

Electronic Supporting Information

Metal-free photocatalysts with charge-transfer excited states enable visible light-driven atom transfer radical polymerization

Yuchen Huang,^{a,b} Yangxin Liu,^{a,b} Yingde Yan,^{a,b} Yanjun Gong,^c Yifan Zhang,^{a,d*}
Yanke Che,^{a,b} and Jincai Zhao^{a,b}

^a Key Laboratory of Photochemistry, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

^b University of Chinese Academy of Sciences, Beijing 100049, China.

^c School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, P. R. China.

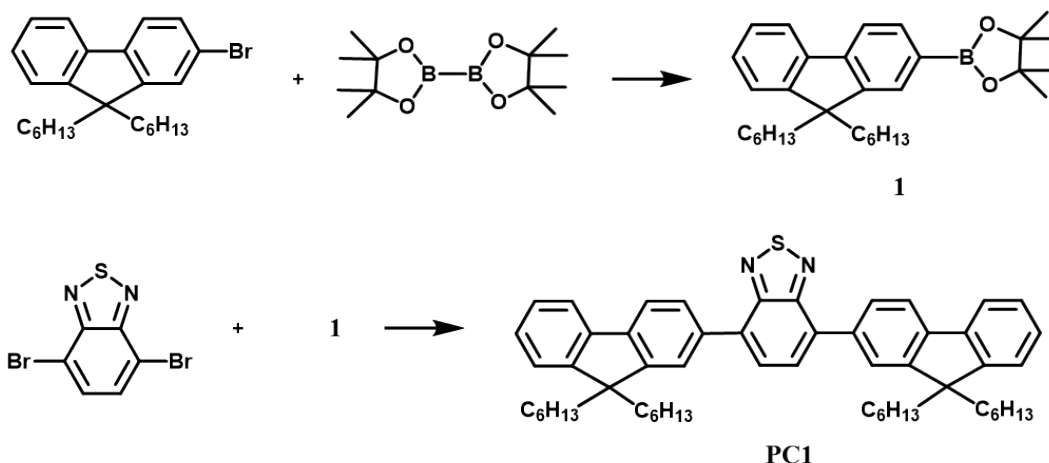
^d Key Laboratory of Green Catalysis of Higher Education Institutes of Sichuan, School of Chemistry and Environmental Engineering, Sichuan University of Science and Engineering, Zigong 643000, P. R. China.

Table of contents

1. Synthesis of photocatalysts **1-3**
2. Experimental methods
3. Other supporting figures and tables
4. Atom coordinates
5. References

1. Synthesis of photocatalysts PC1-PC3

1.1 Synthesis of photocatalyst 1 (PC1).



2-(9,9-dihexyl-9H-fluoren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1). A mixture of 2,7-bromo-9,9-dihexyl-9H-fluorene (580 mg, 1.40 mmol), bis(pinacolato)diboron (540 mg, 2.1 mmol), potassium acetate (410 mg, 5.6 mmol) and Pd(dppf)Cl₂ (100 mg, 0.14 mmol) in deoxygenated 1,4-dioxane (50 mL) was stirred at 85 °C under Ar for 20 h. The solvent was evaporated under vacuum. The residue was poured into water (80 mL) and extracted with ethyl acetate (3 × 40 mL). The combined organic layers were washed with brine (saturated), dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by column chromatography on the silica gel (dichloromethane as the eluent) to afford **1** (540 mg, 1.17 mmol, 84% yield).

4,7-bis(9,9-dihexyl-9H-fluoren-2-yl)benzo[c][1,2,5]thiadiazole (PC1). To a mixture of **1** (320 mg, 0.70 mmol), 4,7-dibromobenzo[c][1,2,5]thiadiazole (89 mg, 0.30 mmol), tetrakis(triphenylphosphine)palladium (35 mg, 0.03 mmol) in deoxygenated 1,4-dioxane (35 mL), an aqueous solution of potassium carbonate (8 mL, 4.0 M) was added. Then the mixture was heated to 85 °C and stirred under Ar for 8 h. The solvent was evaporated under vacuum. The residue was poured into water (80 mL) and extracted with dichloromethane (3 × 40 mL). The combined organic layers were washed with brine (saturated), dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by column chromatography on the silica gel (dichloromethane as the eluent) to afford **PC1** (220 mg, 0.28 mmol, 93% yield).

PC1 ¹H NMR (400 MHz, THF-*d*₈) δ 8.16 (d, *J* = 1.6 Hz, 2H), 8.05 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.98 (s, 2H), 7.88 (d, *J* = 7.9 Hz, 2H), 7.82 – 7.77 (m, 2H), 7.42 (dd, *J* = 6.9, 1.7 Hz, 2H), 7.36 – 7.32 (m, 2H), 7.32 – 7.26 (m, 2H), 2.25 – 1.96 (m, 8H), 1.20 – 1.03 (m, 24H), 0.781-0.79 (m, 8H), 0.76 (d, *J* = 7.2 Hz, 12H). MALDI-MS: (*m/z*) = 800.5.

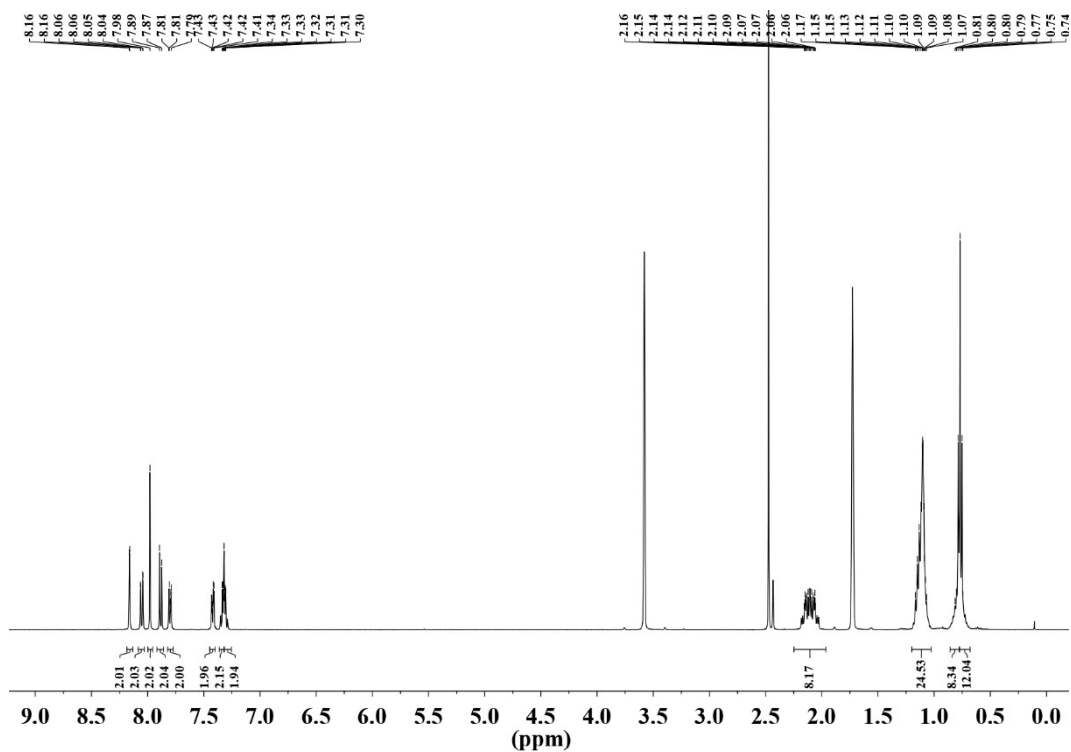


Figure S1. ^1H NMR spectrum of PC1.

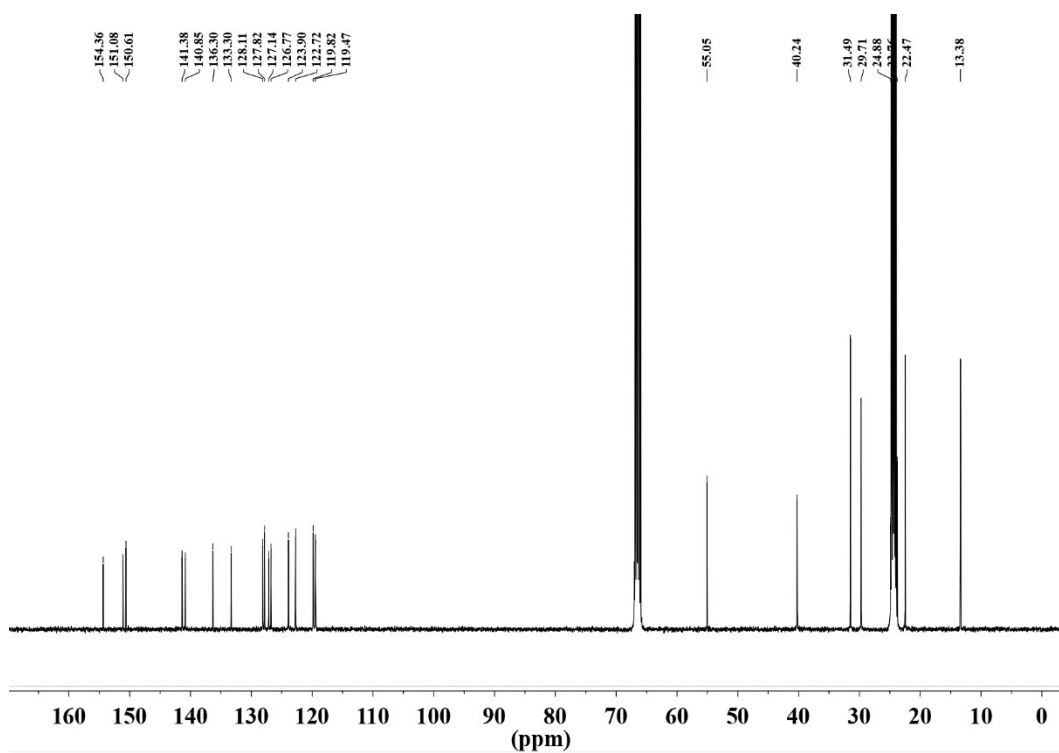


Figure S2. ^{13}C NMR spectrum of PC1.

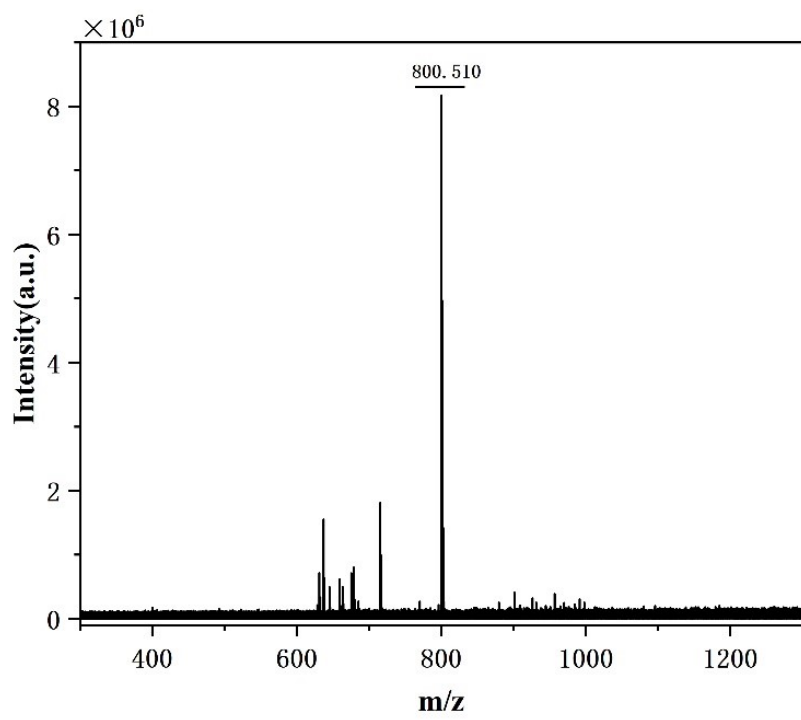


Figure S3. MALDI-TOF mass spectrum of PC1.

1.2 Synthesis of photocatalyst 2 (PC2).

The synthesis of PC2 was performed by following the previously reported method¹.

PC2 ¹H NMR (400 MHz, Chloroform-d) δ 8.06 (dd, $J = 7.8, 1.6$ Hz, 2H), 8.01 (d, $J = 1.6$ Hz, 2H), 7.92 (d, $J = 6.1$ Hz, 4H), 7.86 (d, $J = 7.8$ Hz, 2H), 7.79 (t, $J = 9.2$ Hz, 4H), 7.68 (d, $J = 6.1$ Hz, 6H), 7.66 – 7.59 (m, 6H), 7.59 – 7.52 (m, 4H), 7.07 – 7.00 (m, 4H), 3.89 (s, 6H), 2.22 – 1.97 (m, 16H), 1.20 – 1.04 (m, 49H), 0.85 (d, $J = 36.4$ Hz, 16H), 0.79 – 0.70 (m, 24H). MALDI-MS: (m/z) = 1676.1.

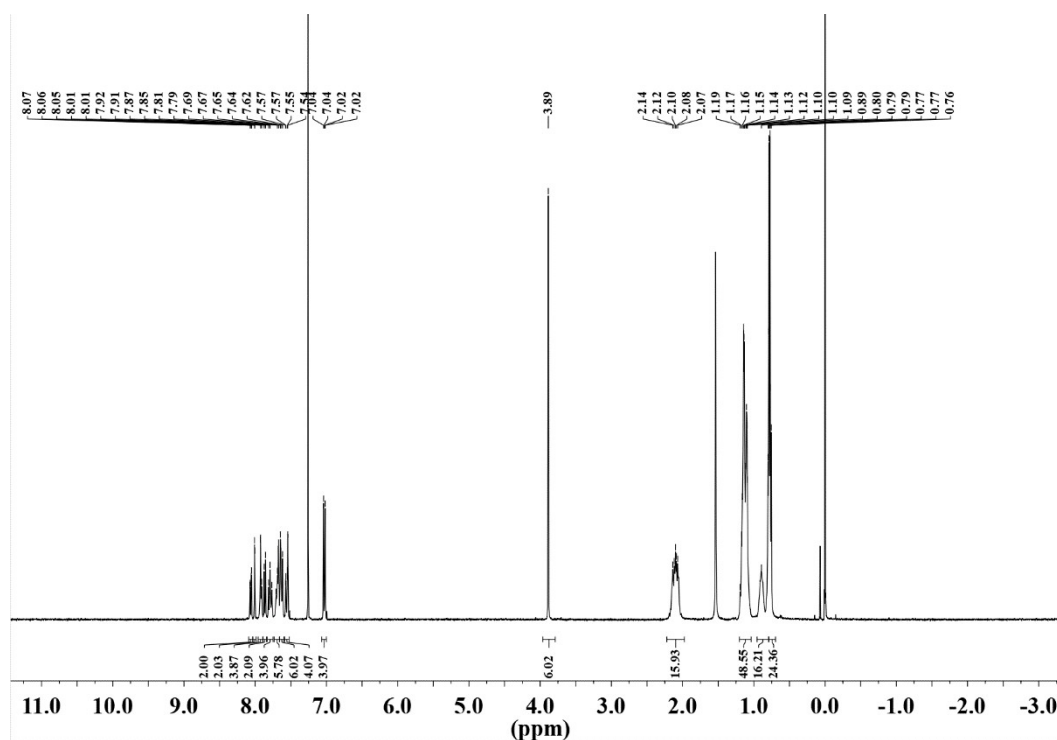


Figure S4. ¹H NMR spectrum of PC2.

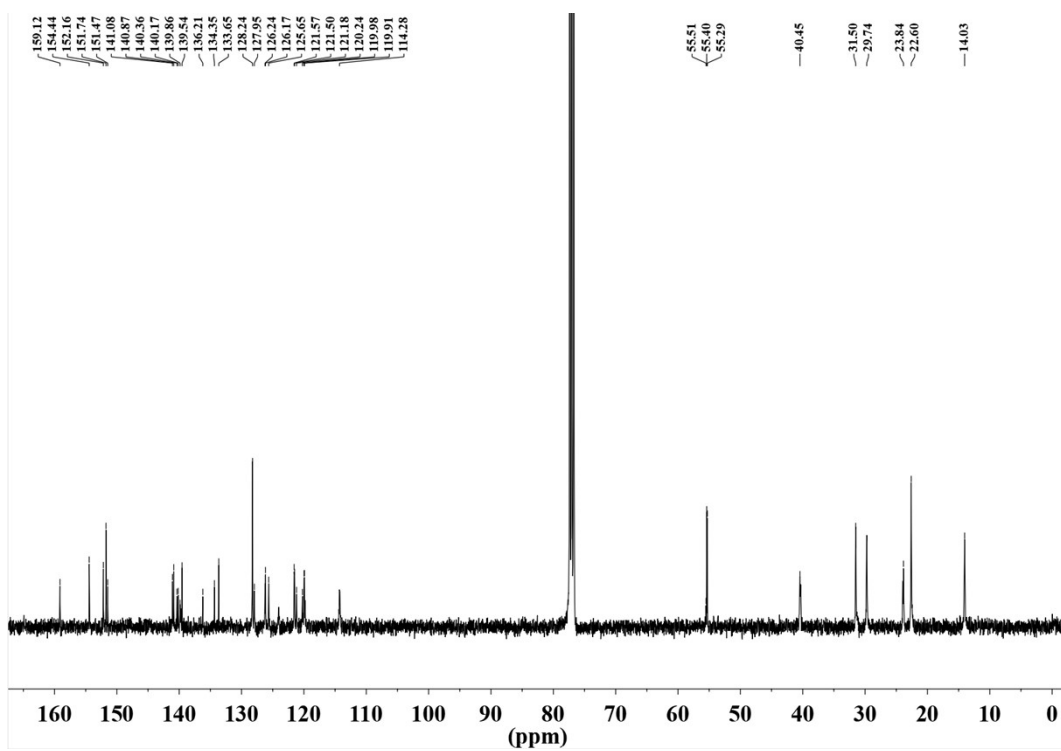


Figure S5. ^{13}C NMR spectrum of PC2.

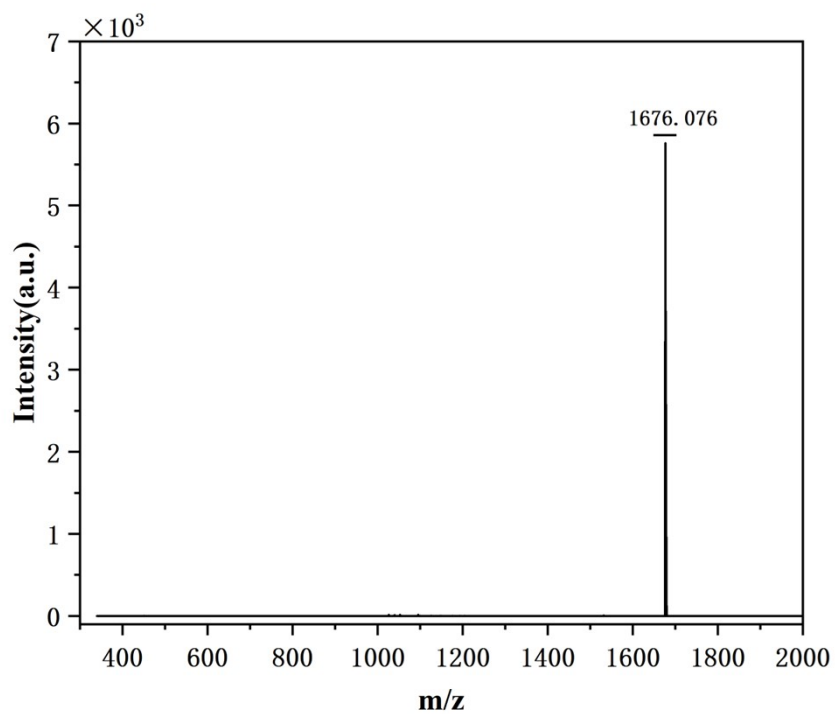
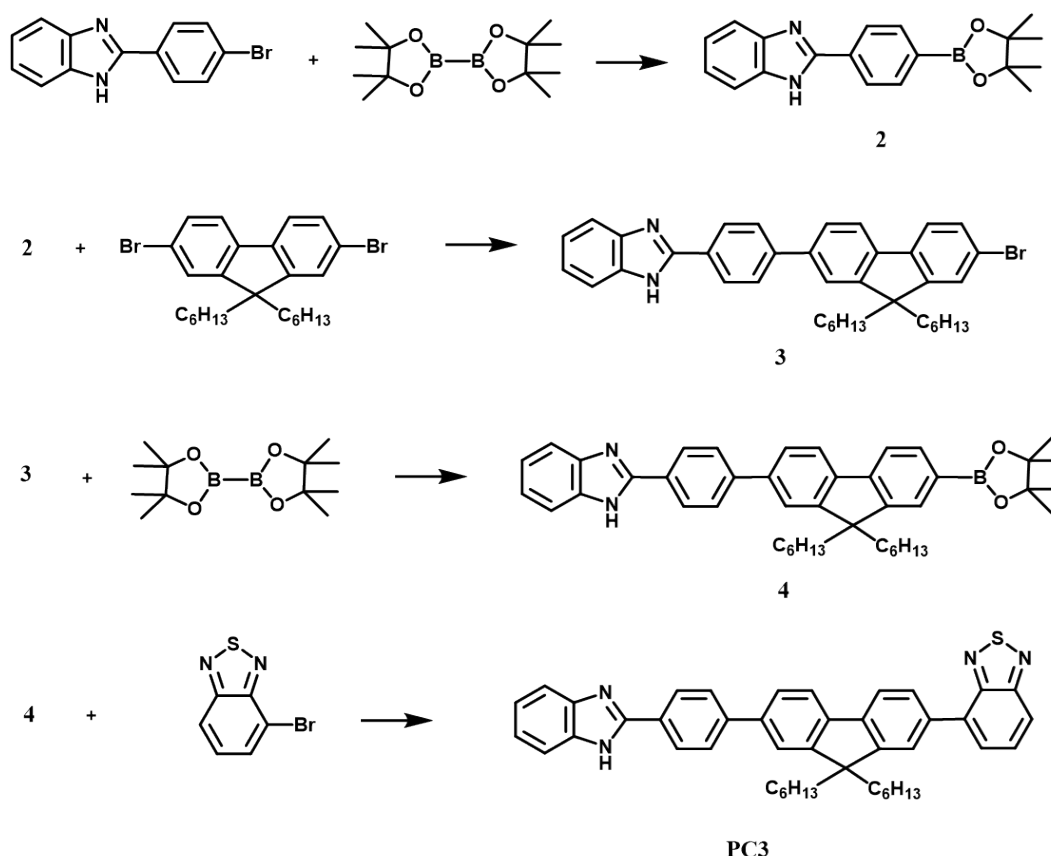


Figure S6 MALDI-TOF mass spectrum of PC2.

1.3 Synthesis of photocatalyst 3 (PC3).



2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (2). A mixture of 2-(4-bromophenyl)-1H-benzo[d]imidazole (2.00 g, 7.32 mmol), bis(pinacolato)diboron (2.70 g, 10.6 mmol), potassium acetate (2.15 g, 21.9 mmol) and Pd(dppf)Cl₂ (260 mg, 0.36 mmol) in deoxygenated 1,4-dioxane (40 mL) was stirred at 85°C under argon overnight. The solvent was evaporated under vacuum. The residue was poured into water (80 mL) and extracted with ethyl acetate (3 × 40 mL). The combined organic layers were washed with brine (saturated), dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by column chromatography on the silica gel (petroleum: ethyl acetate = 10:1 as the eluent) to afford **2** (2.10 g, 6.01 mmol, 86% yield).

Molecule **2** ¹H NMR (400 MHz, DMSO-d₆) δ 8.20 (d, J = 7.7 Hz, 2H), 7.84 (d, J = 7.8 Hz, 2H), 7.60 (s, 2H), 7.22 (dd, J = 6.1, 3.1 Hz, 2H), 1.33 (s, 12H).

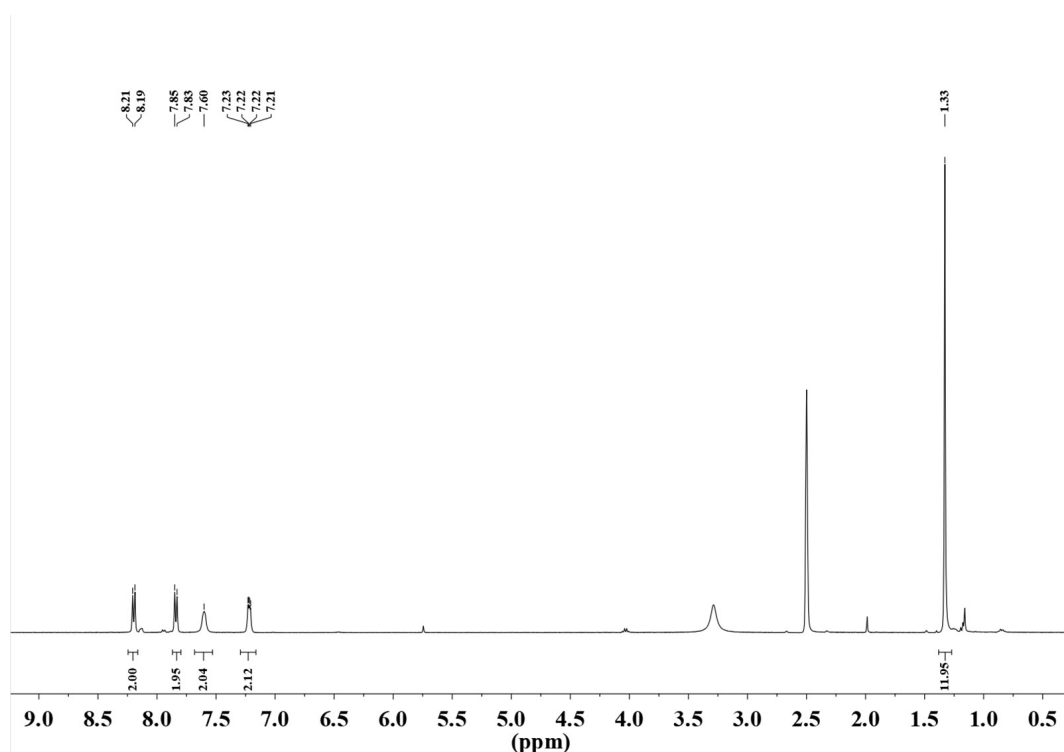


Figure S7. ^1H NMR spectrum of molecule **2**.

2-(4-(7-bromo-9,9-dihexyl-9H-fluoren-2-yl)phenyl)-1H-benzo[d]imidazole (3). To a stirred solution of **2** (2.00 g, 6.25 mmol), 2,7-dibromo-9,9-dihexyl-9H-fluorene (4.6 g, 9.34 mmol), and tetrakis(triphenylphosphine)palladium (360 mg, 0.31 mmol) in deoxygenated 1,4-dioxane (40 mL), an aqueous solution of potassium carbonate (8 mL, 2.0 M) was added. Then the mixture was heated to 85 °C and stirred under argon overnight. The solvent was evaporated under vacuum. The residue was poured into water (80 mL) and extracted with dichloromethane (3 × 40 mL). The combined organic layer was washed with brine (saturated), dried over Na_2SO_4 , and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum: ethyl acetate = 5:1 as the eluent) to afford **3** (2.65 g, 4.38 mmol, 70% yield).

Molecule **3** ^1H NMR (400 MHz, THF- d_8) δ 11.80 (s, 1H), 8.28 – 8.22 (d, 2H), 7.83 (d, $J = 8.5$ Hz, 3H), 7.76 – 7.66 (m, 3H), 7.60 (m, $J = 2.0$ Hz, 2H), 7.49 (m, $J = 8.1, 1.9$ Hz, 2H), 7.15 (m, $J = 6.1, 3.1$ Hz, 2H), 2.10 (td, $J = 9.2, 6.1$ Hz, 4H), 1.12 (q, $J = 7.4$ Hz, 12H), 0.71 (s, 4H), 0.65 (d, $J = 11.3$ Hz, 6H). MALDI-MS: (m/z) = 605.1

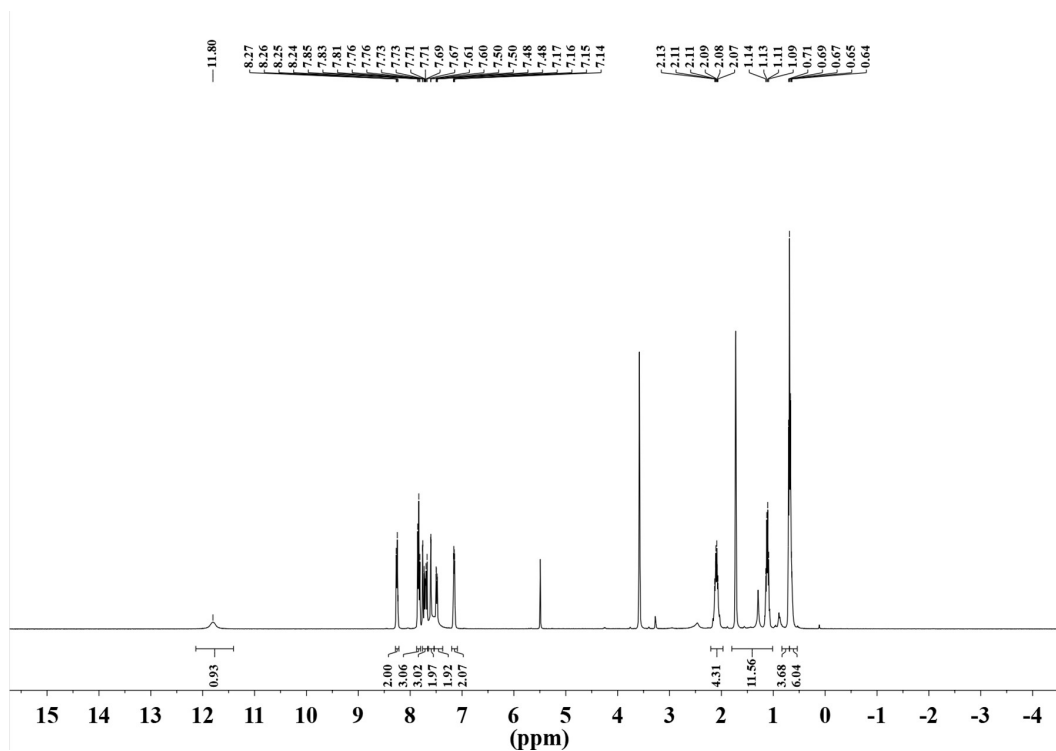


Figure S8. ^1H NMR spectrum of molecule **3**.

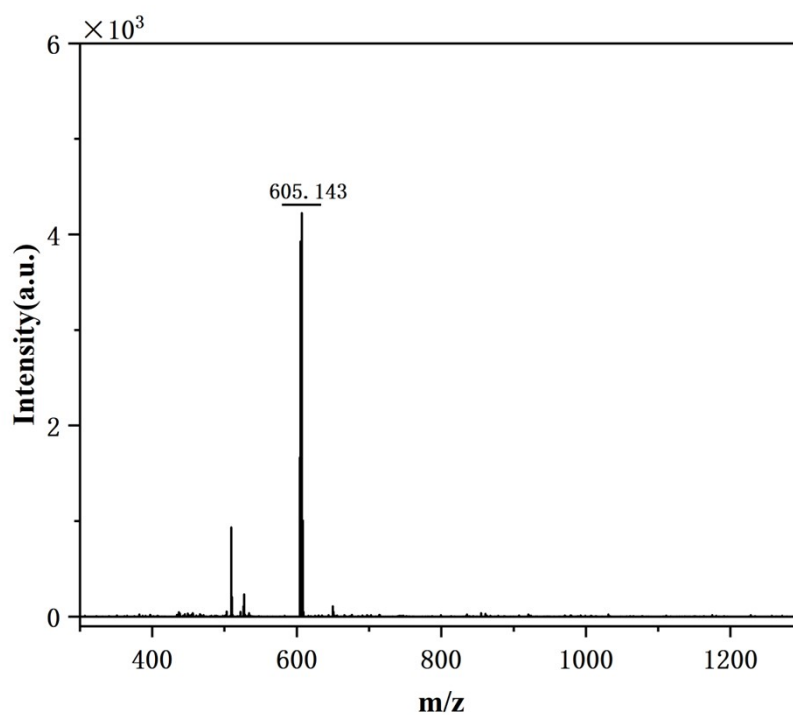


Figure S9. MALDI-TOF mass spectrum of molecule **3**.

2-(4-(9,9-dihexyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-fluoren-2-yl)phenyl)-1H-benzo[d]imidazole (**4**). A mixture of **3** (880 mg, 1.45 mmol),

bis(pinacolato)diboron (550 mg, 2.16 mmol), potassium acetate (430 mg, 4.39 mmol) and Pd(dppf)Cl₂ (50 mg, 0.07 mmol) in deoxygenated 1,4- dioxane (30 mL) was stirred at 85°C under argon overnight. The solvent was evaporated under vacuum. The residue was poured into water (80 mL) and extracted with dichloromethane (3 × 40 mL). The combined organic layers were washed with brine (saturated), dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by column chromatography on the silica gel (petroleum: ethyl acetate = 5:1 as the eluent) to afford **4** (616 mg, 0.99 mmol, 68% yield).

Molecule **4** ¹H NMR (400 MHz, Chloroform-d) δ 8.25 (d, J = 7.9 Hz, 2H), 7.87 – 7.76 (d, 3H), 7.76 – 7.69 (m, 3H), 7.69 – 7.61 (m, 2H), 7.57 (m, J = 7.7 Hz, 2H), 7.30-7.26 (m, 2H), 7.25 (m, J = 1.7 Hz, 2H), 2.01 (td, J = 7.2, 4.0 Hz, 4H), 1.41 (d, J = 12.0 Hz, 12H), 1.01 (tq, J = 8.7, 5.2, 3.5 Hz, 12H), 0.91 – 0.82 (m, 4H), 0.72 (t, J = 7.0 Hz, 6H). MALDI-MS: (m/z) =653.3

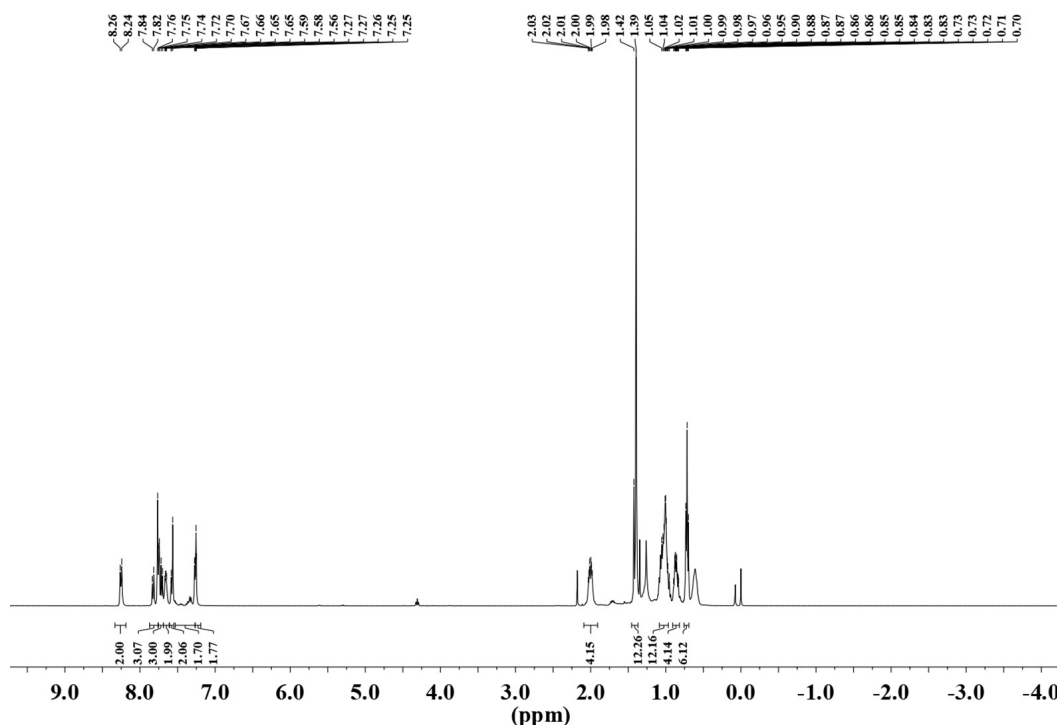


Figure S10. ¹H NMR spectrum of molecule **4**.

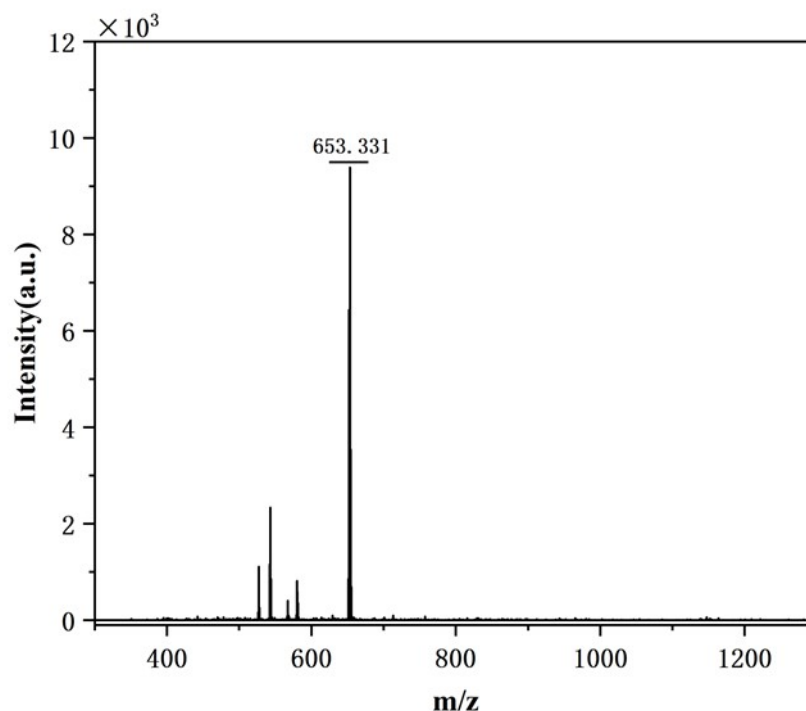


Figure S11. MALDI-TOF mass spectrum of molecule **4**.

4-(7-(4-(1H-benzo[d]imidazol-2-yl)phenyl)-9,9-dihexyl-9H-fluoren-2-yl)benzo[c][1,2,5]thiadiazole (PC3). To a stirred solution of **4** (200 mg, 0.31 mmol), 4-bromobenzo[c][1,2,5]thiadiazole (100 mg, 0.46 mmol), and tetrakis(triphenylphosphine)palladium (50 mg, 0.04 mmol) in deoxygenated 1,4-dioxane (40 mL), an aqueous solution of potassium carbonate (8 mL, 2.0 M) was added. Then the mixture was heated to 80 °C and stirred under argon overnight. The solvent was evaporated under vacuum. The residue was poured into water (40 mL) and extracted with dichloromethane (3 × 40 mL). The combined organic layer was washed with brine (saturated), dried over Na₂SO₄, and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum: dichloromethane = 1:1 as the eluent) to afford **PC3** (237 mg, 0.36 mmol, 78% yield).

PC3 ¹H NMR (400 MHz, THF-*d*₈) δ: 11.86 (s, 1H), 8.31 – 8.23 (m, 2H), 8.14 (d, *J* = 1.6 Hz, 1H), 8.09 – 7.97 (m, 2H), 7.93 (d, *J* = 3.1 Hz, 1H), 7.92 – 7.84 (m, 4H), 7.82 (d, *J* = 1.7 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.71 – 7.61 (m, 1H), 7.50 – 7.38 (m, 1H), 7.23 – 7.08 (m, 2H), 2.28 – 2.06 (m, 4H), 1.11 (m, 12H), 0.83 (dt, *J* = 10.4, 5.8 Hz, 4H), 0.76 (t, *J* = 6.7 Hz, 6H). MALDI-MS: (*m/z*) = 661.3.

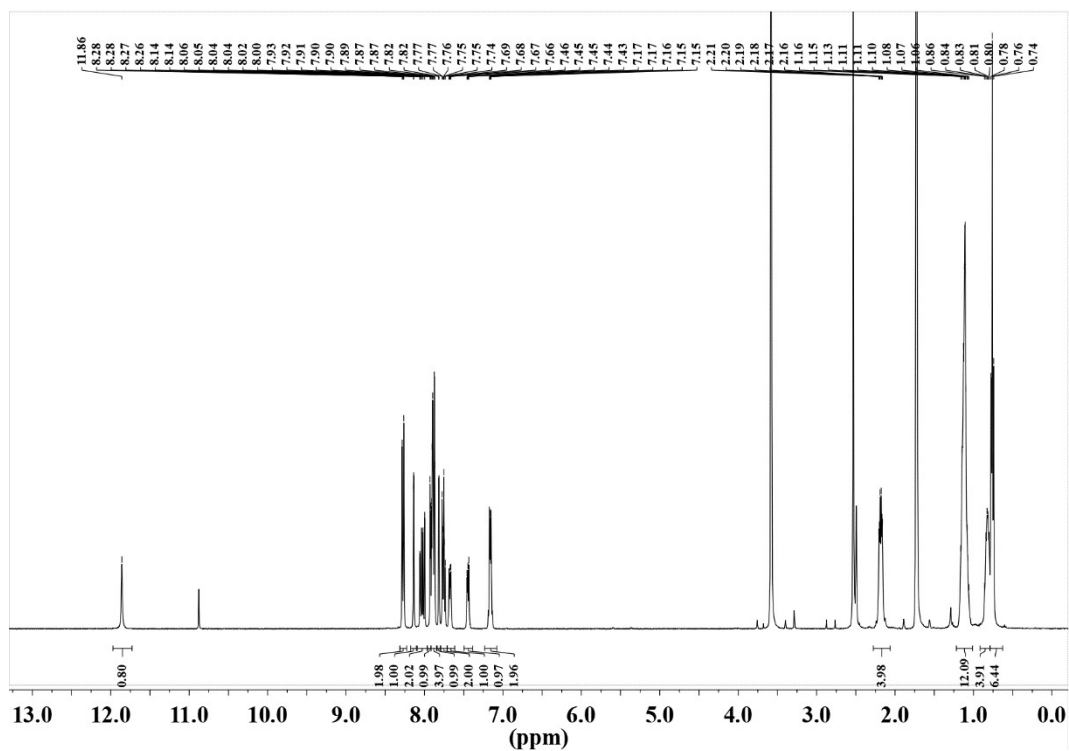


Figure S12. ^1H NMR spectrum of PC3.

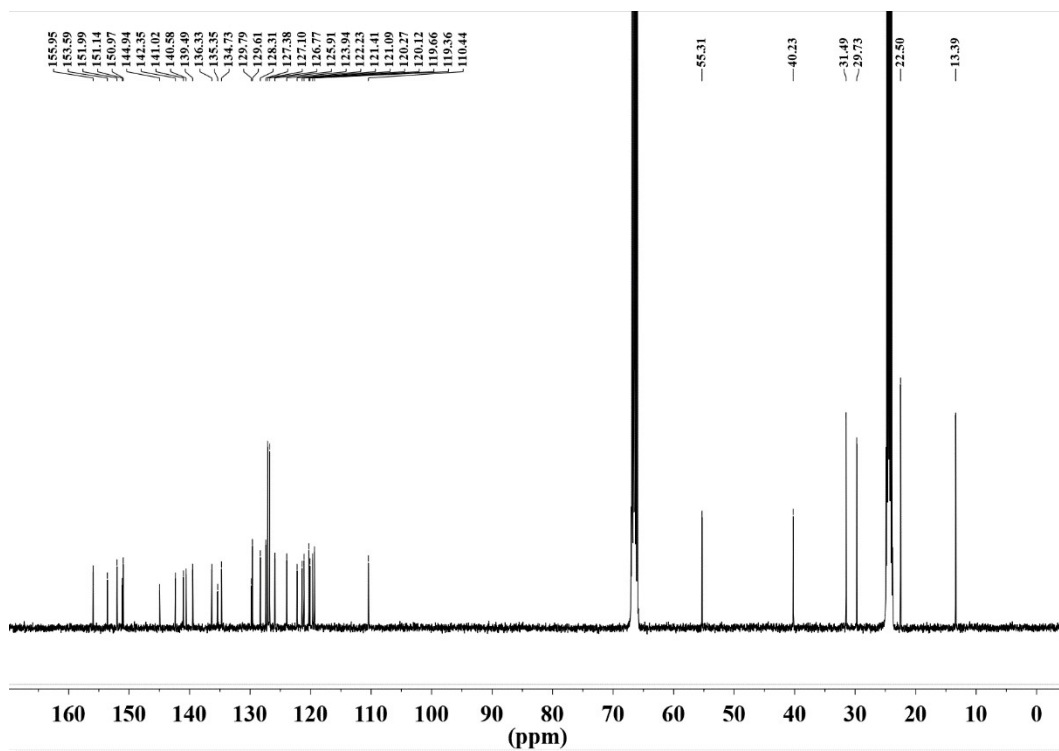


Figure S13 ^{13}C NMR spectrum of PC3.

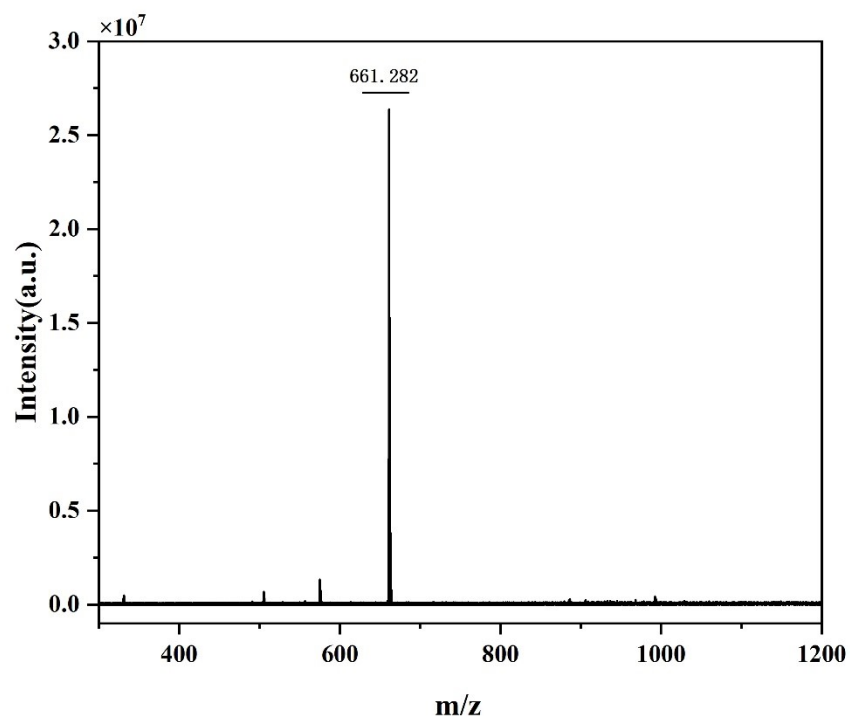


Figure S14. MALDI-TOF mass spectrum of **PC3**.

2. Experimental methods

General considerations All polymerizations were carried out under an argon atmosphere using glove box. **PC1**, **PC2**, and **PC3** were prepared and characterized according to the supporting information above. All other reagents were used as received. NMR spectra were performed in Bruker Avance III 400 HD spectrometer in deuterated solvents. Analysis of polymer molecular weights was performed via Gel permeation chromatography (GPC) coupled with 2414 RI detector, using Styragel HT 3, Styragel HT 4, Styragel HT 5 gel permeation columns. DMF was used as the eluent at a flow rate of 1.0 mL/min. Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry analysis was performed on a Bruker Autoflex III Smartbeam MALDI-TOF mass spectrometer. Absorption spectra of photocatalysts were obtained on a Hitachi U-3900 spectrometer.

Computational details All calculations were carried out with the Gaussian 16 software². The wB97xD functional³ was adopted for all calculations in combination with the SMD solvation model with DMF as the solvent⁴. For geometry optimization and frequency calculations the def2-SVP basis set⁵ was employed, and then single point calculations were performed with the def2-TZVP basis set.

General polymerization procedure A vial equipped with a magnetic stir bar and fitted with a Teflon screw cap septum was charged with methyl methacrylate (213 μ L, 50 equiv.), initiator (1 equiv.), triethylamine (20 equiv.), photocatalyst **PC1** (0.02 equiv.) in DMF (0.8 mL). The reaction mixture was degassed and backfilled with argon using glove box. The reaction was vigorously stirred in front of 470 nm blue LED light for 6 h. An aliquot was taken and analyzed using ¹H NMR in CDCl₃ to give the conversion, and the isolated polymer by methanol was used for GPC to give the M_n and D .

Control experiments The control experiments were the same as the general polymerization procedure, but the feeding ratio depended on the demand. An aliquot was taken and analyzed using ¹H NMR in CDCl₃ to give the conversion. If the conversion is lower than 1%, it will be considered as no polymerization.

The evaluated experiments A vial equipped with a magnetic stir bar and fitted with a Teflon screw cap septum was charged with different kinds and quantities of monomer, initiator, donor, photocatalyst **PC1**, **PC2**, and **PC3** in solvent. the reaction mixture was degassed and backfilled with argon using glove box. The reaction was vigorously stirred in front of 470 nm blue LEDs for 6 h. An aliquot was taken and analyzed using ¹H NMR in CDCl₃ to give the conversion, and the isolated polymer by methanol was used for GPC to give the M_n and D .

Reaction setups for O-ATRP The reactions were performed in a photoreactor, the vial with reaction mixture is placed at the center of a stir plate and surrounded by water to maintain ambient temperature. The parallel blue LED lamp (CEL-100HALED 470 nm) is placed perpendicular to the sidewall of the vial. The reaction temperature can be maintained at 20-25°C during the reaction.

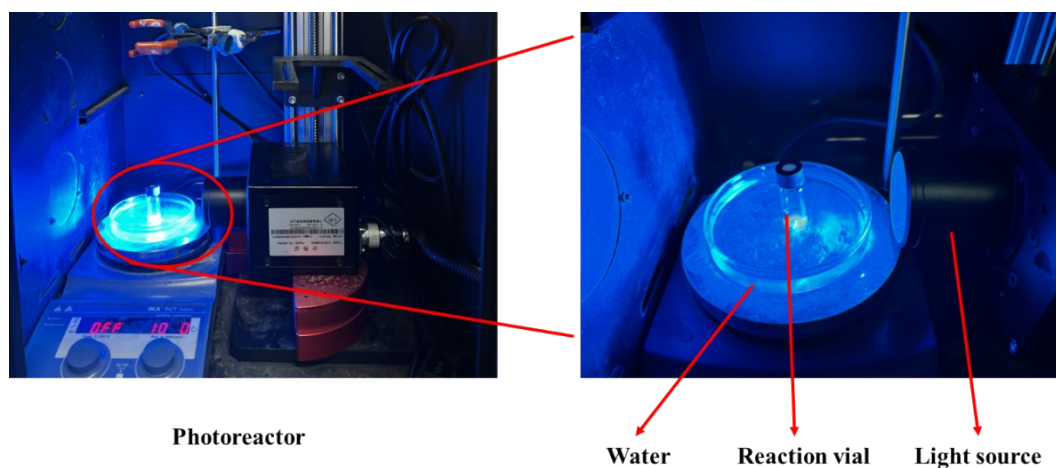


Figure S15. Reaction setup for polymerization.

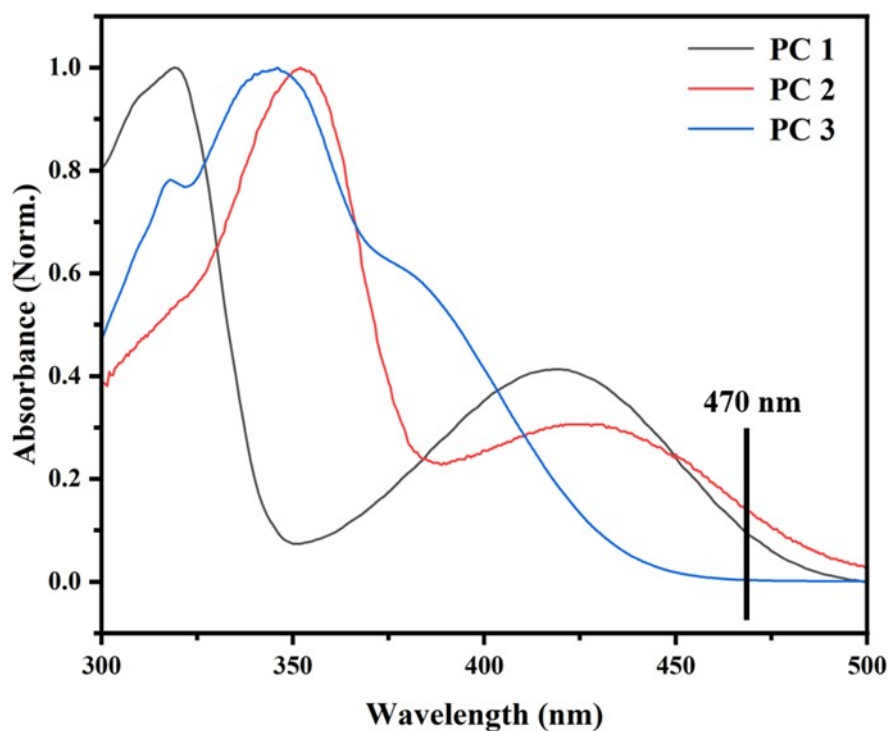


Figure S16. UV-Vis-NIR spectra of PC1, PC2, and PC3 in DMF at 295 K.

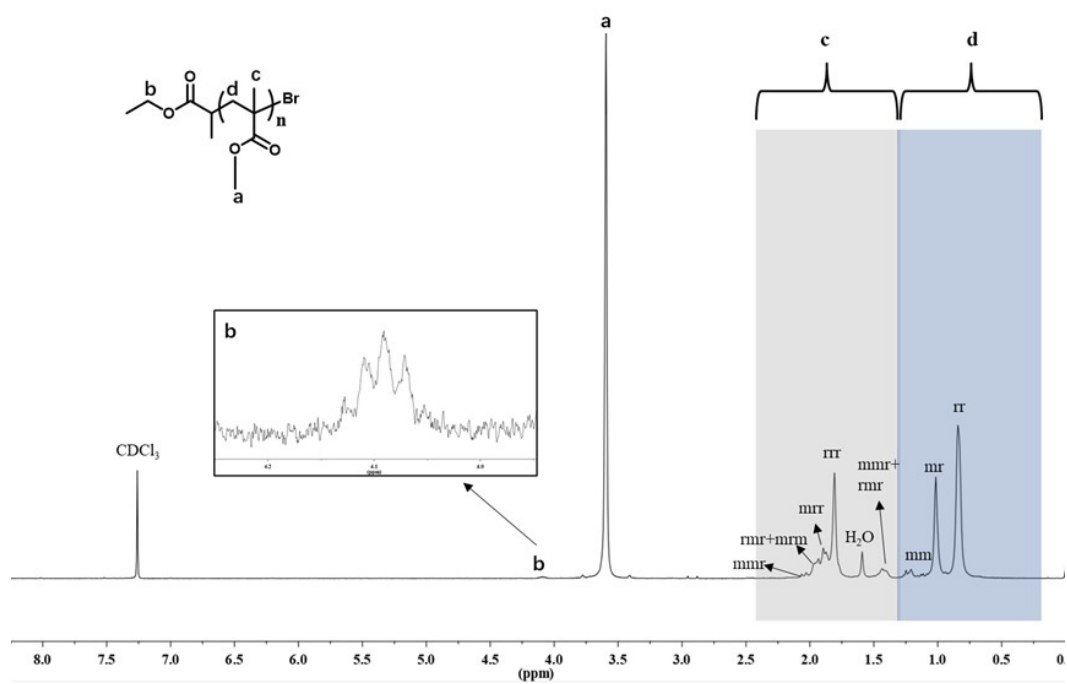


Figure S17. ^1H NMR spectra of the obtained PMMA product. (mmr, rmr, mrm, etc. are tacticity of polymer.)

3. Other supporting figures and tables

Table S1. Control experiments.

Entry ^a	[MMA]:[EBrP]	Photocatalyst	Donor	Light	Conversion (%) ^b
S1	50:1	0.02 eq.	-	470 nm	3.2
S2	50:1	-	20 eq.	470nm	n/a
S3	50:1	0.02 eq.	20 eq.	-	n/a
S4	50:0	0.02 eq.	20 eq.	470 nm	n/a
S5 ^c	50:1	0.02 eq	20 eq.	470 nm	n/a

^a 213 μ L (50 eq.) methyl methacrylate in 800 μ L DMF.

^b Calculated by ¹H NMR in CDCl₃, conversion lower than 1% considered as did not react.

^c In oxygen atmosphere.

Table S2. The results of evaluated experiments

Entry ^a	[MMA]:[EBrP]:[Et ₃ N]:[PC1]	Solvent	Conversion (%) ^b	M_n (kg.mol ⁻¹) ^c	\bar{D} (M_w/M_n) ^c	I^* ^d
S6	50:1:10:0.02	DMF	76.0	13.1	1.31	29.0
S7	50:1:5:0.02	DMF	72.4	15.1	1.39	24.0
S8	50:1:2:0.02	DMF	68.7	15.8	1.58	21.7
S9	50:1:1:0.02	DMF	50.8	22.5	1.63	11.3
S10	50:1:0.5:0.02	DMF	42.7	27.2	1.71	7.8
S11	50:1:20:0.02	DMSO	84.5	11.7	1.37	36.1
S12	50:1:20:0.02	DMA	69.7	10.9	1.34	32.0
S13	50:1:20:0.02	TCM	28.4	14.2	1.29	10.0
S14	50:1:20:0.02	THF	41.6	15.1	1.39	13.8
S15	50:1:20:0.02	DMI	75.4	13.3	1.33	28.3

^a 213 μ L (50 eq.) methyl methacrylate in 800 μ L DMF.

^b Calculated by ¹H NMR in CDCl₃.

^c M_n and M_w are measured by GPC in DMF. $\bar{D} = M_w/M_n$.

^d $I^* = \text{theoretical } M_n / \text{experimentally measured } M_n \times 100$. $M_n(\text{theo.})$ calculated based on [MMA]: [EBrP].

Table S3. Results of the polymerization of different monomers using PC1 as the

Entry ^a	Monomer	Conversion (%) ^b	M_n (kg.mol ⁻¹) ^c	\bar{D} (M_w/M_n) ^c
S16	acrylonitrile	62.8	5.87	1.21
S17	benzyl methacrylate	83.2	9.14	1.57
S18	butyl methacrylate	75.6	5.99	1.32
S19	methyl acrylate	78.4	9.80	1.32

photocatalyst.

^a Entry S16 132 μ L (50 eq.) acrylonitrile in 800 μ L DMF; entry S17 339 μ L (50 eq.) benzyl methacrylate in 800 μ L DMF; entry S18 316 μ L (50 eq.) butyl methacrylate in 800 μ L DMF; entry S19 179 μ L (50 eq.) methyl acrylate in 800 μ L DMF. Entry S16-S19 [Monomer]:[EBrP]:[Et₃N]:[PC1]=50:1:20:0.02.

^b Calculated by ¹H NMR.

^c M_n and M_w are measured by GPC in DMF. $\bar{D} = M_w/M_n$.

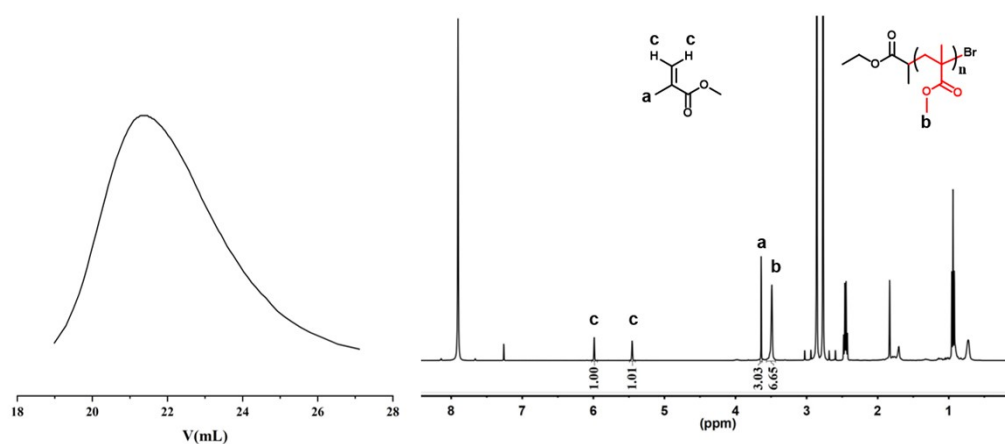


Figure S18. Typical GPC trace (DMF, PS standard, 45°C) and ¹H NMR (400 MHz, CDCl₃, 298 K) spectra for calculating the conversion rate, table 1, entry 1. The conversion = the integration of peak H_b / (the integration of peak H_a + the integration of peak H_b).

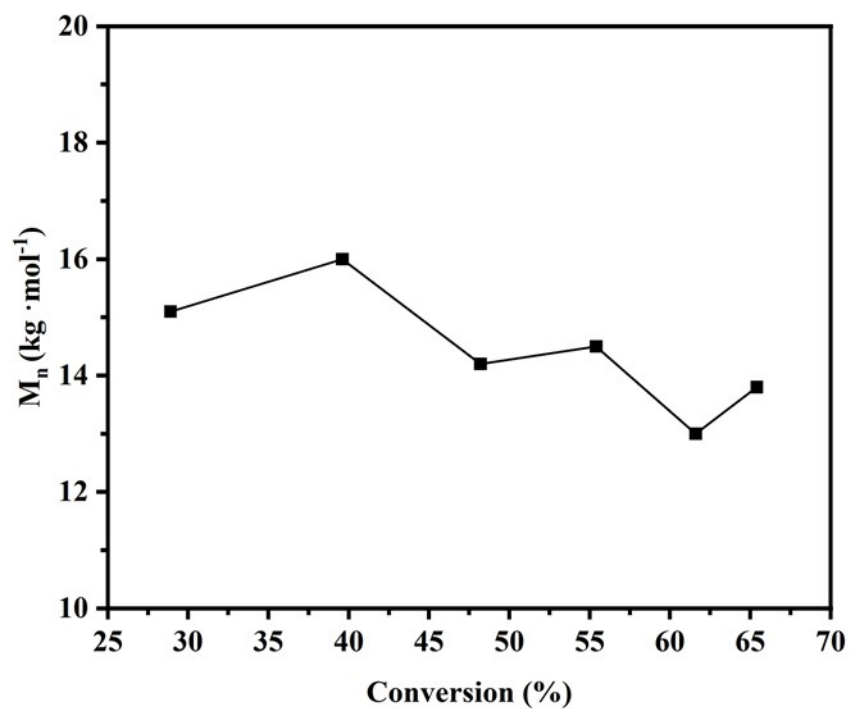


Figure S19. Plot of the M_n as a function of monomer conversion, $[\text{MMA}]:[\text{EBrP}]:[\text{Et}_3\text{N}]:[\text{PC1}] = 50:1:20:0.02$.

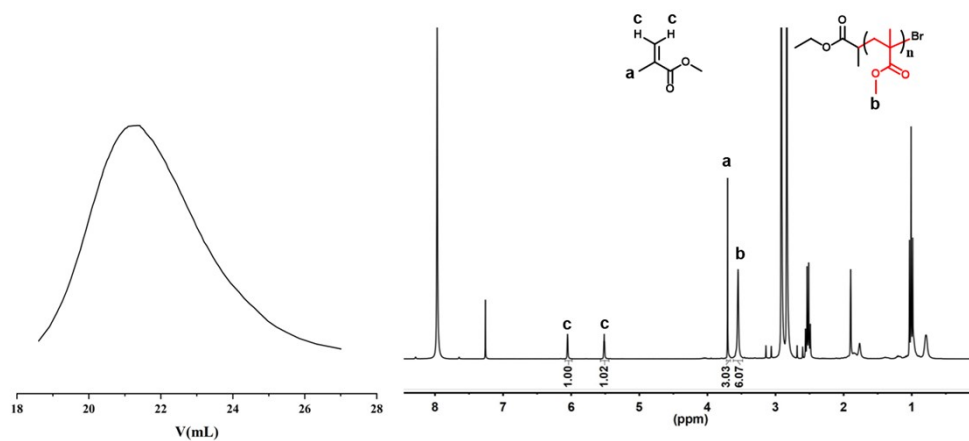


Figure S20. Typical GPC trace (DMF, PS standard, 45°C) and ^1H NMR (400 MHz, CDCl_3 , 298 K) spectra for calculating the conversion rate, table 1, entry 10. The conversion is calculated by integration of peak Hb / (the integration of peak Ha + the integration of peak Hb).

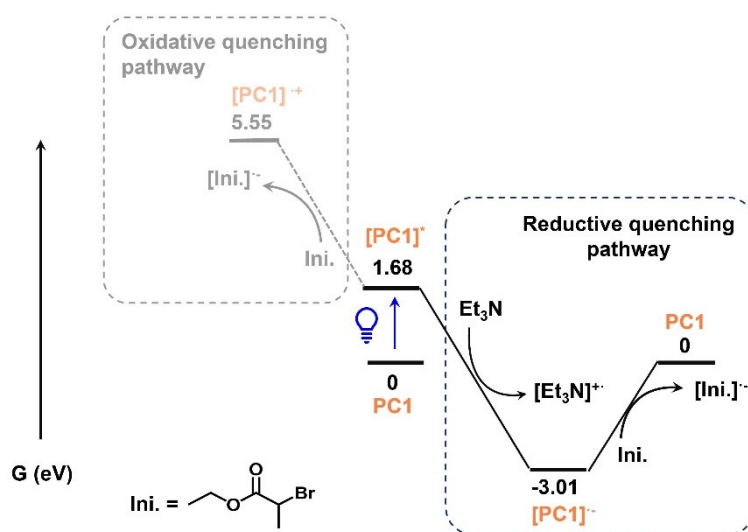


Figure S21. Calculated Gibbs free energy profile of the species involved in the photocatalytic O-ATRP process.

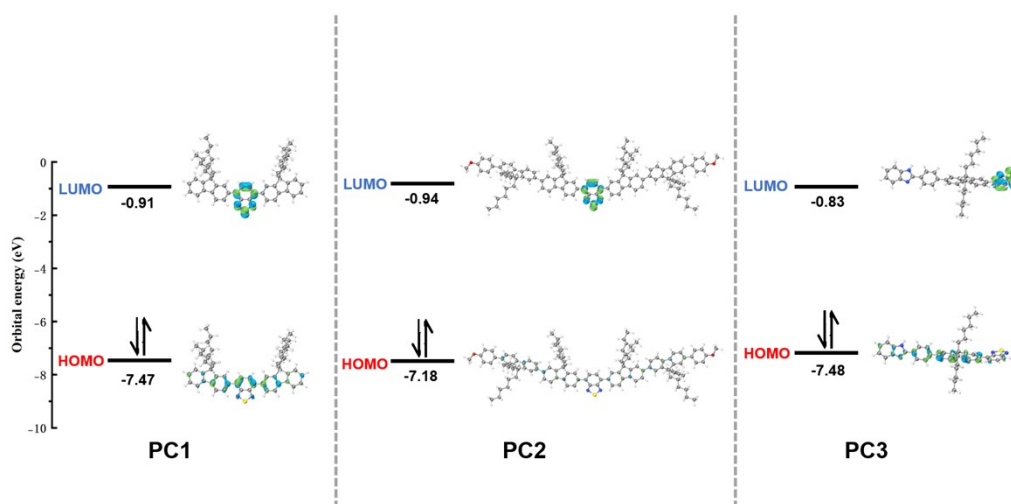
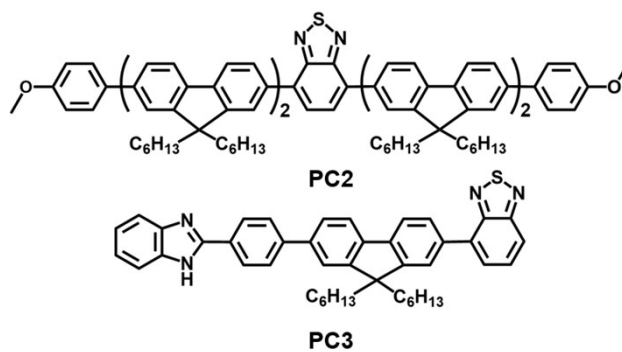


Figure S22. Orbital energy (in eV) and electron cloud distribution of PC1, PC2 and PC3 (HOMO = highest occupied molecular orbital, LUMO = lowest unoccupied molecular orbital).



	Potential (V vs SCE)
PC2/PC2 ⁻	-1.69
PC2 ⁺ /PC2 [*]	-0.93
PC3/PC3 ⁻	-1.57
PC3 ⁺ /PC3 [*]	-0.52

Figure S23. Calculated redox potentials of **PC2** and **PC3**.

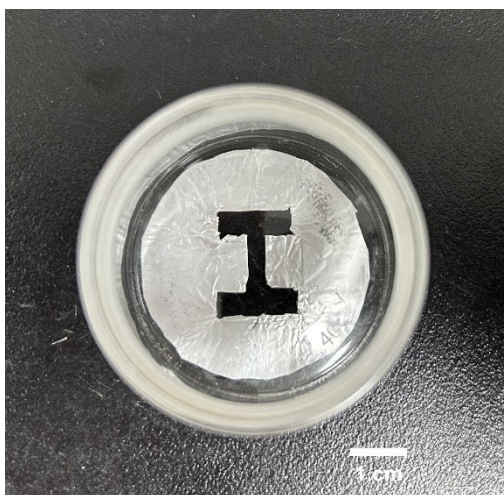


Figure S24. Home-made photomask with pattern “I” from the aluminum foil.

Table S4. Comparison of photocatalytic ATRP performance of state-of-the-art metal-free photocatalysts.

Photocatalyst	M_n (kg·mol ⁻¹)	\mathcal{D}
This work	13.6-25.1	1.29-1.58
Fluorescein ²	20.0-60.0	1.30-1.60
Eosin Y ²	8.70-22.1	1.30-1.90
Erythrosine B ²	13.7-90.0	1.20-2.50
PTDI ¹¹	6.70-87.7	1.22-1.75
1,1'-bisnaphthol ¹³	12.3-19.9	1.19-1.34
N-Aryl phenoxazine ¹⁸	4.60-112.5	1.07-1.38
Thioxanthone ³³	8.90-17.0	1.28-1.45
N,N-diaryl dihydrophenazine ³⁶	9.52-25.5	1.09-1.45
Curcumin ⁴³	60.5-76.3	1.51-1.69
oligopyrene ⁴⁴	12.0-39.1	1.32-1.66
heteroatom-doping of polycyclic arenes ⁴⁵	8.40-19.1	1.25-1.57

M_n represents number-average molecular weight.

\mathcal{D} represents the dispersity of the polymer, $\mathcal{D} = M_w/M_n$.

4. Atom Coordinates

[PC1]

C	3.69171300	-3.82647500	-0.61181000
C	2.95188100	-2.64992600	-0.39332000
C	3.63601400	-1.43941400	-0.18501700
C	5.02382200	-1.41711500	-0.20763000
C	5.74672700	-2.59658600	-0.43181300
C	5.08435700	-3.80685900	-0.63375500
H	3.16838900	-4.76851600	-0.78039000
H	3.07332600	-0.52179000	0.00500800
H	5.64175400	-4.72910600	-0.81395900
C	5.95078600	-0.21801700	-0.02564900
C	7.31783100	-0.88699500	-0.17958200
C	8.59712500	-0.33711300	-0.10410300
C	9.71307600	-1.16685400	-0.25503100
C	9.56218500	-2.53721700	-0.48175100
C	8.28801600	-3.10013800	-0.55929900
C	7.17759000	-2.27024200	-0.40627000
H	8.74429800	0.72956800	0.06688100
H	10.71465900	-0.73428000	-0.19407200
H	10.44540100	-3.16996400	-0.59750100
H	8.16145900	-4.17135800	-0.73405900
C	1.46907300	-2.66032000	-0.42235900
C	0.69431400	-3.72273500	0.16375000
C	0.74479000	-1.64905300	-1.00649200
C	-0.75434000	-3.71273600	0.10312900
C	-0.68123100	-1.63727700	-1.06223600
H	1.27458200	-0.82107700	-1.48273200
C	-1.46367400	-2.63849500	-0.54013500
H	-1.16093300	-0.79999400	-1.57416500
N	1.17349200	-4.77468500	0.82556500
N	-1.30249500	-4.75783800	0.72043400
S	-0.09380800	-5.66309800	1.31452200
C	5.72420300	0.33736100	1.40571400
C	6.46328700	1.60429500	1.82544300
H	5.96776300	-0.47063500	2.11767800
H	4.64197700	0.52290400	1.51593300

C	6.20934000	1.95749300	3.28913000
H	7.54801500	1.48849900	1.67133800
H	6.14488300	2.45132400	1.19583200
C	6.94181900	3.21613600	3.74466100
H	5.12401200	2.08582600	3.45224800
H	6.51423000	1.10832600	3.92702600
H	8.02644600	3.08398000	3.57866700
H	6.63914700	4.06658600	3.10690600
C	6.69830500	3.57271100	5.20884000
C	7.44989500	4.81982800	5.65868900
H	6.99164900	2.71732500	5.84267400
H	5.61562500	3.71463000	5.37260100
H	7.26069900	5.04520400	6.71977700
H	8.53788300	4.69504700	5.53291400
H	7.14815300	5.70228900	5.07084800
C	5.62782600	0.81920000	-1.13749900
C	6.70683300	1.81963900	-1.54928300
H	4.72504100	1.36796600	-0.81594600
H	5.33231200	0.26446600	-2.04386800
C	6.16195300	2.87986300	-2.50262900
H	7.14644300	2.31633200	-0.67118600
H	7.53442100	1.28456400	-2.04355200
C	7.21808900	3.86760100	-2.98910400
H	5.69792000	2.38326200	-3.37408300
H	5.34767600	3.43459500	-2.00203900
H	7.68108700	4.36483900	-2.11733400
H	8.03334700	3.31421600	-3.48982600
C	6.67115100	4.92760000	-3.94172300
C	7.72910700	5.91383800	-4.42135700
H	5.85422300	5.47664700	-3.44092100
H	6.21069800	4.42827300	-4.81235400
H	7.30460800	6.66181700	-5.10905400
H	8.18068800	6.45664500	-3.57482500
H	8.54433400	5.39666500	-4.95367400
C	-2.94399100	-2.60546200	-0.62303800
C	-3.67928700	-3.76073400	-0.94464400
C	-3.62566400	-1.39390700	-0.41445000
C	-5.06619900	-3.71892900	-1.06646100

H	-3.15641300	-4.70264600	-1.11634900
C	-5.00836600	-1.35007200	-0.53338500
H	-3.06557200	-0.49480300	-0.14395900
C	-5.72675200	-2.50869800	-0.85834000
H	-5.62110500	-4.62378500	-1.32559600
C	-5.93540100	-0.15307500	-0.33633200
C	-7.15260500	-2.16515600	-0.91335300
C	-7.29583400	-0.79683300	-0.61082800
C	-5.55624400	0.91066600	-1.40137200
C	-5.76494100	0.36872000	1.11921000
C	-8.25479100	-2.96499300	-1.21449300
C	-8.56958900	-0.22931400	-0.62228100
C	-6.27098100	2.25743300	-1.37478100
H	-5.69091300	0.45099200	-2.39625300
H	-4.47391000	1.09915600	-1.29666800
C	-6.92467000	1.12689700	1.76365800
H	-4.86102500	1.00295500	1.13217800
H	-5.53338000	-0.49302700	1.76723700
C	-9.52361900	-2.38519100	-1.21921500
H	-8.12538800	-4.02548100	-1.44420400
C	-9.67694600	-1.02738500	-0.92752000
H	-8.71977100	0.82614200	-0.39440500
C	-5.80206500	3.17988100	-2.49789200
H	-7.36081500	2.11799000	-1.45839300
H	-6.09084200	2.75967400	-0.41041700
C	-6.52691600	1.77061000	3.08934600
H	-7.31134000	1.90740400	1.09084600
H	-7.76274900	0.43270700	1.94020900
H	-10.40033300	-2.99360500	-1.45428800
H	-10.67386600	-0.58019100	-0.93605400
C	-6.50845700	4.53218600	-2.50378900
H	-4.71201900	3.33696300	-2.40737700
H	-5.95775800	2.68192500	-3.47186400
C	-7.68528100	2.47445800	3.79008000
H	-6.10621900	1.00058000	3.76119700
H	-5.71307800	2.49685900	2.91178900
H	-7.59587800	4.37383600	-2.62116400
H	-6.37733000	5.01599300	-1.51870300

C	-6.01773500	5.47942900	-3.59585800
H	-8.11633100	3.22979100	3.10786500
H	-8.49212400	1.74398600	3.98188800
C	-7.29400500	3.14859400	5.10254500
C	-6.74189200	6.82022600	-3.59867100
H	-6.13842100	4.99231600	-4.57948800
H	-4.93344100	5.64530100	-3.46966600
C	-8.46032400	3.84405500	5.79441500
H	-6.49099800	3.88113500	4.90789900
H	-6.85917800	2.39456000	5.78207700
H	-6.36276200	7.48521400	-4.39022500
H	-7.82369900	6.68795400	-3.76372700
H	-6.61580000	7.34218100	-2.63594200
H	-8.14577100	4.32439100	6.73396400
H	-8.89714500	4.62474000	5.15030100
H	-9.26272500	3.12852400	6.03778300

[PC1]*

C	2.32581400	-2.70105100	-2.06707000
C	2.04569700	-1.93174700	-0.92329800
C	3.01761500	-1.03768500	-0.44195000
C	4.23361300	-0.91949000	-1.10101900
C	4.49443100	-1.68387400	-2.24633700
C	3.54278600	-2.57923100	-2.73394200
H	1.57313600	-3.39380200	-2.44679200
H	2.81648000	-0.45185600	0.45888500
H	3.74062500	-3.17472400	-3.62835100
C	5.41511800	-0.02043500	-0.74600600
C	6.38871000	-0.36996800	-1.87291600
C	7.67491000	0.10661000	-2.12468000
C	8.39074900	-0.38769200	-3.21971000
C	7.83417500	-1.35161500	-4.06413300
C	6.54951100	-1.83921000	-3.82220700
C	5.83906200	-1.34501000	-2.72846700
H	8.13166700	0.86266600	-1.48554300
H	9.39776300	-0.01148300	-3.41569300
H	8.40688400	-1.72530200	-4.91629500
H	6.10873300	-2.59479100	-4.47724500
C	0.73467200	-2.02397600	-0.23636300

C	0.09790200	-3.28510700	0.03629800
C	0.06185200	-0.90854600	0.20133900
C	-1.17229000	-3.34390800	0.73169600
C	-1.19101500	-0.96616000	0.88201200
H	0.49455000	0.07775600	0.01838700
C	-1.84040700	-2.14454000	1.16591100
H	-1.63977800	-0.02336700	1.20176900
N	0.56670700	-4.49057500	-0.28182900
N	-1.61307200	-4.58954000	0.89533900
S	-0.51086800	-5.58654300	0.24195900
C	-3.13712900	-2.19052700	1.87179300
C	-4.19863300	-1.34649200	1.51447200
C	-3.33852000	-3.08443100	2.96722700
C	-5.43983600	-1.37736900	2.25987600
C	-4.34523500	-0.40366400	0.46409200
C	-4.52308000	-3.10552100	3.67484600
H	-2.52573800	-3.75119300	3.26046100
C	-5.59754700	-2.24631700	3.33136100
C	-6.33526800	-0.43515500	1.67994100
C	-5.71151900	0.24800200	0.48259300
H	-3.60397900	-0.18798900	-0.30741200
H	-4.63356200	-3.79404300	4.51599400
H	-6.53323000	-2.27452300	3.89448700
H	-7.33844500	-0.22754700	2.05477000
C	5.93951800	-0.47628500	0.64201300
C	7.09113900	0.29524800	1.27838400
H	6.22590300	-1.53909300	0.55512300
H	5.08387500	-0.44816100	1.33851700
C	7.53777500	-0.32596100	2.59997000
H	7.95441700	0.33218500	0.59461100
H	6.79010900	1.33973500	1.46096300
C	8.70810700	0.40549800	3.25016800
H	6.68432700	-0.34783200	3.30157300
H	7.81718400	-1.38130200	2.42969200
H	9.56110600	0.42008400	2.54752000
H	8.43407600	1.46343600	3.41481200
C	9.15747600	-0.20936500	4.57322000
C	10.34244800	0.51105400	5.20461700

H	9.41530000	-1.27039700	4.40885800
H	8.30816200	-0.21038500	5.27891100
H	10.63834500	0.04450100	6.15705300
H	11.22022800	0.49405700	4.53785800
H	10.10485100	1.56777500	5.40991400
C	4.93075400	1.45670800	-0.75612900
C	5.95289700	2.56432200	-1.00652500
H	4.42231600	1.63807800	0.20721000
H	4.14990300	1.55286800	-1.52895700
C	5.34979700	3.95249600	-0.80615300
H	6.83048500	2.45562600	-0.35101900
H	6.33063000	2.48529200	-2.03914800
C	6.29009700	5.08664500	-1.20281900
H	4.41646100	4.03325300	-1.39242400
H	5.05419300	4.07309700	0.25172700
H	7.23669700	4.99272000	-0.64011600
H	6.55973800	4.97513200	-2.26877000
C	5.70446400	6.47802800	-0.97643900
C	6.63183200	7.60291200	-1.42032600
H	5.46293600	6.59986500	0.09408900
H	4.74392500	6.55825700	-1.51518200
H	6.18232200	8.59214300	-1.24184100
H	7.59043300	7.56826100	-0.87716900
H	6.85878000	7.52920100	-2.49653800
C	-5.53769300	1.77560900	0.70199100
C	-6.80746900	2.62143700	0.70599600
H	-4.86196100	2.14991300	-0.08781100
H	-5.00454700	1.92075700	1.65782400
C	-6.53264000	4.09154100	1.01257400
H	-7.30385400	2.55206300	-0.27616000
H	-7.52418800	2.22368100	1.44572600
C	-7.78688600	4.96030000	0.99211600
H	-6.04477700	4.17619800	2.00031400
H	-5.80457300	4.48456800	0.27989200
H	-8.27995000	4.86334100	0.00772500
H	-8.51087200	4.57331700	1.73223600
C	-7.51819700	6.43612300	1.27544900
C	-8.77808400	7.29315500	1.25213600

H	-6.79606400	6.82066300	0.53373900
H	-7.02385100	6.53291300	2.25809100
H	-8.55292300	8.35201200	1.45364600
H	-9.27750300	7.23934200	0.27089900
H	-9.50363000	6.95612100	2.01048500
C	-6.45991700	-0.06155000	-0.85063600
C	-7.97903200	-0.20449400	-0.76219000
H	-6.05863800	-1.00478100	-1.25934500
H	-6.19994100	0.72141500	-1.58434300
C	-8.62944100	-0.38076700	-2.13138400
H	-8.22674200	-1.07582300	-0.13143400
H	-8.42440700	0.66873100	-0.25960900
C	-10.14468500	-0.54914100	-2.06923000
H	-8.38546300	0.49115400	-2.76511800
H	-8.18387700	-1.25693600	-2.63630600
H	-10.39045600	-1.41375900	-1.42607000
H	-10.58866400	0.33306700	-1.57314200
C	-10.79806600	-0.73841300	-3.43594900
C	-12.31218400	-0.89467600	-3.36417500
H	-10.35811600	-1.62415700	-3.92697600
H	-10.54544300	0.12225500	-4.08011700
H	-12.75399400	-1.03025200	-4.36371300
H	-12.59458500	-1.76842900	-2.75403700
H	-12.78323000	-0.00796100	-2.90920800

[PC1]-

C	2.70708800	-3.40499200	-1.56820600
C	2.17981100	-2.43954500	-0.68252800
C	2.99892400	-1.33961500	-0.34516200
C	4.27229600	-1.21635600	-0.88095200
C	4.77156100	-2.18442800	-1.76322900
C	3.98602000	-3.28375800	-2.10835200
H	2.09447700	-4.26689100	-1.83091300
H	2.63664000	-0.58832300	0.36077200
H	4.36150800	-4.04549300	-2.79682500
C	5.29022500	-0.10302300	-0.63910300
C	6.45356300	-0.58347400	-1.50851700
C	7.71187000	-0.01818500	-1.70915800
C	8.63073800	-0.65832900	-2.54801400

C	8.30092700	-1.85611300	-3.18638800
C	7.04585800	-2.43506400	-2.99100300
C	6.13225600	-1.79599900	-2.15234800
H	7.99188800	0.91881600	-1.22667000
H	9.61603500	-0.21250600	-2.70485500
H	9.02878100	-2.34304600	-3.84008700
H	6.78494500	-3.37468300	-3.48449400
C	0.81230100	-2.54266600	-0.12541700
C	0.16813600	-3.79063400	0.13143300
C	0.08815700	-1.38030900	0.21212800
C	-1.16323700	-3.82969500	0.74801600
C	-1.18807200	-1.41566900	0.76349800
H	0.53561100	-0.40267100	0.01899300
C	-1.86196300	-2.62009100	1.05300400
H	-1.67152000	-0.46831500	1.00720900
N	0.67201700	-5.00898000	-0.11237400
N	-1.61473900	-5.07227000	0.95622800
S	-0.45046700	-6.12597700	0.40333800
C	-3.20069100	-2.61613900	1.67084500
C	-4.20724400	-1.61402800	1.29593300
C	-3.57340400	-3.52621000	2.62695100
C	-5.51317400	-1.58109000	1.99854500
C	-4.22772900	-0.65547100	0.33431000
C	-4.85324000	-3.49221600	3.30192400
H	-2.86660200	-4.30264900	2.92079900
C	-5.79452600	-2.55234500	3.03109000
C	-6.27938300	-0.58959500	1.47444100
C	-5.53252400	0.10037200	0.36295500
H	-3.44155700	-0.42164500	-0.38390300
H	-5.04285600	-4.24910500	4.06820500
H	-6.75168400	-2.53029400	3.55787500
H	-7.28915300	-0.32804800	1.79344500
C	5.64003200	-0.10697500	0.87265300
C	6.55933900	0.98134400	1.41847200
H	6.07296500	-1.09455000	1.11019800
H	4.68685500	-0.05232500	1.42583300
C	6.86082200	0.78578200	2.90262500
H	7.50987800	1.00325500	0.86140900

H	6.09133800	1.96985200	1.28087200
C	7.76211100	1.86925500	3.48727300
H	5.91086400	0.75656500	3.46636400
H	7.33315400	-0.20186900	3.05230900
H	8.71414800	1.89352800	2.92639000
H	7.29279800	2.85761100	3.33051400
C	8.05900800	1.68484600	4.97334600
C	8.96363200	2.76858200	5.54743600
H	8.52401300	0.69547000	5.12925800
H	7.10684500	1.66411800	5.53206100
H	9.15601700	2.60881600	6.61976900
H	9.93817900	2.78897700	5.03273700
H	8.50957200	3.76683500	5.43490500
C	4.66593700	1.23943100	-1.11385800
C	5.59841000	2.38490000	-1.50496200
H	3.98284800	1.57967900	-0.31556600
H	4.02299400	1.02554900	-1.98415900
C	4.84172300	3.68846000	-1.74644300
H	6.36459400	2.55530500	-0.73335700
H	6.14518900	2.11495800	-2.42340700
C	5.74342800	4.83779000	-2.18652200
H	4.05923800	3.52320500	-2.50927700
H	4.30856800	3.97661700	-0.82236200
H	6.52983000	4.99333700	-1.42541700
H	6.27244000	4.55202900	-3.11385300
C	5.00096000	6.15160000	-2.41632000
C	5.91410800	7.29253900	-2.84809600
H	4.47058000	6.43374200	-1.48981500
H	4.21759700	5.99660900	-3.17910700
H	5.35207500	8.22687600	-3.00163000
H	6.68904800	7.49101000	-2.08955600
H	6.42985100	7.05522300	-3.79303300
C	-5.19341300	1.57496400	0.72181300
C	-6.35122800	2.56339900	0.82809300
H	-4.48038900	1.94850600	-0.03356100
H	-4.64771700	1.56390500	1.68182200
C	-5.88751300	3.93346900	1.31783200
H	-6.83727200	2.68439900	-0.15404300

H	-7.12197000	2.17254400	1.51467800
C	-7.01097200	4.95952500	1.43150200
H	-5.39658300	3.82087300	2.30134300
H	-5.11022100	4.31852500	0.63318000
H	-7.50700900	5.07037100	0.45007600
H	-7.78508900	4.57787500	2.12184000
C	-6.53815400	6.32906200	1.91333400
C	-7.66280400	7.34973200	2.03813400
H	-5.76932700	6.71016700	1.21834100
H	-6.03474800	6.21385000	2.88933200
H	-7.28712600	8.32411900	2.38761300
H	-8.16294500	7.51254600	1.06934200
H	-8.42988900	7.01186500	2.75403800
C	-6.25006500	-0.03149900	-1.01203400
C	-7.77348800	0.10889600	-1.00939600
H	-6.00406900	-1.01715700	-1.44096000
H	-5.80731600	0.71397400	-1.69587000
C	-8.35105600	0.24132300	-2.41568300
H	-8.21683400	-0.77361400	-0.51797200
H	-8.08746900	0.97774600	-0.41064600
C	-9.87449300	0.32170900	-2.44157300
H	-7.93024200	1.14309800	-2.89627700
H	-8.01826500	-0.61392300	-3.03161000
H	-10.29581400	-0.58560900	-1.97191500
H	-10.20397600	1.16865200	-1.81227700
C	-10.45994800	0.48047900	-3.84247100
C	-11.98142700	0.56512200	-3.85427700
H	-10.13223700	-0.36681000	-4.47028100
H	-10.03629400	1.38631500	-4.31072100
H	-12.37367200	0.68007100	-4.87679100
H	-12.43474900	-0.34258400	-3.42335200
H	-12.33721800	1.42469000	-3.26279100

[PC1]⁺

C	3.67908400	-3.77403200	-0.87685400
C	2.92748400	-2.62915500	-0.52298100
C	3.60034000	-1.40547700	-0.29731900
C	4.97544900	-1.34747500	-0.41493700
C	5.70477300	-2.49102100	-0.78450600

C	5.05826600	-3.70660700	-1.01981400
H	3.16886500	-4.71650600	-1.07210600
H	3.04168600	-0.51717600	0.00538000
H	5.62241600	-4.59355300	-1.31565000
C	5.89137300	-0.14876500	-0.18960200
C	7.25020800	-0.76420500	-0.52245100
C	8.51962600	-0.18717000	-0.51508100
C	9.63170500	-0.97222800	-0.83392900
C	9.49090200	-2.32506800	-1.15863600
C	8.22862400	-2.91520600	-1.16900700
C	7.12040400	-2.12846800	-0.85097800
H	8.66044300	0.86580300	-0.27052100
H	10.62561700	-0.51853000	-0.82906200
H	10.37374400	-2.91952400	-1.40515000
H	8.10667700	-3.97175100	-1.41896600
C	1.47412400	-2.67726500	-0.41495900
C	0.75323200	-3.85032200	0.02668200
C	0.67767500	-1.56710300	-0.72201900
C	-0.69151400	-3.86959400	0.09574800
C	-0.71292800	-1.58042800	-0.65672800
H	1.15567800	-0.65557600	-1.08238600
C	-1.47503200	-2.70716800	-0.28161600
H	-1.22928300	-0.67516500	-0.97545400
N	1.30428800	-4.97379700	0.46694100
N	-1.16070600	-5.00711200	0.58857300
S	0.10595400	-5.96816400	0.92030600
C	5.77638900	0.23418600	1.31138100
C	6.55752500	1.44056200	1.82080900
H	6.06322700	-0.65291700	1.90289100
H	4.70660100	0.40700100	1.51927300
C	6.38549700	1.63720800	3.32548900
H	7.63024600	1.32881000	1.59490800
H	6.21898700	2.35369700	1.30555400
C	7.16689700	2.82669900	3.87514900
H	5.31227200	1.76702900	3.55437900
H	6.70023300	0.71882600	3.85297200
H	8.24253700	2.68221800	3.66666800
H	6.87252100	3.74159700	3.32940300

C	6.97090100	3.05059300	5.37250100
C	7.77411300	4.22567700	5.91661000
H	7.24873100	2.13012900	5.91555400
H	5.89753500	3.21082600	5.57602600
H	7.60579200	4.36697100	6.99553900
H	8.85515200	4.07323300	5.76446300
H	7.49875100	5.16542600	5.41041400
C	5.45222400	0.99571600	-1.14364700
C	6.46789100	2.07257300	-1.52331600
H	4.56964000	1.47428100	-0.68427200
H	5.09089300	0.53896400	-2.08012000
C	5.80843300	3.23173900	-2.26652600
H	6.98461000	2.46566500	-0.63474000
H	7.24963000	1.63277700	-2.16425600
C	6.79181900	4.30461800	-2.72395500
H	5.26155700	2.83974300	-3.14314400
H	5.04508200	3.69228700	-1.61359900
H	7.34852700	4.68557700	-1.84852300
H	7.54731800	3.84950700	-3.38978800
C	6.12565800	5.47488100	-3.44354500
C	7.11030600	6.54533700	-3.89780200
H	5.37129400	5.92640400	-2.77544600
H	5.56804200	5.09202000	-4.31632500
H	6.59866500	7.37494600	-4.41037000
H	7.65861600	6.97116400	-3.04158700
H	7.85640400	6.13180900	-4.59609000
C	-2.91198000	-2.67168300	-0.28537100
C	-3.68992700	-3.86996600	-0.36778600
C	-3.59478200	-1.41824500	-0.22308500
C	-5.06630700	-3.83115000	-0.38263900
H	-3.18413100	-4.82966400	-0.44862700
C	-4.96476200	-1.38426500	-0.21658900
H	-3.03484000	-0.48662200	-0.13356400
C	-5.71156100	-2.58538900	-0.29528000
H	-5.64312700	-4.75374300	-0.46644400
C	-5.88027700	-0.16948700	-0.12086900
C	-7.11882000	-2.25036300	-0.26711200
C	-7.24835300	-0.84729000	-0.15633200

C	-5.62036200	0.69964800	-1.38143700
C	-5.57442700	0.56717400	1.21271800
C	-8.23468700	-3.09408600	-0.33498500
C	-8.52476900	-0.28995100	-0.11598000
C	-6.35017100	2.03203300	-1.51735300
H	-5.84732100	0.07640400	-2.26398000
H	-4.53589700	0.89830400	-1.41928500
C	-6.65218300	1.46964000	1.81007800
H	-4.65222200	1.15185900	1.05155500
H	-5.32072100	-0.19269400	1.97045000
C	-9.49969000	-2.52150600	-0.29261500
H	-8.10812600	-4.17531300	-0.42178100
C	-9.63874700	-1.13138300	-0.18404600
H	-8.67268500	0.78567800	-0.02452000
C	-6.09599700	2.68348300	-2.87480900
H	-7.43540400	1.89465700	-1.38877600
H	-6.02366400	2.72296800	-0.72327300
C	-6.13870200	2.25461600	3.01447100
H	-7.03948400	2.17564800	1.06010400
H	-7.51112100	0.85550700	2.12665600
H	-10.38890900	-3.15345100	-0.34254200
H	-10.63901000	-0.69341300	-0.14961800
C	-6.78780700	4.03329400	-3.03890500
H	-5.00836300	2.80913200	-3.02383900
H	-6.43536700	1.99990000	-3.67365900
C	-7.19856400	3.15036200	3.64830200
H	-5.75236000	1.54950200	3.77262600
H	-5.27608300	2.87296600	2.70680200
H	-7.87279600	3.90757900	-2.87049700
H	-6.43656800	4.72310600	-2.25017400
C	-6.56353400	4.67531500	-4.40563100
H	-7.57273700	3.86233100	2.89024200
H	-8.06889000	2.53549200	3.94169800
C	-6.69983400	3.92698100	4.86424100
C	-7.26136200	6.02092800	-4.56158300
H	-6.91497500	3.98345400	-5.19114300
H	-5.47941600	4.80024200	-4.57395500
C	-7.75756800	4.83785900	5.47536300

H	-5.81964400	4.52754000	4.57394100
H	-6.34148500	3.21312500	5.62665000
H	-7.08608800	6.45620300	-5.55771200
H	-8.35101700	5.92137300	-4.42797300
H	-6.90176700	6.74594600	-3.81309800
H	-7.36787200	5.37803900	6.35210300
H	-8.10570900	5.58894500	4.74754500
H	-8.63887500	4.26239000	5.80318500

[PC2]

C	-3.69567300	3.68362700	-0.18351400
C	-2.93628300	2.51147900	-0.01602900
C	-3.59328500	1.30330700	0.27392000
C	-4.97649800	1.27978800	0.38677400
C	-5.72163100	2.45348500	0.20655900
C	-5.08461000	3.66117800	-0.07859500
H	-3.19073500	4.62376700	-0.41085200
H	-3.01124200	0.39095800	0.42755600
H	-5.65920900	4.57928700	-0.22179300
C	-5.87436800	0.08776800	0.70724700
C	-7.25213600	0.74962700	0.66047700
C	-8.50989800	0.19583600	0.87507800
C	-9.66212000	0.99925800	0.81008000
C	-9.52598100	2.36745200	0.52134600
C	-8.27218700	2.93525600	0.30605800
C	-7.14079600	2.12424200	0.37798800
H	-8.62059500	-0.87000800	1.07371800
H	-10.41444800	3.00256300	0.48618100
H	-8.17989000	4.00316300	0.09437800
C	-1.46119000	2.52422600	-0.16609700
C	-0.64280800	3.56327200	0.40001500
C	-0.78568300	1.53114500	-0.83287900
C	0.79943900	3.54480800	0.25173300
C	0.63349700	1.51469300	-0.98224500
H	-1.35264800	0.72067400	-1.29651400
C	1.45852400	2.48724200	-0.46980900
H	1.07087700	0.69314600	-1.55384400
N	-1.07326100	4.59537700	1.12318000
N	1.39180800	4.56478300	0.87055900

S	0.22840300	5.45784900	1.56552100
C	-5.50991800	-0.38908200	2.13966600
C	-6.21999200	-1.61457400	2.70638300
H	-5.67359500	0.46340500	2.82193400
H	-4.42391600	-0.58445000	2.15267200
C	-5.87157700	-1.85934000	4.17264000
H	-7.31220200	-1.50109500	2.61858800
H	-5.94919800	-2.51015400	2.12368700
C	-6.57216700	-3.07982200	4.76206800
H	-4.77786200	-1.97746100	4.27696700
H	-6.13872800	-0.96479700	4.76386600
H	-7.66473600	-2.96117500	4.64395400
H	-6.30029600	-3.97640400	4.17558800
C	-6.25100200	-3.32510800	6.23401300
C	-6.96909600	-4.53779000	6.81353300
H	-6.51740200	-2.42537700	6.81627400
H	-5.16032600	-3.45073700	6.35189100
H	-6.72316400	-4.68589200	7.87653100
H	-8.06307400	-4.42556300	6.73715600
H	-6.69351600	-5.45979600	6.27574700
C	-5.65445700	-1.00421200	-0.37516900
C	-6.75382700	-2.04062200	-0.60516600
H	-4.71207900	-1.52231500	-0.12437400
H	-5.47050400	-0.49818900	-1.33773200
C	-6.29951800	-3.16596100	-1.53145100
H	-7.09323700	-2.47864300	0.34551800
H	-7.63586300	-1.54910800	-1.04740000
C	-7.38867000	-4.19776300	-1.80752400
H	-5.94843200	-2.73639100	-2.48726800
H	-5.42344800	-3.67128600	-1.08620300
H	-7.74137000	-4.61902200	-0.84842300
H	-8.26418400	-3.69435500	-2.25624800
C	-6.94065900	-5.33595800	-2.72121000
C	-8.03046800	-6.36982900	-2.97656700
H	-6.05956100	-5.83079100	-2.27607900
H	-6.59777900	-4.91439200	-3.68251200
H	-7.67860300	-7.17263900	-3.64304100
H	-8.36419400	-6.83840300	-2.03628600

H	-8.91430100	-5.90936900	-3.44769300
C	2.93224900	2.43550200	-0.62854200
C	3.68169900	3.59984500	-0.87859400
C	3.59567800	1.19786200	-0.55370400
C	5.06316000	3.54415500	-1.04808000
H	3.17411600	4.56238000	-0.95022400
C	4.97148900	1.13895300	-0.72658700
H	3.02947600	0.28781300	-0.33927000
C	5.70517600	2.30904500	-0.96662700
H	5.62770100	4.45872800	-1.24438000
C	5.87586900	-0.08991900	-0.67511400
C	7.12091100	1.94530400	-1.08415200
C	7.24291300	0.55305900	-0.91478100
C	5.45685100	-1.02374500	-1.84242700
C	5.72299000	-0.75900900	0.71922200
C	8.24017400	2.74041100	-1.32472000
C	8.49959500	-0.03745400	-1.00188900
C	6.14194000	-2.38055500	-1.97250700
H	5.59199800	-0.46249800	-2.78351600
H	4.37165900	-1.19858700	-1.74492800
C	6.86829700	-1.62262500	1.24683600
H	4.79599200	-1.35843000	0.69079000
H	5.54162900	0.03560100	1.46204300
C	9.49347100	2.13731300	-1.40134900
H	8.13818900	3.81959800	-1.46138600
C	9.63934700	0.74866500	-1.24621000
H	8.62181000	-1.11088000	-0.85769900
C	5.70363900	-3.13056900	-3.22805600
H	7.23684900	-2.26028700	-1.99743300
H	5.91353700	-3.00087200	-1.09034200
C	6.47500400	-2.38700800	2.50833200
H	7.21056000	-2.34122000	0.48691100
H	7.73573300	-0.98131800	1.47440400
H	10.37320900	2.75164400	-1.60780600
C	6.36369300	-4.49820900	-3.37603200
H	4.60545800	-3.25321600	-3.21814100
H	5.93334800	-2.51694800	-4.11782800
C	7.62885800	-3.16995400	3.12752300

H	6.07314700	-1.67832400	3.25521800
H	5.64776100	-3.08012800	2.27107500
H	7.46182300	-4.37248700	-3.37741500
H	6.13043800	-5.11349100	-2.48798100
C	5.94256900	-5.25147500	-4.63509800
H	8.04533400	-3.86324600	2.37403800
H	8.44663100	-2.47152700	3.38168600
C	7.23653200	-3.95955800	4.37382400
C	6.61149000	-6.61330200	-4.77727000
H	6.17400500	-4.63337100	-5.52045500
H	4.84559000	-5.37792800	-4.63170800
C	8.40046200	-4.71945600	4.99842400
H	6.42958700	-4.66724000	4.11474800
H	6.80629200	-3.26734100	5.11898900
H	6.28824700	-7.12866000	-5.69506300
H	7.70870400	-6.51532100	-4.81867400
H	6.36922800	-7.26812400	-3.92418600
H	8.08591400	-5.27738200	5.89418000
H	8.83037000	-5.44433500	4.28769100
H	9.20815800	-4.03264100	5.29990200
C	10.97996000	0.11112000	-1.33825800
C	11.14183700	-1.11734700	-2.00397300
C	12.10318800	0.72455100	-0.75685600
C	12.39094000	-1.72640700	-2.10711400
H	10.27493600	-1.59339700	-2.46860800
C	13.34806800	0.11634100	-0.84825500
H	11.98887400	1.66889600	-0.21800500
C	13.49480300	-1.10134000	-1.52782000
H	12.49850700	-2.67530000	-2.63801900
C	14.67708000	0.59909300	-0.27152300
C	14.90871600	-1.48757000	-1.47468900
C	15.61742400	-0.50416000	-0.75909600
C	14.52921500	0.59279600	1.27452000
C	14.99127300	2.00665200	-0.84874600
C	15.56086500	-2.60401200	-1.99435000
C	16.98596400	-0.65677300	-0.56102500
C	15.69080800	1.09205100	2.12815700
H	14.28451000	-0.44074800	1.57652200

H	13.64033900	1.19912700	1.51978500
C	16.44451600	2.47782800	-0.87761200
H	14.38377100	2.73248800	-0.28004800
H	14.61034300	2.04356900	-1.88320300
C	16.93338900	-2.73872400	-1.79769700
H	15.00893700	-3.36128700	-2.55643100
C	17.66284700	-1.77496400	-1.08078700
H	17.54733000	0.08168000	0.01133700
C	15.42743600	0.89745800	3.61971700
H	16.62216500	0.56708600	1.86180600
H	15.86702900	2.16286300	1.93529500
C	16.56847200	3.94009400	-1.29706100
H	16.92355400	2.34661400	0.10459000
H	17.01874100	1.85516200	-1.58314400
H	17.45054100	-3.60077800	-2.22532500
C	16.56362000	1.39478500	4.50808800
H	14.49177200	1.41602700	3.89672900
H	15.25089900	-0.17468200	3.82001000
C	18.01221200	4.42898300	-1.36347000
H	16.08752500	4.08085200	-2.28210100
H	16.00153600	4.57239900	-0.59010200
H	17.49922500	0.87920600	4.22464900
H	16.73818700	2.46835800	4.31226500
C	16.31012600	1.19024100	5.99955500
H	18.48863400	4.28843500	-0.37596100
H	18.58148300	3.79352600	-2.06606500
C	18.14912700	5.89029000	-1.78299400
C	17.45192600	1.68398500	6.87958600
H	16.13294700	0.11744200	6.19176600
H	15.37607100	1.70711600	6.28183200
C	19.59454100	6.37036200	-1.83151100
H	17.57272800	6.52275600	-1.08509700
H	17.68047300	6.02810800	-2.77336300
H	17.23975200	1.52186500	7.94783100
H	18.39267900	1.15995000	6.64382700
H	17.62928400	2.76216900	6.73421800
H	19.66179200	7.42609900	-2.13715500
H	20.07833600	6.27741800	-0.84530100

H	20.18799200	5.77723900	-2.54647800
C	-11.00245100	0.39928300	1.04703000
C	-11.17599600	-0.58633500	2.03585100
C	-12.11377500	0.80361300	0.28674300
C	-12.42220300	-1.16155600	2.27532300
H	-10.32158300	-0.89420200	2.64351900
C	-13.35697800	0.23016700	0.51888800
H	-11.99258900	1.55508500	-0.49816700
C	-13.51347700	-0.74693600	1.51274900
H	-12.53720500	-1.91900800	3.05443500
C	-14.67637500	0.52020400	-0.19326400
C	-14.92227000	-1.15440400	1.53730600
C	-15.61890200	-0.42085600	0.55895500
C	-14.50272000	0.10514900	-1.67909400
C	-15.01658000	2.02724500	-0.02110800
C	-15.58084900	-2.09137900	2.33175300
C	-16.98064300	-0.64078000	0.38017800
C	-15.64683600	0.37489000	-2.65159500
H	-14.26614100	-0.97327500	-1.69612500
H	-13.60388600	0.61967300	-2.05964500
C	-16.48041000	2.45519800	-0.11399500
H	-14.42319300	2.58328600	-0.76805700
H	-14.63901500	2.35248300	0.96278000
C	-16.94733500	-2.29333000	2.14945300
H	-15.03905300	-2.65477500	3.09539000
C	-17.66483700	-1.57605300	1.17695500
H	-17.53174800	-0.09768600	-0.38723100
C	-15.37556500	-0.21347600	-4.03418900
H	-16.58890400	-0.04831100	-2.26792800
H	-15.80794100	1.46100100	-2.75093000
C	-16.64770900	3.97225500	-0.11035700
H	-16.95669300	2.04723300	-1.01856100
H	-17.03687300	2.03556200	0.74004400
H	-17.47032800	-3.00827600	2.78908100
C	-16.50019600	0.03901000	-5.03365500
H	-14.43163400	0.20154300	-4.43177600
H	-15.21195300	-1.30189900	-3.93766500
C	-18.10928200	4.41058100	-0.12688200

H	-16.14815800	4.39578500	0.77965700
H	-16.12685700	4.40119200	-0.98539200
H	-17.44523800	-0.36257900	-4.62448200
H	-16.65606100	1.12759500	-5.14342700
C	-16.24883700	-0.57477500	-6.40860400
H	-18.60803000	3.97557700	-1.01213100
H	-18.62570700	3.98288300	0.75167500
C	-18.30324400	5.92466800	-0.13503900
C	-17.38250600	-0.32975300	-7.39692000
H	-16.08757900	-1.66108700	-6.29405700
H	-15.30709400	-0.16999500	-6.81948200
C	-19.76907800	6.34178700	-0.14624100
H	-17.79131900	6.35143300	-1.01535500
H	-17.80269000	6.35923500	0.74800100
H	-17.17364800	-0.78986000	-8.37523700
H	-18.33114700	-0.75169400	-7.02626700
H	-17.54255100	0.74824700	-7.56234900
H	-19.87978100	7.43732900	-0.15338000
H	-20.28770700	5.94829100	-1.03577600
H	-20.29833100	5.95872900	0.74158400
C	19.12769200	-1.92550300	-0.87322800
C	19.97981400	-0.80599800	-0.85777600
C	19.71228000	-3.18277900	-0.68254700
C	21.34612300	-0.94076800	-0.66076200
H	19.56815300	0.19315700	-1.02151000
C	21.08488000	-3.33602900	-0.48238900
H	19.08376000	-4.07684900	-0.66980000
C	21.91603600	-2.20914600	-0.46872700
H	22.00038100	-0.06620700	-0.65856800
H	21.49008400	-4.33697700	-0.33117400
C	-19.12545400	-1.78642500	0.99361600
C	-19.97445000	-0.72375300	0.66156800
C	-19.70855000	-3.05704300	1.14746400
C	-21.34720800	-0.90274800	0.48575900
H	-19.56542200	0.28396800	0.55202700
C	-21.07090800	-3.25255600	0.97544900
H	-19.08025800	-3.91779800	1.38974500
C	-21.90818800	-2.17618400	0.64188100

H	-21.96544100	-0.04004500	0.23513100
H	-21.51308200	-4.24469400	1.08917000
O	-23.21594200	-2.45709200	0.49419100
O	23.24829600	-2.24747900	-0.28161400
C	23.87127900	-3.49310000	-0.07113300
H	24.94111700	-3.29052500	0.06400800
H	23.48758400	-3.99322700	0.83423100
H	23.74328000	-4.16656100	-0.93548100
C	-24.10571500	-1.41679200	0.16285500
H	-23.85381800	-0.95509900	-0.80683600
H	-25.10251200	-1.86939900	0.08966700
H	-24.12591300	-0.63372400	0.93944800

[PC2]*

C	-3.73484400	3.32113800	-1.75303500
C	-2.93147800	2.24607300	-1.28896300
C	-3.58348800	1.04907400	-0.88915600
C	-4.96128400	0.95513600	-0.94150800
C	-5.73169100	2.03130700	-1.41502700
C	-5.11646600	3.21604100	-1.82578300
H	-3.25320300	4.24237300	-2.07462600
H	-3.00403400	0.20814900	-0.50394100
H	-5.70903500	4.05258500	-2.20308300
C	-5.84324000	-0.22213500	-0.53013500
C	-7.22933000	0.33102000	-0.86665300
C	-8.48060700	-0.25800200	-0.71969700
C	-9.64451300	0.44289900	-1.08146800
C	-9.52836000	1.75127500	-1.58293300
C	-8.28360700	2.35678800	-1.72753500
C	-7.13966000	1.64313800	-1.37011000
H	-8.57613600	-1.26369300	-0.31179200
H	-10.42654900	2.29519900	-1.88443000
H	-8.20598400	3.37127300	-2.12552500
C	-1.48346100	2.34006200	-1.23417500
C	-0.76142200	3.58039500	-1.14218100
C	-0.66416100	1.13960800	-1.27174500
C	0.70662200	3.60937100	-1.12794500
C	0.68865700	1.16302900	-1.27112500

H	-1.16091200	0.17332100	-1.36013900
C	1.47778300	2.39091300	-1.21700100
H	1.20730100	0.20983500	-1.35491800
N	-1.30589900	4.77970600	-1.02253200
N	1.19057800	4.83263400	-0.99926900
S	-0.08238700	5.89930100	-0.90787400
C	-5.65117500	-0.42924700	0.99682500
C	-6.35454800	-1.60302100	1.67119400
H	-5.95129700	0.50665400	1.49965500
H	-4.56744800	-0.53672900	1.17444700
C	-6.13871100	-1.60930600	3.18284800
H	-7.43717600	-1.57706100	1.46788900
H	-5.97871600	-2.55264500	1.25616100
C	-6.81219600	-2.78455500	3.88510700
H	-5.05485200	-1.62681400	3.39748200
H	-6.51823700	-0.66338100	3.60952100
H	-7.89567200	-2.76589200	3.66777200
H	-6.43333400	-3.73035300	3.45670400
C	-6.60361500	-2.79873000	5.39727300
C	-7.28150800	-3.97539700	6.08886500
H	-6.98180800	-1.85293700	5.82370000
H	-5.52077900	-2.81753800	5.61289100
H	-7.11328300	-3.95700600	7.17691700
H	-8.37063800	-3.96389700	5.91918500
H	-6.89755200	-4.93604400	5.70795400
C	-5.44042600	-1.47105800	-1.36307700
C	-6.48180600	-2.57187100	-1.56202000
H	-4.54039600	-1.90013900	-0.88878900
H	-5.11921500	-1.13021100	-2.36143300
C	-5.88409100	-3.84248300	-2.15980200
H	-6.97201300	-2.82770800	-0.61093200
H	-7.27983700	-2.20449900	-2.22806500
C	-6.92416900	-4.93132100	-2.40691300
H	-5.37081500	-3.60078500	-3.10805100
H	-5.10356700	-4.23087900	-1.48072100
H	-7.44988900	-5.14988800	-1.45953100
H	-7.69542500	-4.54809400	-3.09964400
C	-6.34347000	-6.22680200	-2.96791500

C	-7.39468400	-7.30524300	-3.20123400
H	-5.57231800	-6.60674300	-2.27486500
H	-5.82037100	-6.00996100	-3.91584300
H	-6.94702300	-8.22661500	-3.60516600
H	-7.91097000	-7.56791100	-2.26340600
H	-8.16117200	-6.96571000	-3.91700900
C	2.92418500	2.33540000	-1.25861700
C	3.71911400	3.50010000	-1.46109900
C	3.60665800	1.09249500	-1.11241800
C	5.10316300	3.44242700	-1.50765500
H	3.22299000	4.45948900	-1.58577300
C	4.98506500	1.03968200	-1.15602200
H	3.05529300	0.16771900	-0.94259100
C	5.74108300	2.20980400	-1.34827900
H	5.68070400	4.35535100	-1.66975400
C	5.88615200	-0.18612900	-1.01416200
C	7.15579000	1.85128300	-1.33490100
C	7.26713800	0.46159300	-1.13303200
C	5.58093400	-1.12136900	-2.21564600
C	5.61051600	-0.85376900	0.36125500
C	8.28869300	2.65192300	-1.48374500
C	8.53005700	-0.11996500	-1.08654100
C	6.30161000	-2.46317700	-2.30230900
H	5.78265900	-0.54983300	-3.13853100
H	4.49454100	-1.31492900	-2.20951100
C	6.70473100	-1.71915800	0.98412600
H	4.68775700	-1.45024700	0.25207700
H	5.36782100	-0.05776500	1.08482600
C	9.54510600	2.05685400	-1.43032800
H	8.19294800	3.72788700	-1.64650400
C	9.68322200	0.67156200	-1.23305800
H	8.64483100	-1.18868200	-0.90730300
C	6.01248400	-3.18165400	-3.61798000
H	7.39025600	-2.32374700	-2.20903800
H	5.99486400	-3.11137400	-1.46505300
C	6.21865700	-2.46475600	2.22418500
H	7.09567900	-2.44947900	0.25931000
H	7.55799500	-1.08045900	1.26581500

H	10.43670200	2.67393000	-1.56281300
C	6.70387800	-4.53653900	-3.73738000
H	4.92161500	-3.31543400	-3.73256200
H	6.32872400	-2.53715800	-4.45793600
C	7.32443000	-3.24858400	2.92496000
H	5.77514400	-1.74436200	2.93539400
H	5.40315300	-3.15414500	1.94037000
H	7.79137400	-4.40254800	-3.59227900
H	6.36748800	-5.19412700	-2.91531800
C	6.45869800	-5.23273200	-5.07351000
H	7.78247600	-3.95282400	2.20661900
H	8.12971700	-2.55245600	3.22179100
C	6.85104200	-4.02130600	4.15335300
C	7.15626100	-6.58260600	-5.18871500
H	6.79652800	-4.57167300	-5.89088400
H	5.37228600	-5.36496700	-5.22005800
C	7.97028500	-4.78032300	4.85606800
H	6.05729900	-4.72772400	3.85323000
H	6.38020800	-3.31872100	4.86338100
H	6.97061600	-7.05296300	-6.16686600
H	8.24724500	-6.47750300	-5.07087700
H	6.80591500	-7.28109500	-4.41119300
H	7.59772200	-5.32737300	5.73604300
H	8.43958500	-5.51408800	4.18039700
H	8.76131500	-4.09418000	5.20033500
C	11.03151200	0.04767100	-1.16990700
C	11.26810300	-1.20921800	-1.75557600
C	12.08928500	0.70579600	-0.51885000
C	12.52697200	-1.80509500	-1.70744100
H	10.45520700	-1.72074300	-2.27682100
C	13.34324500	0.11321800	-0.46307300
H	11.91642000	1.67321300	-0.04003700
C	13.56528600	-1.13623300	-1.05962400
H	12.69295500	-2.77692900	-2.17843500
C	14.60853100	0.65078000	0.20068100
C	14.97194800	-1.49758500	-0.85275300
C	15.60091500	-0.46369500	-0.13352600
C	14.32377000	0.73668700	1.72479100

C	14.95811200	2.02618500	-0.43104100
C	15.68235500	-2.63194500	-1.24142400
C	16.94691500	-0.58063700	0.19705900
C	15.39067800	1.32475500	2.64302300
H	14.07813900	-0.28239400	2.07165500
H	13.40193900	1.32985100	1.85073100
C	16.40439800	2.51497100	-0.36121700
H	14.29536900	2.77568500	0.03626600
H	14.67129500	1.99526300	-1.49559900
C	17.03259900	-2.73106600	-0.91261800
H	15.19335300	-3.43101800	-1.80392300
C	17.68250000	-1.71446900	-0.19199600
H	17.44334900	0.20081500	0.77194700
C	14.99686400	1.21479900	4.11433500
H	16.35559300	0.81388400	2.49495100
H	15.55622200	2.38657800	2.39731000
C	16.54687100	3.96186200	-0.82543800
H	16.80565500	2.42600900	0.65978400
H	17.03786700	1.87351200	-0.99588000
H	17.59725800	-3.60802000	-1.23789200
C	16.02945500	1.80488700	5.06972700
H	14.02435500	1.71561400	4.27112700
H	14.83390500	0.15136300	4.36609300
C	17.99156400	4.45200000	-0.84139700
H	16.11284300	4.06743200	-1.83635800
H	15.94563900	4.61606600	-0.16834700
H	17.00381300	1.31036800	4.90336800
H	16.18618400	2.87173300	4.82753500
C	15.64518400	1.67413000	6.54148200
H	18.42745100	4.33384200	0.16756900
H	18.58971200	3.80214500	-1.50588400
C	18.14476100	5.90365900	-1.28789500
C	16.68308600	2.25697100	7.49270700
H	15.48529600	0.60747500	6.77796200
H	14.67245200	2.16994500	6.70686600
C	19.59221200	6.37968300	-1.30397400
H	17.54934700	6.55202100	-0.62120400
H	17.70595100	6.02115900	-2.29446000

H	16.37971300	2.13934600	8.54464000
H	17.65931700	1.75983200	7.36995400
H	16.83521000	3.33290800	7.30738400
H	19.67124100	7.42842800	-1.63017400
H	20.04730000	6.30662900	-0.30254600
H	20.20452400	5.77022200	-1.98872200
C	-10.97752700	-0.20284300	-0.94793100
C	-11.13671700	-1.57220000	-1.22858600
C	-12.09974000	0.54539600	-0.55088900
C	-12.37981600	-2.19307700	-1.12657700
H	-10.27422100	-2.15826800	-1.55528400
C	-13.34008700	-0.06931100	-0.44543100
H	-11.98807500	1.60591300	-0.31036800
C	-13.48201900	-1.43398100	-0.73524100
H	-12.48511400	-3.25565600	-1.35817500
C	-14.66683500	0.55162400	-0.01389200
C	-14.89032000	-1.79782400	-0.54861600
C	-15.59839800	-0.65553800	-0.13126800
C	-15.01358600	1.67583900	-1.02515500
C	-14.51429300	1.07923500	1.44266700
C	-15.54142900	-3.01589500	-0.73440400
C	-16.96946300	-0.74296300	0.08720700
C	-16.22389700	2.56203300	-0.74795600
H	-15.12544800	1.21039000	-2.02009400
H	-14.12878000	2.33174100	-1.09306700
C	-15.76844500	1.17894100	2.30962600
H	-14.02669500	2.06806300	1.38318200
H	-13.80106000	0.42497800	1.97103100
C	-16.91273000	-3.09205900	-0.50135300
H	-14.98728300	-3.90254700	-1.05189000
C	-17.64367700	-1.96396500	-0.09115500
H	-17.53842700	0.13710400	0.38768100
C	-16.43269100	3.59915900	-1.84904200
H	-17.13872600	1.95607100	-0.64645600
H	-16.08762100	3.08884200	0.21056700
C	-15.50501300	1.87702400	3.64118100
H	-16.57610000	1.71034400	1.78314400
H	-16.15280400	0.16558200	2.51116000

H	-17.42273700	-4.05045800	-0.62441700
C	-17.59479800	4.55050200	-1.58049800
H	-15.50429600	4.18552200	-1.97318300
H	-16.59589200	3.08355100	-2.81248900
C	-16.72593100	1.89581800	4.55605200
H	-14.66649400	1.37678100	4.15889600
H	-15.17120800	2.91341900	3.45279800
H	-18.52775700	3.96861900	-1.46922400
H	-17.43512300	5.05448000	-0.60991300
C	-17.78550600	5.60539700	-2.66740100
H	-17.56664100	2.38575900	4.03159200
H	-17.05230600	0.85687400	4.74490100
C	-16.48976000	2.59746000	5.89112600
C	-18.93609400	6.56368600	-2.38489200
H	-17.95233400	5.10221800	-3.63602300
H	-16.84808100	6.17767600	-2.78143000
C	-17.71436000	2.59028000	6.79808700
H	-16.17565600	3.63914000	5.70271400
H	-15.64288000	2.11386100	6.40908100
H	-19.04115100	7.31679800	-3.18135800
H	-19.89479500	6.02527100	-2.30633600
H	-18.78148400	7.10168700	-1.43525400
H	-17.51649100	3.10392900	7.75173900
H	-18.56900000	3.09480200	6.31815200
H	-18.02874400	1.56013600	7.03308800
C	19.12543500	-1.82408300	0.15091600
C	19.95428600	-0.68749400	0.18200500
C	19.71254700	-3.05787200	0.45443800
C	21.30089100	-0.78386500	0.49999800
H	19.54184700	0.29383600	-0.06557300
C	21.06546500	-3.17238200	0.77731700
H	19.10022800	-3.96319100	0.45985400
C	21.87384100	-2.02924400	0.80203400
H	21.93775500	0.10338100	0.51240400
H	21.47252800	-4.15613200	1.01269100
C	-19.10610600	-2.05530000	0.16141600
C	-19.70918100	-1.34241700	1.20441700
C	-19.93599800	-2.86280600	-0.63666800

C	-21.07986300	-1.42069500	1.45507700
H	-19.09621800	-0.71776600	1.85959200
C	-21.30029500	-2.95019100	-0.40239400
H	-19.50842300	-3.42046600	-1.47351100
C	-21.88960000	-2.22937500	0.64817700
H	-21.50016300	-0.85367600	2.28629900
H	-21.93799600	-3.57241300	-1.03405200
O	-23.21872600	-2.37269400	0.80351700
O	23.18646800	-2.03051000	1.09889600
C	23.81258000	-3.25143800	1.41673500
H	24.86646000	-3.02142200	1.61756400
H	23.37182800	-3.71446700	2.31585400
H	23.75950000	-3.96926400	0.58070900
C	-23.86574300	-1.66083400	1.83246000
H	-23.74868100	-0.57072400	1.71021000
H	-24.93181600	-1.91133800	1.76473100
H	-23.49338400	-1.95358100	2.82879200

[PC2]-

C	-3.76113100	3.82762100	-0.04744400
C	-2.94489400	2.67787800	0.02783000
C	-3.57517400	1.43238800	0.23637800
C	-4.95560300	1.35135400	0.35090700
C	-5.74614200	2.50568300	0.26213100
C	-5.14740100	3.74979000	0.06382900
H	-3.29031600	4.79867500	-0.19735900
H	-2.97005900	0.52695700	0.32923300
H	-5.75272700	4.65736800	-0.00664000
C	-5.80938300	0.10625200	0.58540900
C	-7.21149700	0.71794200	0.59503000
C	-8.44637600	0.10490000	0.77670700
C	-9.62864900	0.86777000	0.78652600
C	-9.54164800	2.25833400	0.60609700
C	-8.31121600	2.88536300	0.42109600
C	-7.14998000	2.11413400	0.41811400
H	-8.51505200	-0.97643800	0.89347900
H	-10.45066300	2.86405100	0.63085200
H	-8.26039300	3.96906400	0.29059300
C	-1.47435800	2.74631200	-0.12539900

C	-0.70068200	3.85969300	0.31956200
C	-0.76602100	1.67790100	-0.71107000
C	0.75985300	3.85809200	0.17938900
C	0.61844500	1.67746800	-0.84762800
H	-1.32452600	0.82646800	-1.10774900
C	1.43120300	2.74342700	-0.40960800
H	1.08566200	0.82548200	-1.34710900
N	-1.17585800	4.96294400	0.91535700
N	1.33963900	4.96003300	0.67666500
S	0.12838400	5.93463700	1.27702100
C	-5.42215100	-0.46568500	1.97598900
C	-6.05898300	-1.77453500	2.43374600
H	-5.63339400	0.31673700	2.72590500
H	-4.32706900	-0.60125200	1.97954600
C	-5.68859900	-2.12176800	3.87350900
H	-7.15663600	-1.72009700	2.35396900
H	-5.73709400	-2.59773600	1.77476300
C	-6.27472100	-3.44825100	4.34785600
H	-4.58840500	-2.15212000	3.97248900
H	-6.03090500	-1.31194700	4.54268800
H	-7.37324300	-3.42409600	4.22732400
H	-5.91630400	-4.26087300	3.69009100
C	-5.93631100	-3.78584100	5.79746400
C	-6.51582600	-5.11732800	6.25963600
H	-6.30444400	-2.97669000	6.45244000
H	-4.83897300	-3.79882300	5.92020600
H	-6.26745300	-5.32358700	7.31238000
H	-7.61445500	-5.12663400	6.16861600
H	-6.12762900	-5.95309200	5.65474700
C	-5.55526500	-0.89603900	-0.57304800
C	-6.62042800	-1.94632100	-0.88725000
H	-4.59791200	-1.40244500	-0.35730400
H	-5.38318000	-0.31598900	-1.49512900
C	-6.11433200	-2.98714500	-1.88253300
H	-6.95739000	-2.45939600	0.02605100
H	-7.51175600	-1.45162400	-1.30704600
C	-7.17006800	-4.01125500	-2.28756400
H	-5.73582700	-2.47603400	-2.78630400

H	-5.24533300	-3.51205100	-1.44612300
H	-7.56022400	-4.51062700	-1.38202300
H	-8.03242500	-3.48832600	-2.73949000
C	-6.65513000	-5.06734900	-3.26222100
C	-7.71488100	-6.08466000	-3.66701700
H	-5.79560100	-5.59008800	-2.80693800
H	-6.26125300	-4.56612300	-4.16380700
H	-7.31351400	-6.83034500	-4.37096400
H	-8.10149300	-6.62817500	-2.78936800
H	-8.57292200	-5.59397100	-4.15513000
C	2.90334700	2.67019100	-0.54592800
C	3.70050100	3.82412700	-0.71426700
C	3.55435400	1.41707800	-0.52874000
C	5.08335100	3.74488900	-0.86260400
H	3.21660500	4.80014900	-0.72178200
C	4.93093700	1.33445300	-0.67872300
H	2.97419000	0.50452800	-0.37147700
C	5.70092800	2.49468100	-0.84202000
H	5.67055700	4.65762800	-0.99351800
C	5.80484500	0.08059600	-0.66990200
C	7.10850700	2.10077800	-0.95065800
C	7.19341300	0.69844600	-0.84506900
C	5.39580300	-0.77857500	-1.89679200
C	5.60272200	-0.64963900	0.68561800
C	8.25406500	2.87420600	-1.13263900
C	8.43639800	0.08068700	-0.93154100
C	6.06157300	-2.13769600	-2.09154100
H	5.56753000	-0.16519100	-2.79871900
H	4.30497200	-0.93491300	-1.83893800
C	6.68599400	-1.60953500	1.17615300
H	4.64092100	-1.18842700	0.62148200
H	5.46341900	0.11785700	1.46559900
C	9.49328700	2.24225000	-1.21607200
H	8.18379100	3.96108200	-1.22128900
C	9.60202000	0.84523600	-1.12092300
H	8.52820800	-1.00082500	-0.83084200
C	5.72215300	-2.76753300	-3.44048000
H	7.15645700	-2.04432600	-2.01657700

H	5.75102900	-2.82640600	-1.28876100
C	6.25011200	-2.37624000	2.42218800
H	6.96362900	-2.33023900	0.39234600
H	7.60244700	-1.04285200	1.40918900
H	10.39087300	2.84313000	-1.38099500
C	6.37464500	-4.13138100	-3.64500700
H	4.62592600	-2.86475400	-3.54003900
H	6.04187300	-2.08536500	-4.24872200
C	7.31408300	-3.33304800	2.95139400
H	5.97508700	-1.65802200	3.21566200
H	5.32967900	-2.94476600	2.19661100
H	7.46703500	-4.03192600	-3.50852500
H	6.03307000	-4.82291600	-2.85350400
C	6.09622800	-4.75299800	-5.01120500
H	7.57977500	-4.05557600	2.15837700
H	8.23931100	-2.76871900	3.16811800
C	6.88562300	-4.09540500	4.20266800
C	6.76147900	-6.11078000	-5.20080300
H	6.43953600	-4.06006100	-5.79936500
H	5.00540000	-4.85379300	-5.14975100
C	7.94463000	-5.06430400	4.71425600
H	5.95333400	-4.64709100	3.98839200
H	6.63269200	-3.37145800	4.99707000
H	6.55178000	-6.53060000	-6.19690000
H	7.85607900	-6.03495800	-5.09427000
H	6.40646700	-6.83712500	-4.45142000
H	7.60635900	-5.59229700	5.61937700
H	8.18843600	-5.82549200	3.95516700
H	8.87974700	-4.53735300	4.96537100
C	10.92592100	0.17518500	-1.22491800
C	11.05684500	-1.03982700	-1.92227400
C	12.06572700	0.74284600	-0.62886800
C	12.28907700	-1.67952500	-2.04029200
H	10.17904900	-1.48175800	-2.39979600
C	13.29463400	0.10555100	-0.73800900
H	11.97754500	1.67554400	-0.06533800
C	13.40937100	-1.09859000	-1.44704500
H	12.37092000	-2.61757500	-2.59463100

C	14.63698800	0.54207100	-0.15572300
C	14.81259400	-1.52307400	-1.40488200
C	15.54743000	-0.57524300	-0.66799200
C	14.49569300	0.51250300	1.39055400
C	14.98799500	1.95169500	-0.70765600
C	15.43489400	-2.64387500	-1.95139000
C	16.91190200	-0.76732200	-0.47693600
C	15.67037000	0.98067000	2.24392100
H	14.23509800	-0.52137200	1.67777300
H	13.61869500	1.13014400	1.64990200
C	16.45472900	2.37863100	-0.74078100
H	14.40769500	2.68387300	-0.11903500
H	14.59933600	2.02155000	-1.73749800
C	16.80399800	-2.81813500	-1.76136700
H	14.86241900	-3.37280000	-2.53011200
C	17.55907100	-1.88972000	-1.02480500
H	17.49372100	-0.05669300	0.11003000
C	15.41412000	0.77283000	3.73485600
H	16.59143700	0.44416500	1.96497300
H	15.86258100	2.05083200	2.06271200
C	16.62157900	3.84443500	-1.13176200
H	16.93824300	2.21192000	0.23376700
H	17.00259500	1.75334300	-1.46466300
H	17.29895700	-3.68269400	-2.20983300
C	16.56300200	1.24732500	4.61951800
H	14.48695900	1.29992300	4.02405000
H	15.22606200	-0.29914100	3.92523300
C	18.07992600	4.28762700	-1.20084200
H	16.13753600	4.01969800	-2.10968400
H	16.08110300	4.48018400	-0.40743800
H	17.49029400	0.72402300	4.32312900
H	16.74825700	2.32075200	4.43289900
C	16.31950300	1.03101500	6.11095100
H	18.55830500	4.11588600	-0.21925500
H	18.62330600	3.64571100	-1.91792200
C	18.26171300	5.75037900	-1.59766100
C	17.47379300	1.50495700	6.98566100
H	16.13320700	-0.04171000	6.29476700

H	15.39319200	1.55461000	6.40603100
C	19.72155200	6.18453700	-1.64672800
H	17.70975800	6.38961900	-0.88634400
H	17.79247000	5.91875200	-2.58299500
H	17.26892500	1.33552100	8.05419900
H	18.40709400	0.97356200	6.73706000
H	17.66076600	2.58257500	6.84833900
H	19.82102000	7.24241600	-1.93565500
H	20.20718400	6.06073300	-0.66481000
H	20.29211900	5.58456300	-2.37449500
C	-10.94670100	0.20732600	0.98785300
C	-11.06947700	-0.90076100	1.84676300
C	-12.09284700	0.68003700	0.32432700
C	-12.29570300	-1.53118500	2.04804400
H	-10.19096200	-1.26643800	2.38351800
C	-13.31754100	0.05737000	0.52403000
H	-12.01420000	1.52662000	-0.36282700
C	-13.42120500	-1.04584700	1.38318700
H	-12.36857100	-2.38521900	2.72577600
C	-14.66856500	0.42011100	-0.08749300
C	-14.82058400	-1.48572100	1.39644600
C	-15.56531400	-0.64095600	0.55199500
C	-14.55211700	0.24616500	-1.62558100
C	-15.02362900	1.87610000	0.32892300
C	-15.43251600	-2.54065300	2.07134000
C	-16.92752700	-0.86701600	0.38641900
C	-15.73060100	0.66977500	-2.49676900
H	-14.31828200	-0.81422100	-1.82524600
H	-13.66763500	0.81997100	-1.95133100
C	-16.49559500	2.28619800	0.35943700
H	-14.46818600	2.55084000	-0.34595400
H	-14.60958500	2.05406400	1.33538100
C	-16.79981300	-2.74983400	1.90385600
H	-14.85245900	-3.19204500	2.72953600
C	-17.56451700	-1.92153500	1.06484300
H	-17.51584900	-0.23529200	-0.27899100
C	-15.48982900	0.37898900	-3.97619100
H	-16.65278900	0.15741900	-2.17870300

H	-15.91391800	1.74993700	-2.37582800
C	-16.67330000	3.78802800	0.56493900
H	-17.00992200	1.99057000	-0.56747500
H	-17.00698400	1.75196100	1.17719100
H	-17.28617200	-3.56201600	2.44954100
C	-16.64626000	0.81452400	-4.87132400
H	-14.56379100	0.88613900	-4.30218400
H	-15.30870600	-0.70224800	-4.11306800
C	-18.13514100	4.21355600	0.66470800
H	-16.13709800	4.09976200	1.47956700
H	-16.19139500	4.32915900	-0.26945700
H	-17.56975800	0.30033300	-4.54847400
H	-16.83349400	1.89366200	-4.72353600
C	-16.41294100	0.54469100	-6.35552700
H	-18.67044000	3.89095000	-0.24696400
H	-18.61454800	3.67634200	1.50332800
C	-18.32826600	5.71578700	0.85529900
C	-17.57608400	0.98355300	-7.23697200
H	-16.22410300	-0.53315000	-6.50315600
H	-15.49119100	1.06098000	-6.67652800
C	-19.79228000	6.12744400	0.95216400
H	-17.84851900	6.25112700	0.01704600
H	-17.79325800	6.03650600	1.76643600
H	-17.37711700	0.78259000	-8.30116500
H	-18.50430200	0.45450200	-6.96551000
H	-17.76880500	2.06380600	-7.13192000
H	-19.89985500	7.21427200	1.09250400
H	-20.34496100	5.85288200	0.03868600
H	-20.29001700	5.63144400	1.80161700
C	19.02093100	-2.07771000	-0.82783400
C	19.89725700	-0.97729300	-0.80163100
C	19.57905900	-3.35004600	-0.65887200
C	21.26147000	-1.14406400	-0.61540300
H	19.50600800	0.03259800	-0.94894500
C	20.94927800	-3.53533700	-0.46944000
H	18.93089300	-4.23010200	-0.65462900
C	21.80478500	-2.42711200	-0.44534800
H	21.93470700	-0.28411800	-0.60568500

H	21.33408700	-4.54656200	-0.33385400
C	-19.02573800	-2.14091500	0.89872900
C	-19.90749500	-1.06345700	0.75129600
C	-19.57682800	-3.43484800	0.88375700
C	-21.28131600	-1.24986200	0.59285800
H	-19.52349900	-0.04044000	0.77851000
C	-20.94007200	-3.63778200	0.72721500
H	-18.92211000	-4.30493100	0.97666300
C	-21.81049400	-2.54617900	0.58012700
H	-21.92542200	-0.37600400	0.49000400
H	-21.35751600	-4.64679700	0.70705200
O	-23.11683800	-2.83521500	0.43487600
O	23.13711000	-2.49752800	-0.26793300
C	23.73498300	-3.76093800	-0.09311100
H	24.81031200	-3.58431000	0.03443900
H	23.35040800	-4.27369800	0.80477000
H	23.58236400	-4.41040100	-0.97169700
C	-24.03458500	-1.78030700	0.26489000
H	-23.81849400	-1.19461100	-0.64472400
H	-25.02513200	-2.24079300	0.16181900
H	-24.04543600	-1.10254200	1.13522700

[PC2]⁺

C	3.70124000	-3.03714500	-1.67687400
C	2.95355500	-1.92790500	-1.24144600
C	3.62709700	-0.76021200	-0.84232500
C	5.01366200	-0.71294600	-0.88789900
C	5.74466900	-1.82326100	-1.33327800
C	5.09220500	-2.99050200	-1.72924100
H	3.18395000	-3.94432700	-1.99243500
H	3.05664100	0.10030500	-0.48294600
H	5.65700300	-3.85756500	-2.07973700
C	5.93148600	0.44442100	-0.50095800
C	7.30088300	-0.16676800	-0.80081500
C	8.56941500	0.38513700	-0.65444900
C	9.71321300	-0.35669300	-0.99873700
C	9.55564400	-1.66825700	-1.47906600
C	8.29240800	-2.23776900	-1.61809400
C	7.17015500	-1.48334800	-1.28050300

H	8.69080000	1.39554500	-0.26480100
H	10.43576000	-2.24601100	-1.77076700
H	8.18626100	-3.25608000	-1.99963200
C	1.47120900	-1.96206000	-1.23124200
C	0.73374000	-3.11265100	-0.77955700
C	0.71285500	-0.89192500	-1.64069100
C	-0.71577900	-3.12351400	-0.79052400
C	-0.71443400	-0.90249600	-1.65091500
H	1.21440900	0.00648600	-2.00738600
C	-1.46295400	-1.98368600	-1.25237200
H	-1.22356200	-0.01124300	-2.02457600
N	1.25271100	-4.23611600	-0.28724700
N	-1.22567600	-4.25461000	-0.30622800
S	0.01765400	-5.20811200	0.11708300
C	5.72120600	0.71644300	1.01249100
C	6.46819900	1.87796700	1.66035800
H	5.96730700	-0.21387100	1.55382500
H	4.64057500	0.87997700	1.16508400
C	6.20460000	1.96513400	3.16183300
H	7.55312200	1.77992400	1.49491700
H	6.16329700	2.82812300	1.19268500
C	6.95019500	3.10973400	3.84152200
H	5.11950400	2.08078300	3.33577800
H	6.48892500	1.01034300	3.63950000
H	8.03586600	2.98157700	3.67937300
H	6.68163800	4.06299400	3.35104900
C	6.67549400	3.22055100	5.33898300
C	7.44074200	4.35476100	6.00997800
H	6.93155200	2.26344300	5.82637600
H	5.59202400	3.36157700	5.49862700
H	7.21944700	4.41292400	7.08705000
H	8.52915400	4.21935000	5.89987300
H	7.18279000	5.32878600	5.56296300
C	5.58532500	1.67013400	-1.39418700
C	6.66062800	2.73094400	-1.62320100
H	4.68706800	2.14446100	-0.96146500
H	5.27816900	1.29280400	-2.38401000
C	6.13622300	3.93691500	-2.39803100

H	7.08725900	3.07654100	-0.66915300
H	7.49651300	2.28738900	-2.18826800
C	7.20693800	4.99338600	-2.65371400
H	5.71645500	3.59773200	-3.36242100
H	5.29593500	4.39447800	-1.84515000
H	7.60636700	5.34744500	-1.68576600
H	8.06009800	4.52631300	-3.17889100
C	6.71536900	6.19075200	-3.46290900
C	7.79222800	7.24320300	-3.69661900
H	5.85588300	6.65131900	-2.94454200
H	6.32809200	5.83572000	-4.43422200
H	7.40923900	8.09065300	-4.28615300
H	8.17145200	7.64510800	-2.74266200
H	8.65211300	6.81948500	-4.24083700
C	-2.94541400	-1.96854600	-1.28151100
C	-3.67646300	-3.08640100	-1.72409300
C	-3.63544300	-0.80718500	-0.89403400
C	-5.06712500	-3.05454800	-1.79260600
H	-3.14592900	-3.98873300	-2.03154700
C	-5.02151500	-0.77360400	-0.95841700
H	-3.07837200	0.05900400	-0.52779300
C	-5.73624100	-1.89283900	-1.40732200
H	-5.61865100	-3.92829100	-2.14747300
C	-5.95365600	0.37178800	-0.57299500
C	-7.16571500	-1.56805800	-1.36676600
C	-7.31337600	-0.25414000	-0.88274500
C	-5.63300900	1.56922300	-1.50698200
C	-5.73958800	0.69232300	0.93335600
C	-8.27644900	-2.33057200	-1.72570000
C	-8.58588400	0.29378700	-0.77167700
C	-6.35355600	2.89392800	-1.27468000
H	-5.81799100	1.23735600	-2.54364900
H	-4.54781600	1.75553100	-1.43649100
C	-6.86371100	1.39261400	1.69489000
H	-4.81468100	1.29059700	1.00969300
H	-5.52737200	-0.25618300	1.45457400
C	-9.54646200	-1.77362900	-1.60153100
H	-8.15589600	-3.34654100	-2.10865700

C	-9.71763300	-0.46079900	-1.12982700
H	-8.72129500	1.30127100	-0.37949000
C	-6.06811600	3.90812900	-2.37962000
H	-7.44260400	2.73926900	-1.21370900
H	-6.04392500	3.32282600	-0.30760600
C	-6.45351900	1.77700100	3.11417700
H	-7.20076800	2.29503600	1.16277200
H	-7.73864500	0.72459600	1.75031400
H	-10.41861500	-2.36030900	-1.89894100
C	-6.73135200	5.26143400	-2.14213600
H	-4.97657100	4.04760800	-2.48024000
H	-6.41215600	3.49691300	-3.34583300
C	-7.57138800	2.46247800	3.89448600
H	-6.12597000	0.87265500	3.65818900
H	-5.57358700	2.44429900	3.07530000
H	-7.81847900	5.11406300	-2.00710400
H	-6.36324700	5.68523000	-1.19006800
C	-6.49753200	6.26898100	-3.26472100
H	-7.87609600	3.38053200	3.35977500
H	-8.46248800	1.80856500	3.90416600
C	-7.19608300	2.81813400	5.33082200
C	-7.15637400	7.61920500	-3.00975700
H	-6.87529700	5.84693100	-4.21265900
H	-5.41155300	6.40925900	-3.40662600
C	-8.31336200	3.52878300	6.08518200
H	-6.29300600	3.45376900	5.32367700
H	-6.91404200	1.89637400	5.86933800
H	-6.97634200	8.32179100	-3.83824400
H	-8.24732600	7.51388000	-2.89180000
H	-6.76794000	8.08388100	-2.08871000
H	-8.02130900	3.75827300	7.12179800
H	-8.58198700	4.47920500	5.59573100
H	-9.22422900	2.90897800	6.12530400
C	-11.07297800	0.13056500	-1.00487600
C	-11.27531100	1.50461300	-1.27112200
C	-12.16600600	-0.66483500	-0.61724300
C	-12.52888900	2.08307500	-1.16179800
H	-10.43092700	2.11907400	-1.58998700

C	-13.42337600	-0.09341500	-0.49944500
H	-12.01757700	-1.72271300	-0.38904800
C	-13.60786000	1.27539100	-0.77466000
H	-12.67424000	3.14313900	-1.37948200
C	-14.72606500	-0.76236000	-0.07623700
C	-14.99958200	1.59324000	-0.58604100
C	-15.69317400	0.41272500	-0.19352300
C	-14.55052200	-1.21527100	1.39958600
C	-15.02882400	-1.93754000	-1.04620600
C	-15.67385900	2.82061800	-0.73026800
C	-17.04363000	0.47095000	0.04275700
C	-15.68428200	-1.98683800	2.06673900
H	-14.32712500	-0.31451400	1.99742500
H	-13.64175200	-1.83937600	1.43701700
C	-16.47824300	-2.39578500	-1.20254300
H	-14.40800400	-2.78945400	-0.71929800
H	-14.65744600	-1.66056600	-2.04663700
C	-17.02469800	2.87045000	-0.48425000
H	-15.13241100	3.71694700	-1.03754700
C	-17.75655400	1.70185200	-0.09804700
H	-17.57628300	-0.42137500	0.36067000
C	-15.40415000	-2.24556900	3.54534000
H	-16.63527300	-1.43703800	1.97884700
H	-15.83143000	-2.95326100	1.55782900
C	-16.58943500	-3.68377100	-2.01363300
H	-16.95306500	-2.55018900	-0.22159800
H	-17.06000800	-1.60619600	-1.70652900
H	-17.54154300	3.82005700	-0.61750200
C	-16.50930700	-3.03318800	4.24216200
H	-14.44645400	-2.78683400	3.64769200
H	-15.26322700	-1.27914800	4.06190300
C	-18.03088600	-4.12913100	-2.24127400
H	-16.08944500	-3.54710400	-2.98948000
H	-16.03554000	-4.48856200	-1.49747700
H	-17.46831500	-2.49636600	4.12537800
H	-16.64283400	-4.00465800	3.73248300
C	-16.24758400	-3.27614300	5.72635600
H	-18.53118500	-4.25339600	-1.26352000

H	-18.58196200	-3.32616500	-2.76399700
C	-18.15551600	-5.42579600	-3.03700000
C	-17.35949600	-4.05841300	6.41453400
H	-16.11208900	-2.30417400	6.23256900
H	-15.29013600	-3.81369600	5.84223700
C	-19.59908100	-5.86121200	-3.25780700
H	-17.60499000	-6.22668500	-2.51269800
H	-17.65410400	-5.30126700	-4.01291200
H	-17.14338300	-4.21694800	7.48247500
H	-18.32288300	-3.52723100	6.34448300
H	-17.49509100	-5.04943300	5.95106100
H	-19.65553600	-6.80122100	-3.82847500
H	-20.11707700	-6.02253100	-2.29821900
H	-20.16562700	-5.09749200	-3.81543100
C	11.06717200	0.24856100	-0.87881300
C	11.26660300	1.61511200	-1.14880400
C	12.17420600	-0.53923000	-0.51693700
C	12.53229800	2.19326900	-1.07232400
H	10.41806700	2.23437500	-1.44983900
C	13.43767800	0.03089200	-0.44412900
H	12.03532100	-1.59835000	-0.28499900
C	13.61960700	1.39295900	-0.72294100
H	12.66649300	3.25421900	-1.29641800
C	14.75563500	-0.64673700	-0.07691700
C	15.04695500	1.70119900	-0.58489300
C	15.72711700	0.52583900	-0.21515500
C	15.01346000	-1.76396800	-1.12273800
C	14.64520900	-1.18898500	1.37726700
C	15.73785700	2.89613400	-0.77728100
C	17.10827600	0.55568500	-0.05330400
C	16.18744700	-2.71418400	-0.90851100
H	15.11357400	-1.28102300	-2.11055400
H	14.09601400	-2.37483600	-1.17479000
C	15.93572000	-1.38930000	2.17037700
H	14.09142800	-2.14311300	1.32933100
H	14.00547800	-0.49906100	1.95259000
C	17.11946700	2.91531300	-0.59854200
H	15.20697700	3.80923500	-1.05732900

C	17.82256300	1.75294100	-0.23819500
H	17.65262900	-0.35238400	0.20657800
C	16.32918800	-3.71925900	-2.04923000
H	17.13139700	-2.15505900	-0.80451400
H	16.04722400	-3.26987000	0.03291200
C	15.70105700	-2.07377100	3.51427600
H	16.66496600	-1.97830800	1.59379100
H	16.40936700	-0.41041600	2.35041400
H	17.65970900	3.85636600	-0.72576100
C	17.44751300	-4.73289000	-1.82712000
H	15.37216100	-4.25591400	-2.18069700
H	16.50583700	-3.17865600	-2.99644700
C	16.98766700	-2.27720200	4.30900100
H	14.98882400	-1.47696500	4.11226900
H	15.21568700	-3.05271300	3.34937800
H	18.40678900	-4.19826100	-1.70295500
H	17.27198900	-5.26282000	-0.87324400
C	17.58340700	-5.75653300	-2.95135900
H	17.68924000	-2.88510200	3.70908900
H	17.48320000	-1.30013200	4.45562300
C	16.78149400	-2.94390600	5.66668300
C	18.69101600	-6.77488900	-2.71019400
H	17.76759000	-5.22836500	-3.90339100
H	16.62054300	-6.28194100	-3.07855800
C	18.08186400	-3.16147500	6.43105100
H	16.27279700	-3.91305700	5.52102200
H	16.09492000	-2.32768500	6.27335500
H	18.75853200	-7.50331500	-3.53311300
H	19.67286500	-6.28226200	-2.61819600
H	18.51668400	-7.33854100	-1.77901300
H	17.90458900	-3.64180200	7.40589200
H	18.77375000	-3.80458000	5.86286800
H	18.59770900	-2.20548400	6.61868400
C	-19.17684500	1.75638300	0.13565900
C	-19.96238700	0.56708200	0.24581800
C	-19.86396000	2.99832700	0.26831600
C	-21.31240300	0.61966600	0.46609200
H	-19.49950600	-0.41210700	0.12701300

C	-21.21752000	3.06510700	0.50314100
H	-19.31368500	3.93696200	0.21282100
C	-21.96740800	1.87028000	0.60488400
H	-21.90891900	-0.29141300	0.53399200
H	-21.69489600	4.03823400	0.61365000
C	19.29652500	1.78245000	-0.04367200
C	19.91343100	1.00982000	0.94751900
C	20.12446000	2.58762100	-0.84633600
C	21.29514800	1.02635400	1.14280100
H	19.30387600	0.38488200	1.60542900
C	21.49946900	2.61495100	-0.66631400
H	19.68616500	3.19261600	-1.64380500
C	22.10232100	1.83346600	0.33188500
H	21.72626900	0.41206900	1.93394700
H	22.13487700	3.23637600	-1.30106300
O	23.44118500	1.92060500	0.43596800
O	-23.26413900	1.82433400	0.82423400
C	-24.01645900	3.02391700	0.97266500
H	-25.05308100	2.71199600	1.14006400
H	-23.66300500	3.60287500	1.83879500
H	-23.96016000	3.63673400	0.06051600
C	24.10207300	1.14385300	1.40736700
H	23.93576400	0.06478000	1.24946700
H	25.17347400	1.35528200	1.30155900
H	23.78604500	1.41077200	2.43011100

[PC3]

C	4.32978500	-1.16800700	-2.17400400
C	4.73019700	-0.71051100	-0.90639400
C	3.75914500	-0.23525700	-0.00769300
C	2.42137300	-0.21530500	-0.38028900
C	2.03447400	-0.70873700	-1.63822500
C	2.98609200	-1.18052900	-2.54114700
H	5.07985700	-1.54059800	-2.87335100
H	4.06422200	0.12211500	0.97810400
H	2.68740200	-1.56748100	-3.51822800
C	1.21278200	0.25887700	0.41770800
C	0.07809700	-0.11069400	-0.52981400
C	-1.28723600	0.03969200	-0.33375600

C	-2.18519800	-0.35163400	-1.34251000
C	-1.67597700	-0.88495000	-2.54042000
C	-0.30537100	-1.03424200	-2.74277700
C	0.57054600	-0.64600200	-1.72994300
H	-1.66473100	0.43760500	0.61191100
H	-2.36596000	-1.17315400	-3.33669800
H	0.07052700	-1.44722800	-3.68182500
C	6.15478800	-0.75313300	-0.49327200
C	7.21485900	-0.34770300	-1.38098800
C	6.53860900	-1.16612600	0.76030900
C	8.59620200	-0.39427000	-0.94995600
C	7.90590300	-1.21029200	1.18394200
H	5.77374300	-1.49577000	1.46723900
C	8.93245800	-0.84106100	0.36275100
H	8.11982500	-1.55960100	2.19646100
N	7.07908600	0.11242800	-2.62387000
N	9.44837100	0.02440600	-1.88512500
S	8.56730700	0.44132400	-3.18521500
H	9.97642400	-0.87727100	0.67683000
C	-3.65124400	-0.20057900	-1.14752800
C	-4.17902900	0.90398300	-0.46245800
C	-4.55079900	-1.15745400	-1.64491800
C	-5.55051800	1.05155200	-0.28205700
H	-3.50922900	1.67621900	-0.07779500
C	-5.92049200	-1.01405400	-1.46660800
H	-4.17240000	-2.04021100	-2.16520300
C	-6.44159700	0.09409100	-0.78403400
H	-5.91287900	1.93124000	0.25443000
H	-6.60680300	-1.76916700	-1.85364300
C	-7.90040200	0.21080100	-0.61950400
C	-10.00474100	-0.19639000	-0.67952900
C	-9.85955100	1.06307600	-0.05535100
C	-11.28521400	-0.74069300	-0.86457200
C	-10.95298300	1.80988200	0.39395500
C	-12.37570600	-0.00429600	-0.42008200
H	-11.41081000	-1.71344800	-1.34506000
C	-12.21148000	1.25297000	0.19996600
H	-10.82269700	2.78167400	0.87378200

H	-13.38411200	-0.40412200	-0.55117900
H	-13.09556200	1.80043300	0.53545400
N	-8.76608800	-0.69578700	-1.01692300
N	-8.50509400	1.28848300	-0.03395700
H	-8.04815000	2.11190500	0.34207200
C	1.19288300	1.80115500	0.59281500
C	2.32434700	2.43752300	1.39430300
H	0.23076200	2.05806400	1.06910400
H	1.16914000	2.25923400	-0.41088700
C	2.11495000	3.93678600	1.59417700
H	2.41771600	1.95429100	2.38121300
H	3.28527900	2.27902600	0.87819500
C	3.24766600	4.61396100	2.35964100
H	1.99936800	4.42292000	0.60857200
H	1.16190100	4.10415100	2.12759900
H	3.36859300	4.12281800	3.34242500
H	4.19967000	4.45241100	1.82214000
C	3.03630300	6.11120300	2.56934400
C	4.17294300	6.78118000	3.33164500
H	2.08560400	6.27007700	3.10802900
H	2.91230300	6.59972800	1.58679100
H	3.98889300	7.85782700	3.47072700
H	4.30076500	6.33301000	4.33076200
H	5.13080900	6.67244100	2.79706400
C	1.08993000	-0.45547500	1.77872900
C	0.99674700	-1.97660200	1.70874500
H	0.19892500	-0.05506800	2.29320500
H	1.95502500	-0.17759400	2.40323100
C	0.83491000	-2.62413200	3.08088200
H	0.14528700	-2.26935400	1.07041300
H	1.90022800	-2.38196000	1.22098500
C	0.74172200	-4.14617100	3.02765200
H	1.68280800	-2.33202200	3.72661400
H	-0.07085300	-2.22044800	3.56818100
H	-0.09769400	-4.43650000	2.36989800
H	1.65299300	-4.55115900	2.55126000
C	0.55651700	-4.79882100	4.39515800
C	0.46067800	-6.31828900	4.33002900

H	-0.35378000	-4.39149300	4.86914200
H	1.39571700	-4.50904800	5.05183600
H	0.32636500	-6.75982400	5.32985100
H	-0.39151300	-6.63743800	3.70772900
H	1.37197500	-6.75706800	3.89164500
[PC3]*			
C	4.11466300	-1.66587800	-2.74366700
C	4.66026700	-1.08890500	-1.55983300
C	3.75672100	-0.50470200	-0.62786100
C	2.40487800	-0.46236400	-0.89806900
C	1.89415800	-1.04149700	-2.07891700
C	2.75437600	-1.64391700	-3.00344700
H	4.77462700	-2.11159800	-3.48799700
H	4.14499500	-0.10974000	0.30773100
H	2.36405700	-2.09097600	-3.92017500
C	1.28524700	0.13664500	-0.05559300
C	0.06668700	-0.24847700	-0.88416500
C	-1.27126600	-0.01618300	-0.60069900
C	-2.26081700	-0.45153500	-1.49938600
C	-1.87132400	-1.10861900	-2.68242200
C	-0.53048200	-1.34121000	-2.97376300
C	0.43897900	-0.91121400	-2.06583600
H	-1.55560700	0.47686700	0.33239000
H	-2.63339800	-1.43043500	-3.39551600
H	-0.24784600	-1.85040000	-3.89794300
C	-3.69952400	-0.22821800	-1.19970600
C	-4.13350400	0.94485100	-0.56428300
C	-4.66519700	-1.19018400	-1.53768000
C	-5.47866000	1.15130200	-0.27510800
H	-3.41237600	1.72283300	-0.30469100
C	-6.00820200	-0.98840300	-1.24914700
H	-4.36002700	-2.12349400	-2.01582700
C	-6.43535300	0.18518800	-0.61208700
H	-5.76888300	2.08390500	0.21375500
H	-6.74635500	-1.74901400	-1.50874800
C	-7.86875700	0.35348700	-0.31902900
C	-9.98034000	0.00849800	-0.18285200
C	-9.73916700	1.25562300	0.43666300

C	-11.28781600	-0.49750800	-0.24948000
C	-10.76206800	2.02488300	0.99992300
C	-12.30818900	0.26148400	0.30826000
H	-11.48601300	-1.45981500	-0.72652000
C	-12.04865800	1.50463300	0.92418100
H	-10.55935600	2.98574700	1.47660000
H	-13.33566200	-0.10851200	0.27150200
H	-12.87973100	2.07013900	1.35230300
N	-8.79509900	-0.52233300	-0.64091900
N	-8.38259300	1.44242600	0.32925000
H	-7.86538000	2.24187500	0.67766000
C	1.36948700	1.68720100	-0.01652000
C	2.58074400	2.29709800	0.68192000
H	0.44880600	2.05494900	0.46880100
H	1.33599600	2.05391900	-1.05701900
C	2.59866500	3.82193200	0.61765900
H	2.61440500	1.98050500	1.73789400
H	3.50779500	1.92507300	0.21914200
C	3.84583500	4.42601800	1.25682700
H	2.54147300	4.14040600	-0.43891000
H	1.69614600	4.22923300	1.10786200
H	3.88936500	4.13403700	2.32201700
H	4.74206300	3.98158800	0.78658000
C	3.92455400	5.94618000	1.14659700
C	5.18360400	6.53051800	1.77528000
H	3.03247500	6.39251700	1.62017300
H	3.87745500	6.23247800	0.08109500
H	5.22186300	7.62537200	1.66386300
H	5.23566100	6.30275900	2.85259500
H	6.09102800	6.11576700	1.30635100
C	1.23410100	-0.45789400	1.36569800
C	1.05194400	-1.97120800	1.42672000
H	0.41266900	0.03699000	1.91280900
H	2.16253800	-0.18669400	1.89437200
C	0.98564500	-2.50717400	2.85388700
H	0.12960000	-2.25844200	0.89298500
H	1.88296400	-2.46484900	0.89308500
C	0.81498800	-4.02173000	2.92331100

H	1.90262400	-2.21719900	3.39797200
H	0.14859500	-2.02063700	3.38654000
H	-0.09100600	-4.31155700	2.36039300
H	1.66180200	-4.50744200	2.40506300
C	0.71654900	-4.56694600	4.34582600
C	0.55337500	-6.08104300	4.40095000
H	-0.13404100	-4.08501700	4.85929500
H	1.61875800	-4.27209400	4.91027000
H	0.47991000	-6.44370500	5.43808400
H	-0.35760200	-6.40316400	3.87029100
H	1.40888200	-6.59132900	3.92880600
C	6.08391200	-1.08551600	-1.32986300
C	6.74173700	-0.18992500	-0.41226800
C	6.95206100	-2.02511200	-2.05608500
C	8.19156300	-0.26440300	-0.23243900
N	6.18313700	0.76959200	0.30777600
C	8.29646200	-2.08824700	-1.86290900
H	6.48943100	-2.73011600	-2.74569000
C	8.95856500	-1.20852800	-0.94949300
N	8.67773700	0.62602800	0.62477000
S	7.39026500	1.53315200	1.18578900
H	8.88910200	-2.82384700	-2.40982400
H	10.03903900	-1.25131600	-0.80475500

[PC3]-

C	4.13334400	-1.64737700	-2.70909100
C	4.65427600	-1.12335700	-1.50707800
C	3.75085400	-0.56938600	-0.57887100
C	2.39401500	-0.51301200	-0.86461900
C	1.89551700	-1.05821600	-2.05984800
C	2.76766800	-1.63103200	-2.98592700
H	4.81844300	-2.06395800	-3.45131500
H	4.13422300	-0.18179800	0.36382400
H	2.39197100	-2.05327600	-3.92153100
C	1.27140500	0.08223700	-0.02258600
C	0.05520600	-0.27282500	-0.86891900
C	-1.28231900	-0.03260800	-0.59193700
C	-2.27138300	-0.43889600	-1.50613000
C	-1.87692800	-1.07536300	-2.69633800

C	-0.53316200	-1.31452400	-2.98119000
C	0.43436800	-0.91469400	-2.06004700
H	-1.56899100	0.44526100	0.34866500
H	-2.63518800	-1.37703200	-3.42263000
H	-0.25022900	-1.80871700	-3.91373100
C	-3.70968600	-0.20505800	-1.21174600
C	-4.13417000	0.95863000	-0.55258900
C	-4.68609700	-1.14624200	-1.57707700
C	-5.47821000	1.17508200	-0.26547100
H	-3.40502300	1.72156200	-0.27155900
C	-6.02842000	-0.93434200	-1.29175300
H	-4.38982400	-2.07241000	-2.07444500
C	-6.44503600	0.22886000	-0.62911200
H	-5.75934600	2.10054000	0.24203800
H	-6.77408800	-1.67988200	-1.57289800
C	-7.87720400	0.40748900	-0.33663600
C	-9.99391200	0.08720000	-0.21513400
C	-9.73763800	1.31295600	0.43996900
C	-11.30798200	-0.39876800	-0.29861800
C	-10.75130600	2.08005900	1.02229600
C	-12.31947700	0.35811500	0.27818100
H	-11.51820700	-1.34491200	-0.80213700
C	-12.04475300	1.57980500	0.92923600
H	-10.53657700	3.02471700	1.52540500
H	-13.35179100	0.00334000	0.22881500
H	-12.86919500	2.14442300	1.37118500
N	-8.81450400	-0.44629400	-0.68545400
N	-8.37840000	1.48425900	0.34127300
H	-7.85185100	2.26637200	0.71410600
C	1.37355400	1.63087700	0.05597300
C	2.63626200	2.20100300	0.69404000
H	0.48768800	1.99254400	0.60745700
H	1.28229800	2.03213400	-0.96824500
C	2.63396800	3.72358400	0.79623800
H	2.78069500	1.77658800	1.70200100
H	3.51760200	1.89822700	0.10852200
C	3.95377200	4.26824700	1.33627800
H	2.44097400	4.15943600	-0.20070900

H	1.80181600	4.05675400	1.44259900
H	4.15494500	3.81594700	2.32455800
H	4.77552600	3.92944000	0.67924900
C	4.00384300	5.78816600	1.45943900
C	5.33715800	6.29963500	1.99213800
H	3.18703100	6.12695100	2.12088600
H	3.80309900	6.23968600	0.47196100
H	5.34941800	7.39778800	2.07289400
H	5.54833000	5.88858500	2.99296100
H	6.16865500	6.00281500	1.33190700
C	1.19516900	-0.53836100	1.38692000
C	1.02093200	-2.05347100	1.41993900
H	0.35930600	-0.05905700	1.92637900
H	2.11049400	-0.27215900	1.94065600
C	0.91361600	-2.61070500	2.83648500
H	0.11752900	-2.33822000	0.85301800
H	1.87139600	-2.53387600	0.90570200
C	0.75156500	-4.12716500	2.88071200
H	1.81149500	-2.32229000	3.41255600
H	0.05737400	-2.13722300	3.35016700
H	-0.13747300	-4.41538300	2.29041800
H	1.61485100	-4.60007400	2.37821800
C	0.62021000	-4.69251100	4.29266600
C	0.46313400	-6.20795700	4.32321100
H	-0.24510100	-4.22159100	4.79156300
H	1.50674900	-4.40125100	4.88328700
H	0.36804200	-6.58554900	5.35326300
H	-0.43414500	-6.52684200	3.76772400
H	1.33147200	-6.70770500	3.86347900
C	6.10954300	-1.15556700	-1.23091800
C	6.76422200	-0.10063900	-0.52203400
C	6.90351600	-2.22681600	-1.68652700
C	8.20704000	-0.15970500	-0.30505900
N	6.19631500	1.01036800	-0.02172600
C	8.28284400	-2.28358000	-1.46472900
H	6.41960100	-3.05697400	-2.20787200
C	8.94792700	-1.26306400	-0.78164700
N	8.70842500	0.90074000	0.35459300

	S	7.41729200	1.91396500	0.68154200
	H	8.84682500	-3.14724400	-1.82789000
	H	10.02619000	-1.30284300	-0.60850500
[PC2] ⁺				
	C	4.29762900	-1.25819500	-2.12833500
	C	4.70730600	-0.74016200	-0.88647800
	C	3.74480700	-0.21319200	-0.00798900
	C	2.40502600	-0.20418800	-0.37393200
	C	2.00965400	-0.75737100	-1.60383000
	C	2.95277000	-1.27985800	-2.48799700
	H	5.04155700	-1.67038200	-2.81161900
	H	4.05717100	0.19185200	0.95657200
	H	2.64575500	-1.71292600	-3.44272800
	C	1.20344000	0.31170900	0.40815500
	C	0.06311400	-0.09342500	-0.51679800
	C	-1.29828100	0.07539700	-0.32458700
	C	-2.20208300	-0.37747700	-1.30542800
	C	-1.70098700	-0.98074200	-2.47569000
	C	-0.33320700	-1.13469400	-2.67889400
	C	0.54719600	-0.69329700	-1.69101500
	H	-1.66760700	0.52691500	0.59934000
	H	-2.39305700	-1.31323300	-3.25172700
	H	0.03855200	-1.59509100	-3.59680500
	C	6.13329300	-0.77532800	-0.47714700
	C	7.19494900	-0.43947300	-1.39158100
	C	6.51647700	-1.11822000	0.79767300
	C	8.57726400	-0.48252200	-0.96346700
	C	7.88463900	-1.15634500	1.21891700
	H	5.75038000	-1.39524100	1.52536900
	C	8.91259300	-0.85365000	0.37276100
	H	8.09775400	-1.44457200	2.25060600
	N	7.06093800	-0.05166500	-2.65894200
	N	9.43178900	-0.13476200	-1.92513300
	S	8.55172700	0.21872100	-3.24442700
	H	9.95734900	-0.88594600	0.68460700
	C	-3.65756000	-0.21918300	-1.11172800
	C	-4.17381700	0.88464100	-0.39596200
	C	-4.56582500	-1.16310100	-1.63674400

C	-5.53154000	1.04898400	-0.21994500
H	-3.49371300	1.63826400	0.00352600
C	-5.92558000	-1.01437700	-1.45888300
H	-4.19340100	-2.03884500	-2.17055400
C	-6.43659800	0.09953300	-0.75052600
H	-5.89073300	1.92181700	0.32798200
H	-6.62057700	-1.75443500	-1.85715100
C	-7.85188000	0.22745800	-0.59933700
C	-9.94073300	-0.22977000	-0.74515600
C	-9.82489900	1.03059200	-0.04501900
C	-11.23011900	-0.79511900	-0.98845100
C	-10.93278600	1.73887400	0.40535100
C	-12.31395700	-0.09421300	-0.53864600
H	-11.32112000	-1.74762800	-1.51169700
C	-12.16772100	1.15774400	0.14731600
H	-10.83804000	2.69033600	0.92845400
H	-13.32141900	-0.48259400	-0.69700000
H	-13.07188900	1.67177100	0.48057200
N	-8.73813500	-0.68858300	-1.06880400
N	-8.48627100	1.26403900	0.01888300
H	-8.04847600	2.07703300	0.44595300
C	1.19258100	1.85944400	0.52294500
C	2.33514700	2.51726500	1.29081200
H	0.23640600	2.13910600	0.99839200
H	1.16202800	2.27956900	-0.49701200
C	2.12847400	4.02092600	1.45712400
H	2.44314200	2.05871400	2.28790800
H	3.28867700	2.34594700	0.76524600
C	3.26837000	4.71248900	2.19874300
H	2.00520400	4.48515400	0.46192600
H	1.18026000	4.20140900	1.99492000
H	3.39737000	4.23993400	3.18960100
H	4.21556600	4.53963600	1.65631800
C	3.06011300	6.21358300	2.38202600
C	4.20162000	6.89500100	3.12672500
H	2.11250600	6.38351900	2.92283200
H	2.93169700	6.68487400	1.39162900
H	4.01959500	7.97405100	3.24874800

H	4.33400900	6.46338800	4.13250300
H	5.15657100	6.77601900	2.58915400
C	1.08165000	-0.34920300	1.79662500
C	0.98159400	-1.87143900	1.78431400
H	0.19450200	0.07539700	2.29814600
H	1.95052100	-0.05149300	2.40636600
C	0.83510200	-2.46928400	3.18048000
H	0.12096100	-2.18403700	1.16787800
H	1.87726700	-2.29796800	1.30026700
C	0.73166800	-3.99156500	3.17985700
H	1.69437600	-2.16118000	3.80328500
H	-0.06093500	-2.04306200	3.66663100
H	-0.12040800	-4.29772300	2.54585500
H	1.63239600	-4.41782800	2.70203200
C	0.56530500	-4.59853200	4.57057900
C	0.45881700	-6.11860400	4.55583500
H	-0.33422500	-4.17008800	5.04656800
H	1.41750700	-4.29388900	5.20337800
H	0.33863800	-6.52710800	5.57134200
H	-0.40593500	-6.45163700	3.95863100
H	1.35979900	-6.57720100	4.11650900

[EBrP]

C	-0.57951900	0.78933400	-0.51485300
O	-0.86073500	1.27135400	-1.58305800
O	-1.40126700	0.04489000	0.20962600
C	-2.70235200	-0.21984500	-0.33436000
H	-3.21177400	0.73872800	-0.51680400
H	-2.58264000	-0.72530900	-1.30501200
C	-3.45968800	-1.07476300	0.64967800
H	-3.57476400	-0.56001800	1.61516600
H	-4.46217900	-1.28676600	0.25045600
H	-2.94596300	-2.03266000	0.81933300
C	0.76983900	0.98002600	0.15913500
H	1.30466500	1.75165600	-0.40562100
C	0.69209300	1.31245000	1.63331900
H	0.18820100	0.51639800	2.19765600
H	1.69687800	1.46934300	2.04918300
H	0.12035400	2.24594600	1.75744800

[EBrP]⁻	Br	1.80688600	-0.66772800	-0.14376800
	C	0.90547800	0.73429600	0.74545600
	O	1.06531100	0.51093300	1.93452000
	O	1.70540600	0.18403800	-0.19613200
	C	2.68719400	-0.73627500	0.25442100
	H	3.33242400	-0.25509900	1.00783800
	H	2.19311900	-1.58816200	0.75122000
	C	3.49119000	-1.19415300	-0.93975900
	H	3.99346300	-0.34363000	-1.42547000
	H	4.26052800	-1.91245700	-0.61970900
	H	2.84650600	-1.68781000	-1.68274300
	C	-0.09455200	1.61261000	0.19001100
	H	-0.74022600	2.09522800	0.92433700
	C	-0.17432800	1.98345300	-1.24617000
	H	0.05277000	1.12043000	-1.88722300
	H	-1.18063400	2.34586600	-1.49817800
	H	0.54647300	2.78540700	-1.50066700
	Br	-2.23885900	-0.64340400	-0.05715000
[Et₃N]	N	-0.00267700	-0.00353000	0.02954300
	C	-1.18102400	-0.76134800	0.43218100
	C	-2.40289600	-0.48966100	-0.43368200
	H	-1.42617500	-0.57739800	1.50260800
	H	-0.94190300	-1.83279100	0.35890600
	H	-3.24314700	-1.12919500	-0.12169500
	H	-2.74268000	0.55514400	-0.36378600
	H	-2.17929500	-0.70313000	-1.49064600
	C	1.23751900	-0.64481200	0.44970800
	C	1.64288300	-1.81258800	-0.43831600
	H	1.17398200	-0.97829400	1.50980200
	H	2.04176100	0.10504000	0.41908900
	H	2.59523400	-2.24545200	-0.09465100
	H	0.89413300	-2.61962900	-0.43349600
	H	1.77075600	-1.47610100	-1.47904700
	C	-0.07371800	1.39518000	0.43338300
	C	0.77893800	2.31519300	-0.42861500
	H	0.20002400	1.51770200	1.50553000

H	-1.12054400	1.72310400	0.35209900
H	0.63993200	3.36450200	-0.12545500
H	1.85334600	2.08948100	-0.34621600
H	0.49310100	2.21994500	-1.48779600
[Et ₃ N] ⁺			
N	0.11093300	-0.04146700	-0.32682100
C	-0.18367800	1.28419600	0.16774500
C	-1.61127000	1.75748900	0.00190900
H	0.52473700	1.96869200	-0.32675800
H	0.10887800	1.28319100	1.23602500
H	-1.67564600	2.77460300	0.41208100
H	-1.90348400	1.80087200	-1.05714400
H	-2.32710200	1.13003200	0.55061400
C	1.48687600	-0.46608500	-0.48690500
C	2.49792700	0.19892200	0.42552700
H	1.72675800	-0.27075200	-1.55176000
H	1.50085500	-1.55918300	-0.36604100
H	3.47513600	-0.26609600	0.23648100
H	2.59815400	1.27627000	0.23849700
H	2.24222100	0.03903200	1.48298800
C	-0.92509700	-1.00669500	-0.61517600
C	-1.33362500	-1.74699700	0.66243200
H	-0.52333800	-1.71281400	-1.35446500
H	-1.78565400	-0.48745900	-1.05376600
H	-2.10042400	-2.48830800	0.39966100
H	-0.47264100	-2.26947400	1.10284100
H	-1.75178200	-1.05332100	1.40529300

5. References

1. C. Liao, Y. Gong, Y. Che, L. Cui, Y. Liu, H. Ji, Y. Zhang, L. Zang, J. Zhao and Y. Che, *Chem. Eur. J.*, 2023, **29**, e202301747.
2. C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158-6170.
3. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.
4. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
5. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.