

Supporting Information for:

Experimental and Theoretical Insights into Palladium-Mediated Polymerization of *Para-N,N*-disubstituted Aminostyrene

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Contents:

S1. Experiments

S1.1 Materials.

S1.2 Measurements.

S1.3 Polymerization procedures

S2. Polymerization results

S3. Characterization of polymer samples

S4. Computational details.

S5. References

S1. Experiments

General Methods

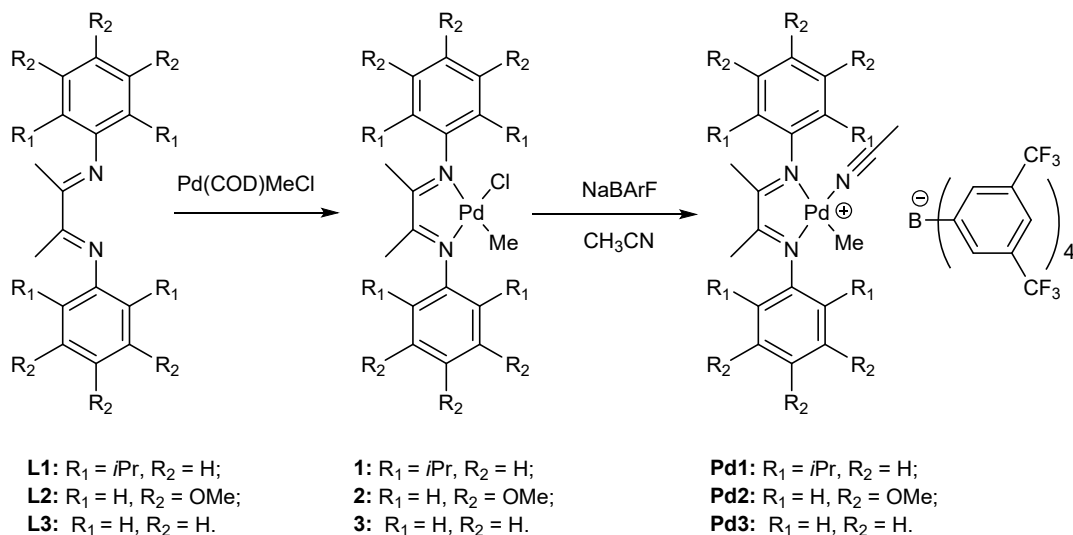
All manipulations involving air- and moisture sensitive compounds were carried out under an atmosphere of dried and purified nitrogen with standard vacuum-line, Schlenk, or glovebox techniques.

S1.1 Materials.

Anhydrous dichloromethane was distilled from P₂O₅ under nitrogen. Anhydrous tetrahydrofuran and methanol were distilled from CaH₂ under nitrogen. Diacetyl and substituted anilines purchased from Energy Chemical and used as received. Methyltriphenylphosphonium bromide, potassium tertbutoxide, *para*-dimethylaminobenzaldehyde, *para*-diethylaminobenzaldehyde and *para*-diphenylaminobenzaldehyde were also purchased from Energy Chemical and used without purification. All α -diimine palladium complexes were prepared by the reaction of Pd(COD)MeCl with the corresponding α -diimine ligand according to the previously reported method.^{1,2} Other commercially available reagents were purchased and used without purification.

The commercial polystyrene ($M_n = 139000$, PDI = 2.07, PS) was directly purchased from SINOPEC.

Synthesis and characterization of cationic α -diimine palladium complexes



Scheme S1. Synthetic route of cationic α -diimine palladium complexes

Pd1, Pd2 and Pd3.

The α -diimine palladium complexes were synthesized by the reaction of Pd(COD)MeCl with the corresponding α -diimine ligand. Then the corresponding α -diimine palladium complexes were treated with NaBARF to obtain the cationic α -diimine palladium complexes (Scheme S2).^{1,2}

Pd1: 1H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.70 (s, 8H, Ar-**H** in BARF⁻), 7.54 (s, 4H, Ar-**H** in BARF⁻), 7.35-7.30 (m, 6H, Ar-**H**), 2.84 (m, 4H, **CH**(CH_3)₂), 2.18 (s, 6H, =**CCH**₃), 1.76 (s, 3H, **CNCH**₃), 1.34, 1.21 (t, 24H, **C**(CH_3)₂), 0.53 (s, 3H, Pd**CH**₃).

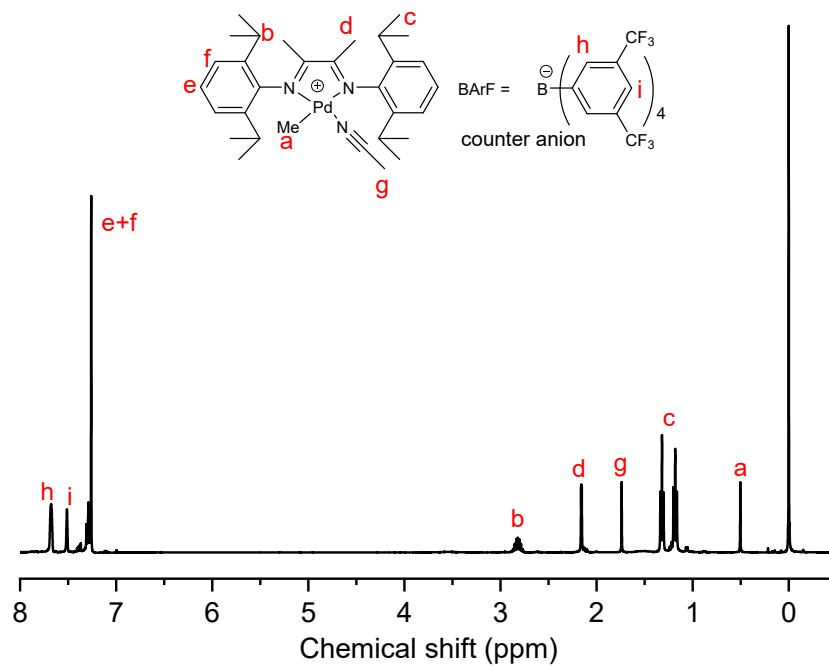


Figure S1. ¹H NMR spectrum of **Pd1**.

Pd2: ¹H NMR (400 MHz, CDCl₃), δ (ppm): 7.68 (s, 8H, Ar-**H** in BArF⁻), 7.52 (s, 4H, Ar-**H** in BArF⁻), 6.13 (s, 2H, Ar-**H**), 6.03 (m, 2H, Ar-**H**), 3.88, 3.79 (d, 18, O**CH**₃), 2.21, 2.18 (s, 6H, =C**CH**₃), 2.01 (s, 3H, CN**CH**₃), 0.67 (s, 3H, Pd**CH**₃).

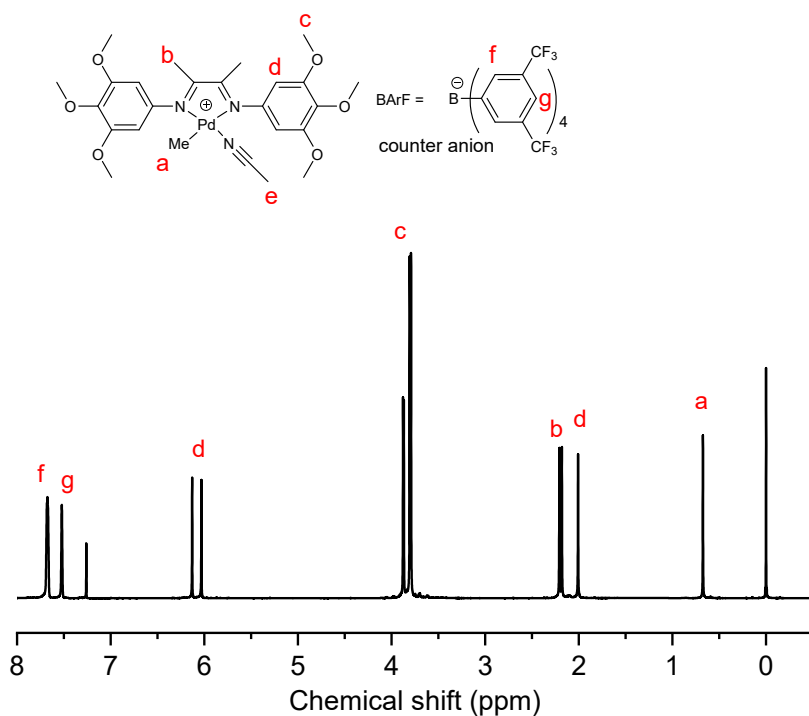


Figure S2. ^1H NMR spectrum of **Pd2**.

Pd3: ^1H NMR (400 MHz, CDCl_3), δ (ppm): 7.70 (s, 8H, Ar-*H* in BArF^-), 7.53 (s, 4H, Ar-*H* in BArF^-), 7.50-7.27 (m, 6H, Ar-*H*), 6.92-6.80 (dd, 4H, Ar-*H*), 2.18, 2.14 (s, 6H, $=\text{CCH}_3$), 1.85 (s, 3H, CNCH_3), 0.54 (s, 3H, PdCH_3).

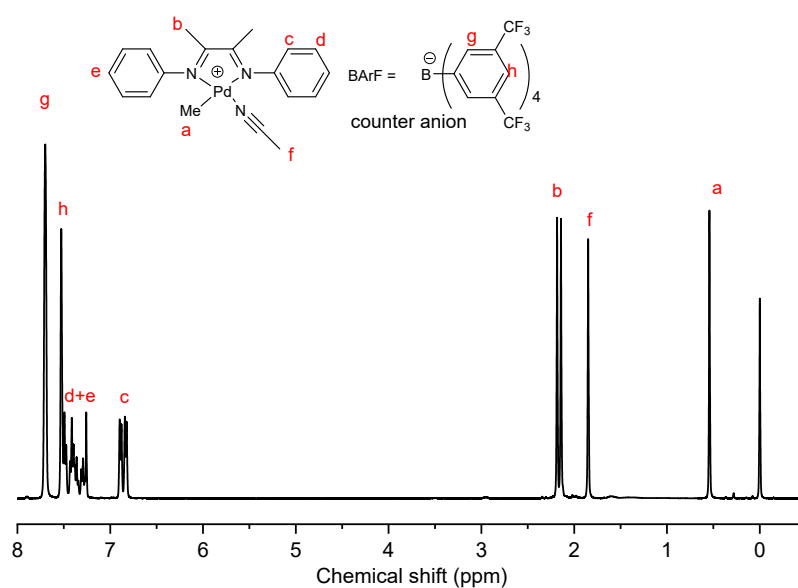
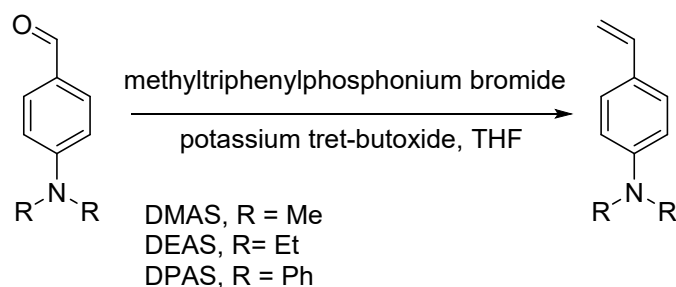


Figure S3. ^1H NMR spectrum of **Pd3**.

Synthesis and characterization of *para*-*N,N*-disubstituted aminostyrene



Scheme S2. Synthetic route of DMAS, DEAS, and DPAS.

DMAS, DEAS, and DPAS were synthesized by Wittig reactions according to the reported literatures.^{1,3} All products after dehydration and purification were stored in brown ampules under dry nitrogen.

DMAS, ¹H NMR (400 MHz, CDCl₃), δ (ppm): 7.33-7.25 (m, 2H, Ar-H), 6.70-6.65 (m, 2H, Ar-H), 6.65-6.57 (q, 1H, CH=CH₂), 5.58-5.49 (dd, 1H, CH=CH₂), 5.04-4.97 (dd, 1H, CH=CH₂), 2.93 (s, 6H, N(CH₃)₂).

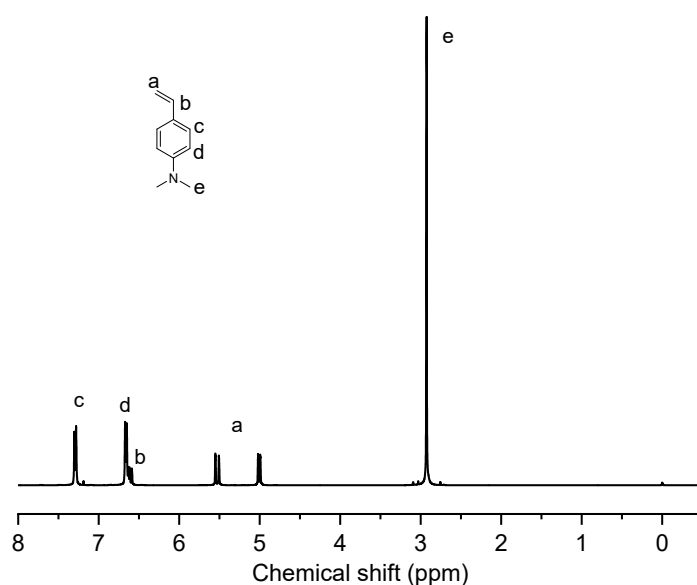


Figure S4. ¹H NMR spectroscopy of DMAS.

DEAS, ^1H NMR (400 MHz, CDCl_3), δ (ppm): 7.36-7.21 (m, 2H, Ar-H), 6.70-6.59 (m, 2H, Ar-H), 6.58 (s, 1H, $\text{CH}=\text{CH}_2$), 5.57-5.44 (dd, 1H, $\text{CH}=\text{CH}_2$), 5.02-4.91 (dd, 1H, $\text{CH}=\text{CH}_2$), 3.36 (q, 4H, $\text{N}(\text{CH}_2)_2$), 1.16 (t, 6H, $(\text{CH}_3)_2$).

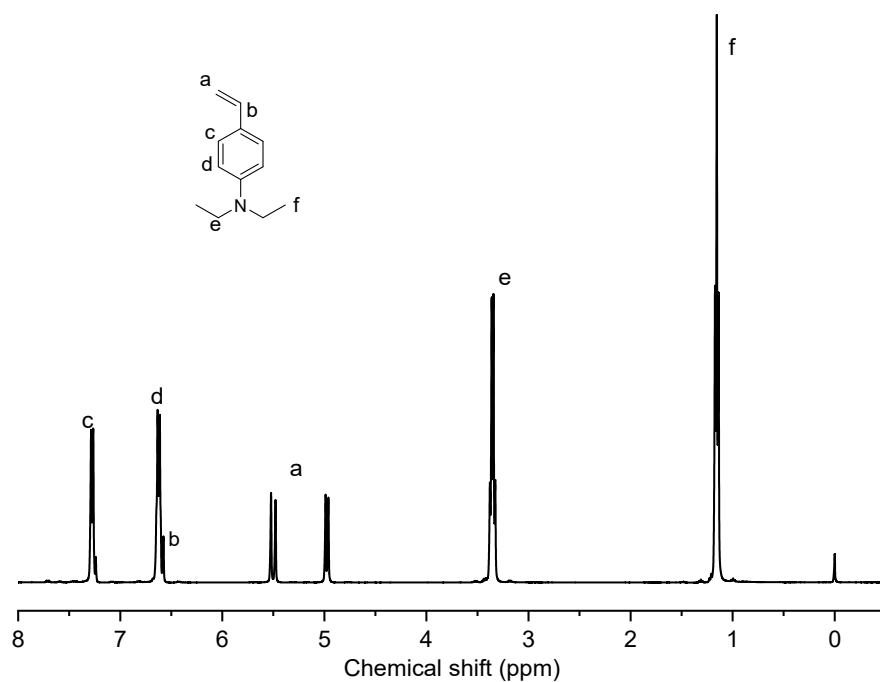


Figure S5. ^1H NMR spectroscopy of DEAS.

DPAS, ^1H NMR (400 MHz, CDCl_3), δ (ppm): 7.33-6.94 (m, 14H, Ar-H), 6.72-6.60 (q, 1H, $\text{CH}=\text{CH}_2$), 5.69-5.57 (dd, 1H, $\text{CH}=\text{CH}_2$), 5.19-5.10 (dd, 1H, $\text{CH}=\text{CH}_2$)

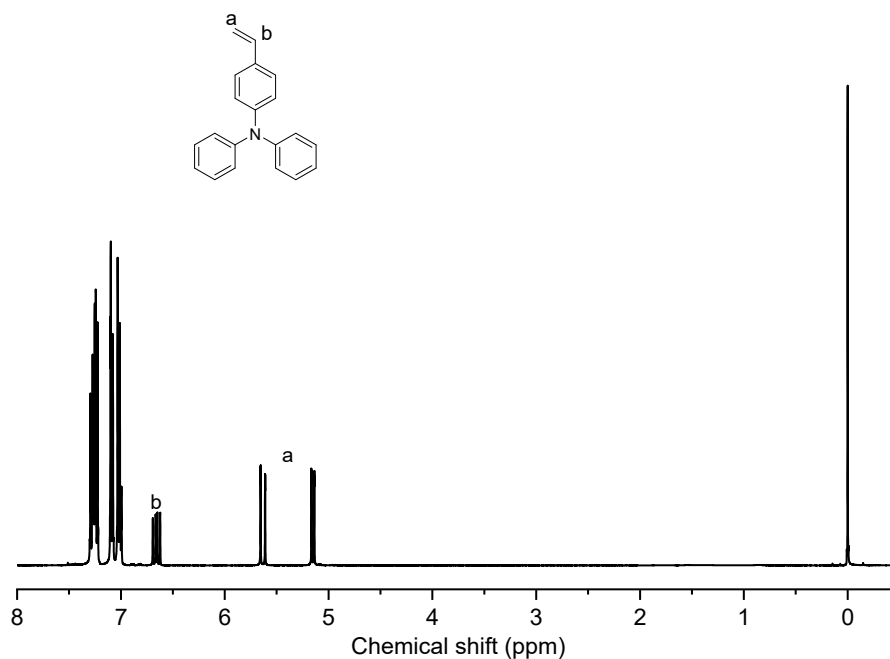
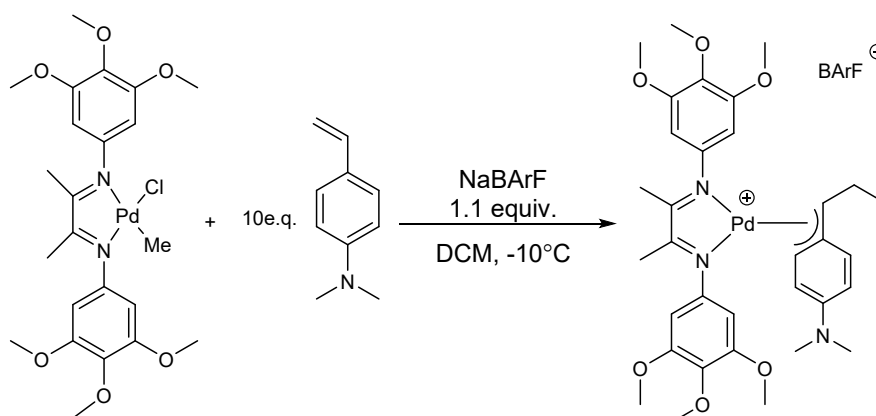


Figure S6. ¹H NMR spectroscopy of DPAS.

Synthesis and characterization of DMAS-treated palladium complexes



Scheme S3. Synthetic route of Pd-DMAS complex.

The Pd-DMAS complex was synthesized referring to previous report,^{1,4} the detailed synthetic process was shown as follows. α -Diimine palladium complex **2** (1.0 equiv, 0.2 mmol, 0.115 g), and NaBARF (1.1 equiv, 0.22 mmol, 0.196g) were added to a Schlenk tube and stir for 30min. DMAS (10.0 equiv., 2 mmol, 0.30 mL) and CH₂Cl₂ (15 mL) were

subsequently added, and the reaction mixture was then stirred for 12 h at -10 °C. After filtration, the filtrate was evaporated to 3 mL under vacuum and then 50 mL hexane was added. After filtered and washed with hexane (3 × 10 mL), the complex was precipitated as a dark red solid in 84 % yield.

Pd-DMAS, ¹H NMR (400 MHz, CDCl₃), δ (ppm): 7.68 (s, 8H, Ar-H in BArF⁻), 7.53 (s, 4H, Ar-H in BArF⁻), 7.21 (d, 1H, γ'), 6.55 (d, 1H, γ), 6.48 (d, 1H, β'), 6.25 (s, 2H, Ar-H in ligand), 5.52 (s, 2H, Ar-H in ligand), 4.0-3.61 (m, 18H, OMe in ligand), 2.78 (s, 6H, N(CH₃)₂), 2.72 (dd, 1H, c), 2.18 (s, 3H, CH₃ in ligand), 2.01 (s, 3H, CH₃ in ligand), 1.28 (d, 1H, H_{b-1}), 0.77 (t, 3H, CH₃), 0.64 (m, 1H, H_{b-1}).

S1.2. Measurements.

NMR spectroscopy of all samples were carried out on Bruker 400 MHz instruments in CDCl₃ using TMS as a reference. GPC analyses of the molecular weights and molecular weight distributions ($PDI = M_w/M_n$) of the polymers were performed on a Waters Breeze 2 GPC chromatograph equipped with a differential refractive-index detector. Tetrahydrofuran (THF) used as the eluent at a flow rate of 1.0 mL/min. DSC analysis of polymers was conducted with a Perkin-Elmer DSC-4000 system. The DSC curves were recorded as second heating curves from 30 to 200 °C at a heating rate of 10 °C/min and a cooling rate of 10 °C/min. Thermogravimetric analysis (TGA) was carried out with a NETZSCH TG209F3 thermal gravimetric analyzer at a heating rate of 20 °C/min from

50 to 800 °C under a nitrogen flow. MALDI-TOF spectroscopy was performed on a Bruker ultrafleXtreme. PL spectra were measured on a GANGDONG F-380 spectrofluorometer, the tested sample was entry 7 from table 2, and the concentration of its THF solution was diluted gradually from 1 mg/mL to 0.00125 mg/mL. The water surface contact angle (WSCA) test was conducted on a goniometer (Krüss, DSA100S)

S1.3. Polymerization Procedure.

The typical polymerization procedure (using the polymerization of DMAS with **Pd2** as an example) is described. A round-bottom Schlenk flask with a stirring bar was heated for 3h at 150 °C under vacuum. After cooling to room temperature, fill with dry nitrogen. 0.54 mL of DMAS (3.5mmol) and 9 mL of CH₂Cl₂ were injected into the round-bottom Schlenk flask at 30 °C. The polymerization was started by the addition of 1 mL of **Pd2** solution in CH₂Cl₂ (2μmol) into the round-bottom Schlenk flask at 30 °C. The reaction mixture was continuously stirred at a polymerization temperature of 30 °C. After a certain polymerization time, the reaction was terminated by injected methanol (1mL) containing a small amount of aqueous NaOH solution (0.1%). Then the quenched mixture was pouring the into 150 mL of methanol containing a small amount of aqueous NaOH solution (0.1%) and stirred for 0.5 h at room temperature to precipitate polymers. The resulting precipitated polymers were collected

and treated by filtration, washed with methanol and water. Dried in a vacuum at 40 °C to a constant weight. The monomer conversion was determined by gravimetry.

S2. Polymerization results

Table S1. Polymerization of DMAS using **Pd2** at different times. ^a

entry	time (min)	yield (mg)	conv. (%)	TOF (mol/mol Pd h)	M_n^b	PDI ^b
1	2	66.9	12.9	6820	6100	1.59
2	5	167.4	32.3	6820	5700	1.60
3	10	325.1	62.7	6627	5300	1.54
4	20	405.9	78.3	4140	4700	1.59
5	30	437.0	84.3	2970	4100	1.62
6	45	439.6	84.8	1990	4000	1.64
7	60	444.3	85.7	1510	4000	1.61

^a Polymerization conditions: 2 μ mol of **Pd2**, $[M]_0/[Pd]_0 = 1750$, 10 mL of CH_2Cl_2 , $T = 30$ °C. ^b Molecular weight and PDI were determined by GPC using tetrahydrofuran as eluent.

Table S2. Polymerization of DMAS using **Pd2** with BQ ^a

entry	$[BQ]_0/[Pd]_0$	yield (mg)	conv. (%)	TOF (mol/mol Pd h)	M_n^b	PDI ^b
1	5	439.3	84.7	2984	3900	1.61

^a Polymerization conditions: 2 μ mol of Pd2, 30 min, $T = 30$ °C, 10 mL of CH_2Cl_2 . ^b Molecular weight and PDI were determined by GPC using tetrahydrofuran as eluent.

ss

Table S3. Polymerization of DMAS by **Pd2** in the presence of methanol at different times ^a

entry	$[MeOH]_0/[Pd]_0$	time (min)	yield (mg)	conv. (%)	TOF (mol/mol Pd h)	M_n^b	PDI ^b
1	1750	5	46.2	8.9	1883	4000	1.18
2	1750	10	143.9	27.8	2932	3900	1.28
3	1750	15	239.1	46.1	3248	3600	1.23
4	1750	20	260.6	49.8	2655	3300	1.23
5	1750	30	303.8	58.6	2628	3200	1.18
6	1750	60	338.5	65.3	1150	2700	1.26
7	1750	120	343.1	66.2	583	2500	1.25

^a Polymerization conditions: 2 μ mol of Pd, $[DMAS]_0/[Pd]_0 = 1750$, 30 °C, 10 mL of CH_2Cl_2 . ^b Molecular weight and PDI were determined by GPC using THF as eluent.

S3. Characterization of polymer samples

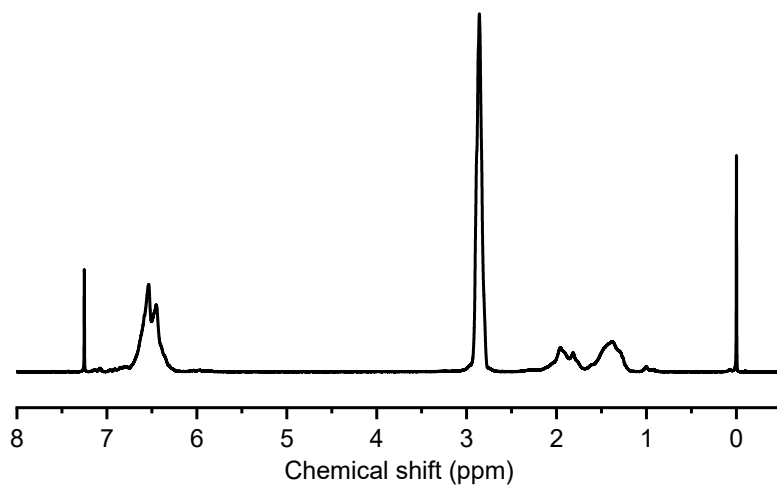


Figure S7. ¹H NMR spectrum of polymeric product of DMAS and ethylene copolymerization.

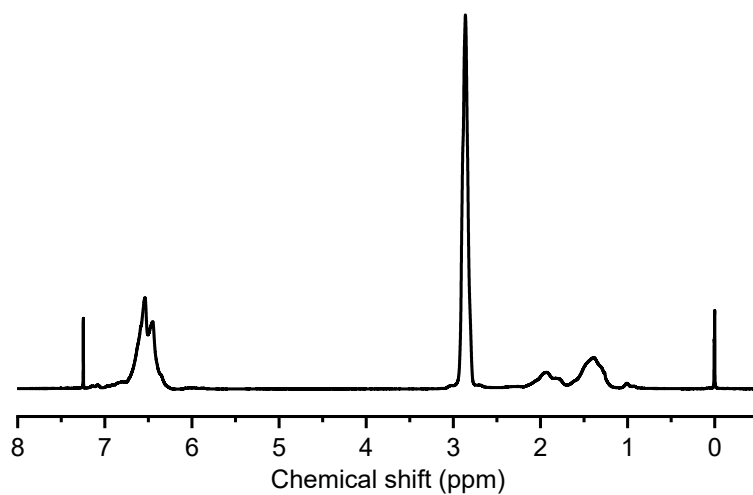


Figure S8. ¹H NMR spectrum of polymeric product of DMAS and CO copolymerization.

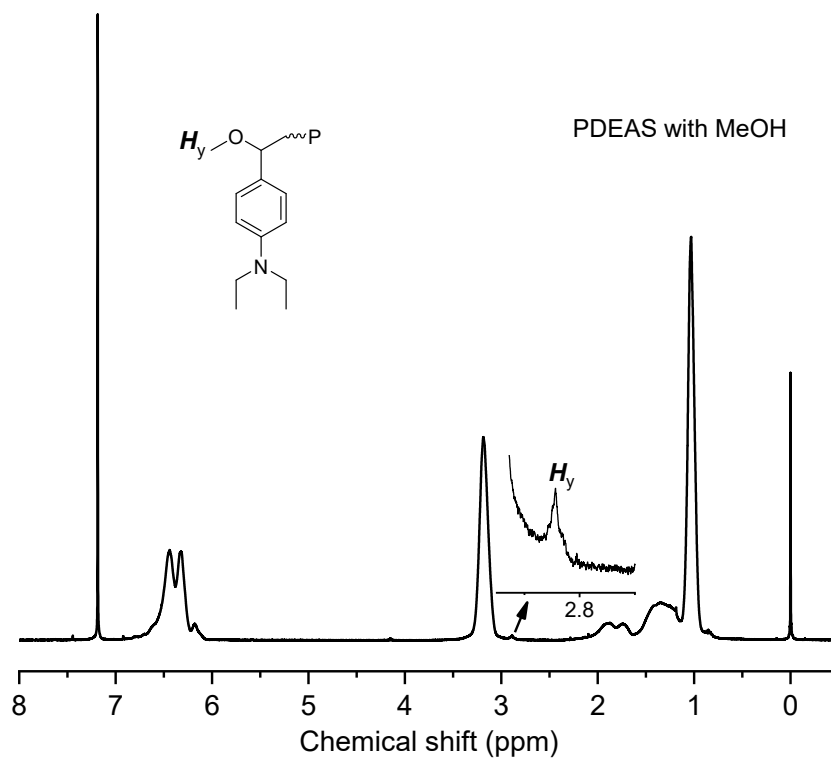


Figure S9. ^1H NMR spectroscopy of PDEAS obtained with MeOH.

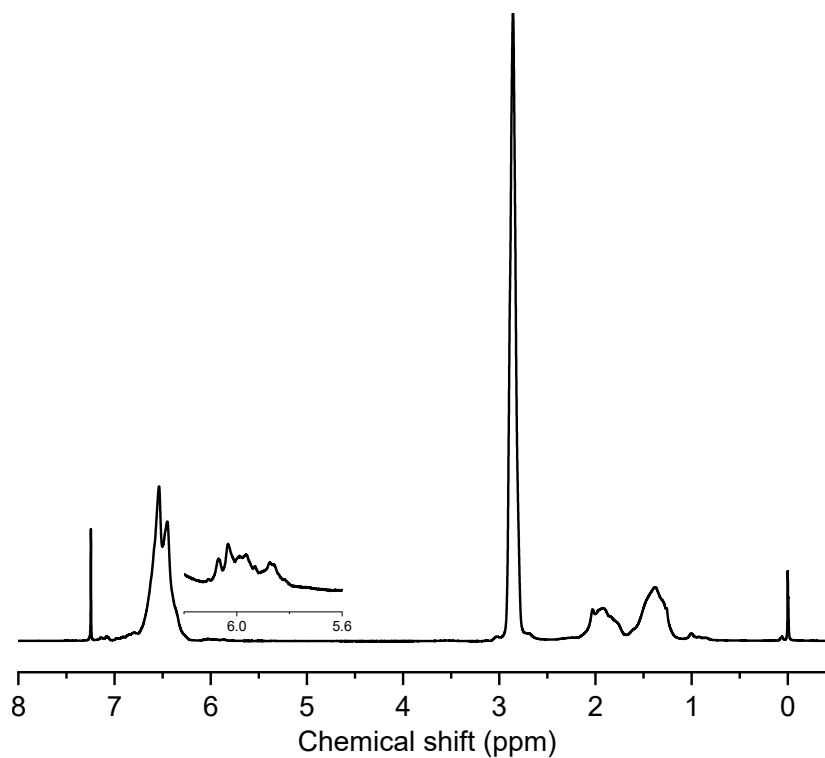


Figure S10. ^1H NMR spectroscopy of PDMAS produced by **Pd1** (entry 2 in Table 1).

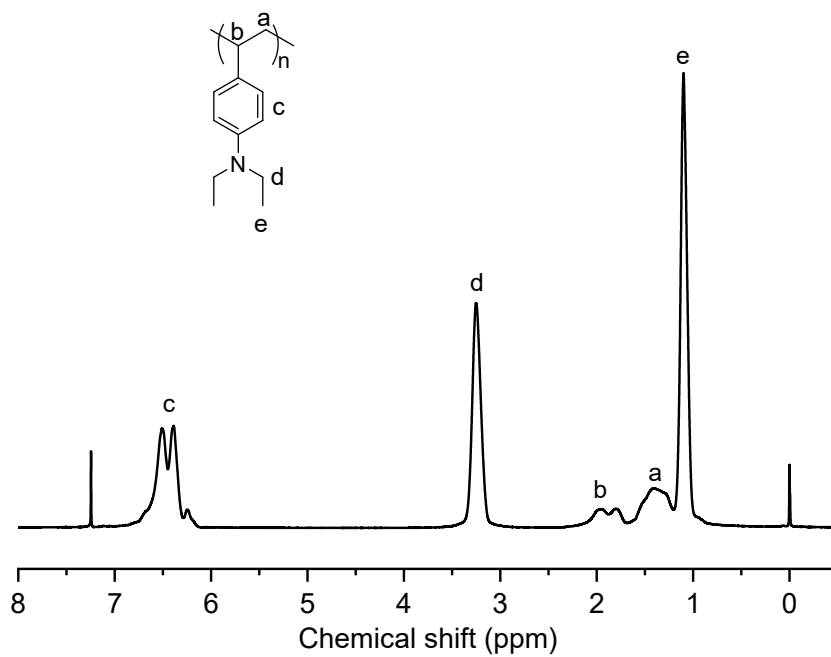


Figure S11. ^1H NMR spectroscopy of PDEAS (entry 3 in Table 2).

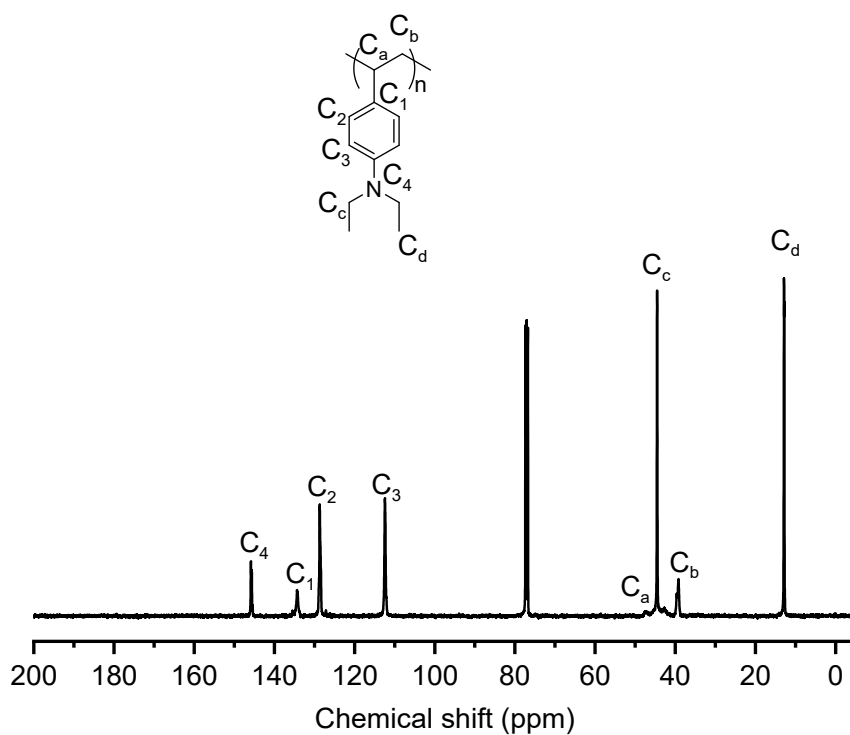


Figure S12. ^{13}C NMR spectroscopy of PDEAS (entry 3 in Table 2).

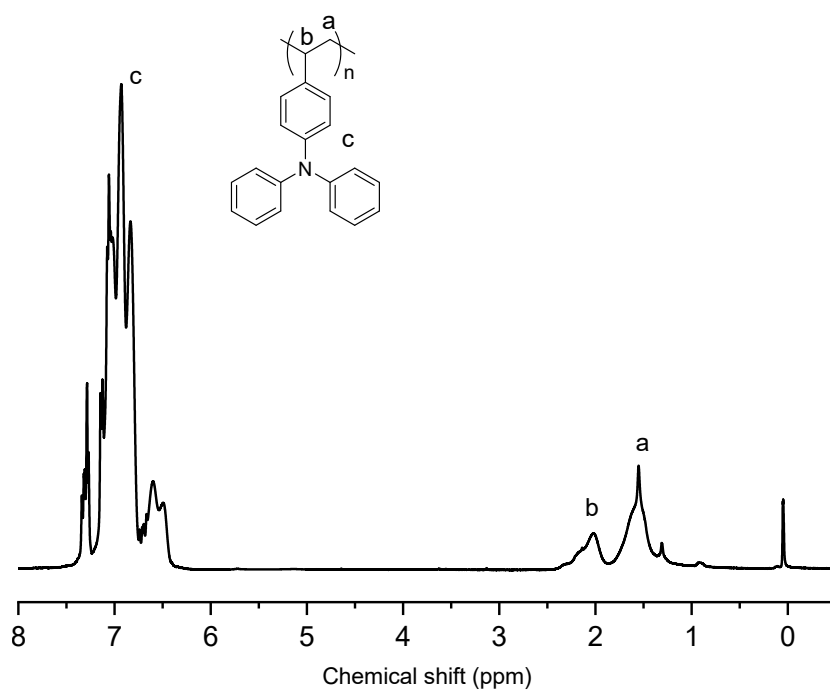


Figure S13. ¹H and spectroscopy of PDPAS (entry 7 in Table 2).

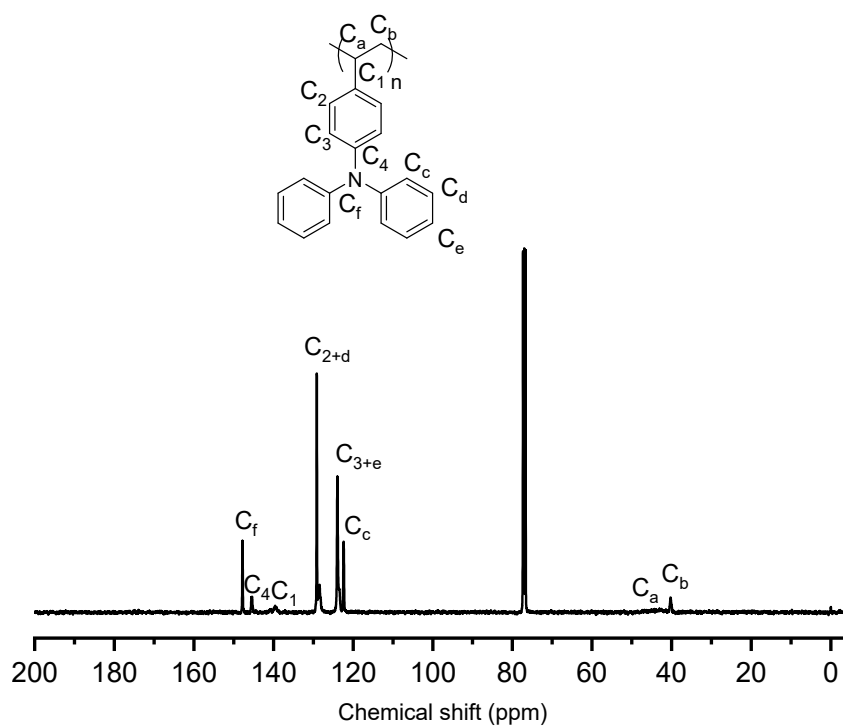


Figure S14. ¹³C NMR spectroscopy of PDPAS (entry 7 in Table 2).

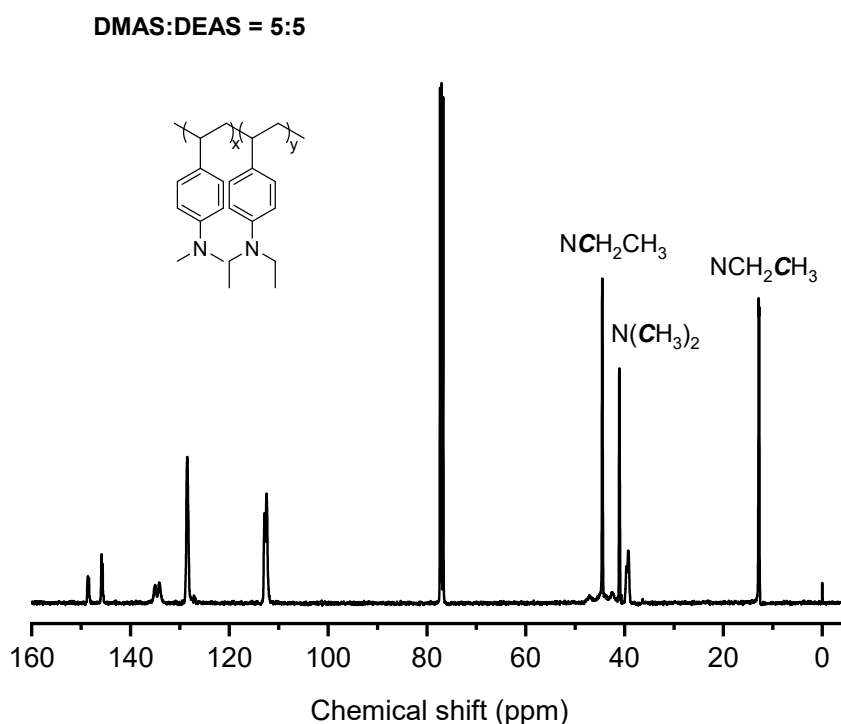


Figure S15. ^{13}C NMR spectrum of poly(DMAS-*co*-DEAS) using **Pd2**.

S4. Computational details

By using the density functional theory^{5,6} (DFT), all the calculations were performed with the Gaussian 16 program⁷. All the structures were carried out at the M06-L⁸ functional and def2-SVP⁹ basis sets. Based on optimized structures, frequency analysis calculations were performed to characterize the structures to be minima (no imaginary frequency) or transition states (one imaginary frequency). IRC calculations were taken to confirm the connection between two correct minima for a transition state. Based on M06-L/def2-SVP optimized geometries, the energy results were further refined by calculating the single-point energy at the M06-L/def2-

TZVP^{5, 6} level of theory. At the M06-L/def2-TZVP level of theory, the bulky solvation effect of dichloromethane ($\epsilon = 8.93$) were simulated by the SMD⁷ continuum solvent model.

The Cartesian coordinates (xyz) for all optimized structures

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IM-Pd1

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H 2.52965500 4.48642600 3.73023900
C -7.42100000 0.42547500 3.32403000
H -6.45305100 0.14284500 3.77026900
H -7.37494100 1.48688300 3.02549300
H -8.20409200 0.30765000 4.07980500
C -9.59015200 -1.64232000 -0.32128500
H -10.37630200 -2.37855600 -0.12166500
H -9.90605400 -0.66837500 0.08804400
H -9.45884800 -1.55124800 -1.41129800
C -6.19938800 -2.45437400 -3.10004700
H -6.72194000 -3.18925500 -3.72051400
H -6.07683700 -1.52371300 -3.67838200
H -5.20137700 -2.84684000 -2.84574100
Pd -1.89183700 -0.22176600 -0.44643800
C 2.22078000 -0.46349100 0.47063900
C 2.94781700 -0.87648300 -0.65766200
C 4.26227900 -0.49283100 -0.86703800
C 4.92433000 0.35836200 0.05346400
C 4.22285300 0.72033700 1.22818400
C 2.90965700 0.32373000 1.41127000

H 2.45625600 -1.50887200 -1.40370100
H 4.76702000 -0.81635800 -1.77914300
H 4.68232200 1.38336100 1.96118900
H 2.37831600 0.66229300 2.30850100
C 0.77494100 -0.80891500 0.66405800
N 6.18746200 0.83226700 -0.19719700
C 0.55679200 -2.04304800 1.65587400
C 1.15533400 -3.24903800 1.09576000
H 0.53224200 -3.88780900 0.45890700
C 2.51910900 -3.49765600 1.09803300
C 3.09083100 -4.40713600 0.15004000
C 3.43659500 -2.73454200 1.89165500
C 4.43521000 -4.43666900 -0.09439900
H 2.42134600 -5.04275000 -0.43523400
C 4.78575200 -2.77135500 1.67080900
H 3.05360100 -2.11311900 2.70112300
C 5.32712000 -3.57722600 0.62635100
H 4.82232500 -5.10518100 -0.86242800
H 5.44209400 -2.16681800 2.29522700
N 6.64546700 -3.54439900 0.33742200
C 6.80972200 1.74121200 0.73569700
H 7.00149700 1.26562400 1.71384500
H 7.77278700 2.07538500 0.33638200
H 6.18361700 2.63004000 0.91466400
C 6.84104800 0.50802100 -1.43860800
H 7.03101200 -0.57580100 -1.54480000
H 6.24696300 0.82003700 -2.31517200
H 7.80792200 1.01877200 -1.49165400
C 7.52187100 -2.62396600 1.03739600
H 8.51523800 -2.64984400 0.58107200
H 7.14227700 -1.59270400 0.97735800
H 7.63047600 -2.88957200 2.09999500
C 7.19950300 -4.39441800 -0.69890700
H 7.02162700 -5.45892700 -0.48999000
H 6.77220000 -4.16179900 -1.68672500
H 8.28059900 -4.24255900 -0.75380400
C -0.01840700 -1.01108500 -0.62717400
H 0.42892800 -0.41320300 -1.43826600
H 0.01069400 -2.06164000 -0.96037400
H 0.34092600 0.02563900 1.24696200
H 1.00115700 -1.76732000 2.62381100
H -0.53082200 -2.14234600 1.78072300
C -2.58408800 -2.13730200 -0.36528700
H -1.87190000 -2.89829600 -0.00900900

H -3.47468700 -2.15284900 0.28425200
H -2.88502500 -2.42434900 -1.38782100

IM-Pd2

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N -2.28961800 -1.05291400 0.16492200
C -1.83052300 -2.27139900 0.11001300
C -0.36430200 -2.41256200 0.25013100
N 0.31550800 -1.34274500 0.53899700
C 1.72911200 -1.33688300 0.60462000
C 2.47057100 -1.39388300 -0.57831600
C 2.34724200 -1.20160000 1.84871000
C 3.86693200 -1.31416500 -0.50946400
C 3.74612800 -1.14247300 1.91036100
C 4.51170100 -1.18658000 0.73184500
C -3.62448100 -0.68294700 0.00390100
C -4.09601400 0.36297300 0.81667600
C -4.47823300 -1.25657800 -0.95090200
C -5.41356200 0.79564900 0.71180000
C -5.79127700 -0.79877600 -1.09203900
C -6.28041600 0.24241100 -0.26824700
C -1.14545800 3.65045200 1.89594400
H -0.41793300 4.44077400 2.12430500
H -2.10543200 4.13904900 1.68600700
H -1.26358700 3.03969400 2.80208300
C 0.58527700 2.03846400 0.95935200
H 0.86883400 1.95278900 2.02072500
C -0.66034500 2.81913400 0.72267800
H -0.60324800 3.41307300 -0.20264500
H -1.56729800 2.12090000 0.45357100
C -2.66050000 -3.50411200 -0.02470000
H -2.70489700 -3.87042000 -1.06289300
H -2.24784700 -4.32656500 0.57269700
H -3.69256100 -3.32640000 0.30066200
C 0.24702800 -3.76193300 0.08194500
H -0.07296300 -4.42891000 0.89671100
H -0.08483400 -4.23833100 -0.85123900
H 1.34025300 -3.72601600 0.08757400
H 1.73067500 -1.13934900 2.74571100
H 1.95145700 -1.46864100 -1.53459800
H -3.41621500 0.79383000 1.55434200
H -4.10207600 -2.02949600 -1.61776700
O 4.44837400 -0.99388900 3.04991800

O 5.85218300 -0.97567600 0.77685700
O 4.67888700 -1.31150700 -1.58598700
O -5.96524300 1.74860000 1.48031800
O -7.51561700 0.74772500 -0.28704000
O -6.66666600 -1.31942400 -1.97979400
C 3.73885600 -0.87042400 4.25782300
H 3.07079900 0.00715900 4.24983700
H 3.13960900 -1.76925400 4.47611900
H 4.48299700 -0.74043100 5.04959300
C 6.64301800 -2.13314400 0.97610400
H 6.51564300 -2.85244400 0.15075500
H 7.68892700 -1.80914700 1.00487400
H 6.40001200 -2.62775900 1.92955900
C 4.09209200 -1.35841000 -2.86214100
H 3.40052600 -0.51346300 -3.02412700
H 4.91039600 -1.29264800 -3.58759100
H 3.54654100 -2.30197700 -3.02838800
C -5.16930200 2.34727900 2.47006300
H -4.79781100 1.60978700 3.20049000
H -4.30778700 2.87954300 2.03319300
H -5.80387800 3.07168500 2.98978400
C -8.31709600 0.78674100 -1.45685200
H -9.04679800 1.58662800 -1.29003300
H -7.72168200 1.02153500 -2.34894200
H -8.85042100 -0.15819000 -1.61746300
C -6.24443100 -2.37587500 -2.80491000
H -7.10562100 -2.65931800 -3.41775500
H -5.42056100 -2.07263200 -3.47133500
H -5.92472500 -3.25180200 -2.21594100
Pd -0.75154800 0.49715100 0.57757400
C 1.72741800 2.04936400 0.06624400
C 3.02537200 1.85168100 0.58032300
C 1.61710600 2.21811700 -1.33162100
C 4.14222300 1.80760800 -0.23015200
H 3.15449800 1.73637600 1.66100300
C 2.72207600 2.17429900 -2.16052900
H 0.63170400 2.37503200 -1.78278400
C 4.02344400 1.95086500 -1.63483000
H 5.11794300 1.64252100 0.22716900
H 2.57924500 2.30703900 -3.23366400
N 5.11585400 1.86430200 -2.45196100
C 4.99636100 2.16981900 -3.85641100
H 5.98595100 2.14126200 -4.32302600
H 4.35653200 1.44761900 -4.39278500

H 4.57614600 3.17420000 -4.02843600
C 6.41457400 1.56299900 -1.88973000
H 6.81061000 2.39183700 -1.27803600
H 6.37222200 0.66196200 -1.25969600
H 7.12673500 1.37617900 -2.70003200

IM-Pd3

I 1

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C 0.01995900 2.51150200 -0.28062000
N 0.69552300 1.42721000 -0.07103800
C 2.09411300 1.36111500 0.05518800
C 2.60864600 0.88277400 1.26438100
C 2.93689000 1.65402000 -1.02364800
C 3.98731500 0.70248400 1.40296500
C 4.31485300 1.43614700 -0.88995300
C 4.84648600 0.94011900 0.31474500
C -3.27100000 0.81375900 -0.29222600
C -3.66185400 -0.28925900 -1.06323400
C -4.21887600 1.50897200 0.47040300
C -4.99593400 -0.68571000 -1.08541000
C -5.55626200 1.09865400 0.47240400
C -5.96494200 -0.01313700 -0.29750600
C -1.05980800 -2.43531200 0.15237400
H -1.60313300 -2.68666300 -0.77202500
C -1.76117800 -2.87304200 1.40691900
H -1.21782900 -2.51093300 2.29517300
C -2.27810900 3.55052300 -0.70942400
H -2.48204200 4.16208400 0.18388200
H -1.76051500 4.20847700 -1.41958100
H -3.24756900 3.26834800 -1.13630900
C 0.62198100 3.87184300 -0.38154000
H 0.62077000 4.23376500 -1.42148200
H 0.04754700 4.60537400 0.19997600
H 1.66026800 3.87907600 -0.03148200
H 2.50759200 2.00970900 -1.96058400
H 1.91758000 0.64797500 2.07422100
H -2.89893300 -0.82758700 -1.62616000
H -3.90352800 2.34393200 1.09381100
O 5.21564900 1.65081200 -1.87153800
O 6.16269500 0.61860200 0.40487000
O 4.58046300 0.26178000 2.53330400

O -5.46320800 -1.72818100 -1.79392600
O -7.21550600 -0.48069400 -0.38827800
O -6.52568500 1.73194600 1.16948400
C 4.75011200 2.13395900 -3.10778300
H 4.04641900 1.42987600 -3.58325800
H 4.25509700 3.11323900 -3.00552100
H 5.62631600 2.24728500 -3.75351700
C 7.03036700 1.68587600 0.75060400
H 6.78117500 2.09756000 1.74120300
H 8.04599200 1.27757100 0.78342700
H 6.99490700 2.49177600 0.00136700
C 3.77343600 0.06035200 3.66949300
H 3.01608800 -0.72416800 3.50281200
H 4.44018000 -0.25531300 4.47793200
H 3.25939400 0.98674600 3.97124400
C -4.56644100 -2.42296600 -2.62191600
H -4.11277500 -1.76224700 -3.37868800
H -3.75990600 -2.90357000 -2.04217300
H -5.14438200 -3.20093000 -3.13007600
C -8.11032200 -0.44879500 0.71109300
H -8.84435200 -1.24053600 0.52441600
H -7.59306500 -0.65479100 1.65855500
H -8.62971100 0.51439400 0.78961200
C -6.17638500 2.85260600 1.94157500
H -7.09953000 3.21807200 2.40189500
H -5.46025300 2.59547300 2.73913600
H -5.74693100 3.65762500 1.32219800
Pd -0.40236800 -0.45535200 0.01310900
C 0.38166000 -2.44666100 0.03240300
C 0.97717000 -2.19249200 -1.24898000
C 1.29359000 -2.58594700 1.12822900
C 2.34142100 -2.07383400 -1.42182600
H 0.32777800 -2.16223800 -2.12844100
C 2.65252800 -2.49103500 0.95728200
H 0.89916900 -2.79425200 2.12584500
C 3.22963000 -2.21360500 -0.32214400
H 2.73027400 -1.90481100 -2.42500400
H 3.30400000 -2.60807600 1.82381000
N 4.57170900 -2.09883000 -0.46163400
C 5.46366300 -2.44825400 0.62971500
H 6.49422900 -2.43330900 0.26461400
H 5.40151700 -1.72895400 1.45958600
H 5.25183200 -3.45863700 1.00920400
C 5.17759100 -1.70468300 -1.71499300

H 5.38598200 -2.56597500 -2.37195900
H 4.53228900 -1.00460600 -2.25804200
H 6.11537400 -1.17540000 -1.50923400
H -1.70032300 -3.97689600 1.46664500
C -3.21333100 -2.44848500 1.49690900
H -3.69409700 -2.86608600 2.39111700
H -3.31424100 -1.35420700 1.54626100
H -3.79352100 -2.78978700 0.62639000

IM-Pd4

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C -0.45876800 -2.63957900 -1.50455100
N -1.17367300 -1.81113400 -0.81214800
C -2.52790500 -2.13789100 -0.53306700
C -2.82582600 -2.79233800 0.66188500
C -3.53774000 -1.70416100 -1.39049200
C -4.16430000 -3.02608300 1.00185800
C -4.87866400 -1.91792200 -1.03669100
C -5.20814000 -2.58777000 0.15858300
C 2.70191500 -0.75844700 -1.51099200
C 3.12935000 0.23714600 -2.38959000
C 3.61994600 -1.42537400 -0.69123100
C 4.49275900 0.54847400 -2.47739300
C 4.96605200 -1.06713400 -0.72762500
C 5.42729700 -0.07830400 -1.62681600
C -3.00916100 -0.09447000 3.24302000
H -3.65569300 -0.85282700 2.77665200
H -2.75637100 -0.44470300 4.25363000
H -3.61386100 0.81728500 3.34727900
C -2.08351700 0.57918000 0.99884700
H -2.61675400 -0.21064100 0.46001100
C -1.75668700 0.15580700 2.41100600
H -1.14848800 -0.76619400 2.38209900
H -1.12348900 0.90646600 2.91562500
C 0.09247300 2.20483100 0.48112200
H -0.54237200 2.79753800 -0.18088700
H -0.13286200 2.28310700 1.54814300
C 1.35293200 1.82074900 0.06465000
H 1.63662300 2.05414200 -0.97075300
H 2.39740900 0.72536900 -3.03250600
H 3.25529000 -2.17233000 0.01431900

H -3.27179900 -1.16605800 -2.30097400
H -2.01231600 -3.10381700 1.31741800
O -5.92371500 -1.49244500 -1.77874800
O -6.46903000 -2.78945700 0.58533500
O -4.55423500 -3.64318200 2.13109300
O 4.98966500 1.45643300 -3.34955200
O 6.74792000 0.18032900 -1.58293200
O 5.90584400 -1.58512100 0.08862300
C -5.66582300 -0.82958800 -2.98972400
H -5.11515400 0.11304100 -2.83371300
H -5.09695300 -1.46065200 -3.69197300
H -6.63848000 -0.59689500 -3.43472300
C -7.43076900 -3.32981500 -0.30252300
H -6.96903700 -4.00503700 -1.03857600
H -8.13550000 -3.90615600 0.30888200
H -7.98169900 -2.54495400 -0.83815700
C -3.56600900 -4.09804000 3.01953300
H -4.08949000 -4.56579400 3.85929500
H -2.90587100 -4.84729400 2.55193600
H -2.94619400 -3.27097200 3.40488700
C 4.08953300 2.18825300 -4.14188100
H 3.51531900 1.53725300 -4.82061700
H 3.38252500 2.77130300 -3.52724600
H 4.68848800 2.87984200 -4.74294700
C 7.25485600 1.48138700 -1.80933200
H 8.21975900 1.52688000 -1.28936700
H 7.41443400 1.68394900 -2.87623400
H 6.59303800 2.25827000 -1.39786800
C 5.51442600 -2.58333200 0.99526800
H 4.71601800 -2.23503800 1.67364600
H 5.16536600 -3.49157800 0.47599300
H 6.39994000 -2.83518000 1.58952000
C 1.84784800 -3.33039600 -2.34290800
H 1.34758700 -3.83680400 -3.17847200
H 2.79088800 -2.90800600 -2.70405600
H 2.09725000 -4.11721900 -1.61410300
C -0.96876300 -3.93172200 -2.04978100
H -0.90322600 -3.94182000 -3.14800500
H -0.35574200 -4.77463800 -1.70048100
H -2.00872000 -4.11985200 -1.76773400
C -2.76881900 1.84598600 0.77916400
C -3.48324300 2.04934200 -0.42091300
C -2.75638900 2.92176000 1.69014600
C -4.13594900 3.23214700 -0.70648500

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C -3.41072000 4.11265100 1.43029500
H -2.22239400 2.82201000 2.63990900
C -4.12202100 4.30817300 0.21889700
H -4.67767500 3.32437200 -1.64838900
H -3.37564400 4.90431600 2.17860600
C 2.44861400 1.37825100 0.91288600
C 2.26996600 0.60918100 2.07722100
C 3.76411100 1.74917200 0.58399300
C 3.34482600 0.18414300 2.83925200
H 1.25746200 0.30128000 2.36197500
C 4.84707300 1.36655200 1.35398200
H 3.93543800 2.36783300 -0.30287000
C 4.67404100 0.53286700 2.48366800
H 3.15575700 -0.43977300 3.71352600
H 5.84557000 1.69356800 1.06346500
N -4.77323600 5.48255600 -0.04302200
N 5.75162600 0.06343600 3.18795300
Pd -0.29756300 0.16044400 -0.19818400
C 7.09078100 0.34973600 2.72785700
H 7.81096100 -0.22578100 3.31857500
H 7.21631700 0.06488600 1.67082100
H 7.35469300 1.41681000 2.82819100
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H 4.95199300 -0.13830300 5.13929400
H 5.04182300 -1.65564800 4.21588700
H 6.51939600 -0.91378900 4.85818500
C -5.48379300 5.65262500 -1.28682600
H -6.29785300 4.91831500 -1.40486100
H -5.93116300 6.65059300 -1.31998600
H -4.81820700 5.55759500 -2.16060800
C -4.76510700 6.54764900 0.93074200
H -5.20998700 6.23524300 1.88976500
H -3.74620800 6.91406100 1.13835500
H -5.35053500 7.39180900 0.55435000

IM-Pd5

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C -1.84871200 -1.45093200 1.60285200
N -2.29831300 -0.61456300 0.70525200
C -3.64242400 -0.27762100 0.53735800

C -4.68427100 -1.21788100 0.62440700
C -3.92476400 1.04820200 0.17479900
C -5.99879800 -0.82271300 0.35904400
C -5.24171200 1.44470200 -0.05844600
C -6.29561500 0.51829700 0.05354900
C 1.56458000 -1.55101300 0.20472100
C 1.97463100 -2.02545700 -1.04581700
C 2.52288300 -1.14898800 1.14584400
C 3.33355400 -2.13689100 -1.34436300
C 3.87918700 -1.20120300 0.82267200
C 4.30765100 -1.70356200 -0.42356700
C -0.74109500 2.16299000 -1.54549300
H -1.44196100 2.22258600 -2.38684000
H -0.83061900 3.00158500 -0.84162500
C 0.51514200 1.52583500 -1.75594700
H 0.68571700 1.06558700 -2.74045000
H 1.20885800 -2.30268100 -1.76944300
H 2.19168700 -0.71227100 2.08741500
H -3.08060700 1.73117700 0.07036200
H -4.45035600 -2.26187700 0.82610600
O -5.60378600 2.70001900 -0.40607900
O -7.58456700 0.89889100 -0.13341200
O -7.06135400 -1.66073700 0.37356200
O 3.79701800 -2.63705400 -2.52058600
O 5.64482700 -1.71916900 -0.64162800
O 4.86449500 -0.76633100 1.64061800
C -4.58185000 3.65350000 -0.55753400
H -4.02432800 3.81009600 0.38062800
H -3.86399300 3.36752600 -1.34383300
H -5.06707000 4.59313000 -0.84149300
C -7.98480300 1.00409800 -1.48252700
H -7.91702100 0.03173500 -1.99917200
H -9.03121400 1.33050000 -1.48634000
H -7.38146300 1.74500800 -2.03146700
C -6.83188900 -3.00286700 0.70272800
H -7.80496600 -3.50526100 0.68545000
H -6.16459600 -3.50095700 -0.02124500
H -6.39574800 -3.11279200 1.71068300
C 2.86068000 -2.93184900 -3.52210800
H 2.17361900 -3.74031800 -3.22146500
H 2.25913300 -2.04854400 -3.79729100
H 3.42809400 -3.26230900 -4.39895200
C 6.16187000 -1.41424100 -1.91889100
H 6.26095000 -2.30900100 -2.54936800

H 5.53816500 -0.68269000 -2.45521700
H 7.15763500 -0.97850400 -1.75862000
C 4.49335300 -0.19682100 2.86589800
H 3.83301200 0.67788200 2.72952400
H 3.98437800 -0.92588900 3.52048100
H 5.41827700 0.12961700 3.35599200
C 0.19954600 -2.64175400 2.57695500
H -0.45773700 -3.47778100 2.85481200
H 1.16193100 -3.05540200 2.25428500
H 0.38216400 -2.07218100 3.50287400
C -2.64587200 -1.99410100 2.74829900
H -2.06274900 -1.95095200 3.67875000
H -3.57264100 -1.42918300 2.90095600
H -2.92331600 -3.05187700 2.61024900
C 1.75704500 1.80300000 -1.01653400
C 1.78560000 2.47978700 0.21651400
C 2.99594800 1.36358100 -1.50957800
C 2.96595000 2.69816200 0.91493800
H 0.84663900 2.83574300 0.65115200
C 4.18739100 1.56979200 -0.82416700
H 3.02490600 0.83307500 -2.46841100
C 4.20477200 2.23239200 0.41862900
H 2.92217500 3.22991500 1.86758200
H 5.11820300 1.20309600 -1.25821100
N 5.37994600 2.40511800 1.13023300
Pd -0.75685700 0.28133200 -0.65479400
C 6.60632200 1.84749400 0.62442900
H 7.39998400 1.97201300 1.37060500
H 6.49983200 0.76716800 0.43215100
H 6.95146700 2.32821100 -0.31164500
C 5.39973800 3.28034000 2.26786600
H 5.04736800 4.30035900 2.02835800
H 4.77103500 2.91315200 3.10087400
H 6.42345300 3.36510500 2.64987500

TS1

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C 0.95346200 -3.10000200 -1.38117600
N 1.66699700 -2.18473300 -0.79509700
C 3.01373900 -2.39845700 -0.42747400
C 3.99018700 -1.56905600 -0.98287800

C 3.34041700 -3.35649700 0.53842600
C 5.32227600 -1.71585000 -0.58102100
C 4.67241100 -3.48200300 0.95555300
C 5.66917100 -2.65090600 0.41230800
C -2.16842100 -1.13151200 -1.52513600
C -3.23501600 -1.84534000 -0.96283300
C -2.41086300 0.04649100 -2.23692200
C -4.53510500 -1.36683400 -1.10306500
C -3.72089500 0.49759100 -2.42708700
C -4.80279200 -0.18844500 -1.83793100
H -3.02923600 -2.73324800 -0.36613200
H -1.56372100 0.57488100 -2.67258100
H 2.55164200 -3.97309900 0.96991200
H 3.68990500 -0.81714400 -1.71222100
C -1.31375900 -3.78711700 -2.33533000
H -2.22762100 -3.35081200 -2.75157200
H -0.76867800 -4.29006700 -3.14424700
H -1.61697000 -4.58080900 -1.63448700
C 1.47334600 -4.43175100 -1.81022000
H 1.31494300 -4.57988900 -2.88795100
H 2.54172700 -4.54323600 -1.60343000
H 0.94055200 -5.25341600 -1.30843900
O -5.61459900 -1.94599100 -0.53801800
O -4.02421600 1.59714200 -3.15951900
O -6.09991200 0.17549000 -1.89433600
O 5.09754500 -4.36597600 1.87963600
O 6.94158700 -2.72202700 0.86733300
O 6.34520900 -0.98748500 -1.07099200
C -6.49103400 1.52915600 -2.01744300
H -7.52001100 1.58202300 -1.64039300
H -5.85508400 2.19844100 -1.41784100
H -6.47376800 1.87242800 -3.05974400
C -2.96918800 2.34654700 -3.70471100
H -2.29127400 2.73090000 -2.92336900
H -2.37757100 1.75970900 -4.42586000
H -3.42269800 3.19389600 -4.22895300
C -5.41926600 -3.11310900 0.21653900
H -5.01370400 -3.93439000 -0.39796100
H -4.74108700 -2.94112700 1.07096100
H -6.40271100 -3.41181500 0.59641600
C 4.14706800 -5.20140100 2.48784400
H 3.38138600 -4.62391500 3.03150600
H 3.64355300 -5.85470600 1.75543400
H 4.68873600 -5.82815100 3.20323300
C 7.77474600 -3.63995200 0.18820300
H 8.76137300 -3.59246700 0.66172900
H 7.39312600 -4.67068000 0.27015800
H 7.88093800 -3.37810400 -0.87720900
C 6.05336100 0.00189000 -2.02332700
H 7.00307100 0.48072900 -2.28255800
H 5.60993200 -0.42452200 -2.93848400
H 5.36622500 0.76576500 -1.62248700
Pd 0.65921900 -0.33956500 -0.27826200
C 2.20753000 0.49695800 0.75446600
H 2.79955700 -0.31465900 1.20565200
H 2.83421100 1.04221300 0.02701500
H 1.90146600 1.20500800 1.54037900
C -2.24713800 0.63730900 1.72449300
C -3.34564600 1.13007600 0.99686800
C -4.63517200 0.69408700 1.23638800
C -4.90332600 -0.29770700 2.21205500
C -3.79987600 -0.79760900 2.94812900
C -2.51881600 -0.32397000 2.71386800
H -3.18654700 1.89942600 0.23301800
H -5.45463900 1.11487900 0.65490500
H -3.95030600 -1.55450300 3.71864100
H -1.69133800 -0.71764900 3.31208900
C -0.89187600 1.17697200 1.54858100
N -6.17739400 -0.74828600 2.43394100
C -1.06675000 2.91504000 2.44832500
C 0.22501500 3.35556200 2.74574800
H 0.67085500 2.98921600 3.67910700
C 1.09342200 4.09586100 1.91032100
C 2.45485200 4.26943700 2.27663600
C 0.68260300 4.68560900 0.68389200
C 3.34227600 4.96458800 1.48981800
H 2.80595100 3.82703400 3.21273100
C 1.55780500 5.38506900 -0.11372300
H -0.35950900 4.59639300 0.36853300
C 2.92103200 5.54970700 0.26326100
H 4.37616700 5.06363300 1.81840300
H 1.19044200 5.82864000 -1.03866800
N 3.78696600 6.25047600 -0.51621300
C -6.43883100 -1.65377000 3.52537100
H -6.14613500 -1.23149500 4.50155500
H -7.50923900 -1.87780700 3.56730600
H -5.90478500 -2.61213200 3.40875300
C -7.27961200 -0.21303000 1.66583100

H -7.45839400 0.85653800 1.87466500
H -7.10559900 -0.33267900 0.58536100
H -8.19525300 -0.75717400 1.91885200
C 3.33580400 6.84809000 -1.75388000
H 4.17312600 7.35657000 -2.23967500
H 2.94884500 6.09333100 -2.45602800
H 2.54207700 7.59313800 -1.58647300
C 5.16053800 6.43217600 -0.09813900
H 5.23019700 6.96485600 0.86305000
H 5.68697200 5.47111600 0.00912800
H 5.69424900 7.02356900 -0.84712400
C -0.35700300 1.42406600 0.21089800
H -1.13931600 1.63148000 -0.53736900
H 0.42823100 2.19103600 0.16557200
H -0.17642800 0.74844700 2.25989300
H -1.63769100 3.43389600 1.67195200
H -1.67850800 2.60121400 3.29659300

TS2(2,1)

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C -0.459483 1.936271 1.225702
N 0.232769 1.188625 0.421946
C 1.652250 1.234076 0.452241
C 2.332668 0.350208 1.277124
C 2.341991 2.135987 -0.364445
C 3.734587 0.367897 1.323291
C 3.739619 2.133140 -0.342702
C 4.452281 1.264072 0.513039
C -3.725671 0.379331 0.507406
C -4.596168 1.274409 -0.132018
C -4.185900 -0.872338 0.928151
C -5.930161 0.916973 -0.336374
C -5.525557 -1.228083 0.741755
C -6.421536 -0.334402 0.113234
C -2.289857 -1.683923 -1.556225
H -3.032334 -0.886230 -1.697696
H -2.492505 -2.457365 -2.299159
H -2.371533 -2.150545 -0.563712
C 0.627670 -0.795518 -2.188394
H 0.757817 0.123356 -2.778043
C -0.515088 -1.603023 -2.523847

H -1.019669 -1.333862 -3.455030
H -0.374558 -2.682993 -2.424141
Pd -0.827530 -0.279332 -0.751309
C -2.783425 2.731342 1.944464
H -2.345416 2.999657 2.914770
H -2.874815 3.672652 1.379451
H -3.795732 2.348140 2.111738
C 0.132755 2.939155 2.155506
H -0.313301 3.931043 1.994701
H -0.079612 2.673606 3.202168
H 1.217122 3.022510 2.038892
H -4.215752 2.231647 -0.488735
H -3.487669 -1.555084 1.411328
H 1.783114 2.799622 -1.024488
H 1.800296 -0.368643 1.901457
O -6.837083 1.695448 -0.949756
O -7.706612 -0.587556 -0.164621
O -6.032818 -2.426250 1.105021
O 4.505031 2.888930 -1.159396
O 5.807052 1.157958 0.444984
O 4.299532 -0.562242 2.121472
C 3.865033 3.739621 -2.079143
H 3.222492 3.176039 -2.775652
H 3.255081 4.505906 -1.573954
H 4.654127 4.237276 -2.651371
C 6.587872 2.309294 0.723640
H 6.684266 2.960978 -0.154478
H 6.158659 2.892280 1.554216
H 7.583122 1.954940 1.020243
C 5.536691 -0.323138 2.765131
H 5.631703 0.723171 3.091910
H 5.548536 -0.967226 3.653129
H 6.396017 -0.575745 2.128891
C -5.178602 -3.363111 1.711746
H -4.345139 -3.646315 1.047623
H -4.766140 -2.987910 2.662412
H -5.782611 -4.252515 1.916569
C -8.521333 -1.364330 0.696981
H -8.421133 -2.438841 0.498517
H -8.291347 -1.172456 1.754235
H -9.553184 -1.055728 0.494871
C -6.426027 2.950077 -1.428535
H -6.057446 3.599516 -0.616711
H -5.639848 2.859425 -2.196283

H -7.306104 3.418198 -1.880257
C 1.859493 -1.321727 -1.629938
C 1.901197 -2.429218 -0.756678
C 3.089103 -0.720053 -1.957351
C 3.088525 -2.890751 -0.224061
H 0.966943 -2.923493 -0.469153
C 4.290722 -1.187399 -1.461456
H 3.095822 0.141567 -2.632213
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H 3.064874 -3.737886 0.461088
H 5.210075 -0.671029 -1.737993
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C 5.497960 -3.747399 0.986129
H 6.513380 -3.891295 1.369147
H 4.849576 -3.487118 1.839032
H 5.154638 -4.715570 0.584159
C 6.748030 -2.102466 -0.423301
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H 6.770804 -1.021231 -0.209703
H 7.577176 -2.576606 0.111378

TS3(1,2)

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N 1.809150 -1.219159 -0.268084
C 3.157234 -0.799017 -0.240596
C 3.823170 -0.463126 -1.415777
C 3.794605 -0.667292 1.001488
C 5.147061 0.002253 -1.380991
C 5.113372 -0.219399 1.044766
C 5.805210 0.135140 -0.142151
C -2.191764 -1.830702 -0.188196
C -2.827050 -3.064166 0.023956
C -2.945562 -0.648679 -0.234521
C -4.213978 -3.115422 0.161289
C -4.338027 -0.699512 -0.137717
C -4.997027 -1.938089 0.046753
C -1.201963 0.505974 2.287858
H -0.943446 0.605949 3.346267
H -2.102192 1.078543 2.038899
H -1.426160 -0.559089 2.098208

C 1.362626 1.359331 1.640548
H 1.814874 1.172123 2.621901
C 0.041940 1.944676 1.643301
H -0.262297 2.438871 2.571108
Pd 0.340861 -0.209946 0.847769
C -0.569368 -3.520139 -1.977597
H 0.006016 -3.524798 -2.912005
H -0.485988 -4.535411 -1.558730
H -1.625796 -3.355244 -2.218292
C 2.306025 -3.104114 -1.785457
H 1.978654 -4.149601 -1.713634
H 2.312683 -2.853206 -2.857376
H 3.340608 -3.032905 -1.432825
H -2.231190 -3.970581 0.118909
H -2.422127 0.302061 -0.363838
H 3.239296 -0.909024 1.908017
H 3.337775 -0.539521 -2.389519
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O -6.314513 -2.103456 0.202986
O -5.130297 0.394715 -0.177366
O 5.812444 -0.040244 2.183515
O 7.038043 0.684254 -0.101110
O 5.666737 0.325510 -2.577740
C 5.192114 -0.347824 3.407918
H 4.305477 0.282220 3.584261
H 4.893239 -1.407037 3.460089
H 5.927688 -0.147686 4.192996
C 8.083501 -0.003951 0.569043
H 8.212403 0.361352 1.595824
H 7.899913 -1.088377 0.596462
H 9.005513 0.184208 0.002960
C 7.063724 0.333521 -2.817814
H 7.556635 -0.550098 -2.385263
H 7.176069 0.299719 -3.907165
H 7.546724 1.239863 -2.432455
C -4.527765 1.654963 -0.332884
H -3.847926 1.889713 0.504027
H -3.954088 1.730988 -1.272233
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C -7.263232 -1.285829 -0.462463
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H -6.930479 -1.021880 -1.475554
H -8.178810 -1.884040 -0.529534
C -4.207097 -5.446835 0.526653

H -3.655021 -5.700910 -0.394087
H -3.498677 -5.419394 1.370736
H -4.951653 -6.225991 0.716148
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C -1.625832 3.456767 0.626656
C 0.006624 2.433849 -0.842802
C -2.262141 4.095819 -0.461035
H -2.008614 3.594707 1.640541
C -0.598918 3.077352 -1.919322
H 0.879385 1.796044 -1.005626
C -1.714790 3.887865 -1.748522
H -0.190724 2.947371 -2.924204
H -2.157583 4.370272 -2.620069
N -3.382155 4.869033 -0.274234
C -3.998773 5.521842 -1.403611
H -4.880738 6.076724 -1.069173
H -3.322721 6.237697 -1.901738
H -4.333409 4.797444 -2.165172
C -3.849798 5.147491 1.060637
H -4.719249 5.810359 1.014354
H -4.162996 4.233110 1.594152
H -3.084618 5.645544 1.680304

TS4

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N -1.02170300 -2.02308900 -0.85093200
C -2.34576500 -2.31307700 -0.47521700
C -2.59542800 -3.20180000 0.57968100
C -3.40386100 -1.65964200 -1.11721600
C -3.90965400 -3.45567600 0.97950600
C -4.72431400 -1.93876300 -0.73837900
C -4.99449800 -2.84353000 0.31019800
C 2.86397500 -0.91955300 -1.38071600
C 3.26337000 0.00889400 -2.34021600
C 3.77303700 -1.40355500 -0.43389400
C 4.59888800 0.43003700 -2.38649500
C 5.08375900 -0.93018600 -0.43485700
C 5.52319600 -0.01304000 -1.41659300

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H -2.19361400 0.23765000 -0.19421400
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H -0.33251400 2.43270400 1.34464700
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H 1.37983900 2.12979000 -1.12990900
H 2.53156500 0.36940700 -3.06270400
H 3.42590100 -2.09295600 0.33604500
H -3.18573200 -0.96361300 -1.92827500
H -1.75453100 -3.67672900 1.08576000
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O -4.24712800 -4.26807200 1.99632100
O 5.06985700 1.28505400 -3.32402900
O 6.81092300 0.36752000 -1.31592200
O 6.00247300 -1.25986600 0.49535400
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H -5.06589100 0.43219300 -2.03723700
H -5.08485300 -0.92568100 -3.21357200
H -6.61384000 -0.15855500 -2.70070900
C -7.28716700 -3.38235200 -0.12622500
H -6.92744800 -3.86254200 -1.04794000
H -7.96702900 -4.07141000 0.38899400
H -7.83530400 -2.46899000 -0.39144600
C -3.21784800 -4.88680300 2.72280000
H -3.69821400 -5.48275200 3.50505700
H -2.61128200 -5.55707900 2.09048100
H -2.55010600 -4.14866500 3.19820400
C 4.16335600 1.83914500 -4.24338100
H 3.69878600 1.06785600 -4.87865000
H 3.36560300 2.41089300 -3.73907100
H 4.73731900 2.51986900 -4.87997500
C 7.24612600 1.65051600 -1.72300000
H 8.17848700 1.84065700 -1.17719300
H 7.44750600 1.69679900 -2.80097100
H 6.51685000 2.43383200 -1.46691700

C 5.62238900 -2.14507400 1.51624800
H 4.76241100 -1.76228700 2.09350900
H 5.36809400 -3.14237500 1.11962400
H 6.48419100 -2.24218300 2.18596200
C 2.15334700 -3.64100600 -1.91561400
H 1.74884500 -4.21481800 -2.76002700
H 3.12096200 -3.22463200 -2.21168100
H 2.33482700 -4.37086300 -1.11164800
C -0.62469000 -4.37240200 -1.51890900
H -0.28918400 -4.69469600 -2.51407500
H -0.16347300 -5.06963800 -0.80282500
H -1.70943400 -4.50412800 -1.46106800
C -2.86213800 2.09933700 0.45463200
C -3.47853500 2.36646200 -0.77940000
C -3.15339200 2.97889400 1.51121300
C -4.36434900 3.41500200 -0.95415800
H -3.23473700 1.72811500 -1.63667400
C -4.04367200 4.02992700 1.36396600
H -2.68196300 2.83131800 2.48773400
C -4.68627700 4.27614300 0.12533600
H -4.81585100 3.56901700 -1.93474800
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C -3.504973 4.18469700 0.718986
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H 0.8778760 1.61838100 1.72842900
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Pd 0.19129000-0.42123600 -0.6802270
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H 7.41147800 2.48328900 2.5627740
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H 4.7541770 1.57586000 4.24700700
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C -6.2720340 5.19054000 -1.6108530
H -7.150142 4.74224200 -1.12268700
H -6.543699 6.19976200 -1.93053100
H -6.0429000 4.60106700 -2.51106700
C -4.573148 6.55522800 -0.38715100
H -4.640263 6.76953600 0.6899290
H -3.516655 6.62523000 -0.68556900
H -5.12463500 7.33444600 -0.91929500

IM-1

1 1

C 4.84928400-0.21669100 0.61477000
H 4.52011500-0.32596400 1.65593500
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H 5.27283300 0.78984900 0.50015300
C 2.62853500 0.53784300-0.25208200
H 2.95987300 1.58567900-0.24527000

C 3.70276600-0.45998900-0.36085500
H 3.32120800-1.48763500-0.28275900
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C 1.26804400 0.33320200-0.16478600
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C 0.66088300-0.97019900-0.14646400
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H 0.81454500 2.46647400-0.10065500
C-0.69003300-1.12794800-0.07091600
H 1.29338600-1.85821300-0.19285800
C-1.56343900 0.01131000-0.00347600
H-1.60130300 2.20455000 0.03680800
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N-2.89157200-0.14368100 0.07065500
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H-4.57588900-1.37787200 0.13999700
H-3.24531100-2.02609300-0.83625300
H-3.15001400-2.05629500 0.94649900
C-3.77270800 1.01405600 0.14371500
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IM-2

1 1

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C 3.88002100 1.22785800 0.20270000
C 4.96486600 0.39969000 -0.17623600
C 4.67890800 -0.96252500 -0.42650700
C 3.38530000 -1.45363800 -0.30376400
H 1.79611600 1.39289200 0.62367900
H 4.04217900 2.28315000 0.41274100
H 5.47325300 -1.64807600 -0.71443400
H 3.20801400 -2.51440600 -0.50025900
C 0.91489200 -1.18836400 0.19724500
N 6.23554500 0.89680600 -0.29188500
C 0.02791100 -0.62227300 -0.96288400
C -1.30040700 -1.25931800 -0.99577300
H -0.02390200 0.47102100 -0.87645800
H -1.29990700 -2.33111300 -1.23281200
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C -3.71217000 -1.51664500 -0.79074300
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C -4.94907700 -1.01713100 -0.53087400
H -3.60364700 -2.57025000 -1.05682400
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H 0.97446300 -2.28178500 0.06167800
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IM-3

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C -3.87636900 -1.87955500 -1.03528200

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H -4.76845800 -1.48641600 -1.51872600
H -2.71238600 -0.17711400 -1.61638800
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