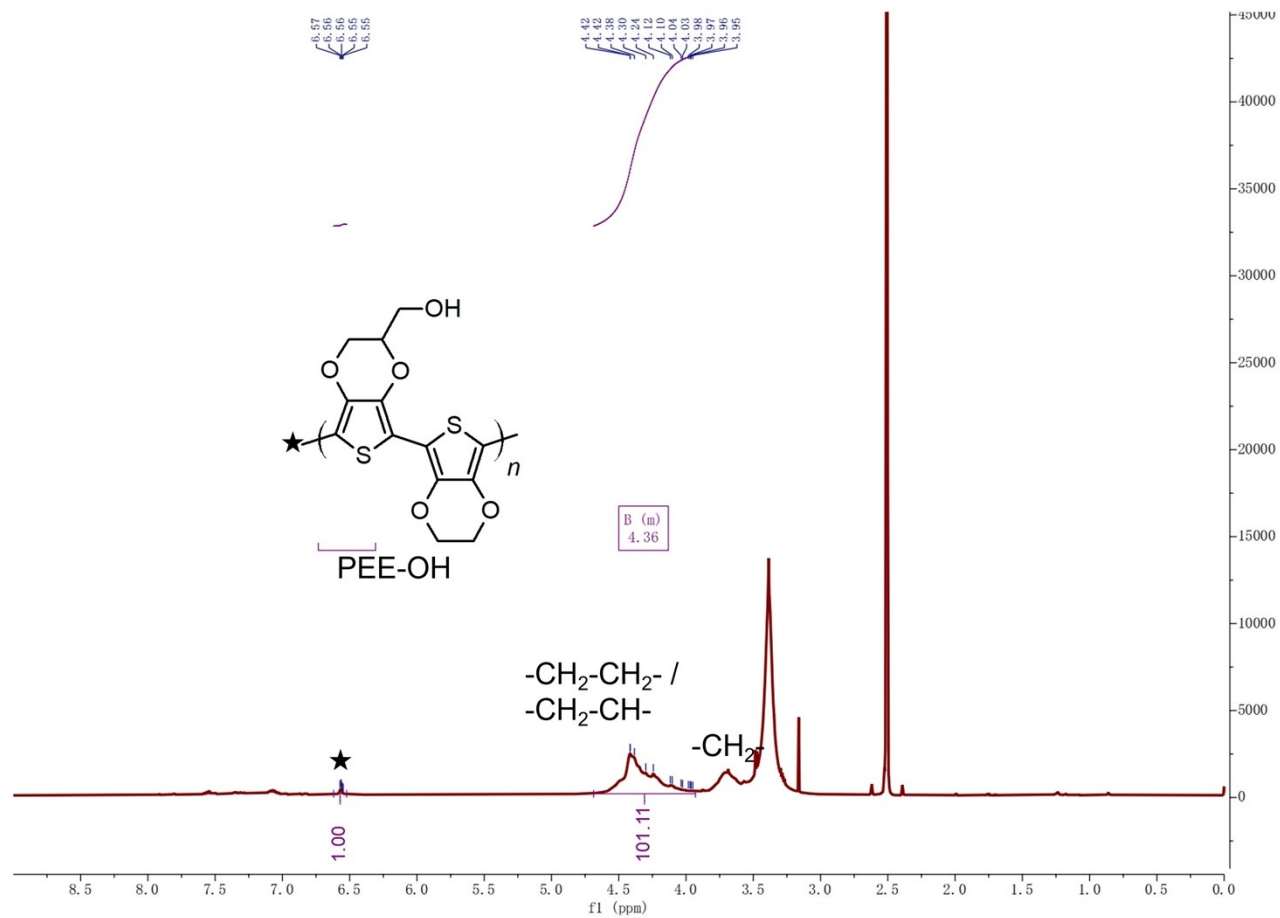
^1H NMR of PEE-OH with entry 16 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



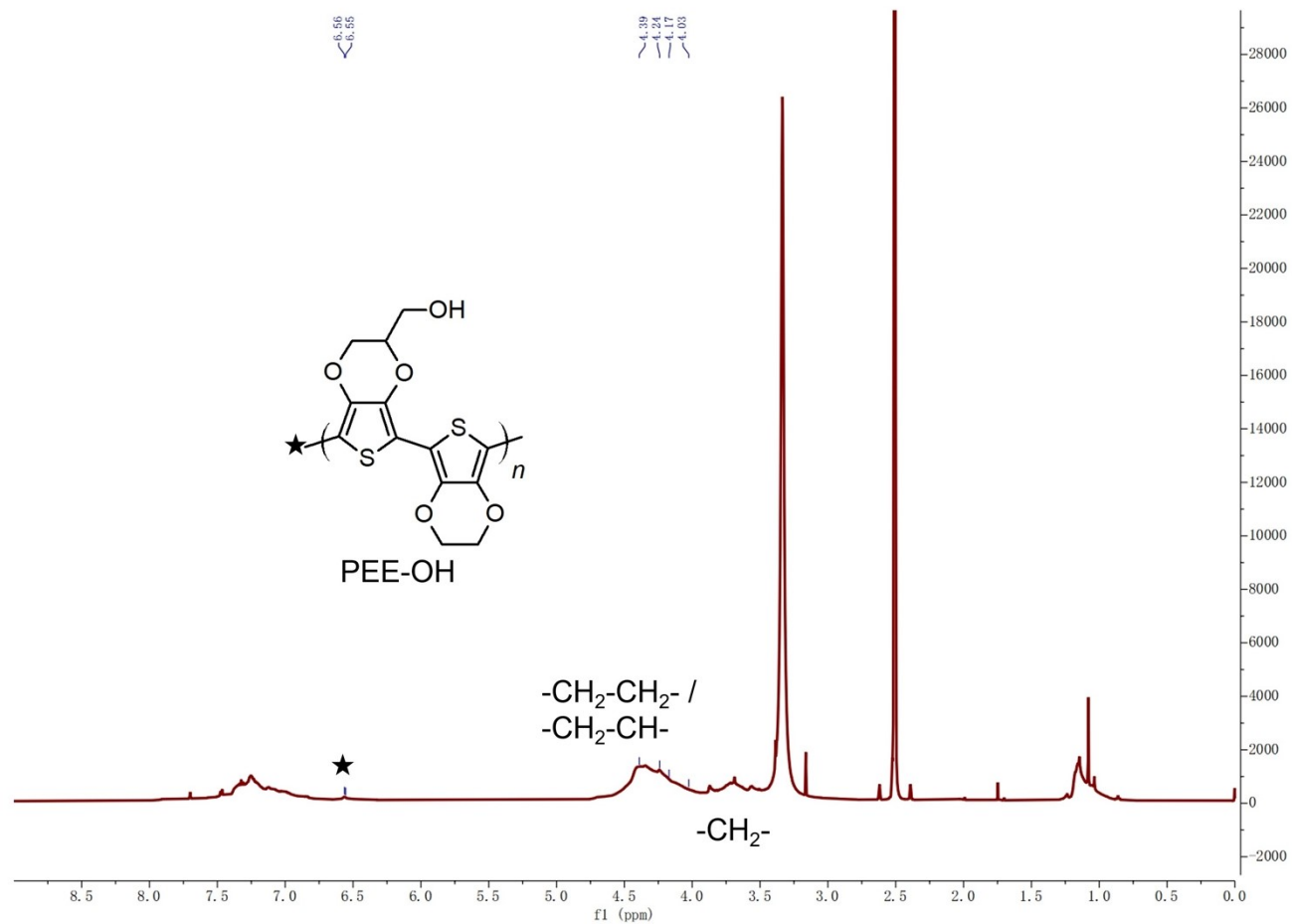
^1H NMR of PEE-OH with entry 17 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



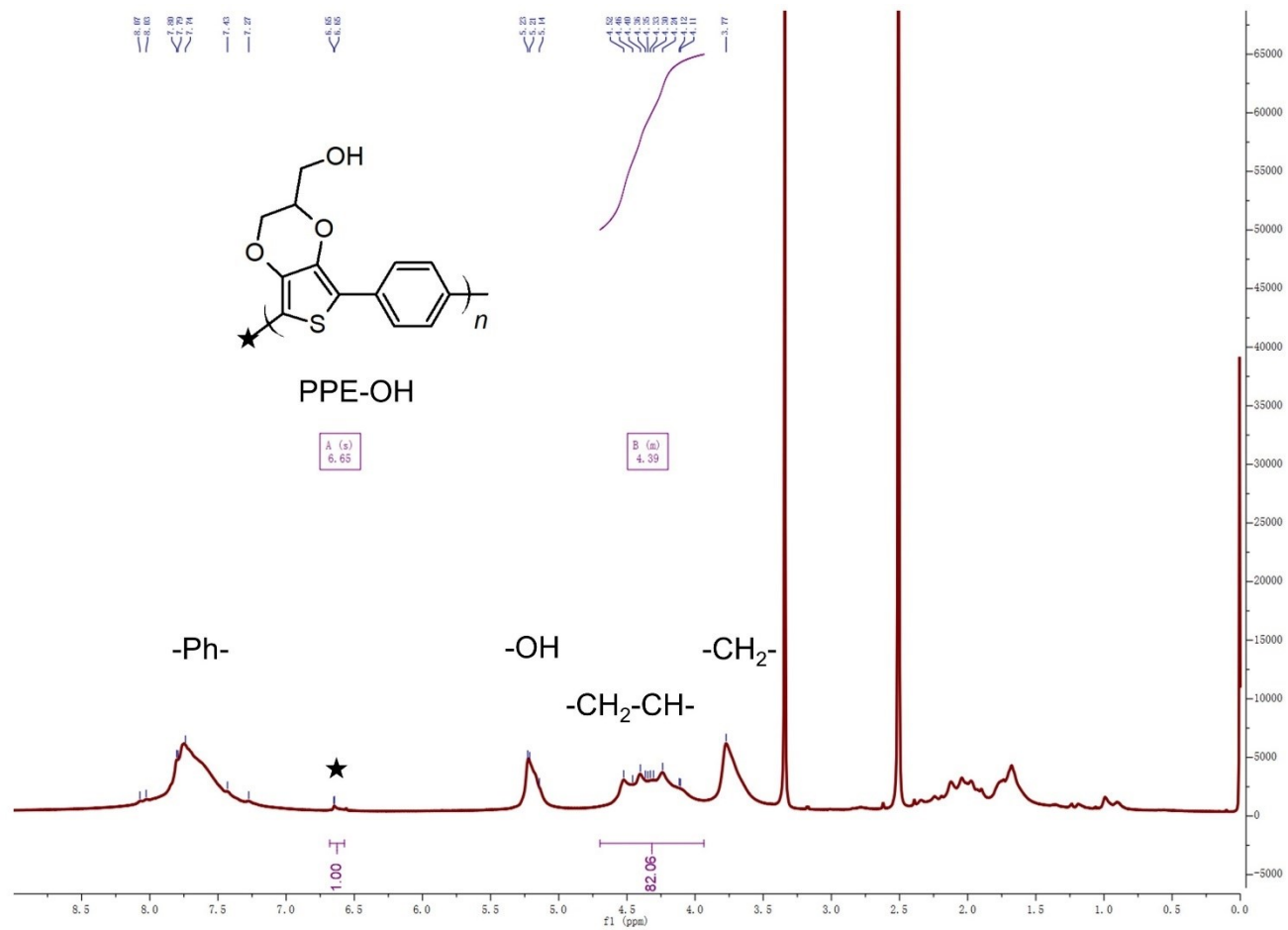
^1H NMR of PEE-OH with entry 18 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



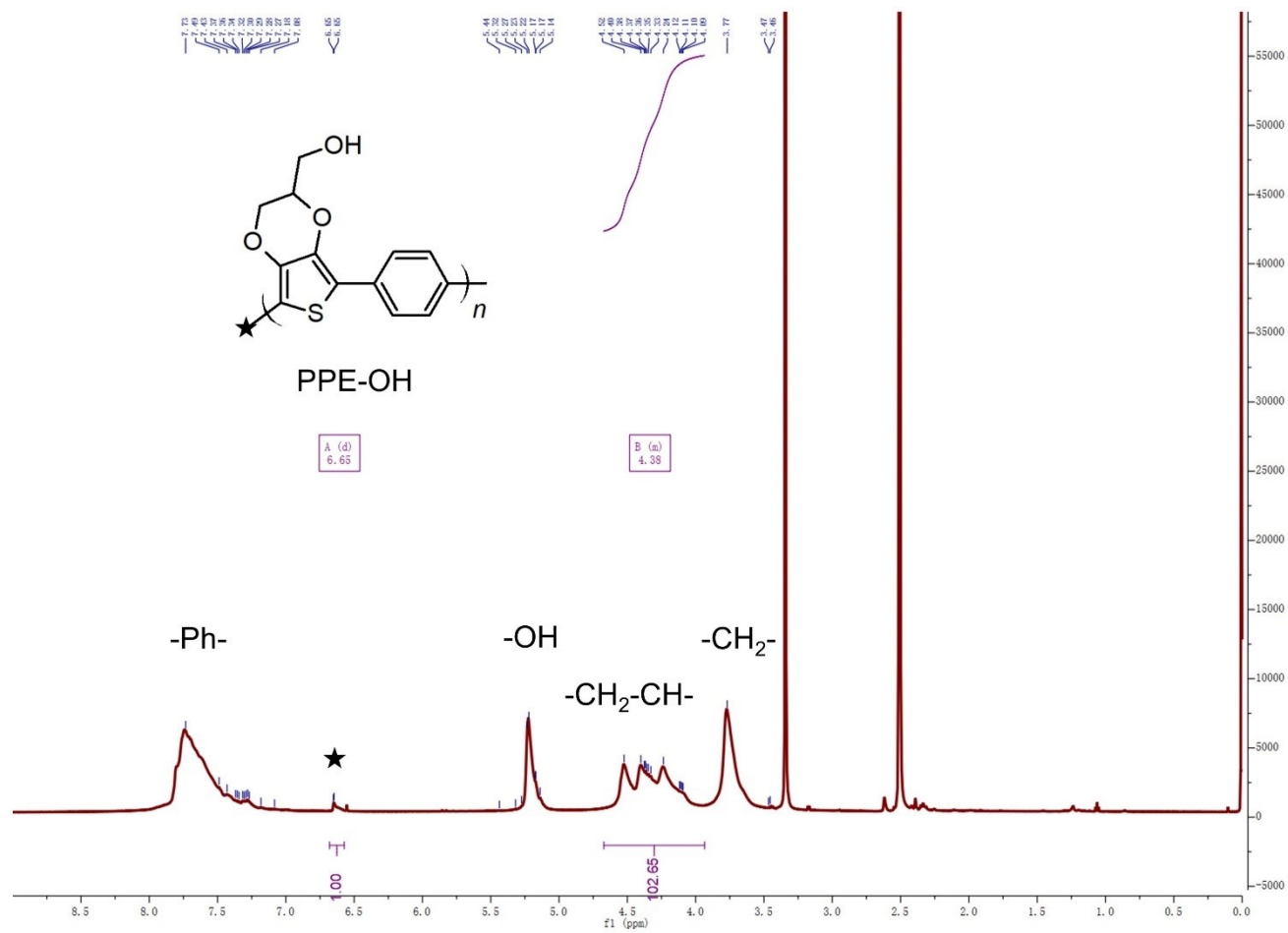
^1H NMR of PEE-OH with entry 19 of Table S3 [600MHz, dimethyl sulfoxide- d_6 / hydrazine hydrate- d_6 (v/v 100:1), 323K]



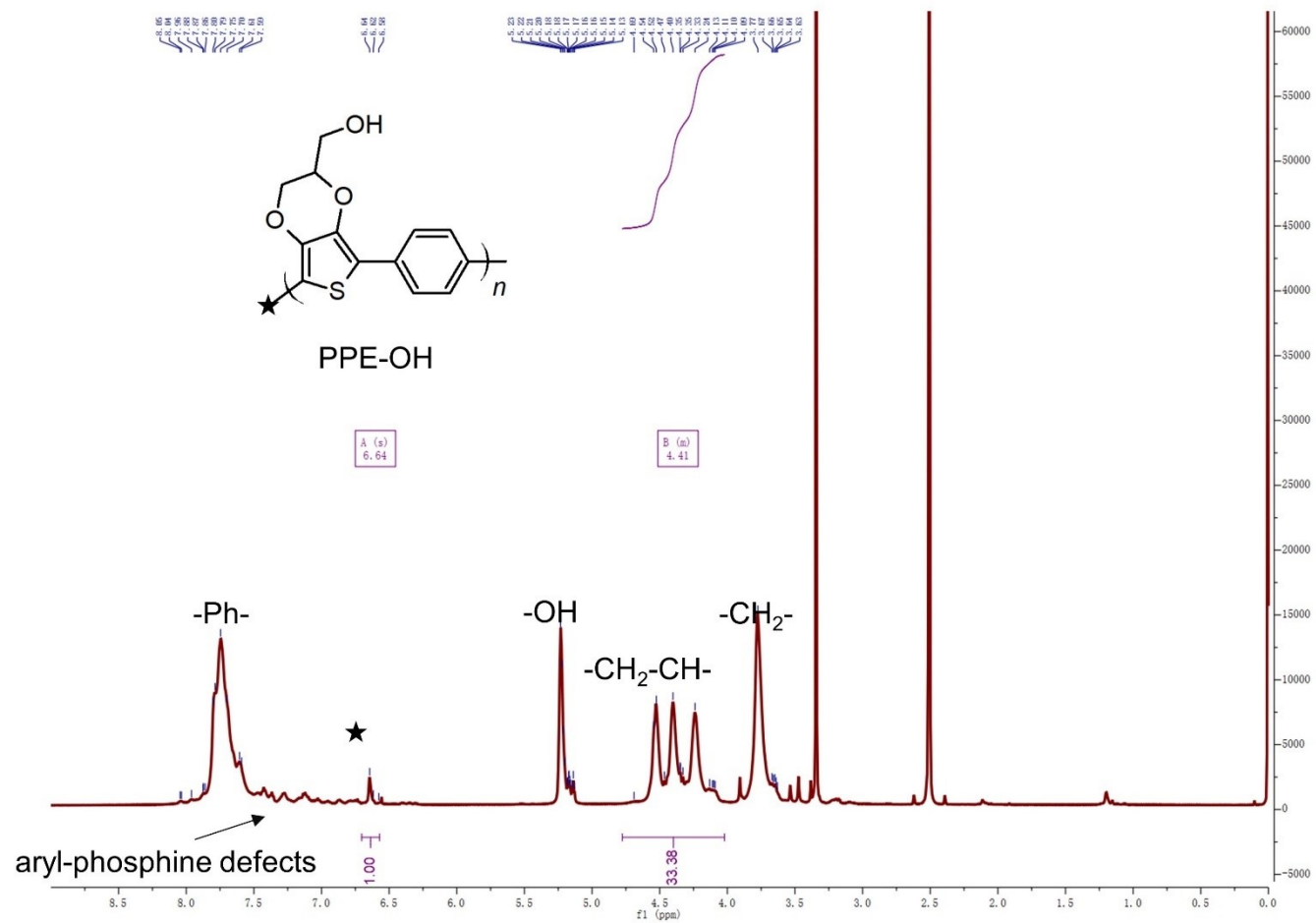
^1H NMR of PPE-OH with entry 3 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



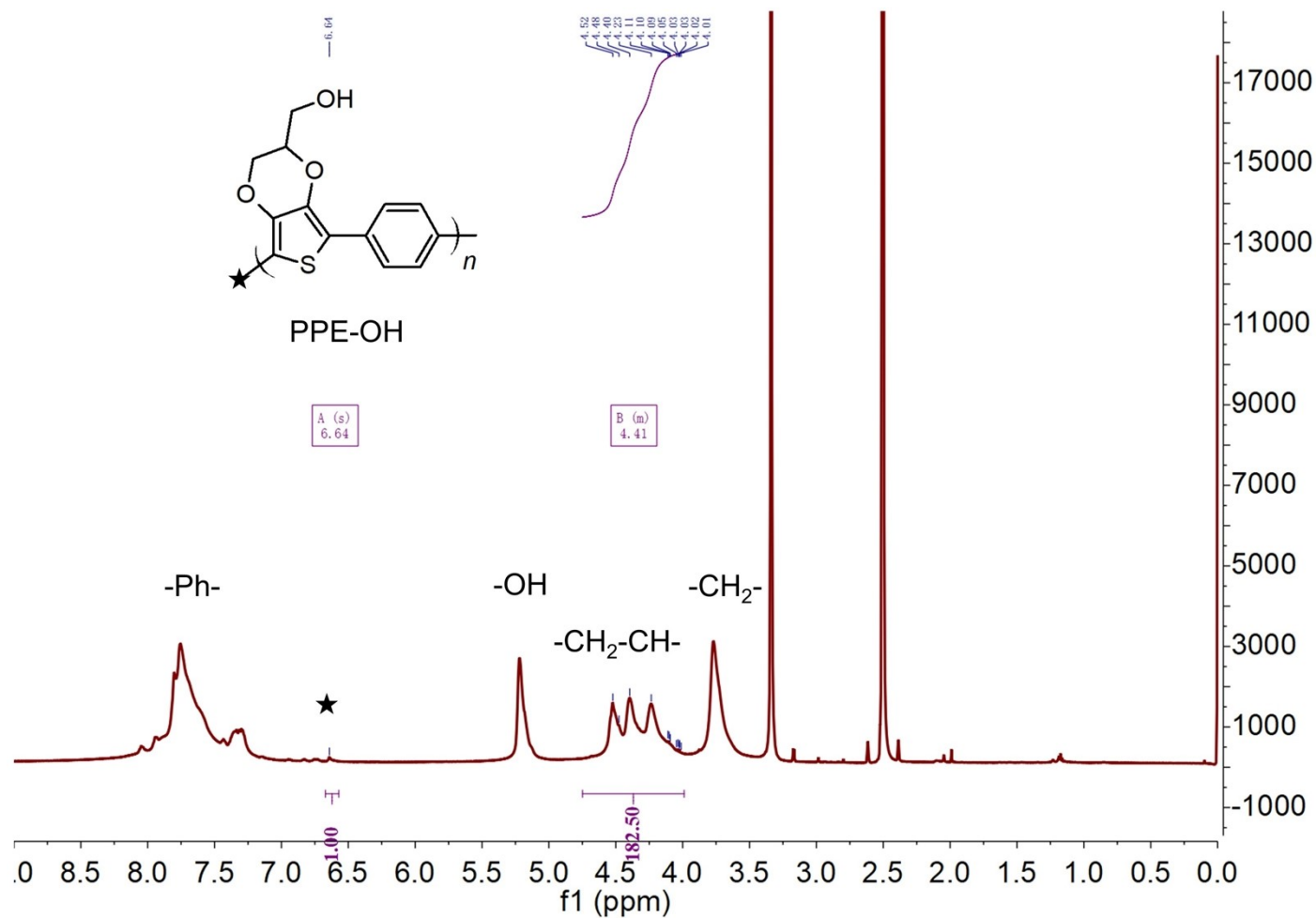
^1H NMR of PPE-OH with entry 5 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



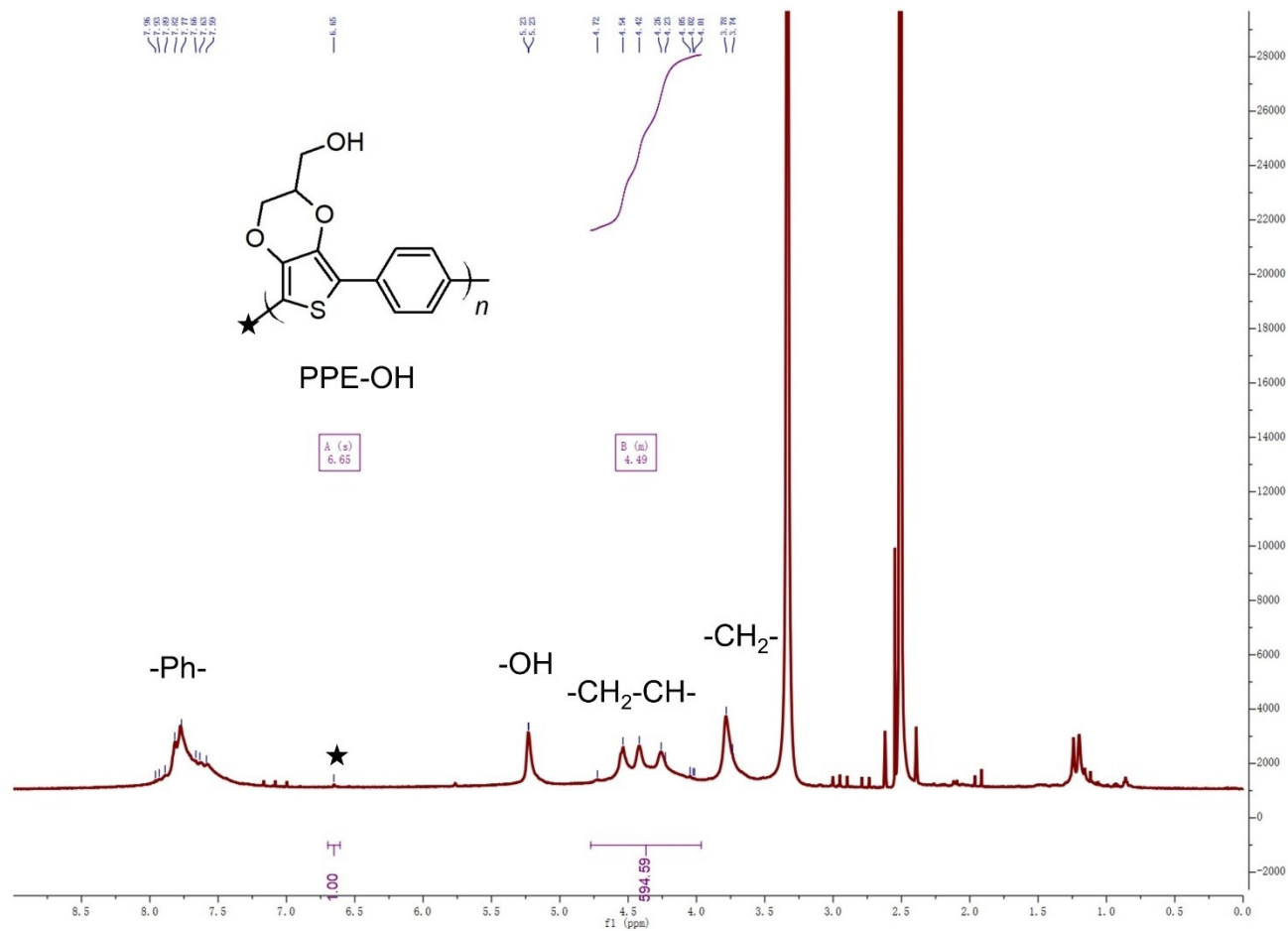
^1H NMR of PPE-OH with entry 6 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



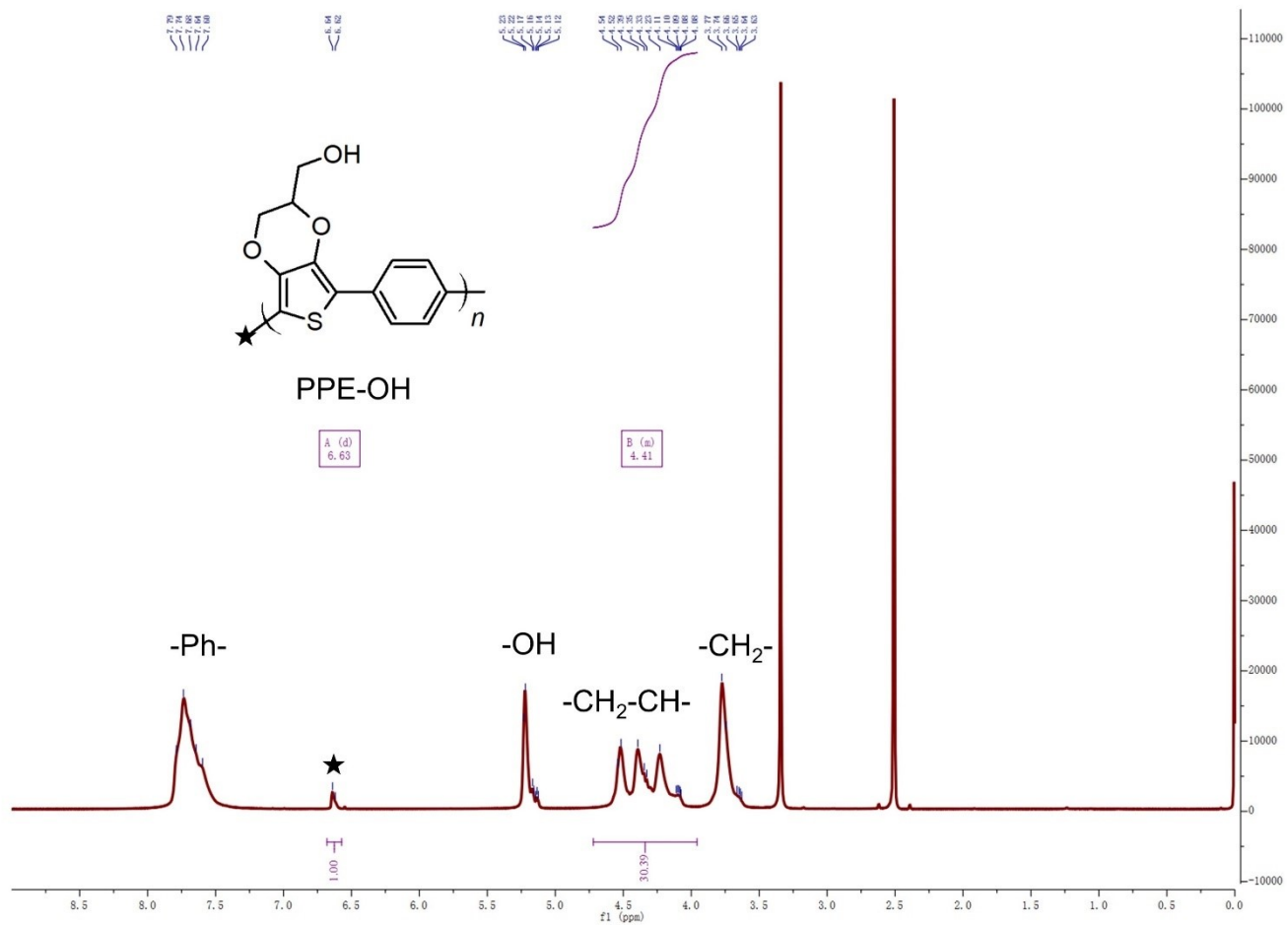
^1H NMR of PPE-OH with entry 7 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



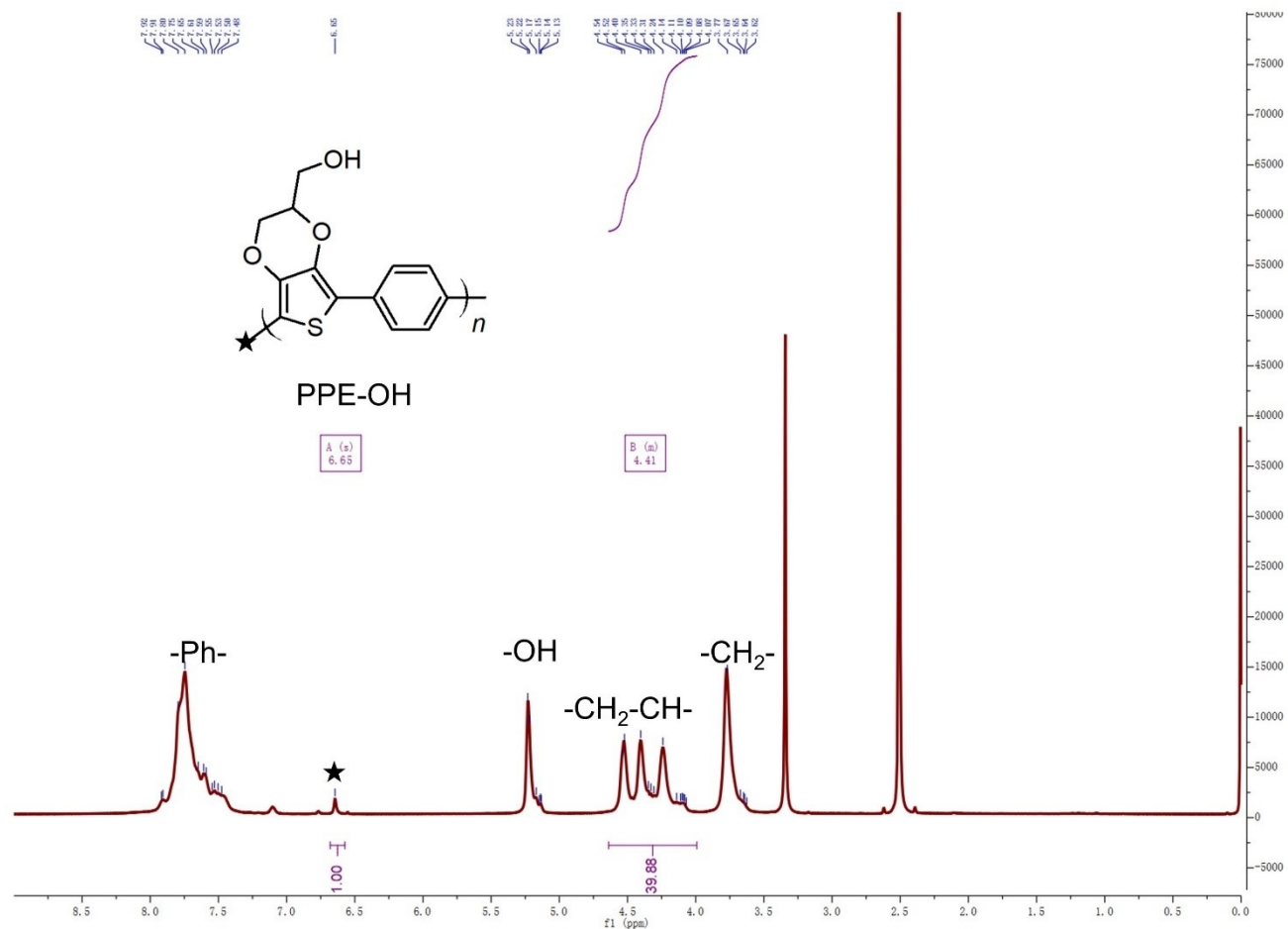
^1H NMR of PPE-OH with entry 8 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



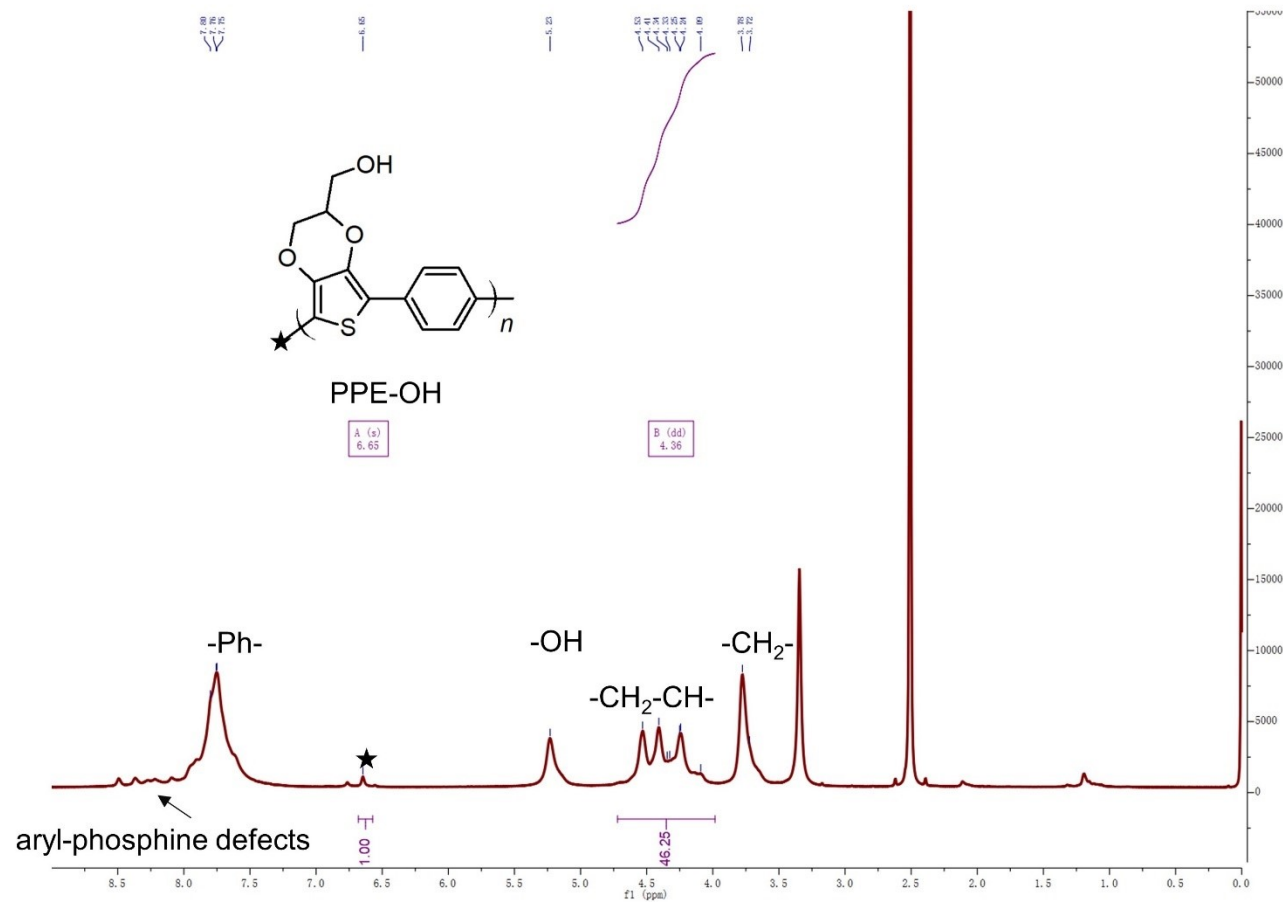
^1H NMR of PPE-OH with entry 9 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



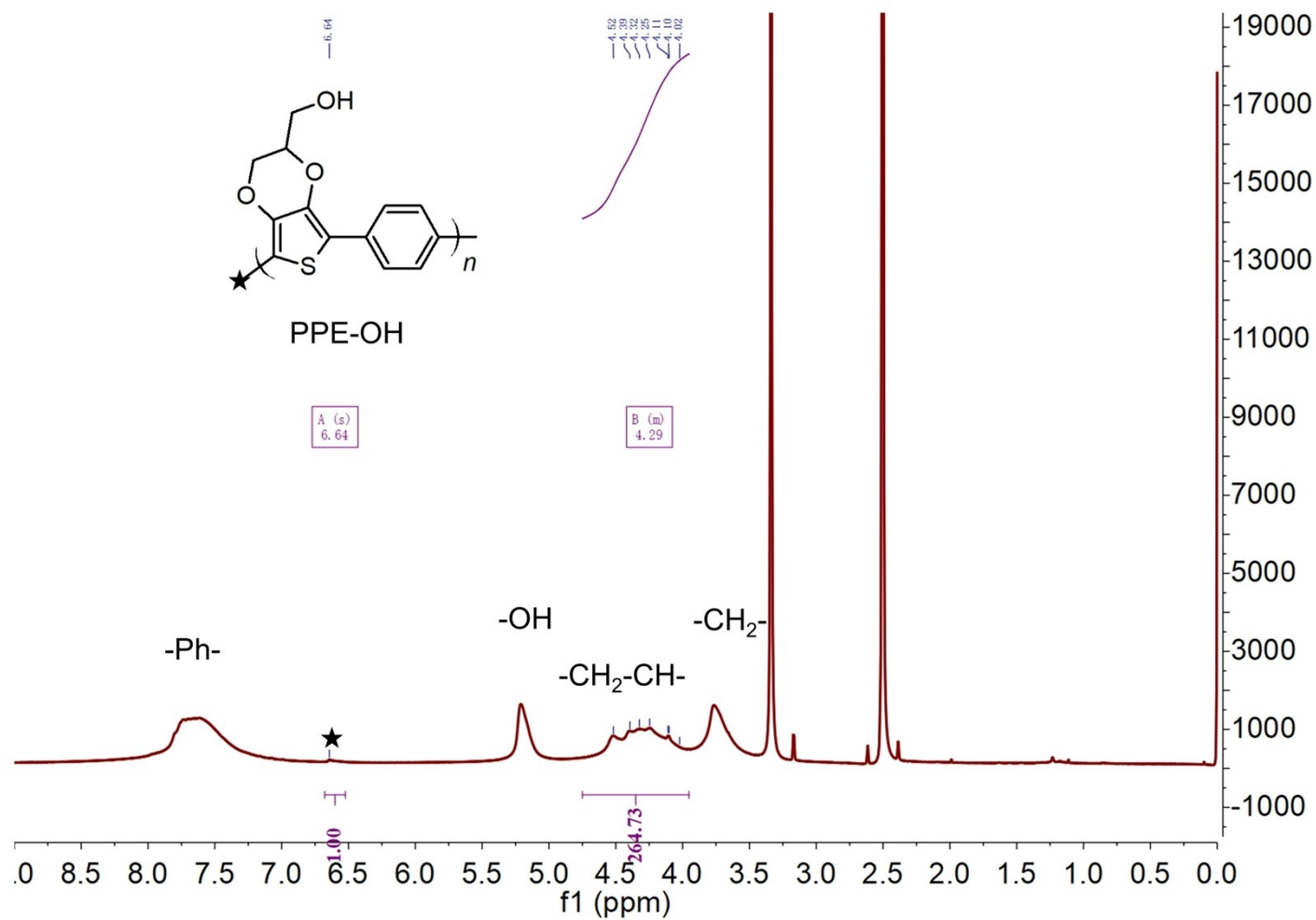
^1H NMR of PPE-OH with entry 10 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



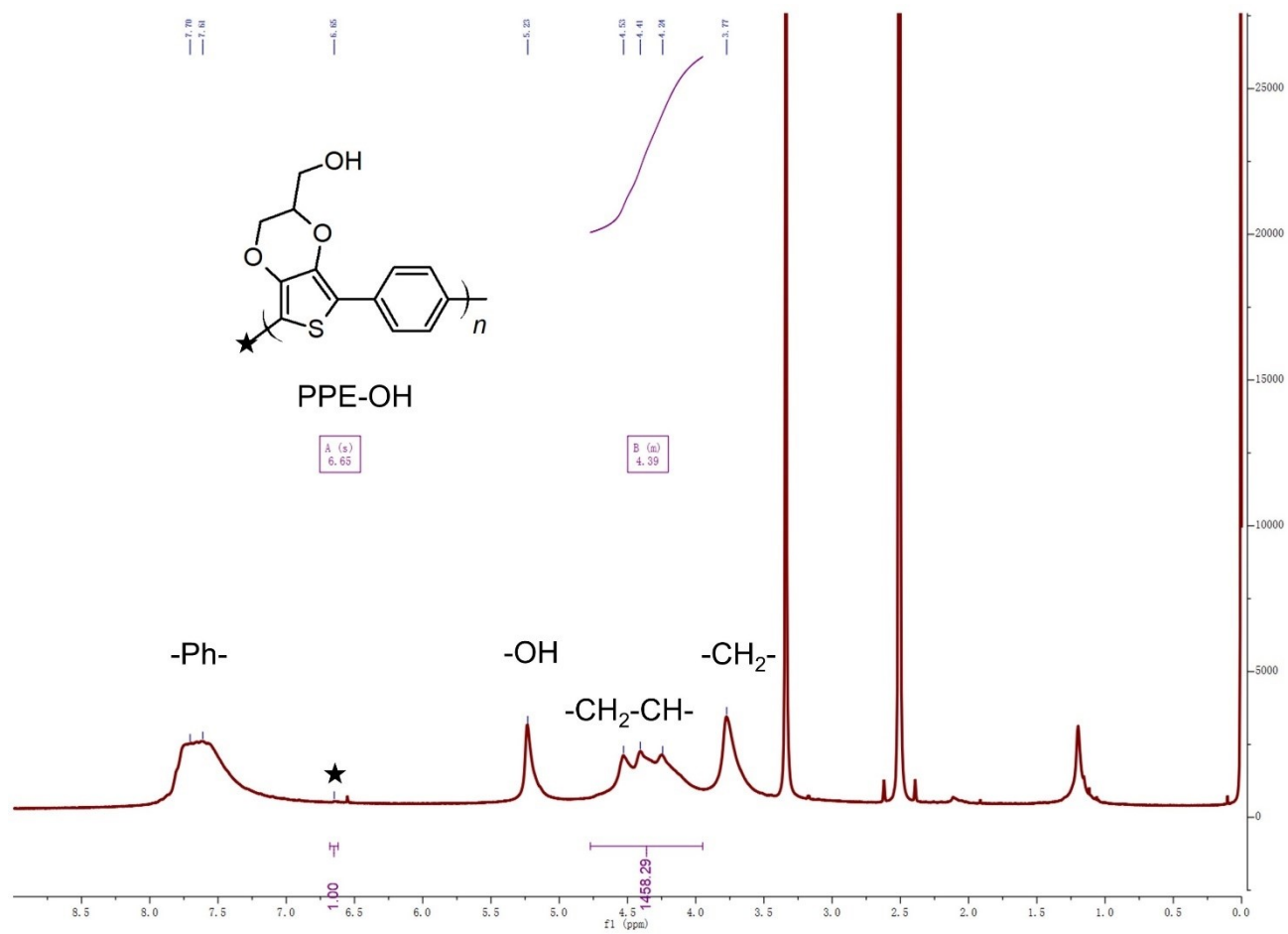
^1H NMR of PPE-OH with entry 11 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



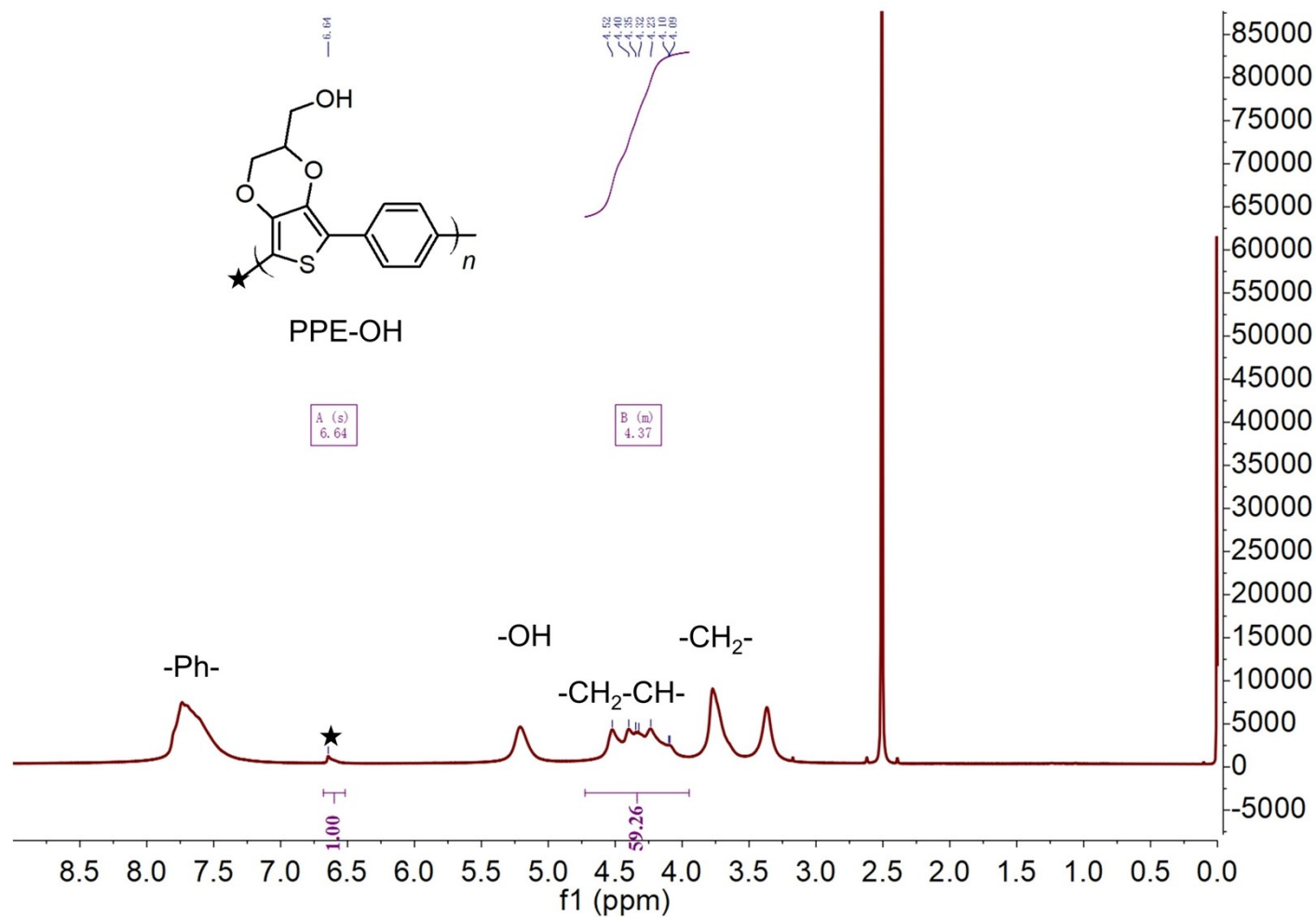
¹H NMR of PPE-OH with entry 12 of Table S4 [600MHz, dimethyl sulfoxide-d6, 323K]



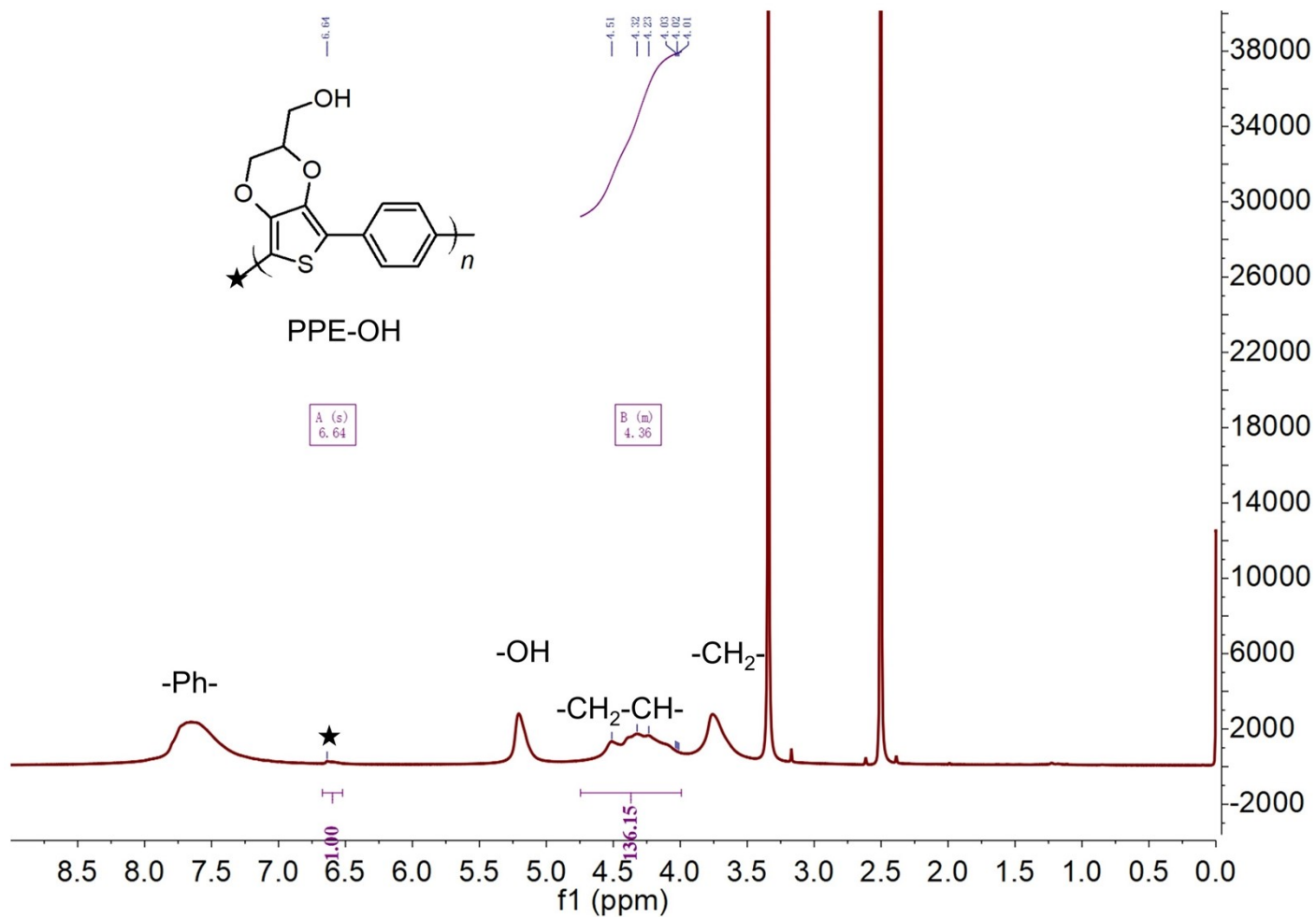
^1H NMR of PPE-OH with entry 13 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



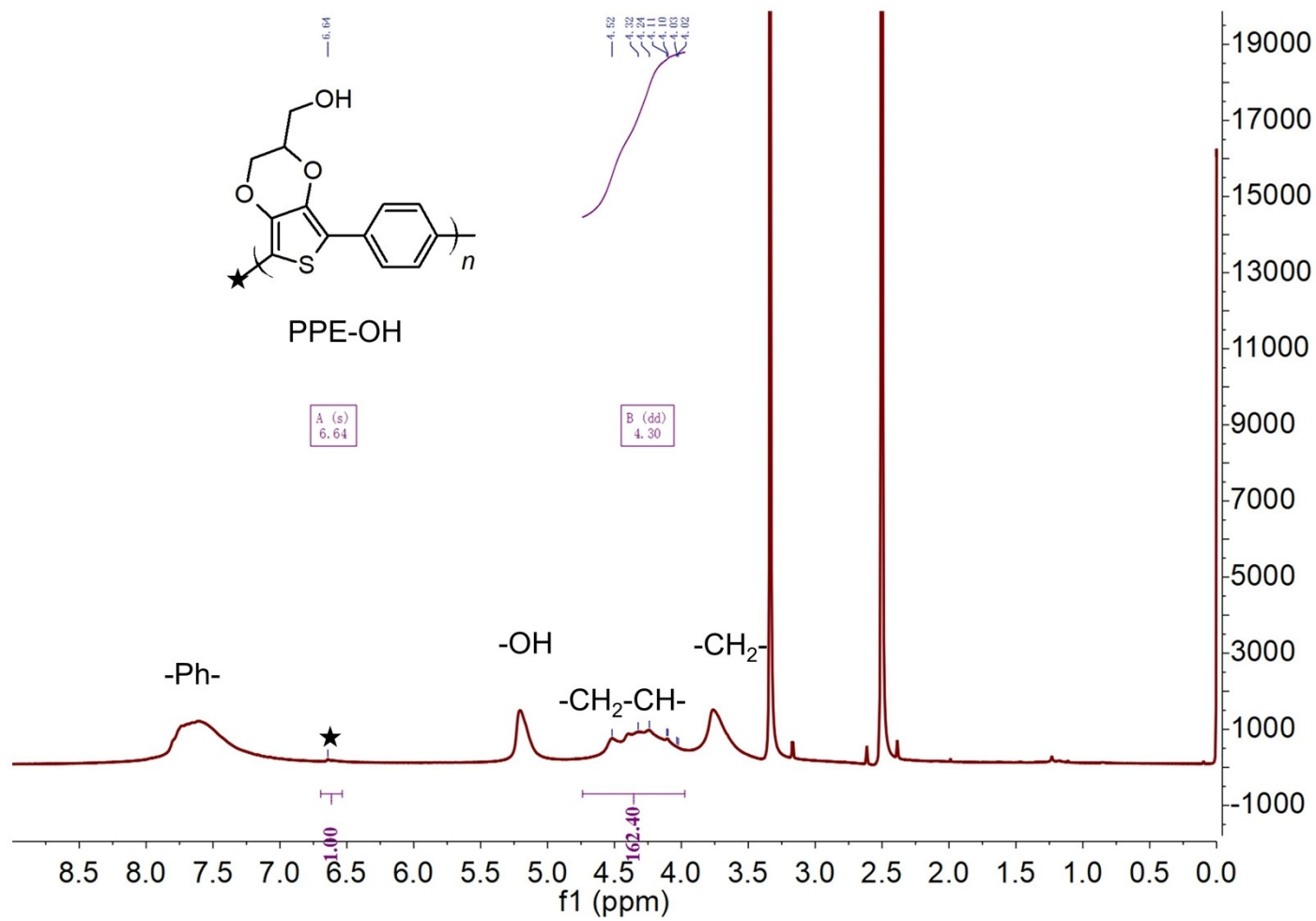
^1H NMR of PPE-OH with entry 14 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



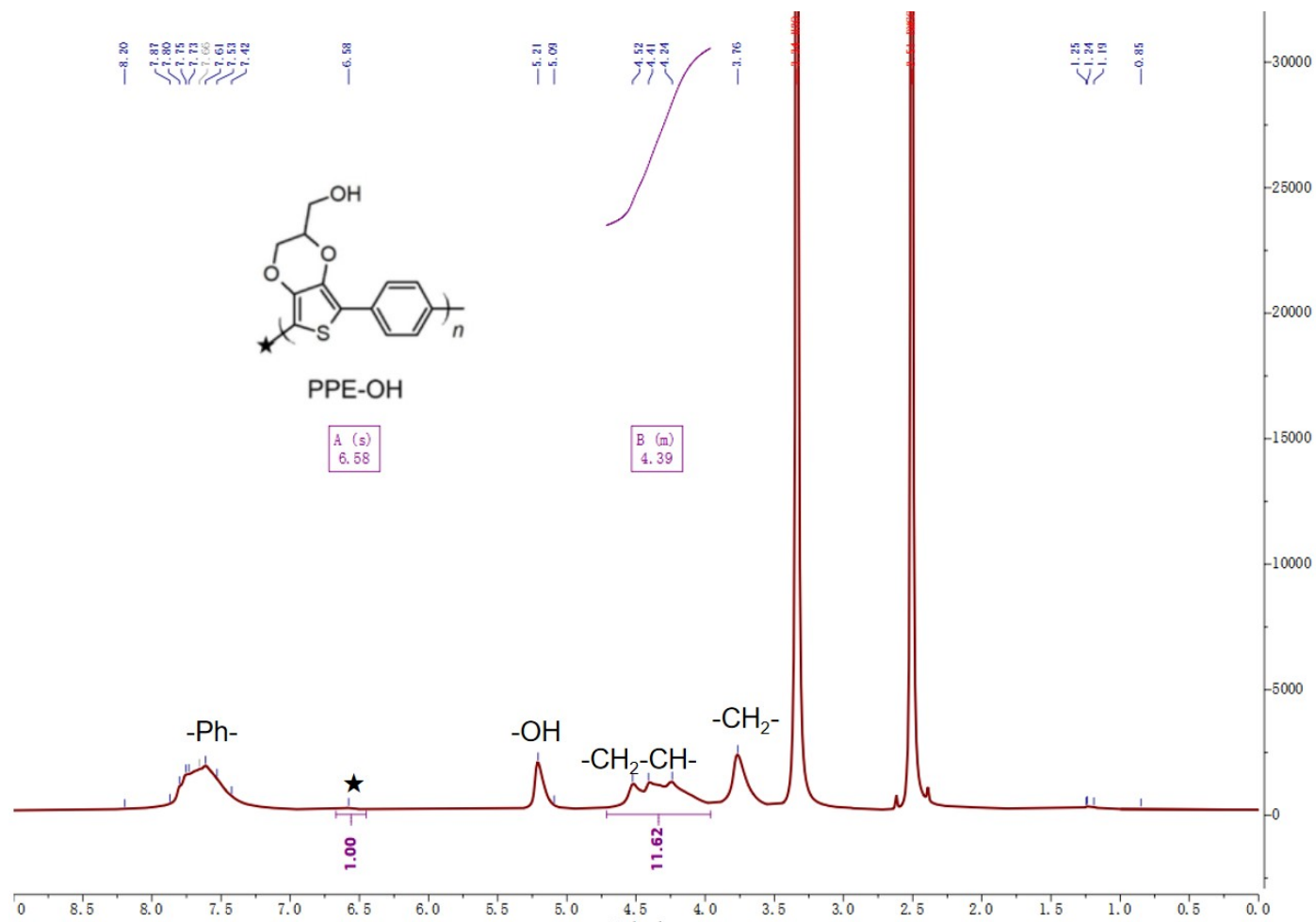
^1H NMR of PPE-OH with entry 15 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



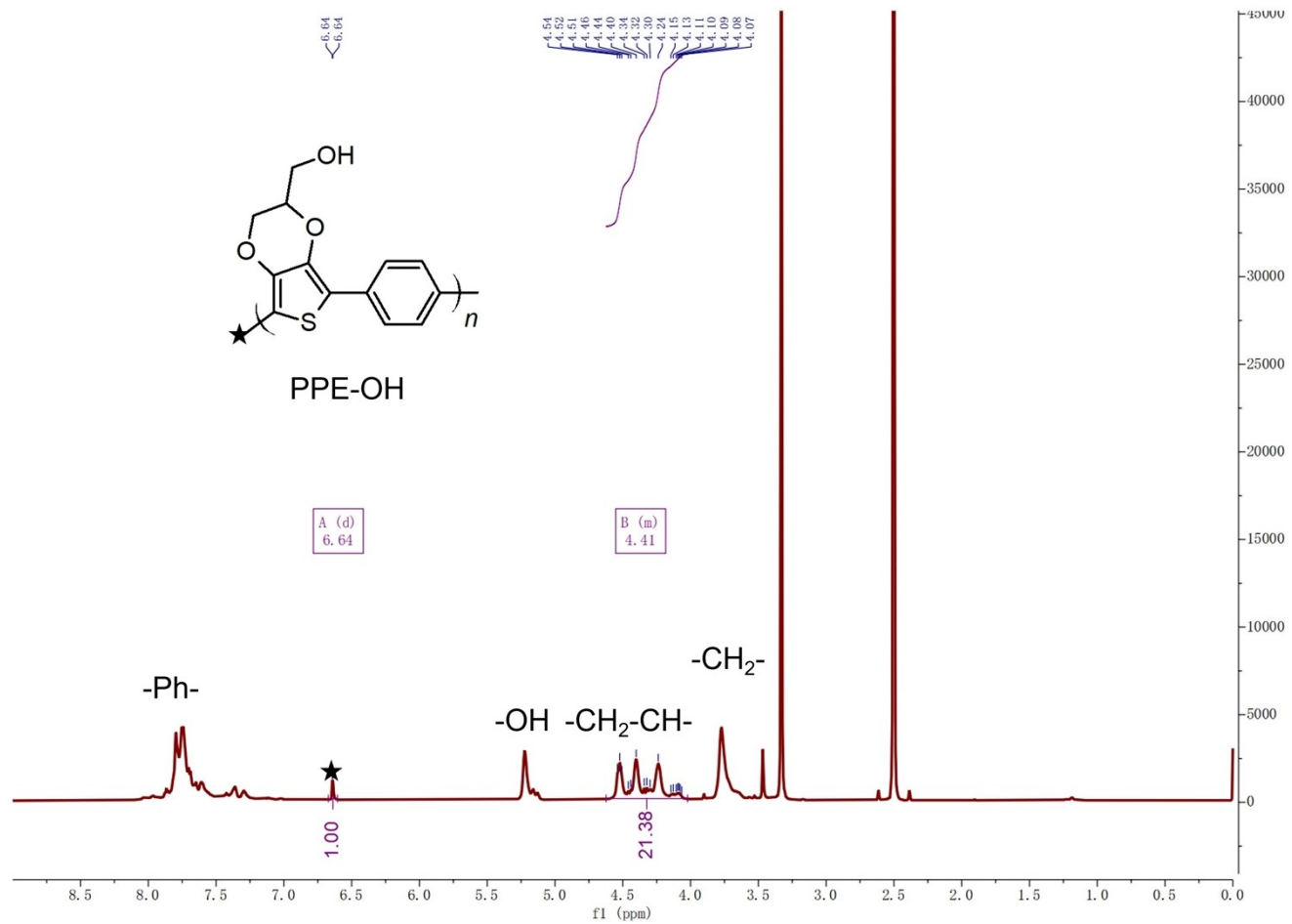
^1H NMR of PPE-OH with entry 16 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



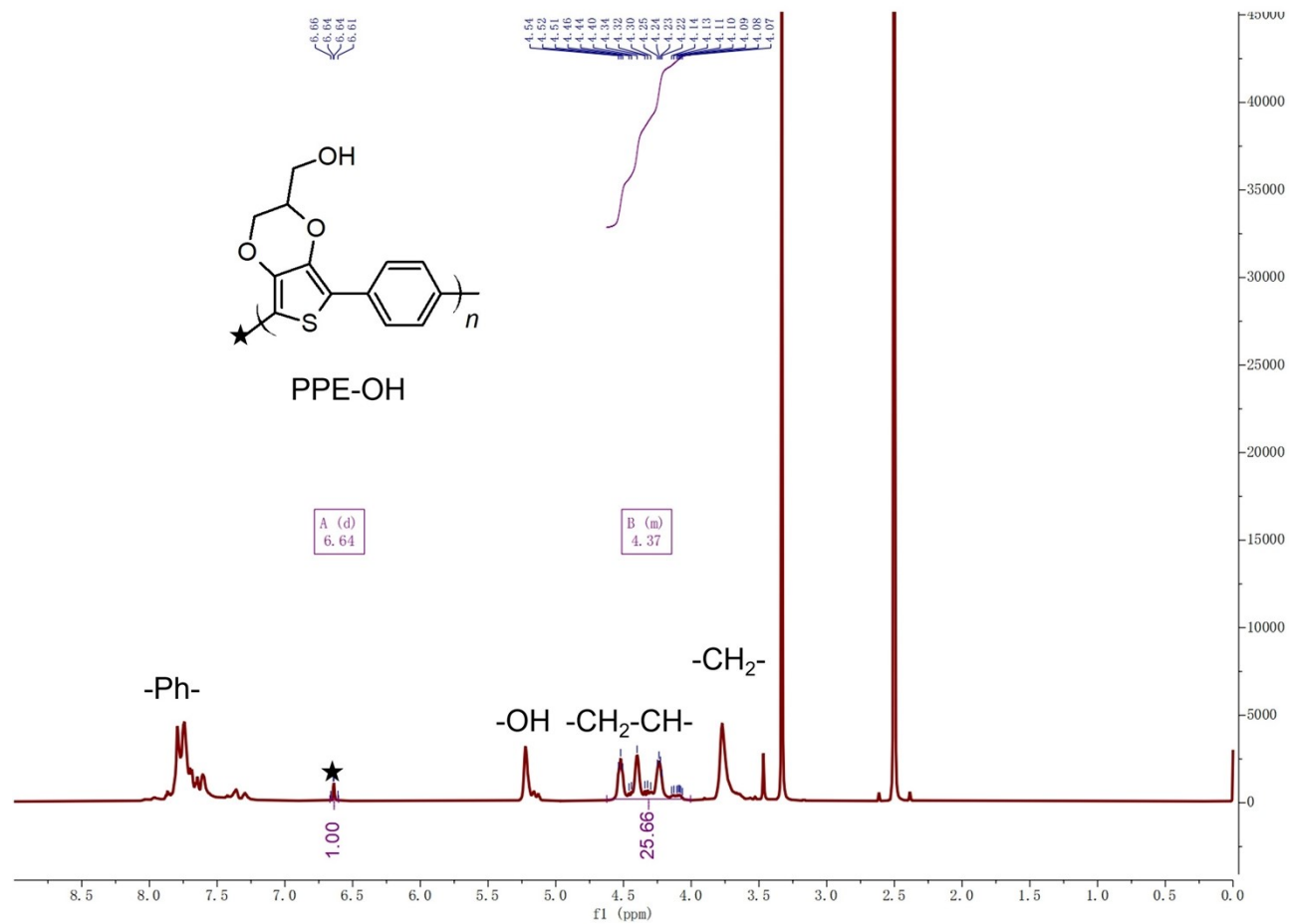
^1H NMR of PPE-OH with entry 17 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



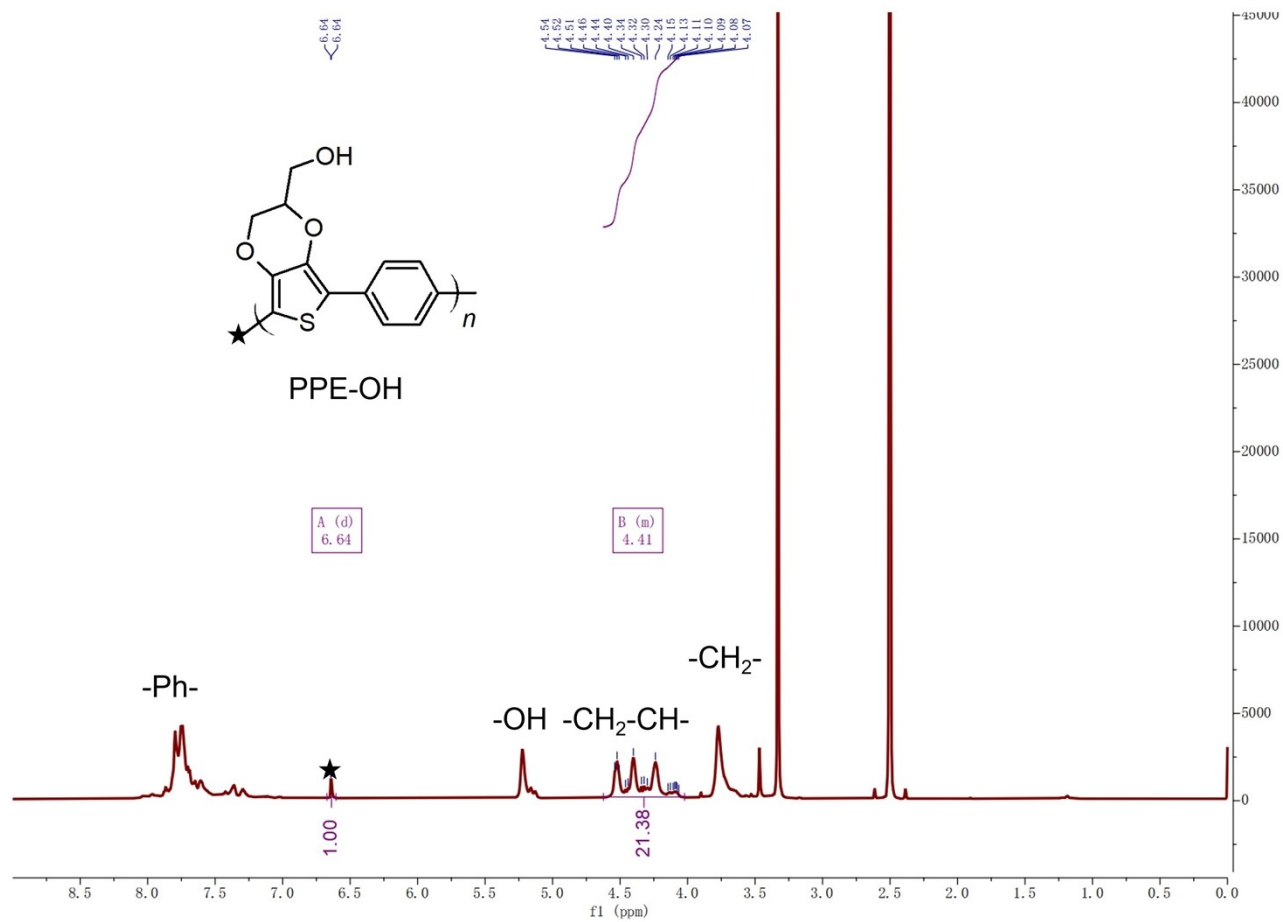
^1H NMR of PPE-OH with entry 19 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



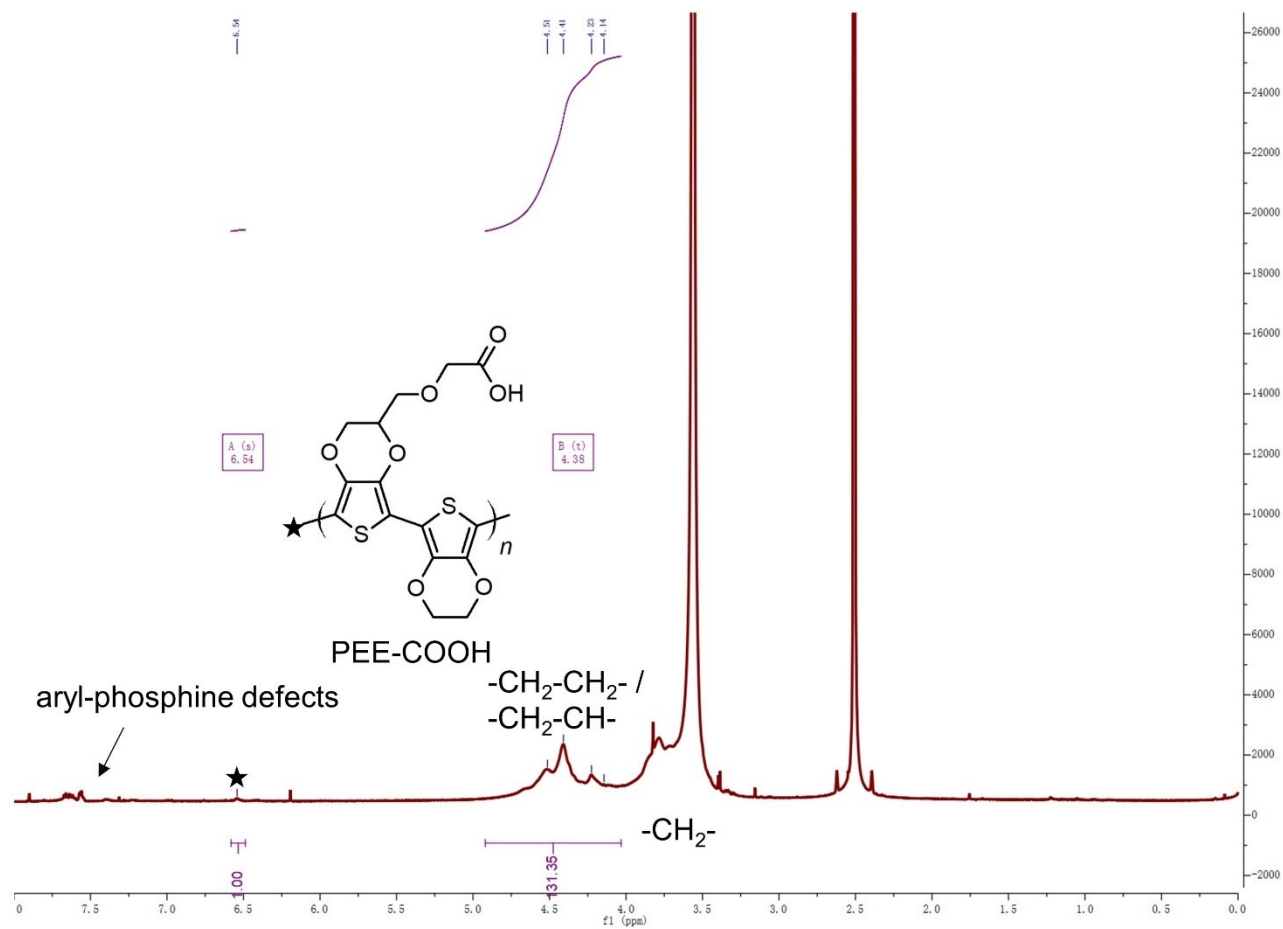
^1H NMR of PPE-OH with entry 20 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



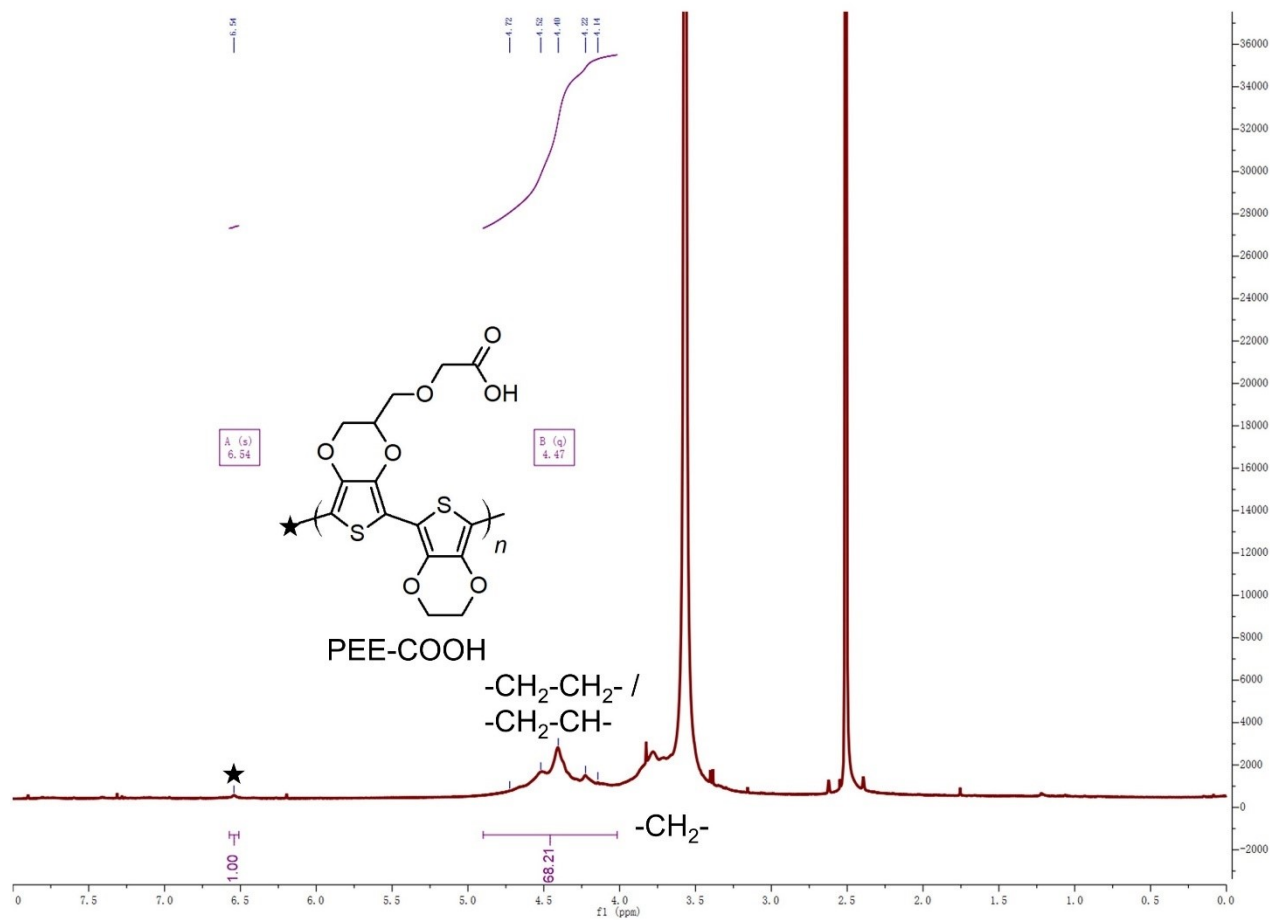
^1H NMR of PPE-OH with entry 21 of Table S4 [600MHz, dimethyl sulfoxide-d₆, 323K]



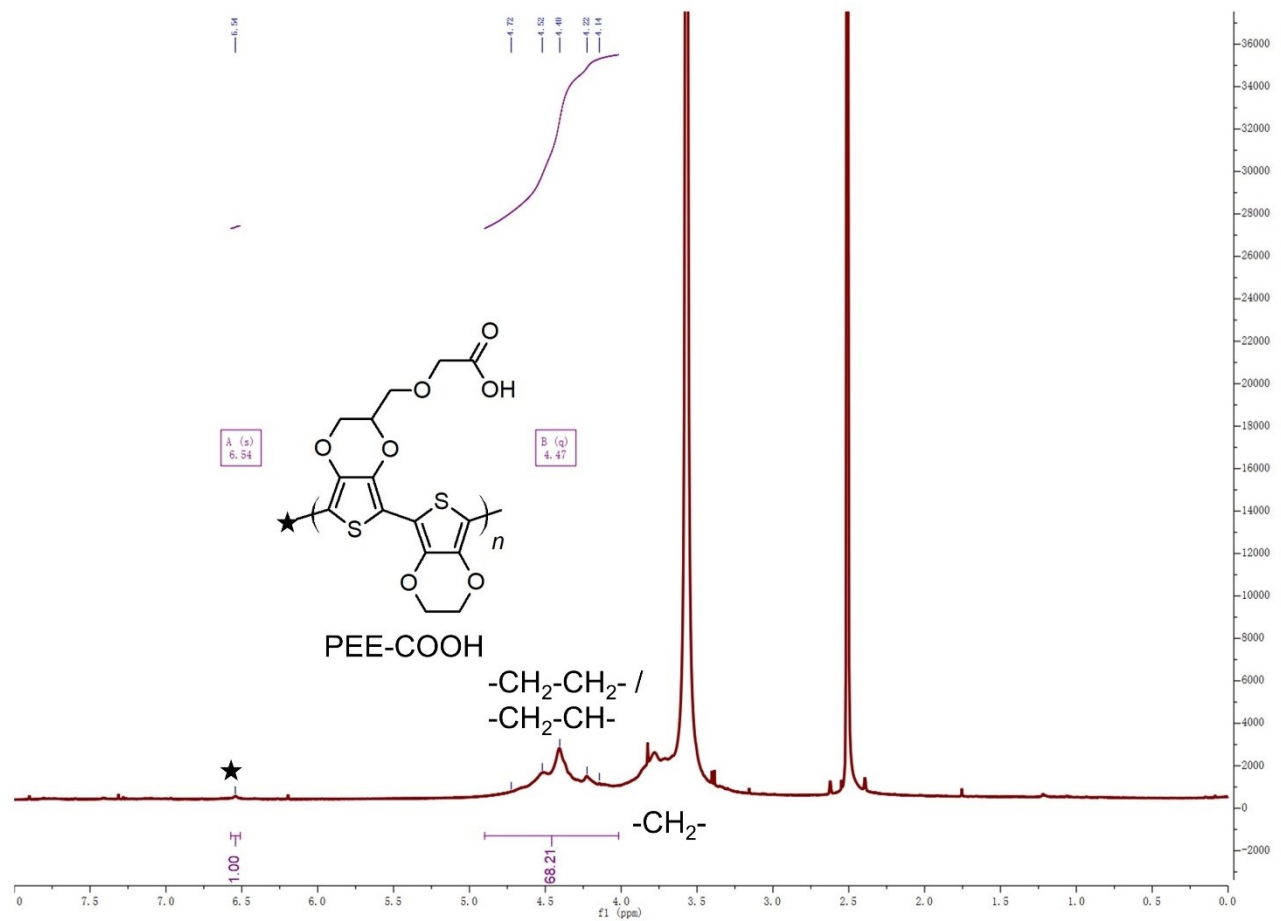
¹H NMR of PEE-COOH with entry 4 of Table S5 [600MHz, dimethyl sulfoxide-d6/deuterium oxide/hydrazine hydrate-d6 (v/v 100:5:1), 323K]



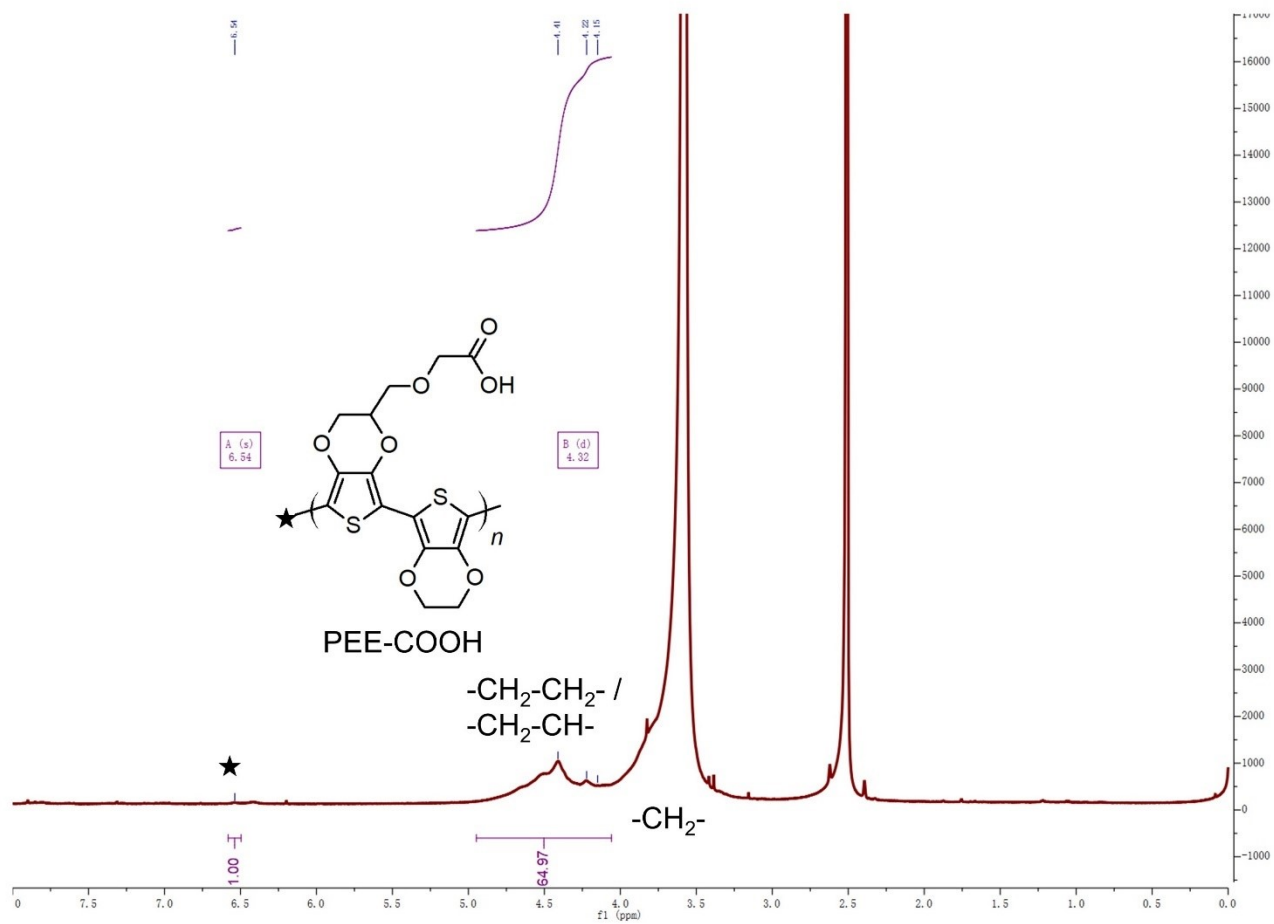
¹H NMR of PEE-COOH with entry 8 of Table S5 [600MHz, dimethyl sulfoxide-d6/deuterium oxide/hydrazine hydrate-d6 (v/v 100:5:1), 323K]



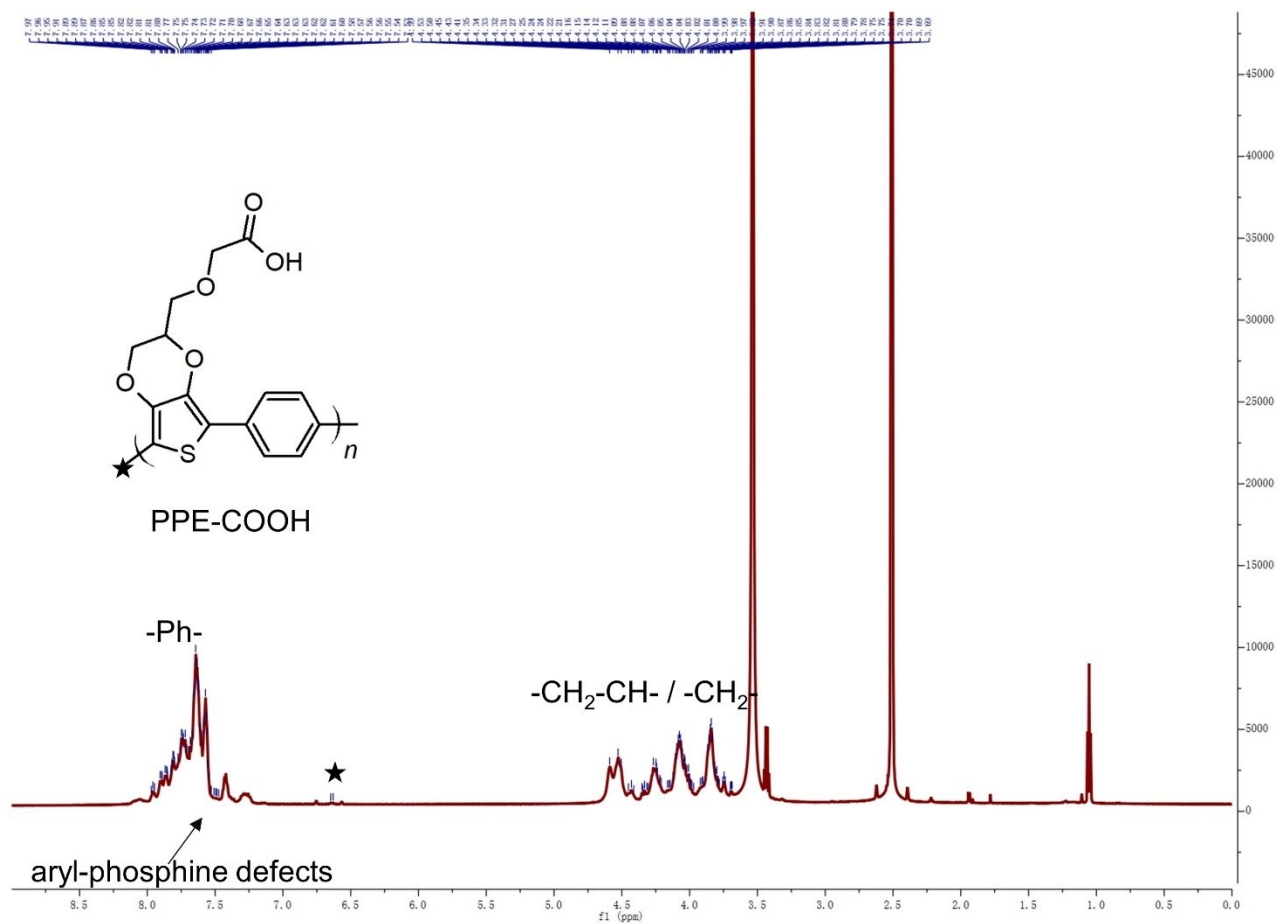
^1H NMR of PEE-COOH with entry 9 of Table S5 [600MHz, dimethyl sulfoxide-d₆/deuterium oxide/hydrazine hydrate-d₆ (v/v 100:5:1), 323K]



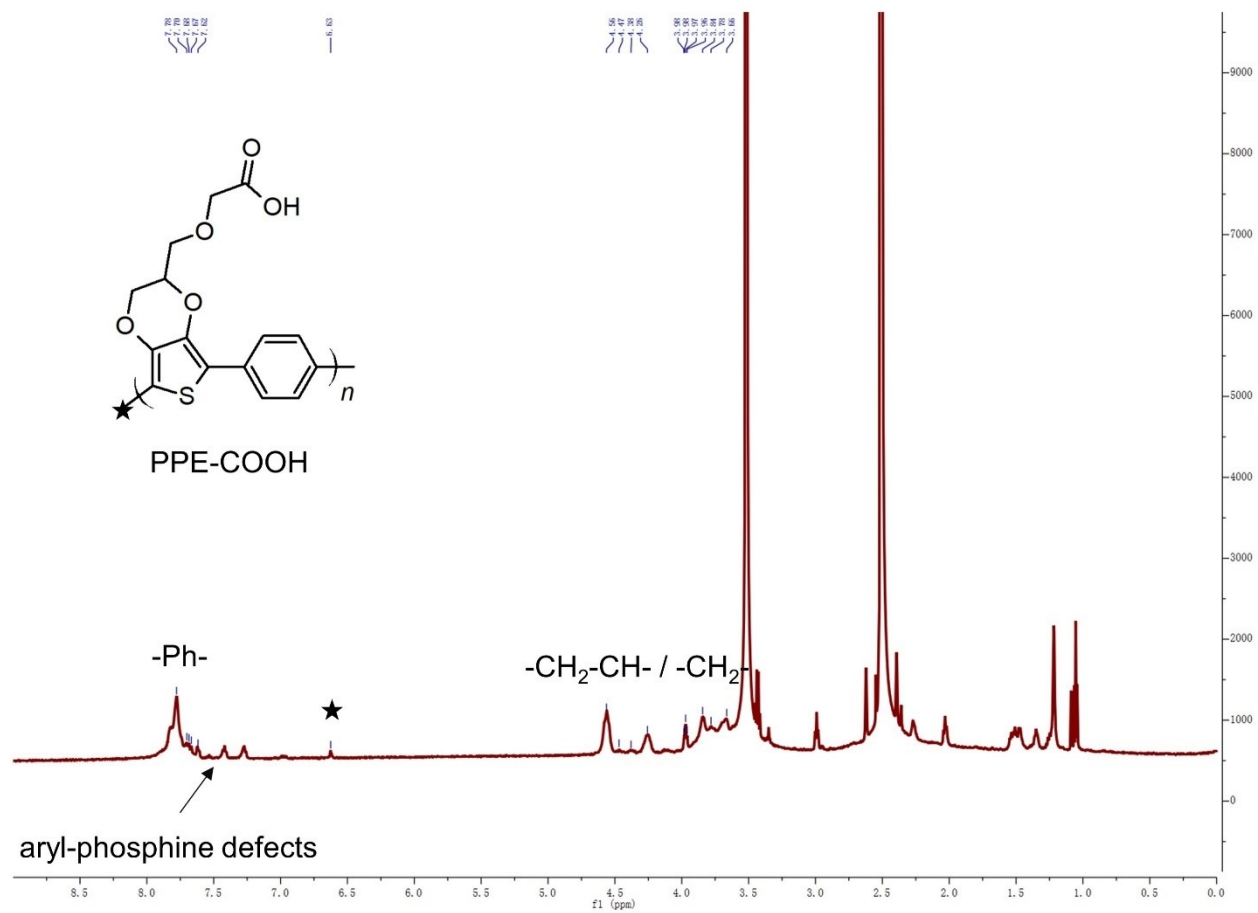
^1H NMR of PEE-COOH with entry 10 of Table S5 [600MHz, dimethyl sulfoxide-d₆/deuterium oxide/hydrazine hydrate-d₆ (v/v 100:5:1), 323K]



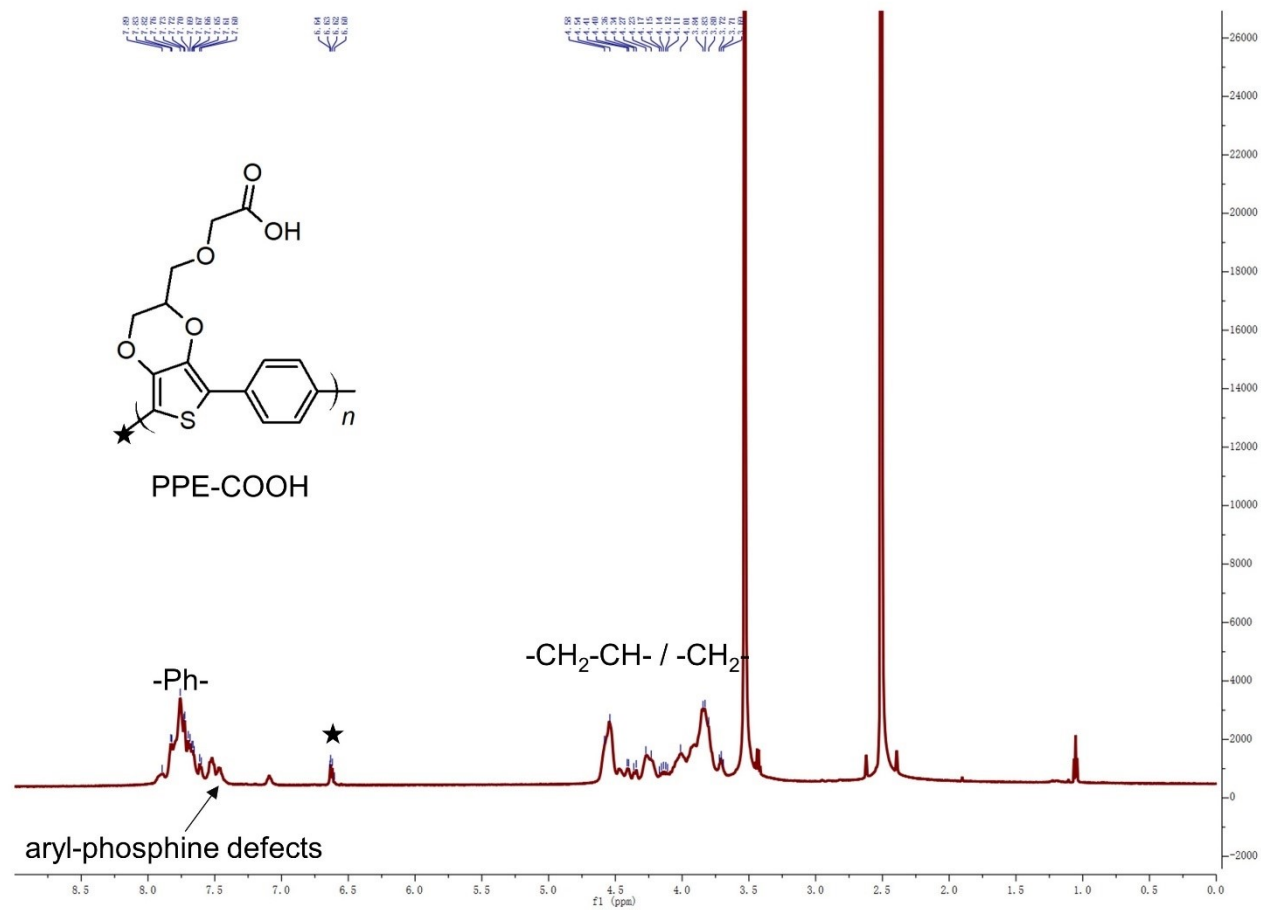
^1H NMR of PPE-COOH with entry 4 of Table S5 [600MHz, dimethyl sulfoxide-d₆/deuterium oxide/hydrazine hydrate-d₆ (v/v 100:5:1), 323K]



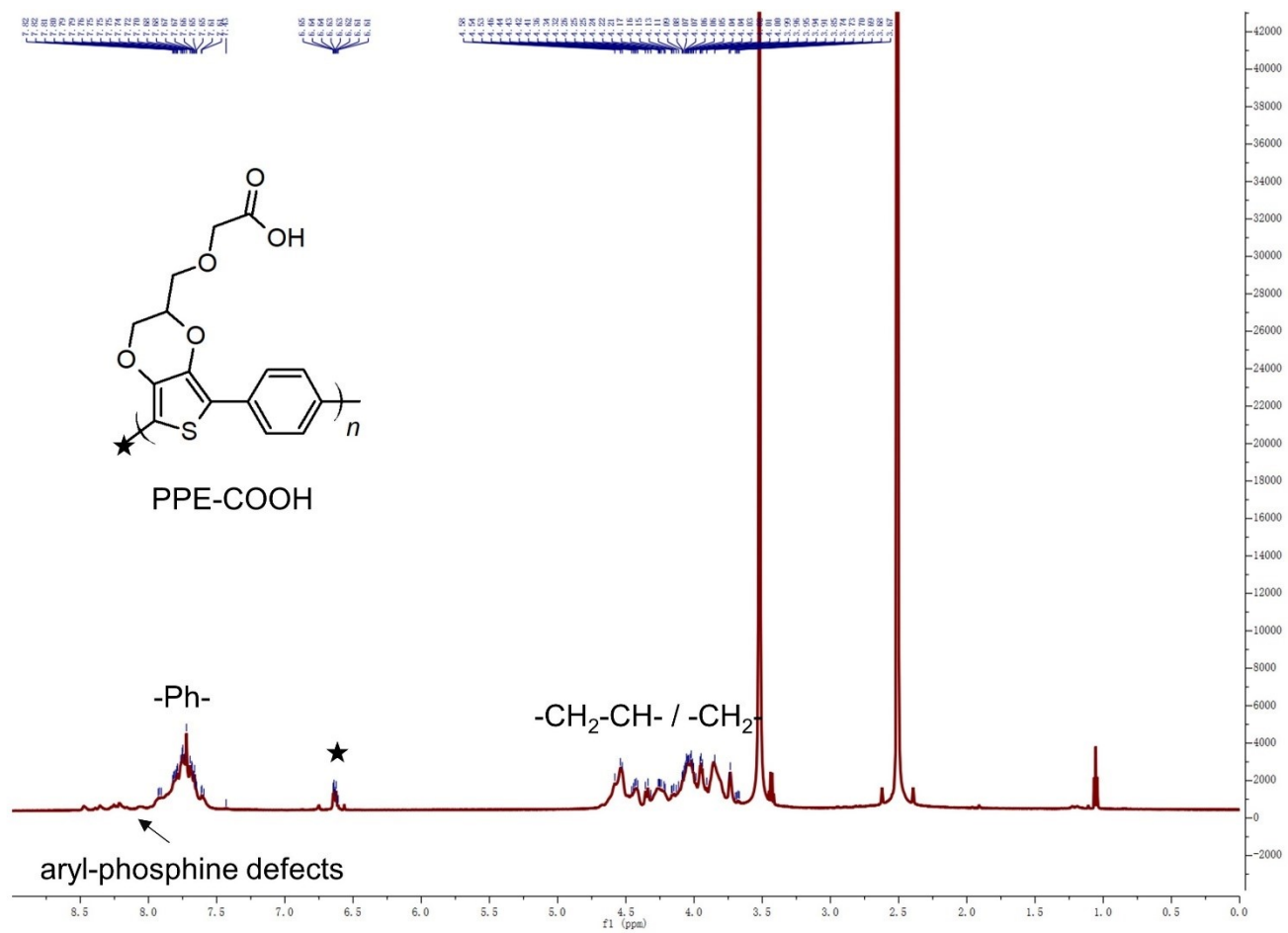
^1H NMR of PPE-COOH with entry 8 of Table S6 [600MHz, dimethyl sulfoxide-d₆/deuterium oxide/hydrazine hydrate-d₆ (v/v 100:5:1), 323K]



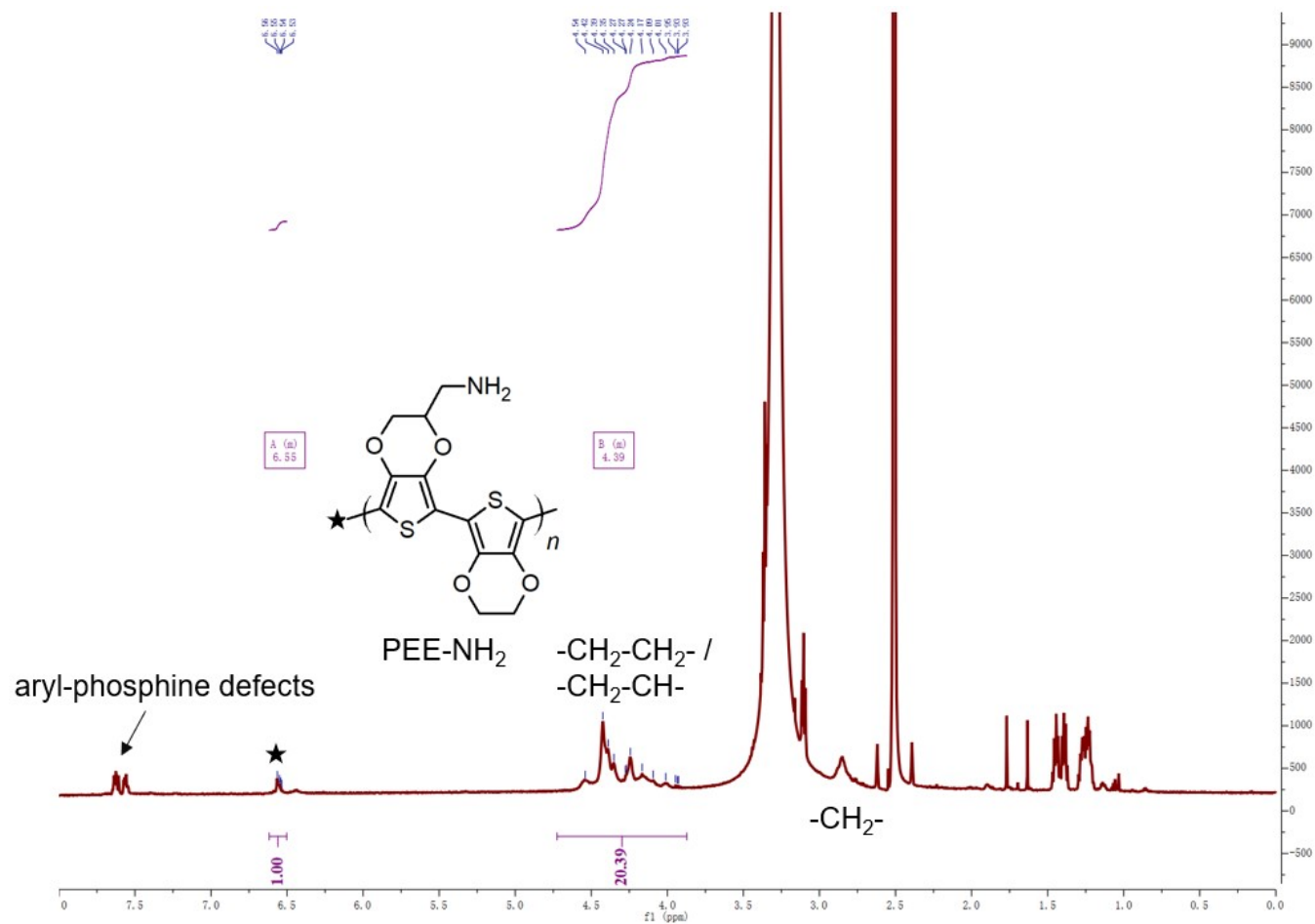
^1H NMR of PPE-COOH with entry 9 of Table S6 [600MHz, dimethyl sulfoxide-d₆/deuterium oxide/hydrazine hydrate-d₆ (v/v 100:5:1), 323K]



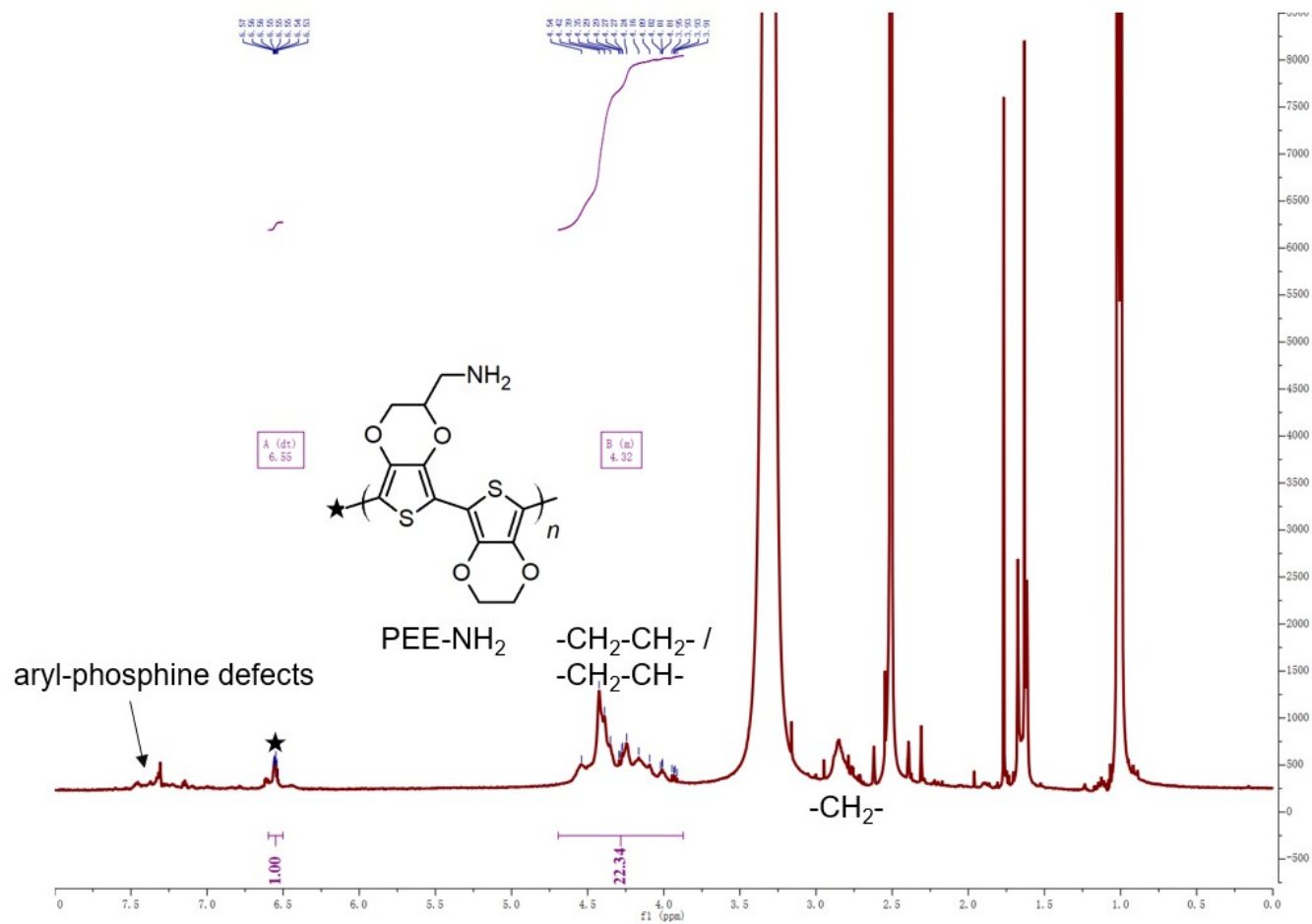
^1H NMR of PPE-COOH with entry 10 of Table S6 [600MHz, dimethyl sulfoxide- d_6 /deuterium oxide/hydrazine hydrate- d_6 (v/v 100:5:1), 323K]



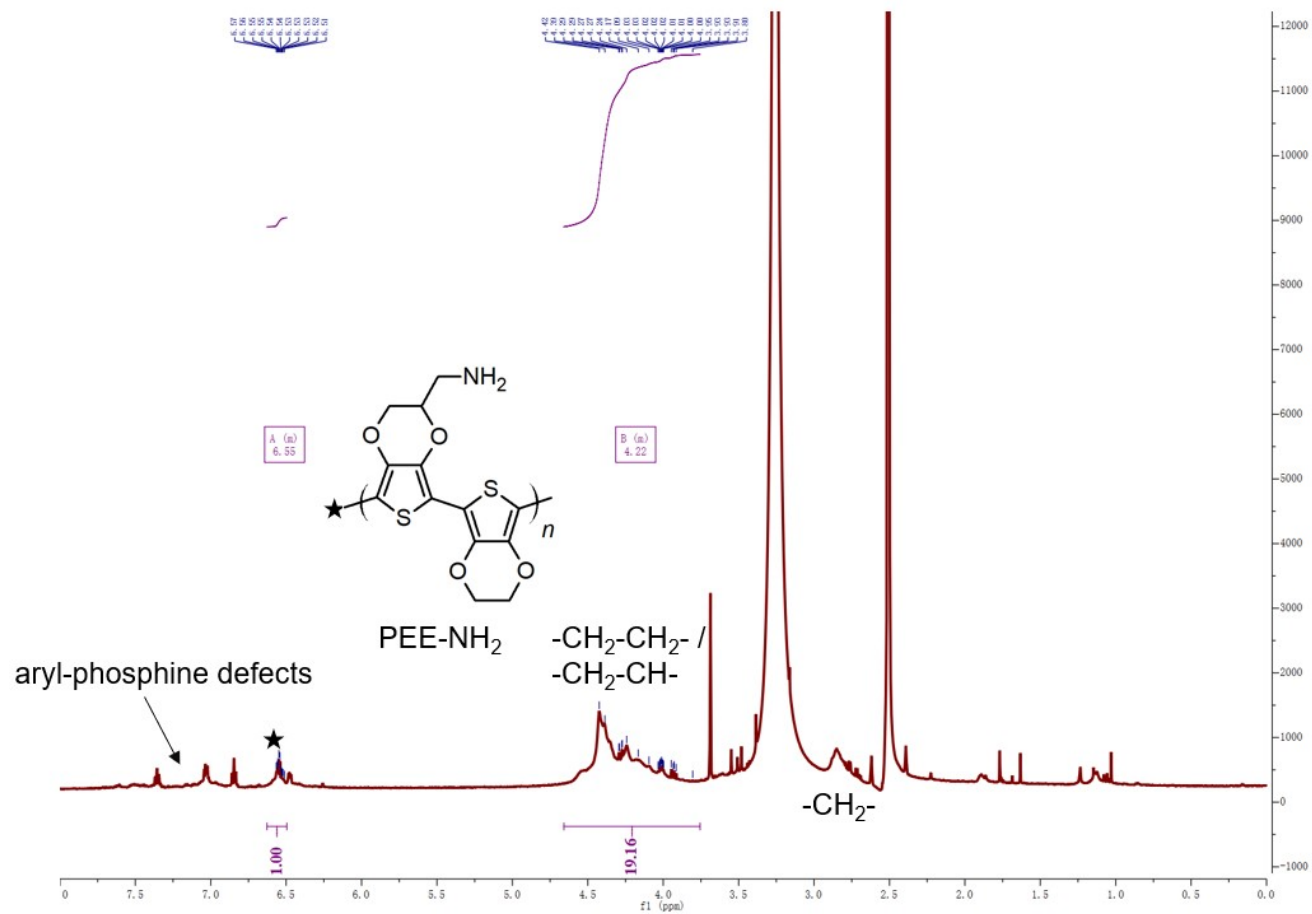
^1H NMR of PEE-NH₂ with entry 4 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



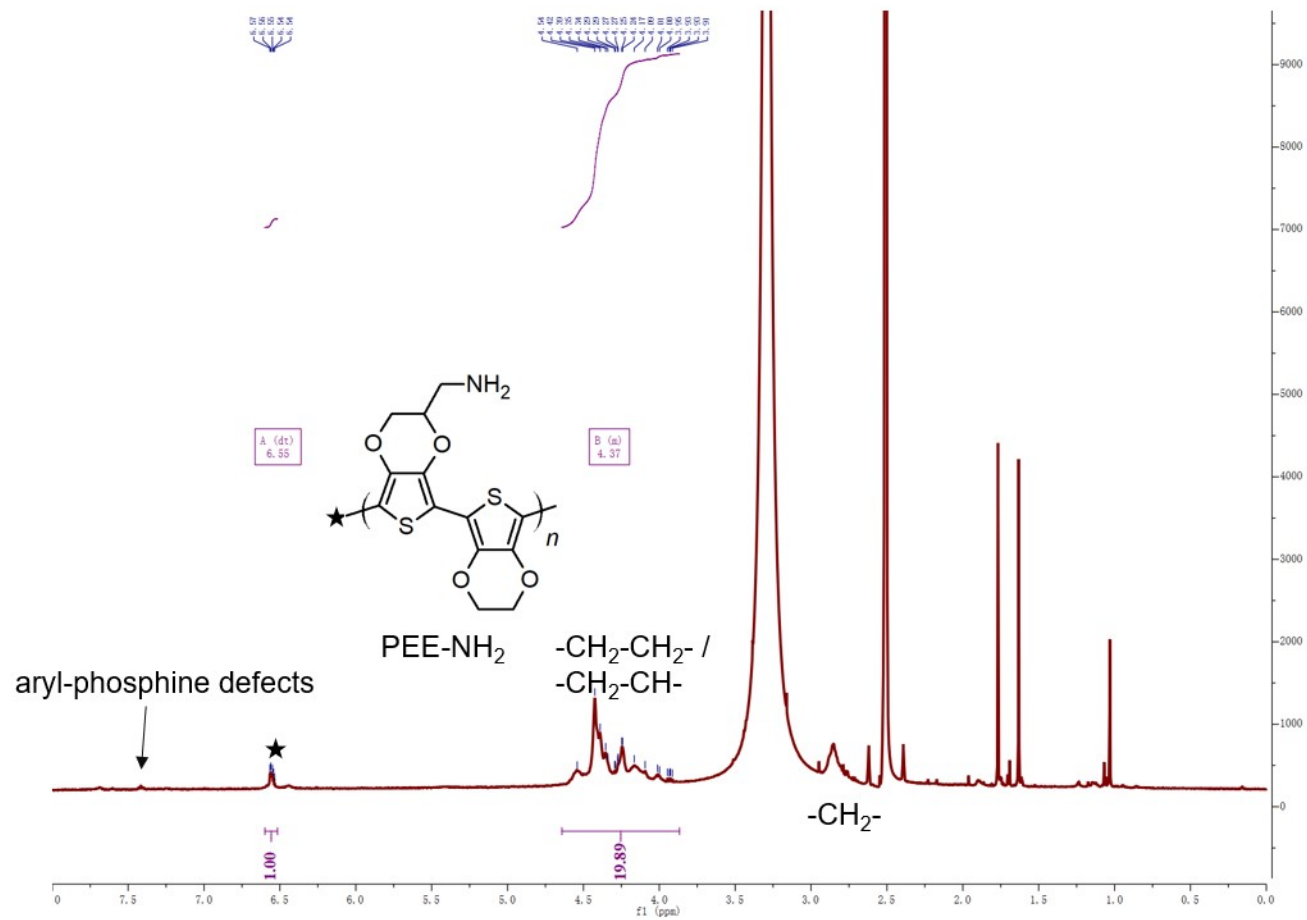
^1H NMR of PEE-NH₂ with entry 5 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



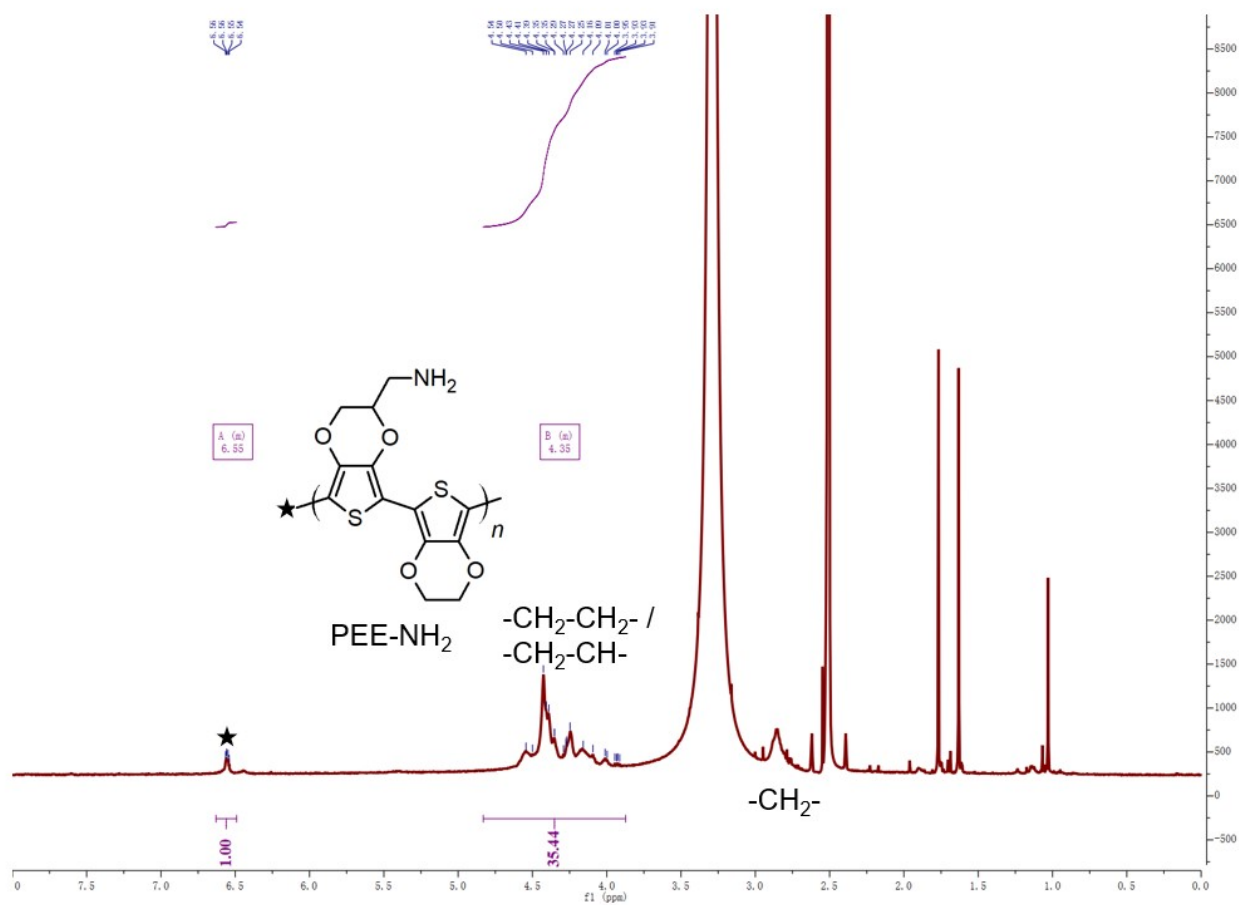
^1H NMR of PEE-NH₂ with entry 6 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



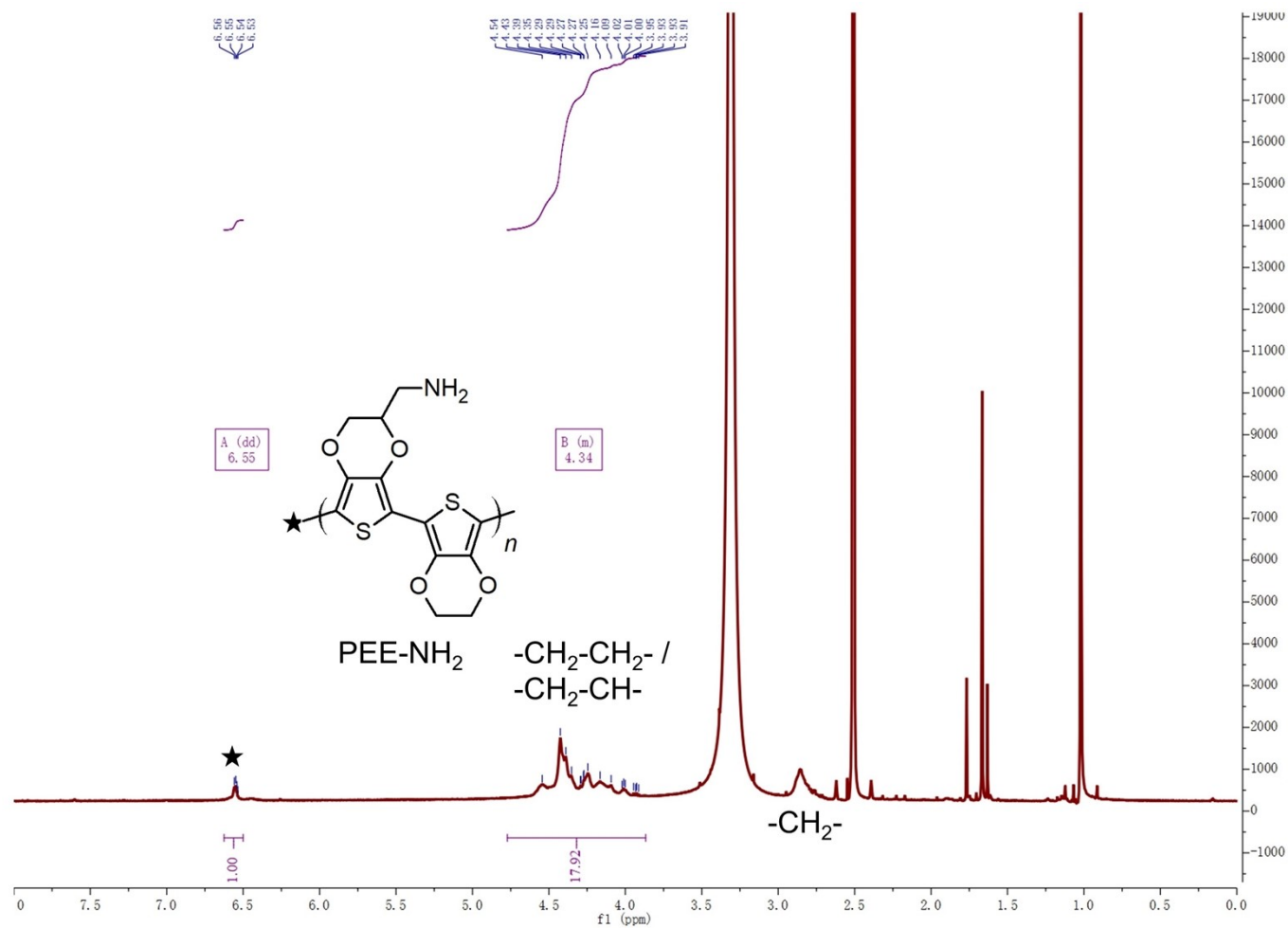
^1H NMR of PEE-NH₂ with entry 8 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



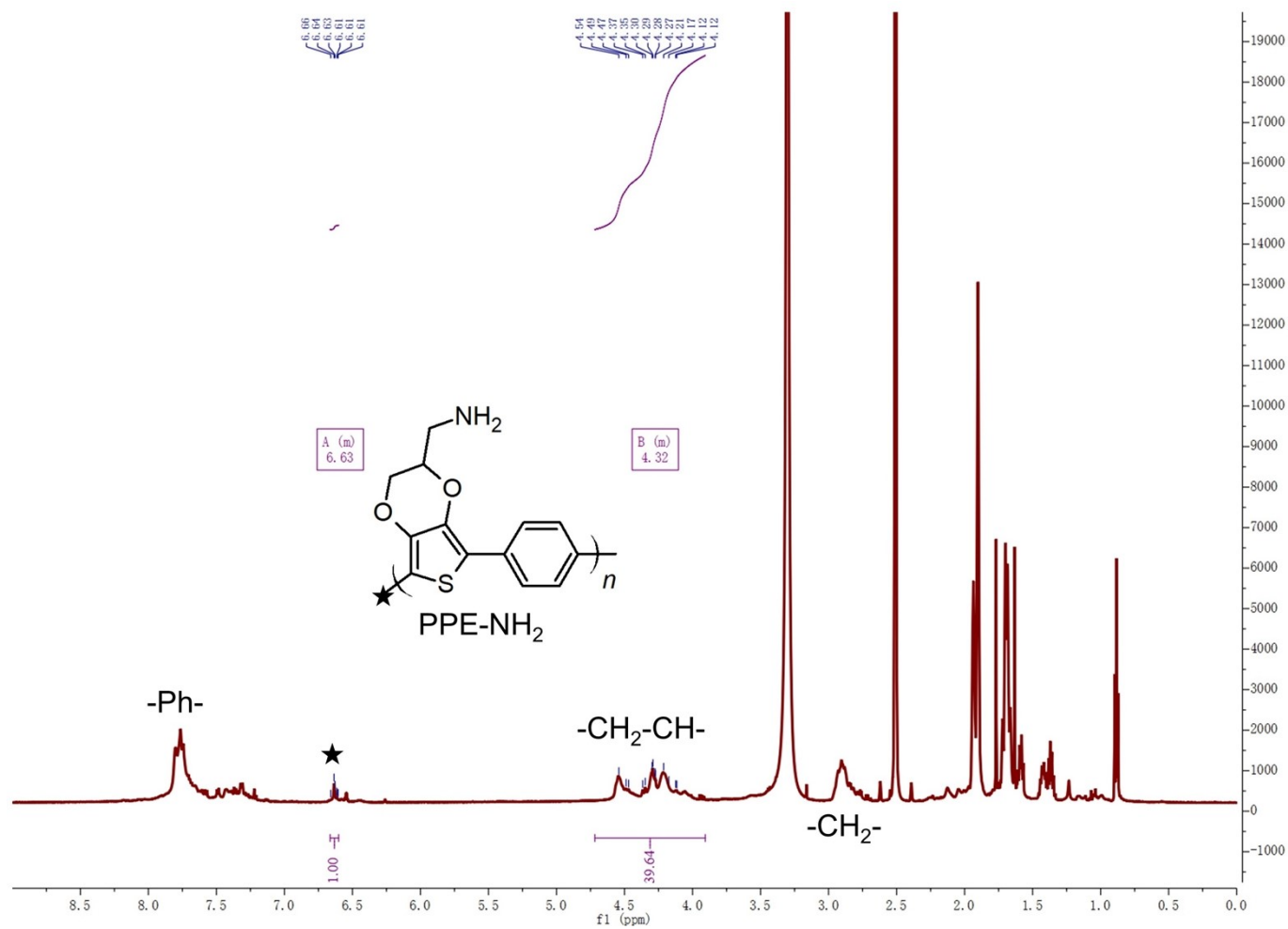
^1H NMR of PEE-NH₂ with entry 10 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



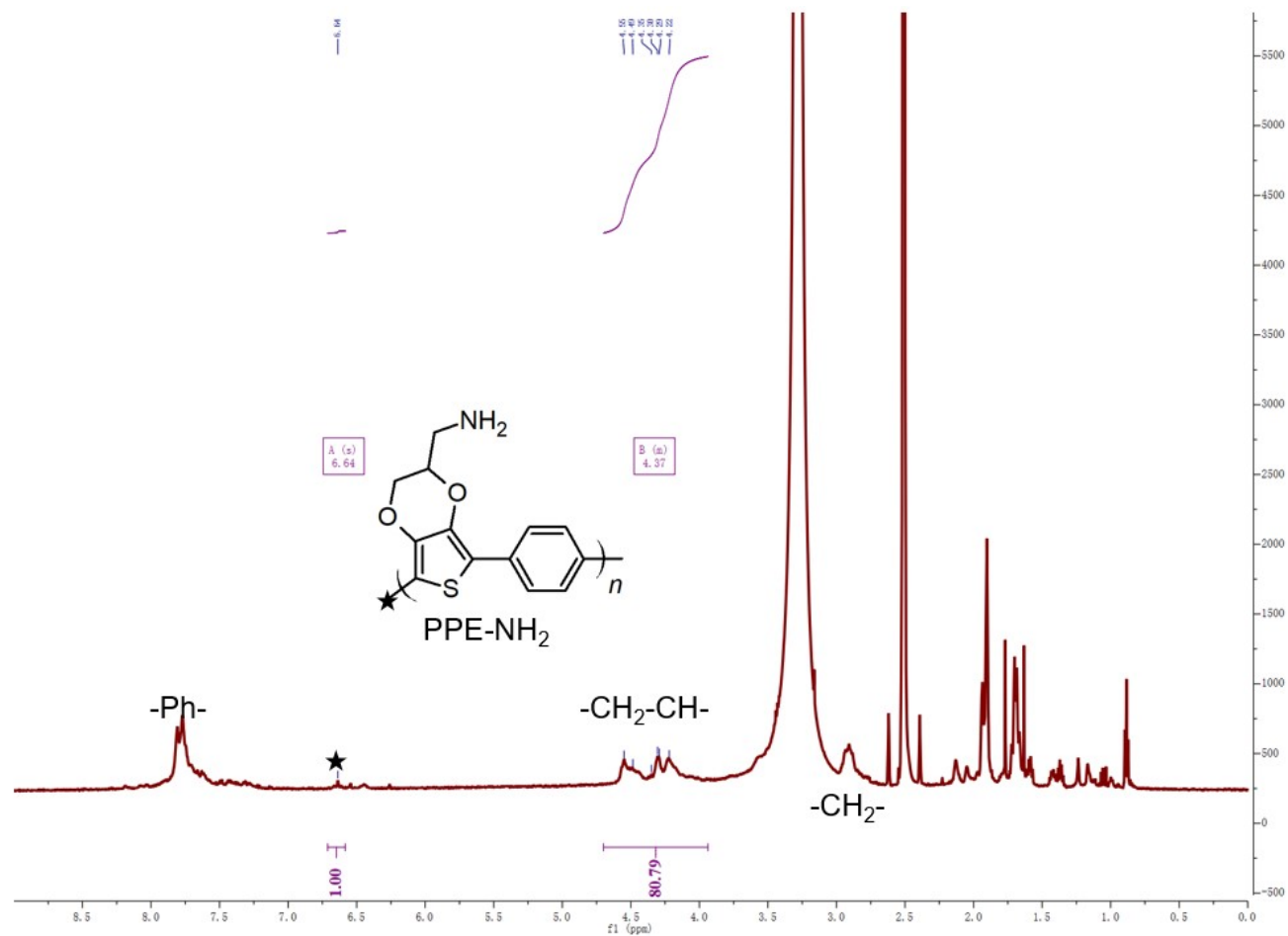
^1H NMR of PEE-NH₂ with entry 13 of Table S7 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



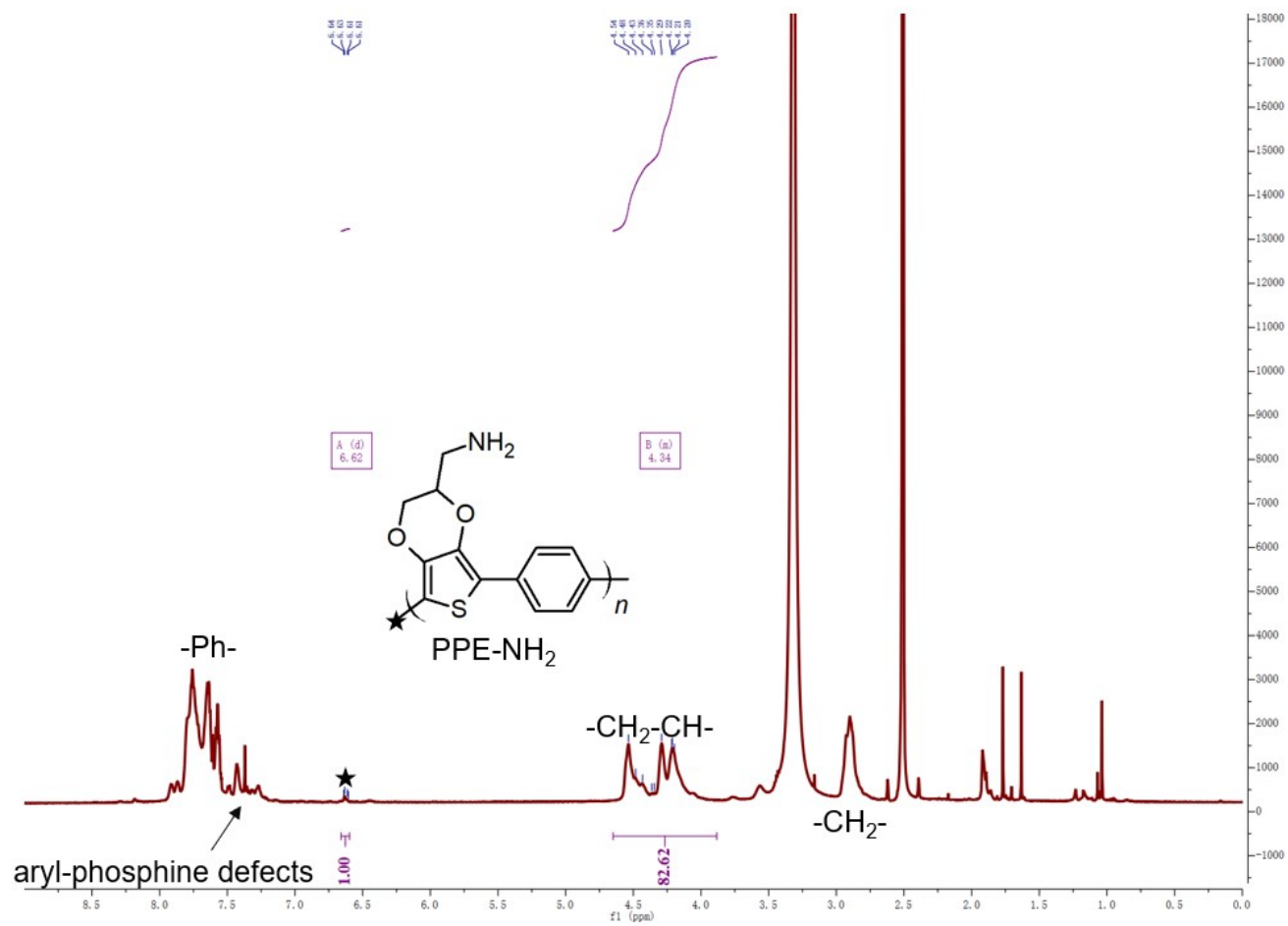
^1H NMR of PPE-NH₂ with entry 4 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



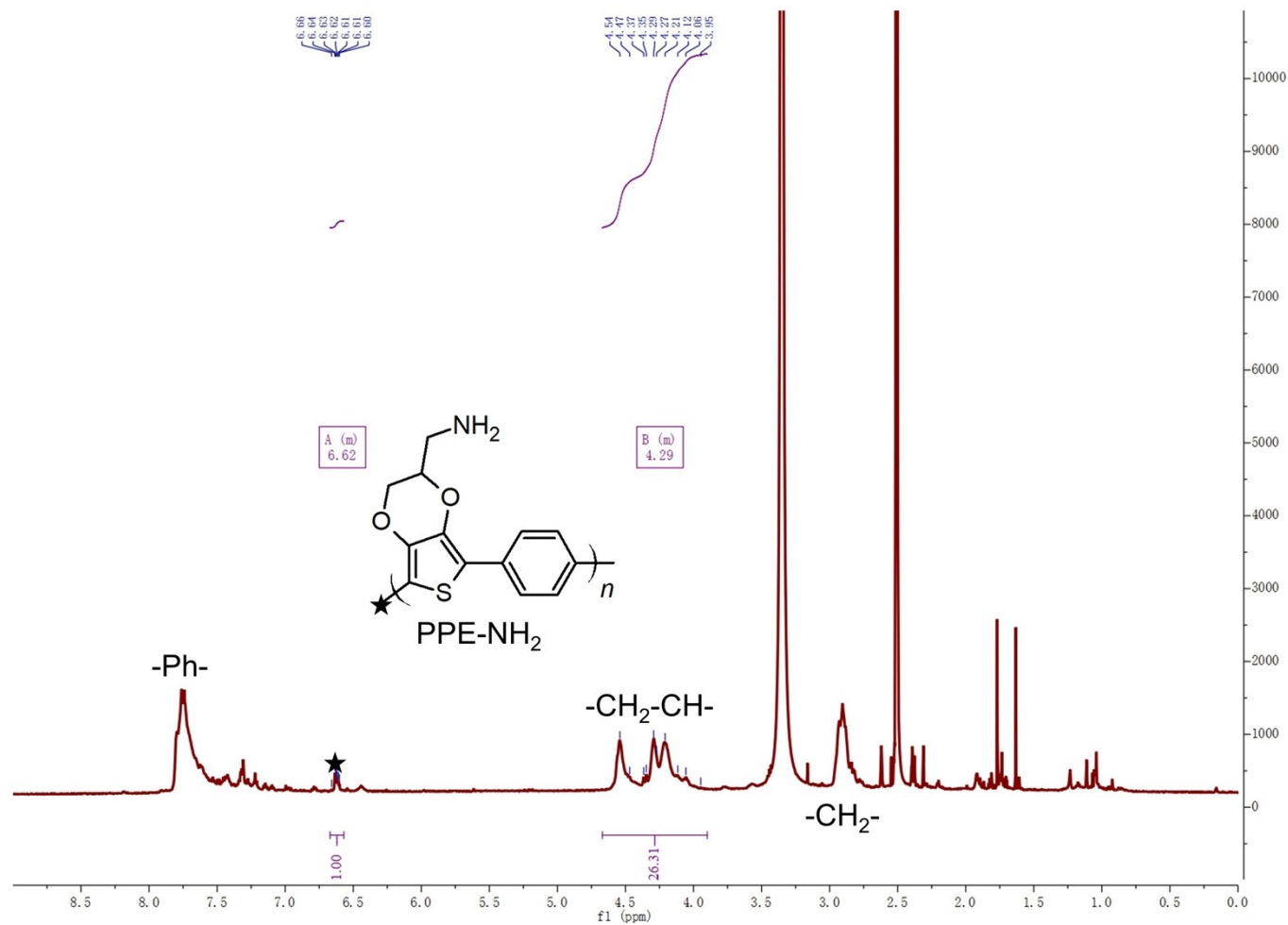
^1H NMR of PPE-NH₂ with entry 5 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



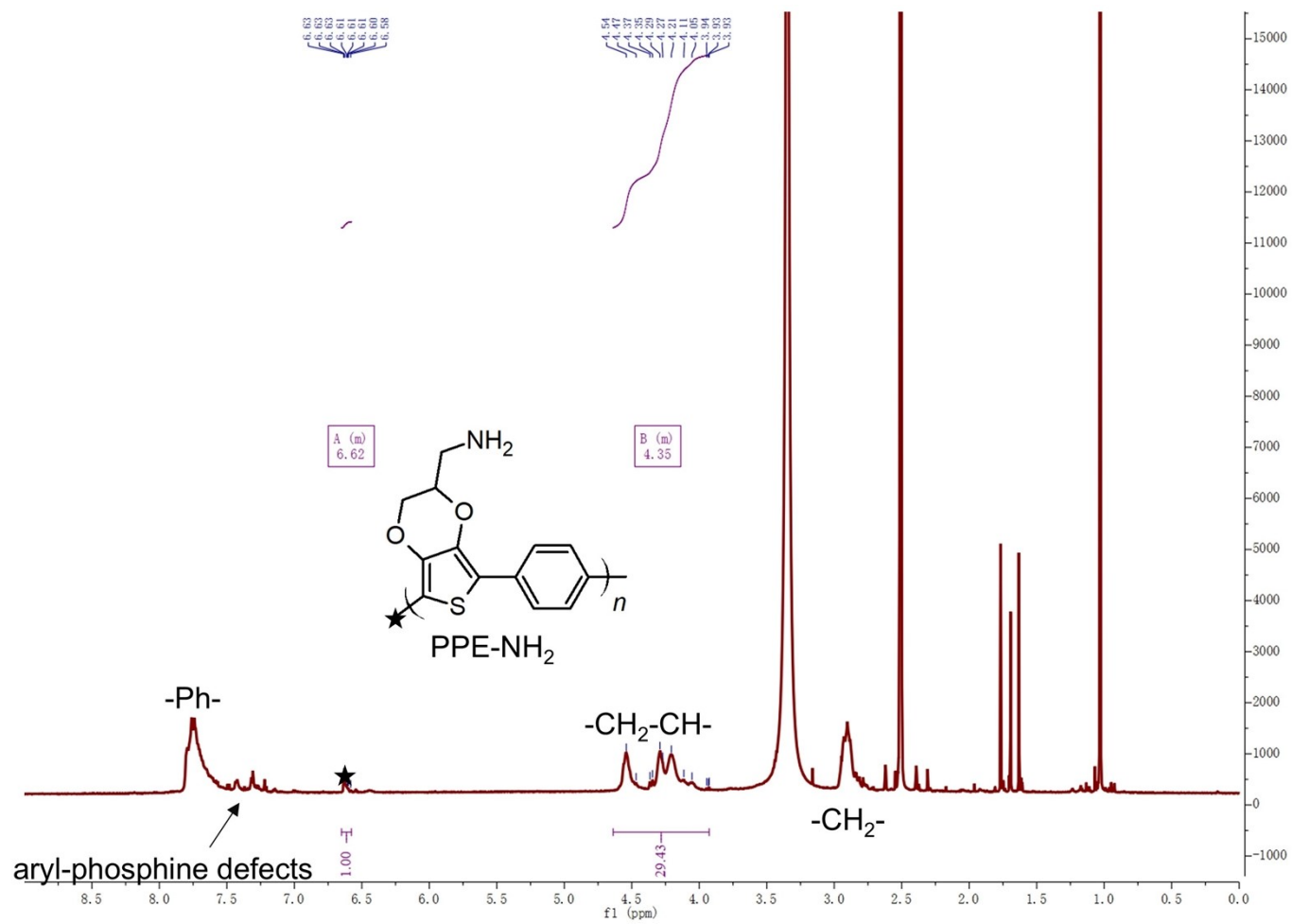
^1H NMR of PPE-NH₂ with entry 7 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



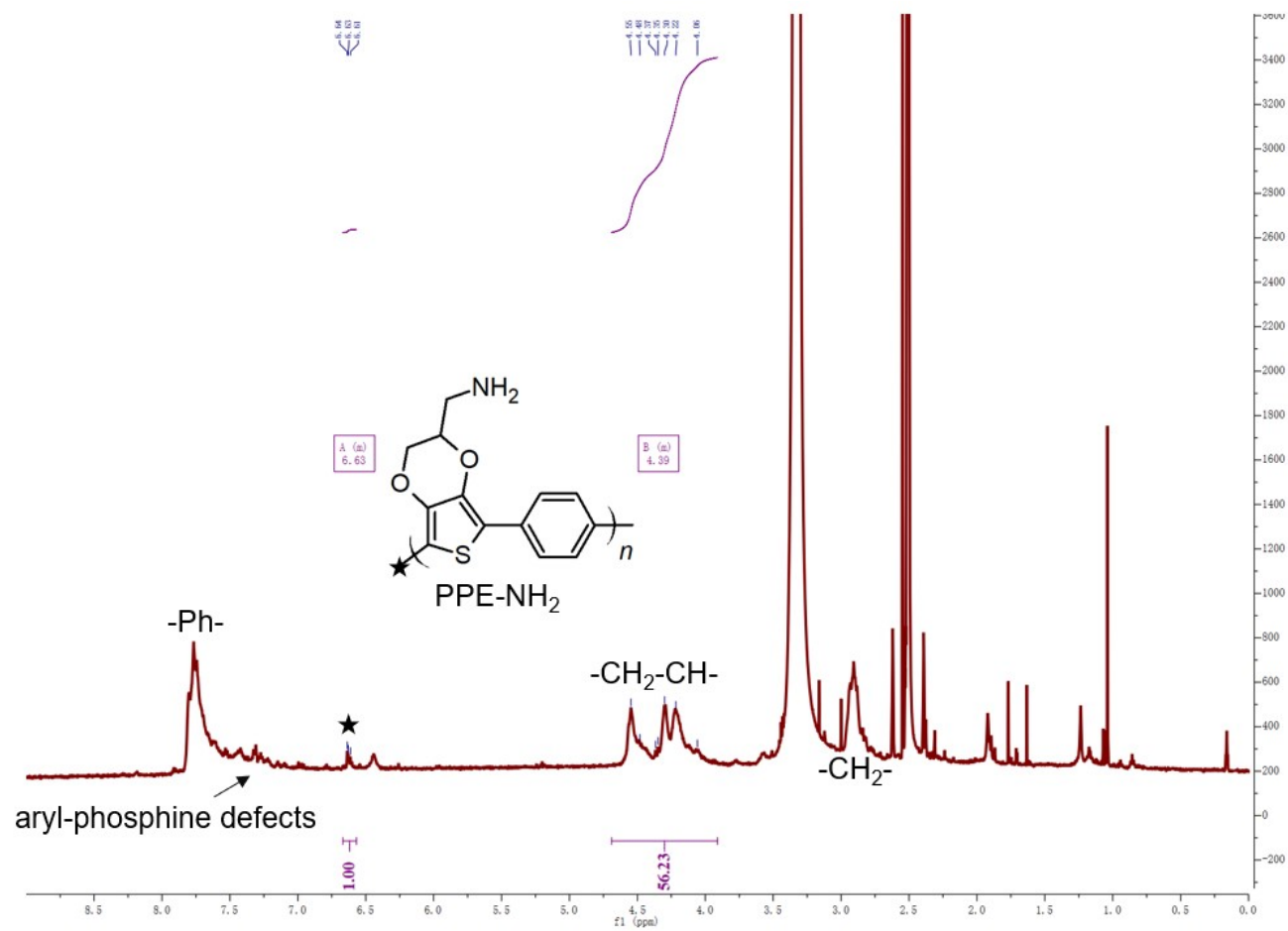
^1H NMR of PPE-NH₂ with entry 8 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



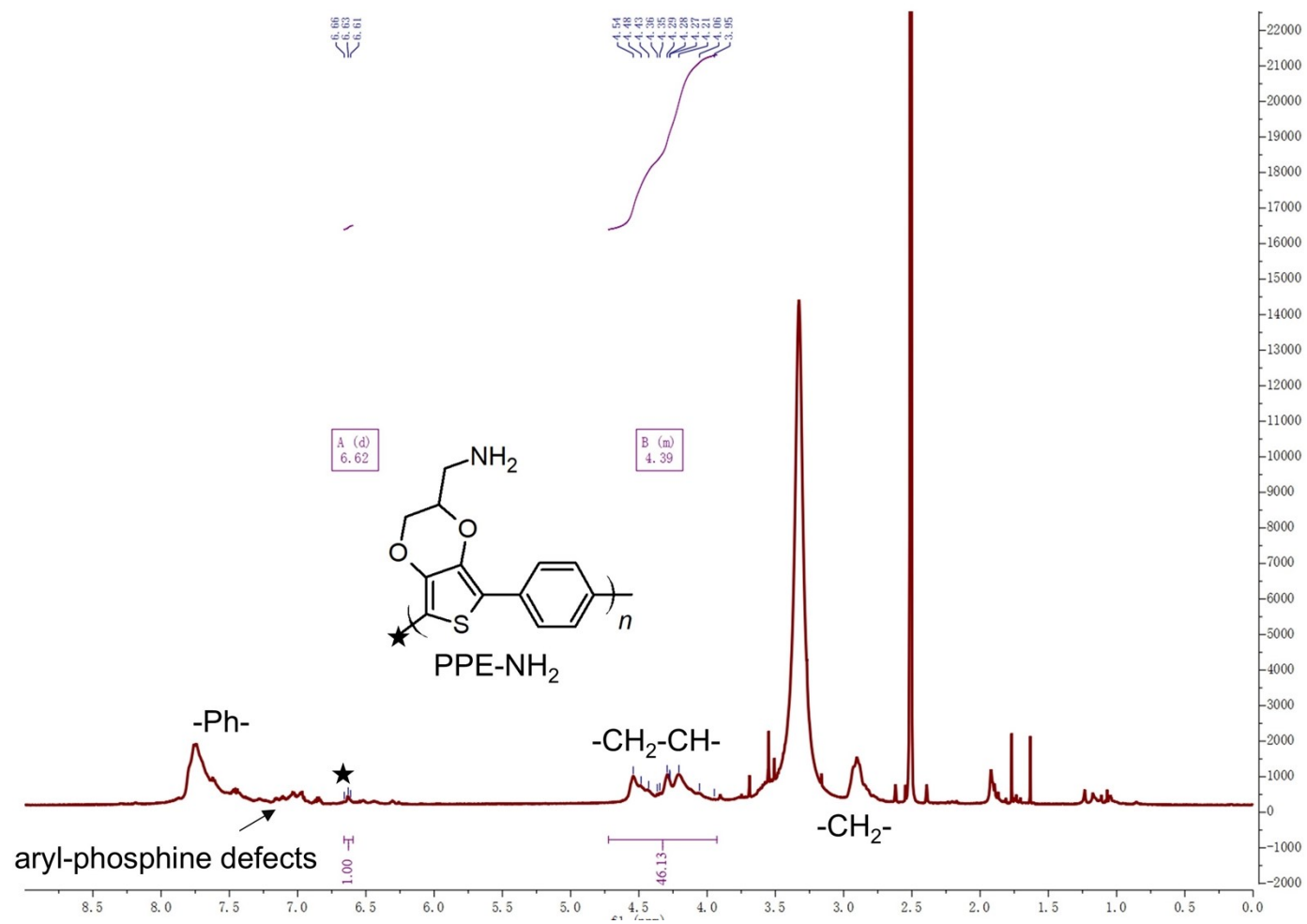
^1H NMR of PPE-NH₂ with entry 9 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



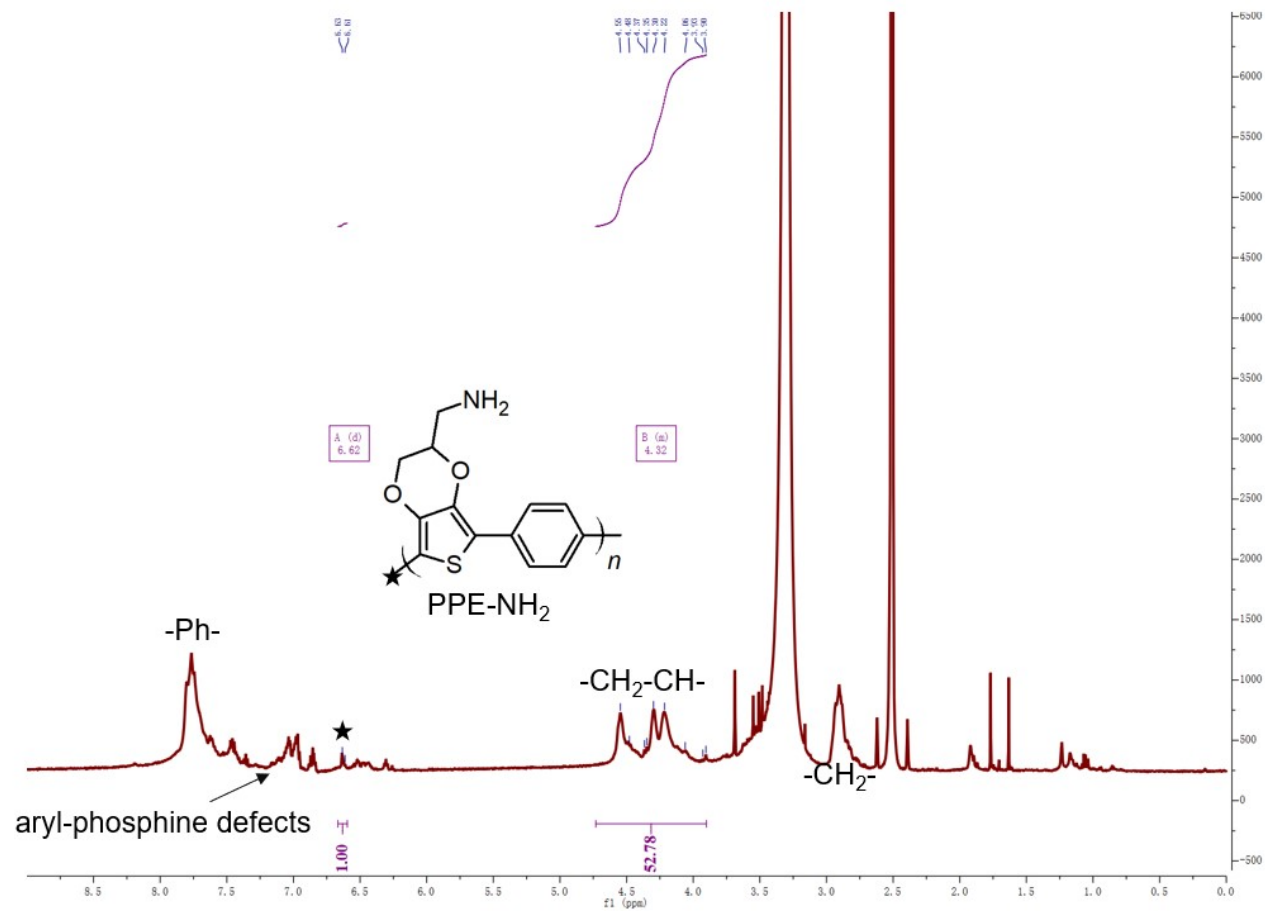
^1H NMR of PPE-NH₂ with entry 10 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



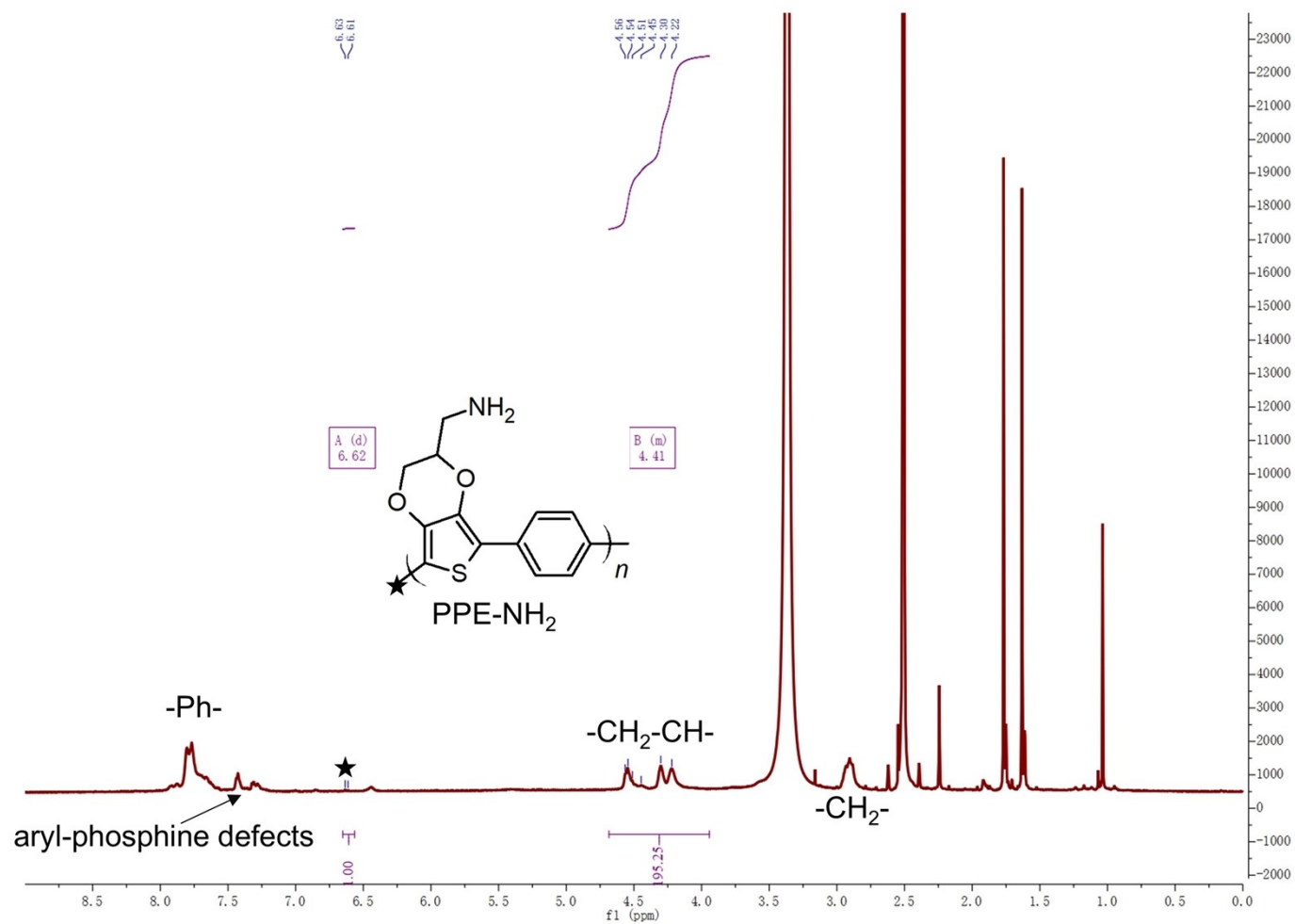
^1H NMR of PPE-NH₂ with entry 12 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



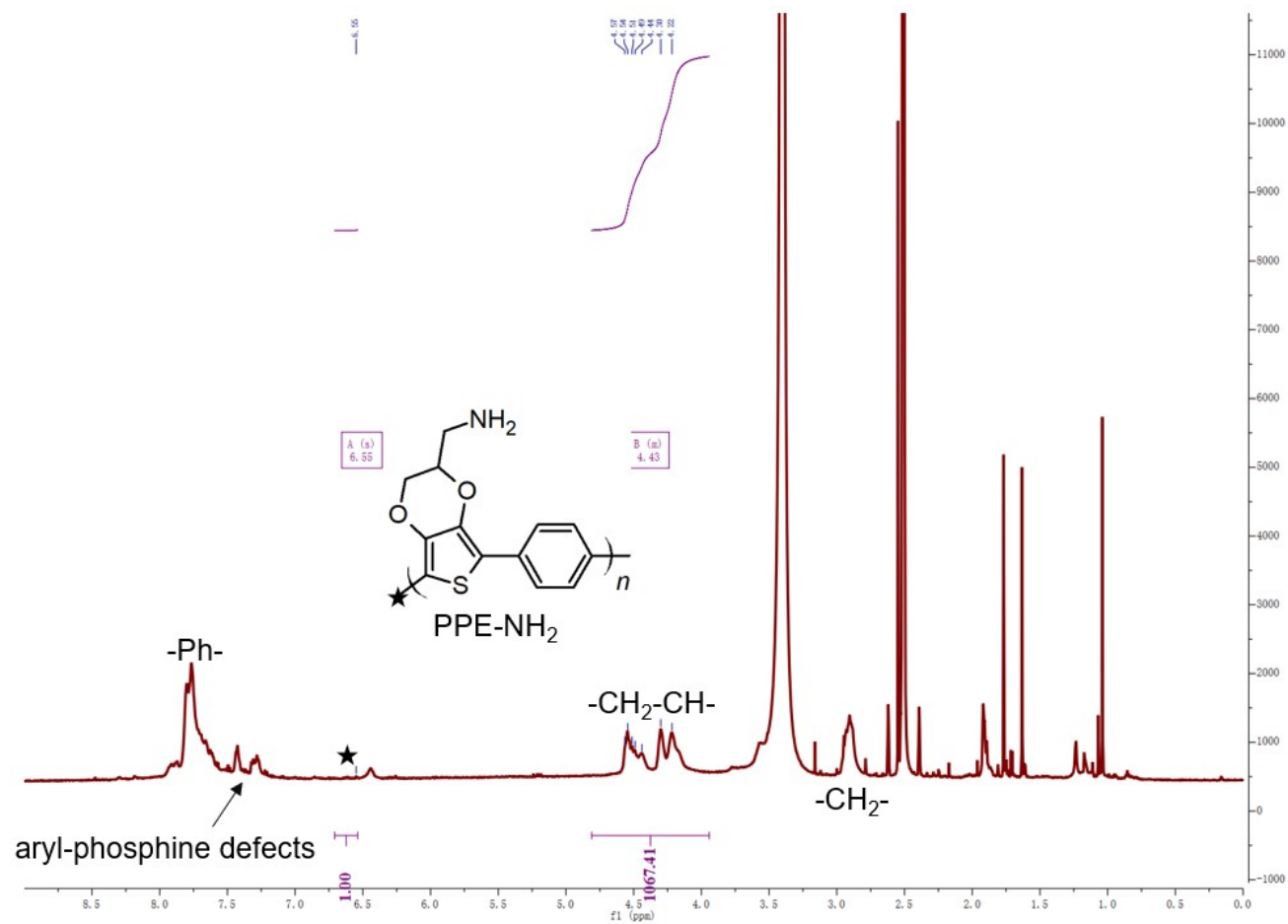
^1H NMR of PPE-NH₂ with entry 13 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



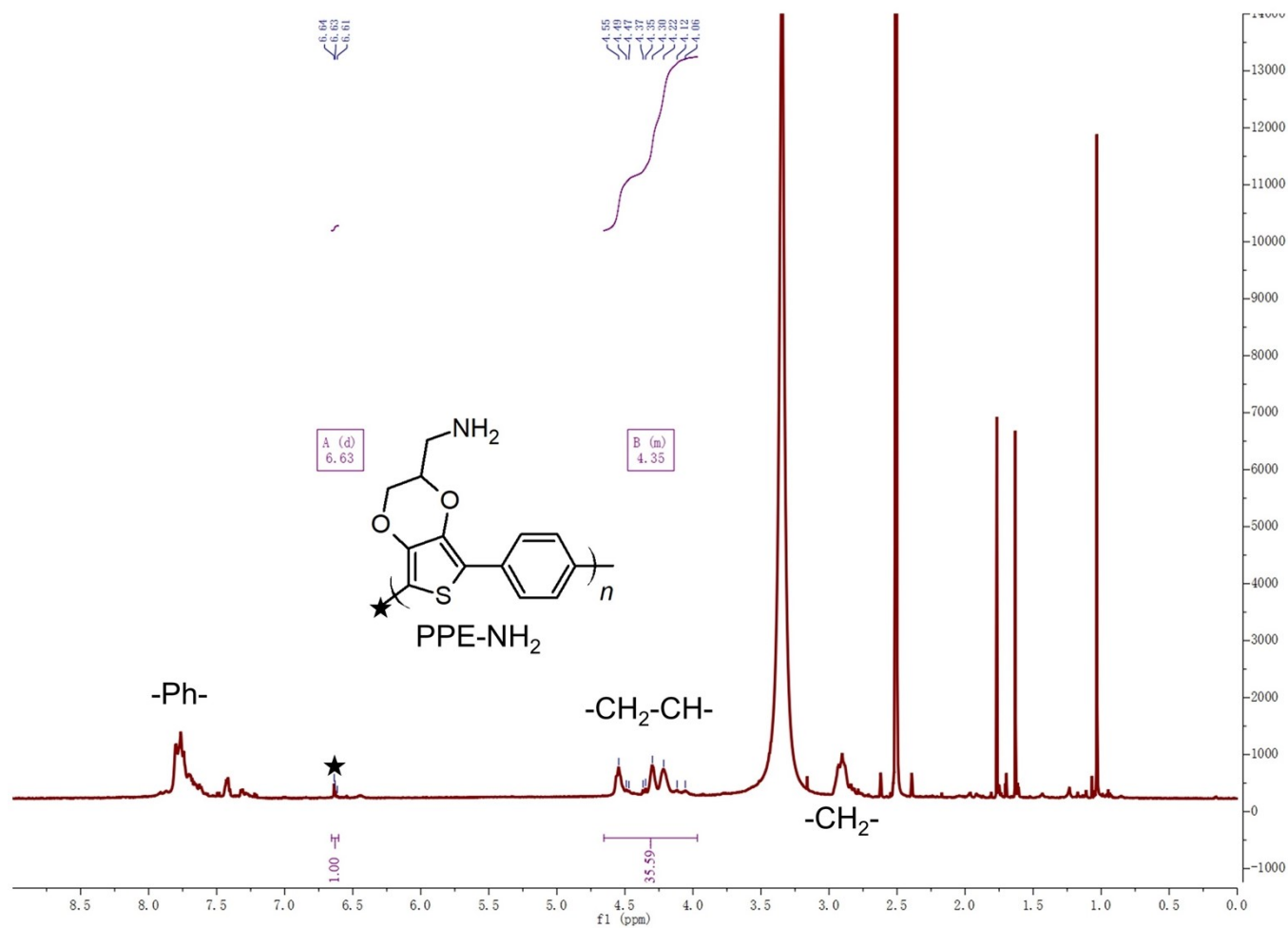
^1H NMR of PPE-NH₂ with entry 16 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



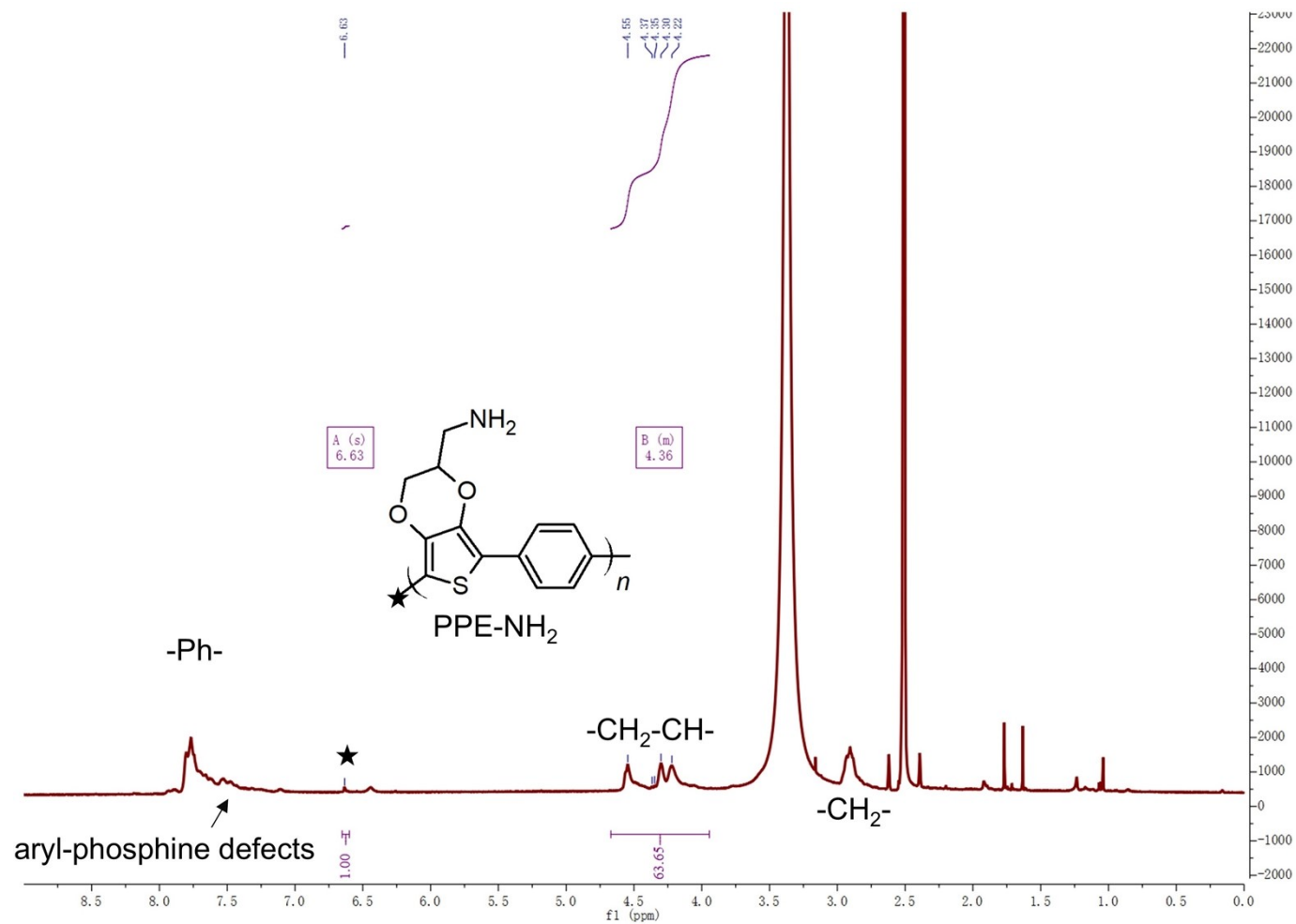
^1H NMR of PPE-NH₂ with entry 17 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



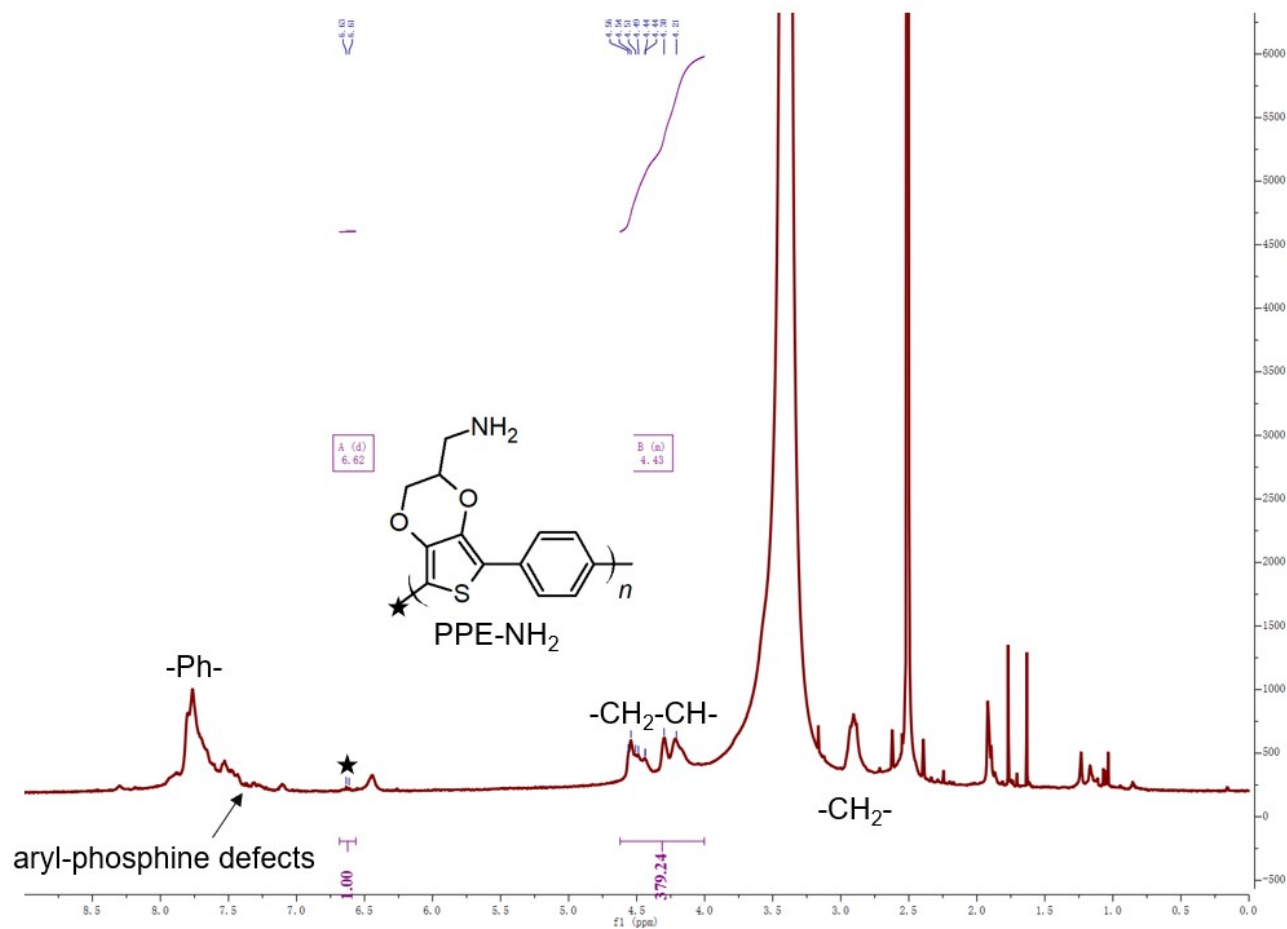
^1H NMR of PPE-NH₂ with entry 8 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



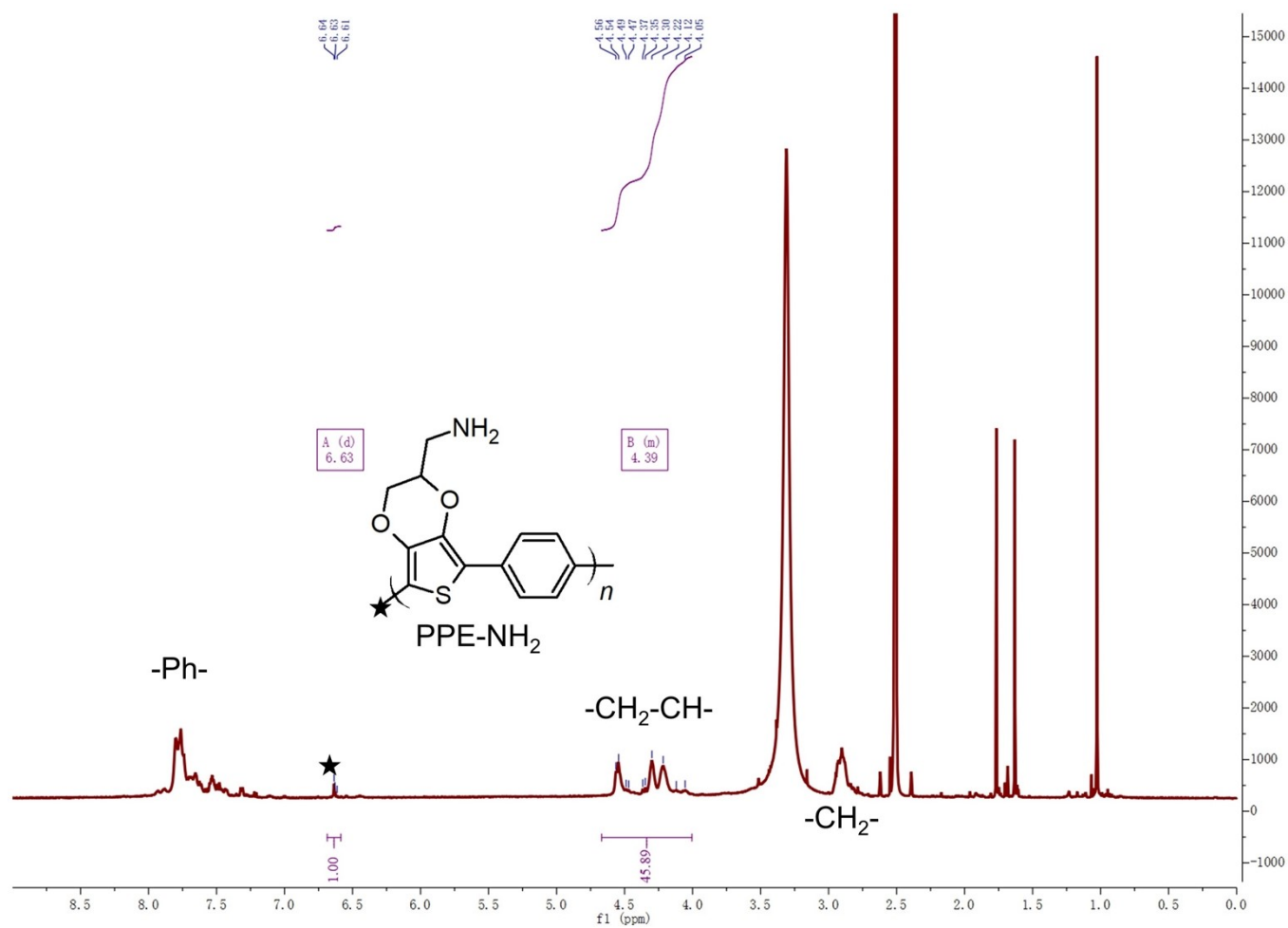
^1H NMR of PPE-NH₂ with entry 19 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



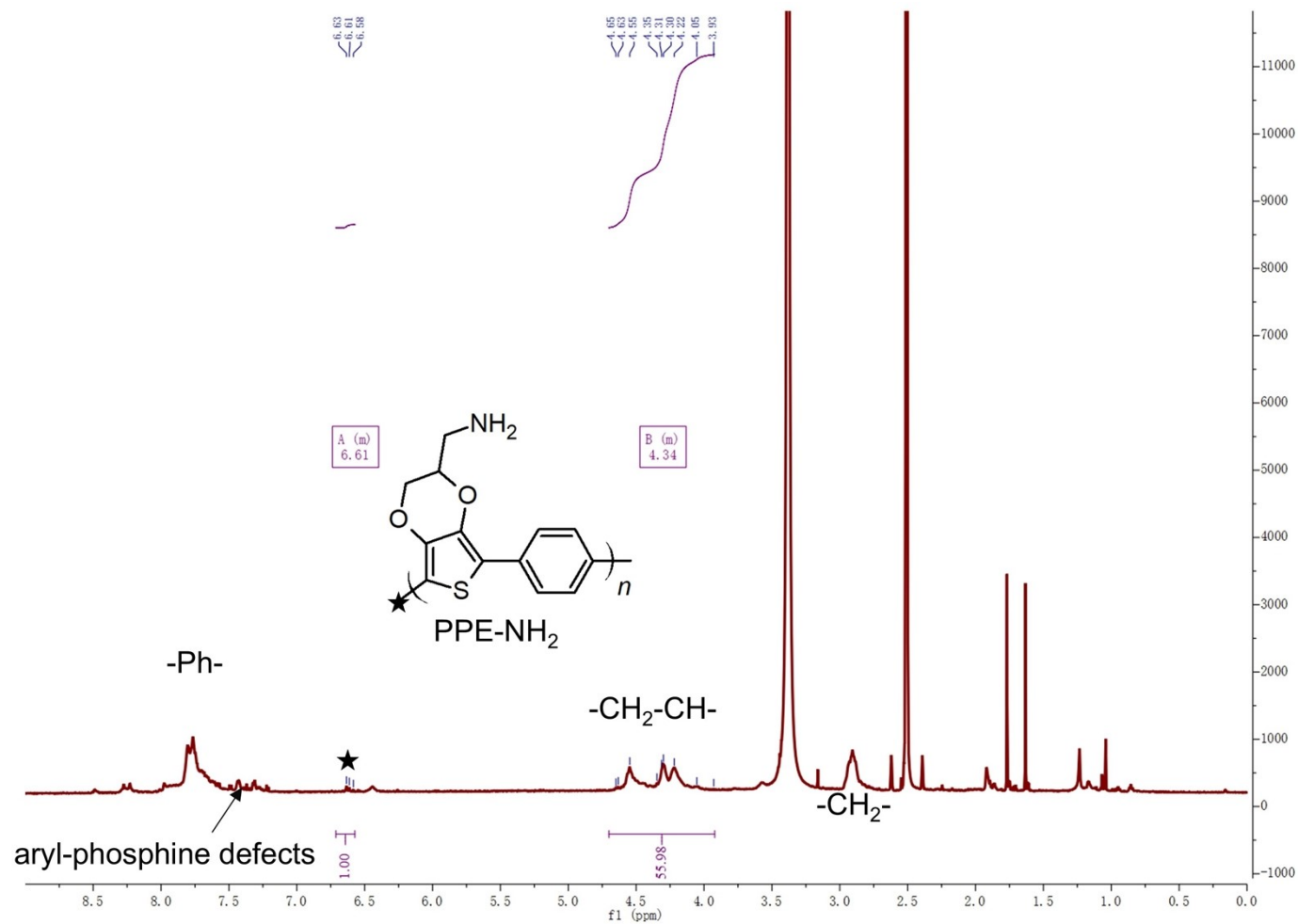
^1H NMR of PPE-NH₂ with entry 20 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



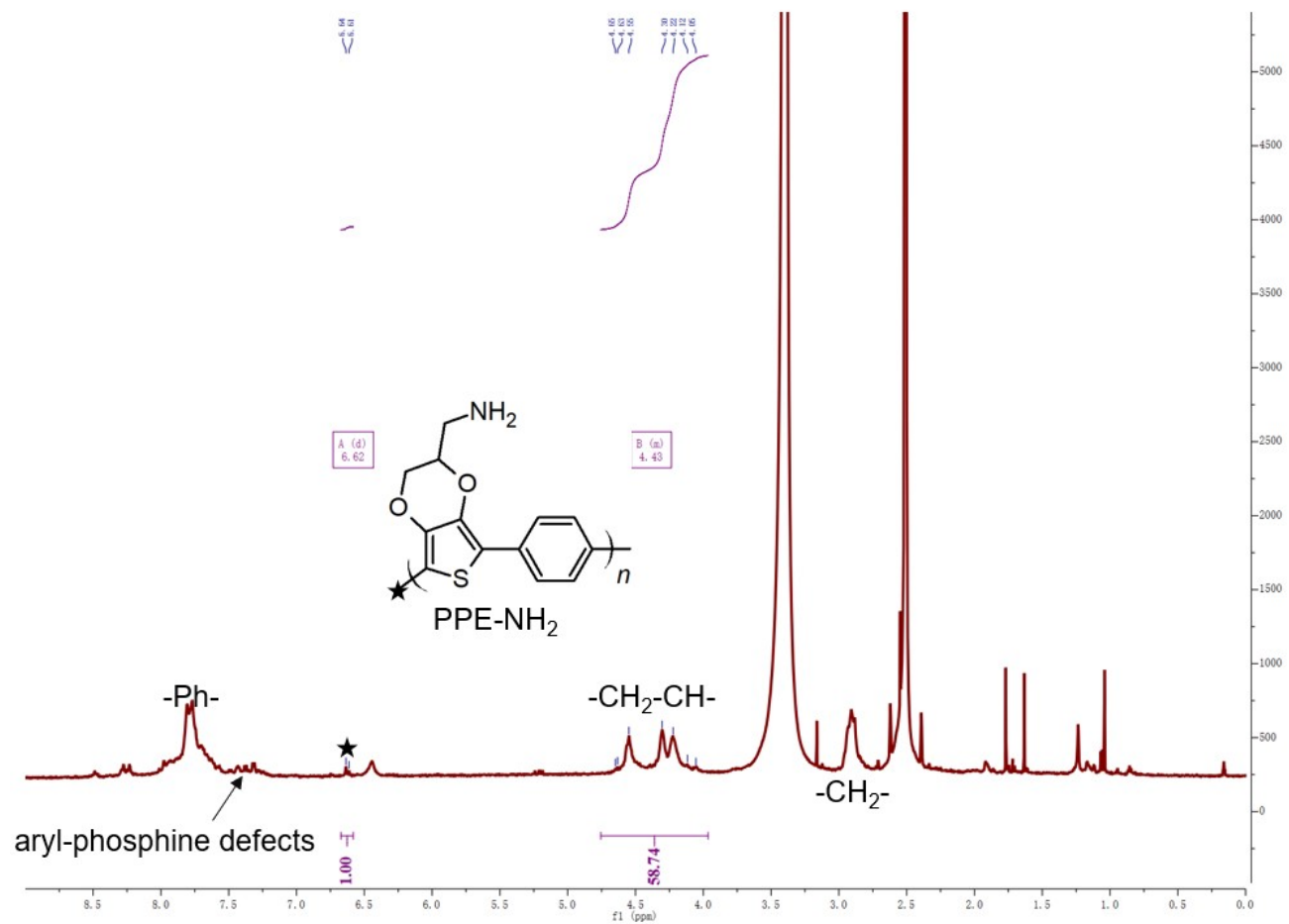
^1H NMR of PPE-NH₂ with entry 8 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



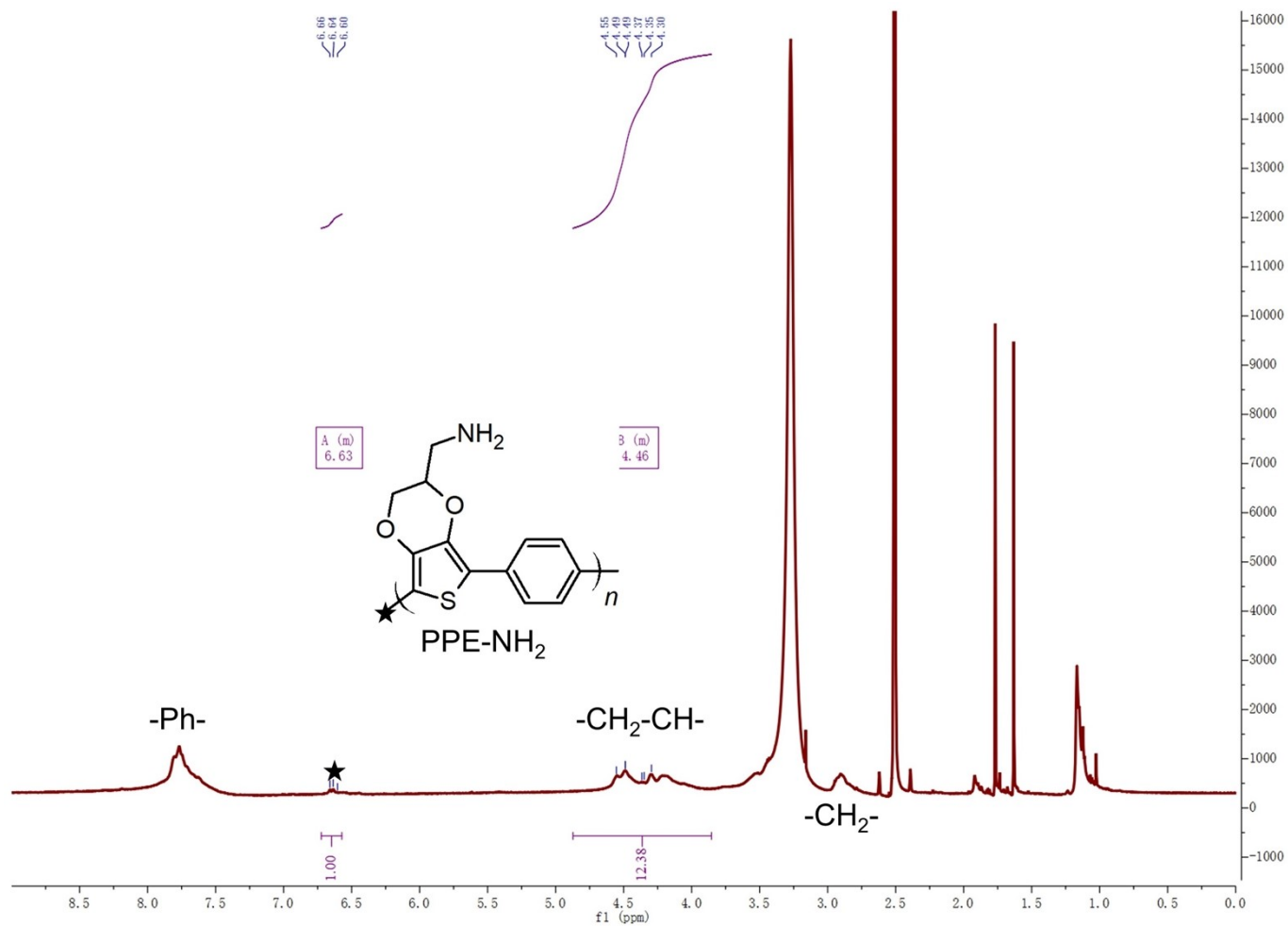
^1H NMR of PPE-NH₂ with entry 22 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



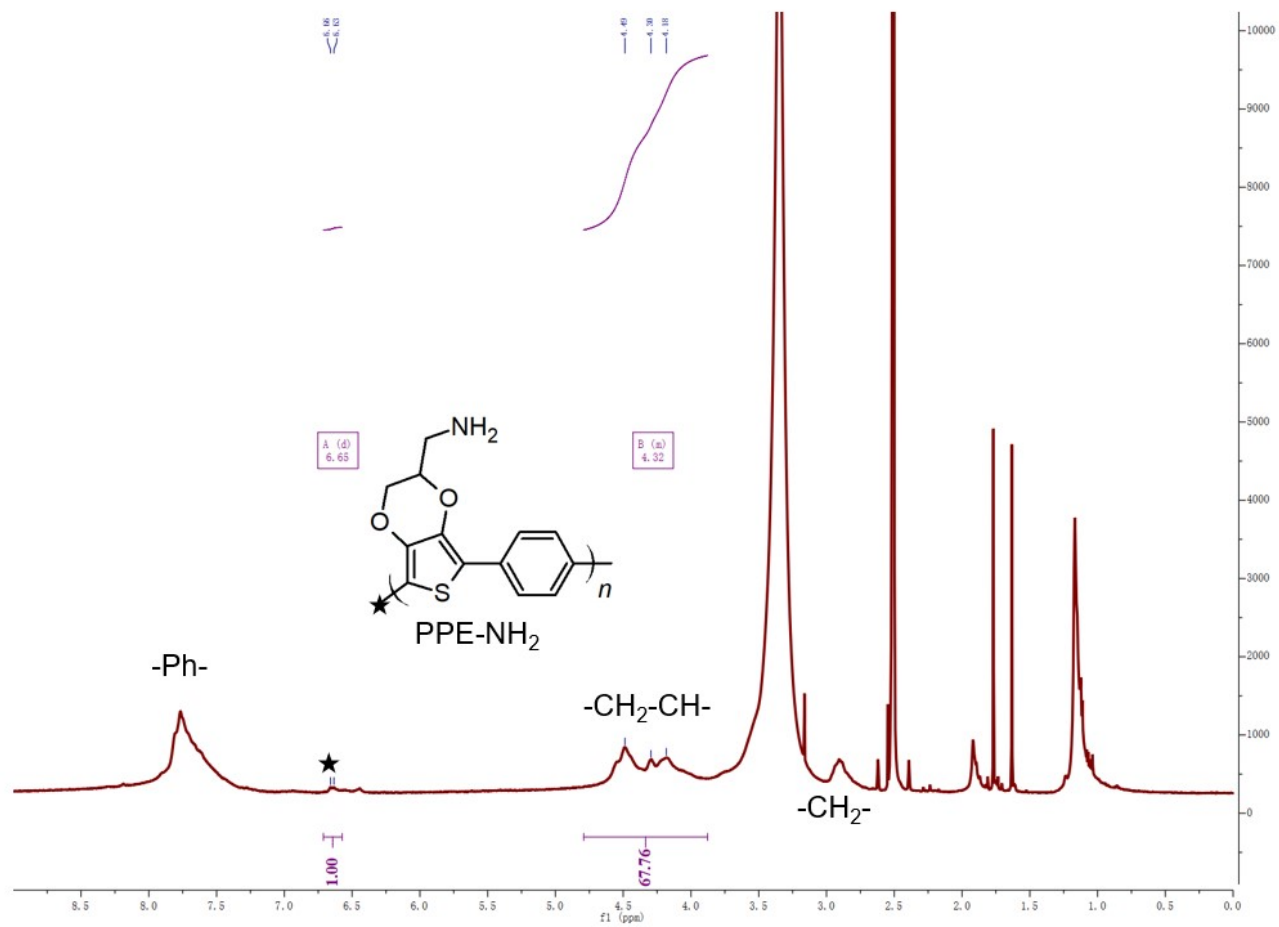
^1H NMR of PPE-NH₂ with entry 23 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



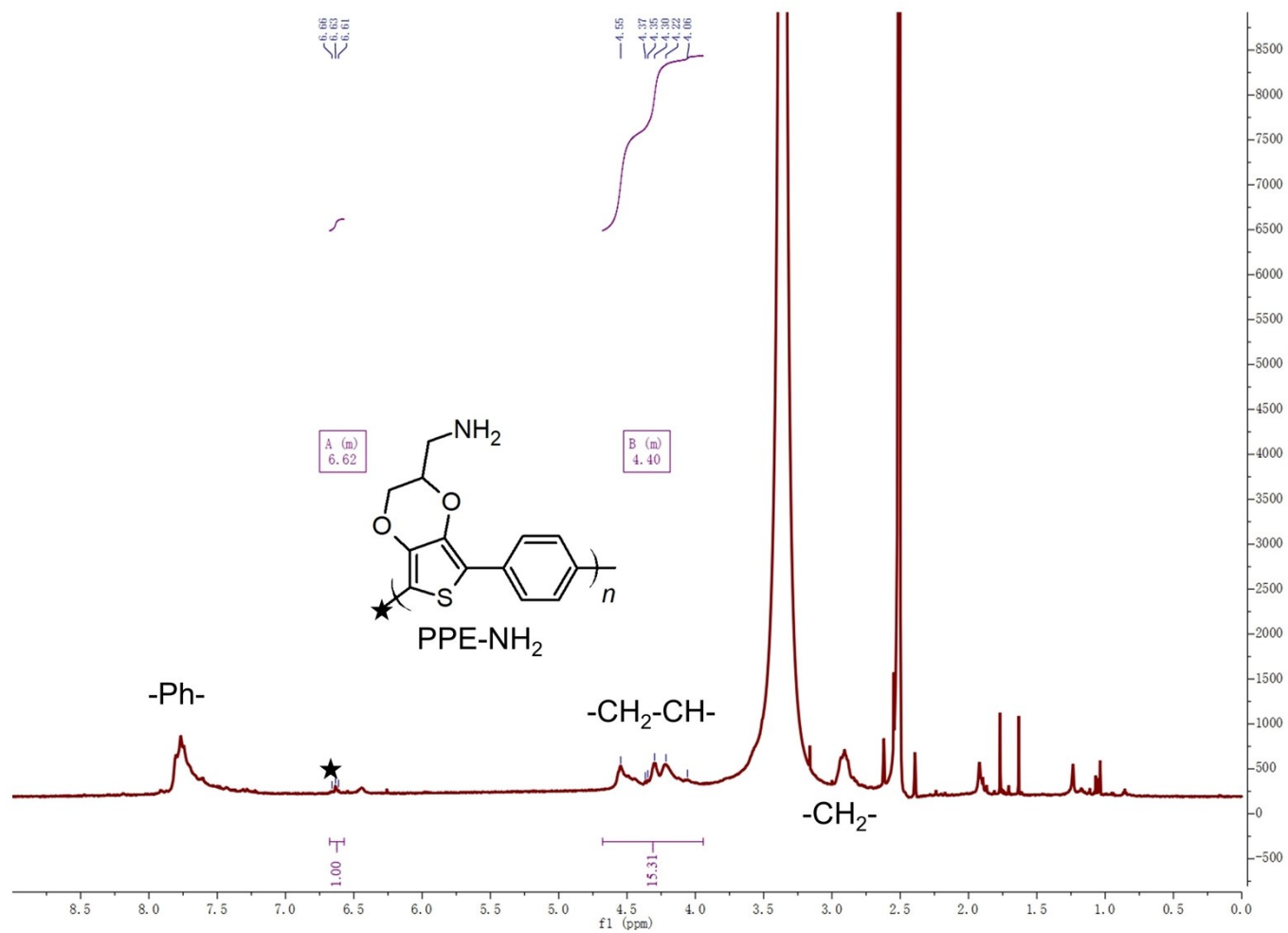
^1H NMR of PPE-NH₂ with entry 25 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



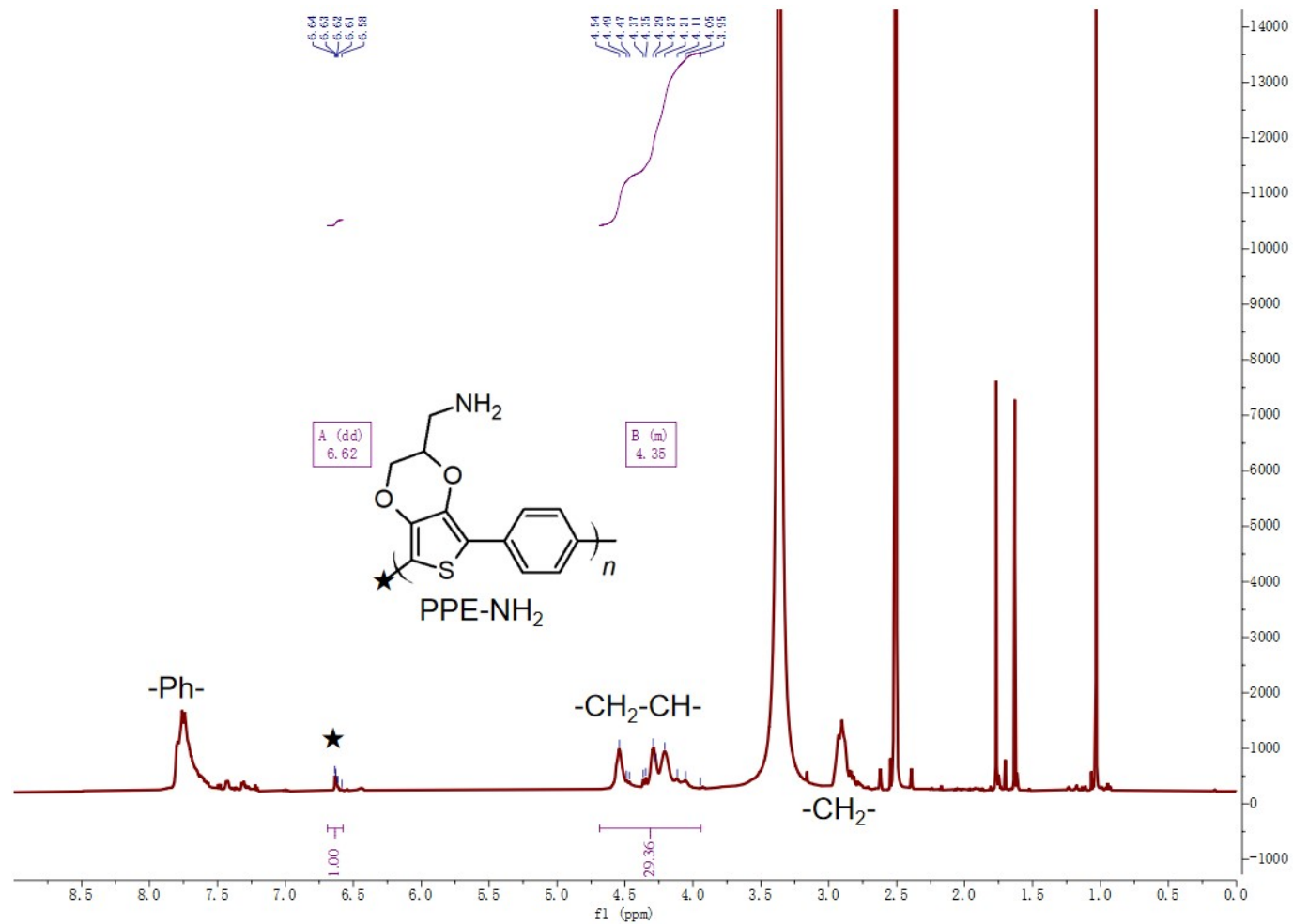
^1H NMR of PPE-NH₂ with entry 26 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]



^1H NMR of PPE-NH₂ with entry 29 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]

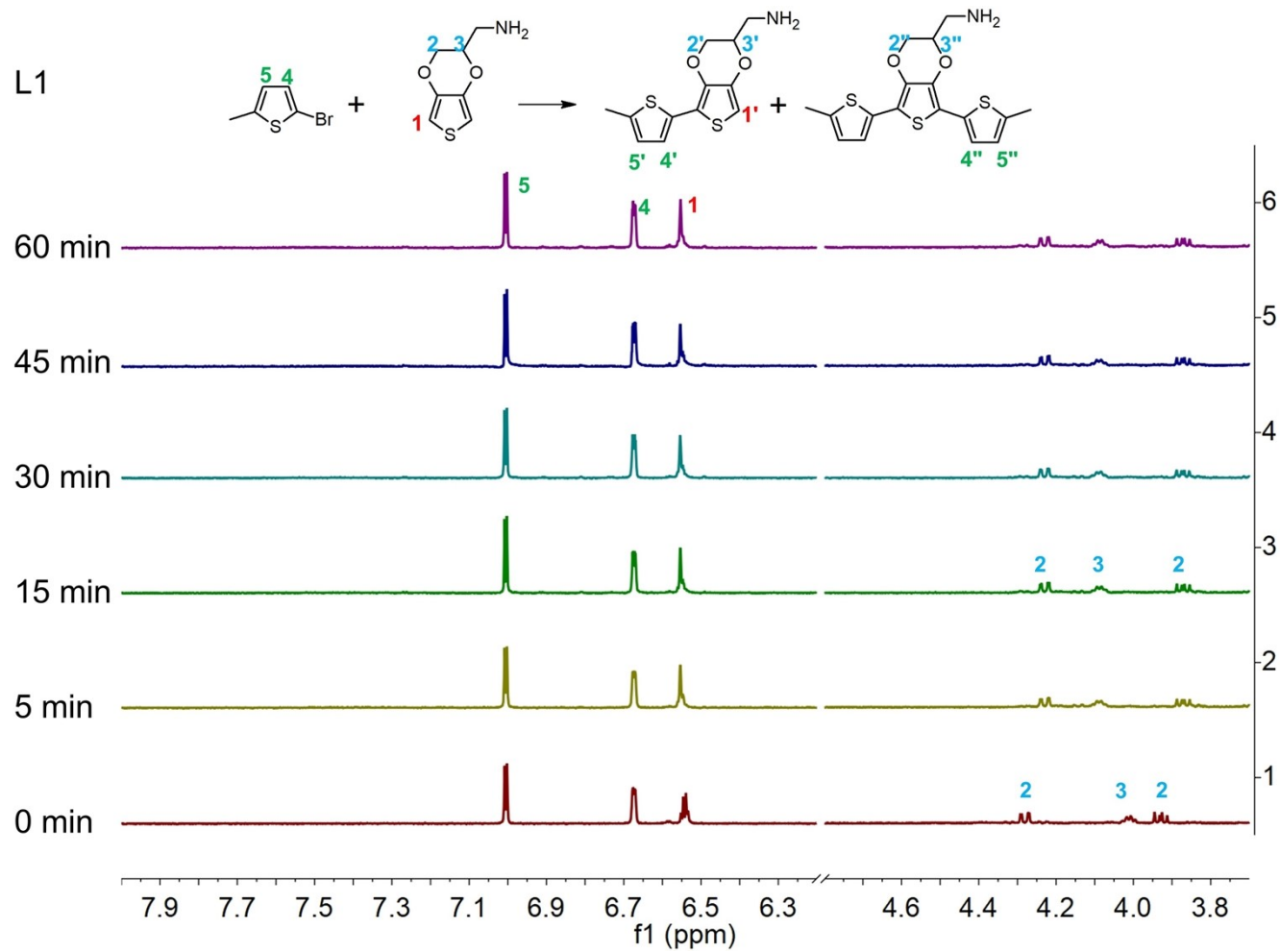


^1H NMR of PPE-NH₂ with entry 30 of Table S8 [600MHz, dimethyl sulfoxide-d₆/hydrazine hydrate-d₆ (v/v 100:1), 323K]

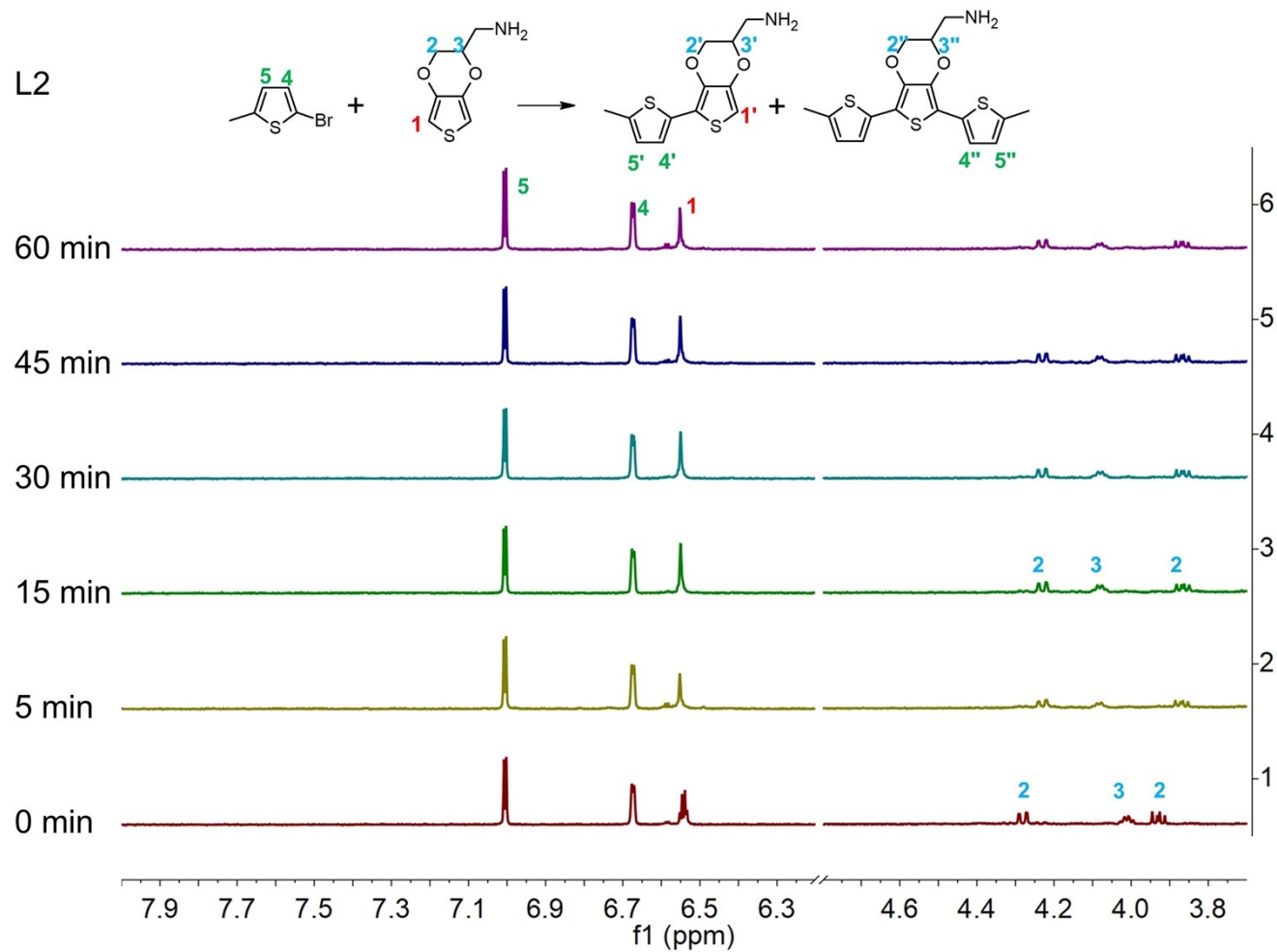


7.2 NMR spectra of Small molecular Model for direct arylation of EDOT derivatives with bromoarenes.

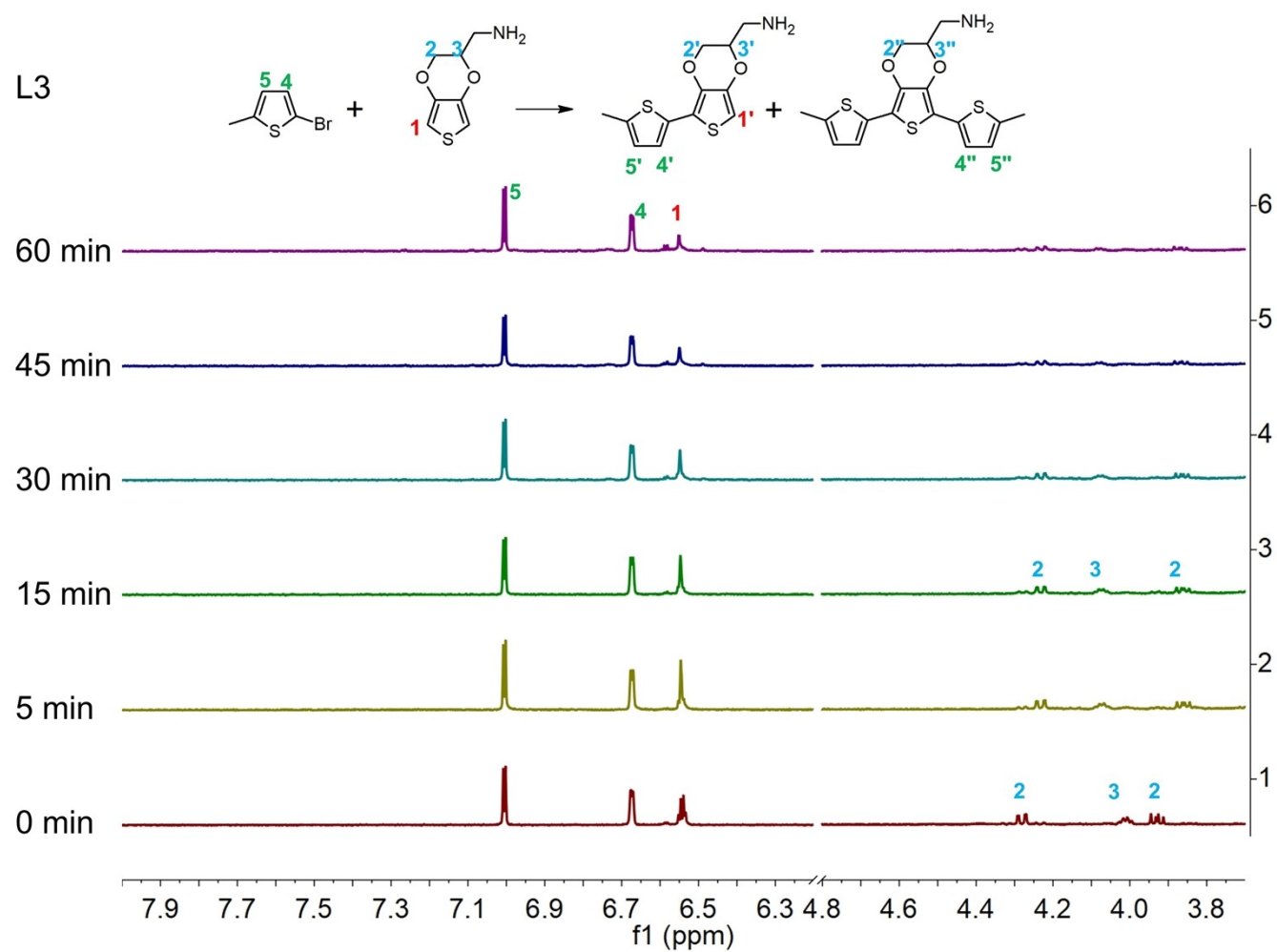
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L1 (DMSO-d₆)



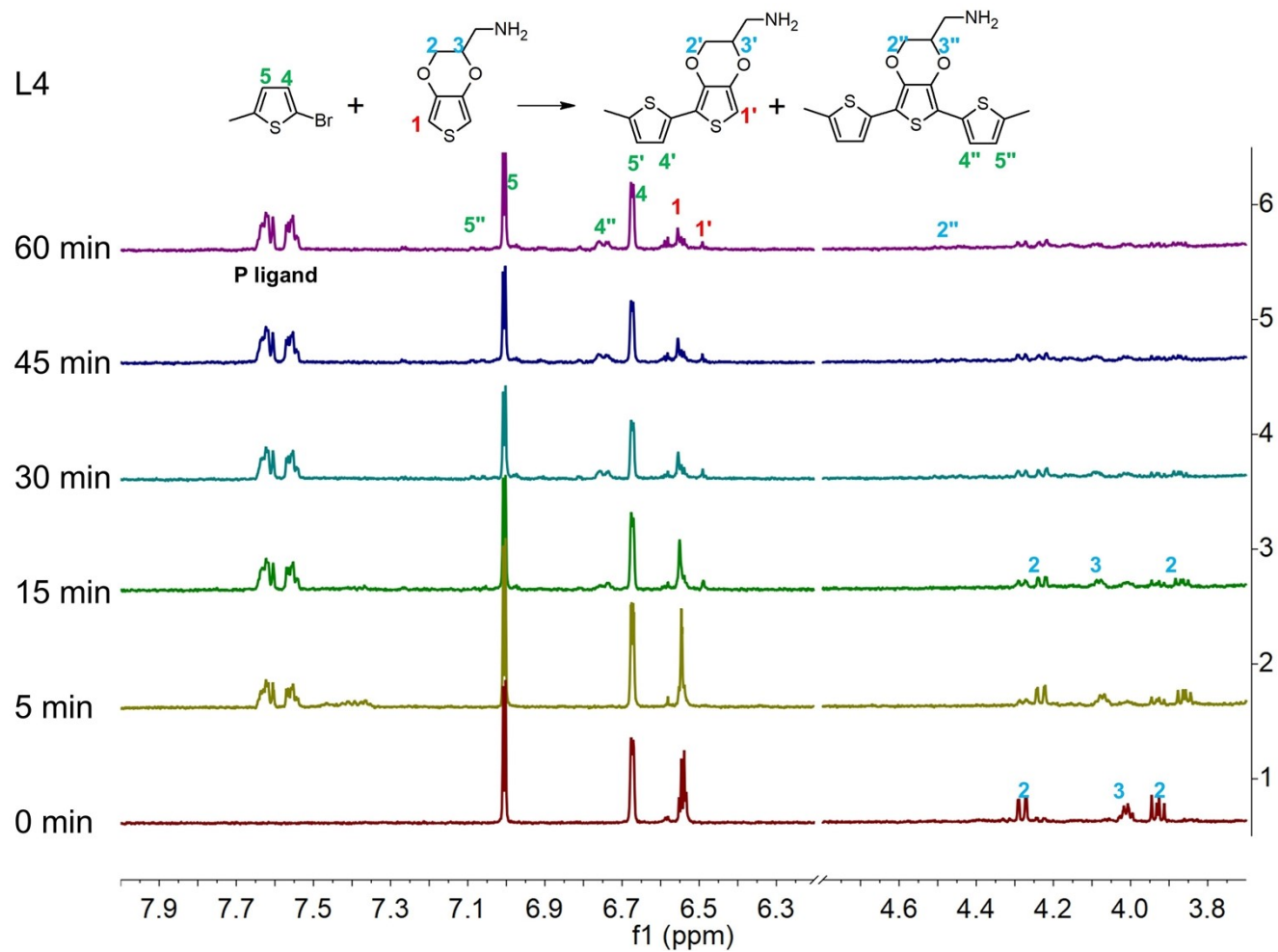
¹H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L2 (DMSO-d₆)



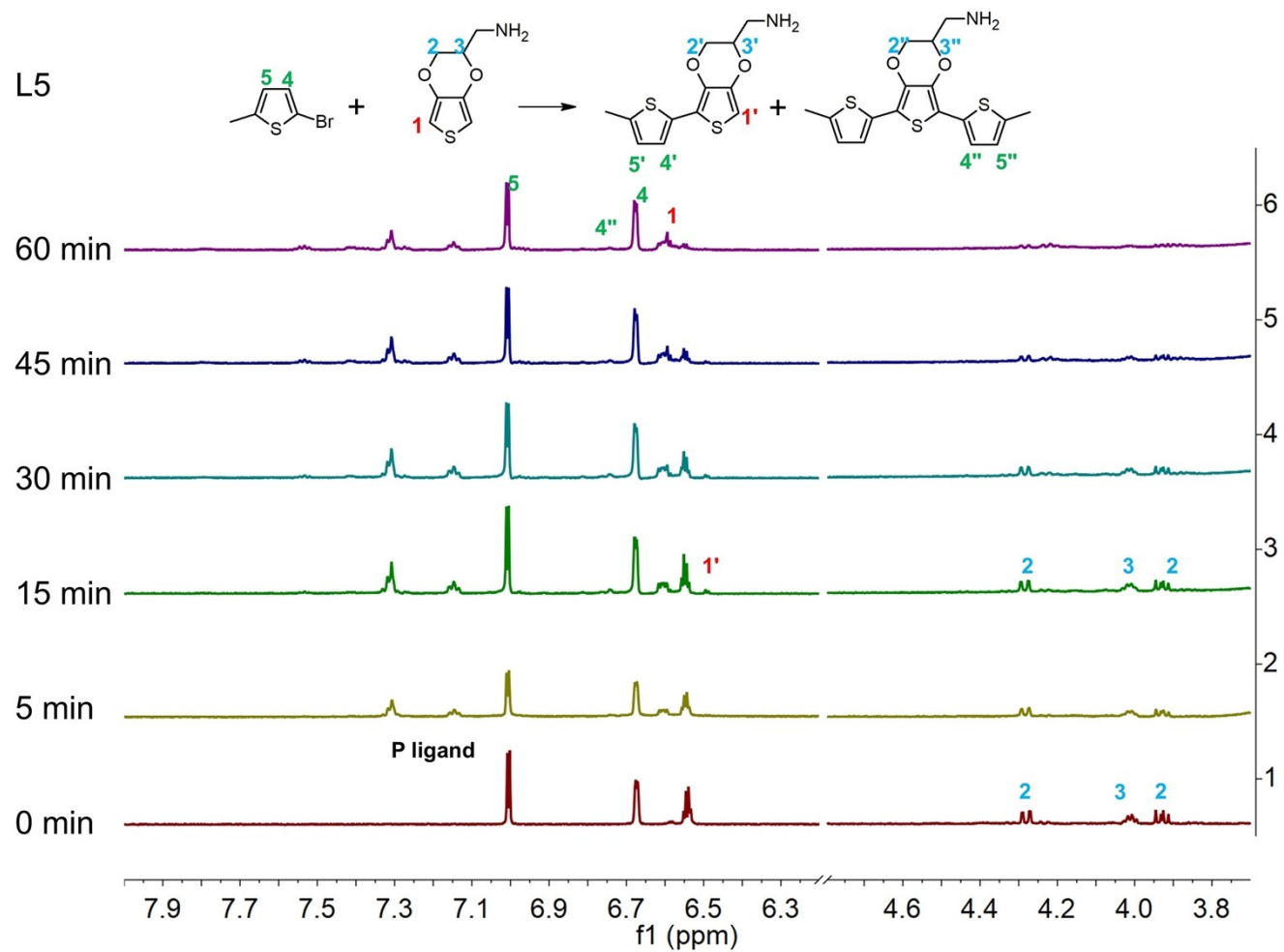
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L3 (DMSO-d₆)



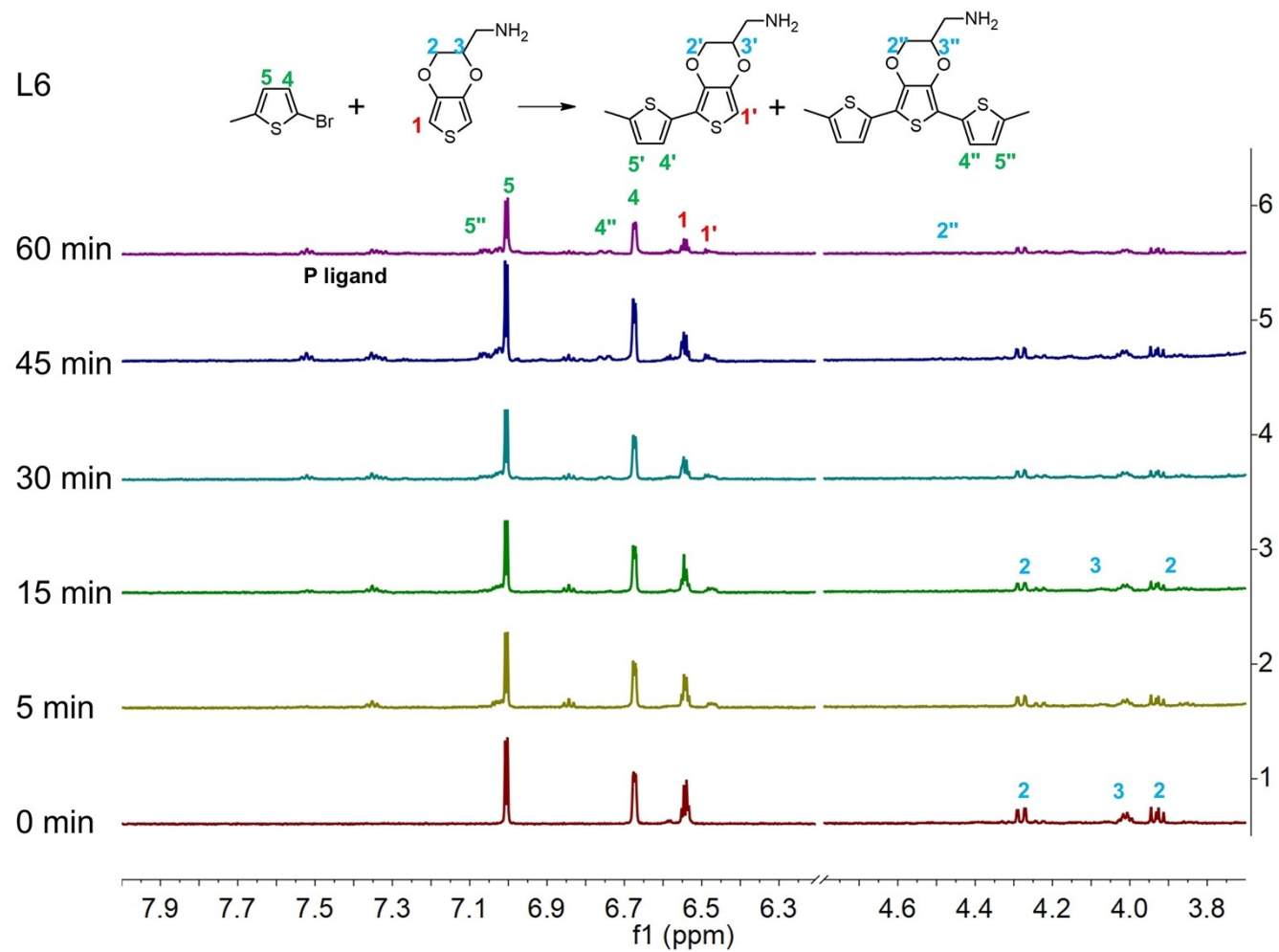
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L4 (DMSO-d₆)



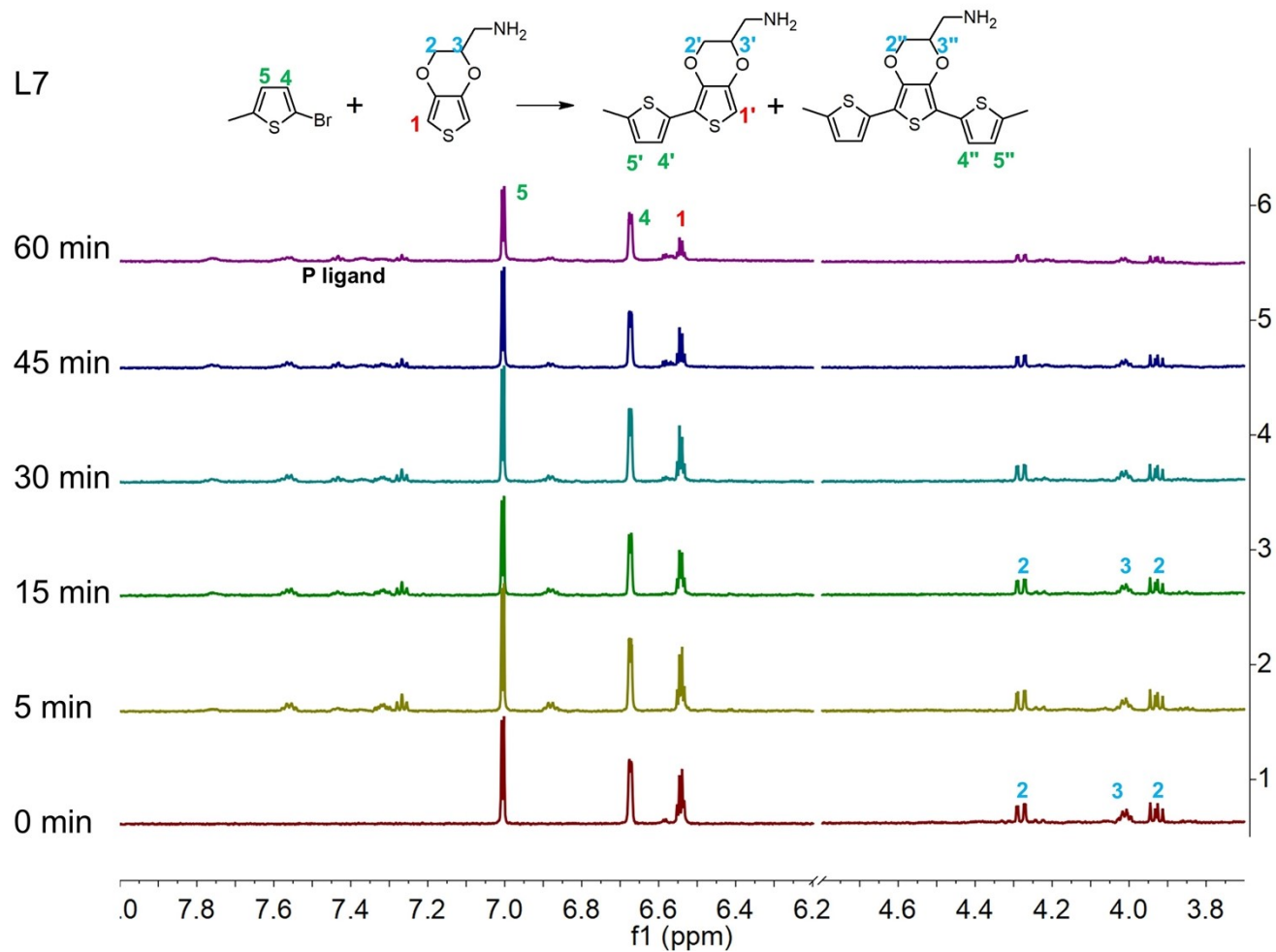
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L5 (DMSO-d₆)



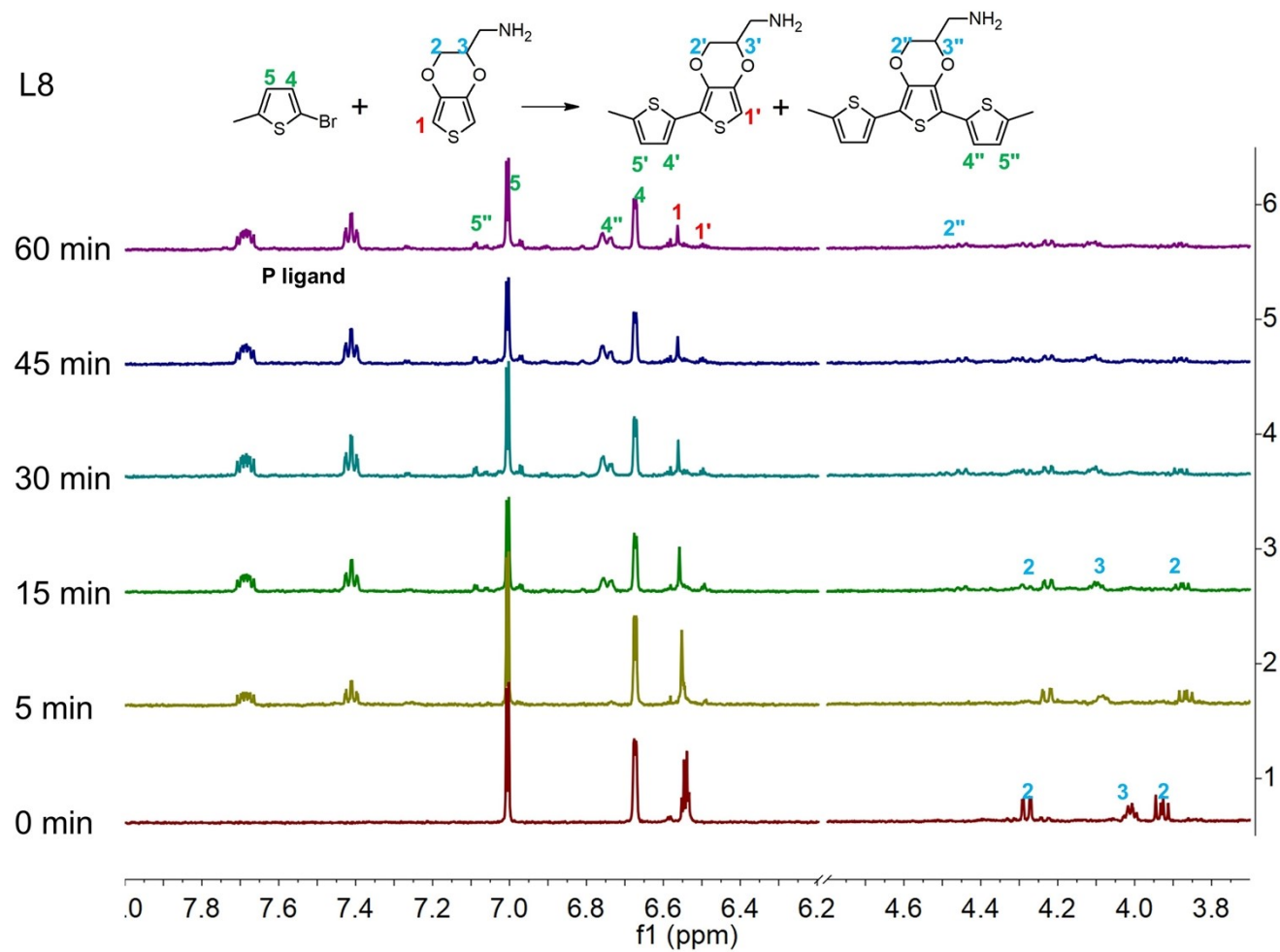
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L6 (DMSO-d₆)



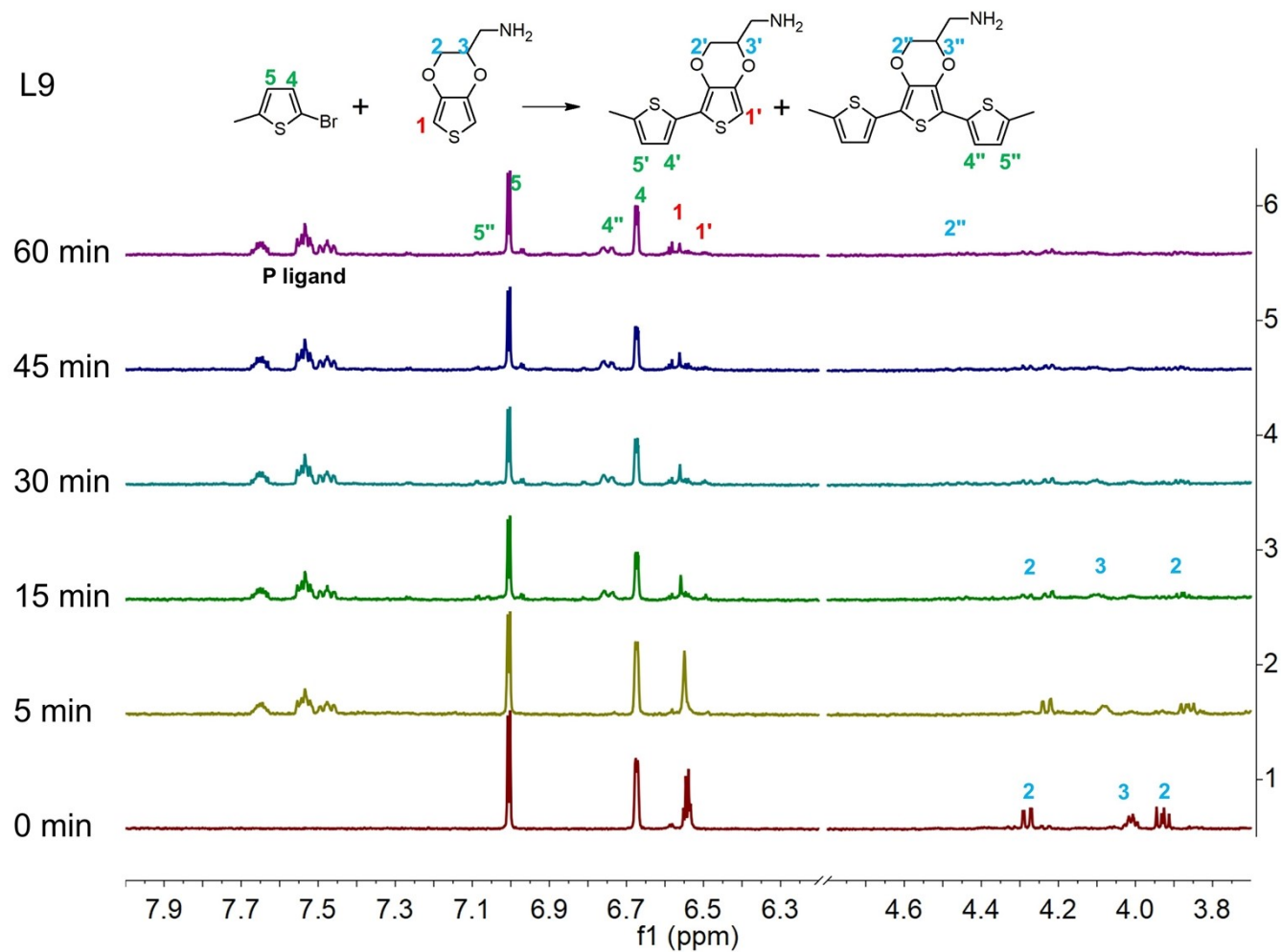
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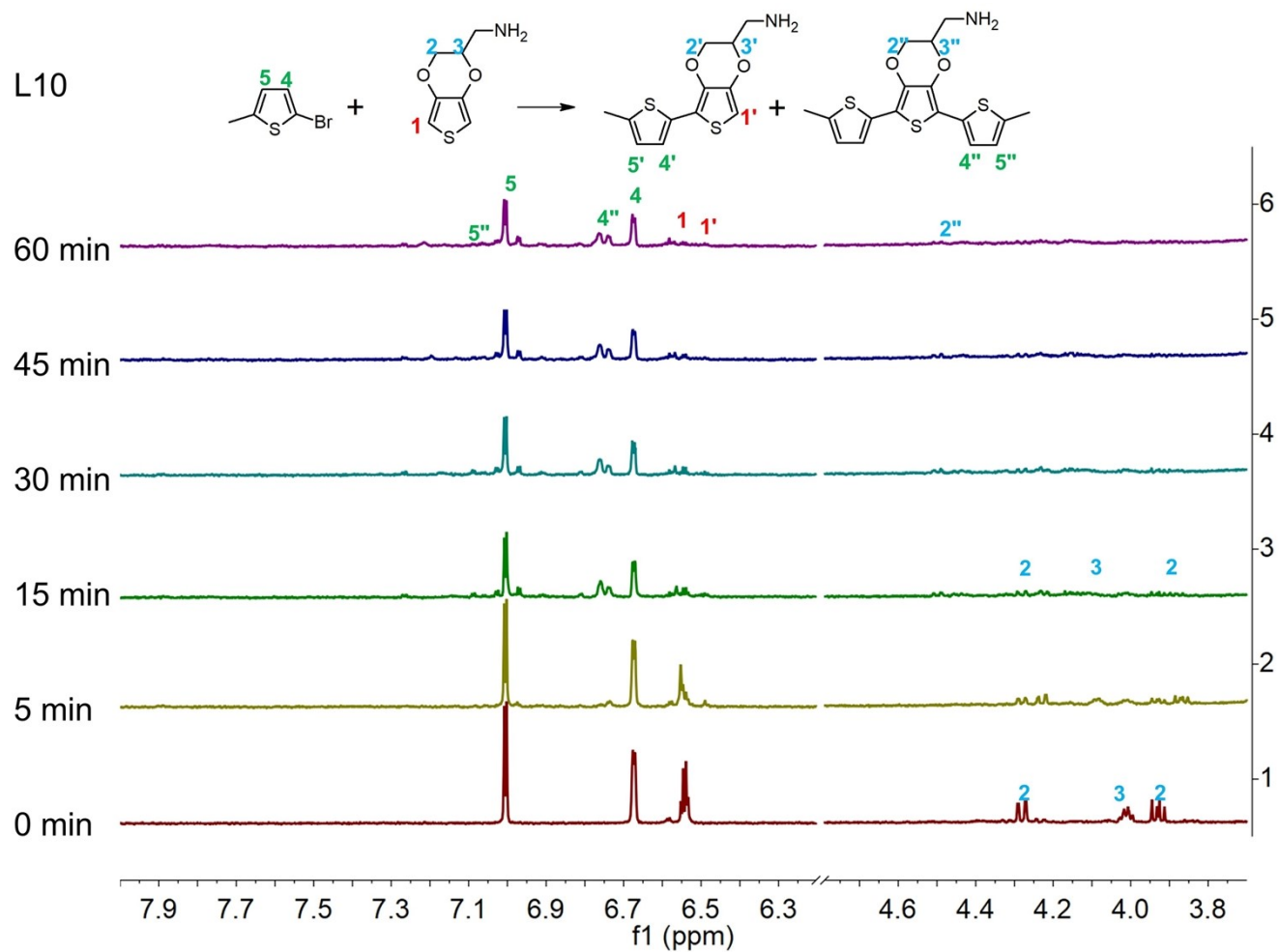
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with 2-bromo-5-methylthiophene assisted by L8 (DMSO-d₆)



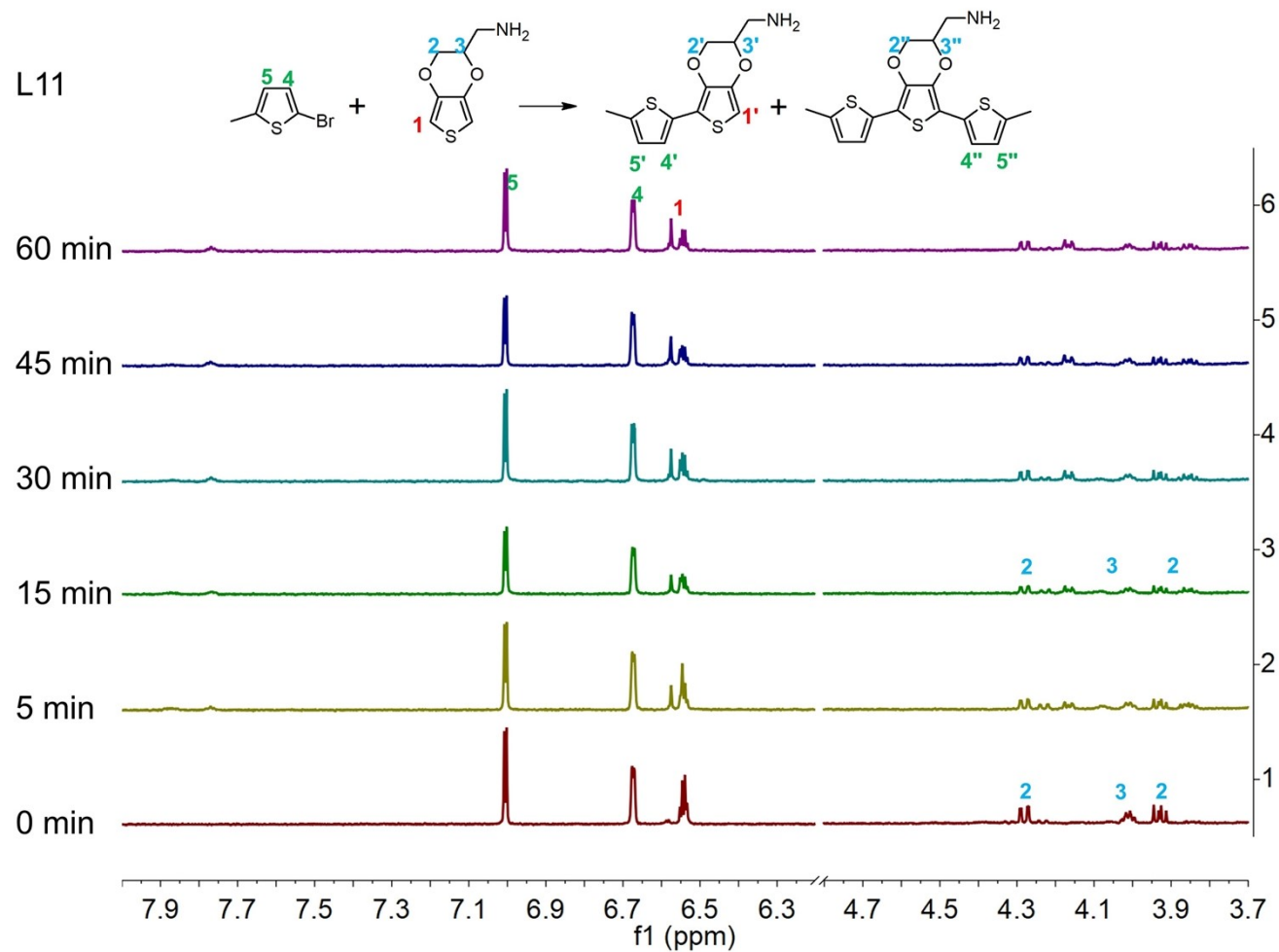
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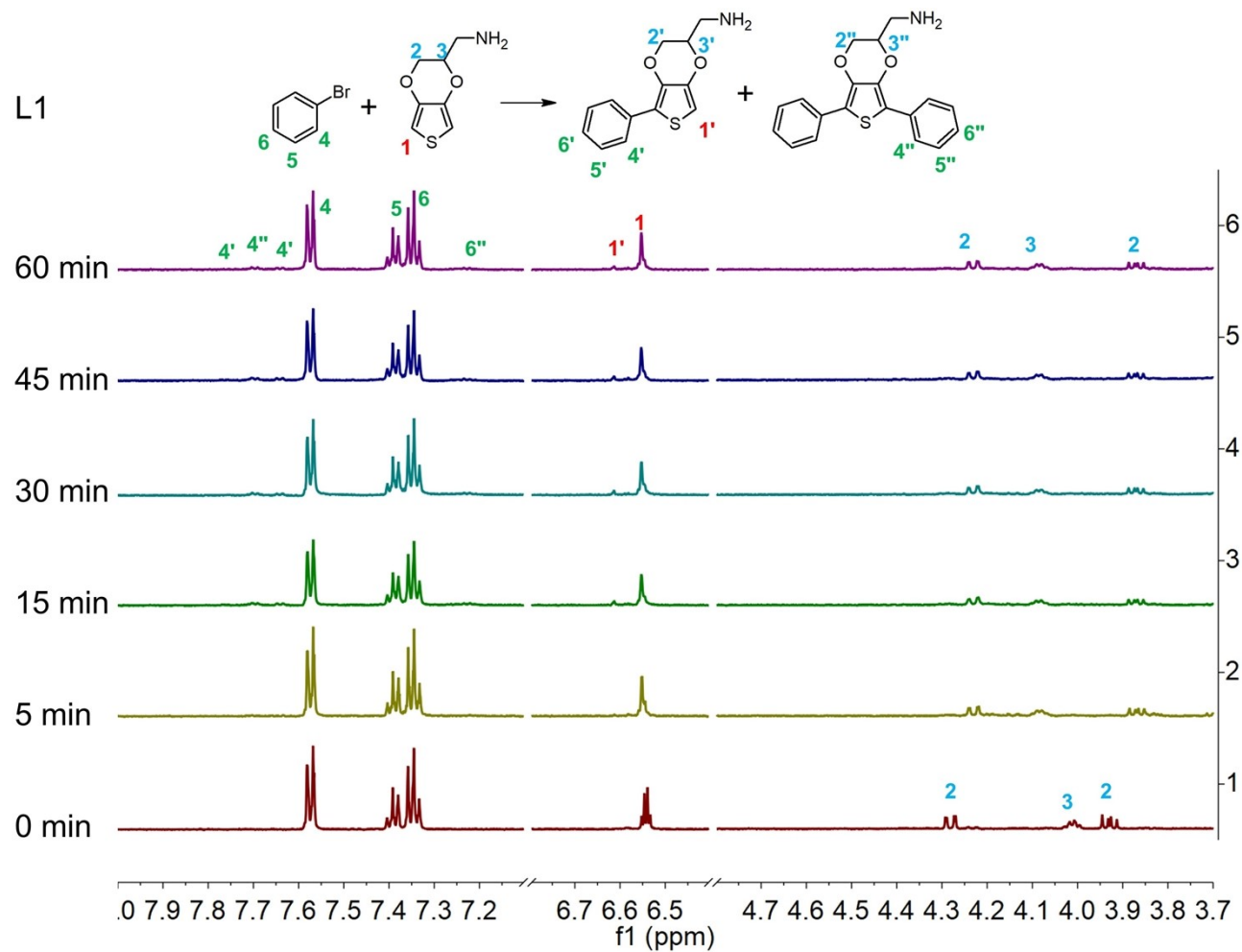
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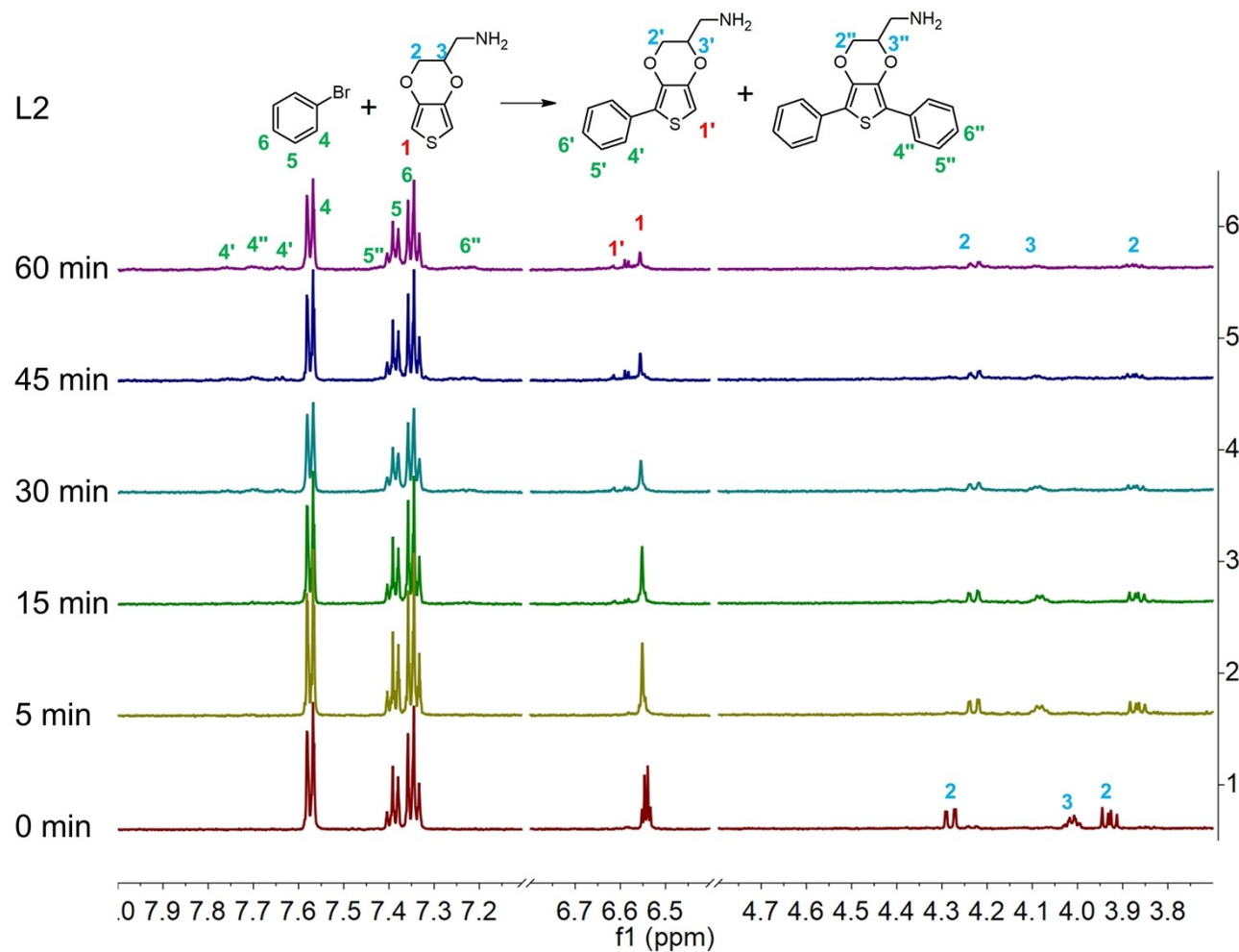
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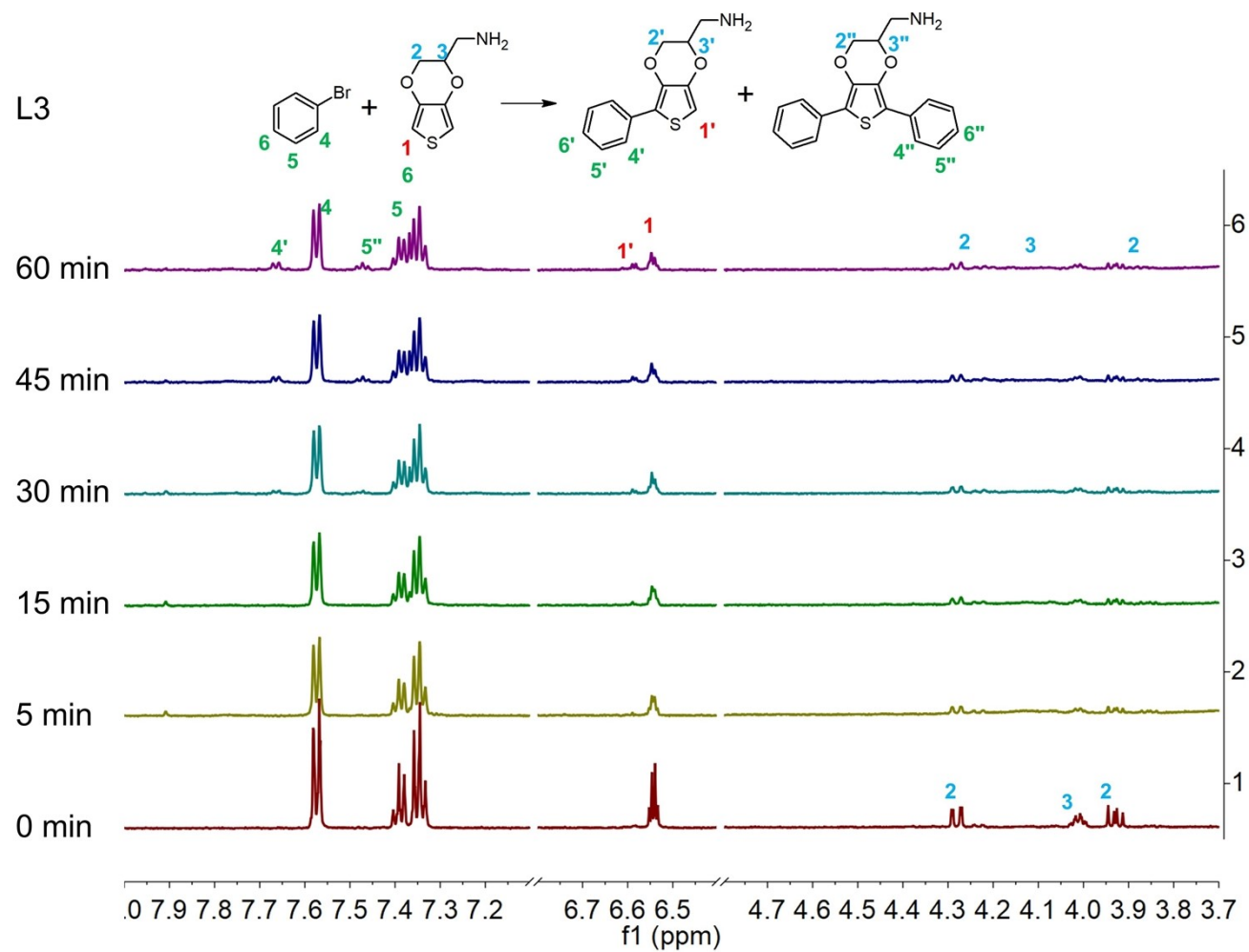
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L1 (DMSO-d₆)



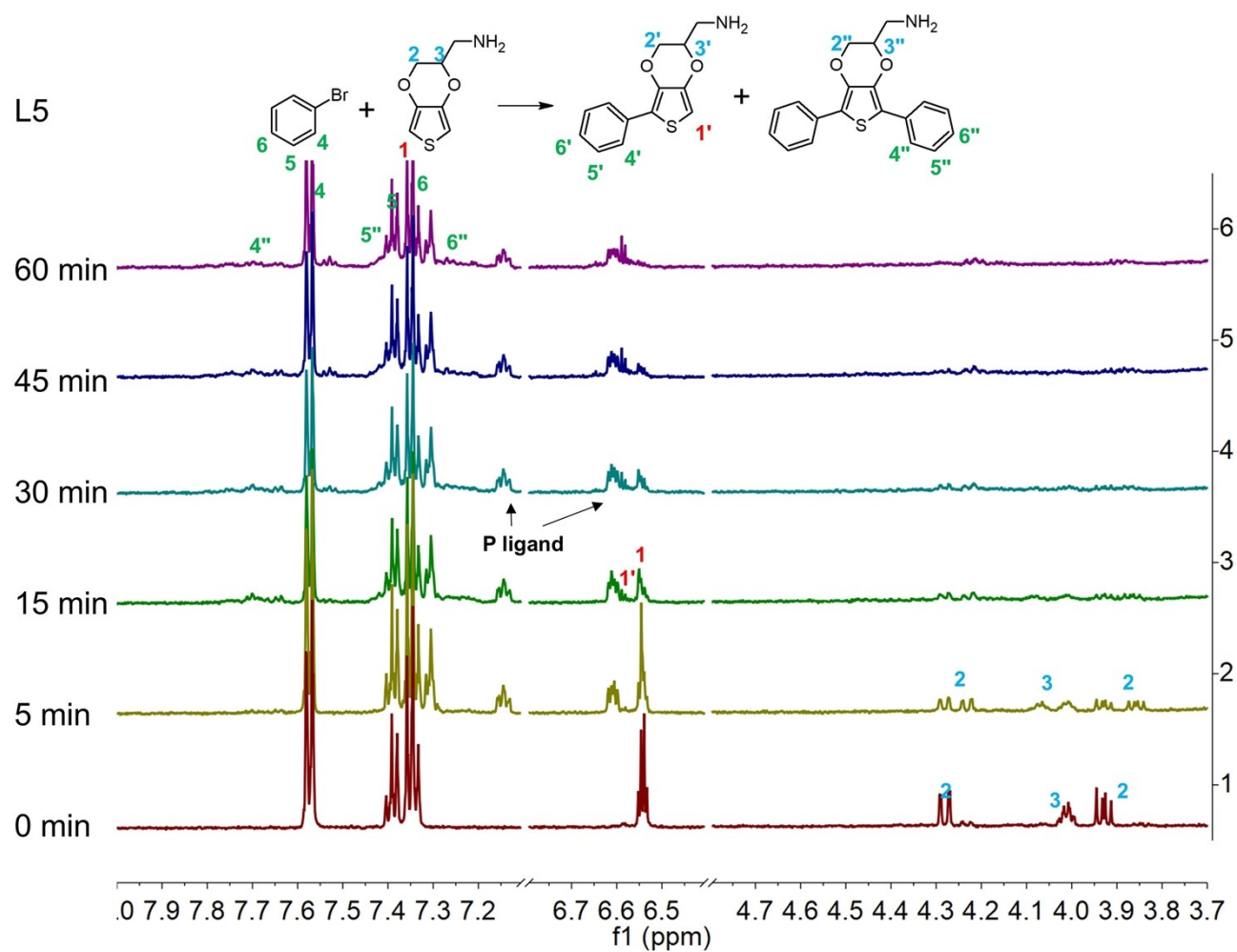
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L2 (DMSO-d₆)



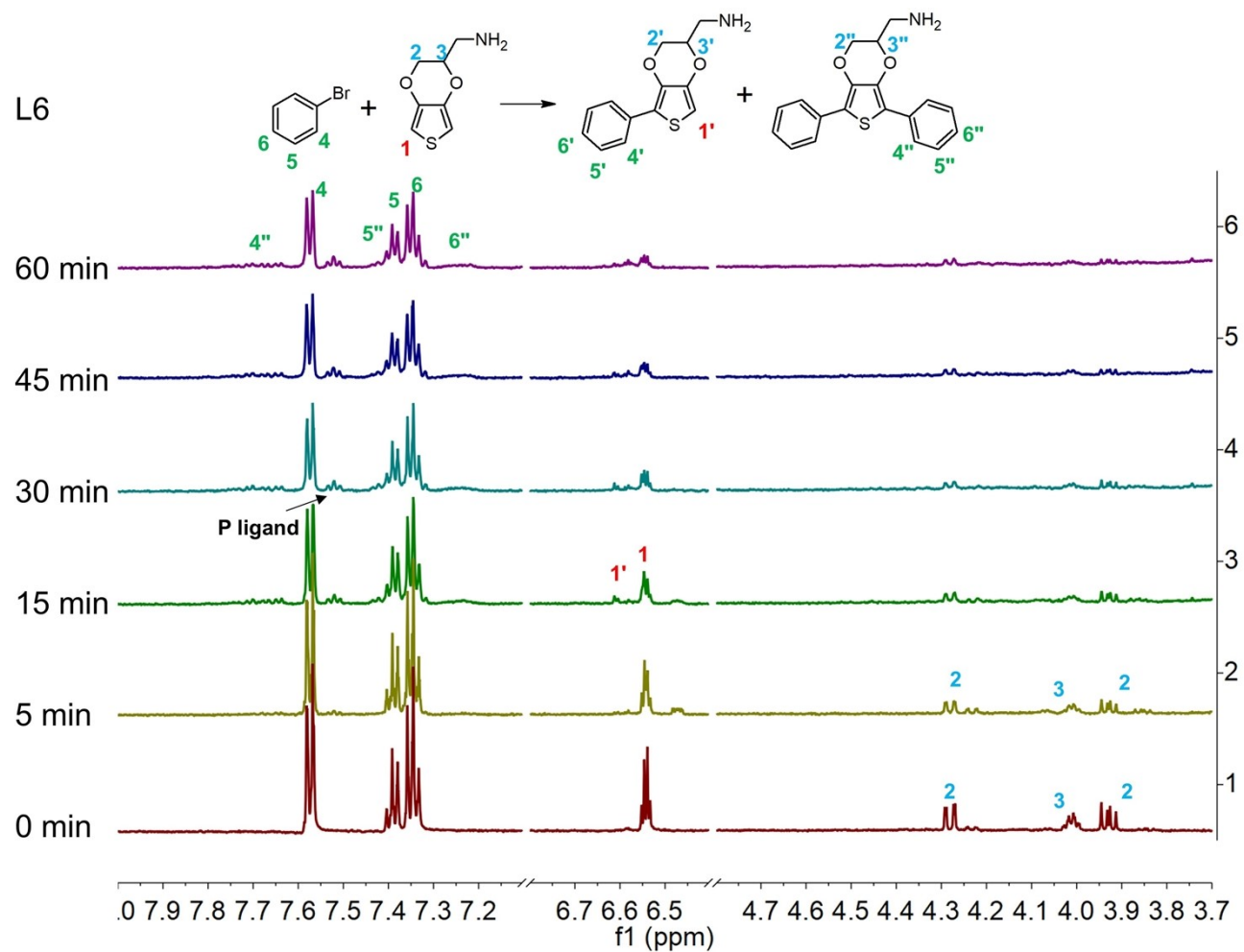
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L3 (DMSO-d₆)



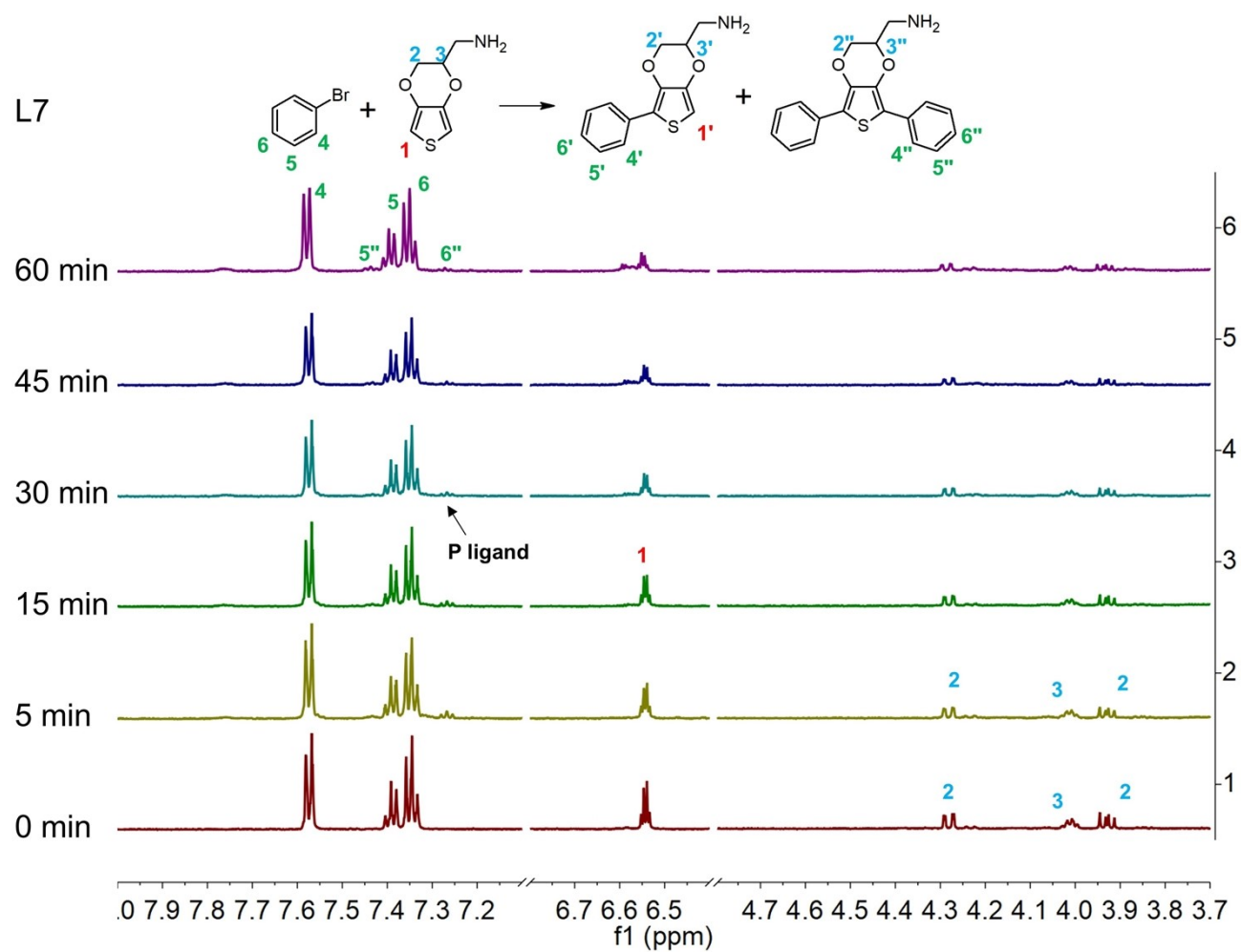
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L5 (DMSO-d₆)



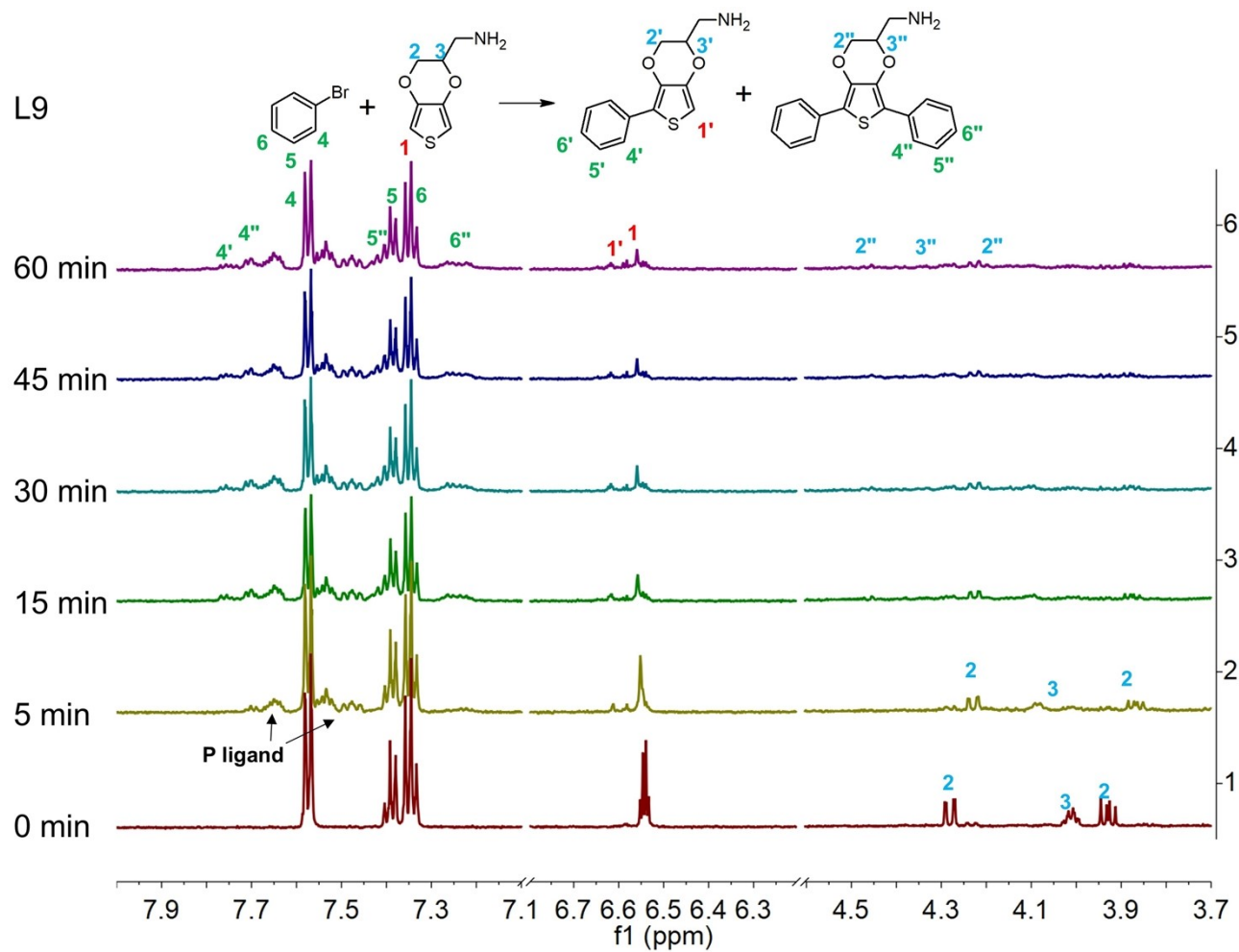
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L6 (DMSO-d₆)



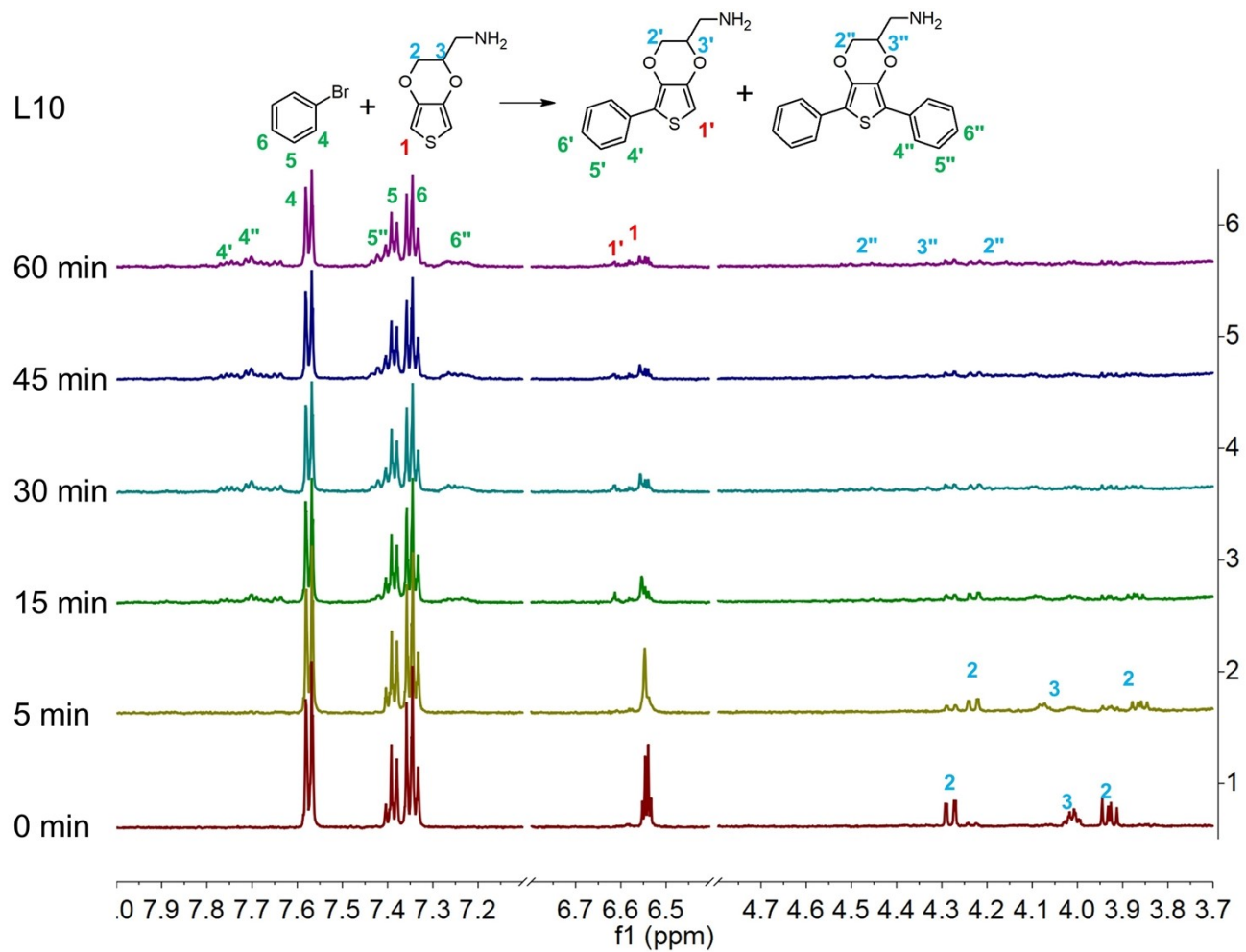
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L7 (DMSO-d₆)



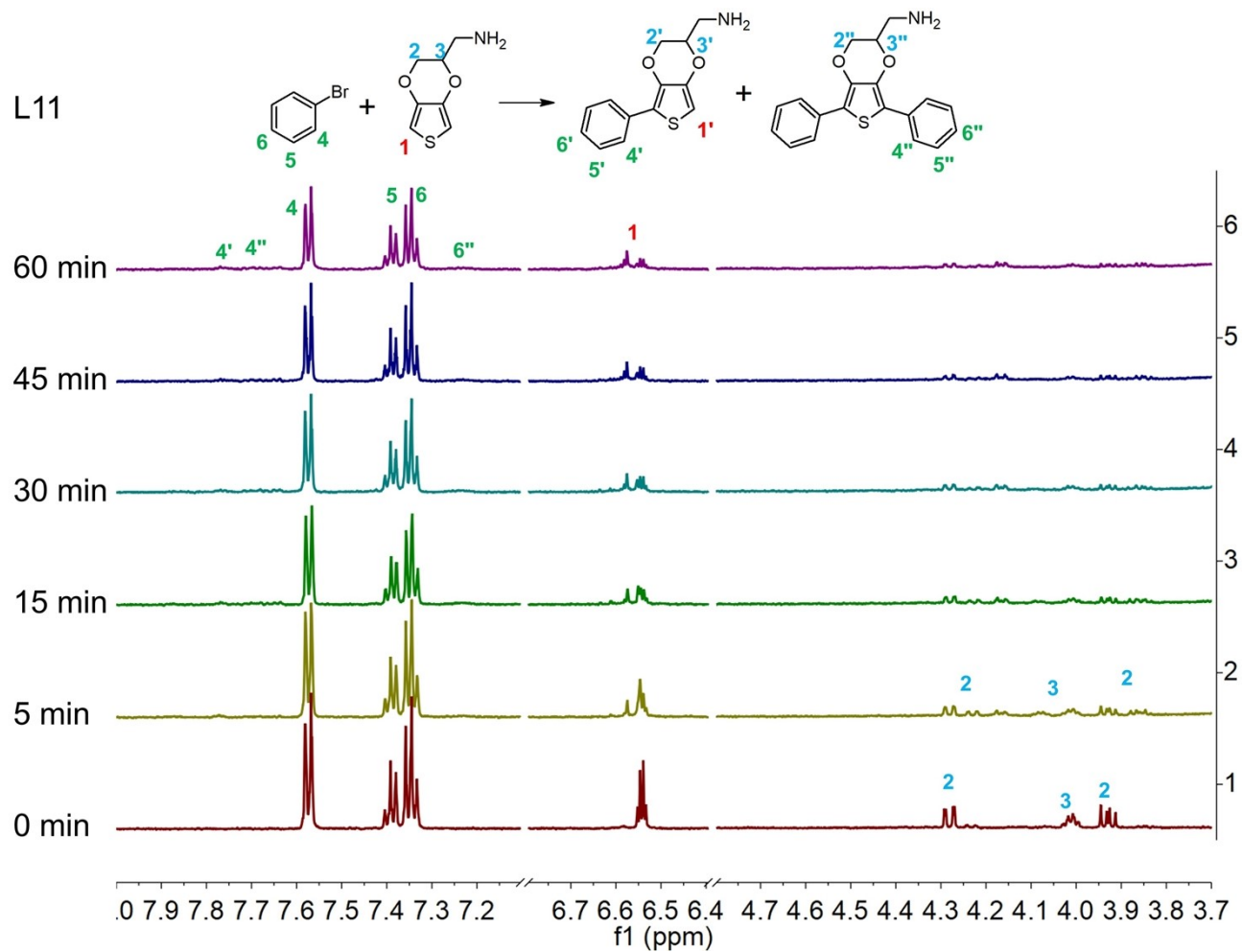
^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L9 (DMSO-d₆)



^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L10 (DMSO-d₆)



^1H NMR collected at different time points direct arylation of EDOT-NH₂ with bromobenzene assisted by L11 (DMSO-d₆)



8. References and Notes

1. H. Meng, D. F. Perepichka, M. Bendikov, F. Wudl, G. Z. Pan, W. Yu, W. Dong and S. Brown, *J. Am. Chem. Soc.*, 2003, 125, 15151–15162.
2. W. Zhang, R. Jamal, R. Zhang, Z. Yu, Y. Yan, Y. Liu, Y. Ge and T. Abdiryim, *Phys. Chem. Chem. Phys.*, 2020, 22, 3592–3603.
3. B. Zhu, S. C. Luo, H. Zhao, H. A. Lin, J. Sekine, A. Nakao, C. Chen, Y. Yamashita and H. H. Yu, *Nat. Commun.*, 2014, 5, 4523.
4. W. Hai, T. Goda, H. Takeuchi, S. Yamaoka, Y. Horiguchi, A. Matsumoto and Y. Miyahara, *ACS Appl. Mater. Interfaces*, 2017, 9, 14162–14170.
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