Supporting Information

Oxime-Based and Catalyst-Free Dynamic Covalent Polyurethanes

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1. Materials and general procedure

All reactions requiring anhydrous conditions were carried out under nitrogen atmosphere using oven-dried glasswares (120 ^{o}C), which were cooled in a desiccator. Piceol (99%), allyl bromide (98%), hydroxylamine hydrochloride (98.5%), hexamethylene diisocyanate (HDI, 99%), propiophenone (99%), octyl isocyanate (97%), phenethyl isocyanate (98%), (*E*)-acetophenone oxime (98%), cyclohexanone oxime (97%), 2,2′-(ethylenedioxy)diethanethiol (95%), trimethylolpropane tris(3-mercaptopropionate) (TTMP, 95%) dibutyltin dilaurate (DBTDL, 97.5%) and 2,2-dimethoxy-2-phenylacetophenone (DMPA, 99%) were purchased commercially and used as received unless otherwise noted. Polyethylene glycol (PEG, M_n=400) was dried under vacuum at 90 ^{o}C for 2 hours before use. All anhydrous solvents (dichloromethane (DCM), toluene (Tol), acetonitrile (MeCN), ethyl acetate (EA), acetone, tetrahydrofuran (THF), *N*,*N*-dimethylformamide (DMF) *N*,*N*-dimethylacetamide (DMAc) and dimethyl sulfoxide (DMSO)) were purchased commercially. All small molecule reactions were monitored by thin-layer chromatography (TLC) on gel GF254 plates, and silica gel (200 ~ 300 mesh) was used for product purification by flash column chromatography.

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Fourier 300 MHz, a Bruker Avance III 400 MHz or a Bruker Avance III 500 MHz spectrometer. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CDCl_3$: 7.27 ppm or TMS: 0.00 ppm for ^{1}H NMR, 77.0 ppm for ^{13}C NMR; DMSO-d6: 2.50 ppm for ^{1}H NMR). DMSO-d6 was dried with 4Å molecular sieves.

Liquid chromatography-mass spectrometry (LC-MS) was performed on an Agilent 6310 Ion Trap LC/MS Systems employing Diamonsil C18(2) 5μ 250×3.0 mm column, MeCN/H_2O (80:20) eluent (0.5 mL/min) and UV detector (254 nm), by means of the ESI technique. High-resolution mass spectral analysis (HRMS) data were determined on a Bruker 9.4T SolariX FT-ICR-MS spectrometer using ESI ion source.

Fourier transform infrared spectra (FTIR) were recorded on a Bruker Tensor27 FTIR spectrophotometer by 64 scans from 4000 to 600 cm^{-1}, with a resolution of 4 cm^{-1}. For small molecule compounds, samples were prepared by solution (CH_2Cl_2) casting onto a KBr window. For polymer samples, the measurements were equipped with a diamond ATR attachment. For kinetics studies, the *in situ* FTIR was performed on a Mettler Toledo ReactIR 15 spectrometer (scan region: 2800-650 cm^{-1}, resolution: 4 cm^{-1}).

Thermogravimetric analysis (TGA) was performed on a TA instruments Q600 Simultaneous Thermal Analyzers. Samples were heated under a nitrogen atmosphere at a rate of 10 ℃/min from 25 to 600 ℃.

Differential scanning calorimetry (DSC) was performed on a TA instruments Q2000 Differential Scanning Calorimeter. Samples were heated from -90 to 150 ^{o}C at a rate of 5 ^{o}C·min^{-1} under a nitrogen atmosphere. For each sample, two cooling-heating runs were performed and the data were obtained from the second heating curves.

Dynamic mechanical analysis (DMA) was conducted on a DMA Q800 apparatus (TA Instrument) in a tension film mode. Rectangular samples (*ca.* 0.5 mm (T) × 3 mm (W) × 8 mm (L)) were tested at a frequency of 1 Hz and a strain of 0.1%. Heating ramps of 3 ^{o}C/min were applied from -120 to 150 ℃. T_g values were calculated from the maximum value of tan δ. The cross-linking density (ν) and molecular weight between cross-links (M_c) were evaluated by the following equation[1]:

$$E = 3\nu RT = \frac{3\rho RT}{M_c} \quad (1)$$

Where E is tensile storage modulus measured at 100 ºC by DMA, ρ is the density of POUs, R is the gas constant and T refers to the absolute temperature (373 K).

Stress-relaxation analysis (SRA) was performed on a TA-Q800 DMA utilizing rectangular films (*ca.* 0.5 mm (T) × 3 mm (W) × 8 mm (L)). The SRA experiments were performed in a strain control (10% strain) mode at a specified temperature. After equilibrating at this temperature for about 5 minutes, the stress decay was monitored. The relaxation modulus (G) was normalized by initial value (G_0). The characteristic relaxation time (τ^*) was defined as the time required for $G/G_0 = 1/e$ with exponential decay function: $G(t) = G_0\exp(-t/\tau^*)$.

Creep-recovery experiments were performed on rectangular samples (*ca.* 0.5 mm (T) × 3 mm (W) × 8 mm (L)) by using TA-Q800 DMA. The samples were equilibrated for 5 minutes at specified temperature, then pulled in a constant stress and held for 30 min. After that, the stress was released and the samples were allowed to relax for another 40 min.

Uniaxial tensile measurements were performed on an Instron 3365 with a 100 mm·min^{-1} strain rate at 26 ℃, equipped with a 5 kN load cell, using a rectangular film with an effective gauge dimensions: 20 mm (L) × 3 mm (W), thickness of 0.4 ~ 0.6 mm. Rectangular tensile bars were cut from large original or reprocessed POU films using a Ray-Ran Cutting Press. Each result was the average from at least three samples.

Reprocessing experiments: The POU networks were cut into pieces (~ 1.5 g), and then placed into a rectangular mould (*ca.* 50 mm (L) × 50 mm (W)) under a hot press (120 ℃, 10 MPa) for required periods of time. The mould was cooled to room temperature by cold water in ~ 10 min and the reprocessed samples were demolded.

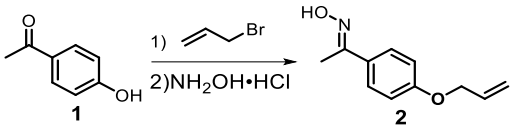
Gel permeation chromatography (GPC) was performed in DMF (1 mL·min^{-1}) at 50 ℃ using a Waters chromatograph instrument equipped with three Styragel columns (HT3, HT4 and HT5; 300 mm × 7.8 mm), 1515 pump and 2414 differential refractive index detector. PS standards were employed for the GPC calibration curve.

Atomic-force microscopy (AFM) was carried out in air at room temperature through a Bruker Multimode 8 system operated in tapping mode using commercial Si cantilevers with a nominal spring constant of 40 N·m^{-1} and resonance frequency at about 300 kHz. Samples for AFM imaging were prepared by a spin-coating method from 7 wt% CH_2Cl_2 solutions on silicon substrates, dried under vacuum at 40 ℃ for at least two days.

The gel fraction and swelling ratio of samples were determined at room temperature by soaking the sample in THF for three days with the THF refreshed each day. After that, the insoluble polymer was dried at 100 ℃ to the constant weight (W_2). The original weight of the sample was expressed as W_0. The weight of the swollen sample immediately taken out of THF was signed as W_1. Therefore, the gel fraction (GF) and the swelling ratio (SR) were calculated according to the formulas: $GF = W_2/W_0$; $SR = (W_1-W_0)/W_0$. Solubility experiments at elevated temperatures (Figure 3C) were conducted in anhydrous DMAc under N_2.

2. Synthesis of small molecule compounds and polymers

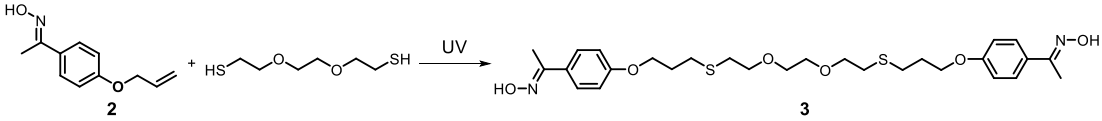
Scheme S1. Synthesis of (*E*)-1-(4-(allyloxy)phenyl)ethan-1-one oxime **2**.



To the stirred solution of Piceol **1** (52.37 g, 385 mmol) in MeCN (300 mL) were added allyl bromide (37.3 mL, 423 mmol) and K_2CO_3 (79 g, 572 mmol), then the mixture was heated to 50 °C for 3 h. The resulting solution was concentrated in *vacuo* and water (200 mL) was added, then the mixture was extracted with EtOAc (3×200 mL). The combined organic phase was washed with brine, dried over Na_2SO_4 and concentrated in *vacuo.* The crude product oxime was used in the next step directly.

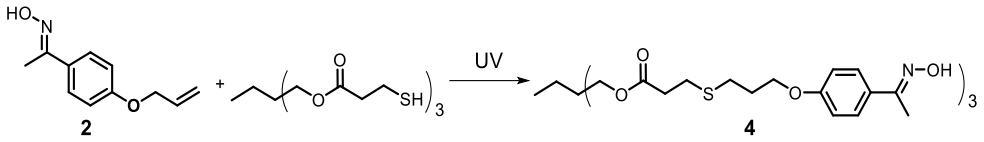
NH_2OH•HCl (40.1 g, 577 mmol) was added to a stirred solution of the crude product and NaOAc (78.9 g, 962 mmol) in 2:1 (*v*/*v*) mixture of water and EtOH (270 mL) at 90 °C. Two hours later, the system was cooled to room temperature, and the solid was obtained via filtration, then washed with H_2O/EtOH (4:1, *v*/*v*) for three times to yield compound **2** as a white solid (71.36g, 373 mmol, 97% yield for 2 steps). The *E*-configuration of acetophenone oxime derivatives was determined from the ^{1}H-chemical shift of the CH_3 group which appears around 2.3 ppm ($CDCl_3$) as a singlet (for *Z*-ketoxime it appeared around 2.6 ppm).[2] **^{1}H NMR** (400 MHz, $CDCl_3$, ppm) δ 9.01 (br s, 1H), 7.58 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.12-6.02 (m, 1H), 5.44 (d, *J* = 17.2 Hz, 1H), 5.32 (d, *J* = 10.4 Hz, 1H), 4.57 (d, *J* = 5.2 Hz, 2H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$, ppm) δ 159.5, 155.6, 133.0, 129.0, 127.4, 117.8, 114.7, 68.8, 12.2; **IR** (neat , cm^{-1}) 3287, 3241, 3095, 2922, 1607, 1512, 1432, 1254, 1000, 951, 840; **ESI-HRMS** Calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$: 192.1019, Found: 192.1019, Error: 0.0 ppm.

Scheme S2. Synthesis of dioxime **3**.



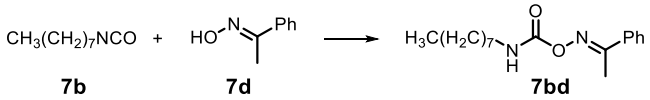
To the stirred solution of oxime **2** (19.37 g, 101 mmol) and 2,2′-(ethylenedioxy)diethanethiol (9.72 g, 50.5 mmol) in THF (100 mL) was added 0.5 mol% (to alkene) DMPA photoinitiator (0.130 g, 0.51 mmol). The solution was then irradiated (365 nm) with stirring for 60 minutes at room temperature. Removal of solvent under vacuum yielded the dioxime **3** as a colorless solid in quantitative yield, which was pure enough for further processing. **^{1}H NMR** (300 MHz, $CDCl_3$, ppm) δ 9.55 (br s, 2H), 7.55 (d, *J* = 9.0 Hz, 4H), 6.87 (d, *J* = 9.0 Hz, 4H), 4.05 (t, *J* = 6.0 Hz, 4H), 3.68-3.61 (m, 8H), 2.73 (t, *J* = 6.6 Hz, 8H), 2.26 (s, 6H), 2.10-2.01 (m, 4H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm) δ 159.7, 155.4, 128.7, 127.4, 114.3, 70.9, 70.2, 66.1, 31.4, 29.2, 28.9, 12.2; **ESI-HRMS** Calcd for $C_{28}H_{40}N_2O_6S_2Na$ $[M+Na]^+$: 587.2220, Found: 587.2224, Error: 0.7 ppm.

Scheme S3. Synthesis of trioxime **4**.



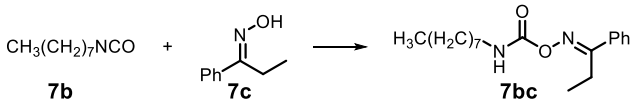
Oxime **2** (13.22 g, 69mmol) and TTMP (9.67 g, 23 mmol) were dissolved in THF (90 mL) and 0.5 mol% (to alkene) DMPA photoinitiator (0.090 g, 0.35 mmol) was added. The solution was then irradiated (365 nm) with stirring for 60 minutes at room temperature. Removal of solvent under vacuum at yielded the trioxime **4** as a colorless viscous liquid in quantitative yield, which was pure enough for further processing. **^{1}H NMR** (300 MHz, $CDCl_3$, ppm) δ 9.10 (br s, 3H), 7.56 (d, *J* = 8.7 Hz, 6H), 6.88 (d, *J* = 9.0 Hz, 6H), 4.06-4.03 (m, 12 H), 2.79 (t, *J* = 7.2 Hz, 6H), 2.72 (t, *J* = 7.2 Hz, 6H), 2.64 (t, *J* = 6.9 Hz, 6H), 2.27 (s, 9H), 2.10-2.05 (m, 6H), 1.49 (q, *J* = 7.5 Hz, 2H), 0.88 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm) δ 171.5, 159.7, 155.5, 128.8, 127.4, 114.3, 66.1, 63.8, 40.6, 34.6, 29.0, 28.5, 26.9, 22.9, 12.2, 7.3; **ESI-HRMS** Calcd for $C_{48}H_{65}N_3O_{12}S_3Na$ $[M+Na]^+$: 994.3623, Found: 994.3623, Error: 0.0 ppm.

Scheme S4 Synthesis of (*E*)-1-phenylethan-1-one O-octylcarbamoyl oxime **7bd**.



Octyl isocyanate (2.620 g, 16.4 mmol) was dissolved in anhydrous CH_2Cl_2 (2.6 mL), and then (*E*)-acetophenone oxime (2.260 g, 16.4 mmol) was added. The solution was allowed to be stirred overnight at room temperature and then solvent was removed in *vacuo*. The residue was purified through column chromatography on silica gel (hexane/EtOAc = 15:1 to 10:1) to yield the compound **7bd** (4.705 g, 99%) as a colorless solid. The configuration of *E*-**7bd** was characterized by two IR absorption at ~ 3350 and 1500 cm^{-1}.[3] In addition, the ^{1}H-chemical shift of the CH_3 group (~ 2.4 ppm) in acetophenone oxime moiety also accord with the reported *E*-oxime-carbamates.[4] **^{1}H NMR** (400 MHz, $CDCl_3$, ppm) δ 7.67-7.65 (m, 2H), 7.47-7.39 (m, 3H), 6.48 (br s, 1H), 3.33-3.28 (m, 2H), 2.41 (s, 3H), 1.61-1.54 (m, 2H), 1.31-1.26 (m, 10H), 0.86 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$, ppm) δ 159.8, 155.4, 134.9, 130.4, 128.5, 126.6, 41.1, 31.6, 29.7, 29.1, 29.1, 26.7, 22.5, 14.3, 13.9; **IR** (neat, cm^{-1}) 3363, 2927, 2856, 1726, 1499, 1445, 1223, 989, 762, 693; **ESI-HRMS** Calcd for $C_{17}H_{26}N_2O_2Na$ $[M+Na]^+$: 313.1886, Found: 313.1888, Error: 0.5 ppm.

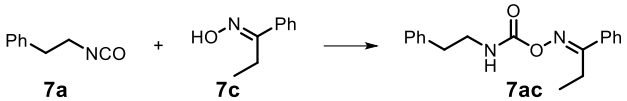
Scheme S5 Synthesis of (*E*)-1-phenylpropan-1-one O-octylcarbamoyl oxime **7bc**.



Prepared according to the same procedure with **7bd** using (*E*)-propiophenone oxime[5] afforded **7bc** as a colorless solid in 98% yield. **^{1}H NMR** (300 MHz, $CDCl_3$, ppm) δ 7.67-7.63 (m, 2H), 7.48-7.40 (m, 3H), 6.47 (br s, 1H), 3.35-3.29 (m, 2H), 2.92 (q, *J* = 7.7 Hz, 2H), 1.62-1.54 (m, 2H), 1.32-1.27 (m, 10H), 1.19 (t, *J* = 7.7 Hz, 3H), 0.87 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm) δ 164.8, 155.6, 133.9, 130.4, 128.7, 126.9, 41.2, 31.7, 29.7, 29.2, 29.1, 26.8, 22.6, 21.6, 14.0, 11.2; **IR** (neat, cm^{-1}) 3361, 2928, 2856, 1726, 1500, 1464, 1222, 949, 764, 694; **ESI-HRMS** Calcd for $C_{18}H_{28}N_2O_2Na$

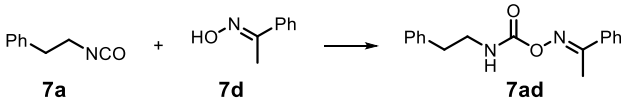
$[M+Na]^+$: 327.2043, Found: 327.2045, Error: 0.5 ppm.

Scheme S6 Synthesis of (*E*)-1-phenylpropan-1-one O-phenethylcarbamoyl oxime **7ac**.



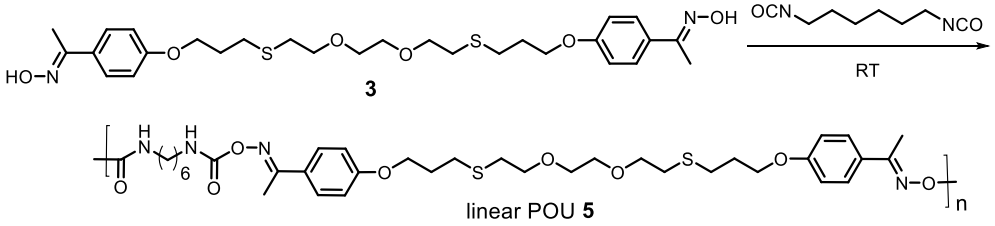
Prepared according to the same procedure with **7bd** afforded **7ac** as a colorless liquid in 98% yield. **^{1}H NMR** (400 MHz, $CDCl_3$, ppm) δ 7.57-7.55 (m, 2H), 7.47-7.38 (m, 3H), 7.33-7.29 (m, 2H), 7.26-7.22 (m, 3H), 6.56 (br s, 1H), 3.61-3.56 (m, 2H), 2.91-2.85 (m, 4H), 1.17 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$, ppm) δ 164.5, 155.4, 138.6, 133.6, 130.4, 128.8, 128.6, 126.8, 126.4, 42.1, 35.8, 21.3, 11.2; **IR** (neat, cm^{-1}) 3398, 3027, 2939, 1731, 1497, 1455, 1227, 947, 751, 697; **ESI-HRMS** Calcd for $C_{18}H_{20}N_2O_2K$ $[M+K]^+$: 335.1156, Found: 335.1158, Error: -0.6 ppm.

Scheme S7 Synthesis of (*E*)-1-phenylethan-1-one O-phenethylcarbamoyl oxime **7ad**.



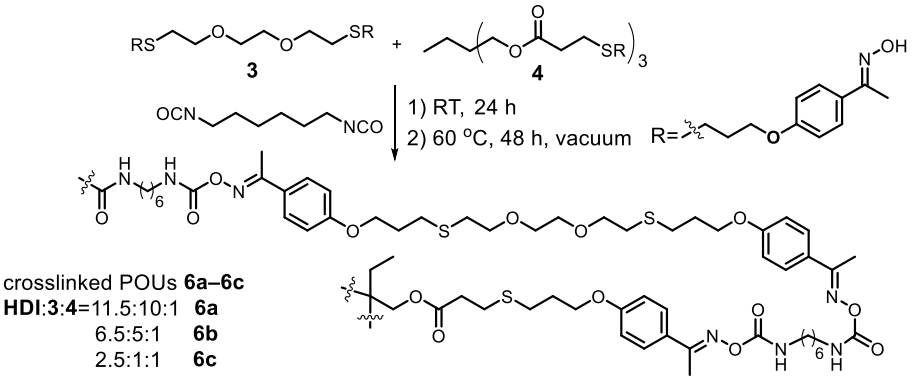
Prepared according to the same procedure with **7bd** afforded **7ad** as a colorless liquid in 98% yield. **^{1}H NMR** (300 MHz, $CDCl_3$, ppm) δ 7.59-7.56 (m, 2H), 7.46-7.23 (m, 8H), 6.54 (br s, 1H), 3.63-3.56 (m, 2H), 2.90 (t, *J* = 6.9 Hz, 2H), 2.40 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm) δ 159.7, 155.4, 138.6, 134.7, 130.5, 128.8, 128.6, 128.5, 126.6, 126.5, 42.2, 35.8, 14.2; **IR** (neat, cm^{-1}) 3399, 3028, 2935, 1732, 1497, 1455, 1230, 949, 762, 695; **ESI-HRMS** Calcd for $C_{17}H_{18}N_2O_2K$ $[M+K]^+$: 321.1000, Found: 321.1001, Error: 0.5 ppm.

Scheme S8 Synthesis of linear poly(oxime-urethane) **5**.



To a solution of dioxime **3** (2.104 g, 1 equiv) in anhydrous CH_2Cl_2 (8.0 mL) was added HDI (0.619 g, 1 equiv) and the mixture was stirred at room temperature for 5 h. Then the solution was poured into a Teflon mould (50 mm L × 50 mm W), and the solvent was evaporated in a fume hood for *ca.* 24 hours. The sample was demolded, and placed under vacuum at 40 ℃ for *ca.* 48 hours, and then kept in a desiccator before measurement. **^{1}H NMR** (400 MHz, $CDCl_3$, ppm) δ 7.60 (d, *J* = 8.4 Hz, 4H), 6.90 (d, *J* = 8.4 Hz, 4H), 6.48 (br s, 2H), 4.07 (t, *J* =5.6 Hz, 4H), 3.65-3.60 (8H), 3.35-3.20 (4H), 2.74-2.70 (8H), 2.36 (s, 6H), 2.07-2.04 (4H), 1.65-1.55 (4H), 1.40-1.30 (4H).

Scheme S9 Synthesis of cross-linked poly(oxime-urethanes) **6**.

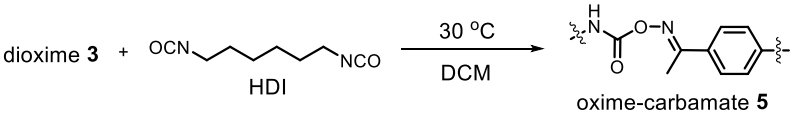


Typical preparation of **6b**: To a stirred solution of trioxime **4** (0.577 g, 1 equiv) and dioxime **3** (1.675 g, 5 equiv) in anhydrous CH_2Cl_2 (2.7 mL) was added HDI (0.640 g, 6.5 equiv). The system was stirred for two minutes, then poured into an aluminum mould (50 mm L × 50 mm W), and allowed to keep in a desiccator at room temperature for *ca.* 24 hours. The film was demolded, and placed under vacuum at 60 ℃ for *ca.* 48 hours to ensure complete removal of the solvent. The films were kept in a desiccator before measurement.

3. Kinetics studies of polyaddition between dioxime 3 and HDI

3.1 Determination of reaction order for the polyaddition

We studied the kinetics of oxime-urethanation reaction by using *in situ* FTIR at various concentrations of the components to observe the initial rate of the reaction.



To a three-necked reaction vessel was added 1.5 mL anhydrous DCM solution of dioxime **3** (0.173 g, 0.3 mmol) via a syringe under N_2. The mixture was stirred at 30 ℃ in an oil bath. Then the IR data collection was started, followed by addition of 0.5 mL DCM solution of HDI (0.051 g, 0.3 mmol) in one portion. I*n situ* FTIR spectra were recorded over the reaction course. Spectra of the NCO group at ~ 2276 cm^{-1} ($A_{2276,\,t}$) was used for the generation of the kinetic profiles. By measuring the initial rate (< 5 min), we have:

$$rate_0 = \frac{-d[NCO]}{dt} = \frac{d[5]}{dt} = k_b[oxime]_0^a[NCO]_0^b \quad (2)$$

$$\alpha = 1 - \frac{A_{2276,\,t}}{A_{2276,\,t=0}} \quad (3)$$

Where $[NCO]_0$ and $[oxime]_0$ represent the initial concentrations of isocyanate and oxime, *a* and *b* are orders of oxime and NCO, respectively. α stands for the reaction conversion.

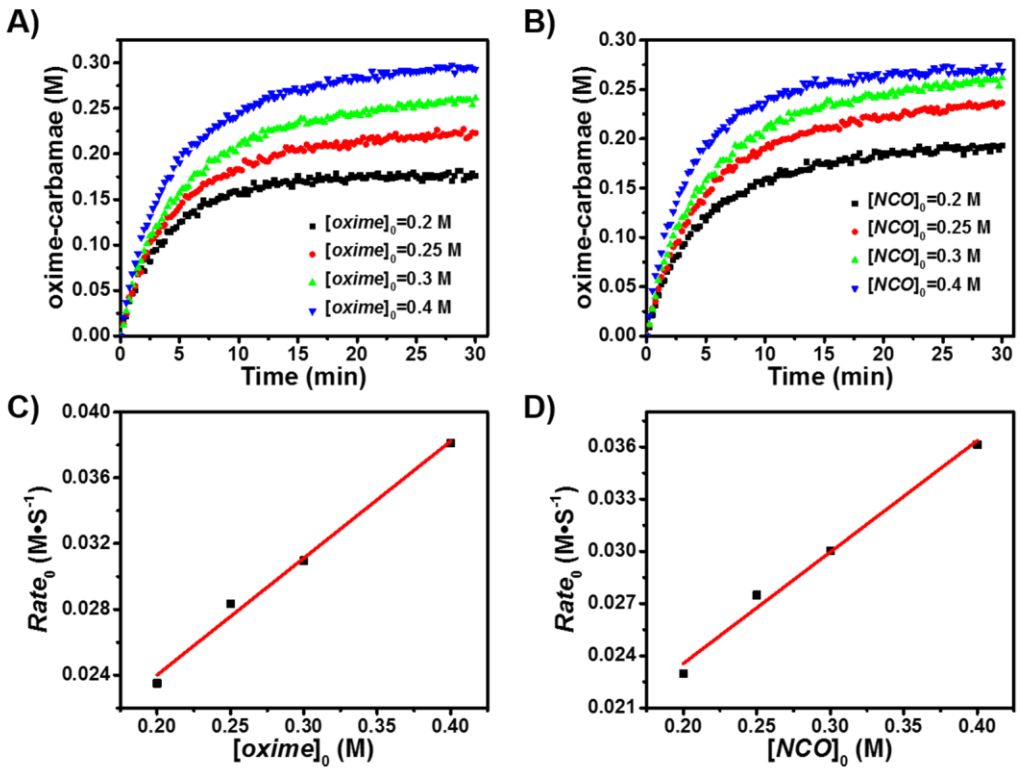


Figure S1 Kinetic profiles of different initial concentrations of (A) oxime (from 0.2 to 0.4 M) and (B) NCO (from 0.2 to 0.4 M). Linear fittings of the initial reaction rates as a function of (C) $[oxime]_0$ and (D) $[NCO]_0$ showing that $a = b = 1$.

3.2 Kinetics of the polyaddition in various aprotic solvents

Kinetics studies were performed with dioxime **3** (0.401g, 0.70 mmol, in 1.5 mL anhydrous solution) and HDI (0.118g, 0.70 mmol, in 0.5 mL anhydrous solution) at a constant temperature, and were monitored by *in situ* FTIR. The NCO group stretching at ~ 2276 cm^{-1} ($A_{2276,\,t}$) was measured at different periods. To counteract the change of concentration during the reaction course, the absorbance is normalized to 1,4-substituted Ar-H stretching at ~ 835 cm^{-1} ($A_{835,\,t}$), which does not change during the reaction. For PEG-HDI-DBTDL (1 mol%) system, C-O stretching at ~ 1106 cm^{-1} ($A_{1106,\,t}$) was used for normalization in the whole process. Isocyanate conversion (α) was calculated as follows:

$$\alpha = 1 - \frac{A_{2276,\,t} / A_{835,\,t}}{A_{2276,\,t=0} / A_{835,\,t=0}} \quad (4)$$

For second-order kinetics:

$$-\frac{d[NCO]}{dt} = k_b[oxime][NCO] = k_b[NCO]^2 \quad (5)$$

Where $[NCO]$ and $[oxime]$ represent the concentrations of isocyanate and oxime at time t, respectively (in our systems, $[NCO] = [oxime]$).

$$\frac{1}{1-\alpha} = k_b[NCO]_0 t + 1 \quad (6)$$

The apparent bonding rate constant k_b was obtained by linear fitting according to equation (6) using the data less 90% conversion ($[NCO]_0$ = 0.70 M). Phase separation and turbid phenomenon were observed owing to the poor solubility of POU **5** in these solvents, such as EA, MeCN, Acetone and Tol. So kinetics data before phase separation were used for calculations in these solvents. Typically, polyaddition reaction in DCM at 30 °C was performed three times to acquire appropriate standard deviation, showing that bonding rate constant (k_b) values are confident and reproducible (k_b = (8.3 ± 0.5) $\times 10^{-3}$ $M^{-1} \cdot s^{-1}$).

For comparison, the reactions of PEG (0.277g, 0.70 mmol, M_n = 400) and HDI (0.118g, 0.70 mmol) without/with catalyst DBTDL (1 mol% to HDI) in anhydrous DMAc were monitored by *in situ* FTIR.

Table S1 The rate constant k_b for the polyaddition in DMAc at different temperatures (Figure 1C).

T (°C)	$k_b 10^4$ ($M^{-1} \cdot s^{-1}$)
30	2.1
41	6.3
55	14.9
65	25.3

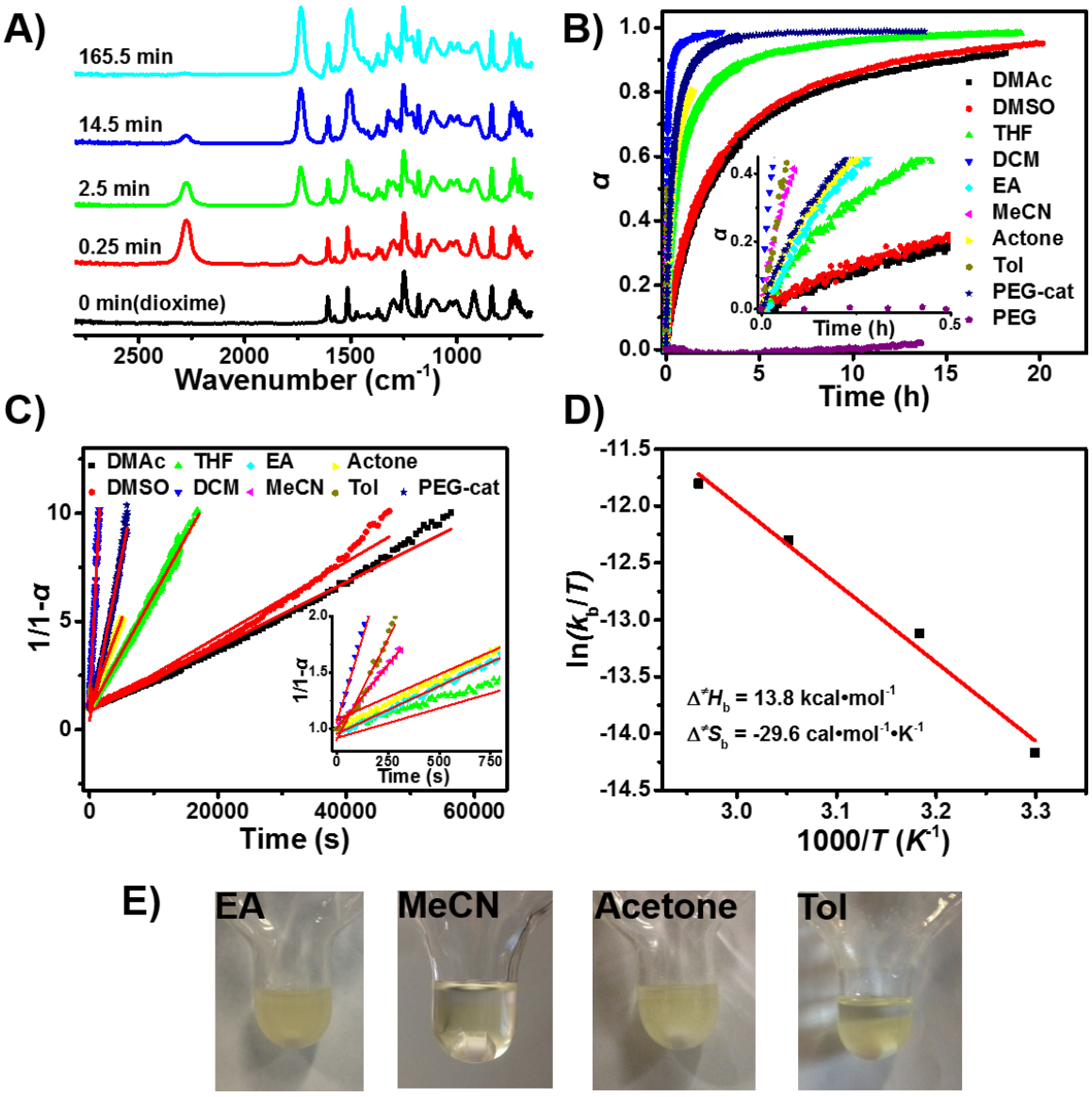


Figure S2 (A) Representative *in situ* FTIR spectra for polyaddition reaction of dioxime **3** and HDI in DCM at 30 °C. (B) Isocyanate conversion α and (C) linear plot of $1/(1-\alpha)$ as a function of time in various aprotic solvents at 30 °C. (D) Eyring plot of the polyaddition reaction in DMAc to determine the activation parameters. (E) Photos showing the poor solubility of POU **5** in EA, MeCN, Acetone and Tol.

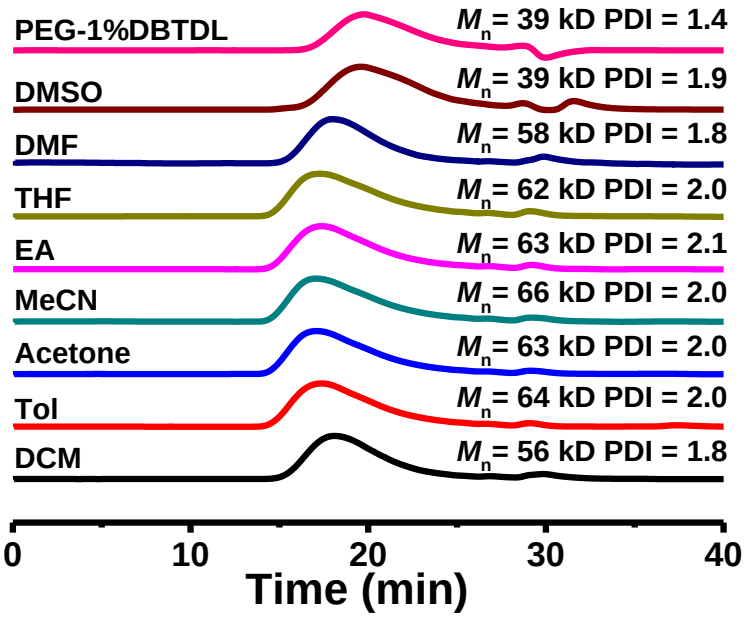
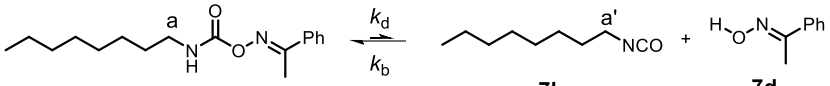


Figure S3 GPC traces of POU **5** prepared in different solvents after the complete conversion of isocyanate. PEG-HDI-DBTDL (1 mol%) system in DMAc was also shown for comparison.

4. Studies of the dynamic nature in model compounds

4.1 Variable-temperature NMR experiments of oxime-carbamate 7bd

Scheme S10 Thermal dissociation reaction of oxime-carbamate **7bd** to **7b** and **7d**



7bd $K_d = k_d/k_b$ **7b** **7d**

To a NMR tube were added oxime-carbamate **7bd** (0.051 g, 0.176 mmol) and anhydrous DMSO-d6 (total volume = 0.70 mL). The ^{1}H NMR spectra were acquired by *in situ* variable-temperature NMR at 100 °C until the dissociation reaction reaching equilibrium (~ 40 min). Then, the temperature was raised for subsequent variable-temperature experiments. Typically, variable-temperature NMR experiment at 120 °C was performed three times to acquire appropriate standard deviation, showing that dissociation equilibrium constant (K_d) values are confident and reproducible (K_d = (3.4 ± 0.5)×10^{-3} M). The first-order dissociation rate constant at 100 °C (k_{d2}) was obtained from the first-order kinetic equation (7). The enthalpy (ΔH_d) and entropy (ΔS_d) of the dissociation reaction were extracted from Van't Hoff equation (8).

$$\ln\frac{c_0}{c} = k_{d2}t \quad (c_0 = 0.25\ \text{M}) \quad (7) \qquad \text{Then} \quad k_{d2} = \frac{\ln 1.05}{43\ \text{min}} = 0.07\ \text{h}^{-1}$$

$$\ln K_d = -\frac{\Delta H_d}{RT} + \frac{\Delta S_d}{R} \quad (8)$$

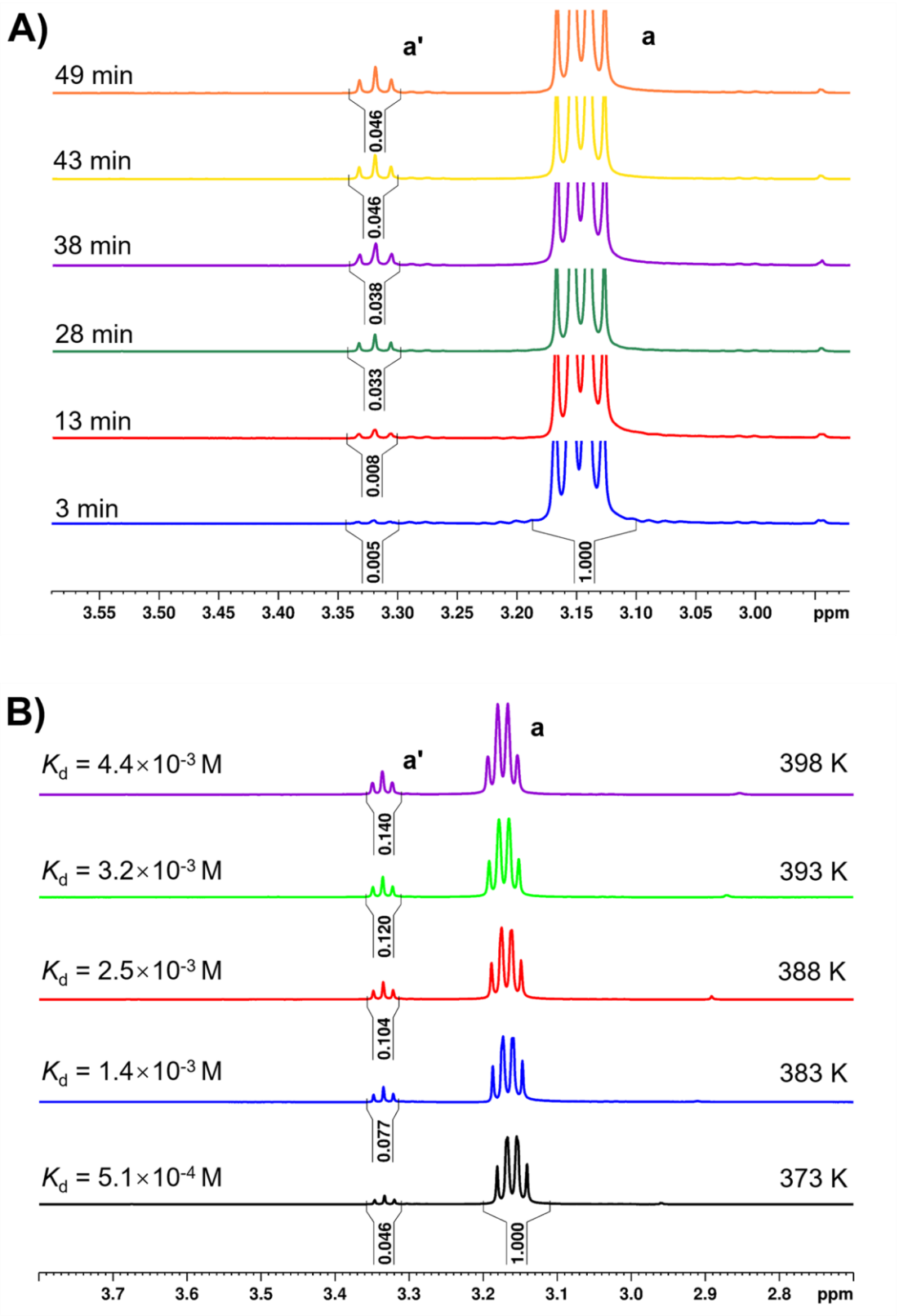


Figure S4 I*n situ* variable-temperature ^{1}H NMR spectra of **7bd**: (A) after being heated at 100 ^{o}C for different periods; (B) thermodynamic equilibrium of **7bd** at different temperatures.

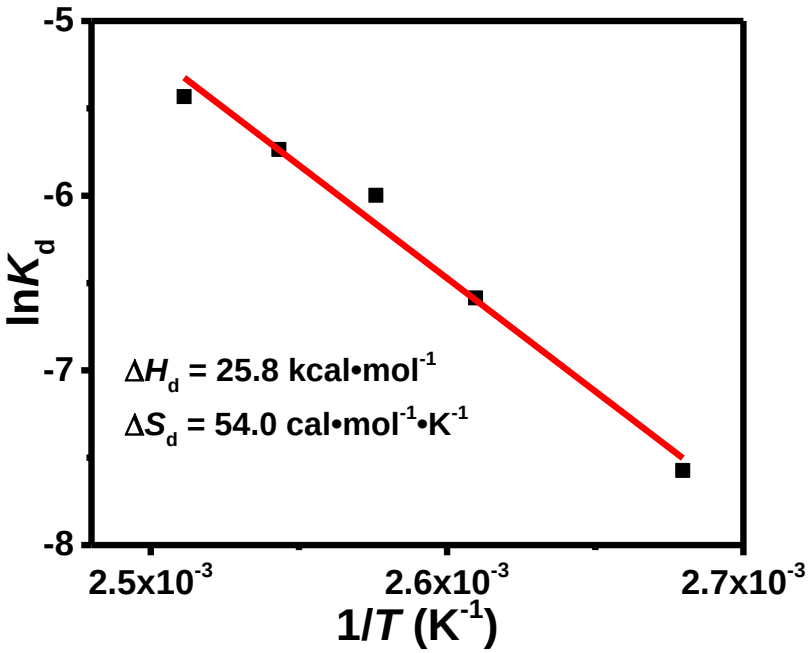
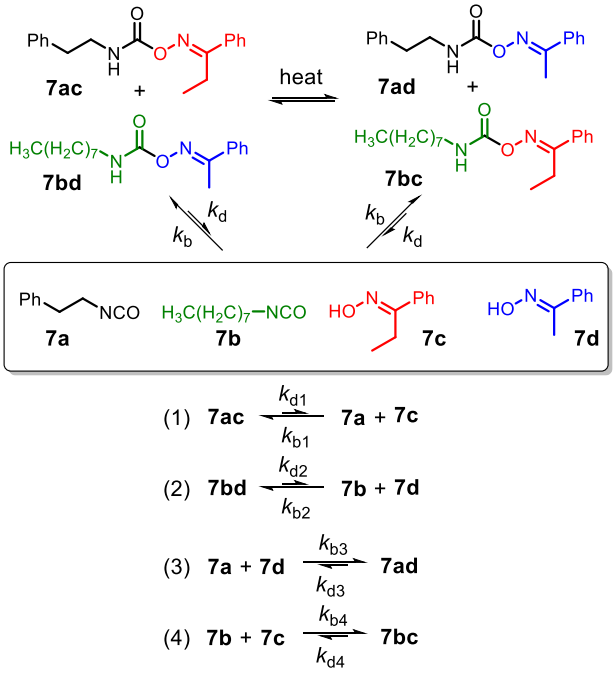


Figure S5 Van't Hoff plot for the dissociation reaction of **7bd**.

4.2 LC-MS analysis of the transcarbamoylation of 7ac and 7bd

Scheme S11 The dissociative transcarbamoylation reaction between **7ac** and **7bd** to yield **7ad** and **7bc**.



The mixture of oxime-carbamates **7ac** (0.206g, 0.69 mmol) and **7bd** (0.201, 0.69 mmol) was immerged in a preheated oil bath (80-120 °C) under N_2 atmosphere. Aliquots were periodically withdrawn and diluted in MeCN, then analyzed via LC-MS. Concentrations of the product **7bc** were calculated from a calibration curve ($y = 1.511\times10^{-7}x + 3.722\times10^{-6}$).

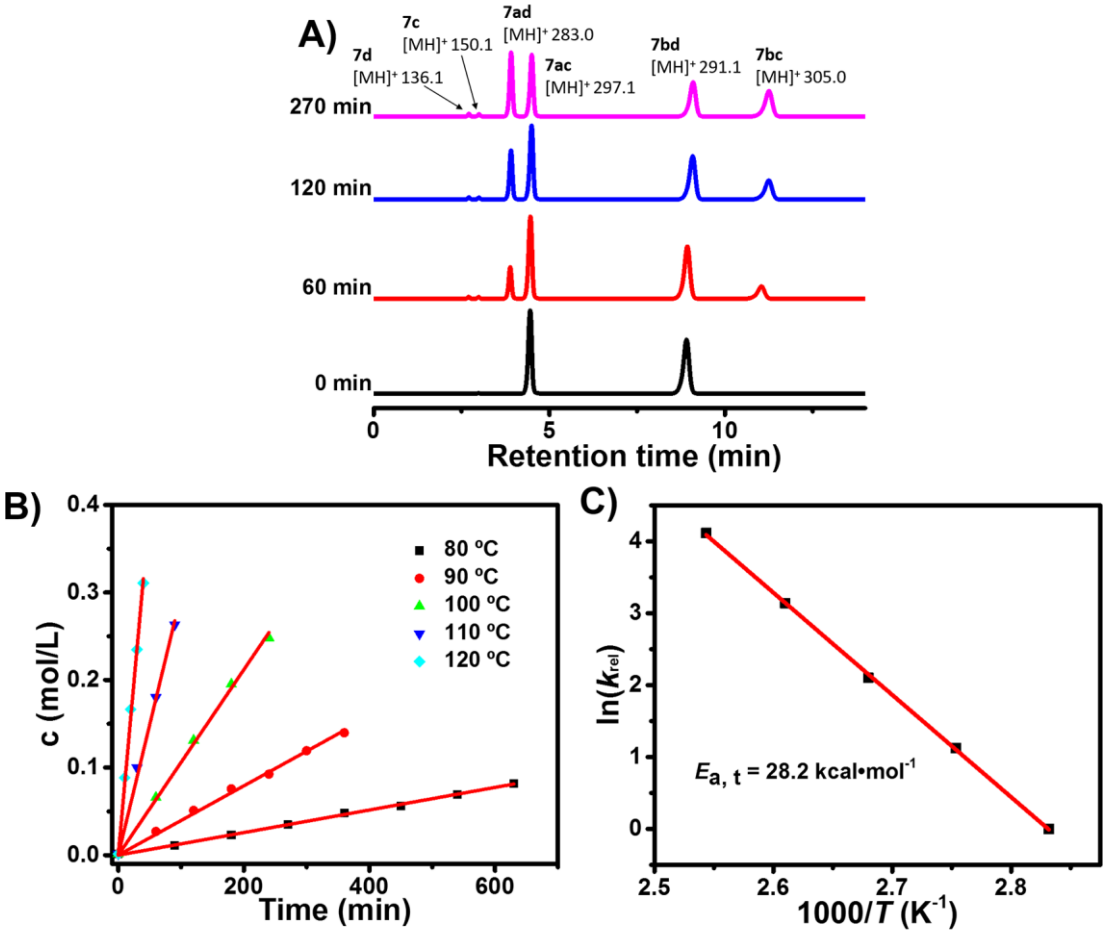


Figure S6 (A) LC-MS analysis of the transcarbamoylation reaction for **7ac** and **7bd** at 120 °C. Similar to variable-temperature NMR experiments, the chromatogram curves show slight dissociation products (the relative contents of **7c** and **7d** by peak area normalization method: $A_{\mathbf{7c}} = A_{\mathbf{7d}} =$ ~ 1%). (B) Concentrations of the transcarbamoylation product **7bc** versus time. Linear fits are shown for initial rates. (C) Arrhenius analysis of this model transcarbamoylation reaction.

Kinetics analysis of oxime-enabled transcarbamoylation reaction to demonstrate the dissociative exchange mechanism, as well as to acquire apparent dissociation rate constants (k_d) and dissociation activation energies ($E_{a,\,d}$).

Based on our proposal, if the transcarbamoylation reaction processes through a dissociative exchange mechanism (Scheme S11), we have:

$$\frac{d[7bc]}{dt} = k_{b4}[7b][7c] - k_{d4}[7bc] \quad (9)$$

In this case, the concentrations of intermediate oxime **7c** and isocyanate **7b** can be regarded as

constants, so we have:

$$[7b]=[7b]_{eq}=\frac{k_{d4}}{k_{b4}}\times\frac{[7bc]_{eq}}{[7c]_{eq}} \quad (10) \qquad [7c]=[7c]_{eq} \quad (11)$$

Then, we get the next relationship:

$$\frac{d[7bc]}{dt}=k_{d4}[7bc]_{eq}-k_{d4}[7bc]=k_{d4}([7bc]_{eq}-[7bc]) \quad (12)$$

By solving equation, we can obtain equations (13) and (14).

$$\int_0^t\frac{d[7bc]}{[7bc]_{eq}-[7bc]}=\int_o^t k_{d4}dt$$

$$\ln([7bc]_{eq}-[7bc])=\text{-}k_{d4}t+\ln[7bc]_{eq} \quad (13)$$

$$\ln(A_{7bc,\ eq}-A_{7bc})=\text{-}k_{d4}t+C \quad (14)$$

Where A and A_{eq} stand for chromatographic peak area at reaction time t and the final equilibrium peak area, respectively. In our system, the equilibrium peak area at 100, 110, and 120 ^{o}C could be obtained experimentally (Figure 2B).

With similar processing, we have another three equations (15-17).

$$\ln(A_{7ad,\ eq}-A_{7ad})=\text{-}k_{d3}t+C \quad (15)$$

$$\ln(A_{7ac}-A_{7ac,\ eq})=\text{-}k_{d1}t+C \quad (16)$$

$$\ln(A_{7bd}-A_{7bd,\ eq})=\text{-}k_{d2}t+C \quad (17)$$

The thermal dissociation rate constants (k_d) of corresponding dissociation reactions were determined by linear regression of ln(A_{eq}-A) or ln(A-A_{eq}) versus time (Figure S7). As a consequence, the apparent dissociation activation energies ($E_{a,\ d}$) of oxime-carbamates were determined to be about 26.7 ~ 30.3 kcal·mol^{-1} (Figure S8), which are in accordance with transcarbamoylation activation energy ($E_{a,\ t}$, Figure S6). Additionally, the dissociation rate constant (k_{d2} = 0.09 h^{-1}, Figure S7) at 100 ^{o}C is also close to that measured by variable-temperature NMR experiments (k_{d2} = 0.07 h^{-1}, equation 7). These results confirm our proposal that the transcarbamoylation of oxime-carbamates occurs via a dissociative process. Typically, LC-MS analysis of the transcarbamoylation at 120 ^{o}C was performed three times to acquire appropriate standard deviations, showing that dissociation rate constant (k_d) values are confident and reproducible (k_{d4} = 0.64 $\pm$ 0.08 h^{-1}, k_{d3} = 0.65 $\pm$ 0.08 h^{-1}, k_{d1} = 0.56 $\pm$ 0.03 h^{-1}, and k_{d2} = 0.60 $\pm$ 0.05 h^{-1}).

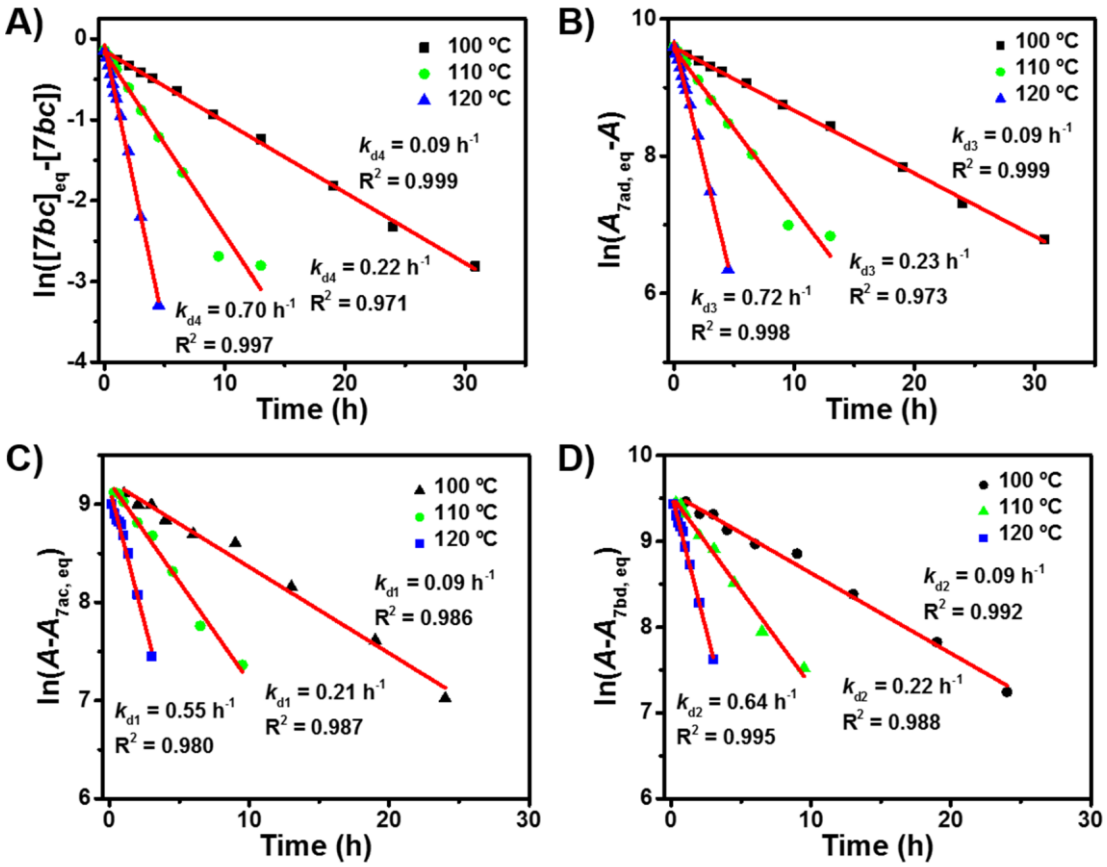


Figure S7 Linear fittings of (A) $\ln([7bc]_{eq}-[7bc]) \sim t$, (B) $\ln(A_{7ad,\,eq}-A) \sim t$, (C) $\ln(A-A_{7ac,\,eq}) \sim t$ and (D) $\ln(A-A_{7bd,\,eq}) \sim t$ at 100, 110 and 120 °C.

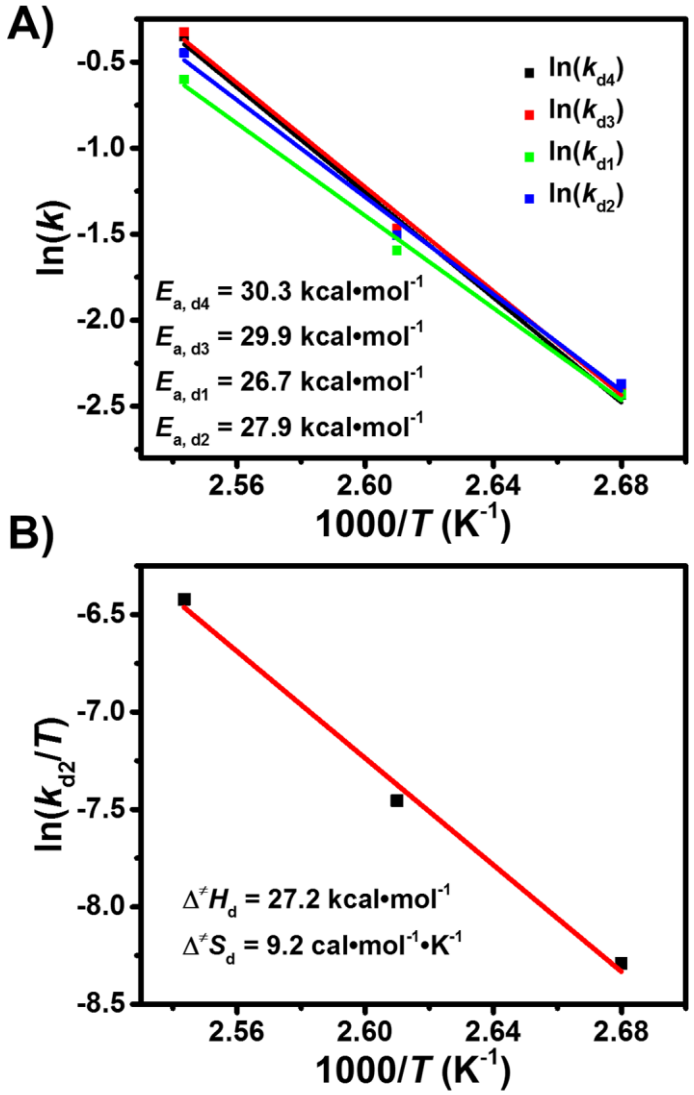


Figure S8 (A) Determination of the dissociation activation energies ($E_{a,\ d}$) for oxime-carbamates through Arrhenius analysis. (B) Eyring plot of the dissociation reaction of **7bd** to determine the activation parameters.

5. Dynamic depolymerization and repolymerization of POU 5

HDI (0.69 mmol) and dioxime **3** (0.69 mmol) were stirred in DMF (1 mL) at 60 °C for 5 h to form the solution of POU **5**. GPC experiment was performed to identify the molecular weight of POU **5**. Then one additional equiv. **3** (0.69 mmol) was added and the solution was heated at 110 °C. After 1 hour, the system was cooled to room temperature and GPC experiment was performed. Finally, one equiv. HDI (0.69 mmol) and DMF (1 mL) were added to the solution. After 5 h reaction at 60 °C, GPC experiment was carried out (Figure 2C).

6. Characterization of POUs

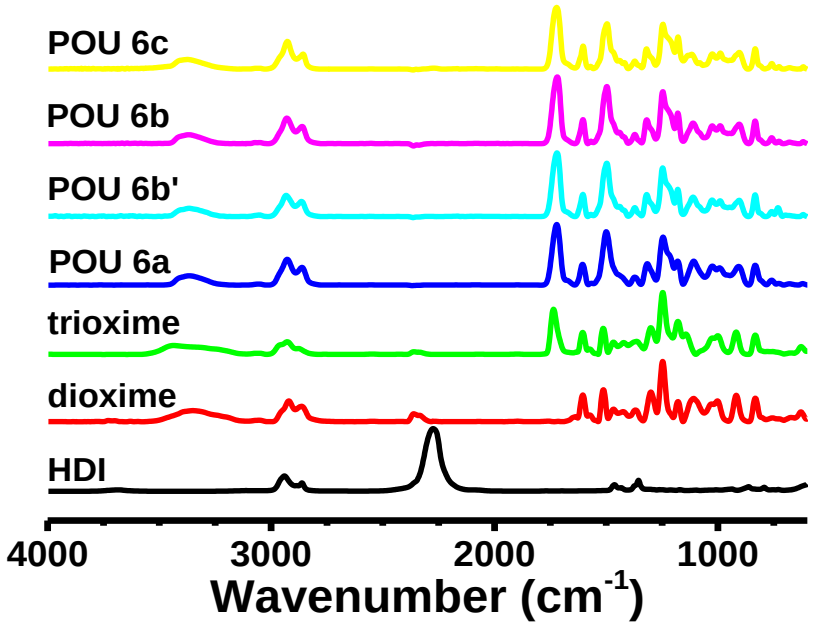


Figure S9 FTIR spectra of HDI, polyoximes and as-synthesized cross-linked POUs (POU **6b'** represent IR spectrum of **6b** before solvent removal at 60 °C under vacuum).

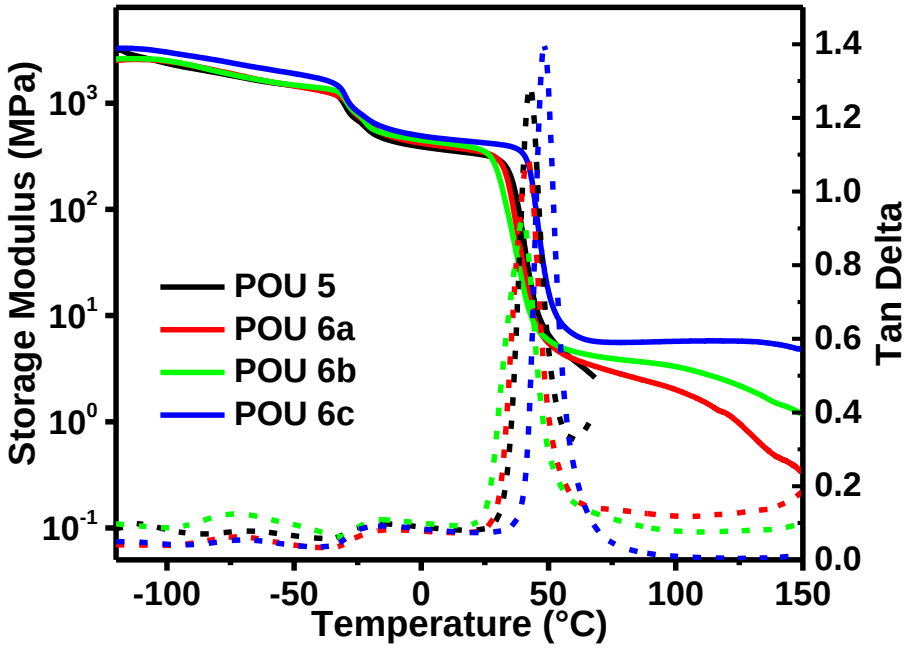


Figure S10 Dynamic mechanical analysis of POUs.

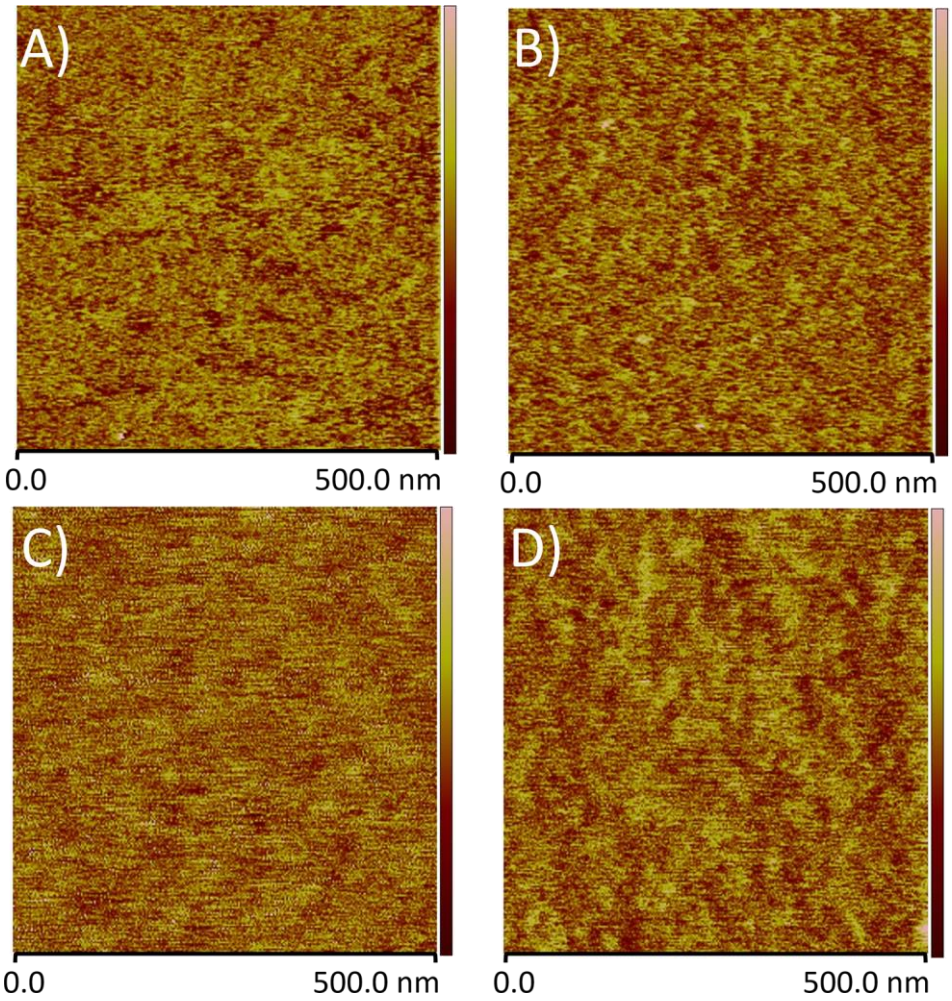


Figure S11 AFM phase images of POUs **5** (A), **6a** (B), **6b** (C) and **6c** (D).

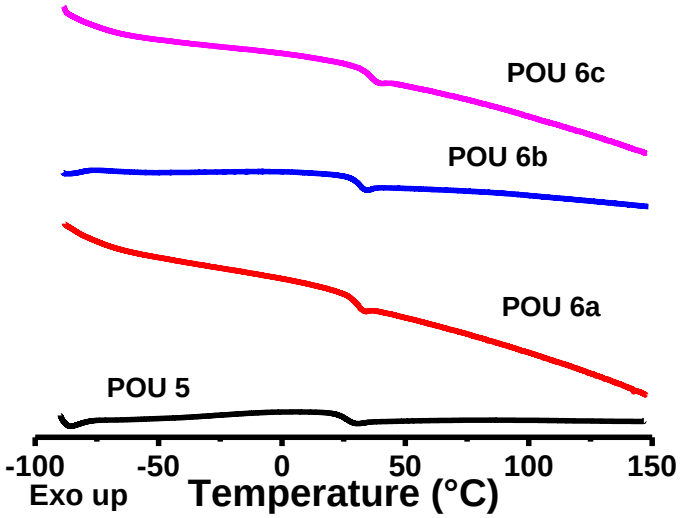


Figure S12 The second DSC heating scans of POUs at 5 ℃/min under N_2.

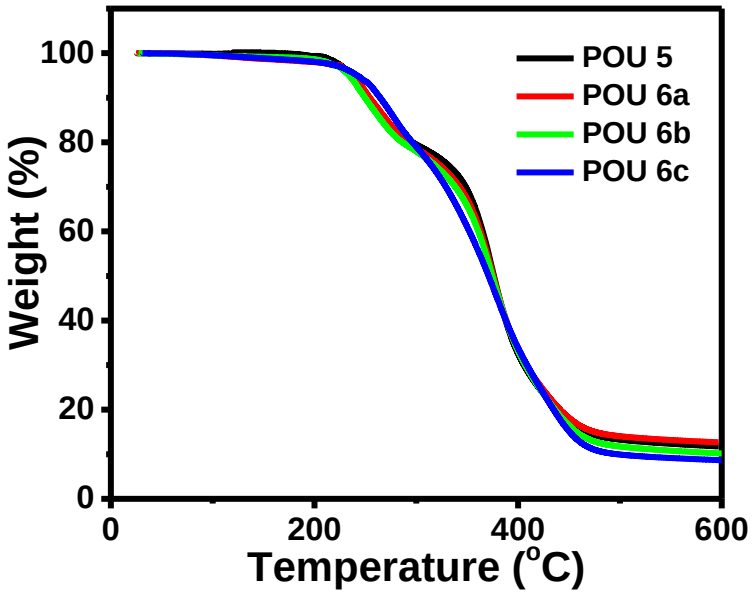


Figure S13 TGA of POUs at 10 ℃/min under N_2.

Table S2 Properties of POUs.

POUs	T_g/°C (DSC)	T_g/°C (DMA)	T_d/ °C (5%)	*SR*/%	*GF*/%	ρ/ g·mL^{-1}	*E*/MPa (100 °C)	ν/ mol·m^{-3}	M_c/ kg·mol^{-1}	T_v/°C
5	25	43	237	/	/	1.18	/	/	/	/
6a	30	42	238	246	84	1.20	2.0	216	5.6	31
6b	30	40	235	210	97	1.21	3.3	356	3.4	37
6c	35	48	242	188	99	1.18	5.7	615	1.9	48

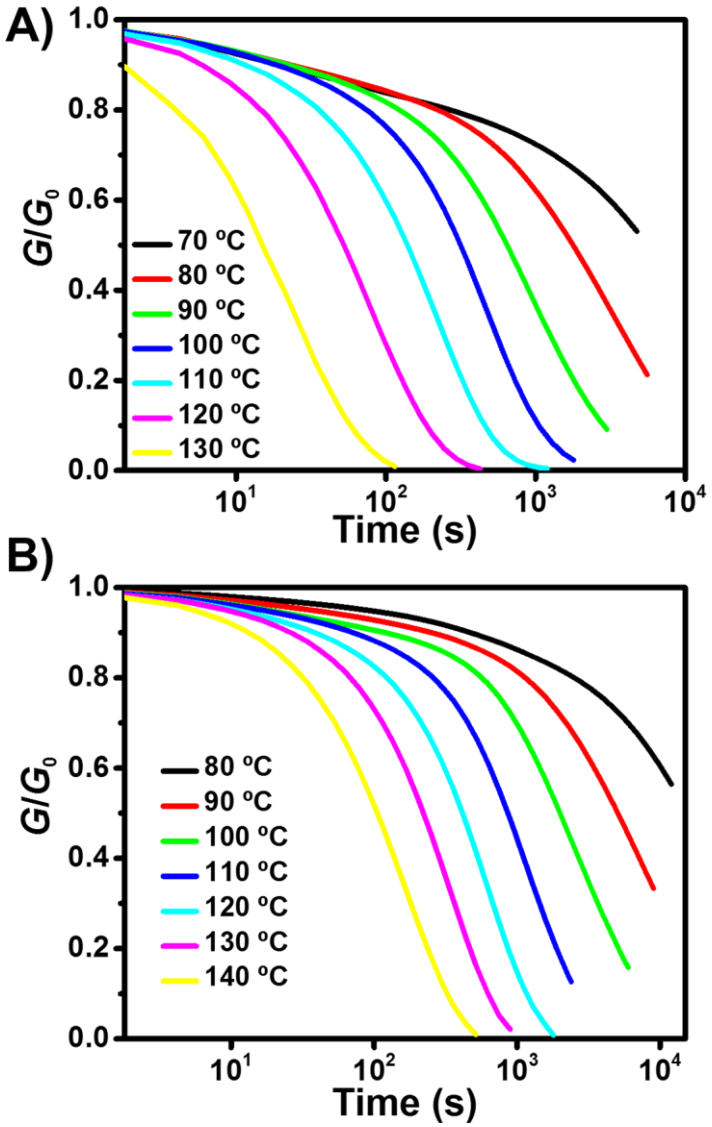


Figure S14 Normalized stress-relaxation analysis of (A) POU **6a** and (B) POU **6c**.

Freezing-transition temperature (T_v) determination:

T_v is regarded as the liquid-to-solid transition temperature, where the viscosity (η) is 10^{12} Pa·s. The values of T_v were determined using Maxwell's relation (equation 18) and Arrhenius relationship (equation 19).[6]

$$\eta = \frac{E \cdot \tau^*}{3} \quad (18)$$

$$\ln \tau^*(T) = \ln \tau_0 + E_a / RT \quad (19)$$

Where E is rubbery plateau modulus measured at 100 ºC by DMA, E_a is the Arrhenius activation energy of the oxime-enabled transcarbamoylation determined by SRA ($E_{a,\,r}$, Figure 3B).

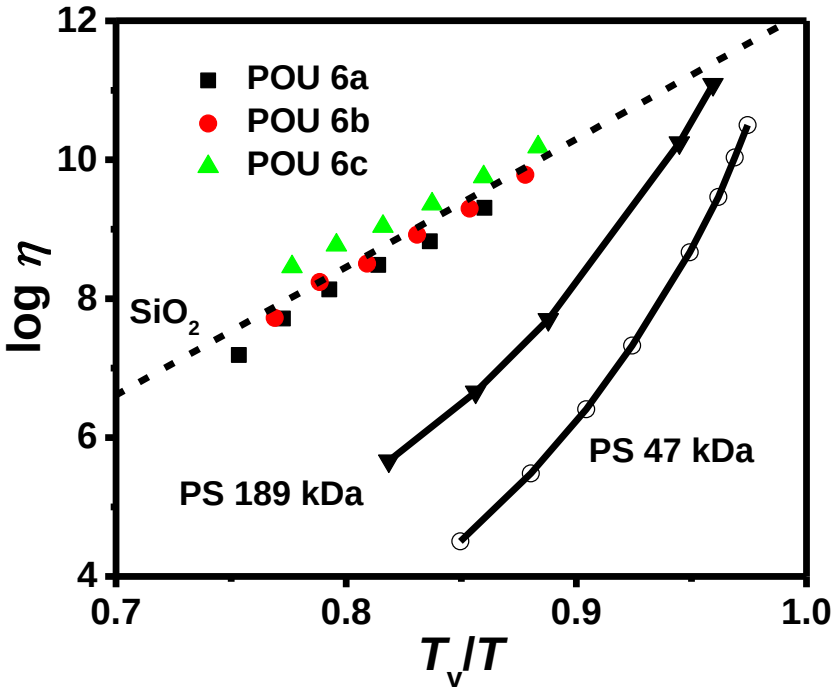


Figure S15 Angell fragility plots of the viscosity with temperature scaled by values of T_v for cross-linked POUs, polystyrene (PS)[7] and silica[8].

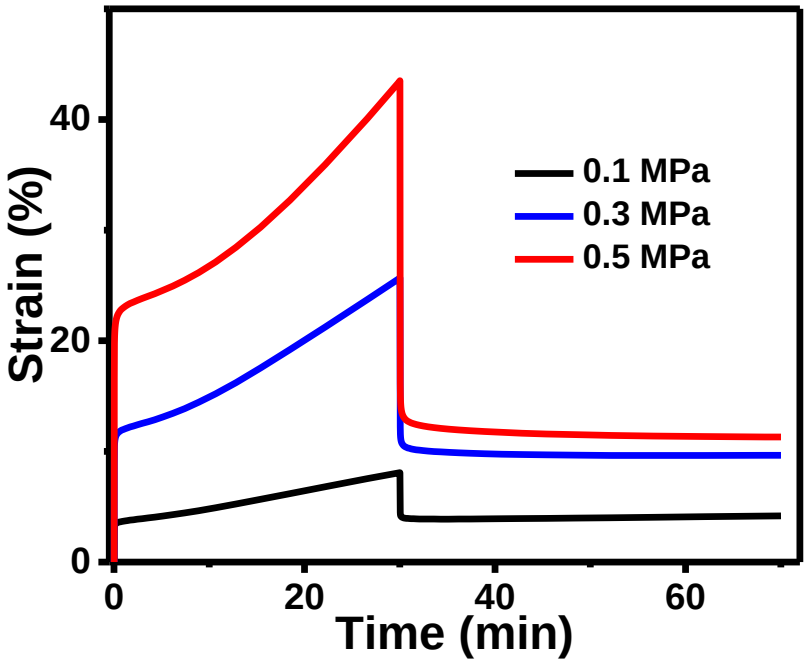


Figure S16 The creep-recovery behavior of POU **6b** at 90 °C with different stress.

Table S3 Mechanical properties of original and recycled POUs.

POUs	Young's Modulus (MPa)	Yield Stress (MPa)	Stress of break (σ_b, MPa)	Strain of break (ε_b, %)
Origin (**6b**)	262.5 ±9.5	10.2 ±0.2	49.1 ±2.2	677 ±11
Recycle 1	200.2 ±6.8	6.9 ±0.4	40.4 ±2.1	606 ±15
Recycle 2	216.0 ±9.1	9.5 ±0.9	39.4 ±2.3	606 ±12
Recycle 3	223.4 ±10.0	11.9 ±3.0	36.5 ±1.7	598 ±17
Recycle 4	220.3 ±1.7	10.0 ±1.9	33.6 ±2.1	614 ±20
Origin (**6a**)	130.2 ±1.7	5.4 ±0.6	31.6 ±2.2	672 ±6
Recycle 1	124.3 ±6.0	5.5 ±0.6	26.7 ±2.0	576 ±20
Origin (**6c**)	344.2 ±4.2	15.0 ±0.8	42.0 ±2.3	491 ±16
Recycle 1	313.9 ±10.6	14.5 ±0.5	42.2 ±1.7	430 ±14
5	77.6 ±9.1	5.9 ±0.9	13.6 ±0.6	645 ±35

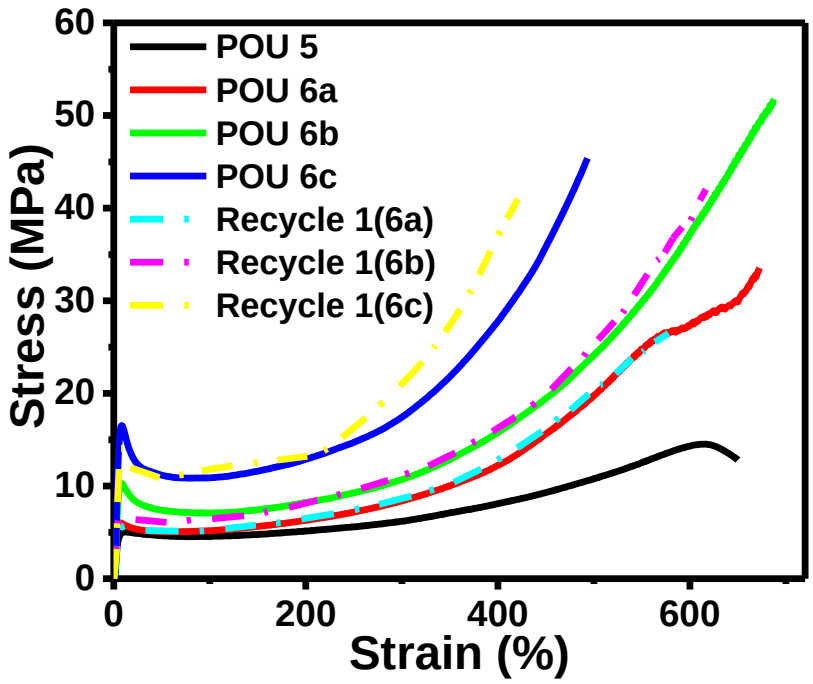


Figure S17 Stress-strain curves of the original POUs and the first recycled cross-linked samples.

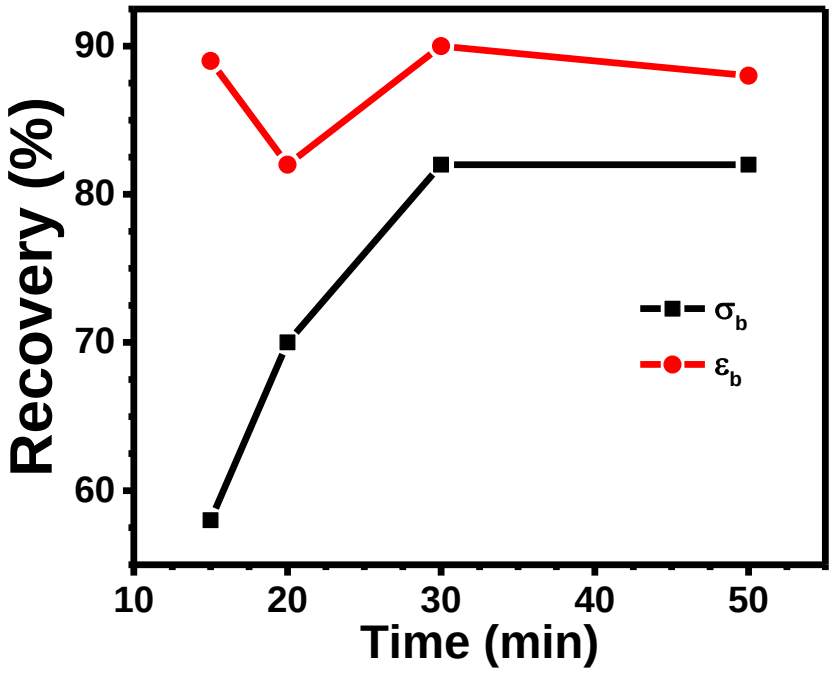


Figure S18 The recovery efficiency of the 1st recycled POU **6b** as a function of reprocessing time at 120 °C under 10 MPa measured by breaking stress (σ_b) and breaking strain (ε_b).

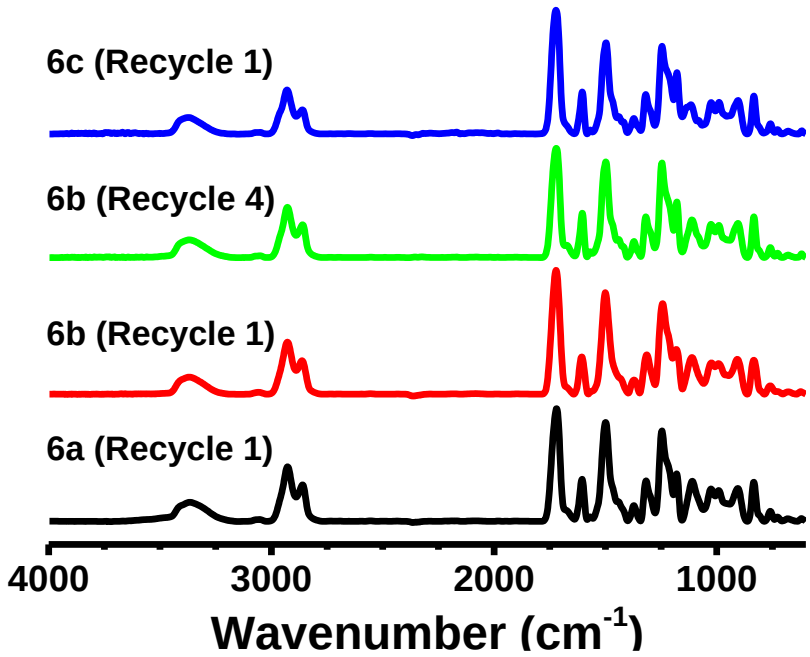


Figure S19 ATR-FTIR spectra of recycled POUs showing that no isocyanate (~ 2276 cm^{-1}) could be detected.

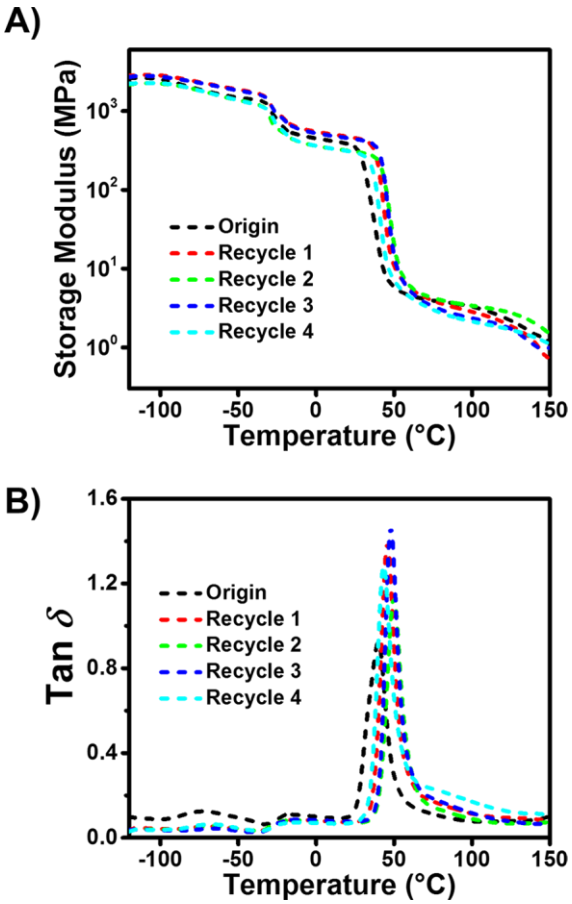


Figure S20 (A) Storage Modulus and (B) tan δ curves of recycled POU **6b** also confirming the recovery of mechanical properties. The recovery of plateau modulus further indicating that the cross-linking density is preserved via dissociative transcarbamoylation after recycle.

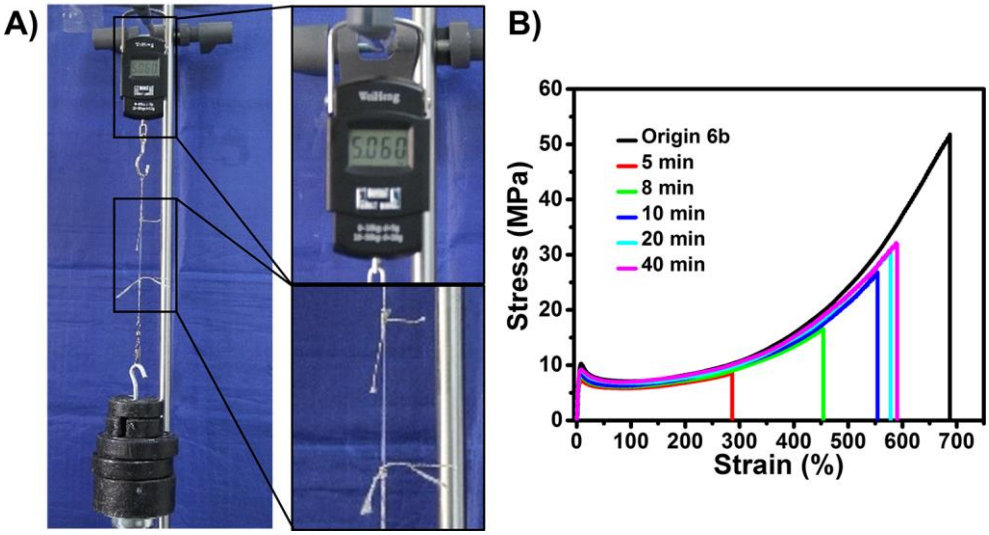


Figure S21 (A) The load-bearing test and of POU **6b** after self-healing at 120 °C for 10 min. The repaired film (32.50 mm (L) × 3.00 mm (W) × 0.60 mm (T) = 0.081 g) could withstand a weight of ~ 5 kg. (B) Stress-strain curves of **6b** with healing time at 120 °C.

7. DFT calculations: details and discussions

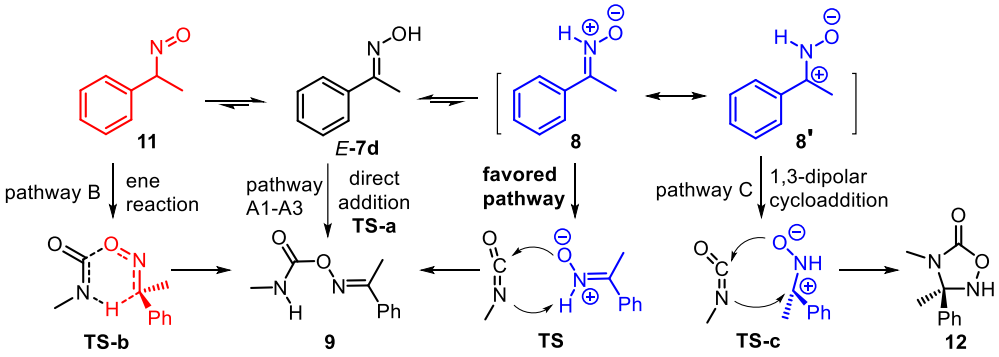
7.1 Computational methods

All calculations were performed with the Gaussian 09 program.[9] Density functional theory (DFT)[10] calculations with the B3LYP functional[11] and the 6-31G+(d) basis set[12] in *N*,*N*-dimethylacetamide (polarizable continuum (PCM) model[13]) were used to locate all the stationary points involved (referred as PCM/B3LYP/6-31+G(d) method). The vibrational frequencies were computed at the same level of theory to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point energy (*ZPE*) and the thermal corrections at 298 K (all ΔG_{sol} and ΔH_{sol} were based on these calculations, together with the mention of calculation methods). For some reactions, we also performed the gas-phase optimization and frequency calculations at the B3LYP/6-31G+(d) level (all ΔG_{gas} were based on these calculations). Intrinsic reaction coordinate (IRC) calculations[14] were used to confirm that the transition states connect the corresponding reactants and products in either the gas phase or solvent calculations. For the favored pathway, structure optimization, vibrational frequencies, and solvation energies were also calculated at the PCM/B3LYP/6-31+G(d,p) (Figures S29 and S30) and PCM/M06-2X/6-31+G(d,p) (Figures S31 and S32) level of theory[15] for comparison, showing that both methods gave similar conclusions. In this article, all discussed energies are enthalpies in *N*,*N*-dimethylacetamide (ΔH_{sol}) unless specified. The Gibbs free energies in gas phase (ΔG_{gas}) and in *N*,*N*-dimethylacetamide (ΔG_{sol}) both at 298 K are also given for reference. All figures (distances in Å) of solvation structures were prepared using CYLview.[16]

7.2 Possible pathways and their energies

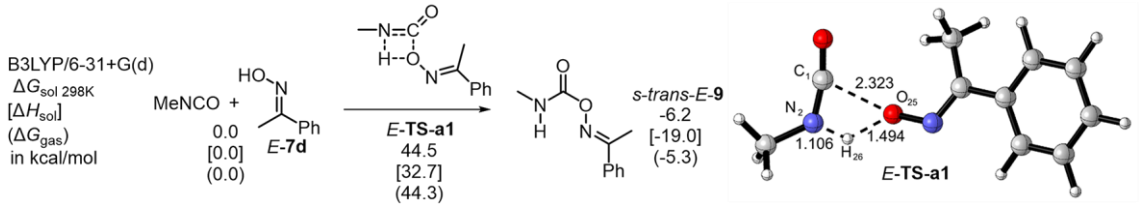
Generally, oxime (especially for ketoxime) is stable (its C=N bond has the fixed configuration) and the *cis*-*trans* isomerization requires acid or base as catalysts.[17] In our preparation process of small molecule oxime-carbamate **7bd** (Scheme S4), the *cis* product was not observed. Consequently, our proposed mechanisms (Figure 5) do not involve the *cis*-*trans* isomerization of oxime. So, herein, we used *E*-acetophenone oxime (*E*-**7d**) as a model substrate for our calculations.

Scheme S12 Possible pathways for oxime-based urethanation of *E*-**7d** and methyl isocyanate (MeNCO).



7.2.1 The direct addition of oxime to MeNCO (pathway A1-A3)

Scheme S13 DFT-calculated relative energies for the addition of one *E*-**7d** to MeNCO through concerted four-membered ring mechanism (pathway A1, Scheme S12).



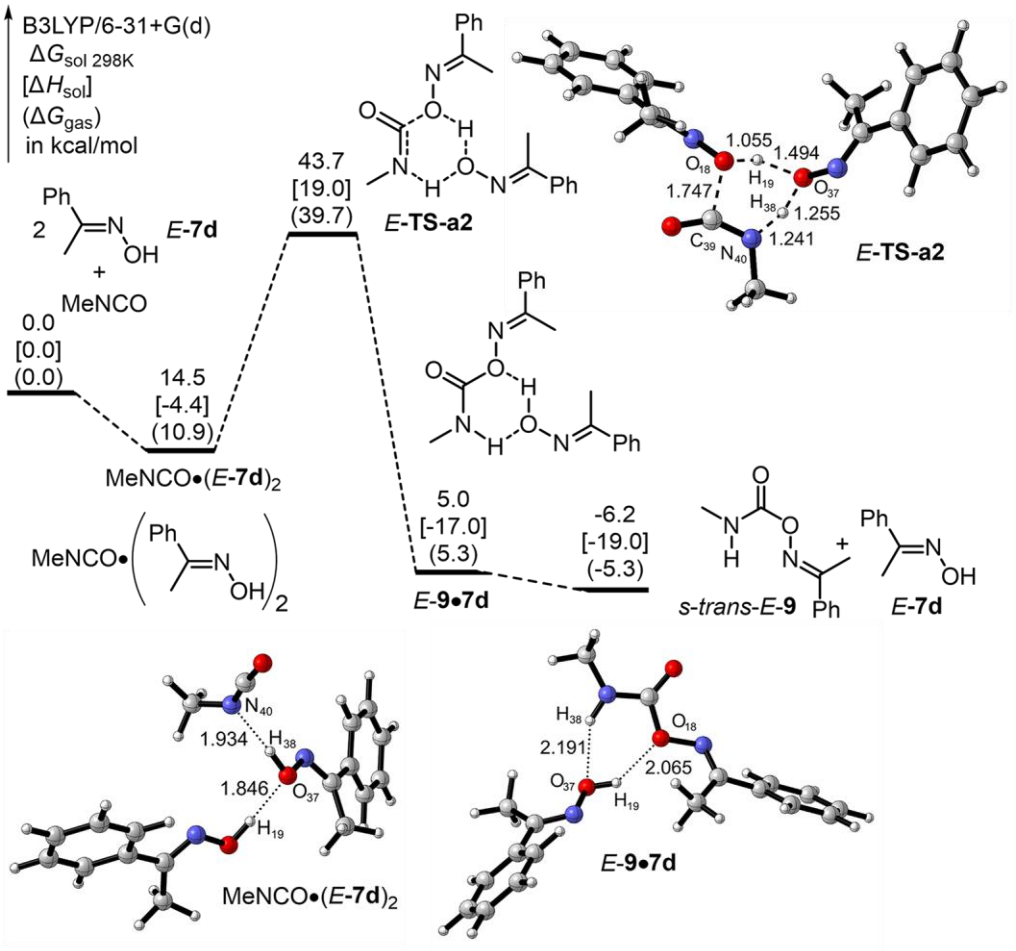


Figure S22 DFT-computed energy surface for the autocatalytic mechanism of two molecules of *E*-**7d** and MeNCO (pathway A2, Scheme S12).

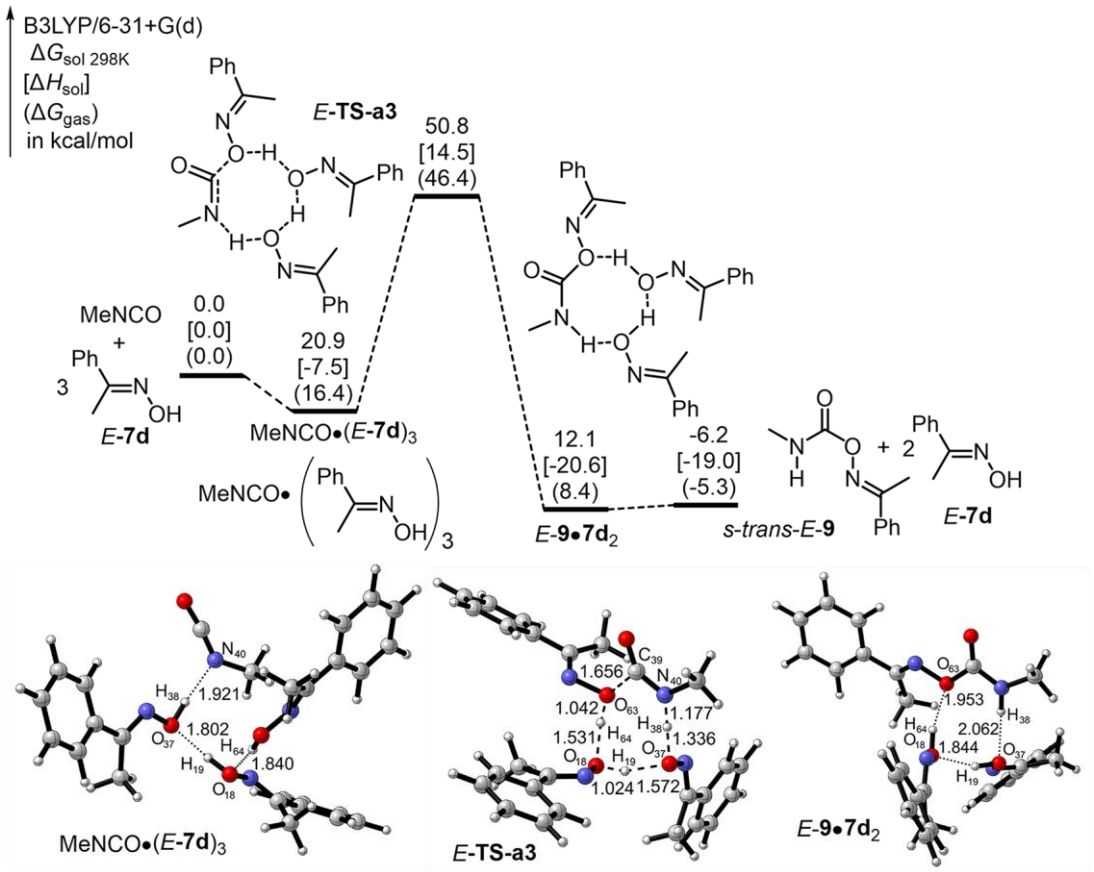


Figure S23 DFT-computed energy surface for the autocatalytic mechanism of three molecules of *E*-**7d** and MeNCO (pathway A3, Scheme S12).

7.2.2 The reaction of oxime and MeNCO through nitroso ene reaction (pathway B)

In addition to nitrone tautomer of oxime, another commonly existed tautomer, nitroso (**11**),[18] could likely yield the corresponding oxime-carbamate through ene reaction[19] (pathway B, Scheme S12). We found computationally this is not favored in terms of the high activation enthalpy (25.4 kcal·mol^{-1} from to **11**) via transition state **TS-b** (Figure S24).

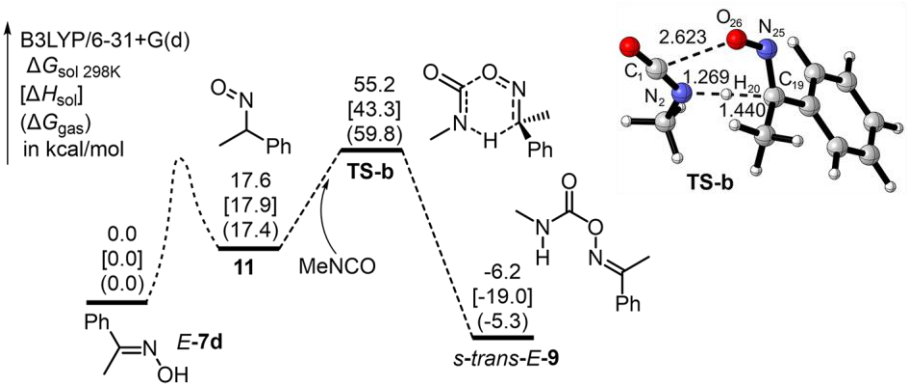


Figure S24 DFT-calculated energy surface for ene reaction of nitroso **11** and MeNCO (pathway B).

7.2.3 The reaction of oxime and MeNCO through cycloaddition reaction (pathway C)

In addition to the favored pathway discussed in the manuscript, the nitrone isomer may also react with isocyanate through stepwise 1,3-dipolar cycloaddition to give 1,2,4-oxadiazolidin-5-one **12**[20] (pathway C, Scheme S12). We found that this pathway requires relatively higher activation enthalpy via **TS-c** ($\Delta H^{\neq}$ = 11.4 kcal·mol^{-1} from *E*-**Int2**) than intramolecular hydrogen transfer transition state *E*-**TS3** to form oxime-carbamate (this is almost a barrierless process). Then, we can exclude this competitive pathway for consideration (Figure S25). This was also supported by experiment, where we did not observe this side product **12** in the oxime-urethanation reaction between octyl isocyanate **7b** and *E*-**7d** (Scheme S4).

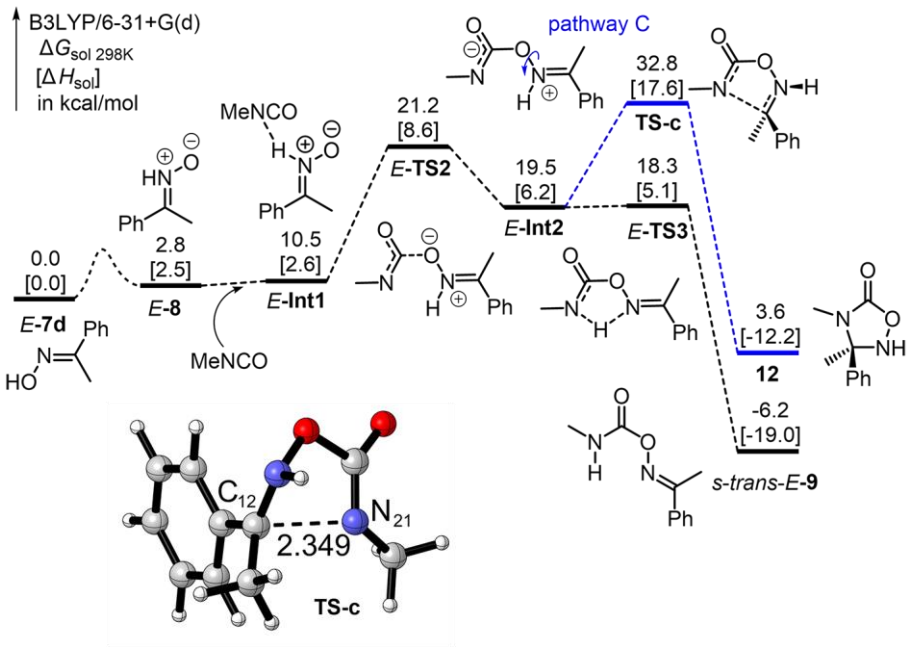
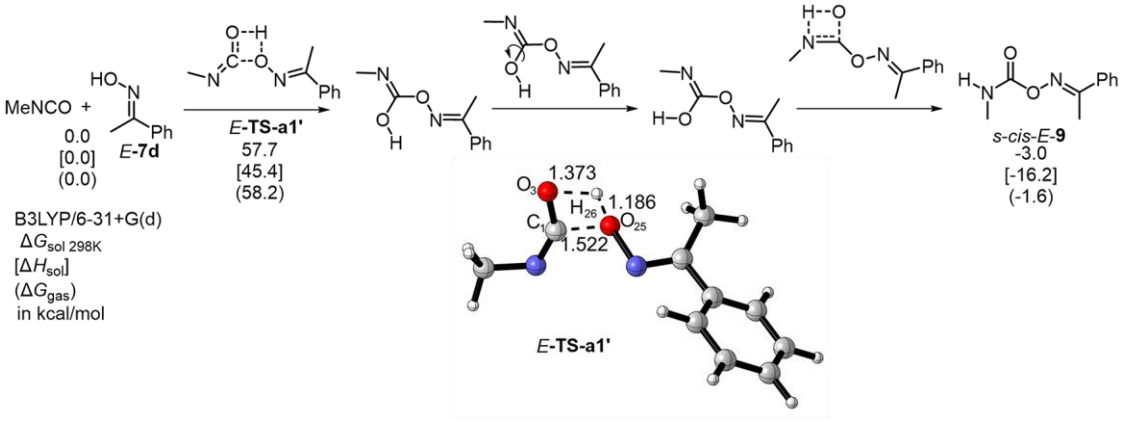


Figure S25 DFT-computed energy surface for the competitive 1,3-dipolar cycloaddition reaction of *E*-**7d** and MeNCO (pathway C; the favored pathway was also shown for comparison).

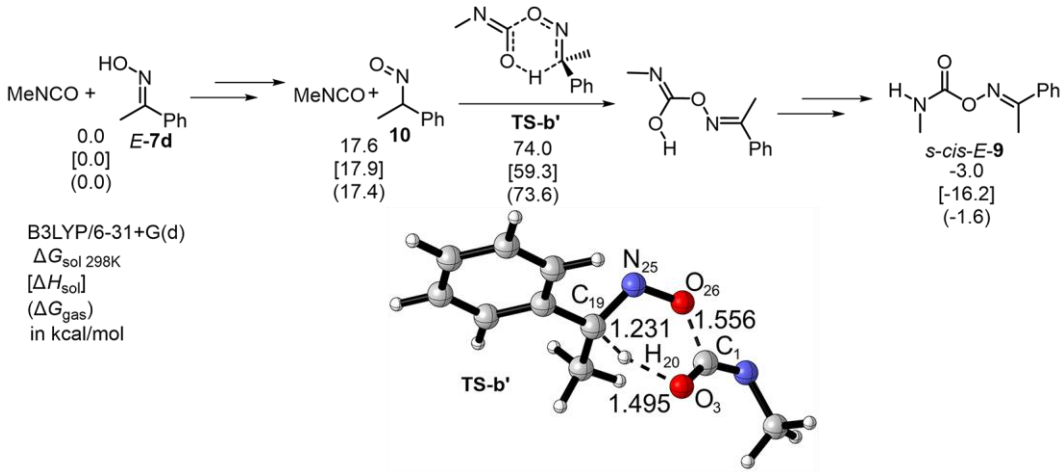
7.3 The reaction of oxime and MeNCO through C=O bond of isocyanate

In principle, the addition of *E*-acetophenone oxime across C=N bond of isocyanate gives *s-trans-E*-**9**, whereas the addition across C=O bond produces *s-cis-E*-**9**. The C=N addition process is the favored pathway in the present investigations (ref. 20 in the manuscript). We also performed calculations of C=O addition to understand why this is not favored. We found that, compared with additions of oxime to C=N bond, the C=O addition processes are all disfavored kinetically in the direct four-membered ring mechanism (Scheme S14), nitroso ene reaction (Scheme S15) and nitrone addition pathway (Figure S26).

Scheme S14 Selectively DFT-calculated relative energies for the addition of one *E*-**7d** to MeNCO through concerted four-membered ring mechanism via C=O bond (pathway A1').



Scheme S15 Selectively DFT-computed relative energies for the nitroso ene reaction via C=O bond (pathway B').



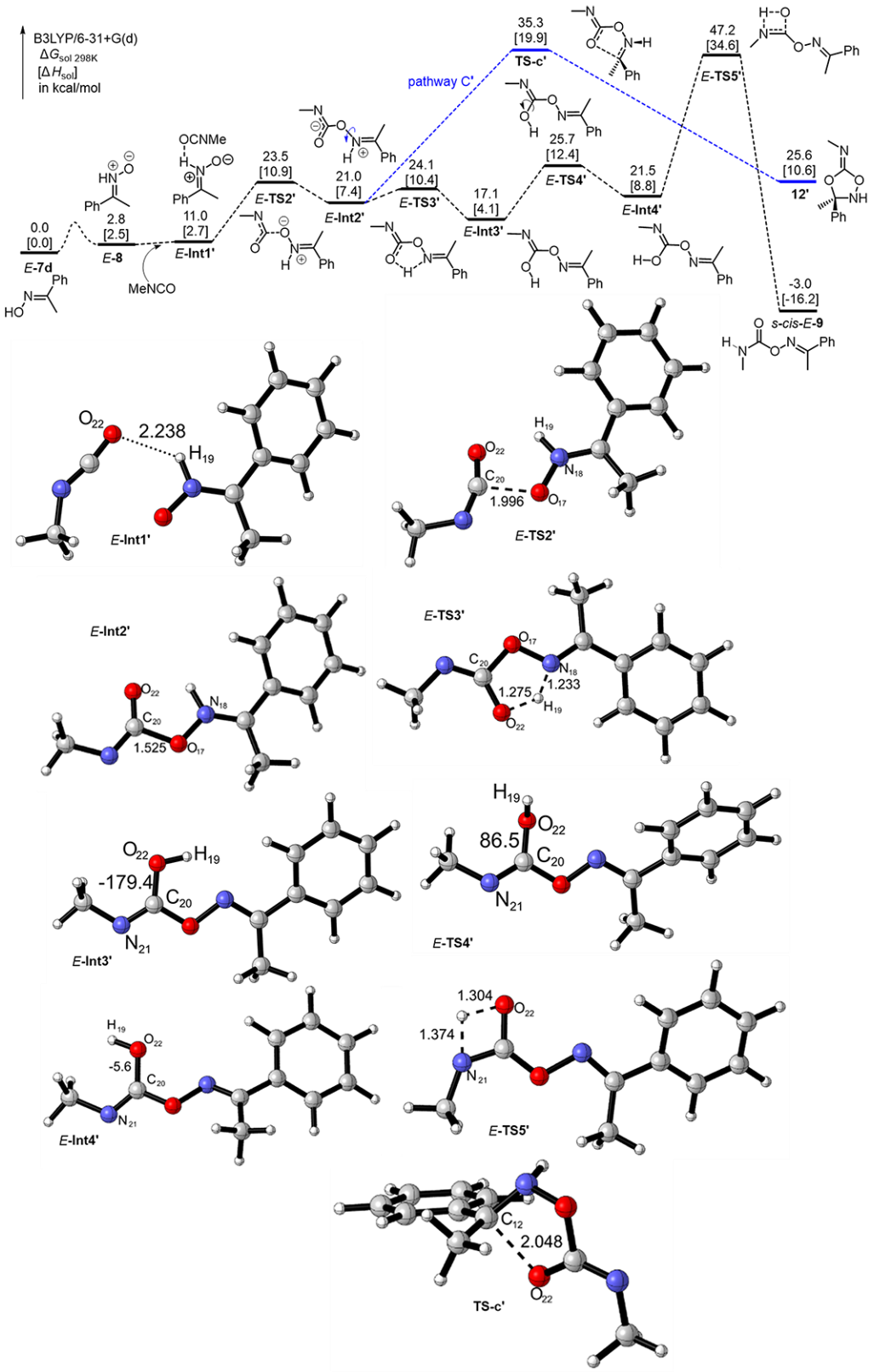
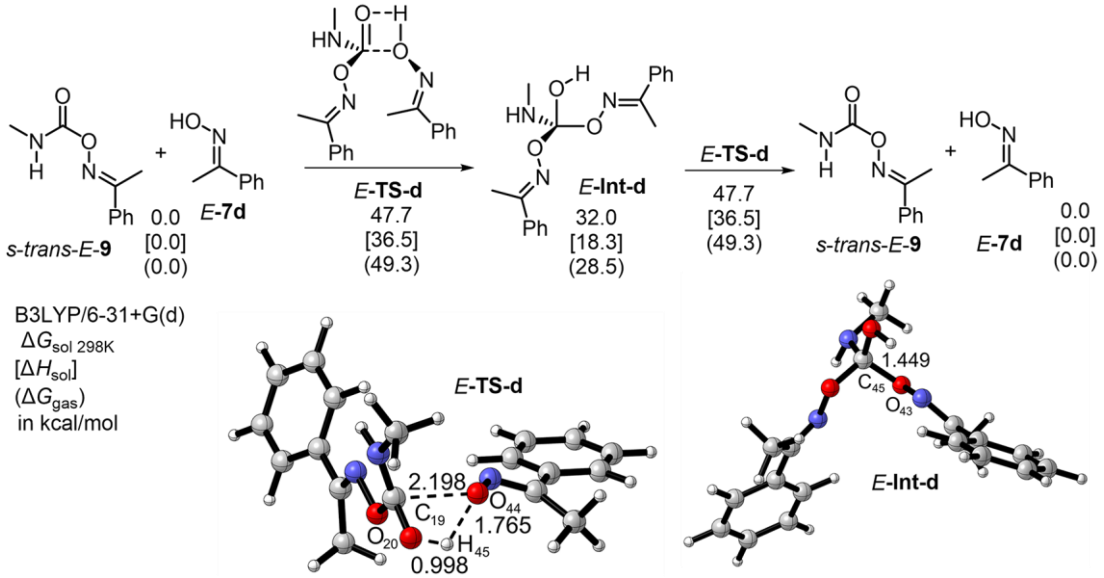


Figure S26 DFT-calculated energy surface for the pathway of nitrone nucleophilic addition/hydrogen transfer and the 1,3-dipolar cycloaddition reaction via C=O bond.

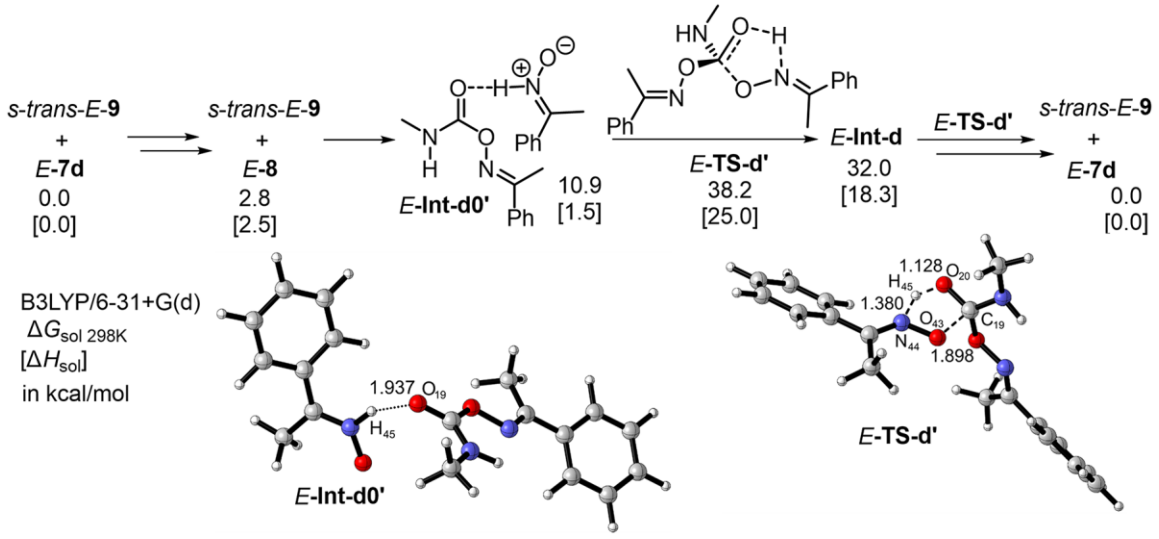
7.4 The exchange reaction of excess oxime with oxime-carbamate

There is a possibility that the generated oxime-carbamate could undergo exchange reaction with oxime (similar to hydroxyl-assisted associative transcarbamoylation, ref. 3d in the manuscript). In our experiments, we used 1:1 ratio of oxime and isocyanate and no excess of oxime existed in our systems. So, we can rule out this possibility. In addition, calculations showed that such process is not favored with an activation enthalpy of as high as 36.5 kcal·mol^{-1} (Scheme S16). Compared with the direct backward reaction of *s-trans-E*-**9** to *E*-**7d** (Figure 5B), the exchange reaction of *s-trans-E*-**9** with excess *E*-**8** is also disfavored in terms of the activation free energy of 38.2 kcal·mol^{-1} (Scheme S17).

Scheme S16 DFT-calculated relative energies for the hydroxyl-assisted associative transcarbamoylation mechanism between *s-trans-E*-**9** and *E*-**7d**.



Scheme S17 DFT-calculated relative energies for the exchange reaction of *s-trans-E*-**9** with *E*-**8** at the PCM/B3LYP/6-31+G(d,p) level.



7.5 Intramolecular tautomerism of oxime to nitrone

The intramolecular [1,3]-H shift is difficult with an activation enthalpy of as high as 48.8 kcal·mol^{-1}, suggesting this is not the pathway of isomerization (Figure S27).

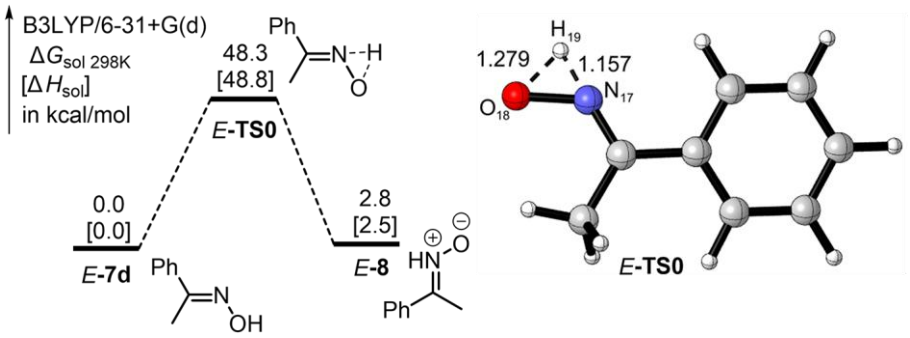


Figure S27 DFT-computed energy surface for intramolecular tautomerism mechanism of *E*-**7d** to nitrone *E*-**8**.

7.6 DFT-computed structures in Figure 5 of the manuscript

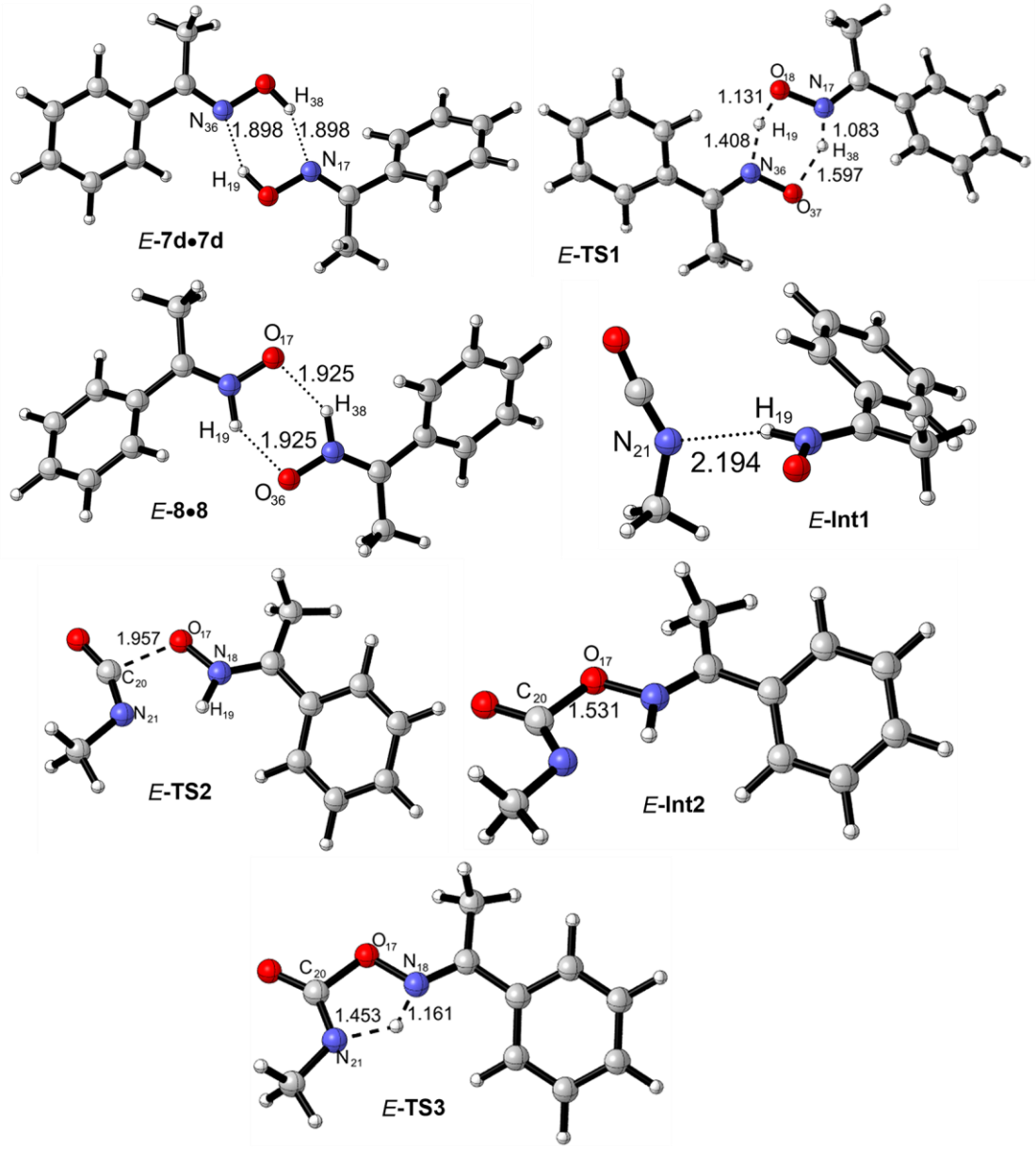


Figure S28 DFT-computed structures of transition states and intermediates in Figure 5 at the PCM/B3LYP/6-31+G(d) level.

7.7 Basis set considerations

Calculations using the B3LYP functional with a bigger basis set of 6-31+G(d,p) (Figures S29 and S30) gave similar energy surfaces with those of B3LYP/6-31+G(d) (Figure 5).

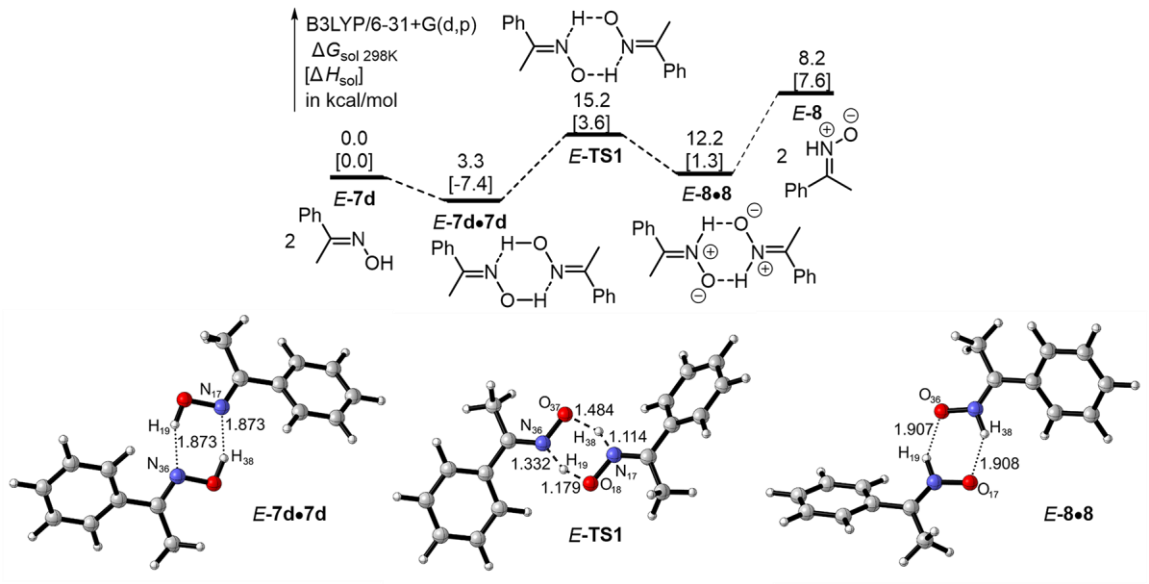


Figure S29 DFT-calculated energy surface for bimolecular tautomerism of *E*-**7d** to *E*-**8** at the PCM/B3LYP/6-31+G(d,p) level.

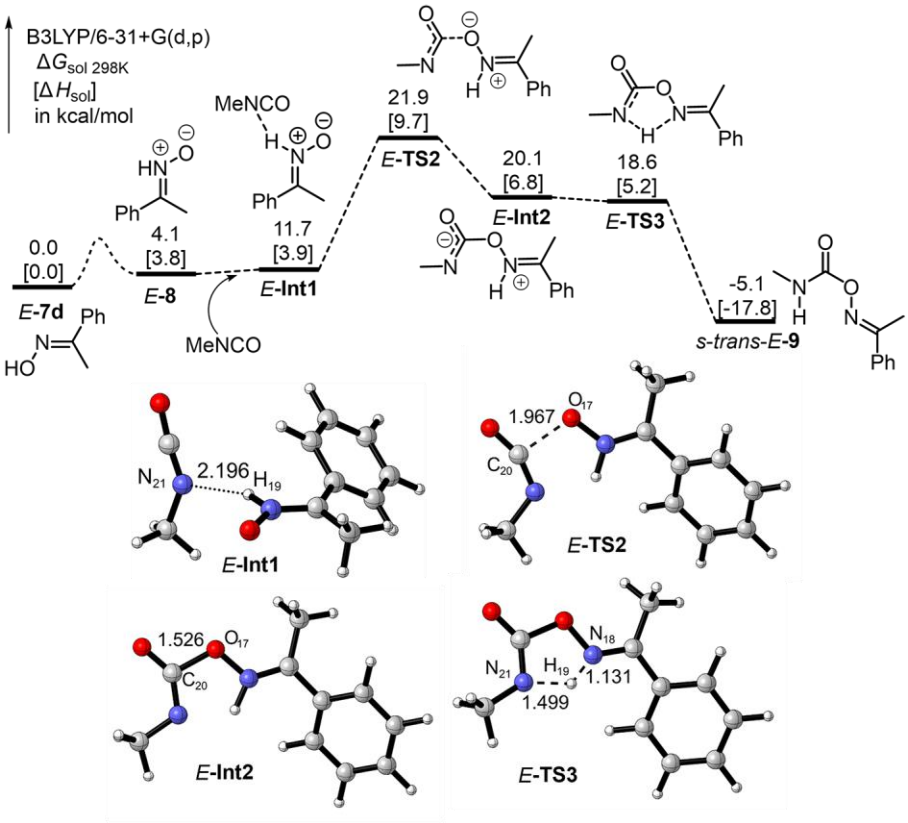


Figure S30 DFT-calculated energy surface for the favored reaction pathway between *E*-**7d** and MeNCO at the PCM/B3LYP/6-31+G(d,p) level (*E*-**TS3** is higher than intermediate *E*-**Int2** by 3.3 kcal·mol^{-1} in terms of single point energy, but with *ZPE* correction, it is lower than *E*-**Int2** by 1.6 kcal·mol^{-1}).

7.8 Density functional considerations

As for the tautomerism of *E*-**7d** to *E*-**8**, calculations using the level of M06-2X/6-31+G(d,p) showed that the proton-transfer process requires an activation enthalpy of 13.2 kcal·mol^{-1} (from *E*-**7d•7d** to *E*-**TS1**, Figure S31), that is close to that of 11.0 kcal·mol^{-1} at the level of B3LYP/6-31+G(d,p).

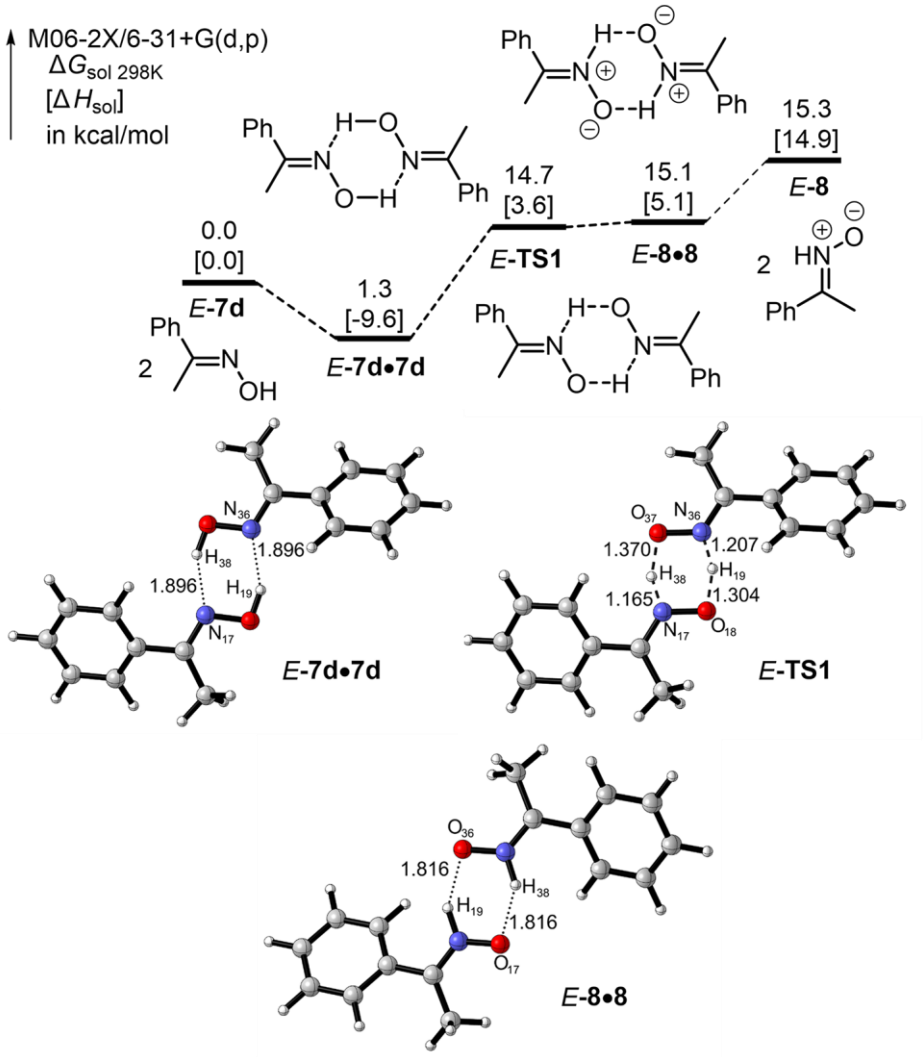


Figure S31 DFT-calculated energy surface for bimolecular tautomerism of *E*-**7d** to *E*-**8** at the PCM/M06-2X/6-31+G(d,p) level (*E*-**TS1** is higher than intermediate *E*-**8·8** by 3.8 kcal·mol^{-1} in terms of single point energy, but with *ZPE* correction, it is lower than *E*-**8·8** by 1.5 kcal·mol^{-1}).

Calculations using the level of M06-2X/6-31+G(d,p) showed that the nitrone nucleophilic addition process requires an activation enthalpy of 5.9 kcal·mol^{-1} (from *E*-**Int1** to *E*-**TS2**) and the intramolecular hydrogen transfer via *E*-**TS3** is barrierless (Figure S32). These results are close to those at the level of B3LYP/6-31+G(d,p).

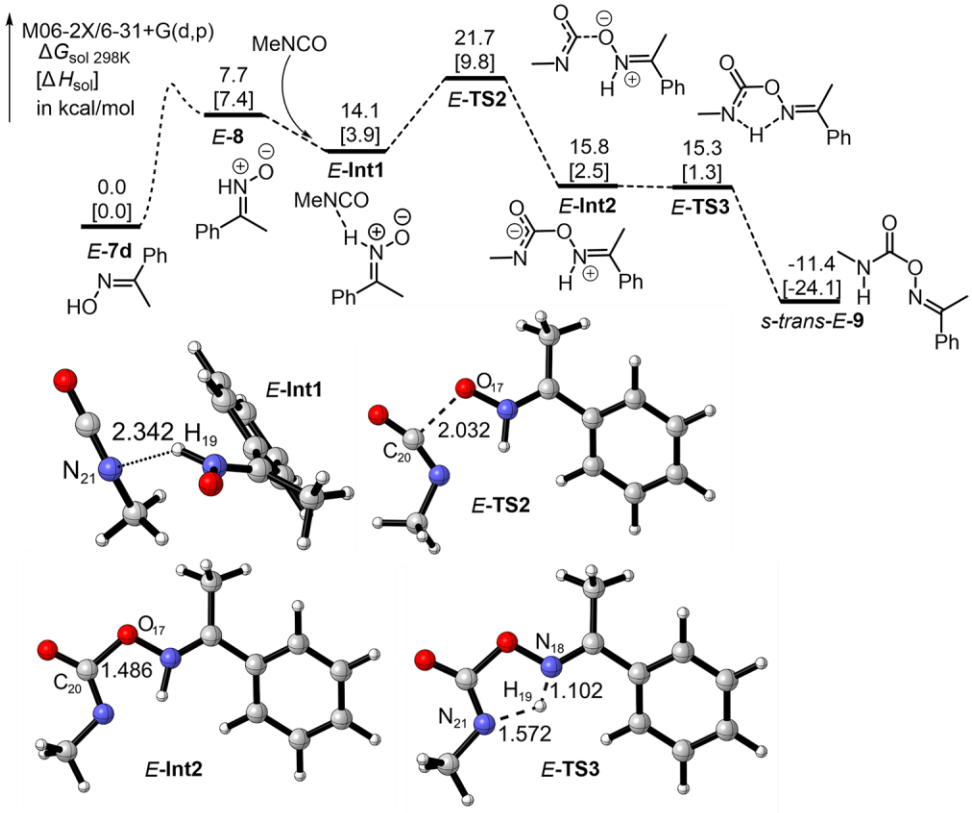


Figure S32 DFT-calculated energy surface for the favored reaction pathway between *E*-**7d** and MeNCO at the PCM/M06-2X/6-31+G(d,p) level (*E*-**TS3** is higher than intermediate *E*-**Int2** by 0.03 kcal·mol^{-1} in terms of single point energy, but with *ZPE* correction, it is lower than *E*-**Int2** by 1.2 kcal·mol^{-1}).

7.9 The reaction of MeOH and MeNCO

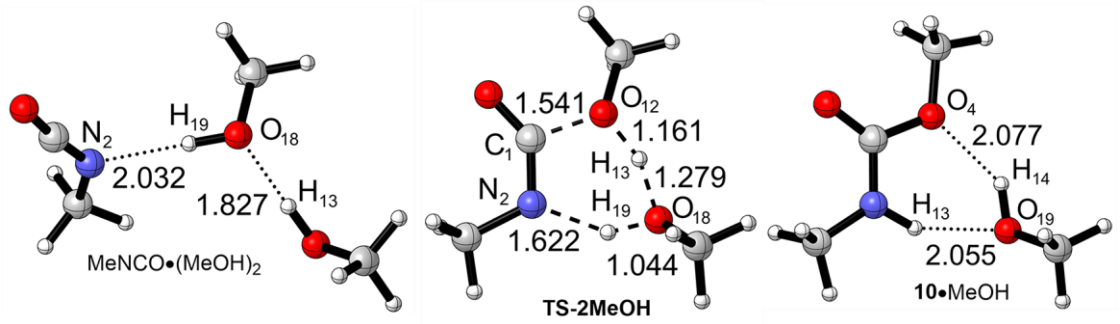
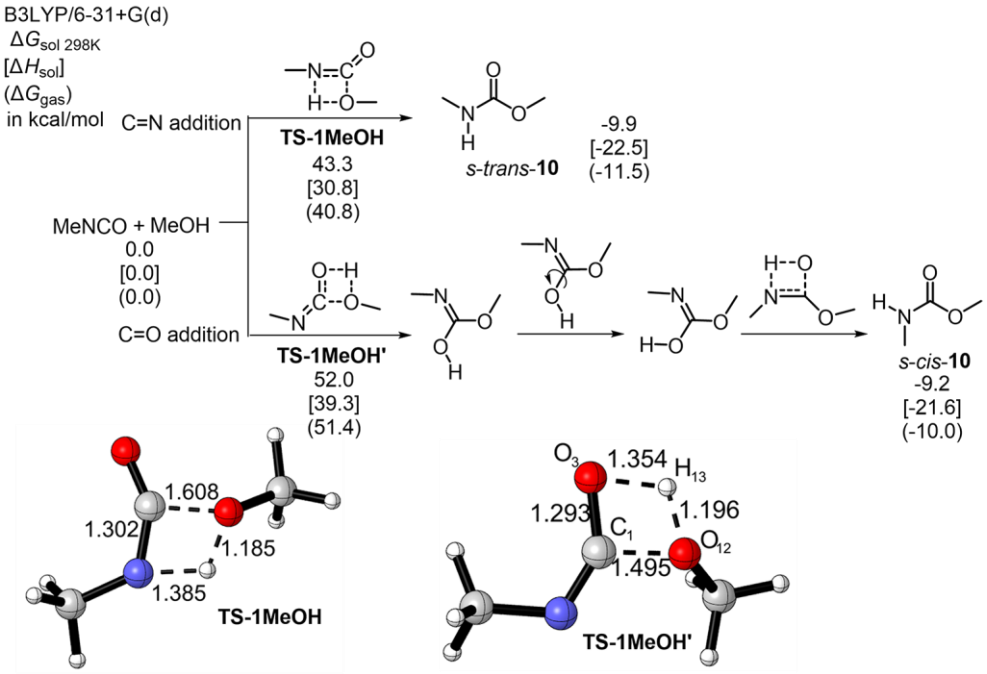


Figure S33 DFT-computed structures (in solution) of transition state and intermediates in Figure 6.

We found that the addition reaction between one MeOH and MeNCO with an activation enthalpy of 30.8 kcal·mol^{-1} and an activation free energy of 43.3 kcal·mol^{-1} is disfavored (Scheme S18) via four-membered ring transition state. If three molecules of MeOH react with MeNCO (Figure S34), the four-molecular process is entropically disfavored with an activation free energy of 37.4 kcal·mol^{-1}. Compared with 6-membered ring transition state (Figure 6), these two pathways are both disfavored.

Scheme S18 Selectively DFT-calculated relative energies for the addition of one MeOH and MeNCO through concerted four-membered ring mechanism (the disfavored C=O addition is also showed).



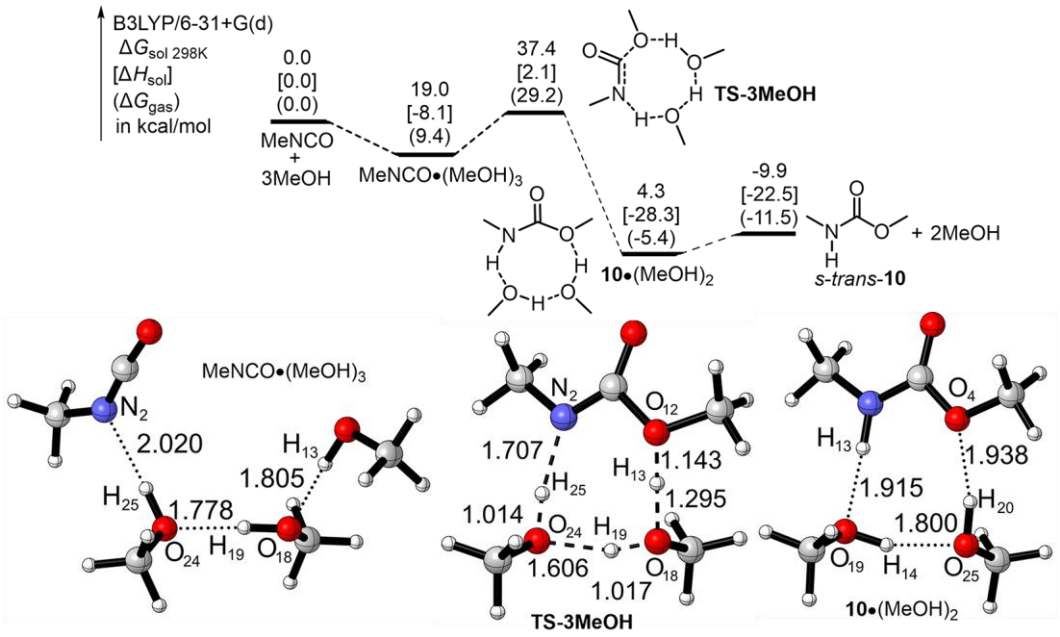
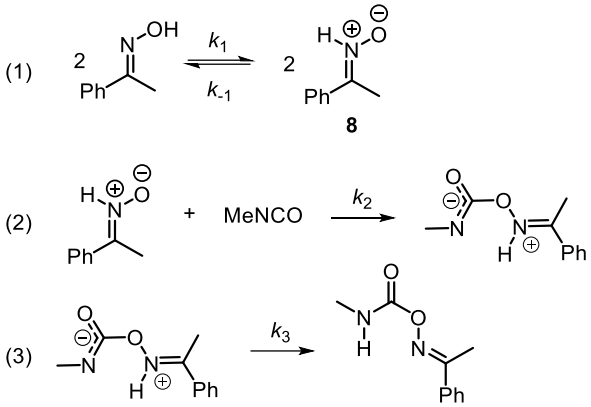


Figure S34 DFT-computed energy surface for the autocatalytic mechanism of three molecules of MeOH and MeNCO.

8. Derivation of the rate equation

Scheme S19 The simplified kinetic model for the reaction of *E*-**7d** and MeNCO.



We assume that the formation of nitrone **8** is a fast equilibrium, but the addition of nitrone to isocyanate and subsequent proton transfer are irreversible. These assumptions are reasonable according to the computed results (Figures 5, S30 and S32). Based on our proposed kinetic model (Scheme S19), the apparent bonding rate constant k_b and Arrhenius activation energy $E_{a,\,b}$ can be calculated.

With equilibrium approximation, we have:

$$k_1[oxime]^2 = k_{-1}[8]^2 \quad (20)$$

$$[8] = \sqrt{k_1 / k_{-1}}[oxime] = \sqrt{K_1^{\Theta}}[oxime] \quad (21)$$

So, we get the following second-order kinetic equation (22) for oxime-based urethanation reaction, that is consistent with the one experimentally measured (equation 5).

$$-\frac{d[NCO]}{dt} = k_2[8][NCO] = k_2\sqrt{K_1^{\Theta}}[oxime][NCO] = k_b[oxime][NCO] \quad (22)$$

Then, the apparent bonding rate constant k_b (equation 23) could be calculated according to Eyring equation (24) and equilibrium relationship (25).

$$k_b = k_2\sqrt{k_1 / k_{-1}} = k_2\sqrt{K_1^{\Theta}} \quad (23)$$

$$k_2 = \frac{k_B T}{hc^{\Theta}} e^{-\Delta G^{\neq}/RT} \quad (24)$$

$$K_1^{\Theta} = e^{-\frac{\Delta G_1^{\Theta}}{RT}} \quad (25)$$

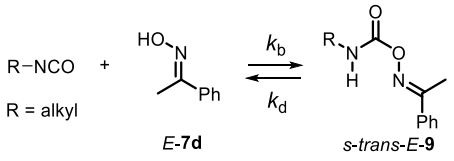
Given the relation between apparent rate constant k_b and elementary reaction rate constant (equation 23), we have the apparent Arrhenius activation energy $E_{a,\,b}$:

$$E_{a,\ b} = E_{a2} + \frac{E_{a1}}{2} - \frac{E_{a\text{-}1}}{2} \quad (26)$$

With the relationship: $E_a = \Delta H^{\neq} + RT$ (27)

$$E_{a,\ b} = \Delta H^{\neq}{}_2 + \frac{\Delta H^{\neq}{}_1}{2} - \frac{\Delta H^{\neq}{}_{-1}}{2} + RT \quad \text{(Taking } T = 338 \text{ K)} \quad (28)$$

Table S4 Kinetics and thermodynamics parameters determined from calculations and experiments.



E-**7d** *s-trans-E*-**9**

	experiment	B3LYP/ 6-31+G(d)	B3LYP/ 6-31+G(d,p)	M06-2X/ 6-31+G(d,p)
k_b10^4 ($M^{-1}\cdot s^{-1}$, 298 K)	1.6[a]	18.0	5.4	7.1
$E_{a,\,b}$ (kcal·mol^{-1})	14.4	9.3[b]	10.4[b]	10.5[b]
$\Delta H^{\neq}_b$ (kcal·mol^{-1})	13.8	8.6[c]	9.7[c]	9.8[c]
$\Delta G^{\neq}_b$ (kcal·mol^{-1})	22.6[d]	21.2[c]	21.9[c]	21.7[c]
$\Delta H^{\neq}_d$ (kcal·mol^{-1})	27.2	27.6[e]	27.5[e]	33.9[e]
$\Delta G^{\neq}_d$ (kcal·mol^{-1})	24.5[d]	27.4[e]	27.0[e]	33.1[e]
ΔH_b (kcal·mol^{-1})	-25.8	-19.0[f]	-17.8[f]	-24.1[f]
ΔG_b (kcal·mol^{-1})	-9.7[g]	-6.1[f]	-5.1[f]	-11.5[f]

[a] Extrapolation from linear regression in Figure 1C. [b] Taking T = 338 K. [c] From MeNCO and *E*-**7d** to *E*-**TS2**. [d] $\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq}$ (T = 298 K) [e] From *s-trans-E*-**9** to *E*-**TS2**. [f] Solvation energies in DMSO were calculated. [g] $\Delta G = \Delta H - T\Delta S$ (T = 298 K).

9. Experiments to exclude the possibility of imine exchange of oxime

The high stability of oximes makes these units inert to realize self-healing or malleable functions in bulk networks through dynamic imine chemistry, as proved by Kuhl and co-workers in aldoxime cross-linked methacrylates system (ref. 9b in the manuscript). Considering the more stable ketoximes in POUs, we could exclude the possibility of imine exchange of oxime in our systems. In addition, experiments were conducted to further verify our proposal.

Scheme S20 The highly thermal stability of oxime ethers.

The mixture of two oxime ethers[21] **S1** (0.247 g, 0.87 mmol) and **S2** (0.208 g, 0.87 mmol) was heated at 120 °C for 12 h and then at 140 °C for 12 h under nitrogen atmosphere. It was found that neither new methylene peak nor m/z corresponding to exchange product could be detected by ^{1}H NMR spectroscopy (Figure S35) and ESI-HRMS (Figure S36), suggesting that the imine exchange of ketoximes can be negligible under 140 °C.

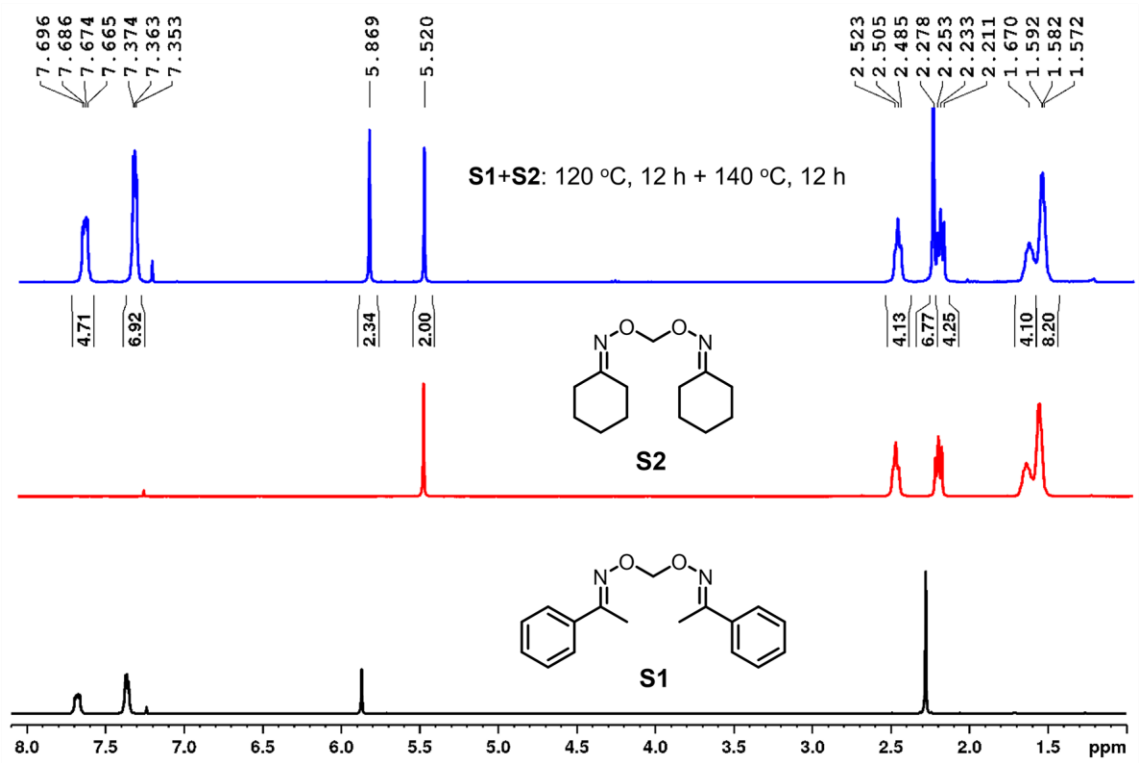
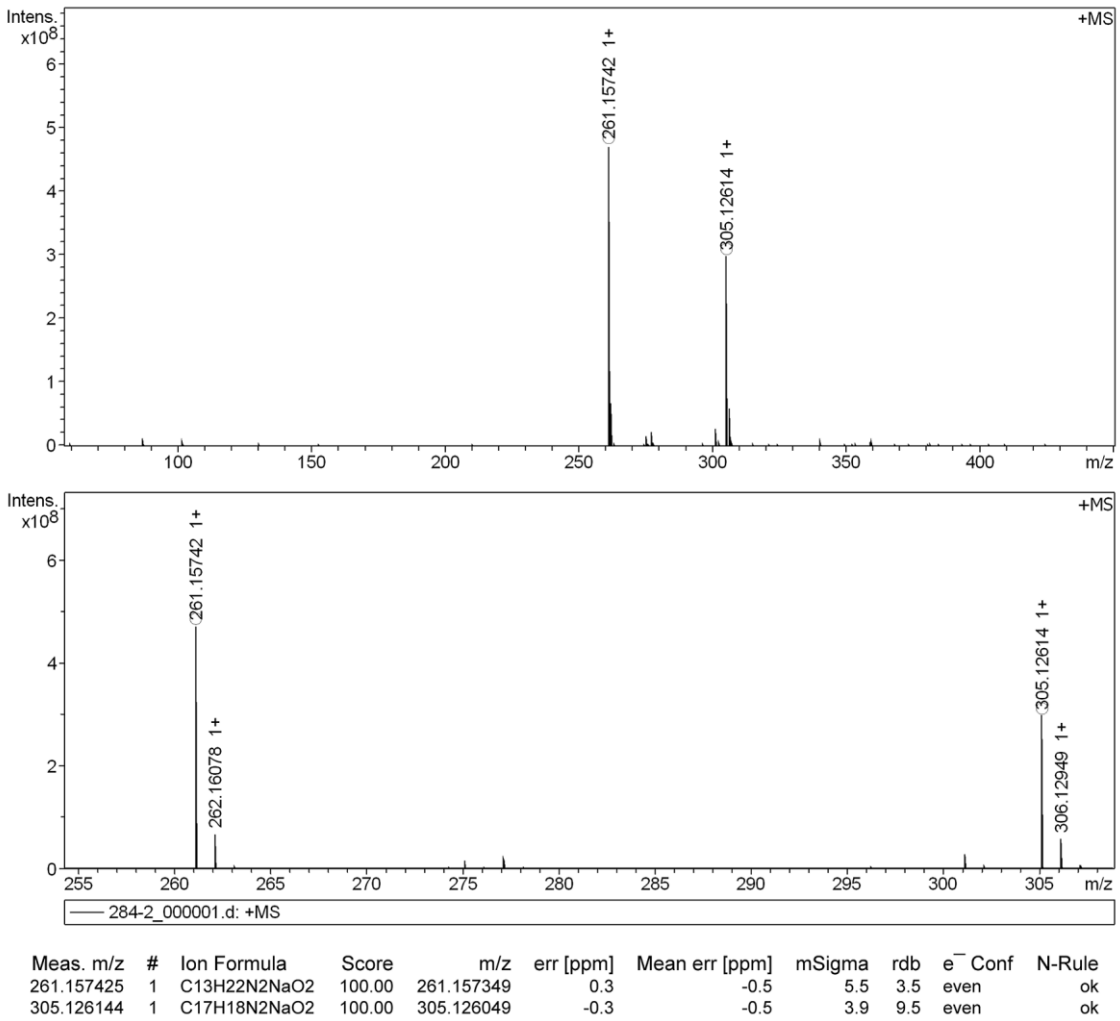


Figure S35 ^{1}H NMR spectra of **S1**, **S2** and the mixture of the two oxime ethers after heat treatments (120 °C, 12 h; then 140 °C, 12 h).



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
261.157425	1	C13H22N2NaO2	100.00	261.157349	0.3	-0.5	5.5	3.5	even	ok
305.126144	1	C17H18N2NaO2	100.00	305.126049	-0.3	-0.5	3.9	9.5	even	ok

Figure S36 ESI-HRMS for the mixture of the oxime ethers (**S1** and **S2**) after heat treatments (120 ^{o}C, 12 h; then 140 ^{o}C, 12 h).

10. Computed energies and the Cartesian coordinates (Å) in DMAc

Table S5 Sum of electronic and thermal Enthalpies (*H*, in Hartree), Sum of electronic and thermal Free Energies (*G*, in Hartree), SCF energy (*E*, in Hartree), Zero-point correction (*ZPE*, in Hartree), Thermal correction to Enthalpy (*TCH*, in Hartree) and Thermal correction to Gibbs Free Energy (*TCG*, in Hartree) at the B3LYP/6-31+G(d) level of theory.

Name	H_{sol}	G_{sol}	E_{sol}	ZPE_{sol}	TCH_{sol}	TCG_{sol}
MeNCO	-207.947881	-207.980435	-208.004147	0.050625	0.056266	0.023713
E-**7d**	-440.058728	-440.103457	-440.222999	0.154169	0.164270	0.119542
E-**TS-a1**	-647.954495	-648.012904	-648.172697	0.202956	0.218203	0.159793
s-trans-E-**9**	-648.036815	-648.093834	-648.260656	0.209049	0.223841	0.166822
E-**TS-a1'**	-647.934196	-647.991865	-648.151314	0.202282	0.217118	0.159449

s-cis-E-**9**	-648.032432	-648.088713	-648.256374	0.209219	0.223942	0.167661
MeNCO•(*E*-**7d**)$_2$	-1088.072340	-1088.164267	-1088.461956	0.362346	0.389616	0.297689
E-**TS-a2**	-1088.035099	-1088.117632	-1088.417640	0.357365	0.382540	0.300008
E-**9•7d**	-1088.092394	-1088.179393	-1088.482720	0.364316	0.390326	0.303327
MeNCO•(*E*-**7d**)$_3$	-1528.136061	-1528.257459	-1528.692214	0.517721	0.556153	0.434755
E-**TS-a3**	-1528.100914	-1528.209798	-1528.649844	0.513331	0.548930	0.440047
E-**9•7d**$_2$	-1528.156923	-1528.271536	-1528.714148	0.520352	0.557225	0.442612
11	-440.030276	-440.075463	-440.194056	0.153703	0.163781	0.118594
TS-b	-647.937533	-647.995873	-648.153818	0.200955	0.216284	0.157945
TS-b'	-647.912057	-647.966038	-648.128581	0.202545	0.216523	0.162543
E-**TS0**	-439.980955	-440.026505	-440.139138	0.147907	0.158183	0.112633
E-**8**	-440.054796	-440.099059	-440.220042	0.155389	0.165246	0.120983
E-**7d•7d**	-880.129377	-880.201158	-880.460503	0.310573	0.331127	0.259346
E-**TS1**	-880.109806	-880.179993	-880.434905	0.305166	0.325098	0.254912
E-**8•8**	-880.118946	-880.190573	-880.451245	0.311894	0.332299	0.260672
E-**Int1**	-648.002508	-648.067146	-648.225877	0.206699	0.223369	0.158731
E-**TS2**	-647.992855	-648.050115	-648.214650	0.207015	0.221796	0.164536
E-**Int2**	-647.996707	-648.052839	-648.219504	0.208175	0.222797	0.166665
E-**TS3**	-647.998436	-648.054795	-648.217070	0.204158	0.218633	0.162275
TS-c	-647.978512	-648.031565	-648.200682	0.208570	0.222170	0.169118
12	-648.025987	-648.078089	-648.251258	0.212039	0.225271	0.173169
E-**Int1'**	-648.002371	-648.066303	-648.225866	0.206915	0.223495	0.159563
E-**TS2'**	-647.989265	-648.046453	-648.211293	0.207191	0.222028	0.164841
E-**Int2'**	-647.994790	-648.050422	-648.218072	0.208785	0.223282	0.167650
E-**TS3'**	-647.990084	-648.045488	-648.208624	0.204303	0.218540	0.163136
E-**Int3'**	-648.000150	-648.056698	-648.223055	0.208260	0.222906	0.166357
E-**TS4'**	-647.986779	-648.042928	-648.207880	0.206599	0.221101	0.164952
E-**Int4'**	-647.992559	-648.049610	-648.215181	0.207810	0.222622	0.165571
E-**TS5'**	-647.951425	-648.008714	-648.169380	0.203330	0.217955	0.160666
TS-c'	-647.974958	-648.027635	-648.197375	0.209039	0.222417	0.169740
12'	-647.989751	-648.043020	-648.214355	0.211167	0.224604	0.171336
E-**TS-d**	-1088.037301	-1088.121250	-1088.424642	0.362328	0.387342	0.303393
E-**Int-d0'**	-1088.093117	-1088.179852	-1088.484157	0.365185	0.391039	0.304305
E-**TS-d'**	-1088.055763	-1088.136386	-1088.440953	0.360890	0.385191	0.304568
E-**Int-d**	-1088.066386	-1088.146323	-1088.456313	0.365694	0.389926	0.309990
MeOH	-115.676017	-115.703098	-115.731393	0.051083	0.055376	0.028295
TS-1MeOH	-323.574791	-323.614502	-323.684072	0.101004	0.109281	0.069570
s-trans-**10**	-323.659685	-323.699253	-323.775628	0.107679	0.115943	0.076375
TS-1MeOH'	-323.561224	-323.600732	-323.670723	0.101387	0.109499	0.069991
s-cis-**10**	-323.658346	-323.698119	-323.774209	0.107552	0.115863	0.076090
MeNCO•(MeOH)$_2$	-439.306393	-439.364558	-439.478817	0.157891	0.172424	0.114259

TS-2MeOH	-439.283526	-439.330900	-439.450506	0.155532	0.166980	0.119605
10•MeOH	-439.337042	-439.390767	-439.510803	0.160620	0.173760	0.120035
MeNCO•$(MeOH)_3$	-554.988899	-555.059495	-555.219321	0.211335	0.230423	0.159826
TS-3MeOH	-554.972530	-555.030192	-555.198398	0.210387	0.225868	0.168206
10•$(MeOH)_2$	-555.021092	-555.082845	-555.253495	0.215544	0.232402	0.170650

Table S6 Sum of electronic and thermal Enthalpies (*H*, in Hartree), sum of electronic and thermal Free Energies (*G*, in Hartree), SCF energy (*E*, in Hartree), Zero-point correction (*ZPE*, in Hartree), Thermal correction to Enthalpy (*TCH*, in Hartree) and Thermal correction to Gibbs Free Energy (*TCG*, in Hartree) at the B3LYP/6-31+G(d,p) level of theory for the favored reaction pathway.

Name	H_{sol}	G_{sol}	E_{sol}	ZPE_{sol}	TCH_{sol}	TCG_{sol}
E-**7d**	-440.076203	-440.120901	-440.240224	0.153912	0.164021	0.119323
E-**7d•7d**	-880.164255	-880.236526	-880.494646	0.309763	0.330391	0.258120
E-**TS1**	-880.146603	-880.217590	-880.470044	0.303384	0.323441	0.252454
E-**8•8**	-880.150270	-880.222336	-880.481522	0.310761	0.331251	0.259186
E-**8**	-440.070194	-440.114444	-440.235067	0.155012	0.164873	0.120623
MeNCO	-207.951928	-207.984493	-208.007990	0.050416	0.056062	0.023497
E-**Int1**	-648.021960	-648.086789	-648.244711	0.206043	0.222751	0.157922
E-**TS2**	-648.012665	-648.070476	-648.233763	0.206231	0.221099	0.163287
E-**Int2**	-648.017256	-648.073359	-648.239095	0.207204	0.221838	0.165736
E-**TS3**	-648.019898	-648.075820	-648.238454	0.204176	0.218556	0.162634
s-trans-E-**9**	-648.056550	-648.113487	-648.279842	0.208506	0.223292	0.166354

Table S7 Sum of electronic and thermal Enthalpies (*H*, in Hartree), sum of electronic and thermal Free Energies (*G*, in Hartree), SCF energy (*E*, in Hartree), Zero-point correction (*ZPE*, in Hartree), Thermal correction to Enthalpy (*TCH*, in Hartree) and Thermal correction to Gibbs Free Energy (*TCG*, in Hartree) at the M06-2X/6-31+G(d,p) level of theory for the favored reaction pathway.

Name	H_{sol}	G_{sol}	E_{sol}	ZPE_{sol}	TCH_{sol}	TCG_{sol}
E-**7d**	-439.873877	-439.918222	-440.039517	0.155649	0.165640	0.121295
E-**7d•7d**	-879.763075	-879.834370	-880.096691	0.313158	0.333616	0.262322
E-**TS1**	-879.742086	-879.812952	-880.067312	0.305093	0.325226	0.254360
E-**8•8**	-879.739642	-879.812366	-880.073346	0.313229	0.333704	0.260980
E-**8**	-439.862031	-439.906006	-440.028437	0.156645	0.166405	0.122431
MeNCO	-207.855456	-207.888398	-207.912132	0.050955	0.056676	0.023734
E-**Int1**	-647.723139	-647.784072	-647.948029	0.208756	0.224889	0.163957
E-**TS2**	-647.713698	-647.771963	-647.936863	0.208211	0.223165	0.164901
E-**Int2**	-647.725302	-647.781406	-647.948824	0.208977	0.223522	0.167418
E-**TS3**	-647.727228	-647.782270	-647.948772	0.207505	0.221544	0.166501
s-trans-E-**9**	-647.767695	-647.824833	-647.993265	0.210835	0.225570	0.168432

The Cartesian coordinates (Å) in DMAc at the B3LYP/6-31+G(d) level of theory (Table S5)

MeNCO

C	0.73908200	-0.04983000	-0.00004600
N	-0.41362700	-0.37930000	0.00002400
O	1.91299500	0.13919200	0.00001900
C	-1.75633700	0.16063100	0.00000400
H	-2.46872700	-0.66670000	0.00000500
H	-1.91820700	0.77177600	0.89369800
H	-1.91810800	0.77168500	-0.89376700

E-**7d**

C	-1.26465000	0.19262700	0.06229700
C	0.21755400	0.05777700	0.03770700
C	0.83819600	-1.18735600	0.25644500
C	1.02821400	1.17814400	-0.21923200
C	2.22762600	-1.30729400	0.20995900
H	0.22759700	-2.05783600	0.47658000
C	2.41967500	1.05432600	-0.26995100
H	0.57561900	2.14933500	-0.39705800
C	3.02507800	-0.18720600	-0.05479800
H	2.68983000	-2.27501700	0.38960000
H	3.02859300	1.93072200	-0.47799000
H	4.10772200	-0.28149600	-0.08669000
C	-1.91933800	1.49468700	0.44305000
H	-1.23053000	2.14428800	0.98672700
H	-2.26696700	2.02953700	-0.45096800
H	-2.79745600	1.30702300	1.06833500
N	-1.92755000	-0.85976600	-0.27866400
O	-3.32439800	-0.64846000	-0.23153100
H	-3.68050700	-1.51474100	-0.49850100

E-**TS-a1**

C	3.35694000	0.51973400	-0.38952600
N	3.67750200	-0.67624300	-0.14575300
O	3.27657100	1.62411700	-0.75433900
C	4.93480400	-1.35277900	-0.52585200
H	4.67486800	-2.26024300	-1.07459100
H	5.53892700	-0.69495600	-1.15202400
H	5.47654800	-1.60751500	0.38779600
C	-0.45371600	0.40010800	0.53986100
C	-1.85160500	0.05576600	0.16828300
C	-2.33675500	-1.26773400	0.25116000
C	-2.73885200	1.05311900	-0.28210300
C	-3.64698800	-1.57772500	-0.11083000
H	-1.67757300	-2.05242000	0.60937600
C	-4.05330600	0.74048000	-0.64577300
H	-2.40372700	2.08288400	-0.36174200
C	-4.51584700	-0.57522000	-0.56347700
H	-3.99556700	-2.60519900	-0.03289400
H	-4.71389300	1.53098800	-0.99475600
H	-5.53816700	-0.81833200	-0.84278100
C	-0.06899000	1.83947700	0.77242300
H	0.06181400	2.38238600	-0.17365900
H	-0.84028800	2.36763300	1.34449700
H	0.87563600	1.88532500	1.31922300
N	0.38573400	-0.58723700	0.63743500
O	1.66261300	-0.28889100	0.97806900
H	2.83118800	-1.05935800	0.45493800

s-trans-E-**9**

O	-1.82756900	0.99747600	-0.05617800
N	-0.63311400	0.22050800	0.01074800
C	0.41569800	0.95909000	-0.12563700
C	1.71262900	0.23058200	-0.06875800
C	2.86730000	0.87906100	0.40450200
C	1.80642100	-1.11626200	-0.46853000
C	4.08110400	0.19212600	0.49194200
H	2.82110600	1.91644300	0.72251400
C	3.02165500	-1.79651800	-0.38723900
H	0.92842300	-1.62230500	-0.85828400
C	4.16332300	-1.14614500	0.09622800
H	4.96184500	0.70568200	0.86925900
H	3.07951900	-2.83335900	-0.70913200
H	5.10992500	-1.67723300	0.15764200
C	0.38064800	2.45256500	-0.30988000
H	-0.45449900	2.73943000	-0.95420200
H	0.23683200	2.95449500	0.65619700
H	1.31074600	2.81638200	-0.75046300
C	-2.99651300	0.26121600	0.02897300
O	-4.04755900	0.88991200	-0.02435700

N	-2.87413600	-1.06869400	0.16477000
H	-1.94194900	-1.46304000	0.19261100
C	-4.03750300	-1.94289700	0.22958500
H	-3.68005600	-2.96819100	0.34502700
H	-4.67444600	-1.69091000	1.08423300
H	-4.63425400	-1.87610300	-0.68685900

***E*-TS-a1'**

C	-3.05636400	0.01874000	0.09787300
N	-3.29745300	-0.77949500	-0.83733000
O	-3.52120500	0.46553300	1.21222600
C	-4.52206400	-1.57874600	-0.74371600
H	-4.78680700	-1.83472100	0.29068600
H	-5.36412400	-1.03372200	-1.19016300
H	-4.38231500	-2.50370700	-1.31101900
C	0.46396600	0.90334500	0.00070800
C	1.77735400	0.20385400	0.01420400
C	1.92880300	-1.01061300	0.70987100
C	2.87830400	0.73690900	-0.67973700
C	3.15364700	-1.67881300	0.70459700
H	1.09176200	-1.41641700	1.26962400
C	4.09907500	0.05869200	-0.68986300
H	2.78422100	1.66737600	-1.23100600
C	4.24142800	-1.14815000	0.00234000
H	3.26041800	-2.60976100	1.25545500
H	4.93913600	0.47614400	-1.23884700
H	5.19571400	-1.66875000	-0.00007700
C	0.37566000	2.40273000	0.02120300
H	1.34106000	2.86285300	-0.19044000
H	-0.36611000	2.76543900	-0.69710500
H	0.06210500	2.73579000	1.01953400
N	-0.55257300	0.10707500	-0.00390100
O	-1.79861700	0.87484100	0.05993600
H	-2.30515500	1.09574000	1.10980400

***s-cis-E*-9**

O	-1.87914500	0.11788100	0.01143700
N	-0.54364900	-0.35661500	-0.08226700
C	0.29058200	0.60061000	0.14975300
C	1.72614000	0.21315000	0.07032000
C	2.69050900	1.14713800	-0.34857100
C	2.14287500	-1.09146000	0.39691600
C	4.03505000	0.78072300	-0.45303700
H	2.39399300	2.15855800	-0.61086800
C	3.48731000	-1.45174900	0.29891200
H	1.41184600	-1.81609200	0.74248400
C	4.43867800	-0.51802000	-0.12867400
H	4.76585900	1.51272500	-0.78763600
H	3.79365300	-2.46042500	0.56507000
H	5.48633500	-0.79921400	-0.20162300
C	-0.10862300	2.01814200	0.46362500
H	-0.91581900	2.02811900	1.20252500
H	0.73285700	2.59165400	0.85574100
H	-0.48572000	2.52130000	-0.43603300
C	-2.82371900	-0.88171700	-0.12076100
O	-2.57524900	-2.07588900	-0.20435700
N	-4.05944300	-0.33272800	-0.13750900
C	-4.38613100	1.08487900	-0.01363900
H	-5.46905300	1.18276300	-0.11531200
H	-4.08702100	1.48605900	0.96127600
H	-3.90580500	1.67275100	-0.80213200
H	-4.82036800	-0.99890000	-0.18077200

MeNCO•(***E*-7d**)$_2$

C	-2.93234500	-1.67277700	0.08920000
C	-4.26162800	-1.02011600	-0.05875500
C	-4.57315700	0.16339900	0.63818600
C	-5.23319200	-1.57170500	-0.91367600
C	-5.81454800	0.77997000	0.47555700
H	-3.84242000	0.59005300	1.31886500
C	-6.47421000	-0.94973300	-1.07891300
H	-5.01735800	-2.48140300	-1.46717600
C	-6.77067300	0.22748800	-0.38532400
H	-6.03963000	1.68836200	1.02944600
H	-7.20824600	-1.38744700	-1.75112600
H	-7.73848600	0.70737100	-0.50858600
C	-2.77858700	-3.16175500	-0.08066800
H	-3.73762400	-3.67648400	0.01060100
H	-2.35018800	-3.40129400	-1.06326300
H	-2.09133800	-3.55807500	0.67340200
N	-1.94449200	-0.88473900	0.34939500
O	-0.72396500	-1.56682500	0.47218500

H	-0.08618200	-0.84285000	0.66376900
C	3.09247200	-0.36468900	0.78725300
C	4.42125500	-0.46324400	0.12094200
C	4.98874600	0.63892400	-0.54763500
C	5.13441600	-1.67498200	0.14672800
C	6.22745400	0.52590700	-1.17925800
H	4.46177900	1.58808600	-0.55931600
C	6.37321200	-1.78698100	-0.49144900
H	4.71991600	-2.54062900	0.65475100
C	6.92475500	-0.68831900	-1.15646600
H	6.65388600	1.38991900	-1.68319300
H	6.90561600	-2.73457100	-0.46620900
H	7.89091300	-0.77368600	-1.64763800
C	2.74526700	-1.29630200	1.91822800
H	2.32391700	-2.23489000	1.53399200
H	3.63615400	-1.54673200	2.50048100
H	2.00446200	-0.84300600	2.58068600
N	2.30015700	0.53777800	0.31799400
O	1.04895800	0.57673400	0.98400100
H	0.61514400	1.36439200	0.58222100
C	-0.30645100	3.86279200	0.29875400
N	-0.26006300	2.82888600	-0.32962000
O	-0.29353900	4.80499900	1.01110100
C	-0.69874100	2.42749100	-1.66791800
H	-1.25544000	1.49168000	-1.58241700
H	-1.33256500	3.19545100	-2.11761500
H	0.18257000	2.26081400	-2.29306900

***E*-TS-a2**

C	2.72802700	-0.10305200	0.73968500
C	3.97287900	-0.79396100	0.29833600
C	4.03222900	-1.46409300	-0.93889000
C	5.11290000	-0.78261700	1.12130400
C	5.20667500	-2.09792200	-1.34329100
H	3.15295600	-1.49988300	-1.57425300
C	6.29017000	-1.41167600	0.70806800
H	5.09258800	-0.27341900	2.07964200
C	6.34128700	-2.07089300	-0.52336900
H	5.23450800	-2.61963200	-2.29653600
H	7.16564200	-1.38676100	1.35180100
H	7.25563600	-2.56614500	-0.84039300
C	2.48007800	0.10437400	2.20615500
H	2.71510300	-0.81359400	2.75439900
H	3.13535400	0.89426900	2.59174600
H	1.44718900	0.38979300	2.40336400
N	1.94754500	0.25839500	-0.22468600
O	0.74456500	0.90721400	0.26296800
H	-0.01926800	0.66326200	-0.42253200
C	-2.89078200	-0.51999100	-0.89509000
C	-4.16354100	-0.84626000	-0.19394600
C	-5.04405600	0.16878100	0.23038300
C	-4.50856000	-2.18418900	0.07191100
C	-6.22247300	-0.14552600	0.90804400
H	-4.80478200	1.20571900	0.01515900
C	-5.68792500	-2.49718000	0.75487500
H	-3.84861500	-2.98865600	-0.24016300
C	-6.54992800	-1.48060700	1.17606000
H	-6.89153100	0.65283400	1.22057600
H	-5.93043000	-3.53769700	0.95709200
H	-7.46967500	-1.72408800	1.70235700
C	-2.25195900	-1.51953300	-1.82419900
H	-1.47148300	-2.09433300	-1.30638500
H	-2.98561100	-2.22678000	-2.21910600
H	-1.76950500	-0.99969200	-2.65639300
N	-2.38045600	0.63966300	-0.64050000
O	-1.18732600	0.90263200	-1.32258200
H	-0.84526500	2.05894100	-0.97489500
C	0.87313700	2.64671700	0.16408900
N	-0.18933900	2.98714300	-0.47677000
O	1.85756500	3.04422500	0.70772300
C	-0.46544100	4.41649800	-0.68048900
H	-0.59843400	4.92851000	0.27870800
H	0.34602000	4.89913500	-1.23645700
H	-1.38937100	4.49602100	-1.25673400

***E*-9•7d**

C	2.61519300	-0.42819300	0.35356300
C	3.88303900	-1.13384600	0.01167500
C	4.61459800	-0.76299900	-1.13251900
C	4.37549700	-2.17099200	0.82402600
C	5.81151400	-1.40737900	-1.44967100
H	4.23184800	0.01944900	-1.78075400

C	5.57768200	-2.80837000	0.50772400
H	3.83720000	-2.47284200	1.71736500
C	6.29884100	-2.43079000	-0.62937600
H	6.35883500	-1.11550700	-2.34256700
H	5.94954200	-3.60100100	1.15213500
H	7.22974700	-2.93441000	-0.87796800
C	1.44919600	-1.18653500	0.92459200
H	0.80650500	-1.54046000	0.10639700
H	1.78280600	-2.06850400	1.47456500
H	0.84519700	-0.55839900	1.58358400
N	2.62298900	0.83380100	0.08485500
O	1.33101300	1.41392200	0.30129200
H	-0.33127300	0.71555500	-0.70540500
C	-3.31022200	0.25362500	-0.83216000
C	-4.31599200	-0.66853200	-0.23743200
C	-4.12624800	-1.21762400	1.04535100
C	-5.47232400	-1.02083800	-0.95657200
C	-5.06183100	-2.10008900	1.58708300
H	-3.24952000	-0.93816400	1.62187100
C	-6.40512600	-1.90915100	-0.41385500
H	-5.64167200	-0.61722000	-1.95079400
C	-6.20483600	-2.45156900	0.85908400
H	-4.90292500	-2.50654800	2.58301400
H	-7.28864600	-2.17603000	-0.98859400
H	-6.93486200	-3.13649600	1.28332900
C	-3.71717600	1.32687300	-1.80750400
H	-3.39712000	1.06750900	-2.82523700
H	-4.79817100	1.47786200	-1.81053600
H	-3.23092300	2.27358100	-1.55000100
N	-2.08946300	0.05810300	-0.46521100
O	-1.19903200	0.97714400	-1.06787300
H	-0.55609300	2.78415900	-0.00865400
C	1.40344600	2.78063300	0.57379000
N	0.19514300	3.34370100	0.38356200
O	2.41309300	3.34312600	0.96303100
C	-0.04873300	4.74888000	0.68152000
H	0.17081000	4.97076000	1.73138700
H	0.56207300	5.40129100	0.04740800
H	-1.10374200	4.95400700	0.48949800

MeNCO•(*E*-**7d**)$_3$

C	-2.13783100	-2.46991200	-1.08853800
C	-3.35044900	-3.07133000	-0.46590700
C	-3.26193900	-3.83558400	0.71388000
C	-4.61508300	-2.88309400	-1.05177200
C	-4.40597800	-4.38467800	1.29330000
H	-2.29100000	-4.00762000	1.16819700
C	-5.76068100	-3.43081800	-0.46672700
H	-4.71363200	-2.29742900	-1.96098000
C	-5.66156800	-4.18361500	0.70666700
H	-4.31640500	-4.97826000	2.19990200
H	-6.72984200	-3.26840300	-0.93200600
H	-6.55171800	-4.61544500	1.15741500
C	-2.12085400	-2.15251400	-2.56057400
H	-2.73979600	-2.85988500	-3.11904400
H	-2.51591100	-1.14468600	-2.74562900
H	-1.10131500	-2.18813900	-2.95110800
N	-1.15361800	-2.24509700	-0.28618500
O	-0.03011200	-1.67426700	-0.93025100
H	0.64473400	-1.65130700	-0.20951200
C	3.82800800	-1.53564300	0.16234800
C	5.11976400	-0.87052300	-0.16642100
C	5.66008900	0.12624400	0.66887100
C	5.82361300	-1.22995700	-1.32958300
C	6.86346100	0.75143700	0.34196900
H	5.14010500	0.39950800	1.58190800
C	7.02685500	-0.59818800	-1.65735700
H	5.42860300	-1.99446100	-1.99216600
C	7.55144800	0.39385200	-0.82406600
H	7.26991600	1.51313700	1.00292100
H	7.55268400	-0.88400100	-2.56499800
H	8.49031300	0.88064700	-1.07621700
C	3.53664000	-2.91728900	-0.35974000
H	3.10866900	-2.86760000	-1.36986100
H	4.45320600	-3.51065200	-0.41813400
H	2.81939100	-3.43161700	0.28339000
N	3.01718100	-0.84445400	0.88859000
O	1.80266800	-1.52692800	1.16569900
H	1.35955900	-0.92049600	1.80418700
C	1.06994700	1.05617600	3.55435100
N	0.37786000	0.26093700	2.95842200
O	1.84843100	1.76458600	4.08993900

C	-1.06789900	0.06695100	2.82345200
H	-1.60340400	0.56766500	3.63374500
H	-1.39141800	0.46906000	1.85962400
H	-1.27711600	-1.00416600	2.84973600
C	-1.04218500	2.92988900	-1.48094000
C	-2.07652100	3.73977400	-0.78141000
C	-3.30172400	3.16976700	-0.38391400
C	-1.84193800	5.09628600	-0.49147400
C	-4.25584000	3.93135600	0.29232800
H	-3.50855700	2.13039500	-0.62056600
C	-2.79718900	5.85611600	0.19001400
H	-0.90374900	5.56043400	-0.78221300
C	-4.00752000	5.27801300	0.58446400
H	-5.19911000	3.47527700	0.58340100
H	-2.59271700	6.90065800	0.41224800
H	-4.75315900	5.87118900	1.10817200
C	-0.07619800	3.57149800	-2.44312600
H	0.90759000	3.71052400	-1.97478500
H	0.07218600	2.92599000	-3.31435500
H	-0.43489200	4.54563400	-2.78263700
N	-1.02287800	1.67173600	-1.19466000
O	-0.02371100	0.97356300	-1.88954300
H	-0.12180900	0.05127100	-1.56112900

***E*-TS-a3**

C	-2.10288500	-2.17249900	-0.93658100
C	-3.12157700	-3.22696600	-0.66789100
C	-2.74955800	-4.48861200	-0.16530100
C	-4.48222800	-2.97335800	-0.91591400
C	-3.71446300	-5.46298000	0.09090100
H	-1.70068500	-4.70656800	0.01117900
C	-5.44747900	-3.94965300	-0.65285900
H	-4.79534000	-2.00872400	-1.30403100
C	-5.06822700	-5.19709200	-0.14912100
H	-3.40850700	-6.43491700	0.47029600
H	-6.49552800	-3.73270300	-0.84396700
H	-5.81848200	-5.95872900	0.04836500
C	-2.38811800	-1.10375900	-1.95648300
H	-2.91718500	-1.52771500	-2.81530600
H	-3.02811500	-0.32265400	-1.52633400
H	-1.46545700	-0.63285900	-2.29922300
N	-1.01990700	-2.26223600	-0.24239200
O	-0.07498600	-1.23899200	-0.54281600
H	0.77112200	-1.52716000	-0.04335700
C	3.83813800	-1.41835000	-0.17980800
C	5.08034800	-0.68387500	-0.54522700
C	5.66604600	0.25260800	0.33146400
C	5.70251000	-0.90780500	-1.78806500
C	6.82147200	0.94634600	-0.02882400
H	5.21440600	0.42496700	1.30370800
C	6.86007800	-0.21041500	-2.14872500
H	5.27697600	-1.62133500	-2.48800700
C	7.42526800	0.72035400	-1.27255300
H	7.25854000	1.65884900	0.66710600
H	7.31820600	-0.39677600	-3.11731100
H	8.32797700	1.25905600	-1.55029000
C	3.52091800	-2.73793600	-0.83670200
H	2.96467900	-2.59548900	-1.77411000
H	4.43375800	-3.29221900	-1.07594800
H	2.89738600	-3.34423500	-0.17461000
N	3.07237300	-0.85575400	0.70009900
O	1.92293100	-1.54868400	1.02643800
H	1.27022500	-0.77541700	1.89847000
C	-0.19964400	0.77254800	2.41662100
N	0.64805100	-0.16708400	2.69155400
O	-0.94073100	1.53488900	2.96781700
C	0.82906200	-0.52748300	4.10553900
H	-0.10867500	-0.88479100	4.54456000
H	1.56996600	-1.32847600	4.14814100
H	1.19478900	0.32739300	4.68452100
C	-0.98933800	3.00986100	0.21348500
C	-2.10158500	3.86741300	-0.28105800
C	-3.44259300	3.48268500	-0.09013900
C	-1.82528400	5.07784200	-0.94185800
C	-4.48082300	4.28546300	-0.56258400
H	-3.66737600	2.56652200	0.44659900
C	-2.86846500	5.87430600	-1.41869200
H	-0.80013900	5.39706800	-1.09986800
C	-4.19733400	5.48146900	-1.23163300
H	-5.51174000	3.98148500	-0.40047200
H	-2.64064600	6.80271600	-1.93594900
H	-5.00750800	6.10697000	-1.59788400

C	0.31119400	3.64512900	0.60714200
H	0.78252100	4.08477100	-0.28032000
H	0.12555400	4.46000800	1.31470400
H	1.01281400	2.93694200	1.04487800
N	-1.27532800	1.74992800	0.23927800
O	-0.16240900	0.95879000	0.77201300
H	-0.24088600	0.05057100	0.26626300

***E*-9•7d$_2$**

C	-2.89234800	-1.83317600	-1.12021200
C	-4.31812400	-2.19439600	-0.88941300
C	-5.23110900	-1.25766800	-0.36857600
C	-4.77423200	-3.49204500	-1.18236300
C	-6.56037200	-1.61436600	-0.13863700
H	-4.89835600	-0.24567400	-0.15832500
C	-6.10472700	-3.84829900	-0.94463300
H	-4.08927500	-4.23388700	-1.58279300
C	-7.00248100	-2.91193500	-0.42343200
H	-7.25423300	-0.87594300	0.25568200
H	-6.43766700	-4.85869300	-1.16885700
H	-8.03913700	-3.18762300	-0.24633900
C	-2.08949800	-2.52746300	-2.18832400
H	-1.51679500	-3.36188600	-1.76113200
H	-2.73923300	-2.92892600	-2.96923500
H	-1.37480700	-1.83508200	-2.64116700
N	-2.41800700	-0.92072300	-0.34256000
O	-1.05507700	-0.62905100	-0.62150500
H	0.21931400	-1.82664000	-0.03601400
C	3.15799800	-2.44427300	0.34186300
C	4.44025400	-2.16782000	-0.36291300
C	4.47271300	-1.94065400	-1.75252200
C	5.64874700	-2.12056600	0.35500100
C	5.67711900	-1.66403300	-2.40021700
H	3.55119100	-1.99384700	-2.32429700
C	6.85358300	-1.83843300	-0.29550500
H	5.65223300	-2.28949600	1.42791600
C	6.87344200	-1.60999800	-1.67446400
H	5.68341200	-1.49923600	-3.47499900
H	7.77611900	-1.79871700	0.27848700
H	7.81174400	-1.39780900	-2.18107000
C	3.13957300	-3.24337400	1.61855700
H	4.01632800	-3.89086100	1.69310500
H	3.13135500	-2.57814900	2.49256600
H	2.23725600	-3.85897400	1.66811400
N	2.10209300	-1.94494600	-0.20502500
O	0.92281500	-2.23946700	0.51499300
H	0.51456300	-0.97865100	2.09498300
C	-0.18621800	0.85916000	2.68519900
N	0.11997200	-0.43906400	2.86373900
O	-0.59147300	1.63586800	3.53155500
C	0.02111700	-1.06482400	4.17631800
H	0.71130300	-0.60322200	4.89202300
H	-0.99802300	-0.98881200	4.56905300
H	0.27898800	-2.11981600	4.06436000
C	0.31514900	3.00332300	0.02441700
C	-0.03814200	4.39635200	-0.37200400
C	-0.56075500	5.30872700	0.56464200
C	0.15254800	4.82171400	-1.69847200
C	-0.89030000	6.60817400	0.17976500
H	-0.69416000	5.00014200	1.59680700
C	-0.18491700	6.12273300	-2.08205700
H	0.55330000	4.13766800	-2.44028100
C	-0.70597600	7.02007000	-1.14579900
H	-1.28450200	7.30310600	0.91711000
H	-0.03779900	6.43269700	-3.11359300
H	-0.96149400	8.03404400	-1.44334400
C	1.34145800	2.24480300	-0.77267300
H	2.16001600	2.90927500	-1.06469100
H	1.74596300	1.40408300	-0.20779300
H	0.89185900	1.85265800	-1.69438300
N	-0.32489300	2.55588900	1.05219800
O	0.04328600	1.20278700	1.34585800
H	-0.84705600	0.08867700	0.01114800

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C	0.11250800	0.00349100	0.23259500
C	0.89974300	-1.05854400	0.70444800
C	2.27985200	-1.07644400	0.48058000
C	2.88742500	-0.03996200	-0.23564000
C	2.10775700	1.01464200	-0.72334600
C	0.72950100	1.03794100	-0.49097400
H	0.43042700	-1.86934800	1.25708600

H	2.87734200	-1.90037100	0.86328300
H	3.95990800	-0.05402600	-0.41384900
H	2.57238900	1.82207400	-1.28411300
H	0.13761000	1.86520300	-0.87318400
C	-1.38524700	-0.00952600	0.48688200
H	-1.65510700	-0.87128600	1.10669500
C	-1.95247600	1.28650000	1.08279500
H	-3.03028100	1.18742200	1.25538000
H	-1.46554000	1.48476100	2.04384400
H	-1.78303800	2.14368000	0.42315600
N	-2.04409800	-0.18451100	-0.85509300
O	-2.72617500	-1.18314000	-0.95208600

TS-b

C	3.17169100	0.51273600	-0.08264200
N	2.07939200	0.94046700	0.30921200
O	4.24371000	0.18366500	-0.41712400
C	1.83254700	2.23645800	0.98512500
H	1.16984200	2.82953000	0.35143600
H	1.34722100	2.03095600	1.94133100
H	2.77428400	2.76302500	1.14448000
C	-1.30911600	-0.33250100	-0.01805300
C	-1.70111300	0.44699900	-1.12664800
C	-3.00660700	0.92553900	-1.24466500
C	-3.95480900	0.65108900	-0.25095400
C	-3.57790400	-0.10937000	0.85916300
C	-2.27097900	-0.59576600	0.97495500
H	-0.97171900	0.68477200	-1.89545200
H	-3.28177100	1.52427800	-2.11010300
H	-4.96994700	1.03047300	-0.33946000
H	-4.30113100	-0.33034800	1.64084200
H	-2.00837200	-1.18990900	1.84483900
C	0.08884700	-0.84504600	0.10092600
H	1.03144700	0.24235500	0.15510400
C	0.52268100	-1.56375500	1.36880400
H	1.59288200	-1.77904300	1.33807700
H	0.31211100	-0.96516500	2.26071000
H	-0.01138000	-2.51923500	1.46741300
N	0.70298900	-1.11478400	-1.10034300
O	1.88984500	-1.56613600	-1.04004600

TS-b'

C	2.61014800	-0.31384700	-0.05180700
N	3.80687100	-0.15850300	0.33177100
O	1.96785600	-0.39569000	-1.13020600
C	4.81190800	0.03589300	-0.71260800
H	5.16048600	-0.93554300	-1.08901100
H	4.43586000	0.61757100	-1.56492400
H	5.67182000	0.55246100	-0.27625600
C	-1.57097500	0.13263500	0.04243400
C	-2.48786900	1.19344600	-0.04502100
C	-3.85033700	0.93602900	-0.21640300
C	-4.31591900	-0.38032500	-0.30845300
C	-3.40854400	-1.44246000	-0.23593500
C	-2.04578600	-1.18697100	-0.07241900
H	-2.14946100	2.22181000	0.02992300
H	-4.54933100	1.76659100	-0.27492100
H	-5.37651200	-0.57600800	-0.44533600
H	-3.75844800	-2.46814400	-0.32123900
H	-1.34066200	-2.01416700	-0.04815200
C	-0.09837300	0.35892300	0.22484900
H	0.56652900	-0.09002800	-0.70911900
C	0.42190100	1.81461700	0.20906300
H	1.49893000	1.87005400	0.37279300
H	0.19143600	2.28015700	-0.75164100
H	-0.07641000	2.36910700	1.01109400
N	0.43614100	-0.51123700	1.16075300
O	1.73561400	-0.57847500	1.20732100

E-**TS0**

C	-1.25332300	0.25201800	-0.02578400
C	0.21672400	0.07446700	-0.01559700
C	0.80310200	-1.20545400	-0.09461200
C	1.05927700	1.19737400	0.07582500
C	2.18853600	-1.35312400	-0.07536700
H	0.17099400	-2.08424600	-0.18010700
C	2.44853200	1.04459700	0.09746100
H	0.63658000	2.19501100	0.13823500
C	3.01880500	-0.22863300	0.02255800
H	2.62301000	-2.34748500	-0.14132500
H	3.08269900	1.92429700	0.17291100
H	4.09936100	-0.34668000	0.03651800

C	-1.89504400	1.60164900	-0.14788200
H	-1.68834700	2.20949800	0.74177700
H	-1.50163300	2.13889400	-1.01767300
H	-2.97694700	1.49180800	-0.25039500
N	-1.99599700	-0.79691000	0.07665300
O	-3.42127600	-0.76778800	0.09010600
H	-2.62318900	-1.75779200	0.22304200

***E*-8**

C	1.01046600	1.18548400	0.25713500
C	2.39892600	1.05245700	0.31251400
C	3.00119000	-0.18491900	0.06022900
C	2.20146500	-1.28906900	-0.25390200
C	0.81273500	-1.16058700	-0.31413200
C	0.19305400	0.07823300	-0.04681400
H	0.55797800	2.14994400	0.46957300
H	3.01047400	1.91762800	0.55651400
H	4.08286900	-0.28576600	0.09852300
H	2.65963200	-2.25086000	-0.47079900
H	0.21461500	-2.02212300	-0.60107400
C	-1.27301900	0.23646500	-0.07867400
C	-1.96461600	1.49257500	-0.50386600
H	-2.73961600	1.25810800	-1.24393800
H	-2.47530300	1.96886900	0.34452200
H	-1.26308000	2.20623600	-0.93913100
O	-3.32378000	-0.80028200	0.31011700
N	-2.02541300	-0.76894600	0.29714100
H	-1.56063400	-1.62099200	0.62995500

***E*-7d•7d**

C	-2.48682400	1.30686300	0.07272200
C	-3.67741600	0.42092200	-0.02056000
C	-3.65180100	-0.75278800	-0.79772700
C	-4.85485700	0.74056600	0.67985700
C	-4.76731500	-1.58951300	-0.85886200
H	-2.76236600	-0.99724800	-1.37110200
C	-5.96835200	-0.10166700	0.62119200
H	-4.90024400	1.64066800	1.28646600
C	-5.92933300	-1.26941800	-0.14718900
H	-4.73246000	-2.48714700	-1.47150900
H	-6.86635700	0.15648000	1.17710200
H	-6.79860000	-1.92042000	-0.19798500
C	-2.63279300	2.79417400	0.25206000
H	-3.64833200	3.12625700	0.02809000
H	-2.38944000	3.08675700	1.28216500
H	-1.93362400	3.32179700	-0.40471600
N	-1.33825300	0.72349700	0.00789100
O	-0.25271700	1.60840100	0.09530900
H	0.51611000	0.98748200	0.04456400
C	2.48674800	-1.30679100	0.07267000
C	3.67740100	-0.42093000	-0.02058400
C	3.65185100	0.75288100	-0.79760200
C	4.85485500	-0.74076800	0.67972200
C	4.76743900	1.58950800	-0.85869900
H	2.76240900	0.99749800	-1.37089900
C	5.96843000	0.10136500	0.62109200
H	4.90019800	-1.64095300	1.28621100
C	5.92947400	1.26921600	-0.14713900
H	4.73263200	2.48722200	-1.47123200
H	6.86644500	-0.15694100	1.17691100
H	6.79880000	1.92014100	-0.19791000
C	2.63267800	-2.79409100	0.25213800
H	3.64802200	-3.12630700	0.02746700
H	2.39011400	-3.08644500	1.28249900
H	1.93295600	-3.32177600	-0.40398400
N	1.33821200	-0.72336200	0.00778800
O	0.25260100	-1.60816000	0.09528500
H	-0.51615200	-0.98711500	0.04482200

***E*-TS1**

C	2.34898200	1.28260700	-0.00484300
C	3.55921900	0.43563900	0.01180900
C	3.60038500	-0.76884200	0.74029300
C	4.69440900	0.83430800	-0.71816800
C	4.74841400	-1.56141800	0.72441000
H	2.75091000	-1.07298000	1.34569400
C	5.83698400	0.03303300	-0.73613000
H	4.67846400	1.75954100	-1.28683600
C	5.86787400	-1.16563400	-0.01571200
H	4.77187900	-2.48283200	1.30022800
H	6.70331900	0.34666300	-1.31259300
H	6.76206600	-1.78357000	-0.02369200

C	2.39907900	2.77538900	-0.09479900
H	3.40945500	3.14838500	0.07529700
H	2.05638600	3.11103900	-1.08256200
H	1.72299100	3.21580200	0.64602200
N	1.19813100	0.69441700	0.05490800
O	0.02915700	1.39359200	0.06894100
H	-0.71750700	0.54409600	0.07641700
C	-2.37197400	-1.32938900	-0.00753000
C	-3.55299300	-0.43584700	0.01353200
C	-3.53820600	0.79257800	0.70685500
C	-4.72978900	-0.79332200	-0.67484300
C	-4.64835300	1.63858300	0.69151100
H	-2.66209600	1.07601700	1.28323700
C	-5.84104900	0.05384600	-0.68670600
H	-4.77306500	-1.73235800	-1.21984500
C	-5.80617700	1.27565200	-0.00678400
H	-4.61397400	2.57748000	1.23929000
H	-6.73420400	-0.24165500	-1.23229700
H	-6.67215200	1.93297200	-0.01295000
C	-2.50549300	-2.82204000	-0.12599100
H	-3.52673200	-3.15487100	0.07406100
H	-2.21632100	-3.17156800	-1.12726400
H	-1.82577500	-3.30926200	0.58234200
N	-1.19455100	-0.78052800	0.06334400
O	-0.08997200	-1.55170500	0.04197000
H	0.97995900	-0.36608700	0.05897900

***E*-8•8**

C	-4.71595700	0.73367100	-0.89888300
C	-5.81362900	-0.12289100	-0.99876400
C	-5.88287100	-1.27724700	-0.21119000
C	-4.84637200	-1.56515300	0.68304000
C	-3.74724900	-0.71059300	0.78792300
C	-3.65894300	0.44681100	-0.01220400
H	-4.67129400	1.61966600	-1.52599900
H	-6.61494200	0.11187300	-1.69495800
H	-6.74050600	-1.94084400	-0.28680300
H	-4.89884800	-2.44930100	1.31341000
H	-2.97259100	-0.93151800	1.51747800
C	-2.49674300	1.35459200	0.05989700
C	-2.60163000	2.83851500	-0.10270200
H	-2.11600600	3.34121900	0.74290300
H	-2.07787700	3.17293800	-1.00847900
H	-3.64282100	3.16114200	-0.15424300
O	-0.20046800	1.53961600	0.37884000
N	-1.31086900	0.84852400	0.27021800
H	-1.15713900	-0.17619600	0.33438300
C	4.71607200	-0.73376400	-0.89874500
C	5.81373600	0.12280900	-0.99861000
C	5.88285600	1.27727300	-0.21118000
C	4.84625000	1.56526800	0.68289600
C	3.74713500	0.71069300	0.78776300
C	3.65894600	-0.44680400	-0.01223400
H	4.67150100	-1.61984600	-1.52574600
H	6.61513700	-0.11202500	-1.69467900
H	6.74048200	1.94088300	-0.28678300
H	4.89863500	2.44949700	1.31316100
H	2.97239900	0.93167600	1.51721500
C	2.49675400	-1.35460200	0.05985300
C	2.60173100	-2.83855600	-0.10239600
H	2.11592900	-3.34110100	0.74320100
H	2.07819800	-3.17318900	-1.00822500
H	3.64294700	-3.16114900	-0.15363200
O	0.20041900	-1.53962800	0.37831500
N	1.31081800	-0.84852000	0.26978500
H	1.15703300	0.17620900	0.33375400

***E*-Int1**

C	2.70786300	0.07030900	0.56731700
C	3.30206400	-1.18282200	0.72598400
C	2.69339400	-2.32587500	0.19610000
C	1.48648600	-2.20314800	-0.50061200
C	0.88933900	-0.95161600	-0.66404900
C	1.48464300	0.20567000	-0.11976100
H	3.18728700	0.94617900	0.99513500
H	4.24134400	-1.26559600	1.26726600
H	3.15960200	-3.30052100	0.31643600
H	1.01467800	-3.08145700	-0.93433500
H	-0.02741300	-0.87488700	-1.24325900
C	0.86250300	1.53639500	-0.25649200
C	1.64116600	2.80382300	-0.41570200
H	1.30406200	3.33689700	-1.31413400

H	1.46916500	3.48070800	0.43219100
H	2.71092900	2.60727800	-0.50399000
O	-1.13463000	2.72384300	-0.37365600
N	-0.44434500	1.63129400	-0.23679200
H	-1.00448000	0.78068300	-0.08008200
C	-3.15308000	-1.11209500	-0.37519900
N	-2.75273900	-0.40493200	0.51377900
O	-3.43061200	-1.76670200	-1.32390100
C	-3.15067800	-0.02442600	1.86021600
H	-3.38630900	-0.91333900	2.45298200
H	-2.32411700	0.51312400	2.32831400
H	-4.02542300	0.63196900	1.81820400

***E*-TS2**

C	2.82619200	0.76285800	0.56430400
C	3.95074200	-0.05971500	0.64864900
C	3.93443100	-1.33732600	0.07923100
C	2.78500800	-1.78787400	-0.57915300
C	1.65669000	-0.97119500	-0.66413900
C	1.65990500	0.31280700	-0.08334400
H	2.84900200	1.74818300	1.02047400
H	4.83981000	0.29893000	1.16094800
H	4.81362900	-1.97360600	0.13991500
H	2.77001100	-2.77191500	-1.04044700
H	0.78519500	-1.32293700	-1.20994800
C	0.47089400	1.18714000	-0.13579900
C	0.54713500	2.67851400	-0.22503700
H	-0.08445500	3.03419100	-1.04777000
H	0.16425900	3.14176400	0.69395300
H	1.57044200	3.01601200	-0.39365700
O	-1.85505000	1.28129900	-0.15670500
N	-0.70531400	0.63486700	-0.09566200
H	-0.85993200	-0.38628000	0.01356800
C	-3.30922800	-0.01021300	0.05746600
N	-2.67320900	-1.08210900	0.15584600
O	-4.28176000	0.68558900	0.01911900
C	-3.40997600	-2.33785900	0.35680900
H	-4.10711100	-2.53119700	-0.46886400
H	-2.68965100	-3.15852600	0.40126000
H	-3.97780900	-2.32186200	1.29604100

***E*-Int2**

C	2.81469000	-0.83277100	-0.49562200
C	3.98724400	-0.08230600	-0.58562000
C	4.02725700	1.22367900	-0.08696800
C	2.88672000	1.78000200	0.50297500
C	1.70802300	1.04032400	0.58707500
C	1.65836600	-0.27401000	0.08088600
H	2.79507500	-1.84251100	-0.89326000
H	4.86996600	-0.52016000	-1.04371500
H	4.94516500	1.80237500	-0.14932200
H	2.91690300	2.78766300	0.90838800
H	0.84150800	1.47574200	1.07673000
C	0.42033400	-1.07437600	0.13261300
C	0.41319300	-2.56652100	0.23467000
H	-0.31729000	-2.88830400	0.98399500
H	0.11011700	-3.00584100	-0.72490800
H	1.39670000	-2.94938000	0.50696400
O	-1.90663600	-1.09420700	0.14008100
N	-0.71035900	-0.44712700	0.07065100
H	-0.89051500	0.57450100	-0.06370900
C	-3.07266300	-0.11463400	-0.02076500
N	-2.64524800	1.09495800	-0.18616600
O	-4.14288800	-0.71648300	0.04269600
C	-3.66982400	2.11800800	-0.35650100
H	-4.31114500	1.92312600	-1.22963700
H	-4.32628000	2.20059900	0.52330700
H	-3.18480700	3.08852200	-0.50491800

***E*-TS3**

C	2.79075600	0.85941200	0.43962600
C	3.95979200	0.10053100	0.51646900
C	3.97006800	-1.22383100	0.06813200
C	2.80247800	-1.79020200	-0.45676000
C	1.62935300	-1.04036000	-0.52830900
C	1.61021100	0.29350200	-0.07557500
H	2.79540700	1.88408200	0.79774600
H	4.86248000	0.54645700	0.92554200
H	4.88421600	-1.80961300	0.11987600
H	2.80753200	-2.81421500	-0.82052300
H	0.73758200	-1.48356400	-0.96188000
C	0.37315500	1.10198700	-0.12229900

C	0.39092000	2.59773700	-0.21388200
H	-0.41963600	2.95029300	-0.85774400
H	0.23355600	3.03298200	0.78229500
H	1.34375700	2.95807400	-0.60410400
O	-1.94686900	1.14242400	-0.11839700
N	-0.74826000	0.46758100	-0.06109300
H	-1.13658700	-0.61708400	0.08005400
C	-3.04099000	0.12852200	0.02276300
N	-2.51791400	-1.05817200	0.16807800
O	-4.16387700	0.62010200	-0.02554300
C	-3.39844600	-2.20355000	0.32348100
H	-4.05049400	-2.34218500	-0.55092300
H	-2.79124700	-3.10626300	0.44005800
H	-4.04115200	-2.10752700	1.21034600

TS-c

C	-2.25254100	0.96386700	0.64951800
C	-3.55400500	0.46300400	0.64444900
C	-3.86059200	-0.69236100	-0.08213800
C	-2.85825600	-1.35115900	-0.80279400
C	-1.55694300	-0.85231800	-0.80652500
C	-1.24079600	0.31918700	-0.08859700
H	-2.03231200	1.86388600	1.21351000
H	-4.32860700	0.97527900	1.20857100
H	-4.87457700	-1.08376200	-0.07892000
H	-3.08669900	-2.26082900	-1.35144700
H	-0.78022900	-1.40022300	-1.33212800
C	0.13243700	0.85802500	-0.09604600
C	0.58509200	1.80511500	0.97229600
H	1.64735500	2.03274700	0.89009400
H	0.02398600	2.74324900	0.85425700
H	0.36989600	1.40273100	1.96404700
O	2.17886800	0.80459000	-1.17940500
N	0.79697000	0.81065500	-1.25042800
H	0.45484600	0.21080500	-1.99972600
C	2.65634200	-0.24814200	-0.22064400
N	1.67989700	-0.77123300	0.45368700
O	3.88514800	-0.37151200	-0.26330600
C	2.02204700	-1.67409900	1.53833500
H	2.58477100	-2.54993200	1.17938300
H	2.63161700	-1.18322300	2.31316900
H	1.10304600	-2.03803300	2.01093600

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C	-2.06370100	1.10498700	0.25676200
C	-3.39487500	0.67497000	0.21343200
C	-3.69892000	-0.64561900	-0.12524700
C	-2.66242400	-1.53848300	-0.41999100
C	-1.33475400	-1.10890300	-0.37691600
C	-1.01908000	0.21840200	-0.03901300
H	-1.85480000	2.13531200	0.52305700
H	-4.19172700	1.37714500	0.44556000
H	-4.73347900	-0.97818600	-0.15736900
H	-2.88617900	-2.57008200	-0.68010000
H	-0.53660100	-1.81289600	-0.59862200
C	0.44530900	0.66358400	-0.04159800
C	0.71104300	2.01473100	0.63027900
H	1.78254500	2.23852900	0.58989100
H	0.17829500	2.81709500	0.11256400
H	0.40001700	2.00192800	1.67943000
O	2.32135100	0.29283100	-1.37854700
N	0.92383300	0.71647900	-1.45476700
C	2.48797000	-0.42993300	-0.21729500
N	1.34345200	-0.37593100	0.50917600
O	3.54352500	-0.98836200	0.03490200
C	1.30828800	-0.81356000	1.89802000
H	1.88236000	-1.73831500	1.98825000
H	1.73443300	-0.06039500	2.57261500
H	0.27369200	-1.01228600	2.18665400
H	0.48830200	-0.05849400	-1.96424700

***E*-Int1'**

C	-2.97020400	0.86479800	-0.50737000
C	-4.14440200	0.11477700	-0.59366000
C	-4.18964000	-1.18883000	-0.08789200
C	-3.04988000	-1.73442900	0.51265800
C	-1.87451400	-0.98712200	0.60532500
C	-1.81140900	0.32220900	0.08339800
H	-2.94938700	1.87042000	-0.91732100
H	-5.02458700	0.55019900	-1.06025600
H	-5.10608700	-1.76991300	-0.15192900
H	-3.07856900	-2.73916800	0.92689400

H	-1.01525100	-1.41683000	1.11407900
C	-0.57424400	1.12376000	0.14209600
C	-0.55351500	2.61224300	0.28826200
H	-1.55169400	3.00980800	0.47906600
H	0.10585900	2.89451800	1.11858400
H	-0.14514900	3.08976100	-0.61302600
O	1.75460800	1.06504500	0.11100300
N	0.58018700	0.51140800	0.05343800
H	0.59120200	-0.50634600	-0.08986400
C	3.30130100	-1.29011400	-0.23144700
N	4.40408600	-0.82218500	-0.15113600
O	2.30129800	-1.92945800	-0.33296800
C	5.05750900	0.45728100	0.02788200
H	6.13641900	0.29515400	0.07529600
H	4.83142400	1.11809300	-0.81448000
H	4.72264800	0.92761000	0.95705300

***E*-TS2'**

C	-2.99221600	0.85465200	-0.45789700
C	-4.17998100	0.12819000	-0.55575800
C	-4.23599600	-1.19639000	-0.10989700
C	-3.09487300	-1.79088400	0.43942500
C	-1.90401100	-1.07043000	0.53832100
C	-1.83430000	0.26098300	0.08028200
H	-2.96243400	1.87831400	-0.81883500
H	-5.06200200	0.59865600	-0.98257500
H	-5.16388000	-1.75805100	-0.18113200
H	-3.13369600	-2.81332000	0.80615700
H	-1.04023700	-1.53759100	1.00407000
C	-0.58018800	1.03689100	0.14932400
C	-0.52979400	2.51557900	0.36739200
H	-1.51368600	2.91694400	0.61282500
H	0.16327500	2.74455700	1.18574000
H	-0.14642800	3.02564800	-0.52628400
O	1.74631300	0.95523300	0.08210600
N	0.55031500	0.40552000	0.01038400
H	0.58115800	-0.60555900	-0.18398000
C	3.09113400	-0.50240800	-0.14524300
N	4.13599300	0.14925400	0.00461700
O	2.40622600	-1.47201900	-0.34739600
C	5.42169800	-0.56566700	-0.07612600
H	6.22768600	0.17246000	-0.08216100
H	5.56065300	-1.22197500	0.79257800
H	5.49628700	-1.17230900	-0.98803100

***E*-Int2'**

C	-2.89256000	0.91171500	-0.46322800
C	-4.11630300	0.25229400	-0.57897600
C	-4.24921500	-1.06785400	-0.13655300
C	-3.15126500	-1.72964600	0.42434500
C	-1.92191900	-1.08138800	0.53439500
C	-1.77857100	0.24607900	0.08310300
H	-2.79978200	1.93311200	-0.81883100
H	-4.96579400	0.77117100	-1.01468200
H	-5.20600600	-1.57660500	-0.22044200
H	-3.25369600	-2.74896500	0.78665400
H	-1.08842100	-1.59864200	1.00207700
C	-0.48425300	0.94661600	0.16085800
C	-0.35074700	2.41690800	0.39085400
H	0.26632700	2.59198600	1.28061000
H	0.15988100	2.89276000	-0.45540500
H	-1.32284400	2.88556900	0.54026500
O	1.83090000	0.79040400	0.13088100
N	0.59542100	0.24207100	0.02602800
H	0.66214000	-0.76973200	-0.18077800
C	2.88739900	-0.28538000	-0.09430600
N	4.04167200	0.26630400	0.01287000
O	2.41853700	-1.41623000	-0.32201100
C	5.16621900	-0.65163600	-0.16137000
H	5.18487400	-1.43857800	0.60889900
H	5.15390400	-1.15354900	-1.14146600
H	6.10156100	-0.08679700	-0.08488600

***E*-TS3'**

C	2.87812700	0.89928800	0.43111000
C	4.08966100	0.21493700	0.54455000
C	4.18666500	-1.11817300	0.13390200
C	3.06374000	-1.76821200	-0.39123900
C	1.84835500	-1.09337000	-0.49831800
C	1.74156800	0.24821800	-0.08266100
H	2.81672300	1.93150300	0.76198400
H	4.95748200	0.72546400	0.95363700

H	5.13323600	-1.64627600	0.21537400
H	3.13617900	-2.79949700	-0.72650500
H	0.99072400	-1.60035700	-0.93067200
C	0.45421900	0.97262000	-0.16191900
C	0.37091000	2.45877200	-0.34402100
H	0.07318200	2.93831000	0.59768800
H	1.32713300	2.87326200	-0.66433300
H	-0.39196000	2.70298900	-1.09012000
O	-1.85154800	0.88372900	-0.14047700
N	-0.61764800	0.26417000	-0.05308300
H	-1.06959100	-0.86447700	0.15470300
C	-2.82851600	-0.17315600	0.06045200
N	-4.03555600	0.22289300	0.00593300
O	-2.25827200	-1.31511100	0.25677900
C	-5.05558700	-0.80642300	0.20220900
H	-5.00278000	-1.25259300	1.20625400
H	-6.04448000	-0.35158600	0.08774100
H	-4.96970300	-1.62213700	-0.53051100

***E*-Int3'**

C	-2.89412900	0.96571600	-0.38651100
C	-4.15126900	0.36494800	-0.49075700
C	-4.32451800	-0.97384600	-0.12724000
C	-3.23117600	-1.71238500	0.34096500
C	-1.97277800	-1.11891900	0.43948100
C	-1.78818900	0.22783500	0.07212800
H	-2.77518000	2.00431300	-0.68090400
H	-4.99441300	0.94592300	-0.85564700
H	-5.30485200	-1.43771400	-0.20176300
H	-3.36058000	-2.75025400	0.63744600
H	-1.13274400	-1.69268400	0.81909600
C	-0.44631400	0.86215500	0.14804700
C	-0.28722800	2.33819500	0.38602800
H	-1.22036400	2.79112800	0.72329600
H	0.48389100	2.51640100	1.14207000
H	0.03718700	2.84265400	-0.53317000
O	1.79992600	0.72964300	0.08289300
N	0.55025100	0.05932700	-0.01584200
H	1.56128700	-1.49200300	-0.23996300
C	2.86093500	-0.14098400	-0.05837900
N	4.02615100	0.35016500	-0.00573800
O	2.54744900	-1.43167200	-0.23420200
C	5.15242800	-0.57131000	-0.14288500
H	6.08270300	-0.00009300	-0.07431800
H	5.15967300	-1.33246100	0.64982300
H	5.14300600	-1.09385400	-1.10969100

***E*-TS4'**

C	-2.87804800	0.90058400	-0.47827900
C	-4.13726100	0.30087800	-0.56194800
C	-4.33946900	-0.98704500	-0.05618200
C	-3.27230400	-1.67493700	0.53281700
C	-2.01124600	-1.08215800	0.61088200
C	-1.79718800	0.21277000	0.10199500
H	-2.73666400	1.89865600	-0.88284500
H	-4.95966300	0.84213700	-1.02290400
H	-5.32175100	-1.44923500	-0.11457800
H	-3.42351900	-2.67178300	0.93968700
H	-1.19052900	-1.61450800	1.08208000
C	-0.44807700	0.83957800	0.15533400
C	-0.28352400	2.32641800	0.32502100
H	-1.24345000	2.82183300	0.47676300
H	0.35564900	2.53516700	1.19022700
H	0.20859900	2.76553900	-0.55126700
O	1.78566300	0.70410300	0.16862500
N	0.53779800	0.01572900	0.04313600
H	2.43549000	-1.82751900	-0.92277200
C	2.84820600	-0.10713000	-0.12643800
N	3.91636600	0.06765800	0.52603500
O	2.65810500	-0.92026400	-1.20503500
C	5.11938100	-0.66234000	0.14649200
H	5.98267800	0.00267900	0.25552700
H	5.26647200	-1.50317500	0.83693600
H	5.09457700	-1.05391600	-0.87792600

***E*-Int4'**

C	-2.90077400	0.99345900	-0.33576700
C	-4.16640300	0.42413800	-0.50027700
C	-4.36149100	-0.93996800	-0.26365100
C	-3.28068000	-1.73483800	0.13623200
C	-2.01389600	-1.17159300	0.29356300
C	-1.80758600	0.20056600	0.05592100

H	-2.76455300	2.05345600	-0.52938000
H	-4.99942000	1.04919300	-0.81207800
H	-5.34847200	-1.37984500	-0.38318400
H	-3.42635500	-2.79378600	0.33481300
H	-1.18259700	-1.79038900	0.61743600
C	-0.45685000	0.80952200	0.20393300
C	-0.30531300	2.25542600	0.59381000
H	-1.20665400	2.62729500	1.08490400
H	0.54632000	2.38304400	1.26751200
H	-0.11521700	2.87394000	-0.29333700
O	1.77753000	0.69815700	0.09813700
N	0.52620100	0.01258600	-0.04474600
H	3.44563500	-1.88232700	0.47060000
C	2.85778700	-0.12258800	0.00527500
N	3.91367500	0.34134500	-0.52545100
O	2.65215200	-1.32458100	0.58366500
C	5.12592700	-0.47404500	-0.48424500
H	5.94621700	0.08994200	-0.93609100
H	5.42635500	-0.72892900	0.54386800
H	5.01783100	-1.40818600	-1.05685700

***E*-TS5'**

C	-2.75988500	1.10946800	-0.39519200
C	-4.09131200	0.69536300	-0.48169700
C	-4.45303900	-0.59908300	-0.09557000
C	-3.47409200	-1.48151600	0.37574700
C	-2.14155600	-1.07516900	0.45536100
C	-1.76886100	0.22526600	0.06674600
H	-2.49394500	2.11611400	-0.70405500
H	-4.84512300	1.38671200	-0.84978600
H	-5.49120500	-0.91620500	-0.15450800
H	-3.74942300	-2.48523800	0.68968200
H	-1.38777600	-1.75766100	0.83618500
C	-0.34764300	0.66201900	0.12914600
C	0.01064400	2.09539500	0.41456600
H	-0.85198300	2.65311700	0.78173700
H	0.80632100	2.14427700	1.16419400
H	0.38618900	2.58550400	-0.49265700
O	1.85005100	0.25015400	0.01065200
N	0.50855700	-0.27818700	-0.08925000
H	3.91523500	-1.77083700	-0.29930100
C	2.79814600	-0.67389500	-0.13367700
N	4.07953000	-0.42097700	-0.10267100
O	2.62372700	-1.94866400	-0.31739600
C	4.73457200	0.86441200	0.07488500
H	4.44316400	1.33944200	1.02110300
H	5.81502900	0.70028600	0.09218500
H	4.50483300	1.55315500	-0.74927500

TS-c'

C	2.39513100	0.94380700	-0.56491600
C	3.65972300	0.37107400	-0.69837500
C	3.90173500	-0.91938200	-0.21612100
C	2.87204100	-1.64007300	0.39868000
C	1.60797300	-1.07024200	0.54119200
C	1.35773800	0.23427900	0.06999200
H	2.22493800	1.94795800	-0.93825500
H	4.45547400	0.93297600	-1.17965800
H	4.88657400	-1.36582600	-0.32682200
H	3.04970000	-2.65051200	0.75649600
H	0.81122100	-1.66171800	0.98274200
C	0.02245900	0.84480800	0.23128900
C	-0.35283900	2.06595800	-0.55418300
H	-1.39613100	2.34171200	-0.39714500
H	0.27285300	2.89976200	-0.20811600
H	-0.16988200	1.91749900	-1.61987300
O	-1.98604800	0.62104200	1.30883500
N	-0.59948700	0.63826700	1.41921800
H	-0.27917100	-0.15191200	1.97972700
C	-2.33934600	-0.16857700	0.12731900
N	-3.58841300	-0.45716500	0.08663800
O	-1.35162300	-0.39493700	-0.64525000
C	-4.02198300	-1.18426400	-1.10582000
H	-3.71281200	-0.68945400	-2.03925500
H	-3.62657300	-2.21123200	-1.13096200
H	-5.11532300	-1.25013500	-1.10288500

12'

C	2.32788500	0.92250400	-0.47815600
C	3.60382300	0.34974500	-0.45174500
C	3.77788500	-0.96335100	-0.00762000
C	2.66849900	-1.70366000	0.41503700

C	1.39510800	-1.13200000	0.39409400
C	1.21197400	0.18627000	-0.05663600
H	2.21638700	1.94281500	-0.82893800
H	4.45933800	0.93374900	-0.78128300
H	4.76964900	-1.40831700	0.00834600
H	2.79236800	-2.72732600	0.75916400
H	0.54169500	-1.72094200	0.71853900
C	-0.18138100	0.79485100	-0.04172000
C	-0.38611900	2.02676300	-0.91264100
H	-1.43044100	2.35081900	-0.86056400
H	0.24111800	2.85119800	-0.56325900
H	-0.14084400	1.80384500	-1.95507200
O	-2.04422900	0.82083600	1.28873400
N	-0.61288600	1.05688500	1.34220800
C	-2.26868200	-0.08329000	0.27674700
H	-0.26535800	0.30518900	1.94667600
N	-3.39240500	-0.63966400	0.13362700
O	-1.15745100	-0.22872700	-0.47657700
C	-3.58226400	-1.51730200	-1.02143000
H	-4.65032600	-1.72716500	-1.12999100
H	-3.22005500	-1.06897400	-1.95647400
H	-3.06342200	-2.47549600	-0.88082800

***E*-TS-d**

O	-0.90081600	2.02022700	0.89838800
N	-1.71045200	1.08147200	0.16751500
C	-2.16808600	0.16644100	0.95422000
C	-3.00461700	-0.86280000	0.28222400
C	-4.03225900	-1.51190500	0.98956900
C	-2.79348600	-1.19237100	-1.07048600
C	-4.83964900	-2.45752200	0.35274700
H	-4.21812700	-1.26981600	2.03163300
C	-3.59705000	-2.14297900	-1.69966400
H	-1.98805100	-0.71503100	-1.61997100
C	-4.62442500	-2.77729000	-0.99126300
H	-5.63595600	-2.94460500	0.90963300
H	-3.41546300	-2.39541100	-2.74130100
H	-5.24815600	-3.52011600	-1.48216800
C	-1.91163500	0.11512300	2.43488800
H	-2.52091300	0.86711400	2.95303800
H	-2.15224900	-0.86755400	2.84267500
H	-0.86282900	0.33975900	2.64851100
C	-0.40742700	2.99346600	0.12364100
O	0.25403900	3.93373700	0.78890200
N	-0.92284000	3.24750400	-1.06244800
H	-1.51990800	2.51982800	-1.44614000
C	-0.40904800	4.27220200	-1.96861000
H	0.54033100	3.95377200	-2.41257500
H	-1.14884600	4.41729800	-2.75750600
H	-0.26582400	5.21222500	-1.43359500
C	2.96425500	0.38764000	0.10535700
C	3.13839200	-1.08281600	-0.00035300
C	2.03482600	-1.96552400	0.01166000
C	4.42356900	-1.64883600	-0.12797100
C	2.21052900	-3.34340400	-0.10988000
H	1.03433500	-1.55989100	0.12420900
C	4.59861000	-3.03183300	-0.24886500
H	5.29911500	-1.00652200	-0.14878600
C	3.49510800	-3.88902600	-0.24167300
H	1.34129300	-3.99746000	-0.09249300
H	5.60329100	-3.43608800	-0.35162200
H	3.63067800	-4.96408700	-0.33190900
C	4.12864800	1.27086800	0.47922100
H	4.81505900	0.76764300	1.16792700
H	4.70986700	1.57693100	-0.40358700
H	3.75904700	2.18567700	0.95179400
N	1.78195800	0.86347300	-0.16944300
O	1.62383900	2.19293300	-0.13000100
H	1.14863200	3.51740300	0.93597300

***E*-Int-d0'**

O	0.96281800	0.03740000	0.64541600
N	2.35978100	-0.22040700	0.48693100
C	2.97616600	0.81966100	0.03755900
C	4.43749900	0.63987600	-0.17700600
C	5.31515100	1.72482100	-0.00368000
C	4.96658000	-0.61228400	-0.54242000
C	6.69153800	1.55605700	-0.17432600
H	4.92878900	2.69899700	0.28191200
C	6.34089400	-0.77451000	-0.72156400
H	4.29618100	-1.45121900	-0.70303600
C	7.20867300	0.30793500	-0.53506900

H	7.35832000	2.40170200	-0.02641300
H	6.73358900	-1.74469400	-1.01551900
H	8.27894300	0.18060100	-0.67712000
C	2.31200200	2.13960600	-0.24746600
H	1.36025100	1.98335300	-0.76344800
H	2.09191500	2.66935700	0.68852600
H	2.94778800	2.77666000	-0.86474300
O	-0.96597900	-0.85217400	1.29478800
N	0.91923100	-2.13658300	1.46439900
H	1.91845000	-2.15186400	1.29882600
C	0.25476700	-3.31268700	2.01142200
H	1.01989900	-4.06490700	2.21268100
H	-0.26227200	-3.07172200	2.94597300
H	-0.47081800	-3.72350100	1.30107700
C	0.24661700	-1.02262900	1.15450700
C	-5.83326900	0.13770100	-0.32232400
C	-6.55907500	0.85017400	0.63385700
C	-5.92199000	1.79615600	1.44480900
C	-4.55193100	2.02918200	1.28495300
C	-3.82265700	1.32171500	0.32701400
C	-4.44943600	0.35269200	-0.48309600
H	-6.33949800	-0.60332400	-0.93484100
H	-7.62395500	0.66227900	0.74759400
H	-6.48925400	2.35251200	2.18675500
H	-4.05032000	2.77634900	1.89514000
H	-2.76883000	1.54830300	0.18938800
C	-3.69331500	-0.42345200	-1.48452200
C	-4.25312500	-0.82625700	-2.81241400
H	-3.60432300	-0.45985500	-3.61886700
H	-4.28664000	-1.91958700	-2.91185100
H	-5.25640400	-0.42327200	-2.96161300
O	-1.67302400	-1.44355500	-2.00568800
N	-2.46464000	-0.78700900	-1.20984800
H	-2.06346200	-0.58408000	-0.27832600

***E*-TS-d'**

O	0.90321600	0.78289200	-1.12252100
N	2.10038500	0.56235000	-0.38951400
C	2.85286900	-0.30795600	-0.97275300
C	4.13382600	-0.60573500	-0.27577100
C	5.27056700	-0.98118600	-1.01378000
C	4.23756900	-0.50384900	1.12465600
C	6.48400100	-1.23377300	-0.36830500
H	5.21779500	-1.06054800	-2.09565600
C	5.44847300	-0.76500100	1.76653900
H	3.36212800	-0.23549200	1.70832800
C	6.57735600	-1.12862200	1.02271600
H	7.35558100	-1.51309900	-0.95502400
H	5.50881000	-0.69291100	2.84971300
H	7.51961600	-1.33359500	1.52484500
C	2.50730500	-0.98248500	-2.27378100
H	1.45152300	-1.26809700	-2.28467900
H	2.66820600	-0.29838200	-3.11733800
H	3.11680800	-1.87393000	-2.43189700
C	0.05017700	1.66974800	-0.49655200
O	-1.03868200	1.88260300	-1.18589300
N	0.63900300	2.69607100	0.18443300
H	1.49253200	2.41711800	0.65869200
C	-0.19259500	3.65042700	0.91379300
H	0.46348300	4.41978400	1.32885400
H	-0.90008700	4.12685200	0.23110400
H	-0.74980200	3.17603400	1.73195200
C	-5.17563900	-0.99382900	1.13516900
C	-6.43996700	-1.16666800	0.56537200
C	-6.61228200	-1.05571700	-0.81776500
C	-5.50638600	-0.77256300	-1.62847600
C	-4.24316800	-0.59796900	-1.06210100
C	-4.05817800	-0.69712300	0.33169500
H	-5.06306100	-1.07319900	2.21279500
H	-7.29076400	-1.38706200	1.20557700
H	-7.59498600	-1.19569800	-1.26118200
H	-5.62537300	-0.69959800	-2.70685700
H	-3.39034000	-0.40508300	-1.70674800
C	-2.72706500	-0.49455000	0.95153800
C	-2.34761300	-1.15117700	2.25015700
H	-1.30209200	-1.47443600	2.21246600
H	-2.43574600	-0.44599100	3.08862700
H	-2.98003400	-2.01594300	2.46393700
O	-0.67918500	0.52839700	0.83307800
N	-1.89636700	0.29037700	0.34232800
H	-1.76364900	1.14873000	-0.72966900

E-**Int-d**

O	-0.90081600	2.02022700	0.89838800
N	-1.71045200	1.08147200	0.16751500
C	-2.16808600	0.16644100	0.95422000
C	-3.00461700	-0.86280000	0.28222400
C	-4.03225900	-1.51190500	0.98956900
C	-2.79348600	-1.19237100	-1.07048600
C	-4.83964900	-2.45752200	0.35274700
H	-4.21812700	-1.26981600	2.03163300
C	-3.59705000	-2.14297900	-1.69966400
H	-1.98805100	-0.71503100	-1.61997100
C	-4.62442500	-2.77729000	-0.99126300
H	-5.63595600	-2.94460500	0.90963300
H	-3.41546300	-2.39541100	-2.74130100
H	-5.24815600	-3.52011600	-1.48216800
C	-1.91163500	0.11512300	2.43488800
H	-2.52091300	0.86711400	2.95303800
H	-2.15224900	-0.86755400	2.84267500
H	-0.86282900	0.33975900	2.64851100
C	-0.40742700	2.99346600	0.12364100
O	0.25403900	3.93373700	0.78890200
N	-0.92284000	3.24750400	-1.06244800
H	-1.51990800	2.51982800	-1.44614000
C	-0.40904800	4.27220200	-1.96861000
H	0.54033100	3.95377200	-2.41257500
H	-1.14884600	4.41729800	-2.75750600
H	-0.26582400	5.21222500	-1.43359500
C	2.96425500	0.38764000	0.10535700
C	3.13839200	-1.08281600	-0.00035300
C	2.03482600	-1.96552400	0.01166000
C	4.42356900	-1.64883600	-0.12797100
C	2.21052900	-3.34340400	-0.10988000
H	1.03433500	-1.55989100	0.12420900
C	4.59861000	-3.03183300	-0.24886500
H	5.29911500	-1.00652200	-0.14878600
C	3.49510800	-3.88902600	-0.24167300
H	1.34129300	-3.99746000	-0.09249300
H	5.60329100	-3.43608800	-0.35162200
H	3.63067800	-4.96408700	-0.33190900
C	4.12864800	1.27086800	0.47922100
H	4.81505900	0.76764300	1.16792700
H	4.70986700	1.57693100	-0.40358700
H	3.75904700	2.18567700	0.95179400
N	1.78195800	0.86347300	-0.16944300
O	1.62383900	2.19293300	-0.13000100
H	1.14863200	3.51740300	0.93597300

MeOH

C	0.04795000	0.67101700	0.00000000
H	1.09481200	0.98666900	0.00000000
H	-0.44487000	1.07467800	0.89511300
H	-0.44487000	1.07467800	-0.89511300
O	0.04795000	-0.76241000	0.00000000
H	-0.87637600	-1.06285100	0.00000000

TS-1MeOH

C	0.14351700	0.46197800	-0.11962700
N	0.94156200	-0.56539900	-0.06431500
O	0.05173200	1.65731800	0.01545400
C	2.37295200	-0.44366100	0.17628100
H	2.76500900	-1.42525000	0.45485000
H	2.89935000	-0.10297300	-0.72514400
H	2.58299600	0.25954000	0.99211600
C	-2.24596800	-0.40257000	0.37741500
H	-2.99813000	-1.09253800	-0.01044300
H	-2.64934400	0.61229700	0.40619500
H	-1.91873600	-0.71328700	1.37555400
O	-1.13222100	-0.41754400	-0.54829900
H	-0.25116900	-1.19267700	-0.38457100

s-trans-**10**

O	-0.07043100	1.32862600	0.00019600
C	-0.01446700	0.10042000	0.00023800
N	1.12669900	-0.62446000	0.00045000
O	-1.10743600	-0.70921700	0.00025700
C	-2.38563100	-0.04701900	-0.00036500
H	-2.50319900	0.56985400	-0.89583900
H	-3.12528100	-0.84941500	-0.00024800
H	-2.50373300	0.57059300	0.89452900
C	2.44126000	-0.00143200	-0.00037100
H	3.19132700	-0.79521700	0.00005400
H	2.58604200	0.62063900	-0.89104500

H	2.58640900	0.62187500	0.88935000
H	1.05751000	-1.63419400	-0.00059200

TS-1MeOH'

C	0.16011800	0.31846600	-0.11639200
N	0.90626200	-0.68715400	-0.22130700
O	0.18261000	1.57108400	0.20213500
C	2.32383900	-0.51864700	0.10297500
H	2.52100100	0.34481000	0.75159300
H	2.68308600	-1.42413900	0.60280400
H	2.90420000	-0.39656000	-0.82074100
C	-2.08040600	-0.81940700	0.26364100
H	-1.91833900	-0.75664800	1.34287400
H	-1.75782800	-1.78492300	-0.12775000
H	-3.12304600	-0.62815100	0.00890400
O	-1.30028100	0.21070900	-0.41614800
H	-1.13284300	1.31887700	0.00222800

s-cis-**10**

O	0.71476400	1.56638800	0.00011500
C	0.05752700	0.52496100	-0.00009300
N	-1.29505500	0.46805700	-0.00022900
H	-1.76471900	1.36412600	0.00026100
O	0.60935200	-0.71369700	-0.00032700
C	-2.10403100	-0.74525400	0.00017800
H	-1.91470300	-1.35427900	0.89098500
H	-3.15388700	-0.44386500	0.00016900
H	-1.91482700	-1.35472800	-0.89034300
C	2.04897700	-0.76503800	0.00015300
H	2.45332400	-0.28473700	0.89537800
H	2.29852400	-1.82736200	0.00042500
H	2.45391100	-0.28508900	-0.89500200

MeNCO•$(MeOH)_2$

C	2.73213300	0.00053400	-0.52722000
N	1.86516200	-0.52093600	0.13588000
O	3.48157000	0.60412100	-1.21445100
C	1.80369800	-1.68873100	1.01362300
H	2.20557500	-2.56832100	0.50272400
H	2.37631100	-1.49766200	1.92608700
H	0.76022900	-1.86907500	1.27587000
C	-3.81241000	-0.54700100	-0.90881500
H	-3.32830400	-0.66672000	-1.89004400
H	-4.21565600	0.47483400	-0.83955300
H	-4.64689500	-1.25332500	-0.84769500
O	-2.92199300	-0.84162300	0.16427100
H	-2.15990900	-0.22290900	0.11088000
C	-0.76027000	1.96715400	1.00198200
H	0.05382500	2.68357600	0.83428300
H	-0.66553000	1.53804600	2.00809400
H	-1.71571900	2.49265900	0.92597600
O	-0.75993300	0.94474800	-0.00650400
H	0.10388100	0.48574200	0.01827000

TS-2MeOH

C	1.08334300	0.06541500	-0.14220800
N	0.52774000	-1.08871400	0.08514700
O	2.21225800	0.50793600	-0.30820700
C	1.43298500	-2.23329400	0.14199800
H	2.00608900	-2.35181500	-0.78881000
H	2.15284100	-2.15086700	0.96944700
H	0.84116700	-3.14066400	0.29592400
C	0.26498700	2.44296500	0.25887300
H	0.44306400	2.40429400	1.33772500
H	-0.60284500	3.06476900	0.03244500
H	1.14421500	2.81582300	-0.26481700
O	-0.03828100	1.11623000	-0.24753800
H	-1.02469000	0.63667100	0.13449500
C	-2.90415000	-0.56579800	-0.39105300
H	-3.40745400	-1.48058800	-0.06612300
H	-2.50573700	-0.69905200	-1.40342300
H	-3.61046000	0.26693100	-0.37736300
O	-1.84222900	-0.25828800	0.54210600
H	-1.04734100	-0.92725400	0.43792200

10•MeOH

O	-2.34833500	0.10785500	0.24365200
C	-1.14353700	0.01548800	0.02422200
N	-0.45160800	-1.13448100	-0.10796100
O	-0.32153200	1.10342200	-0.11831300
C	-0.95190300	2.39535100	0.00067500
H	-1.39282100	2.51904900	0.99344400

H	-0.14983500	3.12046400	-0.14611800
H	-1.71859300	2.52220000	-0.76830400
C	-1.09413800	-2.43538000	-0.00289400
H	-0.32650300	-3.20108200	-0.13494800
H	-1.56192600	-2.57037300	0.97905600
H	-1.86018700	-2.56630700	-0.77604300
H	0.54865700	-1.07780100	-0.29382400
H	1.68609000	0.69586900	-0.46069200
C	3.25176400	-0.06642900	0.46982700
H	3.90290000	-0.92857700	0.30226700
H	2.75864300	-0.17720400	1.44532000
H	3.86376000	0.84522800	0.47716300
O	2.29961200	-0.04806100	-0.60191100

MeNCO•$(MeOH)_3$

C	-2.37036800	-1.57765000	0.05022200
N	-2.70634200	-0.43347000	0.25681800
O	-1.92487800	-2.64235400	-0.20496500
C	-3.89198900	0.19283400	0.84121100
H	-4.77743400	-0.05455200	0.24837600
H	-4.02903900	-0.15030500	1.87079700
H	-3.74828300	1.27410500	0.83868800
C	3.97051700	-1.54413200	-0.62451800
H	4.76650600	-0.91816600	-0.19284900
H	3.76667800	-1.19339800	-1.64781100
H	4.33585900	-2.57504000	-0.68038400
O	2.79685600	-1.54437500	0.18216100
H	2.46382600	-0.61863500	0.23275900
C	2.17961800	1.72706100	1.57103100
H	1.53680000	1.28978500	2.34763900
H	2.00045300	2.80971700	1.52593200
H	3.22554100	1.55501900	1.84108800
O	1.95750100	1.11314200	0.29763600
H	1.01958300	1.27060700	0.03263000
C	-0.77727300	1.98383400	-1.83683200
H	-1.79353800	2.32935500	-2.06281100
H	-0.52767400	1.13616000	-2.48794800
H	-0.07481100	2.79974700	-2.02528300
O	-0.65323100	1.63228800	-0.44929600
H	-1.29309000	0.91860200	-0.24950700

TS-3MeOH

C	-1.41098500	0.65163700	-0.04310400
N	-0.33160600	1.31419800	0.24096400
O	-2.62182700	0.82628700	0.05549900
C	-0.57544300	2.61874600	0.85920900
H	-1.17576100	3.27875100	0.21553600
H	-1.09867100	2.53083200	1.82309700
H	0.38698500	3.10831300	1.04118600
C	-2.08170400	-1.65096600	-0.89624900
H	-2.50623900	-1.96379900	0.06028100
H	-1.61938300	-2.49614400	-1.40975700
H	-2.84664600	-1.20156300	-1.52768700
O	-1.02129600	-0.67942200	-0.68966800
H	-0.06218700	-1.16503900	-0.30194700
C	0.93530100	-2.34681100	1.38072100
H	0.59335800	-1.61601500	2.12119100
H	1.91293500	-2.74317700	1.66699900
H	0.21593500	-3.16410700	1.30133100
O	1.03941400	-1.73494700	0.07051200
H	1.68864300	-0.95333600	0.10011500
C	2.93948400	0.96126300	-1.10610600
H	3.12396300	2.04301700	-1.08966700
H	2.35938400	0.71001800	-2.00462100
H	3.89934200	0.43832300	-1.14643800
O	2.26430100	0.54591600	0.08810600
H	1.32492300	0.92865600	0.10120900

10•$(MeOH)_2$

O	-2.88350900	-0.26396400	0.10974500
C	-1.67837600	-0.05610100	-0.00194800
N	-1.03470300	1.07086400	0.35364800
O	-0.81046700	-0.98943100	-0.52128000
C	-1.41767400	-2.19965300	-1.02610000
H	-2.12831300	-1.96724900	-1.82313200
H	-0.59268000	-2.79233200	-1.42511500
H	-1.91797000	-2.74551200	-0.22228300
C	-1.74681500	2.18870800	0.95562600
H	-1.01533600	2.96379600	1.19525000
H	-2.49191600	2.60840600	0.26936000
H	-2.25390500	1.88629600	1.87870700
H	-0.02911700	1.16874400	0.18125700

H	2.10755600	0.51021700	0.03041500
C	2.25647500	2.04454000	-1.21760900
H	1.91884700	3.08502000	-1.21560500
H	1.79911800	1.52557900	-2.07171600
H	3.34878600	2.02808200	-1.33362600
O	1.85630700	1.46373700	0.02743300
H	1.04230600	-1.33526800	-0.07202600
C	2.36182600	-1.91181500	1.29120300
H	3.43973800	-1.78526500	1.42061100
H	2.12700900	-2.98346900	1.27257300
H	1.84201700	-1.44001900	2.13522000
O	2.01194000	-1.28748600	0.04629500

The Cartesian coordinates (Å) in DMAc at the B3LYP/6-31+G(d,p) level of theory for the favored reaction pathway (Table S6)

E-**7d** (B3LYP/6-31+G**)

C	-1.26463700	0.19365800	0.06180300
C	0.21757700	0.05825200	0.03743800
C	0.83724300	-1.18756000	0.25456300
C	1.02869000	1.17861400	-0.21716800
C	2.22634300	-1.30807600	0.20822100
H	0.22586100	-2.05704600	0.47289600
C	2.41986400	1.05390300	-0.26766300
H	0.57697000	2.14977300	-0.39285900
C	3.02432200	-0.18815300	-0.05455100
H	2.68778800	-2.27558200	0.38623800
H	3.02910000	1.92955500	-0.47378900
H	4.10614800	-0.28291200	-0.08631200
C	-1.91829200	1.49637800	0.43910500
H	-1.23022200	2.14404900	0.98369100
H	-2.26150300	2.02941800	-0.45620500
H	-2.79807900	1.30932100	1.06017600
N	-1.92728800	-0.85982000	-0.27645500
O	-3.32410400	-0.64953100	-0.22961000
H	-3.67887500	-1.51367600	-0.49225200

E-**7d•7d** (B3LYP/6-31+G**)

C	2.48053300	1.30291900	-0.06422600
C	3.67392400	0.41994000	0.02080500
C	3.65052500	-0.76404300	0.78212000
C	4.85147500	0.75286200	-0.67294000
C	4.76847900	-1.59762900	0.83403700
H	2.76135600	-1.01861000	1.35009200
C	5.96747800	-0.08628200	-0.62313000
H	4.89500200	1.66079800	-1.26654900
C	5.93068500	-1.26417500	0.12920400
H	4.73561700	-2.50295700	1.43395100
H	6.86517400	0.18200000	-1.17319600
H	6.80138000	-1.91247600	0.17300700
C	2.62190500	2.79064800	-0.23716500
H	3.63254400	3.12532300	-0.00072300
H	2.38942100	3.08371500	-1.26849900
H	1.91199200	3.31119100	0.41168600
N	1.33360700	0.71602100	0.00071200
O	0.24425300	1.59526800	-0.08054200
H	-0.52039500	0.97097600	-0.03316200
C	-2.48053600	-1.30292200	-0.06421200
C	-3.67392500	-0.41994000	0.02081500
C	-3.65051600	0.76406000	0.78210500
C	-4.85148300	-0.75287200	-0.67291300
C	-4.76846600	1.59765000	0.83401500
H	-2.76133900	1.01863600	1.35006200
C	-5.96748300	0.08627800	-0.62311100
H	-4.89501800	-1.66081800	-1.26650400
C	-5.93067900	1.26418600	0.12920000
H	-4.73559500	2.50299100	1.43391000
H	-6.86518400	-0.18201100	-1.17316500
H	-6.80137200	1.91249100	0.17299700
C	-2.62190800	-2.79065600	-0.23711100
H	-3.63254900	-3.12532300	-0.00066900
H	-2.38941400	-3.08375400	-1.26843400
H	-1.91200100	-3.31117900	0.41176200
N	-1.33360800	-0.71602500	0.00070800
O	-0.24425900	-1.59528200	-0.08050300
H	0.52039500	-0.97100100	-0.03308600

E-**TS1** (B3LYP/6-31+G**)

C	2.33124800	-1.29100200	-0.00188700
C	3.53827200	-0.43705500	-0.01121700
C	3.57212500	0.77568900	-0.72621600
C	4.67746400	-0.83455600	0.71286300
C	4.71404300	1.57672800	-0.70161100

H	2.71978900	1.08066600	-1.32583200
C	5.81507200	-0.02618500	0.73829600
H	4.66896900	-1.76568900	1.27076200
C	5.83735600	1.18092900	0.03241700
H	4.73016000	2.50452400	-1.26610800
H	6.68364100	-0.34051100	1.30975900
H	6.72648300	1.80478100	0.04688600
C	2.39309700	-2.78338700	0.09200800
H	3.40205400	-3.15057600	-0.09348800
H	2.06959000	-3.11872500	1.08530500
H	1.70613500	-3.22791900	-0.63452300
N	1.17874700	-0.70688100	-0.07012300
O	0.01526500	-1.41183700	-0.08554600
H	-0.75165200	-0.51613400	-0.09268500
C	-2.33888800	1.31308700	-0.00200100
C	-3.53308100	0.43685000	-0.01222900
C	-3.54203800	-0.79071500	-0.70553600
C	-4.69564900	0.81594500	0.68707800
C	-4.66618000	-1.61737900	-0.68026500
H	-2.67604800	-1.08868700	-1.28852900
C	-5.81986800	-0.01300600	0.70949500
H	-4.71719700	1.75579800	1.23042600
C	-5.81053600	-1.23451000	0.02870700
H	-4.65319600	-2.55594400	-1.22774100
H	-6.70265200	0.29635900	1.26245900
H	-6.68671700	-1.87665500	0.04249500
C	-2.44783600	2.80632000	0.11210900
H	-3.45873900	3.15388400	-0.10674800
H	-2.17242300	3.14741900	1.11872700
H	-1.74511800	3.27810800	-0.58177000
N	-1.17210700	0.74772900	-0.07939300
O	-0.04806000	1.49796900	-0.07144500
H	0.92519800	0.37777700	-0.07892100

E-**8•8** (B3LYP/6-31+G**)

C	-4.68915700	-0.73283100	0.91543100
C	-5.78728800	0.12201000	1.02144700
C	-5.86816800	1.26997700	0.22607600
C	-4.84318200	1.55327600	-0.68244900
C	-3.74363600	0.70047400	-0.79393200
C	-3.64356400	-0.45021700	0.01424800
H	-4.63520400	-1.61372200	1.54773400
H	-6.57947900	-0.10882000	1.72811900
H	-6.72577500	1.93176300	0.30664800
H	-4.90543100	2.43168400	-1.31860000
H	-2.97904300	0.91671000	-1.53437400
C	-2.47984400	-1.35547300	-0.06384000
C	-2.57936200	-2.83719600	0.11448400
H	-2.08843700	-3.34451700	-0.72374600
H	-2.05566000	-3.15827700	1.02390100
H	-3.61850500	-3.16236200	0.16780000
O	-0.18823700	-1.53876300	-0.41006700
N	-1.29897500	-0.84730200	-0.29388200
H	-1.14784900	0.17798000	-0.36542500
C	4.68917800	0.73294100	0.91528000
C	5.78733000	-0.12186600	1.02134600
C	5.86821300	-1.26990600	0.22608100
C	4.84320800	-1.55331200	-0.68239000
C	3.74363900	-0.70054600	-0.79392100
C	3.64356300	0.45021800	0.01415700
H	4.63522400	1.61389000	1.54750200
H	6.57953600	0.10904900	1.72797300
H	6.72583700	-1.93166500	0.30669000
H	4.90545800	-2.43177800	-1.31846100
H	2.97903300	-0.91686600	-1.53432400
C	2.47982300	1.35544400	-0.06398300
C	2.57931900	2.83718400	0.11420900
H	2.08835200	3.34442400	-0.72404500
H	2.05564600	3.15833300	1.02361900
H	3.61845800	3.16237300	0.16745800
O	0.18820400	1.53867200	-0.41015400
N	1.29895400	0.84723400	-0.29394200
H	1.14783900	-0.17805500	-0.36539700

E-**8** (B3LYP/6-31+G**)

C	1.01031200	1.18612100	0.25251600
C	2.39857600	1.05323900	0.30760100
C	3.00057700	-0.18490700	0.06000800
C	2.20089300	-1.29018900	-0.24940100
C	0.81242100	-1.16213100	-0.30963500
C	0.19297500	0.07767000	-0.04663500
H	0.55814300	2.15081800	0.46068500

H	3.00993000	1.91871200	0.54756800
H	4.08150300	-0.28552600	0.09814200
H	2.65885300	-2.25204000	-0.46258000
H	0.21474300	-2.02440800	-0.59259300
C	-1.27297900	0.23626700	-0.07777100
C	-1.96253700	1.49493500	-0.49577000
H	-2.75218000	1.26071300	-1.21839800
H	-2.45410100	1.97698600	0.35937500
H	-1.26390300	2.20087000	-0.94528700
O	-3.32448900	-0.79935100	0.30512900
N	-2.02565300	-0.77063300	0.29246500
H	-1.55892700	-1.62290600	0.61932200

MeNCO (B3LYP/6-31+G**)

C	0.73924800	-0.04968300	-0.00004800
N	-0.41348900	-0.37896300	0.00002400
O	1.91326100	0.13909200	0.00002000
C	-1.75663700	0.16041200	0.00000400
H	-2.46855600	-0.66633000	0.00002700
H	-1.91942600	0.77104300	0.89288600
H	-1.91934600	0.77092400	-0.89297200

E-**Int1** (B3LYP/6-31+G**)

C	2.70720600	0.06973100	0.56792100
C	3.30036100	-1.18359100	0.72692900
C	2.69148700	-2.32610900	0.19670300
C	1.48555000	-2.20285600	-0.50115000
C	0.88944500	-0.95122700	-0.66548500
C	1.48473000	0.20542000	-0.12011900
H	3.18647300	0.94492900	0.99545300
H	4.23849900	-1.26701500	1.26854200
H	3.15667100	-3.30032400	0.31747000
H	1.01425700	-3.08039100	-0.93505900
H	-0.02603700	-0.87372700	-1.24523200
C	0.86274400	1.53611200	-0.25685400
C	1.64175500	2.80297000	-0.41104500
H	1.30377300	3.33759300	-1.30687900
H	1.46757000	3.47608900	0.43799200
H	2.71035200	2.60607800	-0.49861100
O	-1.13266700	2.72378900	-0.38153200
N	-0.44400600	1.63004000	-0.24239700
H	-1.00137200	0.77816300	-0.08787000
C	-3.15289700	-1.11459100	-0.37134900
N	-2.74978300	-0.40573200	0.51516400
O	-3.43253300	-1.77220600	-1.31734700
C	-3.14991700	-0.01470700	1.85839400
H	-3.39072400	-0.89781200	2.45620000
H	-2.32311600	0.52188100	2.32537000
H	-4.02100300	0.64481200	1.81061200

E-**TS2** (B3LYP/6-31+G**)

C	2.83201600	0.77144700	0.53680500
C	3.95403400	-0.05419200	0.62208900
C	3.92390600	-1.34309400	0.08016200
C	2.76341500	-1.80167800	-0.55250900
C	1.63782500	-0.98193300	-0.63901900
C	1.65454300	0.31337000	-0.08421900
H	2.86549600	1.76551400	0.97111100
H	4.85139400	0.31079500	1.11341900
H	4.80031600	-1.98182400	0.14186800
H	2.73779200	-2.79442700	-0.99242800
H	0.75831500	-1.34106900	-1.16539300
C	0.46873900	1.19200900	-0.13535200
C	0.55236500	2.68210900	-0.22730600
H	-0.11728200	3.04215100	-1.01547100
H	0.21909200	3.14515000	0.70991600
H	1.56829900	3.01068500	-0.44437400
O	-1.85642400	1.29611500	-0.14181400
N	-0.70943700	0.64489600	-0.08685600
H	-0.87091100	-0.37604900	0.02235400
C	-3.31060700	-0.01290400	0.06119000
N	-2.66120100	-1.07674200	0.15220400
O	-4.28656900	0.67724700	0.02575200
C	-3.37811400	-2.34740500	0.33504800
H	-4.07597100	-2.53732000	-0.48955200
H	-2.64611000	-3.15728100	0.36190900
H	-3.94075600	-2.35667800	1.27638200

E-**Int2** (B3LYP/6-31+G**)

C	2.81036100	0.83778500	0.48259800
C	3.98082400	0.08383700	0.56874300
C	4.01161800	-1.22637600	0.08150400

C	2.86381900	-1.78382400	-0.49273800
C	1.68749300	-1.04057000	-0.57327700
C	1.64739300	0.27846600	-0.07914700
H	2.79793800	1.85058000	0.87075900
H	4.86862800	0.52205400	1.01475600
H	4.92737800	-1.80744400	0.14059700
H	2.88671500	-2.79468500	-0.88855700
H	0.81491200	-1.47675400	-1.04965500
C	0.41123000	1.08244700	-0.12903700
C	0.40965900	2.57435600	-0.22660200
H	-0.33106100	2.90064800	-0.96211000
H	0.12341400	3.00968600	0.73882100
H	1.39009600	2.95289100	-0.51144900
O	-1.91527500	1.10804200	-0.13757500
N	-0.71933700	0.45634500	-0.06972300
H	-0.92977400	-0.56861000	0.06374000
C	-3.06360200	0.11545700	0.02014100
N	-2.61232800	-1.08804600	0.18090100
O	-4.14685300	0.69375300	-0.03943700
C	-3.61019900	-2.13684200	0.35168700
H	-4.24727900	-1.96488000	1.23145900
H	-4.27246000	-2.22852500	-0.52159100
H	-3.10141400	-3.09582500	0.48784600

E-**TS3** (B3LYP/6-31+G**)

C	2.79465700	0.85725300	0.43761200
C	3.96233300	0.09703100	0.51518600
C	3.97040500	-1.22796800	0.06940400
C	2.80220400	-1.79382700	-0.45398600
C	1.63011200	-1.04303400	-0.52651800
C	1.61324000	0.29149700	-0.07566300
H	2.80066900	1.88207300	0.79309400
H	4.86530600	0.54202700	0.92256600
H	4.88318100	-1.81444300	0.12173000
H	2.80610500	-2.81764600	-0.81596100
H	0.73889400	-1.48603000	-0.95978700
C	0.37848800	1.10229300	-0.12225500
C	0.39693200	2.59647900	-0.21410100
H	-0.41441100	2.94745500	-0.85614500
H	0.23964100	3.02974200	0.78182900
H	1.34917000	2.95507000	-0.60397300
O	-1.94393100	1.14307700	-0.11794800
N	-0.74624600	0.47247500	-0.06026100
H	-1.10115600	-0.59282400	0.07633900
C	-3.04084700	0.12502600	0.02312400
N	-2.52206300	-1.06210300	0.16590800
O	-4.16085000	0.62480200	-0.02456600
C	-3.42124300	-2.19454100	0.32159700
H	-4.09468500	-2.30873400	-0.53921600
H	-2.83004000	-3.11010800	0.41120300
H	-4.04394600	-2.10348100	1.22250000

s-trans-E-**9** (B3LYP/6-31+G**)

O	-1.82768500	0.99918100	-0.05307000
N	-0.63373300	0.22220300	0.01267500
C	0.41579200	0.96011900	-0.12280600
C	1.71209000	0.23023200	-0.06713800
C	2.87026900	0.88108900	0.39358600
C	1.80178700	-1.11980900	-0.45670000
C	4.08357700	0.19338200	0.47900600
H	2.82754400	1.92055400	0.70263200
C	3.01644900	-1.80067800	-0.37716900
H	0.92114500	-1.62726800	-0.83652100
C	4.16170300	-1.14792600	0.09391800
H	4.96670000	0.70854900	0.84621400
H	3.07112300	-2.83943200	-0.69076700
H	5.10737900	-1.67927900	0.15375600
C	0.38260100	2.45313200	-0.30447200
H	-0.46049800	2.74236400	-0.93526600
H	0.25398800	2.95226900	0.66397000
H	1.30723100	2.81346500	-0.75650500
C	-2.99664600	0.26172100	0.02897000
O	-4.04771800	0.89017800	-0.02391600
N	-2.87224900	-1.06792500	0.16170600
H	-1.93956500	-1.45866300	0.18845200
C	-4.03530500	-1.94295100	0.22278600
H	-3.67902700	-2.96779200	0.33777100
H	-4.67448800	-1.69327100	1.07544700
H	-4.63033300	-1.87617200	-0.69386500

The Cartesian coordinates (Å) in DMAc at the M06-2X/6-31+G(d,p) level of theory for

the favored reaction pathway (Table S7)

E-**7d** (M06-2X/6-31+G**)

C	-1.26303400	0.18641600	0.06625200
C	0.21855700	0.05469700	0.04093700
C	0.83513900	-1.18561800	0.26018300
C	1.01759300	1.17507000	-0.21930100
C	2.22160400	-1.30162700	0.21068300
H	0.22281700	-2.05437700	0.48113100
C	2.40608000	1.05505200	-0.27357000
H	0.55724900	2.14287700	-0.39599000
C	3.01206800	-0.18196200	-0.05775500
H	2.68744400	-2.26613200	0.38994700
H	3.01280100	1.93055500	-0.48466000
H	4.09352900	-0.27354800	-0.09286200
C	-1.91415200	1.48449200	0.44890800
H	-1.22395000	2.12176400	1.00195700
H	-2.24693300	2.02118900	-0.44664600
H	-2.79686800	1.29176500	1.06214400
N	-1.92321700	-0.85638500	-0.27902900
O	-3.29739700	-0.64281600	-0.23908400
H	-3.66751700	-1.49598100	-0.50717700

E-**7d•7d** (M06-2X/6-31+G**)

C	-2.42788000	-1.31774600	-0.05009500
C	-3.61418900	-0.42579300	0.02648300
C	-3.57573400	0.76234000	0.76985600
C	-4.78606600	-0.76027700	-0.66389000
C	-4.68344200	1.60533200	0.80825100
H	-2.68302500	1.01309500	1.33535600
C	-5.89203400	0.08803800	-0.62780000
H	-4.83183800	-1.67786400	-1.24361400
C	-5.84399200	1.27241800	0.10709100
H	-4.64391300	2.51868700	1.39428500
H	-6.79133100	-0.17790400	-1.17519300
H	-6.70791700	1.92948700	0.13958400
C	-2.57950800	-2.80076700	-0.22058200
H	-3.58973300	-3.12510000	0.02913500
H	-2.36193300	-3.08753600	-1.25552900
H	-1.86339800	-3.32140200	0.41923100
N	-1.28443300	-0.74177100	0.01094200
O	-0.21734300	-1.61727200	-0.07324200
H	0.55019600	-1.00630200	-0.03070500
C	2.42788200	1.31775000	-0.05004900
C	3.61418900	0.42579200	0.02650800
C	3.57573100	-0.76235800	0.76985400
C	4.78606700	0.76029000	-0.66385700
C	4.68343800	-1.60535300	0.80823000
H	2.68302100	-1.01312300	1.33534800
C	5.89203300	-0.08802800	-0.62778600
H	4.83184000	1.67788900	-1.24356100
C	5.84398800	-1.27242500	0.10707800
H	4.64390700	-2.51872100	1.39424400
H	6.79133100	0.17792400	-1.17517300
H	6.70791200	-1.92949600	0.13955700
C	2.57951300	2.80077300	-0.22050600
H	3.58973900	3.12510000	0.02921500
H	2.36193500	3.08756400	-1.25544600
H	1.86340500	3.32139700	0.41932100
N	1.28443400	0.74177500	0.01097500
O	0.21734600	1.61727900	-0.07319600
H	-0.55019500	1.00630800	-0.03068100

E-**TS1** (M06-2X/6-31+G**)

C	-2.28864000	-1.30219300	0.00020000
C	-3.48718100	-0.43410900	0.01863400
C	-3.47278500	0.80877500	0.66881200
C	-4.65485200	-0.85407900	-0.63169200
C	-4.60229700	1.62256700	0.65030100
H	-2.58839300	1.13069800	1.21230400
C	-5.78233000	-0.03528900	-0.64925200
H	-4.67753000	-1.81528500	-1.13727600
C	-5.75882800	1.20446800	-0.01034500
H	-4.58300900	2.57924000	1.16326500
H	-6.67921500	-0.36710900	-1.16337600
H	-6.63990100	1.83893700	-0.01959800
C	-2.37547500	-2.79161900	-0.07539500
H	-3.35650900	-3.14428500	0.24302200
H	-2.19421700	-3.12883000	-1.10254200
H	-1.60011900	-3.23333800	0.55465600
N	-1.13833300	-0.72894500	0.03016500
O	0.00618000	-1.43299000	0.01817100
H	0.83176000	-0.42375900	0.03268000

C	2.29310300	1.30998300	0.00145800
C	3.48657000	0.43405400	0.02004600
C	3.46650800	-0.80638900	0.67526700
C	4.65649000	0.84059800	-0.63538500
C	4.58921400	-1.62978900	0.65609800
H	2.58142900	-1.11850100	1.22325400
C	5.77796400	0.01323100	-0.65286400
H	4.68566200	1.79923700	-1.14566000
C	5.74735600	-1.22408500	-0.00955400
H	4.56357200	-2.58437100	1.17287100
H	6.67570900	0.33627800	-1.17124500
H	6.62328700	-1.86565100	-0.01927600
C	2.39278500	2.79945300	-0.07750000
H	3.38049100	3.14524600	0.22839100
H	2.20029400	3.14060300	-1.10136400
H	1.62929200	3.24770300	0.56272700
N	1.13847700	0.74356000	0.03417400
O	0.00467800	1.46099400	0.01860300
H	-0.86607400	0.40338900	0.02962200

E-**8•8** (M06-2X/6-31+G**)

C	-4.81497300	-0.82137300	0.48181600
C	-5.90351300	0.04778700	0.45315600
C	-5.77007500	1.32262800	-0.09707300
C	-4.54145900	1.72311800	-0.62470300
C	-3.45119800	0.85762100	-0.60032900
C	-3.57474900	-0.42137500	-0.03456200
H	-4.92520600	-1.80838100	0.92149600
H	-6.85658400	-0.27266500	0.86277600
H	-6.62007000	1.99770900	-0.12268900
H	-4.43393100	2.70717900	-1.07067600
H	-2.51193900	1.17348600	-1.04761600
C	-2.42698000	-1.34841300	0.03247900
C	-2.56799400	-2.83301200	0.01523100
H	-1.78006000	-3.26360600	-0.60830200
H	-2.44180800	-3.24157800	1.02484800
H	-3.54427300	-3.13047000	-0.36731300
O	-0.12938700	-1.53329100	0.19441500
N	-1.23948300	-0.84501100	0.13182100
H	-1.08662700	0.18419600	0.17545300
C	4.81495800	0.82142800	0.48177000
C	5.90353700	-0.04768000	0.45308500
C	5.77015900	-1.32251100	-0.09718500
C	4.54156200	-1.72304300	-0.62482700
C	3.45126100	-0.85759800	-0.60042700
C	3.57475400	0.42138600	-0.03462200
H	4.92514100	1.80842800	0.92148100
H	6.85659400	0.27280200	0.86271600
H	6.62018600	-1.99755100	-0.12282000
H	4.43408200	-2.70709600	-1.07083100
H	2.51201600	-1.17349000	-1.04772600
C	2.42693900	1.34836600	0.03244200
C	2.56786300	2.83297200	0.01516000
H	1.77998600	3.26349500	-0.60849600
H	2.44150800	3.24156600	1.02474300
H	3.54417200	3.13048100	-0.36726700
O	0.12934500	1.53313500	0.19442900
N	1.23947200	0.84490300	0.13182500
H	1.08667900	-0.18430700	0.17547700

E-**8** (M06-2X/6-31+G**)

C	-0.99737000	1.18103500	-0.26229100
C	-2.38309900	1.05519100	-0.32132700
C	-2.98873700	-0.17545000	-0.06372500
C	-2.19951700	-1.27981900	0.25899700
C	-0.81326100	-1.15827600	0.32275800
C	-0.19619800	0.07260100	0.04979700
H	-0.53328700	2.13966400	-0.47604600
H	-2.99020300	1.92006500	-0.57118400
H	-4.06945500	-0.27116700	-0.10502000
H	-2.66404500	-2.23625700	0.47896200
H	-0.21563300	-2.01821100	0.61418400
C	1.27102500	0.22581700	0.08412900
C	1.96212900	1.47234500	0.52229600
H	2.75261800	1.21753300	1.23500800
H	2.44827500	1.96249800	-0.32942300
H	1.26297900	2.16769600	0.98610600
O	3.30391200	-0.78408400	-0.32345500
N	2.01434600	-0.76528700	-0.30607400
H	1.54720500	-1.61280700	-0.64624000

MeNCO (M06-2X/6-31+G**)

C	-0.74706500	-0.04209700	-0.00000300
N	0.40809700	-0.32561800	-0.00000900
O	-1.92046000	0.11986400	0.00000400
C	1.77172100	0.13723900	0.00000200
H	2.43732000	-0.72545700	-0.00068800
H	1.96069600	0.73810100	-0.89216200
H	1.96105200	0.73691700	0.89288100

E-**Int1** (M06-2X/6-31+G**)

C	1.10871000	-1.84371600	0.53149400
C	0.20434100	-2.90241900	0.54514700
C	-0.93745200	-2.86173800	-0.25753800
C	-1.16045600	-1.76332000	-1.08899800
C	-0.25348200	-0.70588200	-1.11178400
C	0.87914700	-0.72568400	-0.28415100
H	1.98396800	-1.87234300	1.17467800
H	0.38758600	-3.75732700	1.18906600
H	-1.64261600	-3.68736100	-0.24459100
H	-2.03449800	-1.73440300	-1.73313700
H	-0.41939600	0.12875700	-1.78906700
C	1.80676000	0.41955300	-0.22598700
C	3.28012300	0.29017900	-0.03904300
H	3.79632400	0.87935700	-0.80400500
H	3.58086600	0.69788400	0.93312800
H	3.59508200	-0.75074000	-0.10908200
O	1.98648900	2.71780700	-0.27366500
N	1.31258300	1.61846900	-0.30797200
H	0.29218900	1.71535900	-0.38428400
C	-2.52407100	1.44930600	0.01301300
N	-1.67119900	1.39420200	0.85218300
O	-3.30067500	1.61350000	-0.86013900
C	-1.25213500	0.56775200	1.96557100
H	-1.33969200	-0.49034800	1.70468800
H	-0.21248600	0.80011400	2.20020100
H	-1.87244800	0.78771900	2.83701500

E-**TS2** (M06-2X/6-31+G**)

C	2.83308800	0.77309100	0.50929600
C	3.94876800	-0.05584700	0.59855400
C	3.90223500	-1.35212800	0.08464500
C	2.73540500	-1.81592100	-0.52447100
C	1.61652400	-0.99204100	-0.61550400
C	1.65349000	0.30703400	-0.08700600
H	2.87214300	1.77830700	0.91883800
H	4.85446600	0.31202700	1.07080600
H	4.77442900	-1.99539900	0.14998600
H	2.69942300	-2.81725200	-0.94230000
H	0.72588800	-1.35302800	-1.12348400
C	0.47421100	1.19502800	-0.13928300
C	0.57280400	2.67864700	-0.25420600
H	-0.17183000	3.03924900	-0.96890200
H	0.35119500	3.14773000	0.71149700
H	1.56872800	2.98087900	-0.57657900
O	-1.82998500	1.31498400	-0.09556100
N	-0.69945500	0.66380000	-0.05675700
H	-0.84245500	-0.35658100	0.06061600
C	-3.34556300	-0.02793000	0.06897700
N	-2.67412400	-1.06754400	0.14458100
O	-4.28230200	0.69423900	0.02593500
C	-3.35378000	-2.35810300	0.29696400
H	-2.91585600	-3.07122500	-0.40432100
H	-3.19634800	-2.73390400	1.31140200
H	-4.42952900	-2.28936100	0.10688200

E-**Int2** (M06-2X/6-31+G**)

C	2.78775700	0.84692500	0.46166900
C	3.95907600	0.09995000	0.55273900
C	3.98864400	-1.21466400	0.08740700
C	2.84262000	-1.78561700	-0.46875500
C	1.66548300	-1.04913100	-0.55374900
C	1.63216800	0.27119800	-0.08190900
H	2.76894600	1.86812200	0.82929700
H	4.84867600	0.54682700	0.98499400
H	4.90605200	-1.79192300	0.15042000
H	2.86729900	-2.80280300	-0.84633500
H	0.78745400	-1.49323500	-1.01429400
C	0.39432600	1.07355500	-0.13692100
C	0.40082900	2.56097200	-0.24135500
H	-0.42453700	2.89869100	-0.87065800
H	0.25901700	2.99019400	0.75752800
H	1.34699100	2.91422900	-0.64838100
O	-1.90893800	1.09935200	-0.11919500

N	-0.72390500	0.44755400	-0.06170900
H	-0.95574600	-0.58689700	0.07398200
C	-3.02124000	0.12424600	0.02453100
N	-2.56962000	-1.08268100	0.16940600
O	-4.11503300	0.67279300	-0.02161700
C	-3.58324000	-2.10967600	0.32923100
H	-4.23261900	-1.91412300	1.19287500
H	-4.22779800	-2.19156800	-0.55618600
H	-3.09584600	-3.07532700	0.48205800

E-**TS3** (M06-2X/6-31+G**)

C	2.78137700	0.85308100	0.44302200
C	3.94949800	0.10004400	0.52959700
C	3.96569500	-1.22051500	0.08103500
C	2.80936800	-1.79121900	-0.45402200
C	1.63612100	-1.04812000	-0.53480900
C	1.61612100	0.27835200	-0.07994100
H	2.77335400	1.87918700	0.79725100
H	4.84684900	0.54682400	0.94567800
H	4.88017100	-1.80276400	0.14081600
H	2.82312200	-2.81350000	-0.81824200
H	0.74887800	-1.49198100	-0.97752400
C	0.38073900	1.08660700	-0.13271300
C	0.40125600	2.57509500	-0.23078700
H	-0.45921900	2.93056300	-0.79930600
H	0.33875800	2.99958200	0.77811800
H	1.32364200	2.91555600	-0.69977600
O	-1.92232900	1.11838500	-0.11376800
N	-0.73620600	0.46079200	-0.06006600
H	-1.03215600	-0.59223500	0.07512500
C	-3.01263900	0.12774600	0.02470100
N	-2.52673900	-1.07034800	0.16108600
O	-4.12264700	0.64026000	-0.01536400
C	-3.49367900	-2.13974100	0.31963900
H	-4.12679000	-1.98865600	1.20352600
H	-4.15537000	-2.22534900	-0.55215100
H	-2.96395000	-3.08747800	0.43807100

s-trans-E-**9** (M06-2X/6-31+G**)

O	-1.80861900	0.99284100	-0.03338700
N	-0.63706400	0.22800900	0.02184800
C	0.40858200	0.95653300	-0.11987000
C	1.70282100	0.22484300	-0.06500700
C	2.86144000	0.88639800	0.35945800
C	1.77813000	-1.12972700	-0.42022500
C	4.07262200	0.20018800	0.44315600
H	2.82036200	1.93464300	0.64022300
C	2.99010800	-1.80929000	-0.34270400
H	0.88698800	-1.64229100	-0.76921800
C	4.14056000	-1.14717600	0.09181100
H	4.96255600	0.72163700	0.78224100
H	3.03897300	-2.85576600	-0.62835100
H	5.08559900	-1.67875100	0.15063000
C	0.38230100	2.44545400	-0.30315200
H	-0.48364100	2.74075900	-0.89671800
H	0.30384000	2.94065100	0.67130600
H	1.29222600	2.78931300	-0.79490300
C	-2.96962700	0.25935800	0.03475500
O	-4.01794300	0.87865000	-0.00825000
N	-2.84843000	-1.06973700	0.14397600
H	-1.92457300	-1.47856100	0.17139300
C	-4.03115600	-1.91087900	0.19296000
H	-3.70460600	-2.94626100	0.28540200
H	-4.65683600	-1.65567400	1.05237800
H	-4.62460800	-1.80373200	-0.71915100

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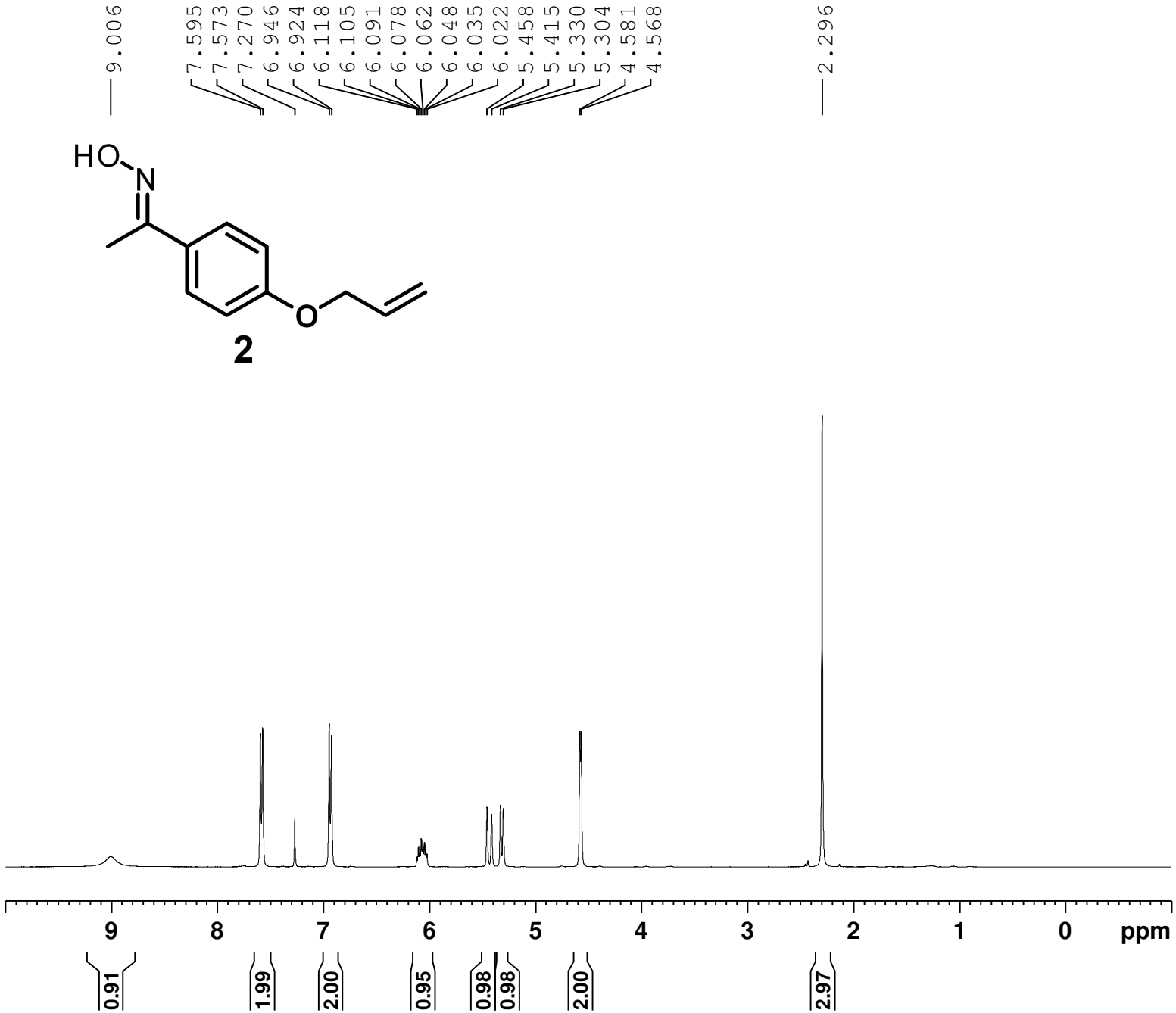
12. NMR spectra

See the next page.

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PROCNO                       1

F2 - Acquisition Parameters
Date_                20151221
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INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                 12019.230 Hz
FIDRES               0.183399 Hz
AQ                   2.7262976 sec
RG                       70.53
DW                      41.600 usec
DE                       6.50 usec
TE                      296.8 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                        1H
P1                       14.00 usec
PLW1               12.00000000 W

F2 - Processing parameters
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SF                 400.1300066 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
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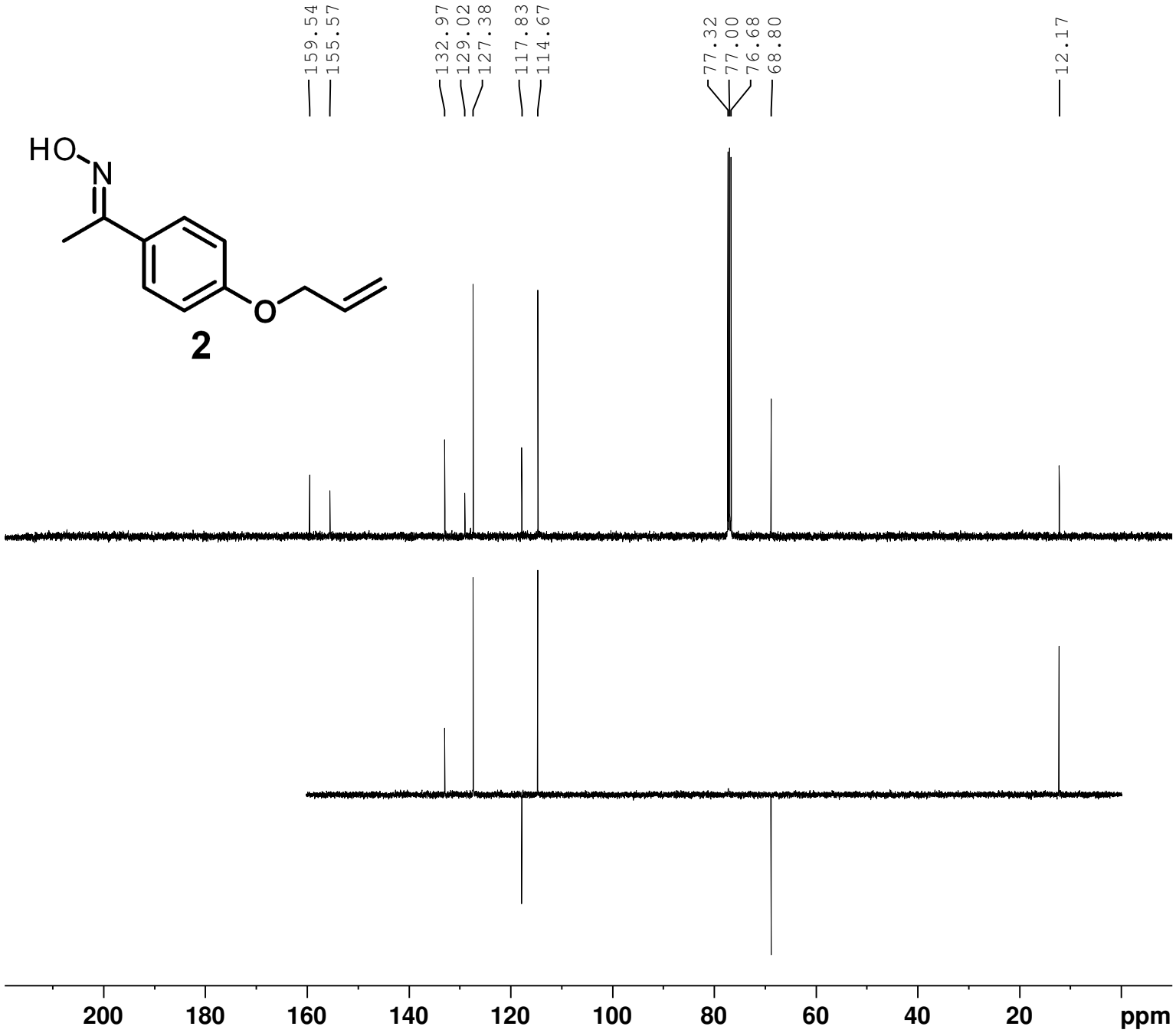


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EXPNO                  3
PROCNO                 1

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INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    70
DS                     4
SWH            16129.032 Hz
FIDRES          0.246110 Hz
AQ             2.0316160 sec
RG                208.31
DW                31.000 usec
DE                 6.50 usec
TE                297.7 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6208171 MHz
NUC1                 13C
P1                  9.80 usec
P13              2000.00 usec
PLW0      0 W
PLW1        47.97299957 W
SPNAM[5]     Crp60comp.4
SPOAL5             0.500
SPOFFS5   0 Hz
SPW5          7.03950024 W

======== CHANNEL f2 ========
SFO2          400.1312797 MHz
NUC2                 1H
CPDPRG[2          waltz16
P3                14.60 usec
P4                29.20 usec
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.31566000 W

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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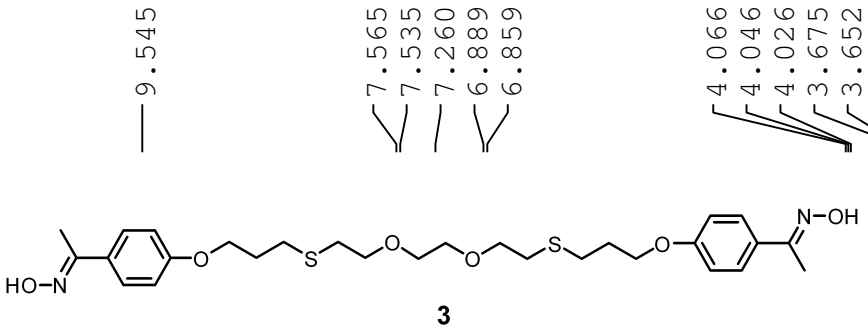

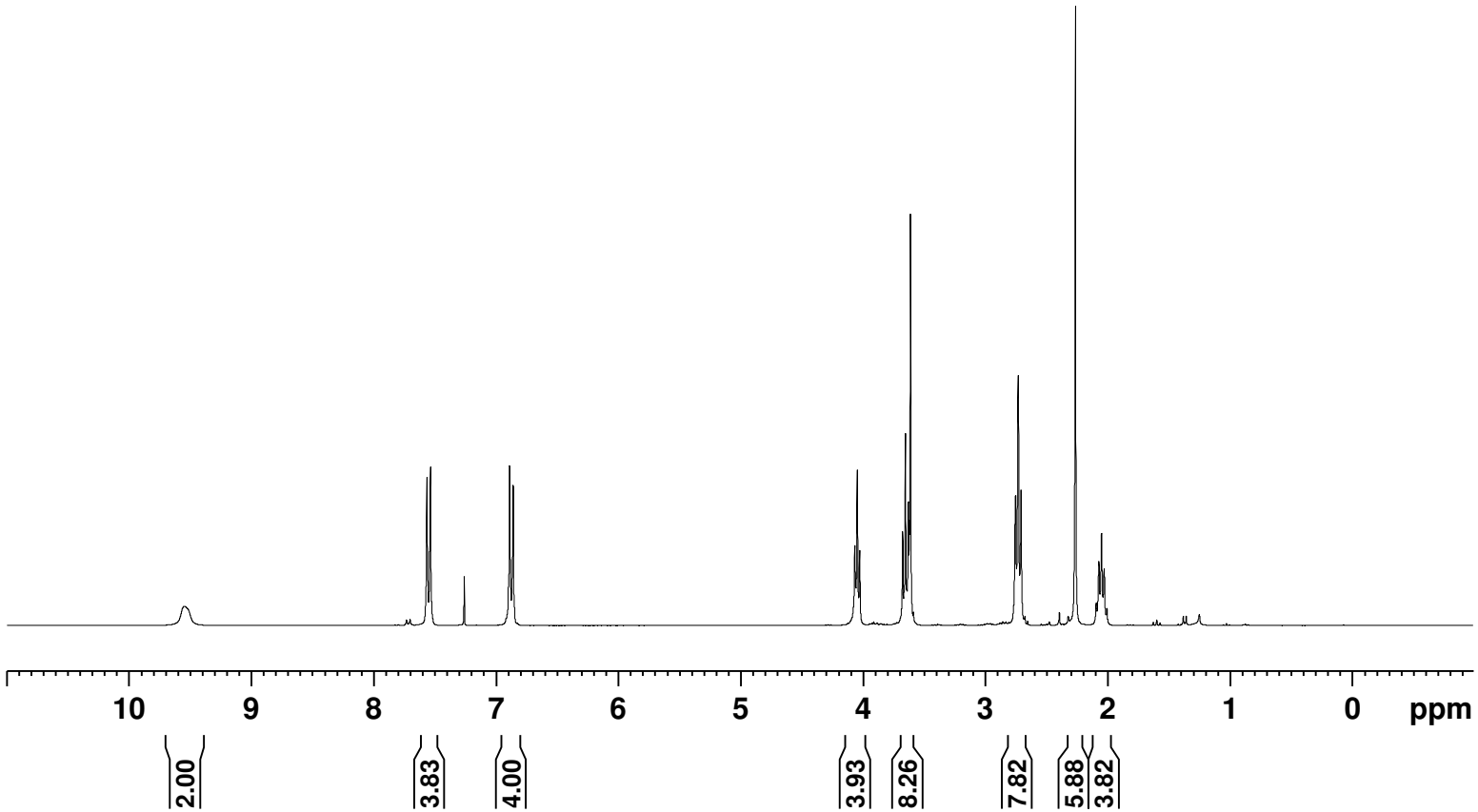


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EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20160106
Time                     21.27
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          10
DS                           2
SWH                   6009.615 Hz
FIDRES                0.091699 Hz
AQ                    5.4525952 sec
RG                       50.51
DW                      83.200 usec
DE                       6.50 usec
TE                      295.1 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                300.1818537 MHz
NUC1                        1H
P1                       12.00 usec
PLW1                18.00000000 W

F2 - Processing parameters
SI                       65536
SF                  300.1800074 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
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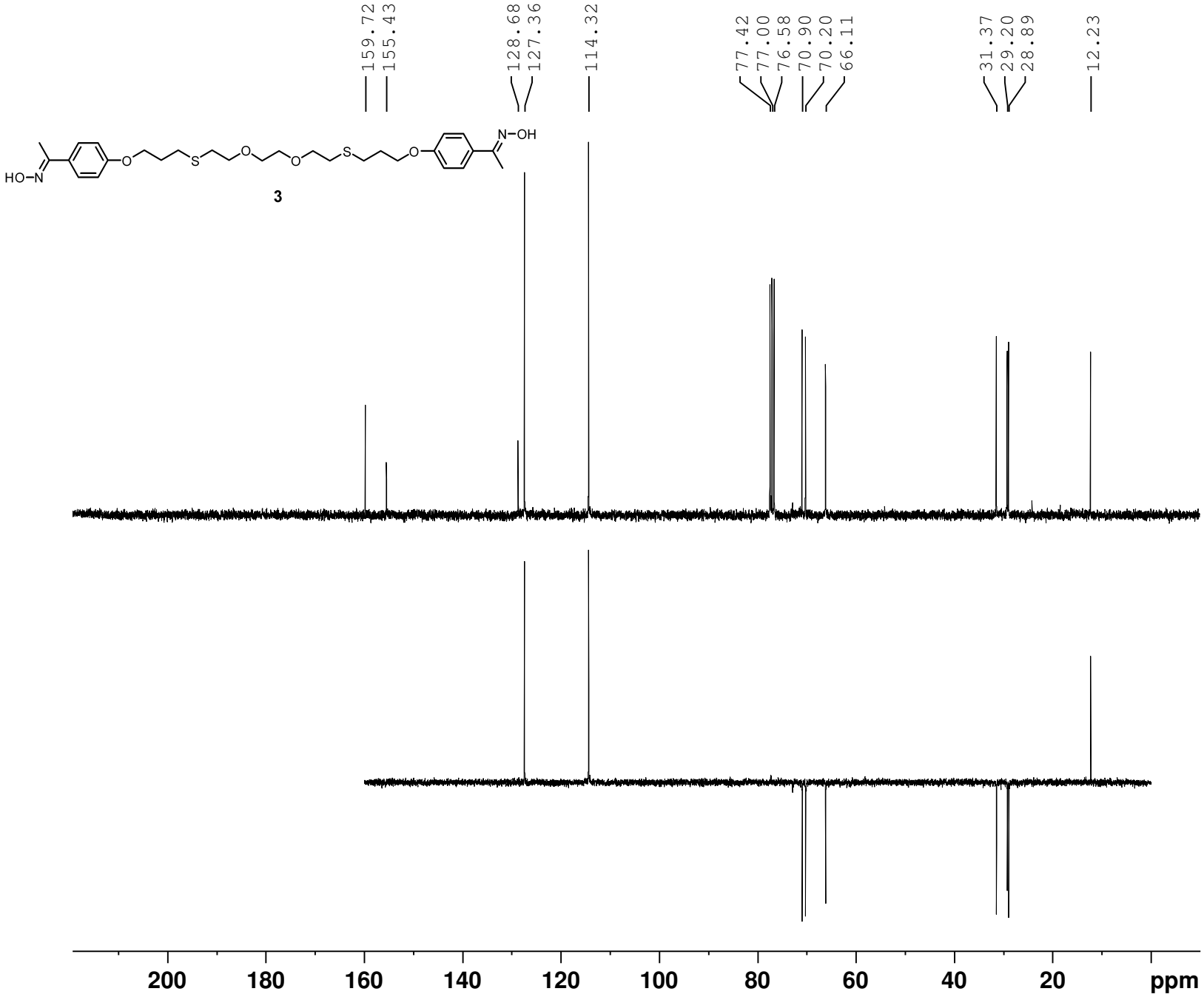


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Current Data Parameters
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EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160106
Time               21.49
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    40
DS                     4
SWH           12077.295 Hz
FIDRES         0.184285 Hz
AQ            2.7131903 sec
RG               208.31
DW                41.400 usec
DE                 6.50 usec
TE                295.8 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4863591 MHz
NUC1                  13C
P1                12.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1        42.00000000 W
SPNAM[5]    Crp60comp.4
SPOAL5              0.500
SPOFFS5   0 Hz
SPW5           9.24069977 W

======== CHANNEL f2 ========
SFO2         300.1809600 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                12.00 usec
P4                24.00 usec
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.31999999 W

F2 - Processing parameters
SI                 32768
SF            75.4803210 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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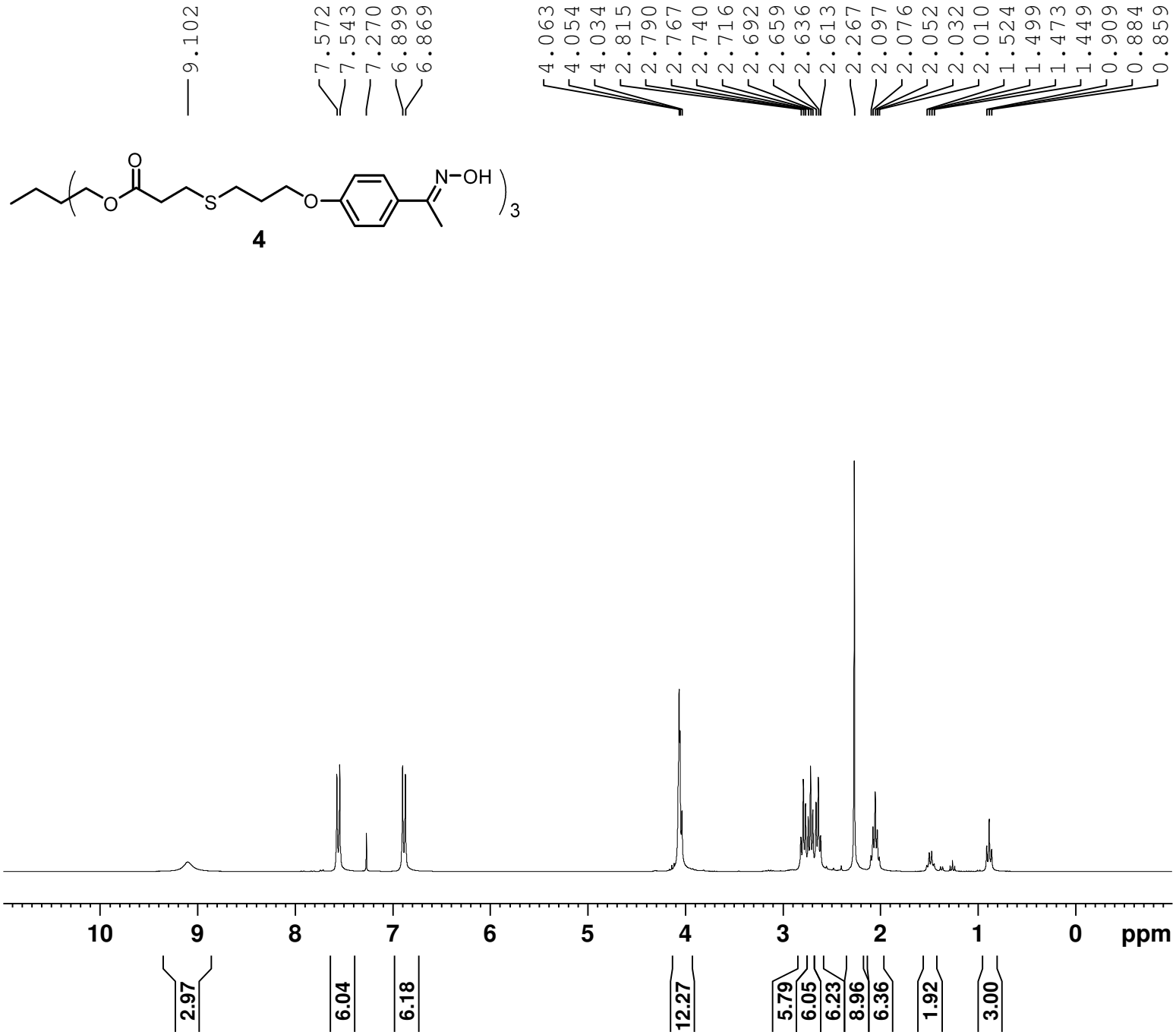


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Current Data Parameters
NAME                  liuwx-42
EXPNO                        1
PROCNO                       1

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Date_                 20151221
Time                     13.09
INSTRUM                  spect
PROBHD    5 mm DUL 13C-1
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          10
DS                           2
SWH                   6009.615 Hz
FIDRES                0.091699 Hz
AQ                    5.4525952 sec
RG                       56.09
DW                      83.200 usec
DE                       6.50 usec
TE                       295.9 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                300.1818537 MHz
NUC1                        1H
P1                       12.00 usec
PLW1                18.00000000 W

F2 - Processing parameters
SI                       65536
SF                  300.1800044 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
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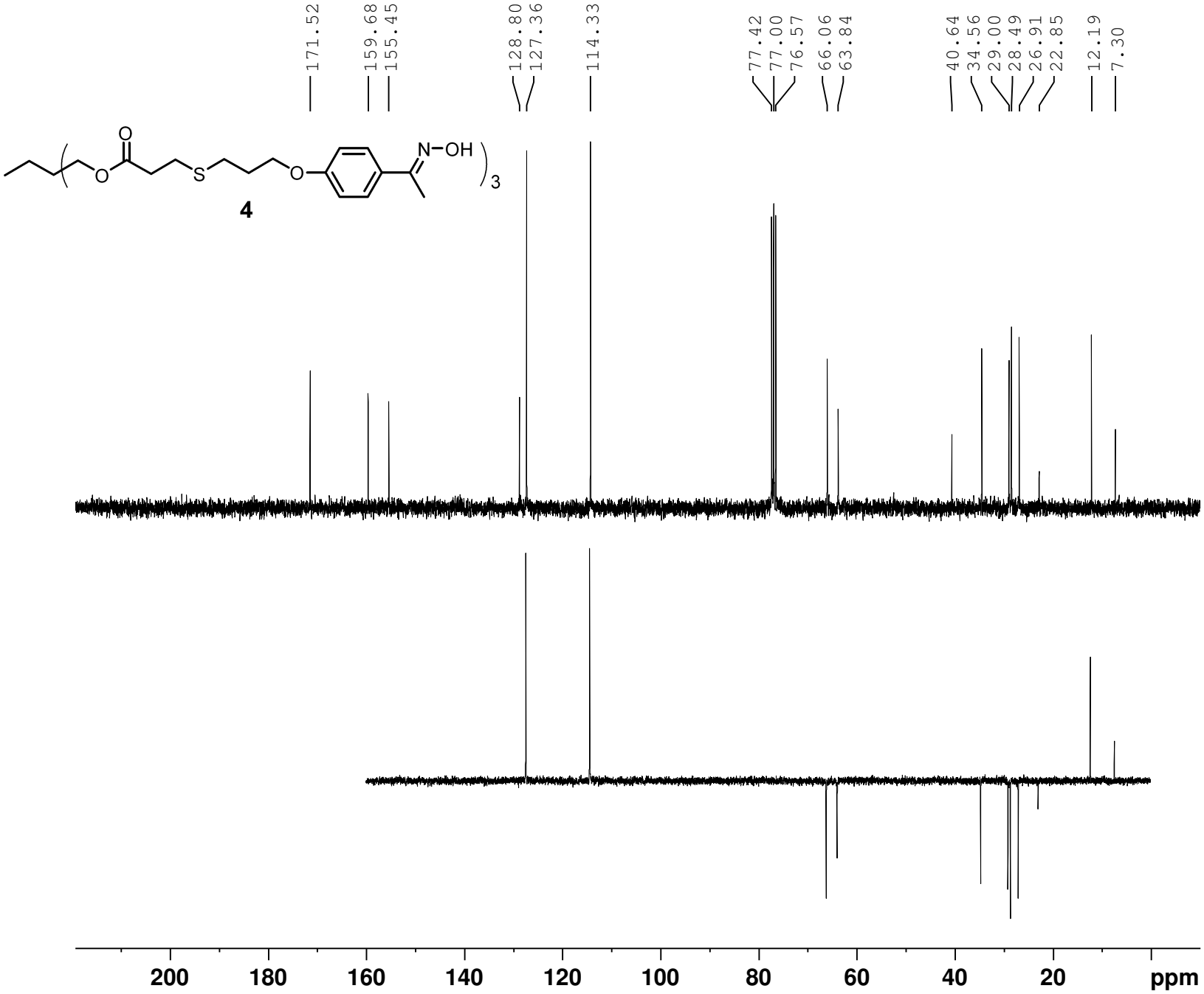


```
Current Data Parameters
NAME            liuwx-42
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151221
Time               13.21
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    60
DS                     4
SWH           12077.295 Hz
FIDRES         0.184285 Hz
AQ            2.7131903 sec
RG               208.31
DW               41.400 usec
DE                6.50 usec
TE                296.5 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4863591 MHz
NUC1                  13C
P1                12.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1        42.00000000 W
SPNAM[5]    Crp60comp.4
SPOAL5              0.500
SPOFFS5   0 Hz
SPW5           9.24069977 W

======== CHANNEL f2 ========
SFO2         300.1809600 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                12.00 usec
P4                24.00 usec
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.31999999 W

F2 - Processing parameters
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SF            75.4803210 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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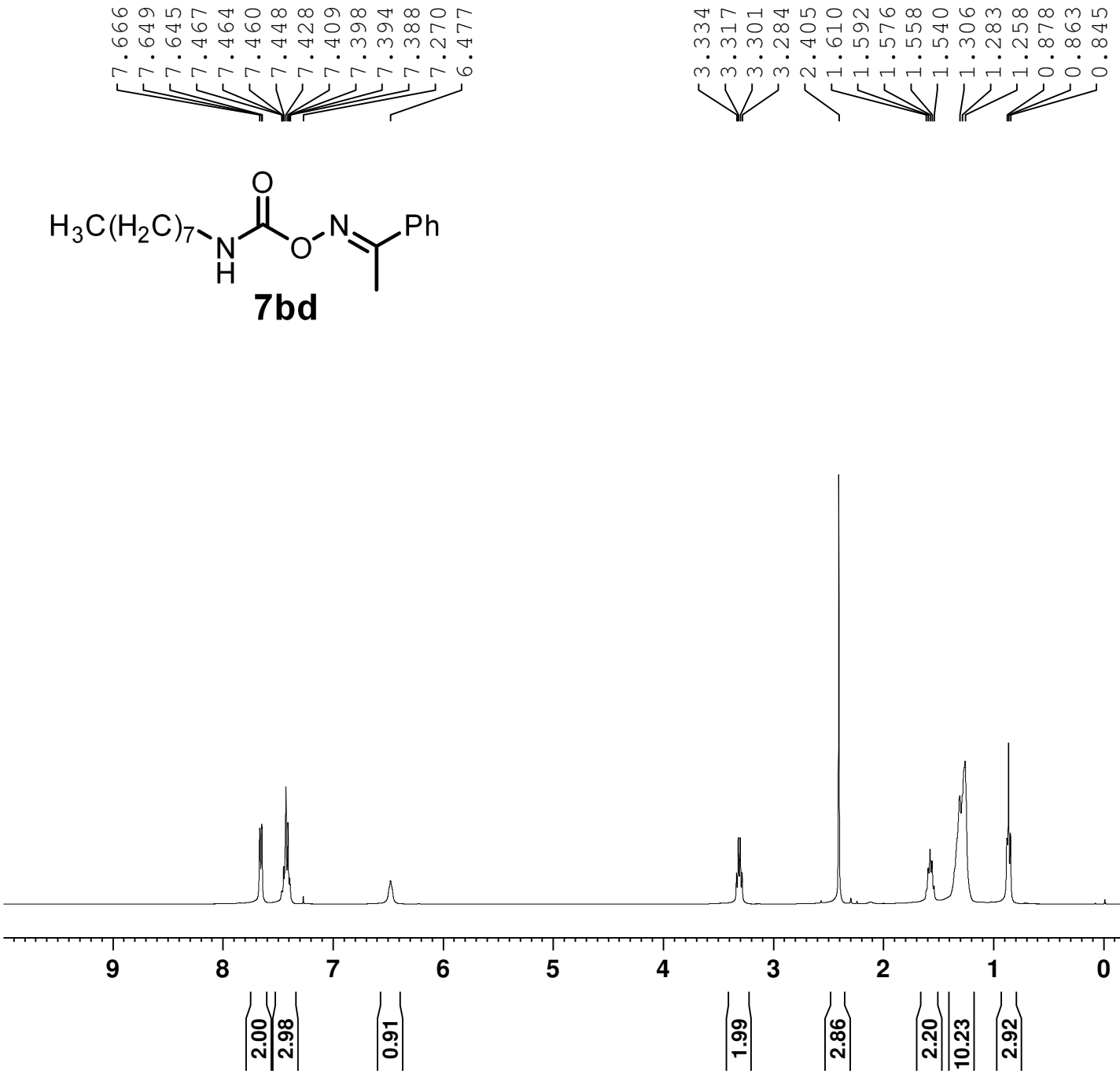


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Current Data Parameters
NAME                  liuwx-3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
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Time                   22.17
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                12019.230 Hz
FIDRES              0.183399 Hz
AQ                 2.7262976 sec
RG                     22.38
DW                    41.600 usec
DE                     6.50 usec
TE                     299.2 K
D1                 2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                     14.00 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                     65536
SF               400.1300059 MHz
WDW                       EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```
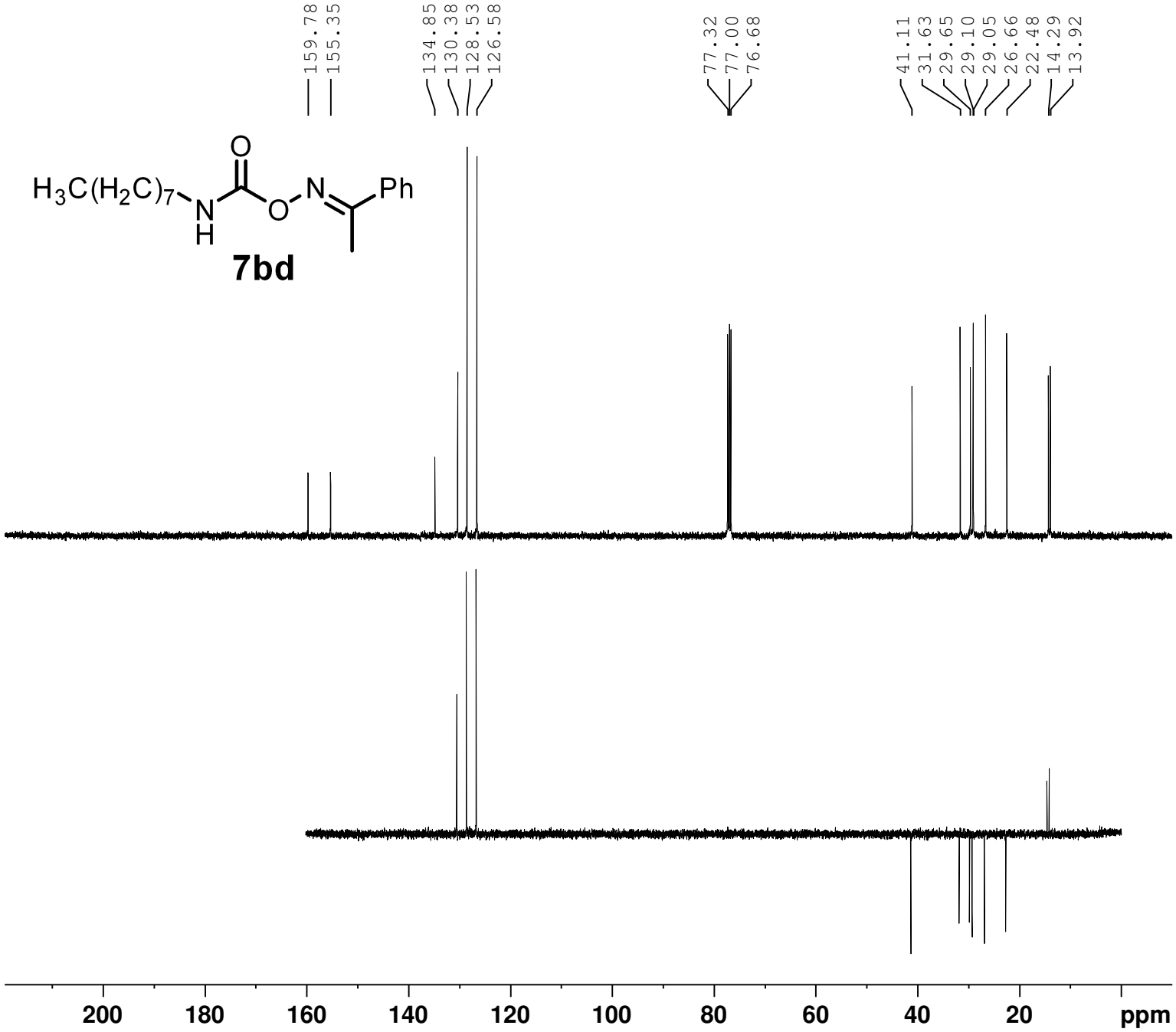
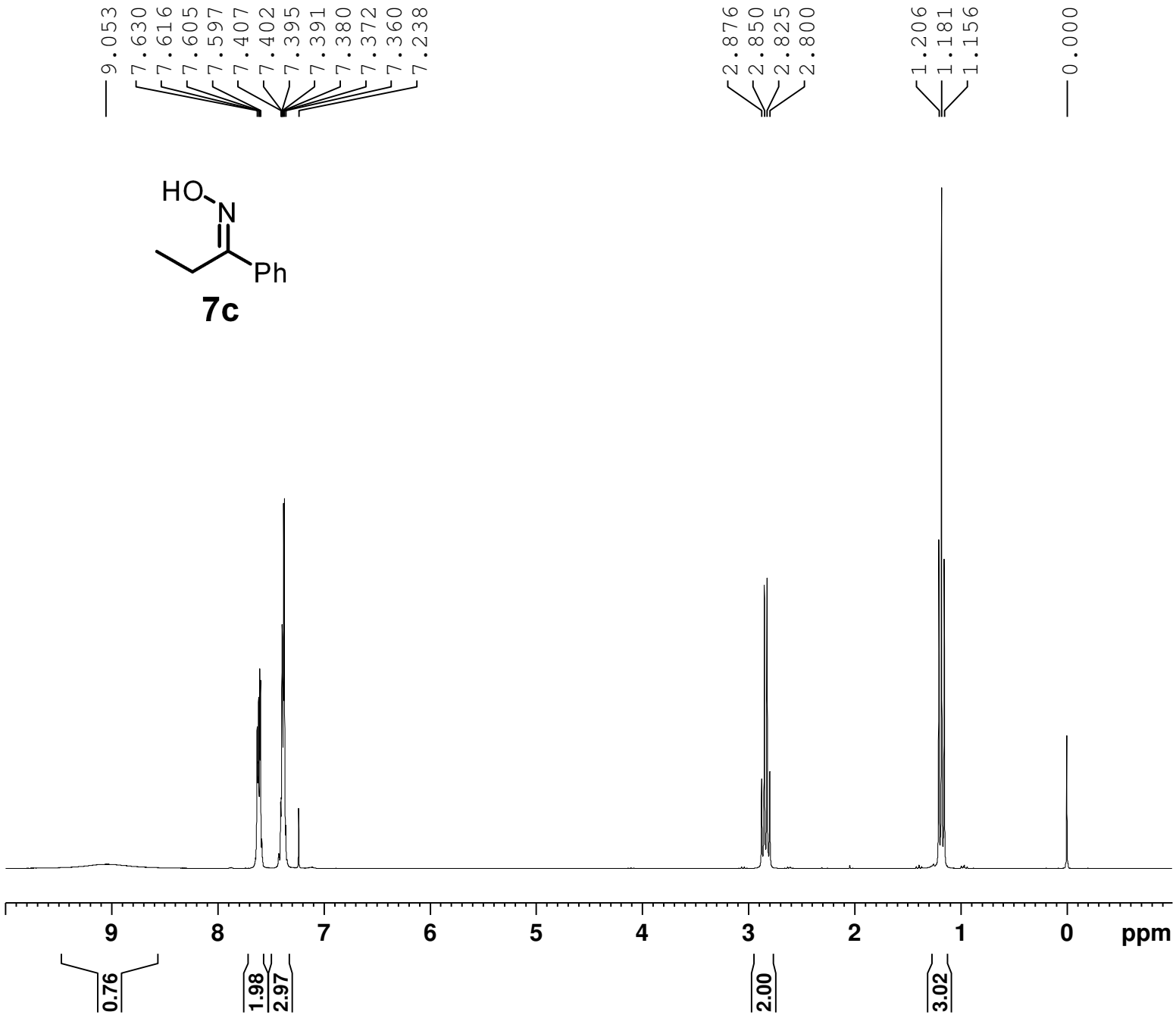
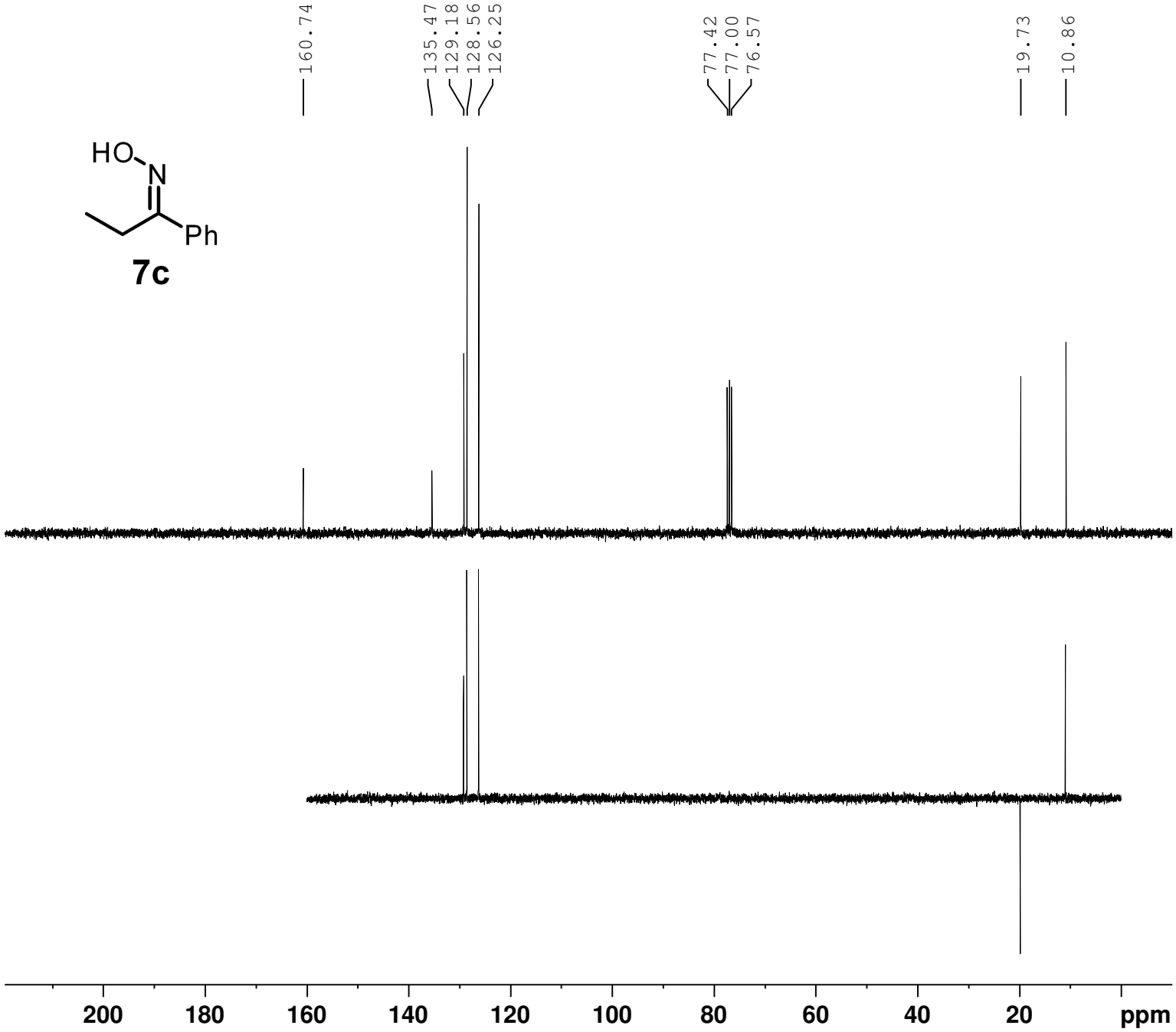



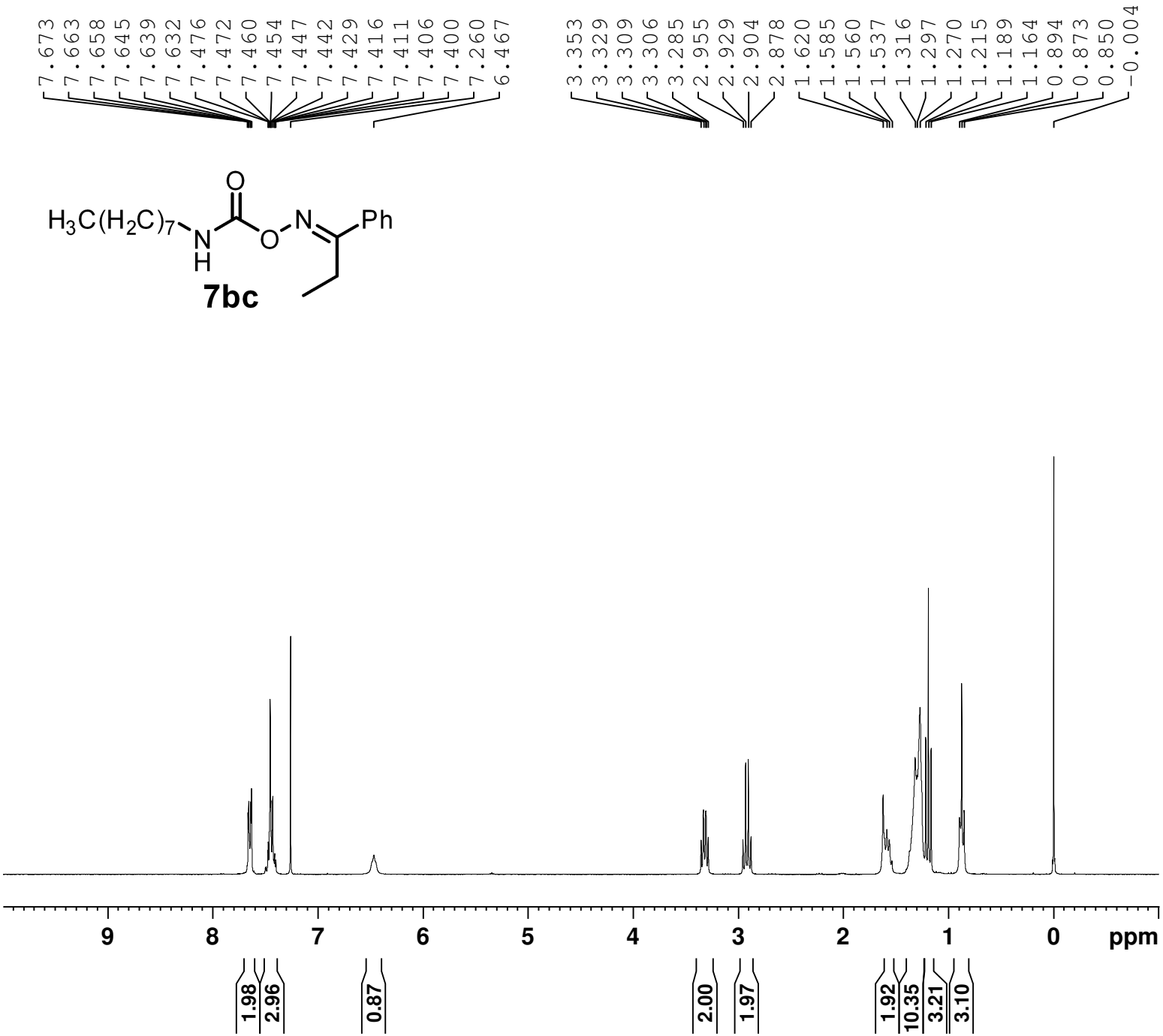

```
Current Data Parameters
NAME                  liuwx-3
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20161128
Time                    3.20
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG            deptsp135
TD                     65536
SOLVENT                CDCl3
NS                       100
DS                         4
SWH                16129.032 Hz
FIDRES              0.246110 Hz
AQ                  2.0316160 sec
RG                     208.31
DW                     31.000 usec
DE                      6.50 usec
TE                     300.2 K
CNST2             145.0000000
D1                  2.00000000 sec
D2                  0.00344828 sec
D12                 0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1              100.6208171 MHz
NUC1                      13C
P1                      9.80 usec
P13                  2000.00 usec
PLW0      0 W
PLW1             47.97299957 W
SPNAM[5]     Crp60comp.4
SPOAL5                 0.500
SPOFFS5   0 Hz
SPW5              7.03950024 W

======== CHANNEL f2 ========
SFO2              400.1312797 MHz
NUC2                       1H
CPDPRG[2              waltz16
P3                     14.60 usec
P4                     29.20 usec
PCPD2                  90.00 usec
PLW2             11.99499989 W
PLW12             0.31566000 W

F2 - Processing parameters
SI                     32768
SF                100.6127690 MHz
WDW                       EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```




```
Current Data Parameters
NAME                  liuwx38
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20161004
Time                   13.20
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        10
DS                         2
SWH                 6009.615 Hz
FIDRES              0.091699 Hz
AQ                  5.4525952 sec
RG                     92.23
DW                    83.200 usec
DE                     6.50 usec
TE                     297.4 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            300.1818537 MHz
NUC1                       1H
P1                    12.00 usec
PLW1            18.00000000 W

F2 - Processing parameters
SI                     65536
SF              300.1800138 MHz
WDW                       EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```




```
Current Data Parameters
NAME                  liuwx38
EXPNO                       6
PROCNO                      1

F2 - Acquisition Parameters
Date_               20161004
Time                   13.33
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG            deptsp135
TD                     65536
SOLVENT                CDCl3
NS                        26
DS                         4
SWH                12077.295 Hz
FIDRES              0.184285 Hz
AQ                 2.7131903 sec
RG                    208.31
DW                    41.400 usec
DE                     6.50 usec
TE                    298.0 K
CNST2             145.0000000
D1                 2.00000000 sec
D2                 0.00344828 sec
D12                0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               75.4863591 MHz
NUC1                      13C
P1                     12.00 usec
P13                  2000.00 usec
PLW0      0 W
PLW1             42.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5                 0.500
SPOFFS5   0 Hz
SPW5              9.24069977 W

======== CHANNEL f2 ========
SFO2              300.1809600 MHz
NUC2                       1H
CPDPRG[2             waltz16
P3                     12.00 usec
P4                     24.00 usec
PCPD2                  90.00 usec
PLW2             18.00000000 W
PLW12             0.31999999 W

F2 - Processing parameters
SI                     32768
SF                75.4803210 MHz
WDW                       EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```

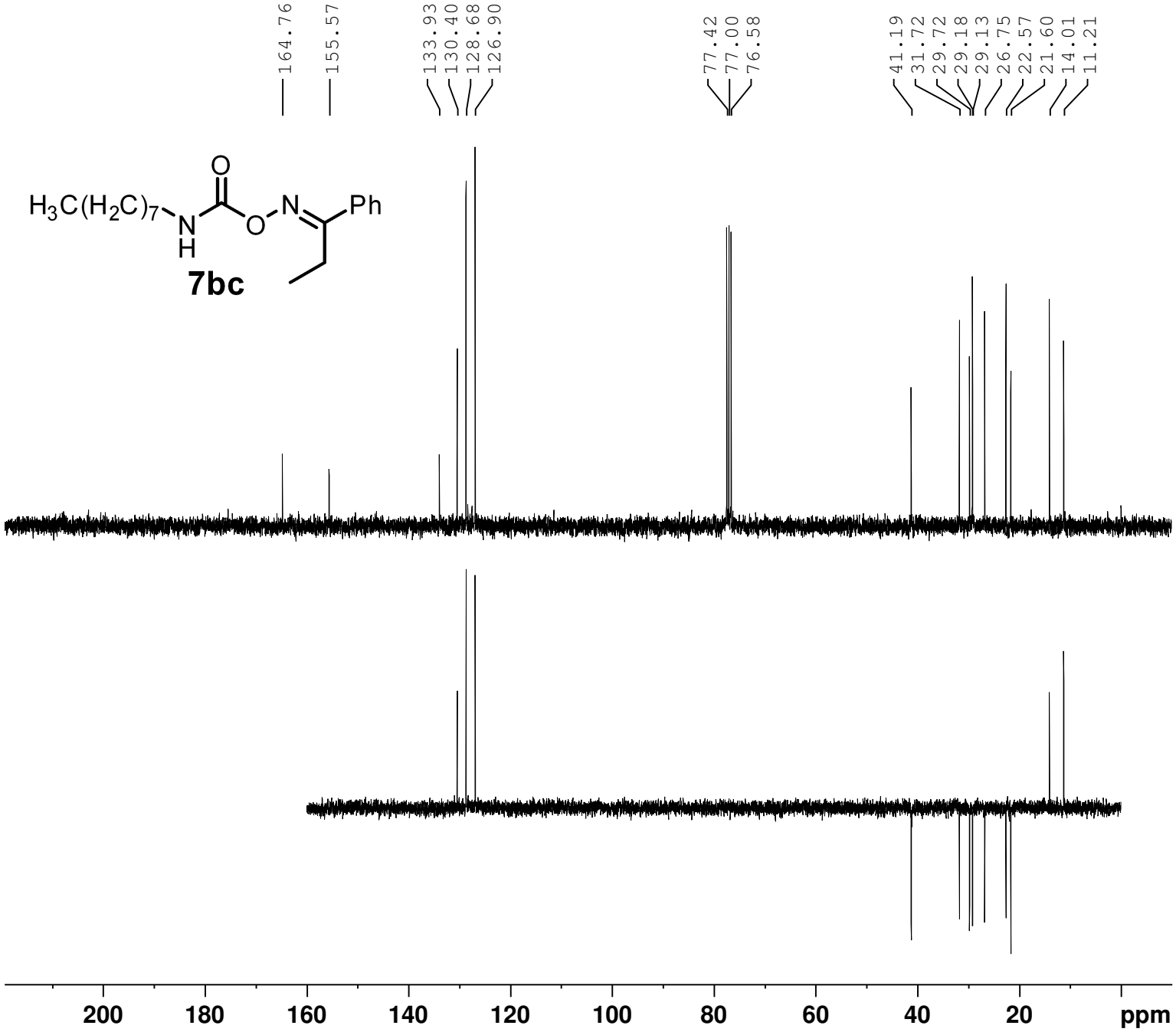


Current Data Parameters
NAME liuwx107
EXPNO 5
PROCNO 1

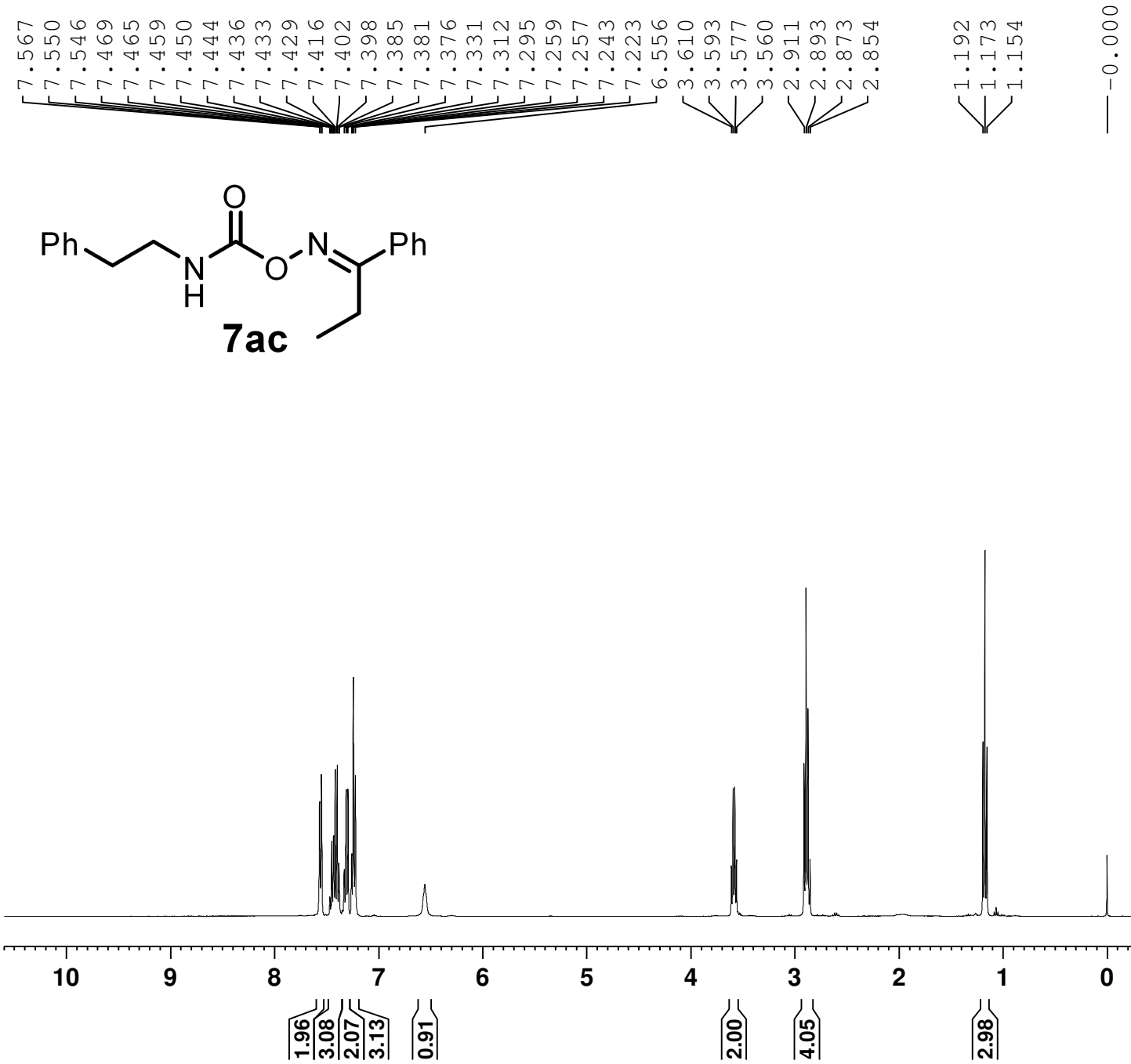
F2 - Acquisition Parameters
Date_ 20161006
Time 11.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 163.23
DW 83.200 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

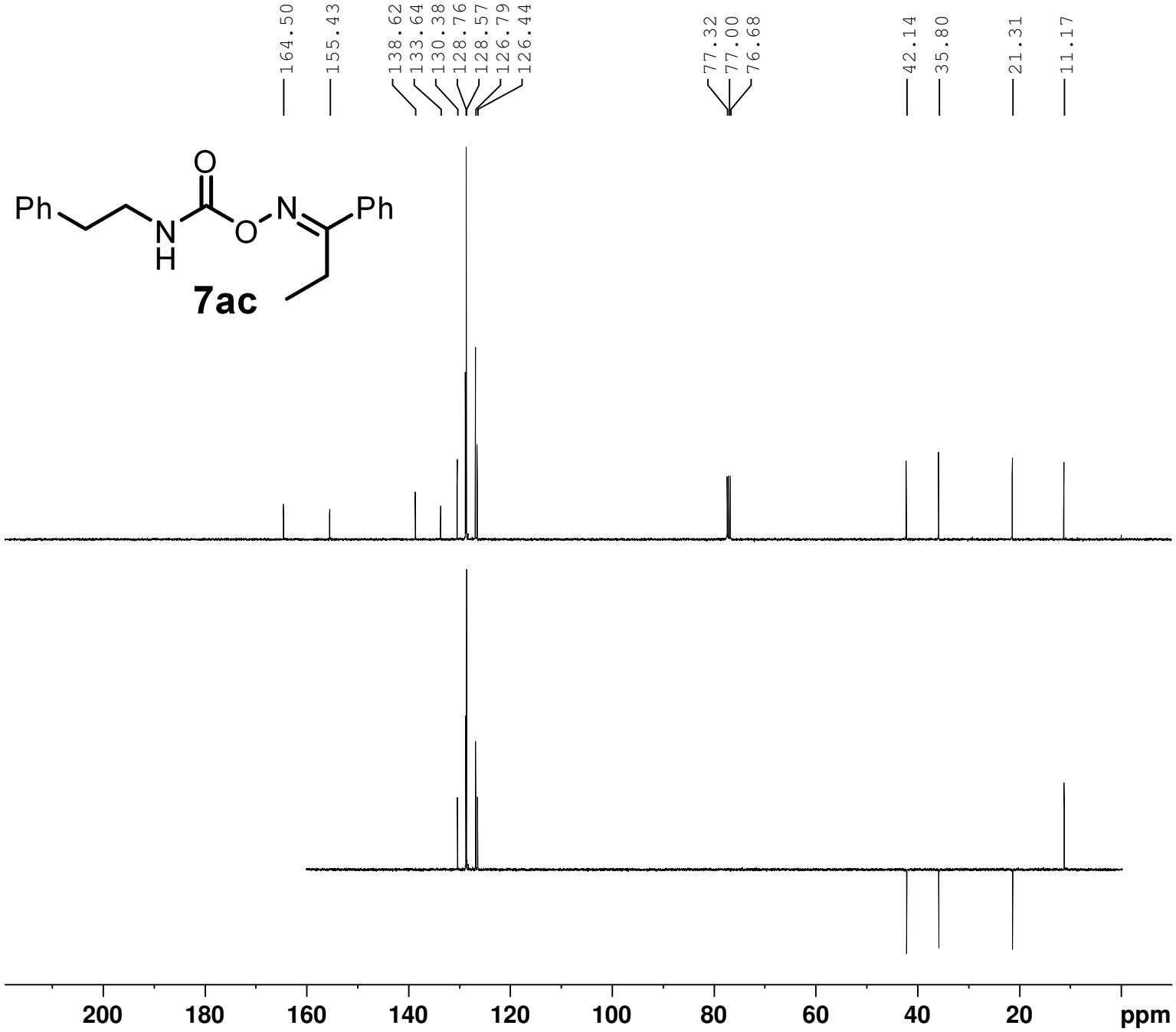
F2 - Processing parameters
SI 65536
SF 300.1800074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



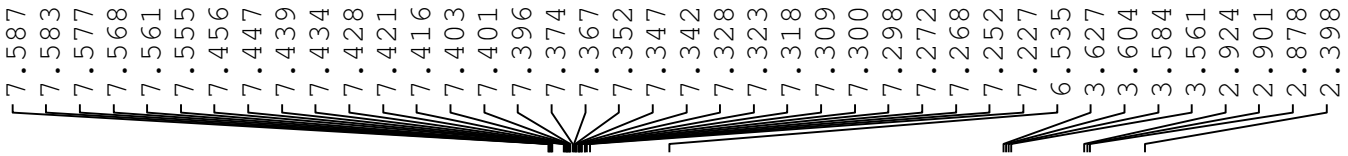

```
Current Data Parameters
NAME            liuwx107
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160926
Time               21.44
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    30
DS                     4
SWH            12077.295 Hz
FIDRES          0.184285 Hz
AQ             2.7131903 sec
RG                208.31
DW                41.400 usec
DE                 6.50 usec
TE                300.2 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4863591 MHz
NUC1                  13C
P1                12.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1        42.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5              0.500
SPOFFS5   0 Hz
SPW5           9.24069977 W

======== CHANNEL f2 ========
SFO2         300.1809600 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                12.00 usec
P4                24.00 usec
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.31999999 W

F2 - Processing parameters
SI                 32768
SF            75.4803210 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

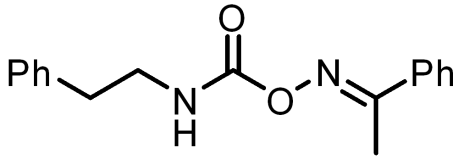



```
Current Data Parameters
NAME                  liuwx201
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20160629
Time                     23.04
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         10
DS                          0
SWH                 12019.230 Hz
FIDRES               0.183399 Hz
AQ                   2.7262976 sec
RG                       32.22
DW                      41.600 usec
DE                       6.50 usec
TE                      299.6 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.00 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                      65536
SF                 400.1300150 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



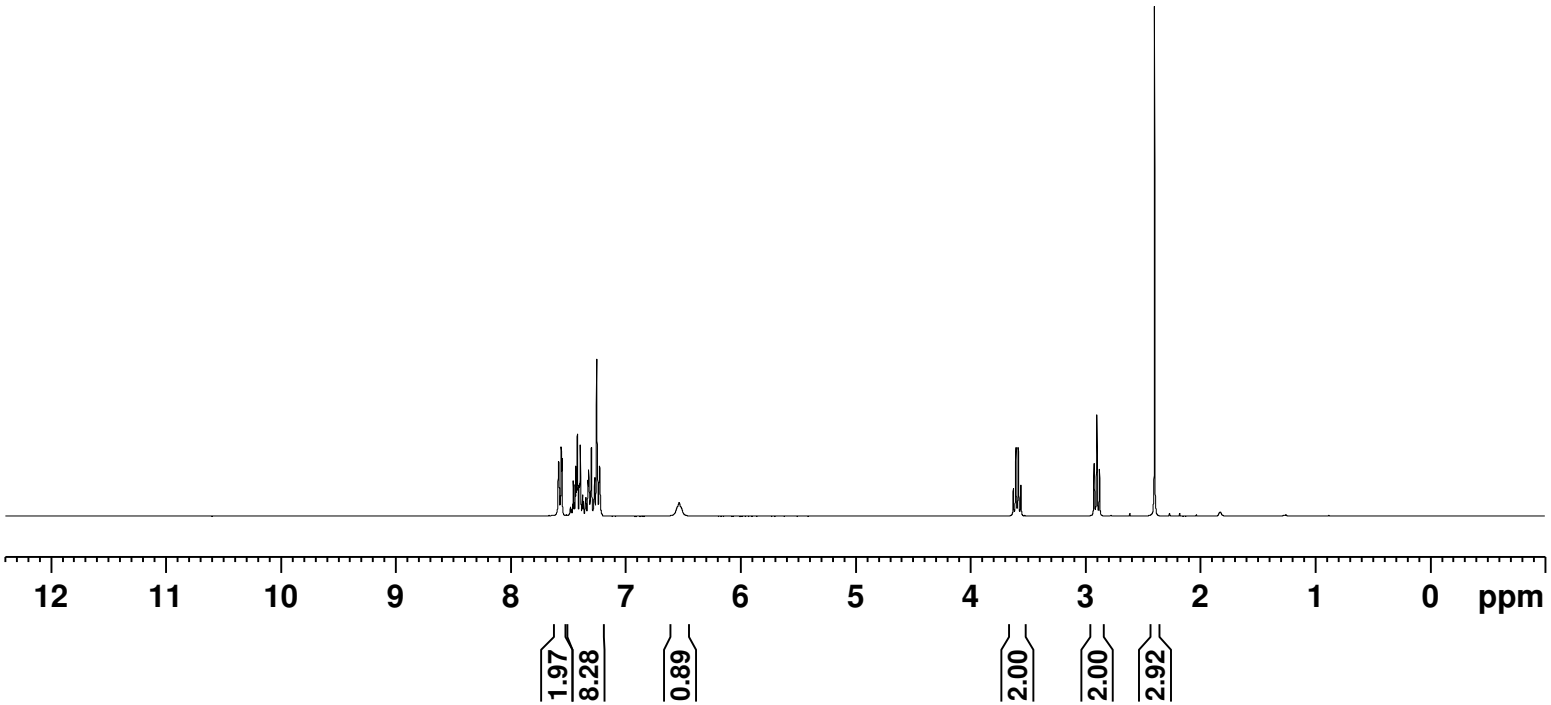

```
Current Data Parameters
NAME            liuwx201
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160629
Time               23.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    30
DS                     4
SWH            16129.032 Hz
FIDRES          0.246110 Hz
AQ             2.0316160 sec
RG                208.31
DW                31.000 usec
DE                 6.50 usec
TE                300.4 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6208171 MHz
NUC1                13C
P1                 9.80 usec
P13             2000.00 usec
PLW0      0 W
PLW1        47.97299957 W
SPNAM[5]    Crp60comp.4
SPOAL5            0.500
SPOFFS5   0 Hz
SPW5          7.03950024 W

======== CHANNEL f2 ========
SFO2         400.1312797 MHz
NUC2                1H
CPDPRG[2         waltz16
P3                14.60 usec
P4                29.20 usec
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.31566000 W

F2 - Processing parameters
SI                 32768
SF           100.6127823 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

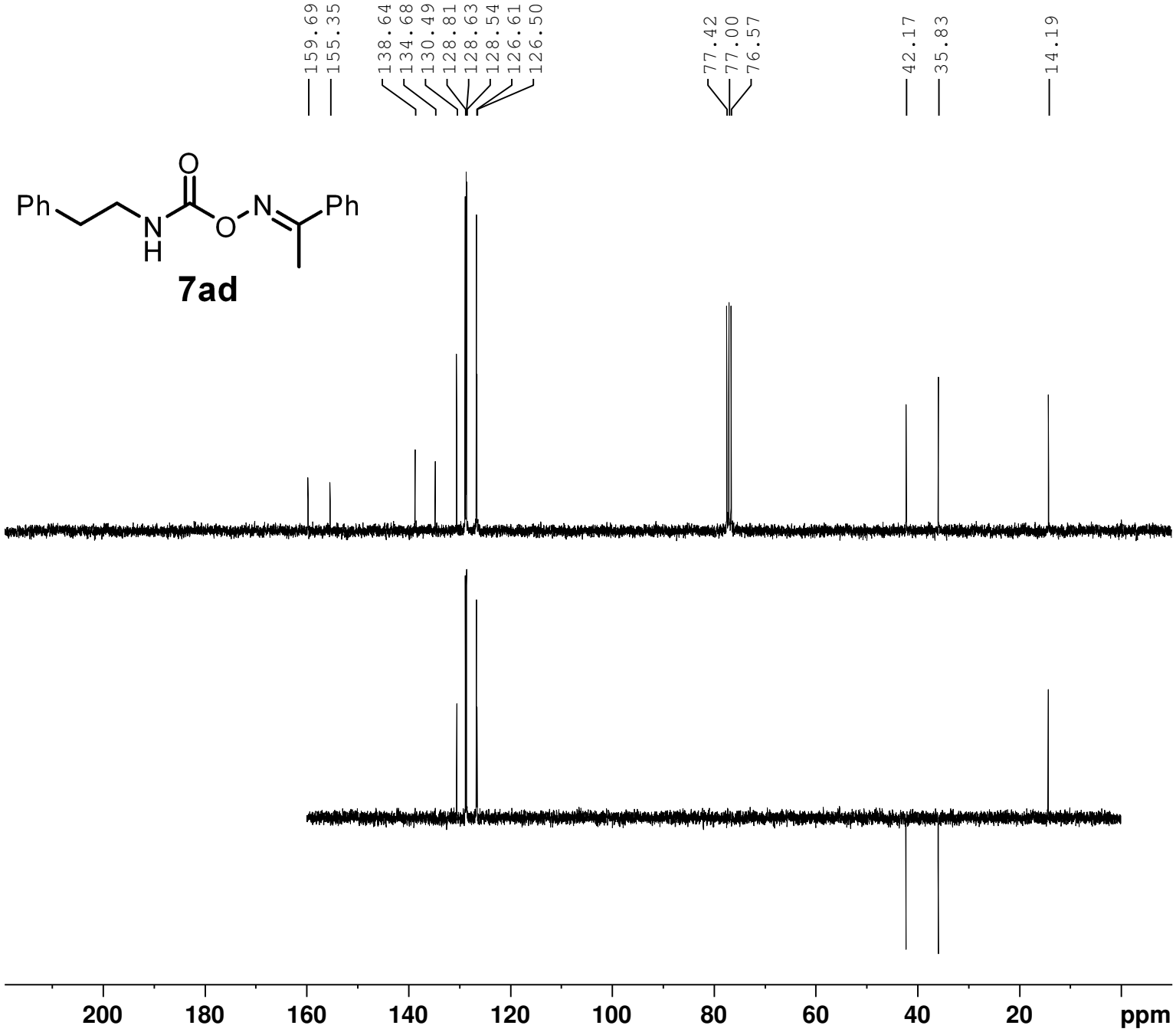




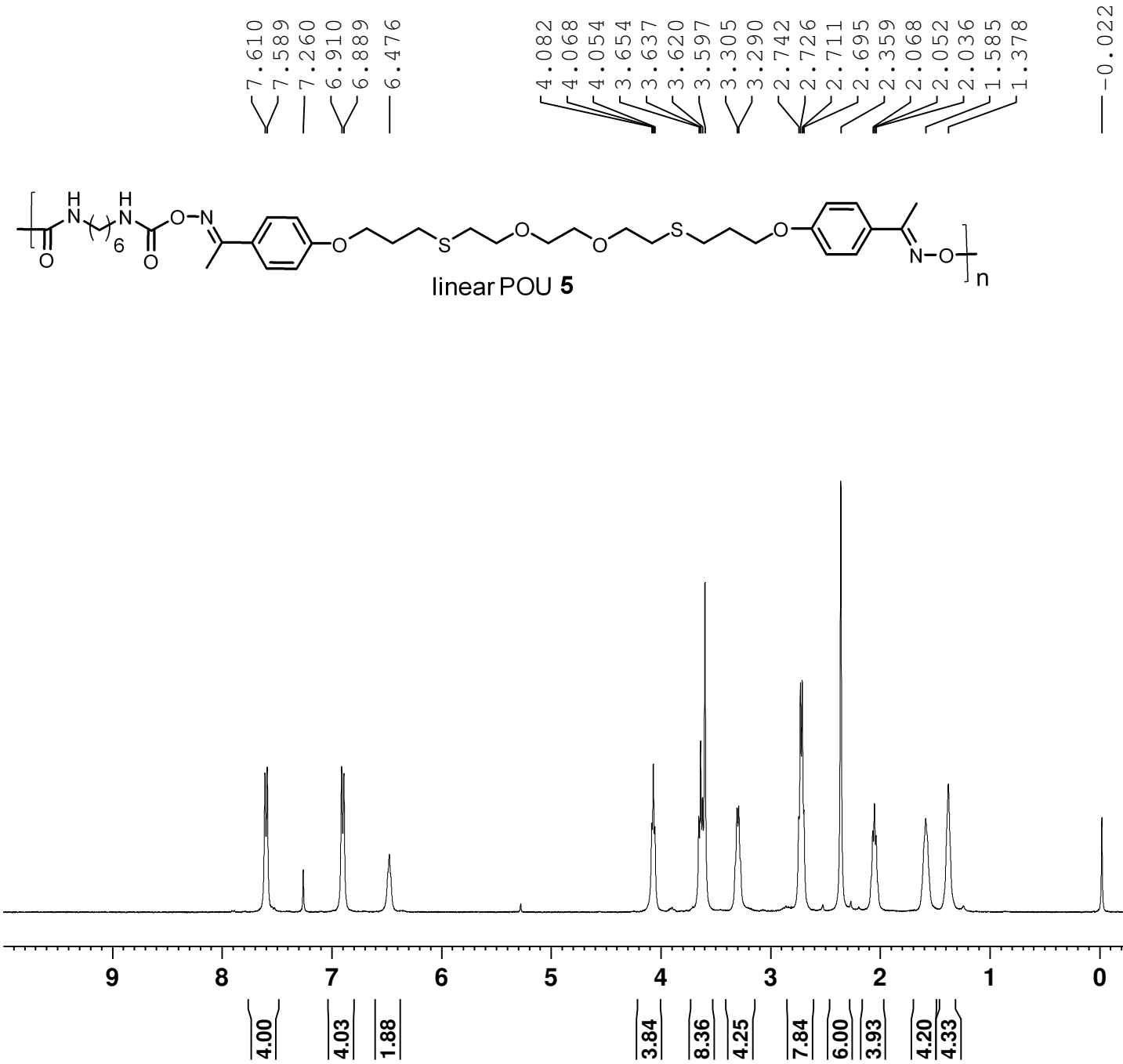
7ad

```
Current Data Parameters
NAME            liuwx191
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160615
Time               11.35
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    10
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ             5.4525952 sec
RG                 92.23
DW                83.200 usec
DE                 6.50 usec
TE                 298.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1818537 MHz
NUC1                   1H
P1                 12.00 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1800097 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```






```
Current Data Parameters
NAME            liuwx191
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160615
Time               11.46
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG        deptsp135
TD                 65536
SOLVENT            CDCl3
NS                    30
DS                     4
SWH            12077.295 Hz
FIDRES          0.184285 Hz
AQ             2.7131903 sec
RG                208.31
DW                41.400 usec
DE                 6.50 usec
TE                299.4 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4863591 MHz
NUC1                  13C
P1                12.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1        42.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5              0.500
SPOFFS5   0 Hz
SPW5           9.24069977 W

======== CHANNEL f2 ========
SFO2         300.1809600 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                12.00 usec
P4                24.00 usec
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.31999999 W

F2 - Processing parameters
SI                 32768
SF            75.4803210 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME                  liuwx215
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20160927
Time                     11.00
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                 12019.230 Hz
FIDRES               0.183399 Hz
AQ                   2.7262976 sec
RG                      208.31
DW                      41.600 usec
DE                       6.50 usec
TE                      298.1 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.00 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                      65536
SF                400.1300100 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```