

Room-Temperature, Ambient-Pressure CO₂ Conversion into Value-Added Pharmaceutical Products quinazoline-2,4(1H,3H)-diones

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1.1. Synthesis details of the ionic liquids

Synthesis of [HDBU⁺] [Cl⁻]ionic liquids. In a N₂ atmosphere, DBU (32.8 mmol, 5.0g) was loaded into a 25 glass bottle, a suitable amount of concentrate HCl (containing HCl 1.20g, 32.8 mmol) was dissolved in 10mL distilled water, the solution was then added dropwise to the bottle with stirring in ice bath. After the mixture was stirred at 25°C for 24 h. The obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 93.8% by mol..

Synthesis of [HDBU⁺] [HSO₄⁻]ionic liquids. In a N₂ atmosphere, DBU (32.8 mmol, 5.0g) was loaded into a 25 glass bottle, a suitable amount of concentrate HSO₄ (containing HSO₄ 3.21g, 32.8 mmol) was dissolved in 10mL distilled water, the solution was then added dropwise to the bottle with stirring in ice bath. After the mixture was stirred at 25°C for 1 h. The obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 92.9% by mol.

Synthesis of [HDBU⁺] [2-Cl-PhO⁻]ionic liquids. In a N₂ atmosphere, DBU (32.8 mmol, 5.0g) was loaded into a 25 glass bottle, 2- Clorophenol (32.8mmol, 4.22g) was dissolved in 5mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 87.3% by mol.

Synthesis of [HDBU⁺] [3-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (20 mmol, 3.0g) was loaded into a 25 glass bottle, 3- Clorophenol (20mmol, 2.53g) was dissolved in 2mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 81.72% by mol.

Synthesis of [HDBU⁺] [4-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (20 mmol, 3.0g) was loaded into a 25 glass bottle, 3- Clorophenol (20mmol, 2.53g) was dissolved in 2mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 86.61% by mol.

Synthesis of [HDBU⁺] [2,4-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (32.8 mmol, 5.0g) was loaded into a 25 glass bottle, 2,4- Diclorophenol (32.8mmol, 5.346g) was dissolved in 5mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 86.56% by mol.

Synthesis of [HDBU⁺] [Im⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (32.8 mmol, 5.0g) was loaded into a 25 glass bottle, Imidazole (32.8mmol, 2.23g) was dissolved in 2L ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 95.26% by mol.

Synthesis of [HDBU⁺] [TFE⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (30mmol, 4.5875g) was loaded into a 25 glass bottle, Trifluoroethanol (TFE) (45mmol, 4.3862g) was then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 81.65% by mol.

Synthesis of [HDBU⁺] [2-F-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (20 mmol, 3.0g) was loaded into a 25 glass bottle, 2- Fluorophenol (20mmol, 2.21g) was dissolved in 2mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 91.69% by mol.

Synthesis of [HDBU⁺] [2-Br-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, DBU (20 mmol, 3.0g) was loaded into a 25 glass bottle, 2-Bromophenol (20mmol, 3.41g) was dissolved in 2mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 90.26% by mol.

Synthesis of [HTMG⁺] [3-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, TMG (32.8 mmol, 3.78g) was loaded into a 25 glass bottle, 3- Chlorophenol (32.8mmol, 4.22g) was dissolved in 2mL ethanol and then added dropwise to the bottle with stirring. After 24 hours reaction, the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 85.01% by mol.

Synthesis of [Ch⁺] [2-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, 2-Cl-Phenol (4.22g, 32.8 mmol) was dissolved in 5mL ethanol, the solution was then added dropwise to the bottle with stirring. After the mixture was stirred at 25°C for 24 h, a light yellow, viscously liquid was obtained. the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 89.71% by mol.

Synthesis of [Ch⁺] [3-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, 3-Cl-Phenol (4.22g, 32.8 mmol) was dissolved in 5mL ethanol, the solution was then added dropwise to the bottle with stirring. After the mixture was stirred at 25°C for 24 h, a light yellow, viscously liquid was obtained. the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 88.52% by mol.

Synthesis of [Ch⁺] [Im⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, Imidazole (2.23g, 32.8 mmol) was dissolved in 5mL ethanol, the solution was then added dropwise to the bottle with stirring. After the mixture was stirred at 25°C for 24 h, a light yellow, viscously liquid was obtained. the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 108% by mol.

Synthesis of [Ch⁺] [2,4-Cl-PhO⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, 2,4-DichloroPhenol (5.346g, 32.8 mmol) was dissolved in 5mL ethanol, the solution was then added dropwise to the bottle with stirring. After the mixture was stirred at 25°C for 24 h, a light yellow,

viscous liquid was obtained. the obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 98.72% by mol.

Synthesis of [Ch⁺] [Cl⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, a suitable amount of concentrate HCl (containing HCl 1.20g, 32.8 mmol) was dissolved in 10mL distilled water, the solution was then added dropwise to the bottle with stirring in ice bath. After the mixture was stirred at 25°C for 24 h. The obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 97.5% by mol.

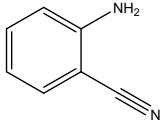
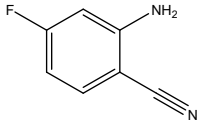
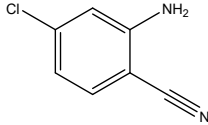
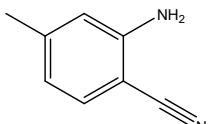
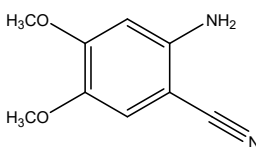
Synthesis of [Ch⁺] [HSO₄⁻]ionic liquids. Typically, in a N₂ atmosphere, Choline hydroxide 45 wt.% aqueous solution (8.833g, 32.8 mmol) was loaded into a 25 glass bottle, a suitable amount of concentrate HSO₄ (containing HSO₄ 3.21g, 32.8 mmol) was dissolved in 10mL distilled water, the solution was then added dropwise to the bottle with stirring in ice bath. After the mixture was stirred at 25°C for 1 h. The obtained Ionic liquids were dried by reduced pressure distillation at 85°C, 0.1kpa for 3h. Yields 98.2% by mol.

Table S1 Synthesis yields of the ionic liquids catalysts.

Entry	Catalysts	Yields(% mol)
1	[Ch ⁺][Cl ⁻]	93.8
2	[Ch ⁺][HSO ₄ ⁻]	92.9
3	[Ch ⁺][Im ⁻]	108
4	[Ch ⁺][2,4-Cl-PhO ⁻]	98.72
5	[Ch ⁺][2-Cl-PhO ⁻]	89.71
6	[Ch ⁺][3-Cl-PhO ⁻]	88.52
7	[HDBU ⁺][Im ⁻]	95.26
8	[HDBU ⁺][TFE ⁻]	81.65
9	[HDBU ⁺][2-Br-PhO ⁻]	90.26
10	[HDBU ⁺][2-F-PhO ⁻]	91.69
11	[HDBU ⁺][2,4-Cl-PhO ⁻]	86.56
12	[HDBU ⁺][4-Cl-PhO ⁻]	86.61
13	[HDBU ⁺][2-Cl-PhO ⁻]	87.3
14	[HDBU ⁺][3-Cl-PhO ⁻]	81.72
15	[HTMG ⁺][3-Cl-PhO ⁻]	85.01
16	[HDBU ⁺][Cl ⁻]	97.5
17	[HDBU ⁺][HSO ₄ ⁻]	98.2

1.2 Substrates scope and scale up investigation catalyzed by [HDBU⁺][3Cl⁻]

Table S2 Substrates scope and scale up investigation catalyzed by [HDBU⁺][3Cl⁻]

Entry	Substrates scope	Substrates (mmol)	Yields(% mol)
1		10	96.4
2		1	98.1%
3		1	98.5%
4		1	95.1%
5		1	92.3%

Reaction conditions for entry 1: 2-aminobenzonitrile, 10 mmol; catalysts, 15 mmol; CO₂ (0.1Mpa), 30 °C and 24 hours. Reaction conditions for entry 2-5: Substrates, 1 mmol; catalysts, 1.5 mmol; CO₂ (0.1Mpa), 30 °C and 24 hours.

1.3 Solubility test of the ILs, substrate and product

The solubility test was conducted to check the substrate, product and ILs' solubility at room temperature, with the following typical procedure. 0.1000 g IL was added to a 25.0 mL glass bottle, and 5 mL solvent was then added into the flask under supersonic vibration for 5 minutes. Table S2 summarizes the solubility results.

Table S3. Solubility test of the ILs, substrate and product(I-insoluble, S-soluble, SS-slightly soluble)..

Entry	Substrates/Products/Catalysts	Water	Ethanol	Ethyl acetate	DMF	DMSO
1	2-aminobenzonitrile	I	S	S	S	S
2	Benzolineurea	I	SS	I	S	S
3	[HDBU ⁺][Im ⁻]	S	S	S	S	S
4	[HDBU ⁺][TFE ⁻]	S	S	S	S	S
5	[HDBU ⁺][2-F-PhO ⁻]	S	S	S	S	S
6	[HDBU ⁺][2-Cl-PhO ⁻]	I	S	S	S	S
7	[HDBU ⁺][2-Br-PhO ⁻]	S	S	S	S	S
8	[HDBU ⁺][3-Cl-PhO ⁻]	I	S	S	S	S
9	[HDBU ⁺][4-Cl-PhO ⁻]	S	S	S	S	S
10	[HDBU ⁺][2,4-Cl-PhO ⁻]	SS	S	S	S	S
11	[Ch ⁺][Im ⁻]	S	S	I	S	S
12	[Ch ⁺][2-Cl-PhO ⁻]	S	S	I	S	S
13	[Ch ⁺][2,4-Cl-PhO ⁻]	S	S	I	S	S
14	[HTMG ⁺][3-Cl-PhO ⁻]	SS	S	S	S	S

Table S3 summarizes the solubility results. All the substrates, products and ILs catalysts had good solubility in DMF and DMSO. That meant DMF and DMSO were ideal solution for this reaction. The substrate, 2-aminobenzonitrile, and most ILs were soluble in ethyl acetate. The product, benzolineurea, was insoluble in ethyl acetate. This means the products could be easily purified by washing with ethylacetate, after the reaction is finished.

1.4 The reusability test of the IL catalyst.

The first round is conducted as the typical procedures as described in the main text. 0.1180 g 2-aminobenzonitrile (1.00 mmol), 0.30 mL DMSO, and 1.50 mmol IL are added to a glass bottle capped with a plastic stopper, the air is flash out with CO₂ at 1 bar. After stirring 24 hours, 10.0 mL water is added, then the solids and liquid were separated by centrifugation and the solids were washed with 5.0 mL ethyl acetate and 1.0 mL ethanol three times. The washed liquids were combined and collected, the obtained solids are dried at 80 °C for 24 hours, and weighed to calculate the product yield.

After the first round, the liquid were collected in a 50 mL glass beaker and then dried at 80 °C until the volume of the left liquid was between 2-3mL, then transfer the liquid to the reaction tube, the beaker was washed with 1mL ethanol for 2 times to prevent the weight loss of the ILs catalyst. The reaction tube was then connected to a vacuum pump and then dried at 80 °C under vacuum for 3 hours with magnetic stirring and ready for reuse for the next round.

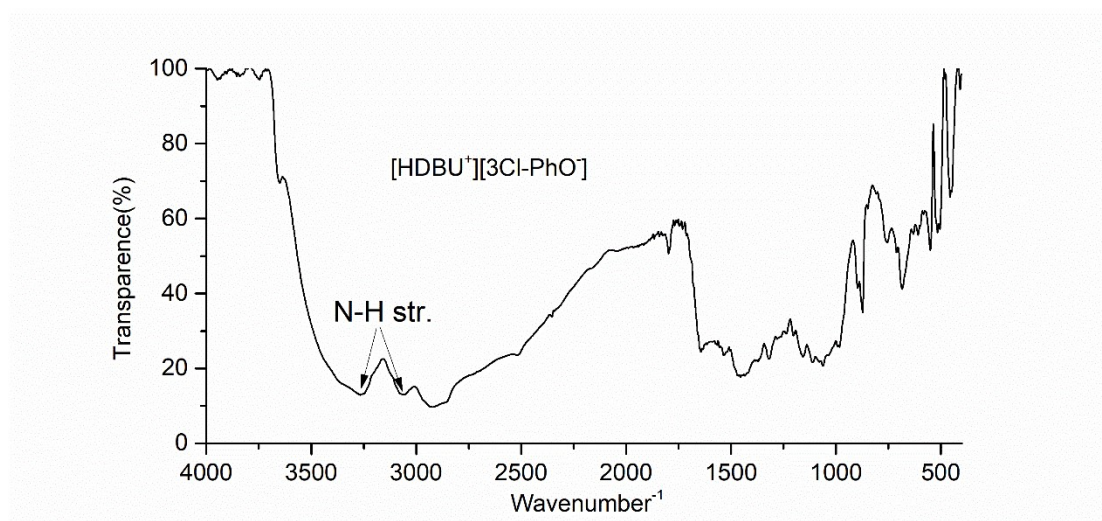
1.5 Thermal stability test of the ILs

1 gram of the specific ILs was added to a crucible (heated and weighed before) and weighed (m_a), the crucible was putted into a furnace and then dried at 200 °C for 30 min. The crucible was weighed (m_b) immediately after cooled to room temperature. The weigh loss of the ILs was simply calculated by m_a minus m_b .

Table S4. Thermal stability test of the ILs

Catalysts	200°C Weight loss (mg)	200°C Weight loss (%)	250°C Weight loss (mg)	250°C Weight loss (%)
[Ch ⁺][Im ⁻]	20.1	2.0	102.4	10.2
[Ch ⁺][2,4-Cl-PhO ⁻]	15.3	1.5	115.3	11.5
[Ch ⁺][2-Cl-PhO ⁻]	18.2	1.8	124.6	12.5
[Ch ⁺][3-Cl-PhO ⁻]	32.5	3.3	127.1	12.7
[HDBU ⁺][Im ⁻]	44.0	4.4	120.5	12.1
[HDBU ⁺][TFE ⁻]	37.3	3.7	172.6	17.3
[HDBU ⁺][2-Br-PhO ⁻]	21.1	2.1	133.2	13.3
[HDBU ⁺][2-F-PhO ⁻]	19.5	2.0	123.1	12.3
[HDBU ⁺][2,4-Cl-PhO ⁻]	33.5	3.4	130.4	13.0
[HDBU ⁺][2-Cl-PhO ⁻]	28.4	2.8	141.2	14.1
[HDBU ⁺][4-Cl-PhO ⁻]	41.1	4.1	133.1	13.3
[HDBU ⁺][3-Cl-PhO ⁻]	27.3	2.7	151.3	15.1
[HTMG ⁺][3-Cl-PhO ⁻]	35.2	3.5	142.6	14.3

1.6 IR spectrum of [HDBU⁺][3-Cl-PhO⁻] ILs.



1.7 HNMR and CNMR data and spectrum:

HNMR and CNMR spectrums were characterized by Agilent 400-MR DD2, d-DMSO as solvent.

[HDBU⁺][Im⁻].¹H NMR (400 MHz, d-DMSO) δ 10.89(s,1H), 7.63(s,1H), 7.0(s, 2H), 3.15-3.09 (m, 6H), 2.28(m, 2H), 1.68-1.62(m, 2H), 1.54-1.45(m, 6H). ¹³C NMR (400 MHz, d-DMSO) δ 161.10, 135.73, 122.10, 52.33, 47.96, 43.29, 36.25, 29.45, 28.35, 26.02, 22.47.

[HDBU⁺][TFE⁻].¹H NMR (400 MHz, d-DMSO) δ 5.38(s,1H), 3.8(s,2H), 3.14(s, 2H), 3.05 (m, 2H), 2.25(m, 2H), 1.65(m, 2H), 1.47-1.56(m, 6H). ¹³C NMR (400 MHz, d-DMSO) δ 174.8, 161.20, 60.6, 52.29, 47.94, 43.41, 36.01, 29.44, 28.34, 26.00, 22.41.

[HDBU⁺][2-Cl-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 9.48(s,1H), 7.1(m,1H), 6.87(m, 1H), 6.67(m, 1H), 6.30(m, 1H), 3.26-3.38(m, 4H), 3.16 (m, 2H), 2.59(m, 2H), 1.79(m, 2H), 1.47-1.59(m, 6H). ¹³C NMR (400 MHz, d-DMSO) δ 164.52, 161.24, 129.37, 127.89, 122.08, 119.07, 113.73, 53.22, 48.13, 39.33, 32.55, 28.93, 27.02, 24.58, 20.30.

[HDBU⁺][3-Cl-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 9.82(s,1H), 6.95(m,1H), 6.54 (m, 1H), 6.48(m, 1H), 6.42(m, 1H), 3.27-3.33(m, 4H), 3.14(m, 2H), 2.47(m, 2H), 1.76 (m, 2H), 1.48-1.59 (m, 6H). ¹³C NMR (400 MHz, d-DMSO) δ 165.68, 163.72, 133.59, 130.44, 116.92, 116.12, 114.07, 53.03, 48.10, 40.27, 33.53, 29.05, 27.31, 24.90, 20.82.

[HDBU⁺][4-Cl-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 10.77(s,1H), 6.97(m,2H), 6.55 (m, 2H), 3.23-3.29 (m, 4H), 3.12 (m, 2H), 2.42 (m, 2H), 1.73 (m, 2H), 1.47-1.57 (m, 6H) ¹³C NMR (400 MHz, d-DMSO) δ 163.19, 162.28, 129.02, 118.40, 118.33, 52.85, 48.06, 40.89, 34.00, 29.05, 29.15, 27.55, 25.16, 21.19.

[HDBU⁺][2,4-Cl-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 8.24(s,1H), 7.08(m,1H), 6.85 (m, 1H), 6.51 (m, 1H), 3.36-3.43 (m, 4H), 3.18 (m, 2H), 2.63 (m, 2H), 1.83 (m, 2H), 1.53-1.61 (m, 6H) ¹³C NMR (400 MHz, d-DMSO) δ 165.04, 161.55, 128.34, 127.69, 122.70, 119.90, 114.26, 53.39, 48.18, 38.75, 32.09, 28.86, 26.79, 24.33, 19.94.

[HDBU⁺][2-Br-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 7.73(s,1H), 7.26(m,1H), 6.91 (m, 1H), 6.66 (m, 1H), 6.25 (m, 1H), 3.33-3.41 (m, 4H), 3.17 (m, 2H), 2.6 (m, 2H), 1.81 (m, 2H) , 1.46-1.61 (m, 6H) ¹³C NMR (400 MHz, d-DMSO) δ 164.75, 161.79, 132.35, 128.60, 118.74, 114.49, 113.12, 53.32, 48.17, 39.11, 32.44, 28.89, 25.91, 24.45, 20.13.

[HDBU⁺][2-F-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 7.47(m,1H), 6.94 (m, 1H), 6.57 (m, 1H), 6.11 (m, 1H), 3.30-3.37 (m, 4H), 3.17 (m, 2H), 2.6 (m, 2H), 1.79 (m, 2H) , 1.51-1.59 (m, 7H) ¹³C NMR (400 MHz, d-DMSO) δ 164.65, 164.50, 138.07, 129.54, 117.16, 115.11, 91.41, 53.28, 48.18, 39.66, 39.43, 32.64, 28.97, 27.08, 24.65, 20.35.

[HTMG⁺][3-Cl-PhO⁻].¹H NMR (400 MHz, d-DMSO) δ 8.59(s,2H), 6.96(m,1H), 6.58 (m, 1H), 6.51(m, 1H), 6.45(m, 1H), 2.72(S, 12H). ¹³C NMR (400 MHz, d-DMSO) δ 165.00, 164.30, 133.57, 130.50, 116.77, 115.98, 114.53, 39.59.

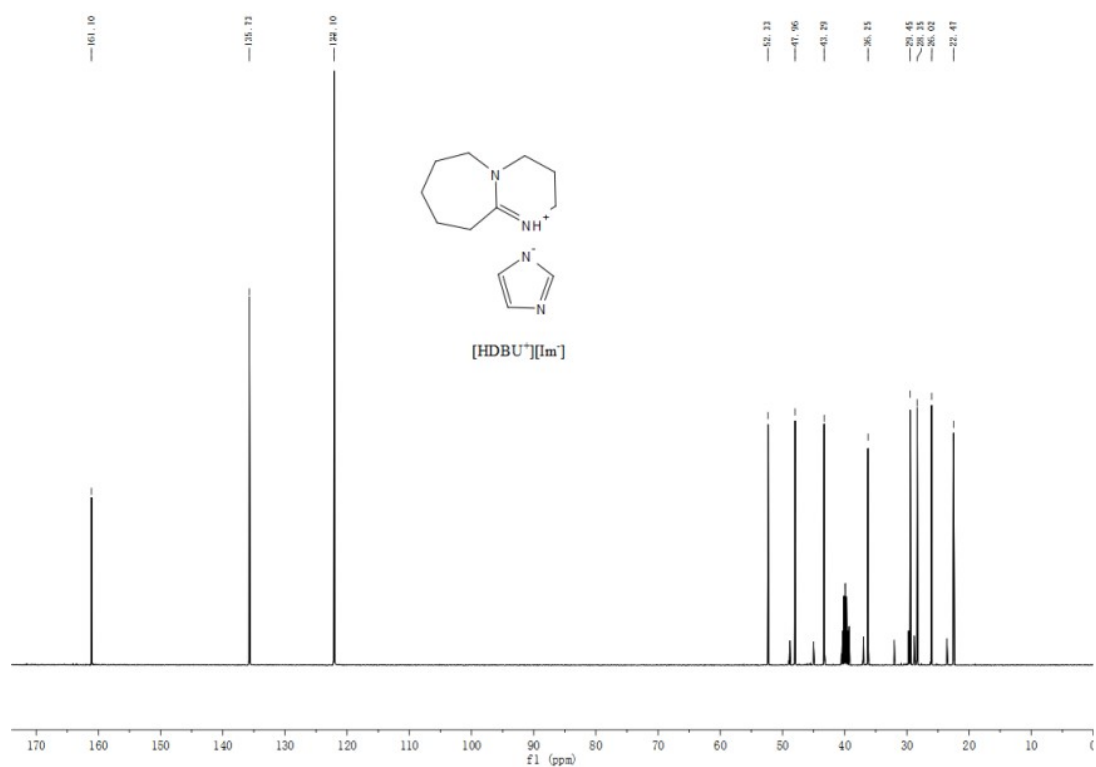
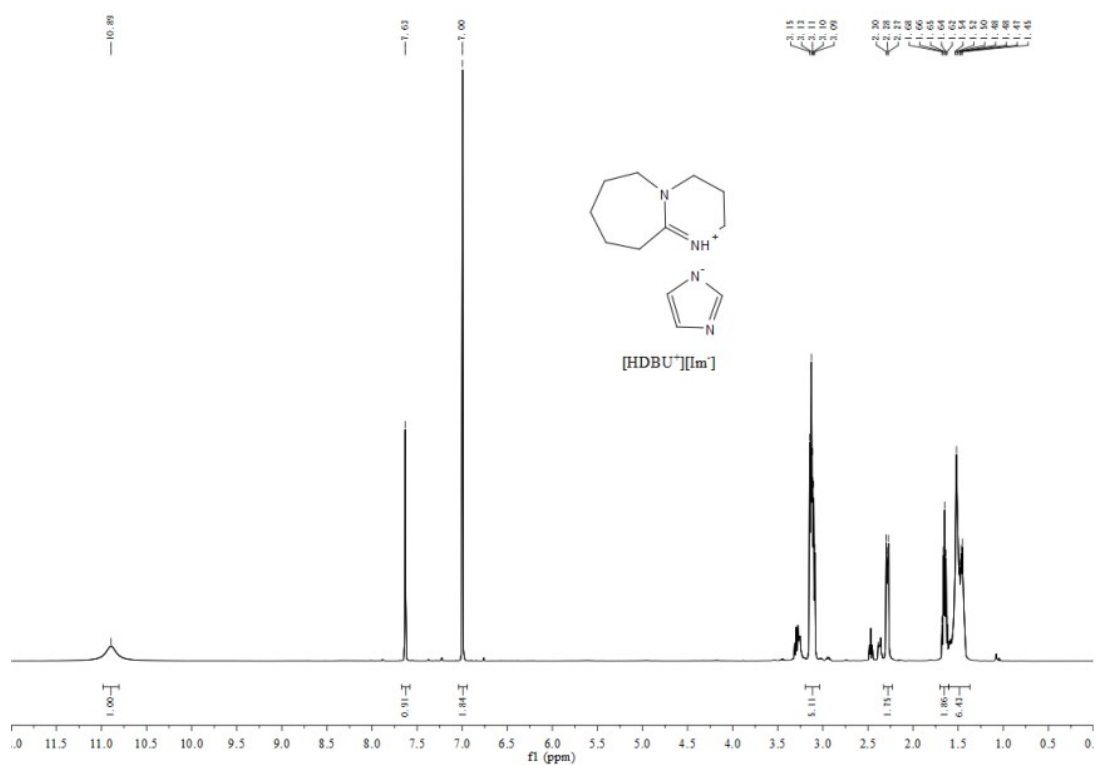
[Ch⁺][Im⁻].¹HNMR (400 MHz, d-DMSO) δ 7.63(s,1H), 7.00 (s, 2H), 3.98 (m, 2H),3.48 (m, 2H), 2.93-3.04 (s, 9H).¹³CNMR (400 MHz, d-DMSO) δ 161.09, 135.73, 68.17, 56.70, 54.54.

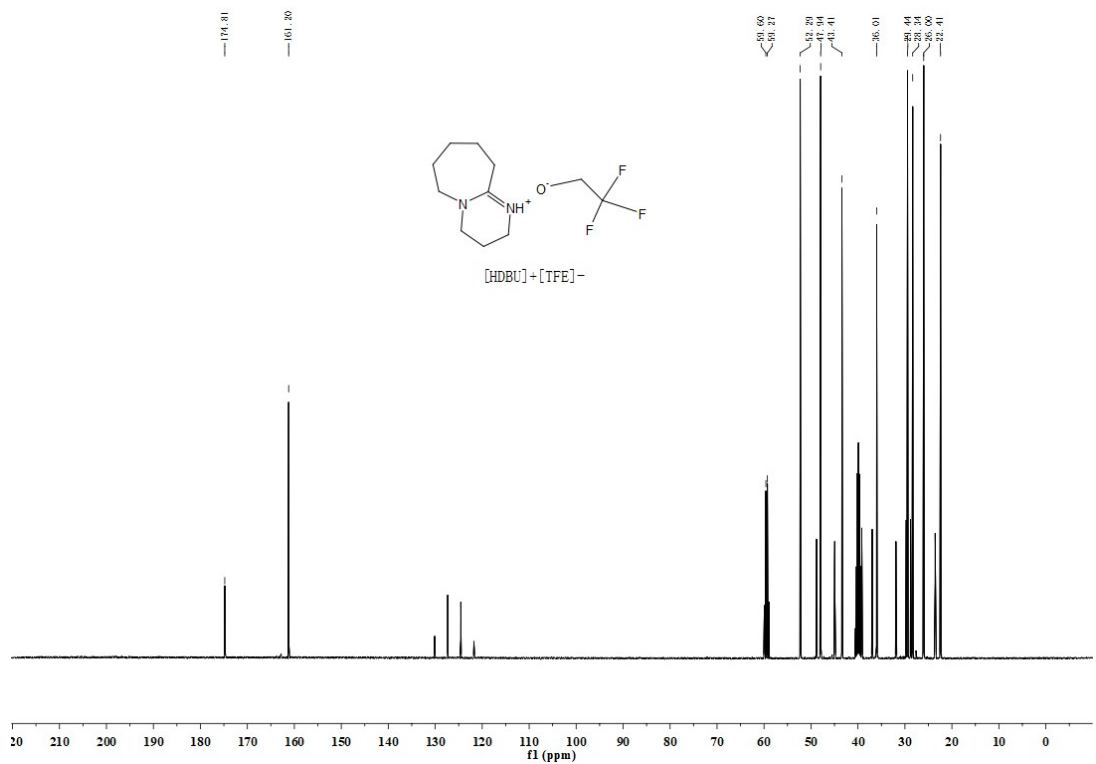
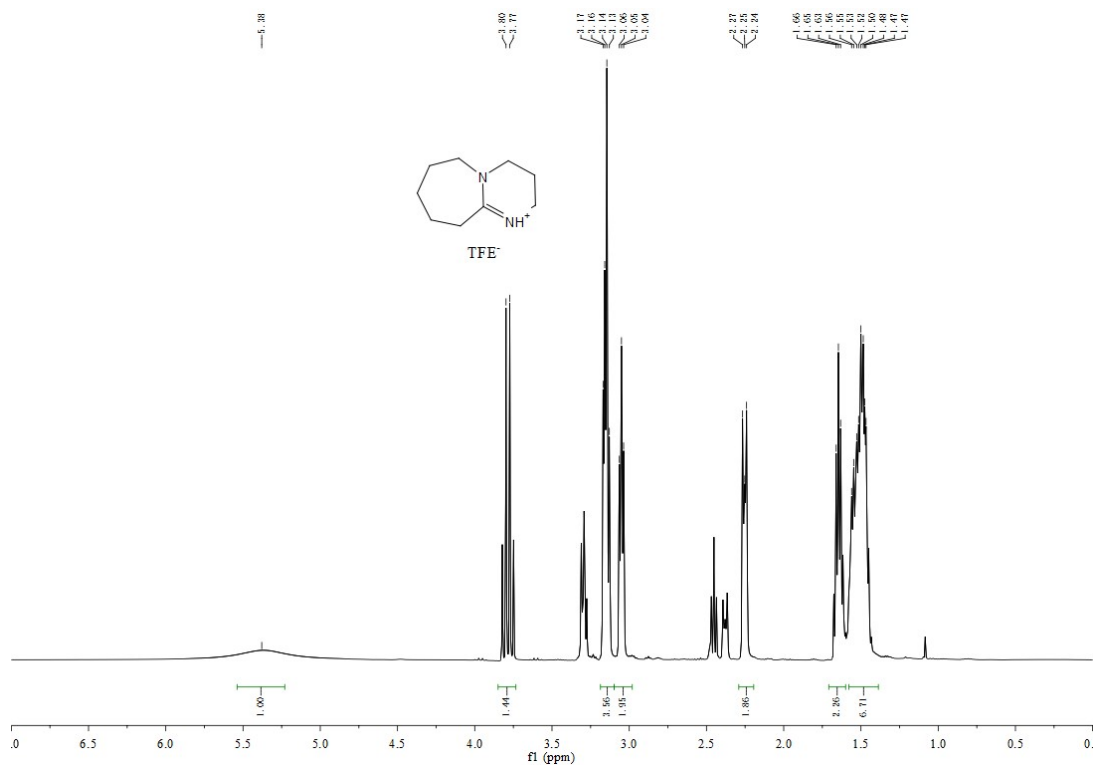
[Ch⁺][2,4-Cl-PhO⁻].¹HNMR (400 MHz, d-DMSO) δ 7.08(s,1H), 6.83 (m, 1H), 6.49 (m, 1H),3.99 (m, 2H),3.48 (m, 2H), 2.93-3.04 (s, 9H). ¹³CNMR (400 MHz, d-DMSO) δ 165.04, 161.55, 128.34, 127.69, 122.70, 119.90, 68.20, 56.73, 54.56.

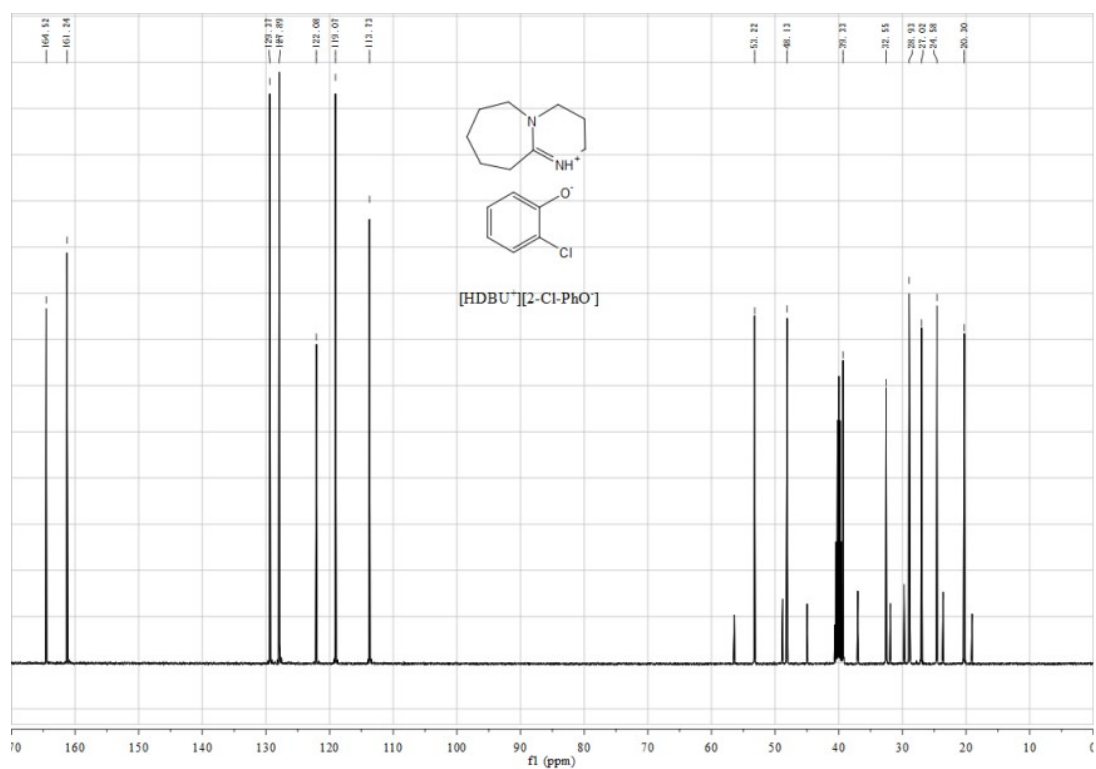
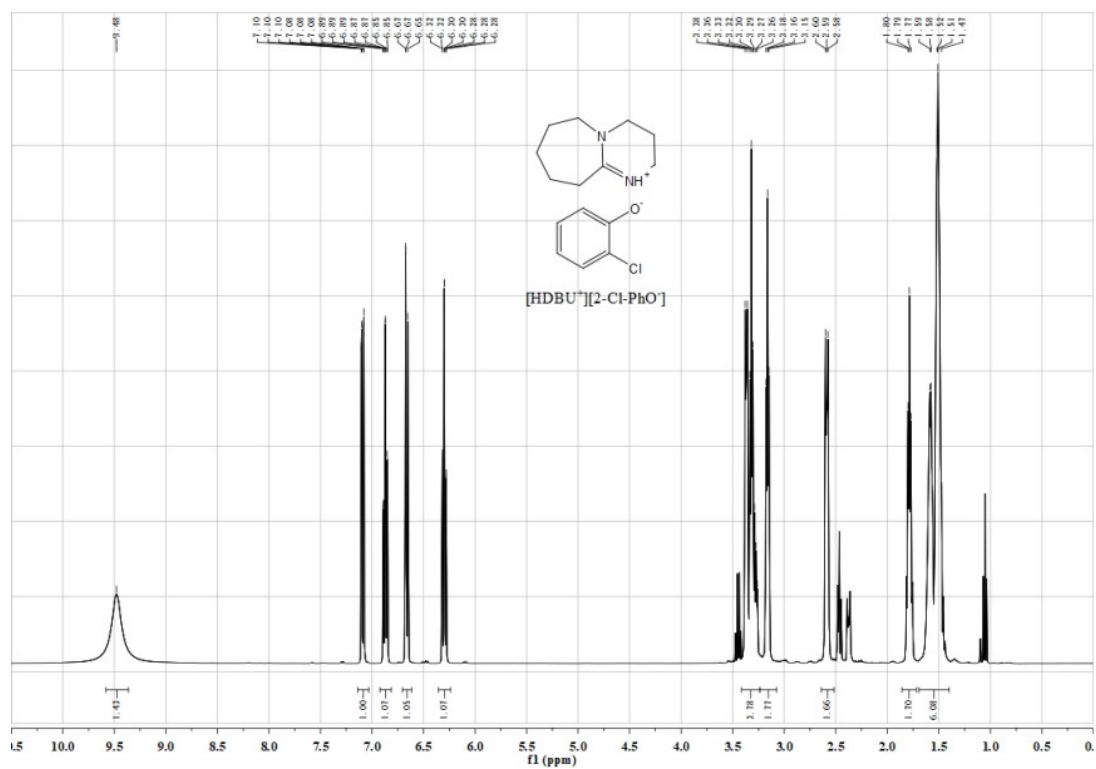
[Ch⁺][2-Cl-PhO⁻].¹HNMR (400 MHz, d-DMSO) δ 7.08(m,1H), 6.84 (m, 1H), 6.67(m,1H), 6.30 (m, 1H),3.99 (m, 2H),3.48 (m, 2H), 2.95-3.04 (s, 9H). ¹³CNMR (400 MHz, d-DMSO) δ 164.54, 161.27, 129.40, 127.92, 122.10, 119.10, 68.32, 56.75, 54.58.

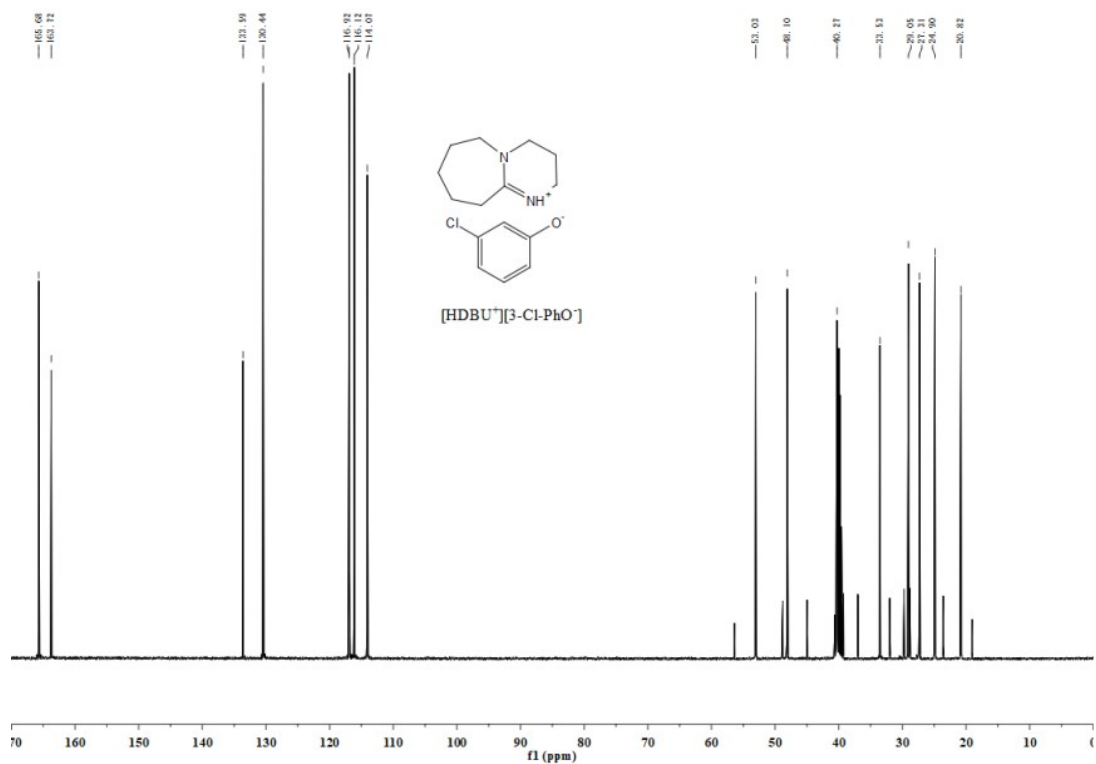
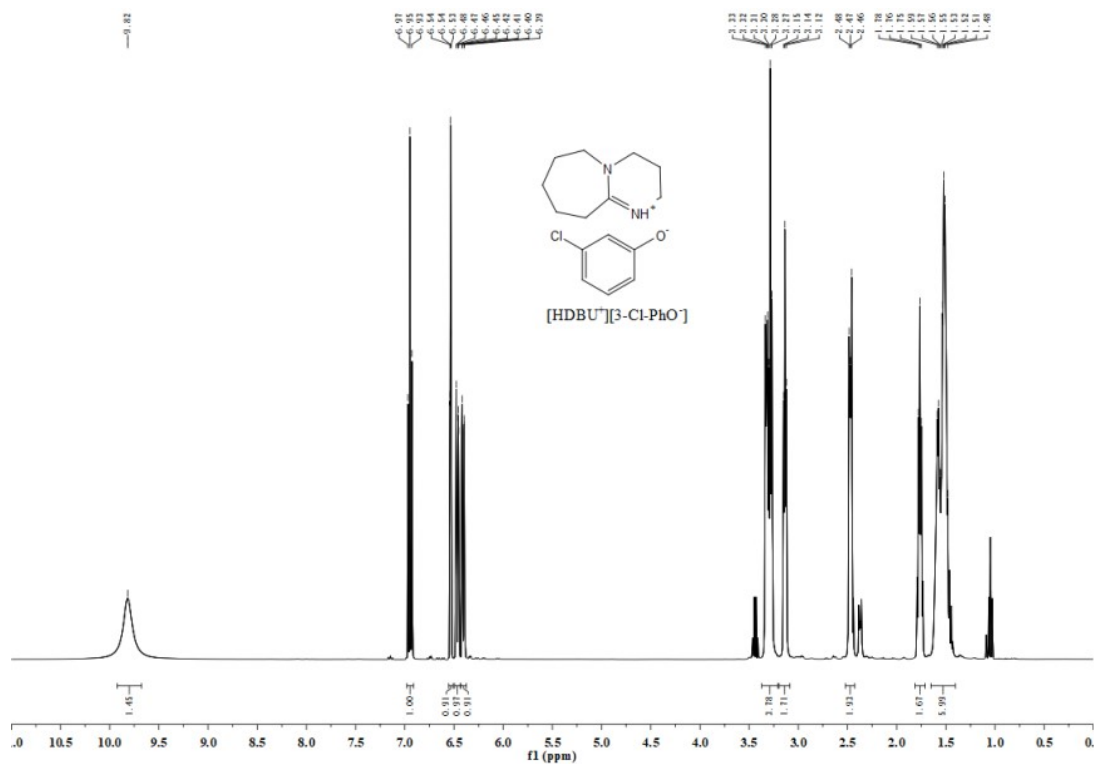
[Ch⁺][3-Cl-PhO⁻].¹HNMR (400 MHz, d-DMSO) δ 6.95(m,1H), 6.54 (m, 1H), 6.45-6.48(m,1H), 6.39-6.42 (m, 1H),3.99 (m, 2H),3.48 (m, 2H), 2.90-3.10 (s, 9H). ¹³CNMR (400 MHz, d-DMSO) δ 165.66, 163.70, 133.58, 130.42, 116.9, 116.1, 114.06, 68.16, 56.69, 54.52.

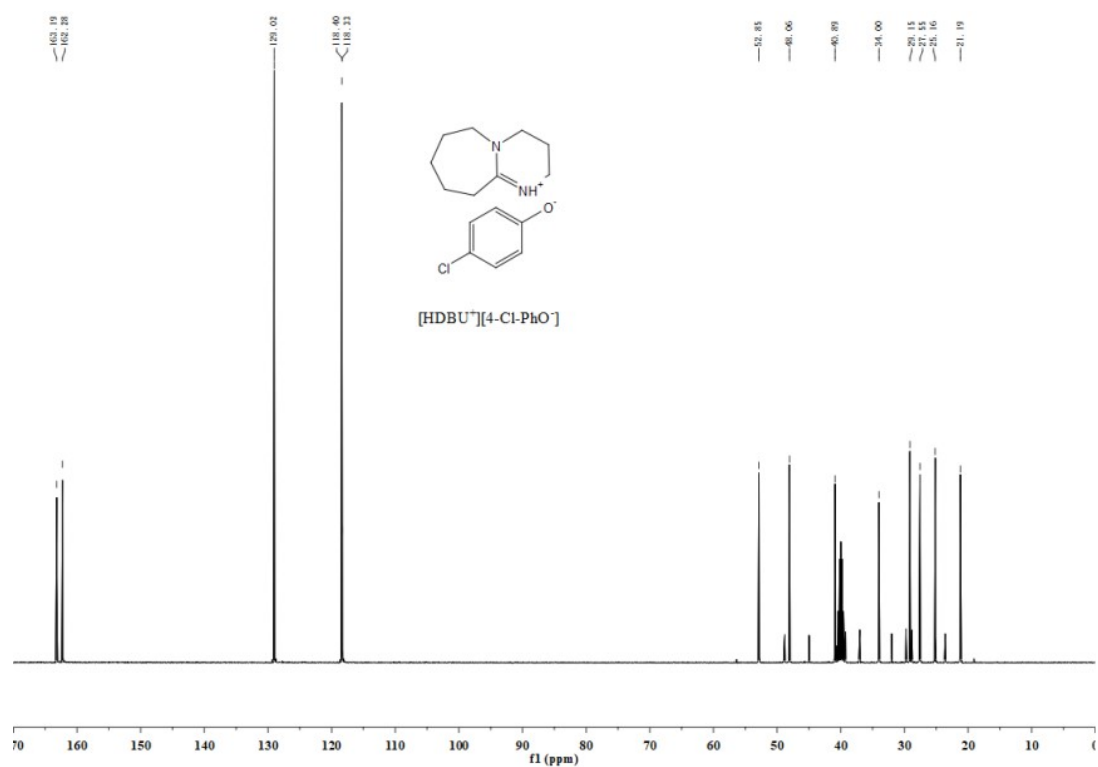
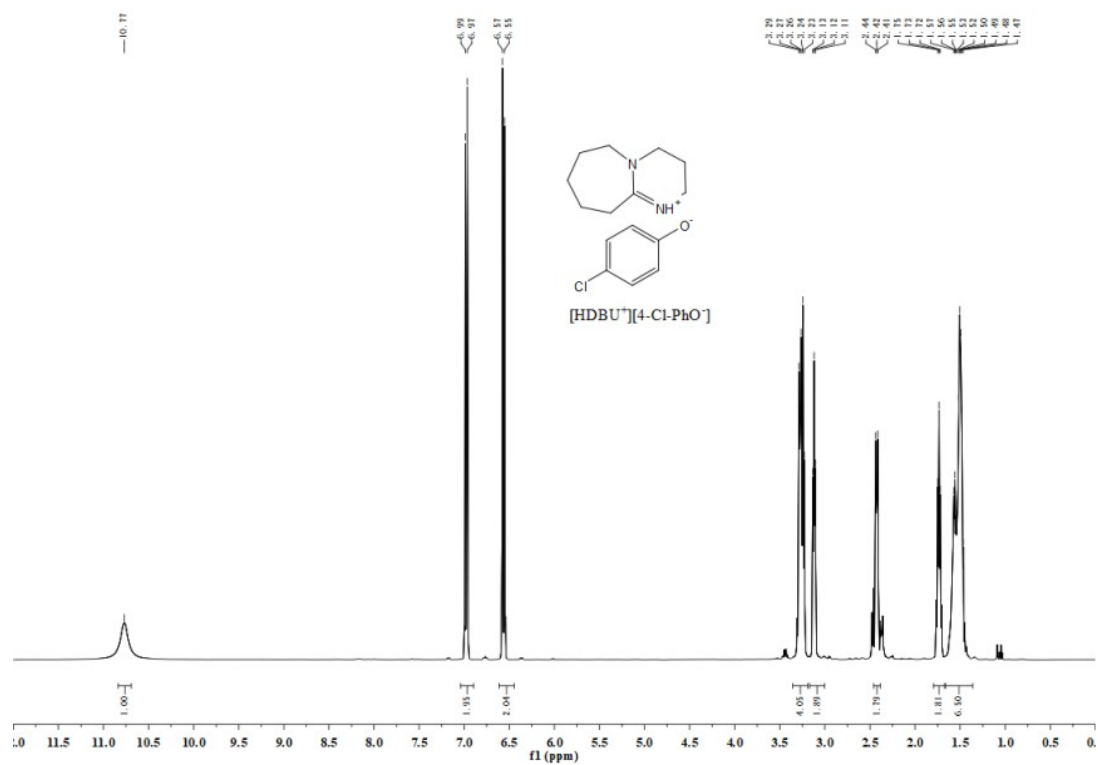
quinazoline-2,4(1H,3H)-diones ¹HNMR (400 MHz, d-DMSO) δ 11.15(s,2H), 7.84 (m, 1H), 7.59 (m, 1H),7.14 (m, 2H) ¹³C NMR (400 MHz, d-DMSO) δ 163.25, 150.74, 141.28, 135.34, 127.36, 122.71, 115.74, 114.75.

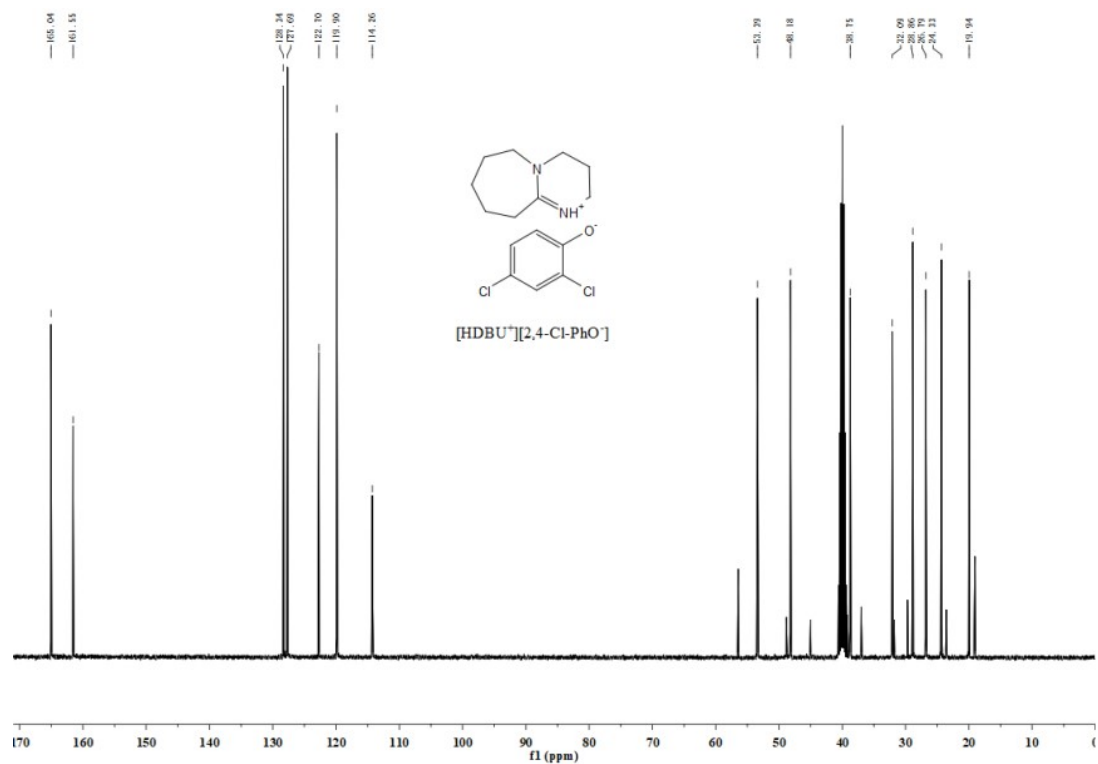
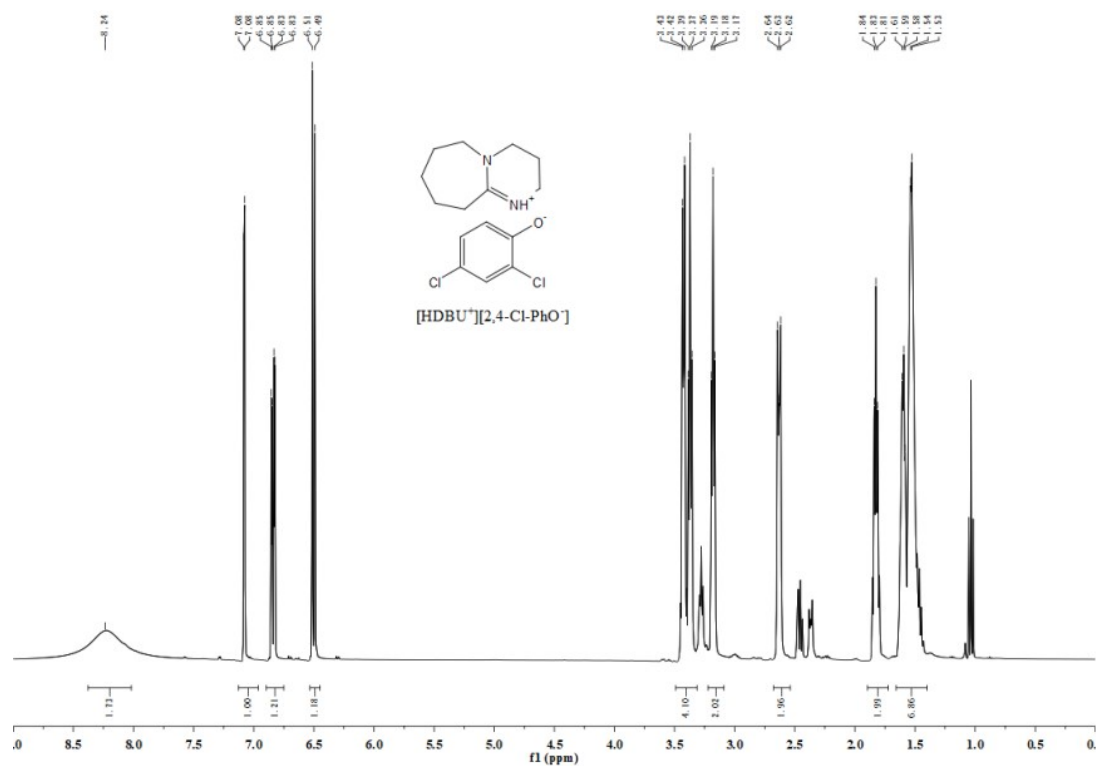


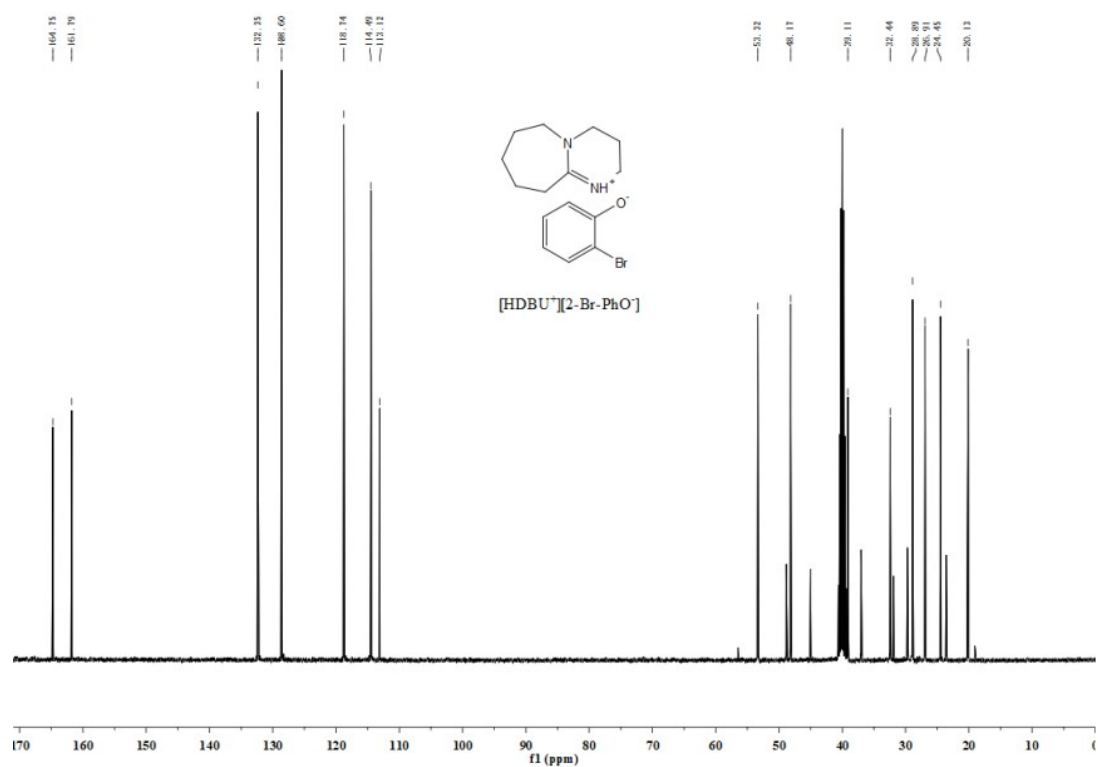
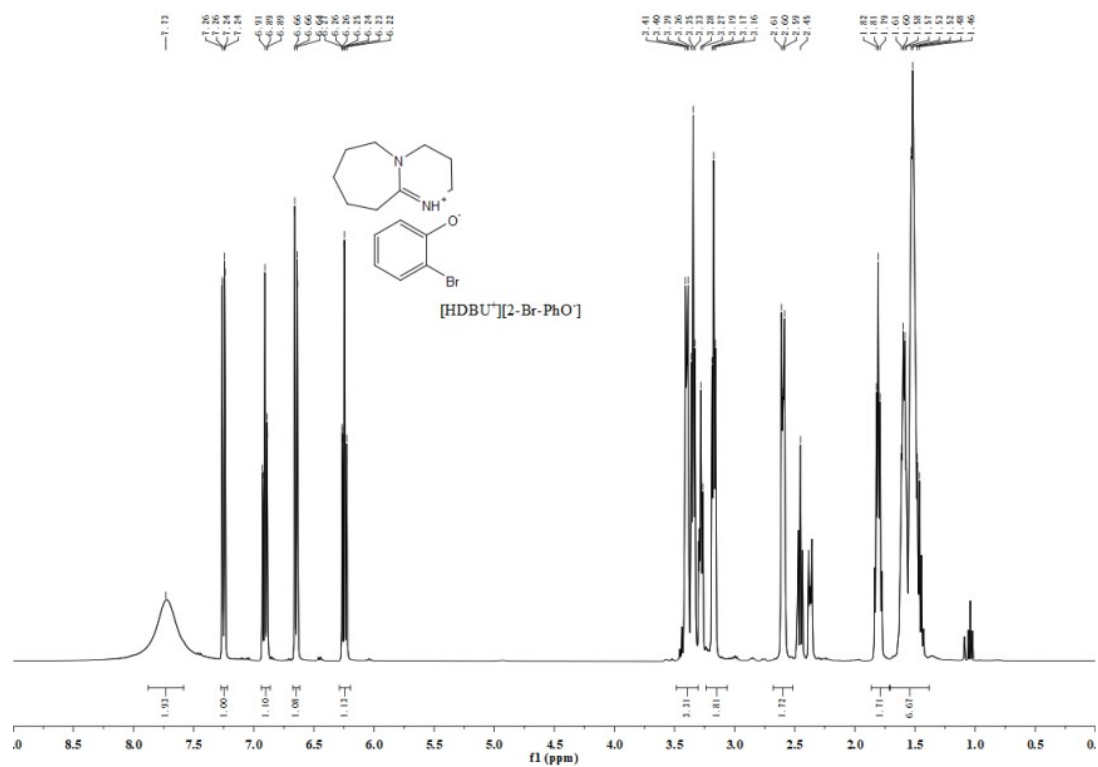


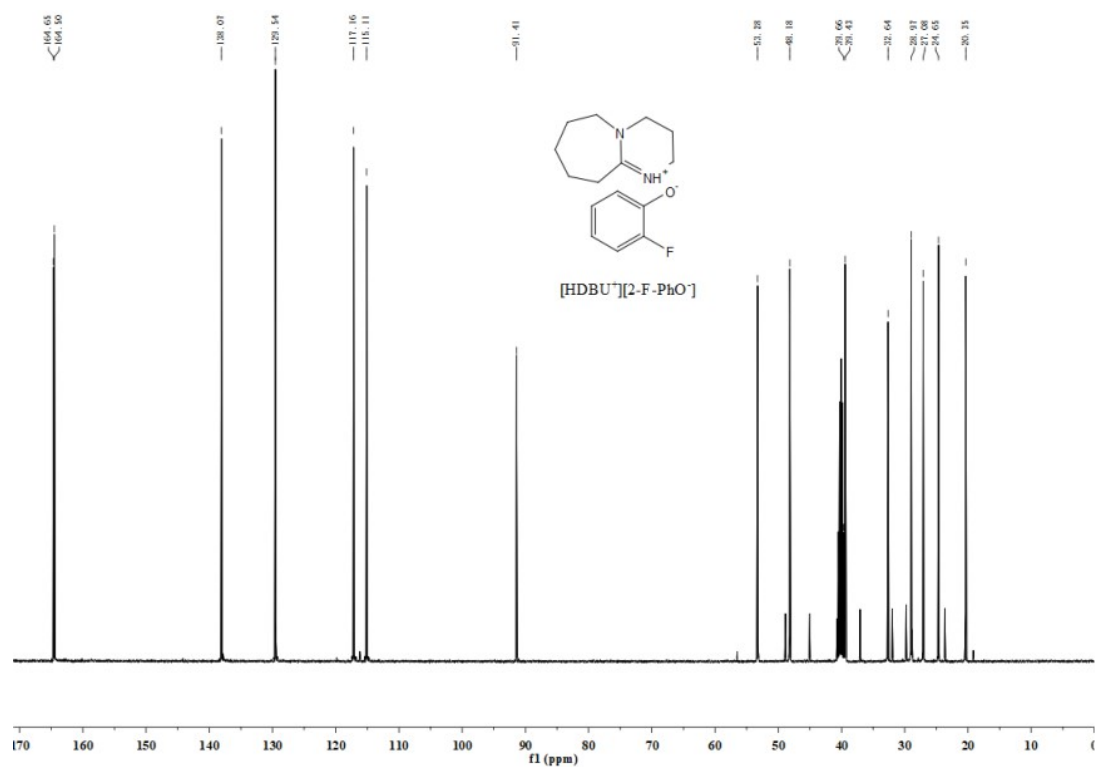
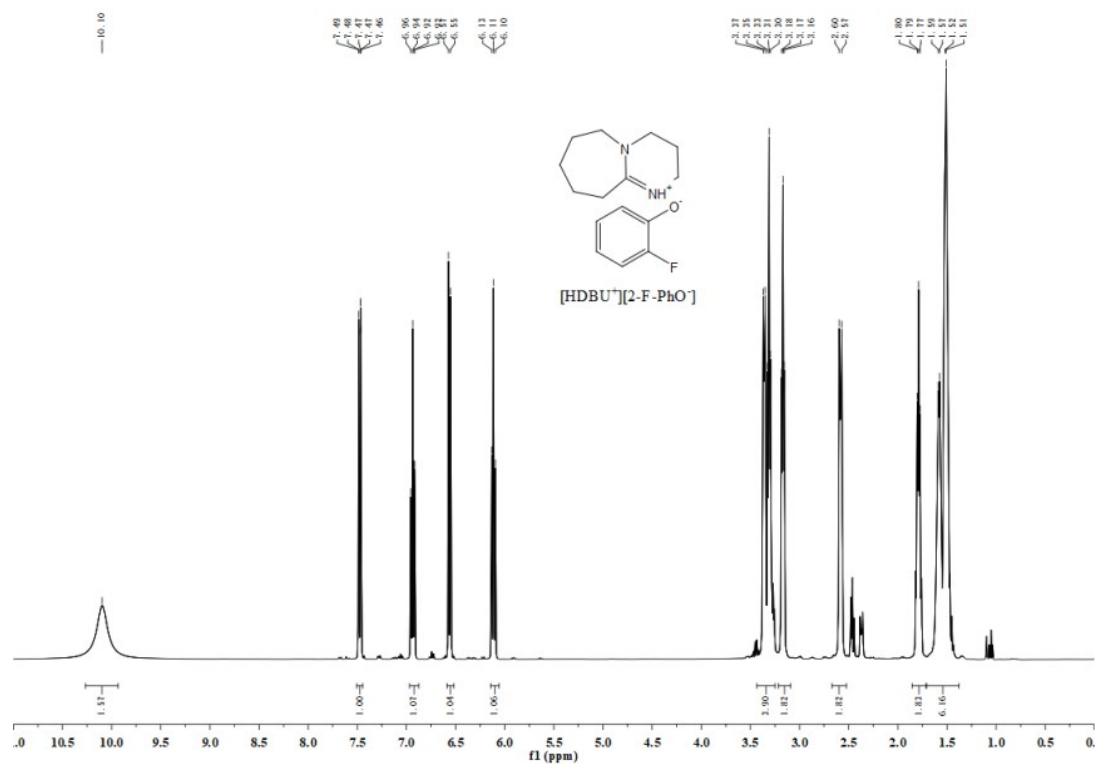


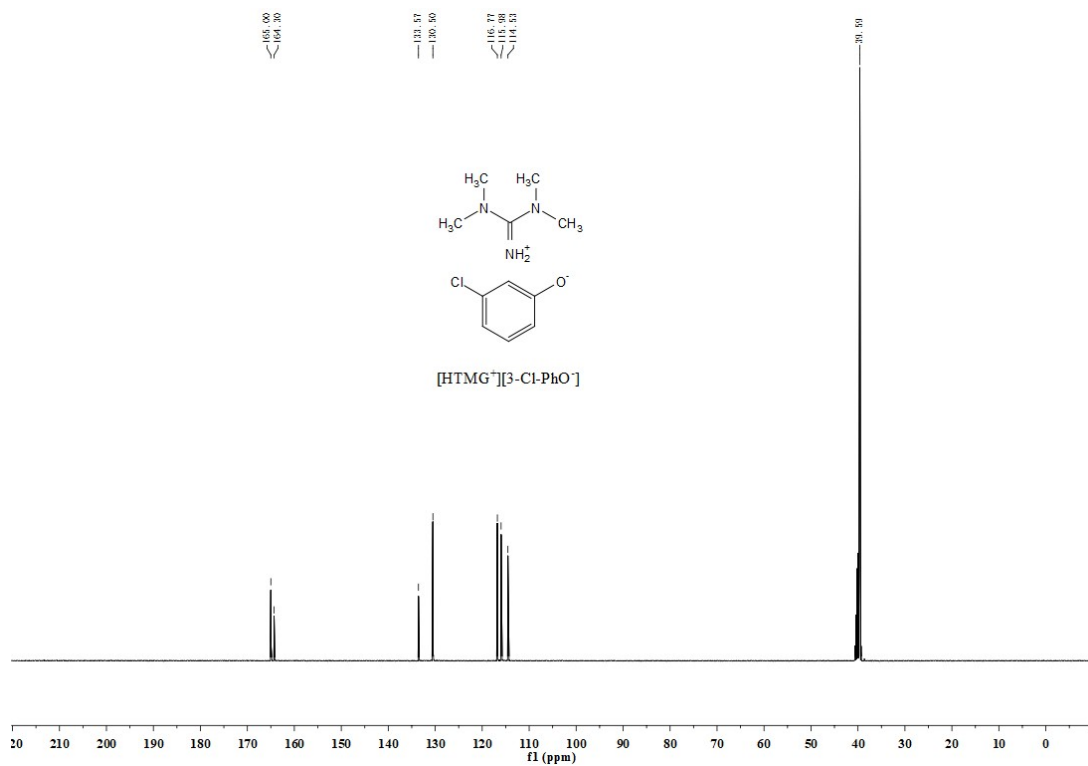
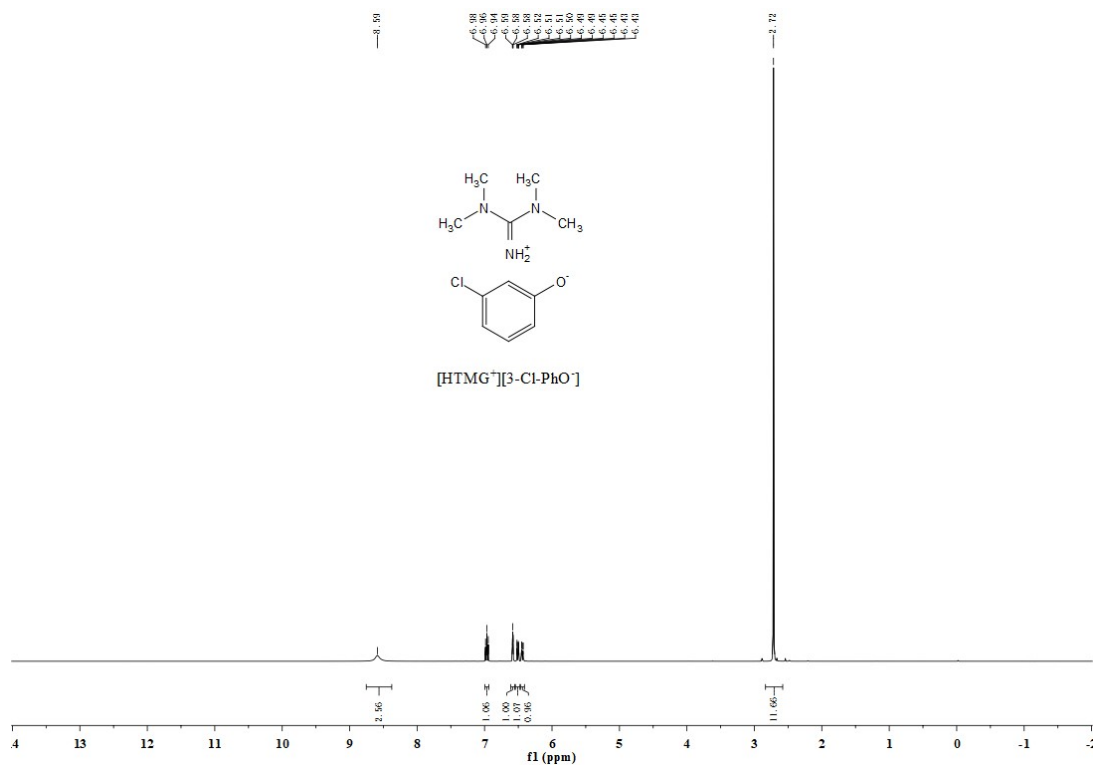


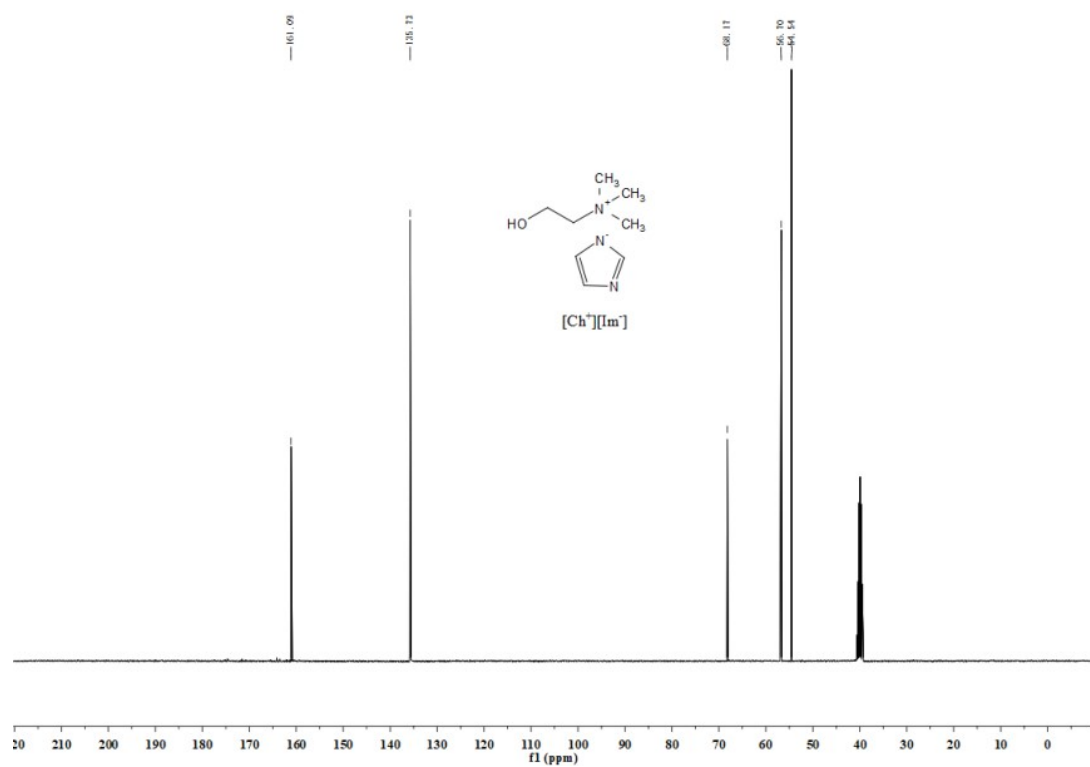
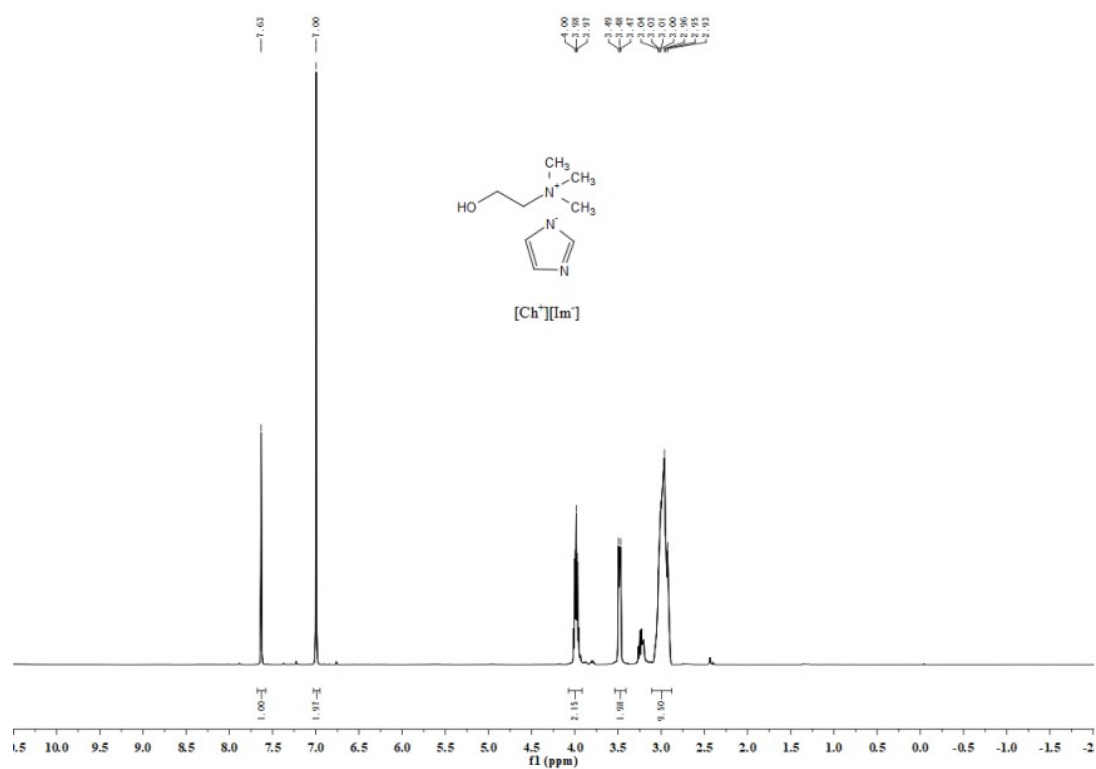


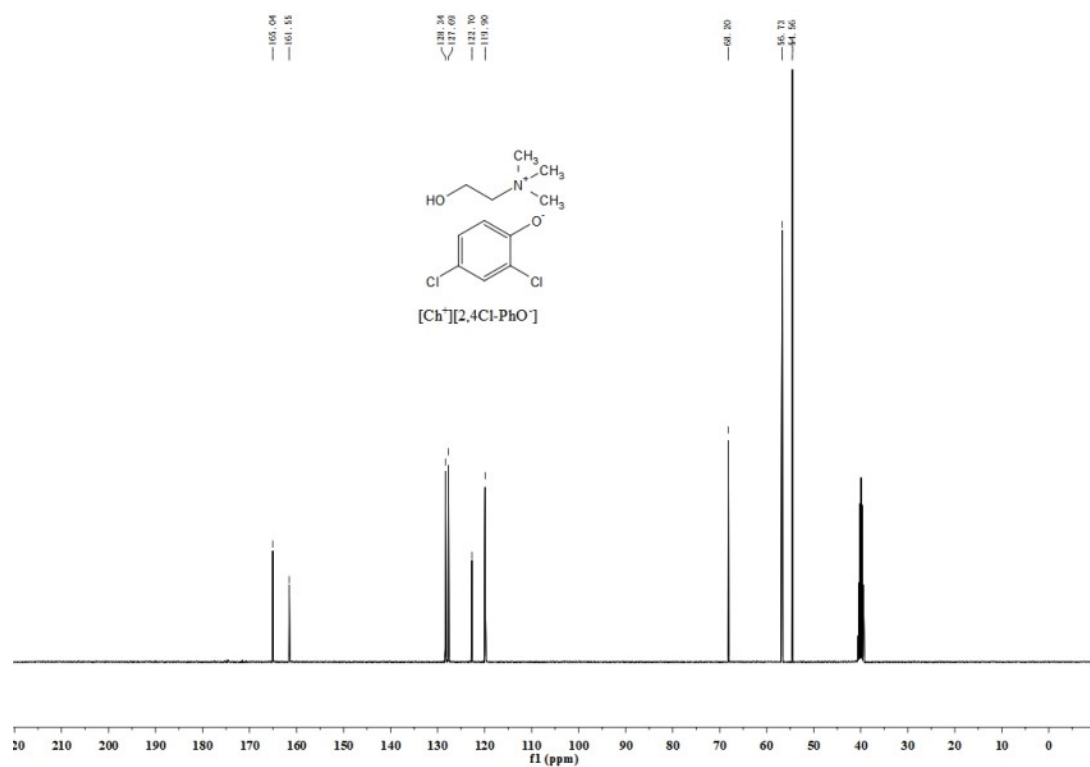
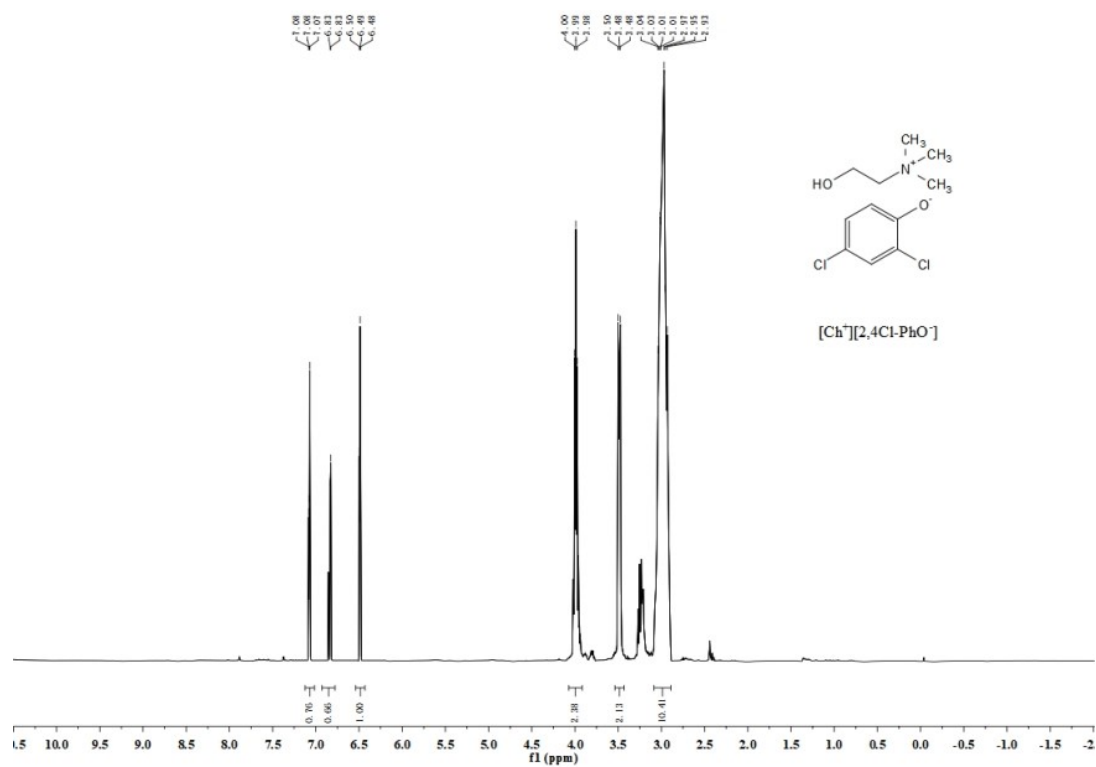


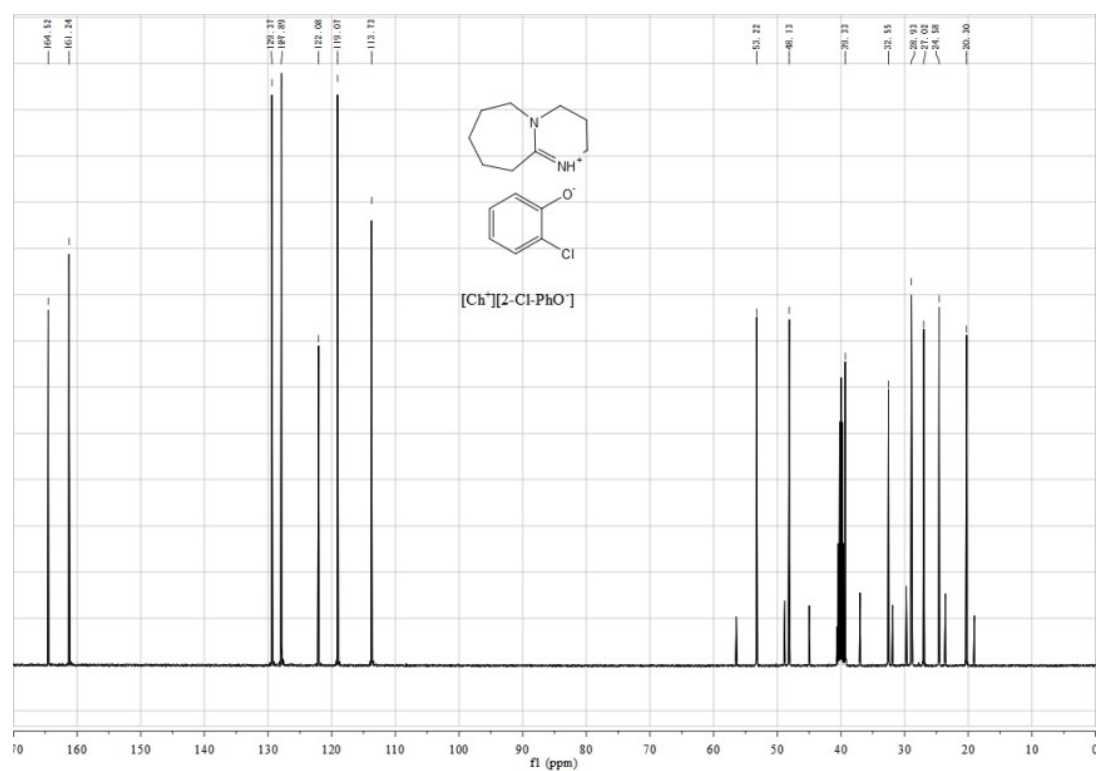
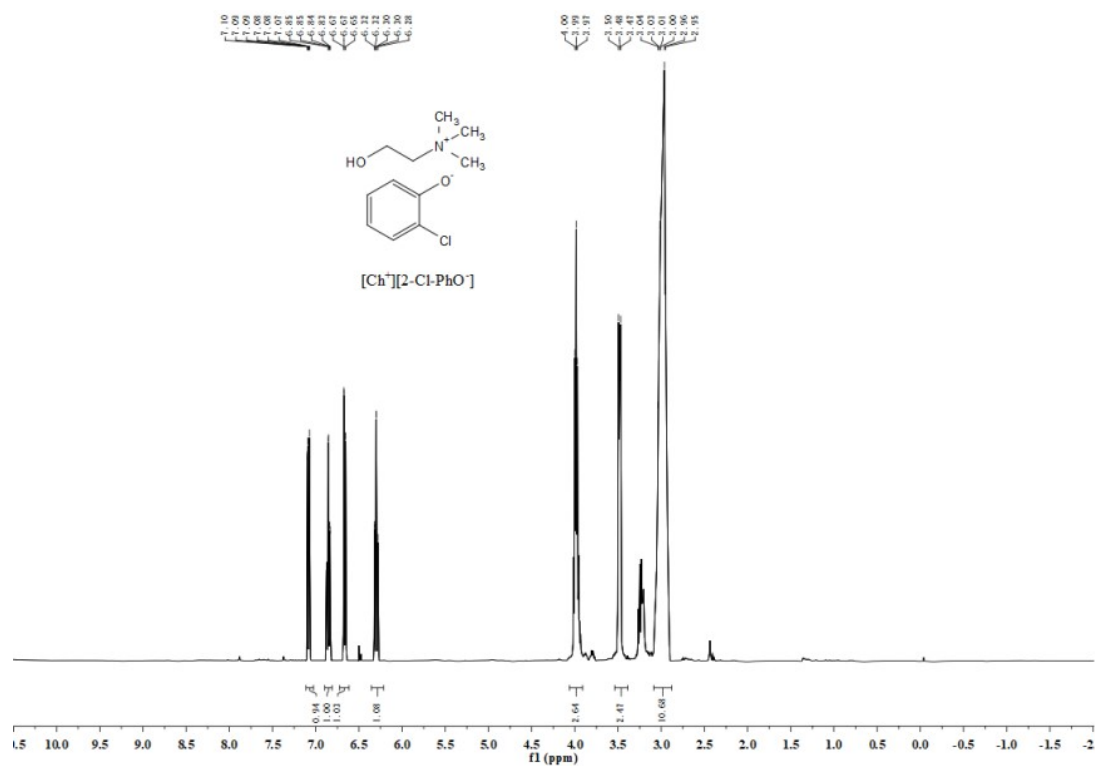


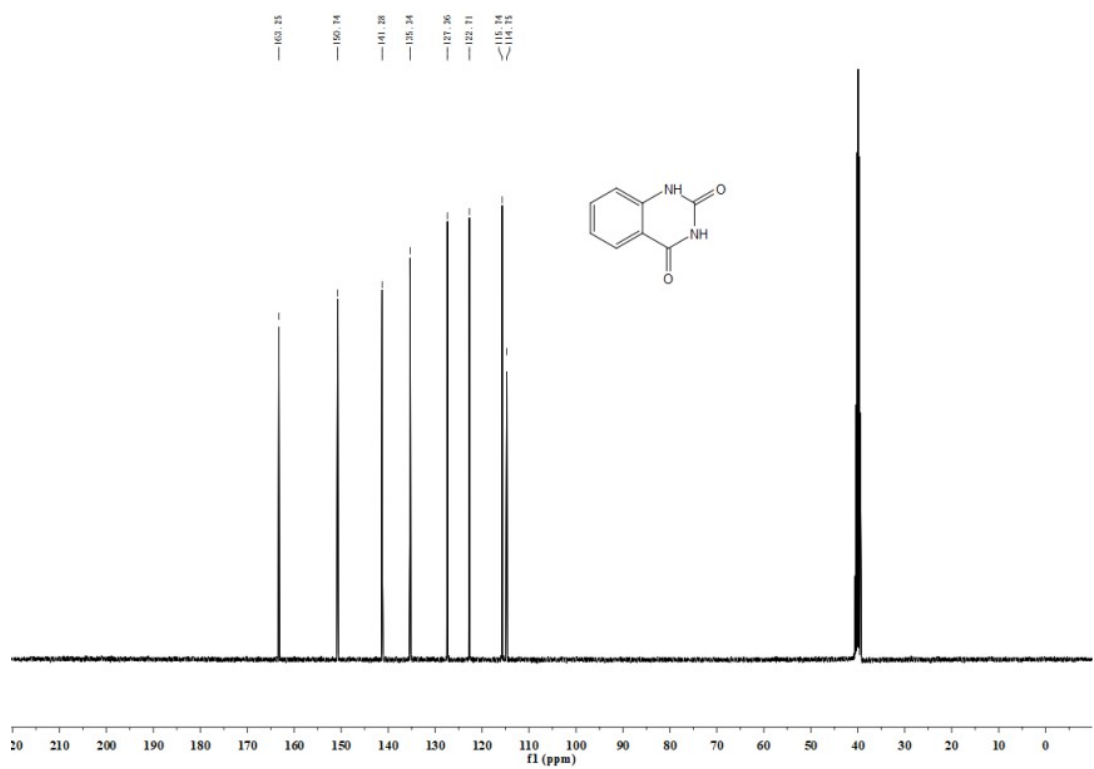
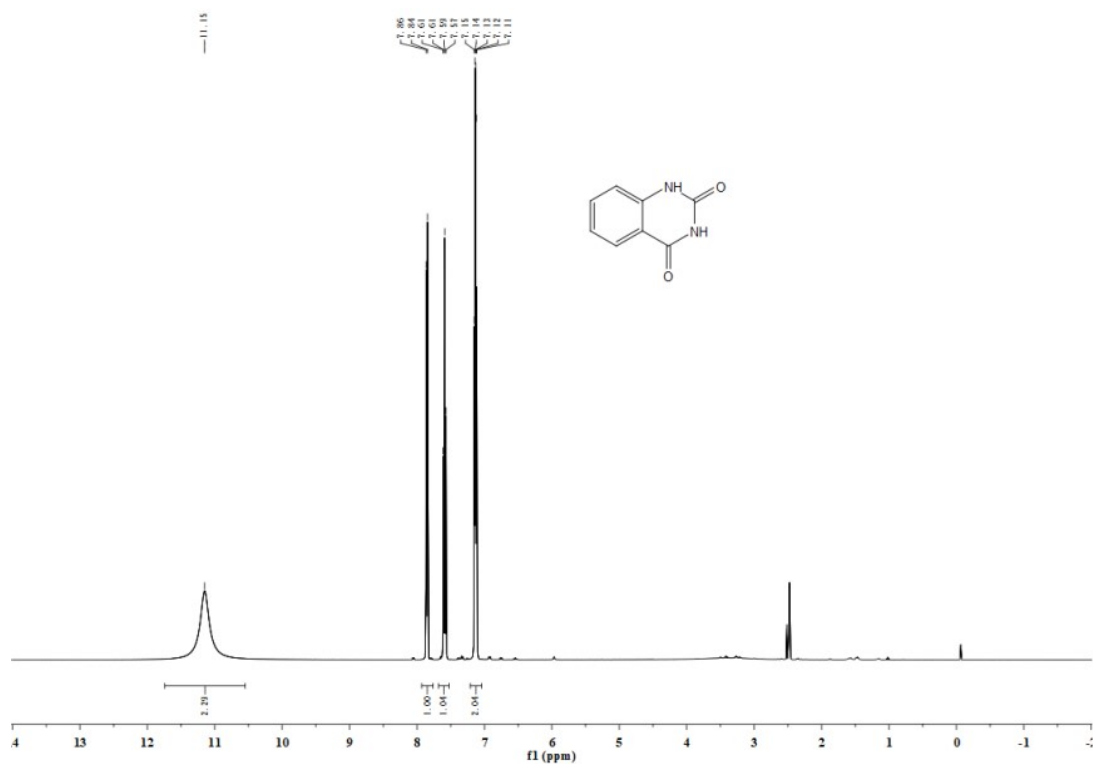












2. Computational section:

To reveal the reaction mechanisms and gain more insight on the reaction, we performed DFT calculations. All calculations were carried out by the Gaussian 16 software package.^[1] All geometries were full optimized with density functional theory methods (DFT) with functionals M06-2X^[2]/6-31g(d).^[3] Vibrational analyses were carried out at the same level to confirm all geometries at their stationary points (either minima for stable intermediate state or saddle point for transition state). With this means, the Gibbs free energy correction was also obtained. More accurate electronic energetics were performed with single point calculation at M06-2X/6-311+G(d,p) level on the full optimized geometries obtained at M06-2X/6-31G(d). Solvent effects on the mechanisms were evaluated with Minisota continuum solvation model (SMD).^[4] Mixed solution parameters of ILs and DMSO were used in the calculation (Equation 1). The required parameters of ILs including the dielectric constant (ϵ), the index of refraction (n), the macroscopic surface tension (γ), the fraction of aromatic carbon atoms (ϕ), electronegative halogen atoms (ψ), and Abraham's hydrogen bond acidity ($\sum\alpha_2\text{ H}$) and basicity ($\sum\beta_2\text{ H}$) were obtained based on the SMD-GIL scheme of Contreras and co-authors.^[5] The required parameters of DMSO was based on the Minnesota Solvent Descriptor Database.^[6] The calculation method of solution parameters can found in the supporting information. The interaction energies calculation was based on the equation:^[7]

$$\Delta E = 627.51 \times [E_{ab}(au) - E_a(au) - E_b(au) + E_{bsse}(au)]$$

where E_{ab} represented the single point energy of ionic liquids cation/anion complexes with CO₂/2-aminobenzonitrile. E_a represented the single point energy of the isolated ionic liquids cations or anions. E_b represented the single point energy of the isolated CO₂ or 2-aminobenzonitrile. E_{bsse} represented the basis set superposition error-corrected energy of the complexes.

2.1 Calculation of the solution parameters

$$\chi = \frac{n_1\chi_1 + n_2\chi_2}{n_1 + n_2} \quad (1)$$

Note: X-mixed solution parameters of ILs and DMSO; n_1 -amount of ILs (mol); x_1 -solution parameters of ILs; n_2 -amount of DMOS (mol); x_2 -solution parameters of DMSO.

Table S5 Mixed solution parameters.

	Eps	Epsinf	HBond Acidity	HBond Basicity	Surface Tension At Interface	Carbon Aromaticity	Electronegative Halogenicity
1	37.57	2.018	0.0600	0.7188	61.64	0.04914	0
2	37.57	2.018	0.0600	0.7188	61.64	0	0.05616
3	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
4	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
5	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
6	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
7	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
8	37.57	2.018	0.0600	0.7188	61.64	0.1048	0.01379
9	37.57	2.018	0.0600	0.7188	61.64	0.1429	0.01638

Note: Entry 1-8 corresponding to the following mixed solution respectively, 1-[HDBU⁺][Im⁻]/DMSO; 2-[HDBU⁺][TFE⁻]/DMSO; 3-[HDBU⁺][2-Br-PhO⁻]/DMSO; 4-[HDBU⁺][2-F-PhO⁻]/DMSO; 5-[HDBU⁺][2,4-Cl-PhO⁻]/DMSO; 6-[HDBU⁺][4-Cl-PhO⁻]/DMSO; 7-[HDBU⁺][2-Cl-PhO⁻]/DMSO; 8-[HDBU⁺][3-Cl-PhO⁻]/DMSO; 9-[HTMG⁺][3-Cl-PhO⁻]/DMSO

2.2 Calculation of pKa data for all the cations and the conjugated acid of the anions

The pKa data were calculated according to Josefredo R. Pliego's work^[8]. All calculations are carried out by the Gaussian 16 software package.^[1] All geometries are fully optimized with density functional theory methods (DFT) with functionals M06-2X^[2]/6-31g(d).^[3] Vibrational analyses are carried out at the same level to confirm all geometries are at their stationary points (either minima for stable intermediate state or saddle point for transition state). With this means, the Gibbs free energy correction are also obtained. More accurate electronic energetics are performed with single point calculation at M06-2X/6-311+G(d,p) level on the full optimized geometries obtained at M06-2X/6-31G(d). IEFPCM (PCM using the Integral Equation Formalism model) where used for evaluation of the Solvent effects.

The pKa value can be calculated by the following equations:

$$pK_a(HA) = pK_a(H_2O) + \frac{\Delta G_{sol}^*}{2.303RT} \quad (2)$$

$$\Delta G_{sol}^* = \Delta G_g^* + \Delta \Delta G_{sol}^* \quad (3)$$

$$\Delta G_g^* = \mu_g^*(A^-) + \mu_g^*(H_2O) - \mu_g^*(HA) - \mu_g^*(OH^-) \quad (4)$$

$$\Delta \Delta G_{sol}^* = \Delta G_{sol}^*(A^-) + G_{sol}^*(H_2O) - G_{sol}^*(HA) - G_{sol}^*(OH^-) \quad (5)$$

Where HA represents cations or the conjugated acids of the anions. A⁻ represents the anions or the conjugated bases of the cations.

Table S6 The calculated pK_a values of the cations and the conjugated acids of the anions.

Entry	Cations and anions	pK _a
1	[Ch ⁺]	24.0
2	[HDBU ⁺]	11.9
3	[HTMG ⁺]	10.5
4	[Im ⁻]	16.8
5	[TFE ⁻]	22.2
6	[2F-PHO ⁻]	13.6
7	[2Br-PHO ⁻]	12.4
8	[2Cl-PHO ⁻]	12.6
9	[3Cl-PHO ⁻]	13.5
10	[4Cl-PHO ⁻]	14.3
11	[2, 4Cl-PHO ⁻]	10.7
12	^e [Cl ⁻]	1.8
13	^e [HSO ₄ ⁻]	1.99
14	^e [OH ⁻]	32

^e-the pK_a value comes from Evan's pK_a table.

2.3 conformation of $[\text{HDBU}^+][\text{Cl}^-]\text{-COO}$ and $[\text{HDBU}^+][\text{HSO}_4^-]$ complexes.

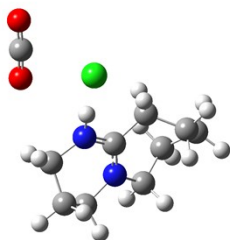


Figure S1 conformation of $[\text{HDBU}^+][\text{Cl}^-]\text{-COO}$ complexes.

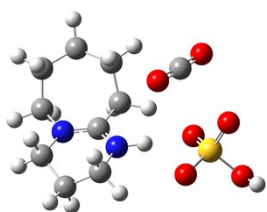


Figure S2 conformation of $[\text{HDBU}^+][\text{Cl}^-]\text{-COO}$ complexes.

2.4 Relationship between the pK_a value of the anions and the catalytic yields of $[\text{Ch}^+]$ ILs.

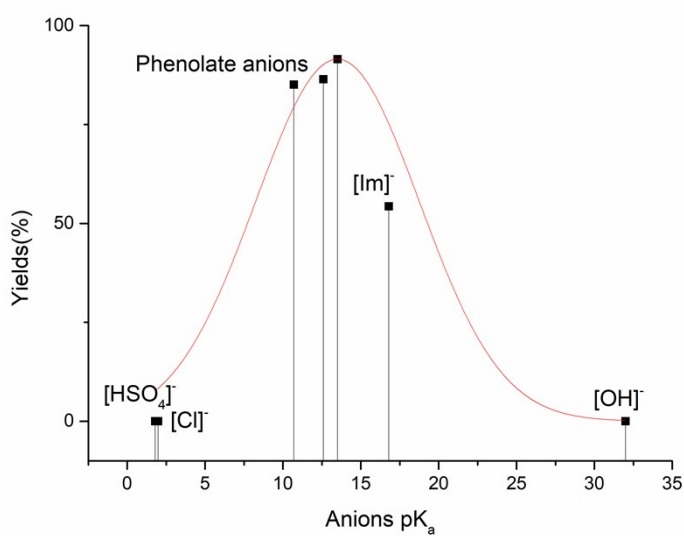


Figure S3 Relationship between the pK_a value of the anions and the catalytic yields of $[\text{Ch}^+]$ ILs.

2.5. Calculated interaction energies for the other [HDBU⁺] ionic liquids complexes

Table S7 Calculated interaction energies for the other [HDBU⁺] ionic liquids complexes.

Entry	Substrates	CO ₂	2-aminobenzonitrile
	Interaction energies (kcal/mol)	kcal/mol	kcal/mol
Anions/cations			
1	[Im ⁻]	-16.7	-4.6
2	[TFE ⁻]	-28.0	-17.1
3	[2-Br-PhO ⁻]	-7.2	-4.9
4	[2-F-PhO ⁻]	-8.5	-5.3
5	[2,4-Cl-PhO ⁻]	-5.2	-4.6
6	[4-Cl-PhO ⁻]	-11.0	-5.9
7	[2-Cl-PhO ⁻]	-8.1	-5.4
8	[3-Cl-PhO ⁻]	-9.5	-5.6
9	[HDBU ⁺]	0.3	-5.1

2.6. Following are the cartesian coordinates of the optimized intermediates, transition states and products

For [HDBU⁺][3-Cl-PhO⁺]

In1

0 1

C	-5.94096900	-1.15606900	-1.51583700
C	-5.02475800	-0.12561800	-1.41817700
C	-4.33932500	0.10860200	-0.21818800
C	-4.55453800	-0.69901000	0.92421600
C	-5.49966400	-1.73827200	0.79801700
C	-6.17051200	-1.95713300	-0.39001000
N	-3.92954400	-0.44062300	2.10589200
C	-3.42566800	1.20259200	-0.13569200
N	-2.72100500	2.12000300	-0.05984100
H	-6.47103100	-1.33769700	-2.44356900
H	-4.82213500	0.52077600	-2.26650600
H	-5.68940300	-2.37343000	1.65876200
H	-6.88722500	-2.77137700	-0.44691100
H	-3.00984400	0.01866800	2.08592400
H	-3.98414700	-1.17781300	2.79521200
N	2.14642100	2.22117600	-0.49623400
N	0.13457700	2.51030200	0.60852000
C	0.72815500	2.64136700	1.93877600
C	2.16149400	3.12087500	1.78585300
C	2.88247700	2.24156600	0.77401200
C	0.81673200	2.30684600	-0.49682500
C	2.89461900	1.88557100	-1.71765800
C	2.64585500	0.46516300	-2.22743200
C	0.05356500	2.15493100	-1.78197100
C	1.34668800	0.30452800	-3.01965300
C	0.06485800	0.70013000	-2.28466600
H	0.12093900	3.35864000	2.49524600
H	0.65847400	1.67276200	2.43817100
H	2.18418300	4.16142900	1.44418900
H	2.67712500	3.06994300	2.74769200
H	2.97690400	1.21407700	1.14224300
H	3.88316100	2.62881500	0.56802800
H	2.66857400	2.62623800	-2.49404200
H	3.94827800	2.00919800	-1.45970400
H	2.66985700	-0.22195400	-1.37512600
H	3.48645400	0.19297400	-2.87600100
H	0.48127900	2.83086700	-2.53231500

H	-0.97172000	2.47482200	-1.59299200
H	1.42374200	0.90560500	-3.93770800
H	1.26154700	-0.74090400	-3.33582800
H	-0.78136200	0.58505100	-2.96989700
H	-0.14130800	0.03627700	-1.43788800
H	-0.88680500	2.43636900	0.54536200
C	1.93553200	-2.95541800	-1.08491400
C	3.27936300	-2.97589000	-0.72282200
C	3.66397400	-2.19853900	0.36346300
C	2.75754900	-1.40831900	1.05215300
C	1.41526700	-1.35481600	0.64194600
C	0.99637500	-2.16596600	-0.42448900
O	0.66778100	-0.47245100	1.35002900
C	-0.77950900	-0.32956200	1.24924800
O	-1.35081000	-0.89662800	0.32140600
O	-1.19063800	0.41176500	2.15235300
H	1.60320400	-3.57496900	-1.91298800
H	4.00468500	-3.58625500	-1.24783800
H	3.06502100	-0.83953900	1.92279500
Cl	5.33560700	-2.21005200	0.88040200
H	-0.04290700	-2.17053400	-0.71590000

TS1-2

0 1

C	-6.16746700	0.48179400	-1.45057000
C	-4.90935000	0.86305500	-1.01146500
C	-4.26807600	0.19046200	0.03487000
C	-4.90702200	-0.89029900	0.67972800
C	-6.18444400	-1.25896600	0.22468000
C	-6.80105900	-0.58893600	-0.81901700
N	-4.35612900	-1.52842900	1.77629200
C	-2.96660400	0.72847900	0.43300700
N	-2.40620500	1.78185500	0.56373400
H	-6.64700500	1.00785700	-2.26843200
H	-4.38517200	1.69384500	-1.47269800
H	-6.69090500	-2.08576200	0.71619300
H	-7.78725900	-0.90726800	-1.14416100
H	-3.34315600	-1.54448100	1.79819800
H	-4.77310700	-2.42463500	1.98860000
N	2.34824000	1.91885400	0.78378500
N	0.07175500	1.52190800	1.12659800
C	0.30471000	0.87873400	2.40999500
C	1.56177400	1.43601800	3.06243800

C	2.72151500	1.34824100	2.07971200
C	1.05188200	1.97372700	0.40232800
C	3.44161200	2.32165400	-0.10288300
C	3.57196600	1.47604700	-1.37171800
C	0.69793200	2.60238300	-0.92489600
C	2.63584200	1.92122600	-2.49282500
C	1.15405300	1.79314800	-2.15201900
H	-0.58146700	1.05189300	3.02802700
H	0.38204100	-0.20507000	2.25963800
H	1.39647300	2.48389700	3.33491400
H	1.80995000	0.88611500	3.97426600
H	3.04803500	0.30859200	1.94288000
H	3.57850500	1.91408400	2.45773900
H	3.33723600	3.38361100	-0.36311300
H	4.35349400	2.23180400	0.49177600
H	3.38434600	0.42688400	-1.11194800
H	4.60909700	1.54145600	-1.72064900
H	1.11216400	3.61878000	-0.96292600
H	-0.39096300	2.68888200	-0.94126800
H	2.86531200	2.96599100	-2.74894900
H	2.84424300	1.32720600	-3.38993600
H	0.56125800	2.13691300	-3.00610500
H	0.88488500	0.74471300	-1.99541000
H	-1.16450700	1.70318800	0.80790700
C	2.49417000	-2.16854100	-2.27078300
C	3.63649000	-2.23172800	-1.47562000
C	3.48893800	-2.08478400	-0.10149300
C	2.24416600	-1.88081300	0.47806700
C	1.11587300	-1.80958500	-0.33907400
C	1.23114100	-1.96219000	-1.72217900
O	-0.06891700	-1.65981300	0.33366400
C	-1.06200600	-0.82074900	-0.16441500
O	-0.99969500	-0.32761800	-1.26805700
O	-1.96622900	-0.67850800	0.74098500
H	2.58951500	-2.28792600	-3.34546800
H	4.61879100	-2.38875800	-1.90628600
H	2.12973700	-1.79900900	1.55344500
Cl	4.89972600	-2.12095800	0.92832000
H	0.35009600	-1.90672300	-2.34614700

In2

0 1

C	-6.60871200	0.44060700	-0.83108200
C	-5.29547200	0.79292300	-0.57594800
C	-4.42758100	-0.04761200	0.13576800
C	-4.90710500	-1.28057700	0.63418600
C	-6.24501700	-1.62419400	0.36225700
C	-7.07781000	-0.78588500	-0.35569000
N	-4.16604600	-2.12494900	1.44235000
C	-3.05169000	0.45800200	0.32465600
N	-2.71418900	1.66423800	0.29701400
H	-7.25669200	1.10322000	-1.39383600
H	-4.89081100	1.73523900	-0.92995400
H	-6.62247400	-2.56881900	0.74582600
H	-8.10282000	-1.09076600	-0.54548500
H	-3.16103600	-2.05734600	1.38807500
H	-4.51433800	-3.07061700	1.50772200
N	2.49625500	2.06906100	0.85191400
N	0.25949500	1.29774800	0.93393500
C	0.39393100	0.91678400	2.33138600
C	1.53050400	1.63874300	3.04704600
C	2.78701700	1.56618600	2.18886500
C	1.25440300	1.83984900	0.31560300
C	3.59176500	2.64489400	0.07887000
C	4.13132500	1.75390600	-1.04498100
C	1.03487000	2.23128500	-1.12832000
C	3.28574800	1.80242300	-2.31644900
C	1.83391000	1.37003100	-2.12104600
H	-0.56264500	1.12315500	2.82536400
H	0.53075800	-0.17249600	2.39331000
H	1.26376700	2.69158000	3.18981000
H	1.71812800	1.20255000	4.03276200
H	3.16635600	0.53346600	2.14037000
H	3.58189800	2.18146200	2.62127000
H	3.28614500	3.61564900	-0.33356000
H	4.39138300	2.85203100	0.79499800
H	4.20021700	0.72494100	-0.67111900
H	5.15221600	2.07698900	-1.28177200
H	1.27150900	3.29378400	-1.27398300
H	-0.03207200	2.09995900	-1.31421400
H	3.30405000	2.82872200	-2.71137200
H	3.74935400	1.16650200	-3.07978500
H	1.31919500	1.39994000	-3.08725900
H	1.79882300	0.32711100	-1.78862600
H	-1.69380600	1.75288900	0.42222400
C	2.22663100	-2.42668600	-2.40179600

C	3.40753300	-2.27253400	-1.67874900
C	3.32699500	-1.90774700	-0.33928400
C	2.10478300	-1.66962800	0.27595300
C	0.94647800	-1.81868800	-0.47647500
C	0.98590500	-2.21163700	-1.80963500
O	-0.24298900	-1.60492100	0.19678000
C	-1.11121800	-0.71082200	-0.33680300
O	-1.03814600	-0.20806700	-1.41911100
O	-2.09524000	-0.57594700	0.56118500
H	2.27603900	-2.71956500	-3.44532100
H	4.37472800	-2.44385400	-2.13744600
H	2.04010100	-1.38217200	1.31884600
Cl	4.78897600	-1.74340900	0.59991300
H	0.06662200	-2.31322200	-2.37237300

TS2-3

0 1

C	-4.24786700	-2.72624000	0.67867700
C	-5.06275900	-3.78801300	1.05700100
C	-6.20273000	-3.55408800	1.82277600
C	-6.51276200	-2.24828600	2.21213300
C	-5.71461400	-1.17965900	1.82194100
C	-4.57900900	-1.42457700	1.05467900
C	-7.08265100	-4.67321200	2.25997800
N	-6.63243200	-5.86335600	2.28925400
H	-3.36226900	-2.90930000	0.07925000
H	-4.83863400	-4.80969400	0.76819300
H	-5.97747600	-0.16922700	2.12297400
H	-3.95230600	-0.59362500	0.74627100
N	-6.24174000	-5.45591100	6.05234300
N	-6.61484500	-3.36537200	5.07004600
C	-5.17528500	-3.12037400	5.06309700
C	-4.41945800	-4.40972500	4.76955300
C	-4.79136400	-5.43229800	5.82875200
C	-7.05307800	-4.48447100	5.58137900
C	-6.75781000	-6.61565400	6.78417900
C	-7.40183600	-6.27406800	8.13052400
C	-8.54152500	-4.66341900	5.71641200
C	-8.84399200	-5.78196400	8.01712300
C	-9.01629800	-4.51961000	7.17406500
H	-4.96066400	-2.35559200	4.31298200
H	-4.87422900	-2.71816900	6.04067300
H	-4.70786700	-4.78373700	3.78207500

H	-3.33836300	-4.24715600	4.77769800
H	-4.28668900	-5.21938400	6.78099100
H	-4.49038000	-6.43452200	5.50725500
H	-7.46059000	-7.17649700	6.15485000
H	-5.89777400	-7.26843400	6.95008200
H	-6.77704600	-5.52573700	8.63485300
H	-7.38392900	-7.17582300	8.75301500
H	-8.84472800	-5.63310000	5.30404700
H	-9.01151100	-3.90409700	5.09342500
H	-9.45158600	-6.58396400	7.57542000
H	-9.24465400	-5.60593300	9.02133800
H	-10.07801100	-4.25262300	7.15847600
H	-8.49099600	-3.67556900	7.63920200
H	-7.38022300	-6.49201700	2.59489300
C	-11.31695600	0.42048400	2.85754100
C	-12.08787200	0.52687300	4.00936800
C	-12.09580100	-0.55093900	4.88915700
C	-11.35598100	-1.69643700	4.64806700
C	-10.58293200	-1.78226000	3.48443400
C	-10.56542800	-0.71869100	2.57457400
O	-9.87667800	-2.93943900	3.36269900
C	-8.83850800	-3.02008400	2.37363900
O	-9.05439700	-2.74214100	1.20398400
O	-8.32570800	-4.36588900	2.68864500
H	-11.30753100	1.24304700	2.14886200
H	-12.67513200	1.41223300	4.22255900
H	-11.36828600	-2.52937300	5.34214300
Cl	-13.05419400	-0.45749400	6.34826700
H	-10.00694600	-0.81285000	1.65244500
N	-7.64682000	-2.12562700	3.06823800
H	-7.29426600	-2.66141200	4.16617300
H	-7.96937900	-1.15868700	3.14082800

In3

0 1

C	-4.00559900	-4.06459600	1.79812500
C	-5.03437500	-4.96067400	2.04892100
C	-6.18728900	-4.54628000	2.71910600
C	-6.32099600	-3.21566600	3.13972900
C	-5.27838600	-2.31324500	2.88524900
C	-4.13652700	-2.73892100	2.22302400
C	-7.26250600	-5.50348400	3.04950900

N	-7.04903700	-6.76574600	3.00034700
H	-3.11335000	-4.38568100	1.27150700
H	-4.97574200	-5.99851000	1.73653100
H	-5.37868500	-1.28027700	3.20794700
H	-3.34038400	-2.02650100	2.02719400
N	-6.87644400	-7.20487000	6.40104300
N	-7.37210400	-4.96108900	6.14530500
C	-5.99131000	-4.52202200	6.32646900
C	-5.05626400	-5.63065000	5.86782100
C	-5.43814500	-6.93449900	6.54949600
C	-7.74111300	-6.22678700	6.14659400
C	-7.30946200	-8.60539600	6.49992700
C	-8.19947900	-8.89613200	7.71058200
C	-9.19781700	-6.53030100	5.93311600
C	-9.66308100	-8.49841300	7.52011700
C	-9.88456500	-7.01591500	7.22290800
H	-5.86607300	-3.61474700	5.73403200
H	-5.82797500	-4.27902000	7.38307900
H	-5.13783300	-5.75534000	4.78439900
H	-4.02108200	-5.37996000	6.11093700
H	-5.18858900	-6.92119800	7.61828800
H	-4.90422000	-7.76693900	6.08520000
H	-7.80304200	-8.89897100	5.56571300
H	-6.39302300	-9.19385200	6.56914200
H	-7.77320100	-8.38977800	8.58605800
H	-8.14869800	-9.97191700	7.91130700
H	-9.29275100	-7.28260500	5.14190100
H	-9.66805000	-5.62191700	5.55349500
H	-10.08055900	-9.08715600	6.69187000
H	-10.22866800	-8.77714100	8.41537700
H	-10.95751400	-6.83211800	7.11520500
H	-9.54806900	-6.40189300	8.06836000
H	-7.92833200	-7.24816300	3.20768800
C	-10.77446000	-0.12073100	5.12227200
C	-10.97450700	-0.06438500	6.49885600
C	-10.67588100	-1.19923000	7.24330500
C	-10.18337800	-2.35270400	6.65394000
C	-9.98738100	-2.39265200	5.26679500
C	-10.29349200	-1.26486800	4.49224500
O	-9.50618200	-3.55910500	4.77481900
C	-8.72199500	-3.52697600	3.44281400
O	-9.30968400	-3.10310500	2.45829700
O	-8.43346600	-5.00194500	3.46464900
H	-11.01175400	0.75017800	4.51850800

H	-11.35605400	0.82608000	6.98434600
H	-9.95114600	-3.22712300	7.25373800
Cl	-10.91180200	-1.17468800	8.97829800
H	-10.16958400	-1.31485300	3.41796100
N	-7.44641100	-2.86331000	3.87845400
H	-8.05134500	-4.29163800	5.75693400
H	-7.61149400	-1.85895500	3.86007400

TS3-4

O 1

C	-3.90007400	-3.01385200	0.70157100
C	-5.04460500	-3.69140500	1.10566800
C	-5.98349500	-3.09664700	1.95120800
C	-5.76385400	-1.77629100	2.37520000
C	-4.61562200	-1.09246700	1.96888700
C	-3.68460200	-1.70917500	1.14163300
C	-7.16629000	-3.88549000	2.45044600
N	-7.09475200	-5.17670600	2.32637500
H	-3.18332200	-3.49526500	0.04401600
H	-5.24189900	-4.71053900	0.78878300
H	-4.45855400	-0.06960700	2.30376000
H	-2.79861700	-1.16334200	0.83158200
N	-6.66963400	-5.55667400	5.65381900
N	-6.06326200	-3.37403100	5.20115200
C	-4.66018300	-3.70808600	4.96521000
C	-4.56113200	-5.12668700	4.42574200
C	-5.33047500	-6.07637400	5.32949400
C	-6.98124200	-4.27486600	5.50674200
C	-7.67380900	-6.54400000	6.07489100
C	-8.14372900	-6.37976100	7.52152400
C	-8.37325100	-3.78483000	5.78917000
C	-9.20151900	-5.29257000	7.70555700
C	-8.75063900	-3.89753800	7.27655100
H	-4.26384700	-2.98553100	4.24894100
H	-4.10872200	-3.60260200	5.90763900
H	-5.00077700	-5.17107000	3.42564800
H	-3.51546500	-5.44072200	4.37716800
H	-4.79902600	-6.27124200	6.27001200
H	-5.47530000	-7.02889000	4.81380600
H	-8.52250500	-6.51080700	5.38159300
H	-7.19991600	-7.51910500	5.95003600
H	-7.26889300	-6.17948100	8.15347100
H	-8.55842700	-7.33935200	7.84946500

H	-9.08090300	-4.31962500	5.14728700
H	-8.41388200	-2.74611700	5.46323500
H	-10.09116600	-5.56733500	7.12293600
H	-9.51226300	-5.26727700	8.75539900
H	-9.56729400	-3.19149000	7.45677900
H	-7.90718700	-3.56374900	7.89516800
H	-7.97636800	-5.55851800	2.68374200
C	-12.20699700	-2.04501500	3.31452500
C	-12.89323500	-1.38725100	4.33326900
C	-12.16172000	-0.61746600	5.22840700
C	-10.78361100	-0.48826200	5.12133600
C	-10.12571500	-1.15577400	4.09020400
C	-10.82606600	-1.94792500	3.18012300
O	-8.75805600	-1.03846900	4.10451200
C	-8.04836900	-1.22177800	2.92529000
O	-8.46783600	-0.92939300	1.83905500
O	-8.10941800	-3.21878100	3.02918800
H	-12.76376000	-2.65368500	2.60892300
H	-13.96940900	-1.46713000	4.43499300
H	-10.21812000	0.12168900	5.81652700
Cl	-12.98884200	0.21462400	6.52521500
H	-10.28656200	-2.47343800	2.40379300
N	-6.64530900	-1.17829200	3.31433800
H	-6.40989200	-2.47785700	4.82746100
H	-6.39917000	-0.19989500	3.46427700

In4

O 1

C	-4.51671300	-6.08263900	0.01137300
C	-5.58659800	-6.84801800	0.45351300
C	-6.65076000	-6.27463200	1.15243000
C	-6.64497500	-4.88408200	1.38333000
C	-5.57833900	-4.10698900	0.91738200
C	-4.52067600	-4.71103700	0.24867500
C	-7.76401200	-7.18116000	1.58060000
N	-8.08846300	-8.16075300	0.84135200
H	-3.69332400	-6.54909300	-0.51915500
H	-5.63032300	-7.91605700	0.26936700
H	-5.58711300	-3.03880300	1.08032400
H	-3.69819600	-4.09371500	-0.09954400
N	-7.19116500	-5.17761400	6.93970900
N	-6.98766600	-5.81684300	4.67597100

C	-5.68463100	-5.16976600	4.55553700
C	-4.99341400	-5.01706800	5.90417400
C	-5.96713900	-4.38508100	6.88750700
C	-7.62583800	-5.79431100	5.80169400
C	-8.08774200	-4.93963100	8.07020200
C	-9.28682100	-4.04137100	7.74375500
C	-8.96931300	-6.48637100	5.85452200
C	-10.45705500	-4.78810400	7.10051000
C	-10.13788000	-5.48945300	5.77889500
H	-5.07665400	-5.76671100	3.86759200
H	-5.80095100	-4.18413400	4.08429100
H	-4.69269000	-6.00012600	6.28232500
H	-4.09527100	-4.39999800	5.81322000
H	-6.19705800	-3.34894500	6.59395600
H	-5.53861200	-4.35794700	7.89423200
H	-8.43069600	-5.89649200	8.48283200
H	-7.47431200	-4.47196100	8.84476100
H	-8.94227600	-3.22728700	7.09435600
H	-9.63883400	-3.57703000	8.67257000
H	-9.04523500	-7.09585800	6.76281700
H	-9.01155100	-7.16492900	5.00145200
H	-10.81948600	-5.54103100	7.81532800
H	-11.28465900	-4.08582800	6.94395100
H	-11.02994500	-6.03029000	5.44594700
H	-9.90842400	-4.75528000	4.99731000
H	-8.83587300	-8.68247700	1.30747500
C	-8.31390300	-0.64777900	6.24732500
C	-9.62414800	-0.49926100	6.68833300
C	-10.62666600	-1.19533400	6.02040200
C	-10.34428100	-2.01509500	4.93768400
C	-9.01990900	-2.15479600	4.52265800
C	-7.98910000	-1.47472300	5.17283200
O	-8.85507600	-3.07339000	3.50999700
C	-7.70714300	-3.14010500	2.75887800
O	-6.84946700	-2.28865500	2.74979300
O	-8.39165600	-6.88506200	2.74176000
H	-7.51887200	-0.10882300	6.75291600
H	-9.87046400	0.13924100	7.52869300
H	-11.12845000	-2.55689400	4.42055100
Cl	-12.27759600	-1.05342200	6.56183700
H	-6.96740900	-1.56873100	4.83567700
N	-7.74110100	-4.30086900	2.05768600
H	-7.74688300	-6.48228900	3.44812500
H	-8.49025400	-4.93757600	2.31342600

TS4-5

0 1

C	-4.33579500	-4.85741100	1.69603000
C	-5.42886700	-5.65803100	2.01677500
C	-6.71551500	-5.28202700	1.64823500
C	-6.91497300	-4.09213200	0.92805100
C	-5.81970000	-3.29026100	0.59095100
C	-4.54249600	-3.67730400	0.98764600
C	-7.90130700	-6.11539400	2.03808300
N	-8.21330400	-7.13602200	1.34957200
H	-3.33436900	-5.15628000	1.98892900
H	-5.29635300	-6.58664900	2.56385600
H	-5.97413500	-2.37702400	0.03369000
H	-3.69906400	-3.04586800	0.72553800
N	-5.80215900	-4.63261700	6.75830300
N	-7.00209900	-4.36918100	4.74052600
C	-6.20345800	-3.20157100	4.38835700
C	-4.80997100	-3.26502200	4.99698000
C	-4.93484300	-3.48715400	6.49552600
C	-6.77268500	-4.97709200	5.85705400
C	-5.76147200	-5.19421400	8.10539900
C	-6.98416800	-4.86517300	8.97048300
C	-7.67255500	-6.13814800	6.21435000
C	-8.17717800	-5.78729000	8.71590000
C	-8.71269100	-5.76118800	7.28425200
H	-6.14124500	-3.14376900	3.29846300
H	-6.72515900	-2.29663900	4.73010400
H	-4.26326700	-4.10077800	4.54650600
H	-4.24928400	-2.34757100	4.79704200
H	-5.33279300	-2.58657700	6.98694000
H	-3.95503000	-3.69694400	6.93758700
H	-5.61990800	-6.28176300	8.05871600
H	-4.86173400	-4.78649200	8.57353500
H	-7.26271500	-3.81733700	8.79809700
H	-6.69435200	-4.94844600	10.02436000
H	-7.07928300	-6.99694200	6.55132500
H	-8.18186300	-6.43065200	5.29478800
H	-7.87590200	-6.81620100	8.95893200
H	-8.98630600	-5.53016300	9.40839500
H	-9.55068300	-6.46199900	7.21160500
H	-9.11526300	-4.76854700	7.04595200
H	-9.04709300	-7.56383600	1.76651000

C	-11.14638500	-0.01206600	-2.37097200
C	-12.36004400	0.31291300	-1.77123600
C	-12.74748400	-0.38255700	-0.63200200
C	-11.95140800	-1.38029300	-0.08420900
C	-10.74557900	-1.68121400	-0.70631300
C	-10.32934200	-1.01109000	-1.85248600
O	-10.03736800	-2.73557800	-0.15965900
C	-8.68522600	-2.61224900	0.02606400
O	-8.04227100	-1.62882600	-0.24605200
O	-8.61767100	-5.65127900	3.07477000
H	-10.83298600	0.52206000	-3.26195900
H	-12.99872200	1.08917200	-2.17652800
H	-12.25270100	-1.92244100	0.80441700
Cl	-14.26544800	0.00396600	0.13525200
H	-9.38329400	-1.25980200	-2.31500400
N	-8.23689500	-3.77872200	0.56404200
H	-8.04332600	-5.04781400	3.67019800
H	-8.94272600	-4.48603700	0.73249800

In5

0 1

C	-5.06528400	-5.63980300	1.79065500
C	-6.19437900	-6.38751200	2.09500100
C	-7.44053400	-6.09125900	1.53567500
C	-7.53796100	-5.03661400	0.59798900
C	-6.40361700	-4.26141100	0.31774300
C	-5.18693600	-4.56278100	0.91613900
C	-8.62231900	-6.89650200	1.97121500
N	-9.60695900	-7.09271200	1.18060500
H	-4.10543000	-5.89371600	2.22904000
H	-6.12700100	-7.22094700	2.78576100
H	-6.48778900	-3.43538800	-0.37391500
H	-4.31970500	-3.95509100	0.67555800
N	-5.66426600	-5.85187500	6.69066400
N	-7.21448000	-5.90905400	4.91194600
C	-7.07475700	-4.47482200	4.69365700
C	-5.70862600	-3.96859500	5.13467500
C	-5.45388100	-4.41146300	6.56731500
C	-6.54173400	-6.48196400	5.85318100
C	-5.13778000	-6.49957800	7.88867200
C	-6.20110400	-6.88439600	8.92438600
C	-6.77123600	-7.96190800	6.05969500

C	-6.89878900	-8.21097500	8.61950900
C	-7.65086000	-8.25059600	7.28894100
H	-7.23020600	-4.27730200	3.62805800
H	-7.87098500	-3.95118100	5.24020300
H	-4.94308300	-4.39478200	4.47682700
H	-5.64844200	-2.87919200	5.06257000
H	-6.11395600	-3.86908700	7.26078000
H	-4.42094700	-4.19523300	6.85923000
H	-4.54956200	-7.38434500	7.61237300
H	-4.43540000	-5.78824400	8.33079200
H	-6.93393300	-6.06986500	8.99328800
H	-5.71654300	-6.96029900	9.90460200
H	-5.81533900	-8.49291000	6.14677800
H	-7.26964900	-8.32828800	5.15956000
H	-6.14067100	-9.00702500	8.61794600
H	-7.59396100	-8.44765900	9.43245800
H	-8.09628900	-9.24325300	7.16788600
H	-8.48230900	-7.53471400	7.29855800
H	-10.32305900	-7.64027200	1.66118800
C	-11.12731100	-1.51865600	-3.88057200
C	-12.45377700	-1.21368200	-3.58778200
C	-13.04627100	-1.81735900	-2.48503900
C	-12.34544900	-2.70304100	-1.67722500
C	-11.02174600	-2.98747200	-1.99473200
C	-10.39916700	-2.40724700	-3.09655800
O	-10.41165600	-3.93558600	-1.19874700
C	-9.12169500	-3.73826900	-0.77365400
O	-8.46257700	-2.76148400	-1.03916000
O	-8.57652300	-7.40484700	3.20601300
H	-10.65239600	-1.05633800	-4.73982500
H	-13.02246300	-0.52366300	-4.20035600
H	-12.80767000	-3.17410200	-0.81774800
Cl	-14.70931600	-1.45589700	-2.09854400
H	-9.36663200	-2.63824300	-3.32163200
N	-8.77008900	-4.81449800	-0.02421700
H	-8.03949200	-6.80835900	3.84706000
H	-9.45832600	-5.56504600	0.10873300

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C	-4.88432200	-5.65702600	1.69864000
C	-6.08013200	-6.25332000	2.06444100
C	-7.27467300	-5.93486900	1.40860900

C	-7.26099300	-5.04890500	0.30818600
C	-6.04717700	-4.42815500	-0.03232500
C	-4.88410200	-4.72207900	0.65775200
C	-8.56530500	-6.47191000	1.86941800
N	-9.56694600	-6.40852400	1.06715200
H	-3.96097600	-5.91928500	2.20431200
H	-6.10816200	-6.97783600	2.87141600
H	-6.03001100	-3.72900200	-0.86387300
H	-3.95724600	-4.23797100	0.36443600
N	-5.81096900	-5.91346000	6.72773900
N	-7.24960000	-5.76884000	4.86844300
C	-6.94631100	-4.35415800	4.69361900
C	-5.54869100	-4.02249000	5.19700900
C	-5.40994500	-4.51088900	6.63088000
C	-6.69848300	-6.43132800	5.83236200
C	-5.41026600	-6.63940600	7.93100700
C	-6.55637800	-6.93522700	8.90518700
C	-7.09923800	-7.87995700	5.98788600
C	-7.37615200	-8.17081000	8.53038000
C	-8.06417300	-8.09583800	7.16724400
H	-7.03983900	-4.11780100	3.62903800
H	-7.69789700	-3.75713100	5.22758300
H	-4.81355000	-4.52841800	4.56111800
H	-5.35486600	-2.94757600	5.14877800
H	-6.02017800	-3.89544700	7.30799200
H	-4.36969800	-4.43473700	6.96367200
H	-4.90108800	-7.57262400	7.65721000
H	-4.66284100	-6.01282500	8.42412800
H	-7.20061400	-6.04855800	8.96706300
H	-6.12841200	-7.08795300	9.90252000
H	-6.21211200	-8.51425100	6.10513200
H	-7.58923100	-8.17003100	5.05576400
H	-6.70872200	-9.04413100	8.53920400
H	-8.13053000	-8.35029900	9.30406300
H	-8.60945500	-9.02966800	6.99782200
H	-8.81135000	-7.29243400	7.15949500
H	-10.45285500	-6.74212800	1.44219200
C	-12.89572800	-8.08659700	-1.41287100
C	-14.04706200	-7.38478300	-1.75222700
C	-13.96990200	-5.99752600	-1.81627400
C	-12.79265000	-5.31807200	-1.55009000
C	-11.64746000	-6.04461800	-1.21122900
C	-11.69219200	-7.44008500	-1.14077100
O	-10.56328700	-5.27296300	-0.91250900

C	-9.31216100	-5.87554600	-0.69990600
O	-8.92463200	-6.82307800	-1.35250700
O	-8.68312600	-6.97714100	3.08444100
H	-12.93096100	-9.17063700	-1.36403600
H	-14.98054500	-7.89168300	-1.96688200
H	-12.74205600	-4.23650700	-1.59447400
Cl	-15.39743500	-5.07998300	-2.23877800
H	-10.79569900	-8.00106500	-0.91615500
N	-8.43008300	-4.75420300	-0.36300900
H	-8.07607800	-6.48975000	3.78729400
H	-8.29353600	-4.17105700	-1.18352600

In6

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C	-5.64101800	-3.85912800	0.46572800
C	-5.54244500	-5.04937100	1.16211100
C	-6.47313800	-6.07145200	0.95065700
C	-7.49271600	-5.90688000	0.00508700
C	-7.59125300	-4.70202100	-0.70402900
C	-6.67918100	-3.69163800	-0.46299400
C	-6.40214900	-7.31894100	1.71803200
N	-7.31164000	-8.27604600	1.33511600
H	-4.92132900	-3.06428200	0.62892800
H	-4.74371800	-5.22373700	1.87759000
H	-8.40081800	-4.56345700	-1.41412000
H	-6.77378800	-2.75631900	-1.00561800
N	-7.74676000	-5.87844900	6.27074100
N	-6.00848500	-5.75488400	4.74083800
C	-6.23662600	-4.35026800	4.41444400
C	-6.90543300	-3.67330500	5.59886300
C	-8.12388200	-4.48069000	6.01981000
C	-6.81795400	-6.45298700	5.51946900
C	-8.72115700	-6.68939800	7.01477500
C	-9.64989300	-7.50989600	6.11490700
C	-6.62184900	-7.94449100	5.54936800
C	-9.03147100	-8.83912200	5.67713900
C	-7.76555100	-8.68814500	4.83402200
H	-5.26989900	-3.89169200	4.18946600
H	-6.88349100	-4.32511100	3.53258000
H	-6.20390800	-3.59675700	6.43674000
H	-7.21517800	-2.66227700	5.32335400
H	-8.88151700	-4.48281000	5.22842000

H	-8.54684500	-4.08322500	6.94594100
H	-8.18528400	-7.33661300	7.71919800
H	-9.29579000	-5.98024400	7.61431700
H	-9.90315900	-6.90773500	5.23488700
H	-10.57212800	-7.71050000	6.67119500
H	-6.52919600	-8.27735900	6.59042900
H	-5.67794600	-8.16041200	5.04601400
H	-8.80747400	-9.44045100	6.57101900
H	-9.77259100	-9.40317700	5.10010900
H	-7.39073600	-9.68097000	4.56104600
H	-8.00406900	-8.13072500	3.92282600
H	-7.29835000	-9.15182100	1.84519100
C	-11.32615100	-6.79293500	1.32258200
C	-11.44310400	-5.63027600	0.55248700
C	-10.57942800	-4.58075600	0.86526500
C	-9.61771800	-4.66178600	1.85342900
C	-9.44423700	-5.86578600	2.60475800
C	-10.37395900	-6.91171600	2.32164100
O	-8.48739400	-5.99706000	3.45433300
C	-8.36208100	-8.14850600	0.42102000
O	-9.14849900	-9.04511200	0.22236100
O	-5.58195300	-7.55523400	2.60320800
H	-11.98480900	-7.63186900	1.11400200
H	-12.19243200	-5.52375600	-0.22263600
H	-8.93502800	-3.83470100	2.02900800
Cl	-10.69761300	-3.08948700	-0.07240000
H	-10.27579900	-7.84315800	2.87606100
N	-8.38405700	-6.93851100	-0.23076500
H	-5.53526800	-6.31651700	4.02868900
H	-9.25874000	-6.73863600	-0.70745400

In7

O	0.23138700	-2.70190300	0.42269800
C	0.81977700	-2.73654500	1.74697800
O	0.05918300	-2.25237800	2.58806500
O	1.94124400	-3.25492200	1.84391600
C	-2.79395600	0.04152700	0.26105700
C	-2.31424800	-1.09179100	0.89535300
C	-2.91969800	-2.32962400	0.64176500
C	-3.99776900	-2.45855200	-0.26019100
C	-4.46227000	-1.29470900	-0.88955000
C	-3.86795200	-0.07076500	-0.62676800
N	-4.53442300	-3.69466900	-0.55762200
C	-2.47285200	-3.51754000	1.30116500

N	-2.23358800	-4.54321400	1.78724700
C	0.79702500	-3.39886500	-0.59523300
C	-0.06349000	-4.19706800	-1.35572000
C	2.15839400	-3.33767900	-0.91360800
C	0.45684000	-4.94792600	-2.40072100
C	2.64792800	-4.10580800	-1.96477000
C	1.80994400	-4.92650500	-2.71798400
H	-2.33322500	1.00530300	0.44574500
H	-1.46758000	-1.07465000	1.57633800
H	-5.28665400	-1.36826400	-1.59322800
H	-4.24713300	0.81485600	-1.12872400
H	-4.37254800	-4.43775900	0.10968700
H	-5.46315600	-3.69600500	-0.95382400
H	2.81047400	-2.71478700	-0.31660200
H	2.18839000	-5.52551400	-3.53845200
N	2.33587400	-5.65629900	3.34190900
N	0.07442300	-5.19980600	3.47737400
C	0.13725600	-4.42631000	4.71880700
C	1.55855500	-3.93504900	4.92442400
C	2.52612000	-5.08734000	4.68538500
C	1.12340500	-5.62691500	2.80107700
C	3.51393700	-5.86705700	2.48552600
C	3.70483500	-7.31583100	2.03264000
C	0.89007000	-6.12834200	1.40520300
C	2.80185400	-7.73625300	0.87458900
C	1.30955500	-7.58629700	1.16419500
H	-0.54172700	-3.58135900	4.59209800
H	-0.20198600	-5.05629400	5.54922900
H	1.75769800	-3.13808500	4.20339200
H	1.68087100	-3.55489000	5.94185900
H	2.38740200	-5.88148600	5.43034900
H	3.55802800	-4.74008500	4.75192800
H	3.44743700	-5.17307100	1.63822100
H	4.37451900	-5.56248500	3.08300900
H	3.55105600	-7.97594300	2.89592100
H	4.75071400	-7.43276500	1.72607100
H	1.44011700	-5.46015200	0.73172800
H	-0.17033300	-5.98900300	1.17755300
H	3.04372000	-7.12532500	-0.00620100
H	3.02022100	-8.77618200	0.60799200
H	0.74452200	-7.95030500	0.30041500
H	1.01914600	-8.21046400	2.01904100
H	-1.11939900	-4.23318800	-1.10787600
H	-0.80099400	-5.14617300	2.95446800

H	3.70538800	-4.06221700	-2.20896000
Cl	-0.62045100	-5.96738100	-3.33134000

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O	0.93737100	0.39620600	-1.22618800
C	1.07360700	-0.89320000	-1.70379700
O	1.99270900	-1.52966900	-1.05778600
O	0.41069600	-1.32777500	-2.62089600
C	5.80619200	-0.02049600	-0.69828700
C	4.50582200	-0.50023500	-0.70654100
C	3.71961100	-0.50198400	0.45148900
C	4.25995400	0.00534200	1.66228300
C	5.58273800	0.48337200	1.65201900
C	6.34041400	0.47008300	0.49452100
N	3.51275600	0.08060300	2.81222700
C	2.34988900	-1.02496400	0.49256800
N	1.49895500	-1.20753300	1.33557200
C	-0.17442700	1.16957800	-1.41864600
C	-0.11962200	2.37910900	-0.71865700
C	-1.30756900	0.83176300	-2.16317700
C	-1.21305200	3.22869200	-0.74617100
C	-2.38894800	1.71313700	-2.16599300
C	-2.36763600	2.90996000	-1.45767600
H	6.39807200	-0.03055400	-1.60694800
H	4.07828800	-0.89917700	-1.61754200
H	5.99879600	0.87618900	2.57636100
H	7.35877700	0.84752200	0.52189200
H	2.65635500	-0.46592700	2.81949400
H	4.02615200	0.14026500	3.67874200
H	-1.33240900	-0.08464100	-2.73260800
H	-3.21046200	3.59161600	-1.46679400
N	-2.95697000	-1.54913400	-0.20032000
N	-0.73410100	-2.02531700	0.30452600
C	-0.71638200	-3.27757800	-0.44324000
C	-1.80622500	-3.28215500	-1.50361500
C	-3.12497800	-2.82985200	-0.89244600
C	-1.78032900	-1.25157800	0.38013200
C	-4.14485600	-0.71798500	0.00595700
C	-4.69476600	-0.76260700	1.43511600
C	-1.66643900	-0.01017000	1.22641900
C	-3.94631600	0.15294800	2.40486800
C	-2.45241900	-0.14224000	2.54359900
H	0.27362000	-3.36608800	-0.89957700
H	-0.84567300	-4.10722500	0.26288500

H	-1.51375700	-2.60149300	-2.30728800
H	-1.92220400	-4.28318800	-1.92743400
H	-3.51000000	-3.57929800	-0.18656900
H	-3.87867800	-2.68935600	-1.67203000
H	-3.91921100	0.31496000	-0.28700000
H	-4.89612000	-1.08903100	-0.69531300
H	-4.67082900	-1.80177500	1.78882300
H	-5.74817000	-0.46148400	1.40694000
H	-2.01916200	0.85991200	0.65959200
H	-0.60308300	0.14196200	1.43040800
H	-4.06561900	1.19107400	2.06431700
H	-4.41847900	0.09278900	3.39161100
H	-2.02209900	0.56199100	3.26207300
H	-2.29615000	-1.14543400	2.96032500
H	0.76920700	2.61586400	-0.14468800
H	-3.27015400	1.45691700	-2.74746000
Cl	-1.14699000	4.72430600	0.15013200
H	0.25856100	-1.68665900	0.81258300

Int8

O	-0.53864900	-3.24590500	-0.10667400
C	-0.09628500	-2.36428400	0.81457300
O	-1.11554900	-1.88684100	1.53492500
O	1.02849600	-1.97914900	0.95846800
C	-3.82053600	0.23618300	-0.71875700
C	-2.95020800	-0.52157800	0.04253200
C	-3.36338300	-1.69409200	0.69509900
C	-4.71756200	-2.11193100	0.58198500
C	-5.58877400	-1.32767600	-0.20392200
C	-5.14985400	-0.18318300	-0.83844500
N	-5.19442700	-3.21465000	1.22083200
C	-2.40007000	-2.49337200	1.45725400
N	-2.62641000	-3.57978000	2.05626800
C	0.30438700	-4.05163900	-0.84707600
C	-0.35939600	-4.74372900	-1.85811400
C	1.65818000	-4.25765200	-0.59465300
C	0.34876400	-5.66711200	-2.61169000
C	2.33635600	-5.19553300	-1.37160000
C	1.69901100	-5.91254900	-2.37861800
H	-3.47680900	1.13828500	-1.21182800
H	-1.91913700	-0.20492900	0.15279400
H	-6.62499800	-1.64260700	-0.29537900
H	-5.85098600	0.39471300	-1.43369500
H	-4.53024900	-3.83196900	1.67523900

H	-6.10885600	-3.55763400	0.97433300
H	2.16545400	-3.71358200	0.18710600
H	2.23176300	-6.64011800	-2.98000700
N	2.00823000	-5.88689600	2.31044600
N	0.16987800	-4.45262000	2.73252200
C	0.97347400	-3.63019000	3.62904600
C	2.46824800	-3.72720100	3.35159600
C	2.86766200	-5.19286100	3.26346900
C	0.70157900	-5.48461200	2.17231500
C	2.47017200	-7.17787800	1.81567600
C	1.83794700	-8.39102100	2.51038300
C	-0.20540600	-6.35591500	1.33103400
C	0.46190000	-8.76094800	1.95437000
C	-0.59159000	-7.65668400	2.05682800
H	0.63679900	-2.59341300	3.52679100
H	0.75982700	-3.93461100	4.66329000
H	2.68878000	-3.22528500	2.40403200
H	3.04610900	-3.22891500	4.13576200
H	2.80458900	-5.66726700	4.25526400
H	3.90312500	-5.29038500	2.92016800
H	2.30696000	-7.23930300	0.73137400
H	3.55350400	-7.19070000	1.96680200
H	1.77520400	-8.18458300	3.58704200
H	2.50799400	-9.25048200	2.39032200
H	0.25622600	-6.58900300	0.36285500
H	-1.09812700	-5.75753000	1.13142600
H	0.57956800	-9.03208300	0.89557400
H	0.09566300	-9.65842500	2.46551700
H	-1.52712400	-8.02869600	1.62609500
H	-0.80193800	-7.42602800	3.10904300
H	-1.41567100	-4.56547700	-2.02323300
H	3.39117700	-5.36808600	-1.18092900
Cl	-0.47917400	-6.54550900	-3.86900900
H	-1.76059200	-3.94717800	2.48490000

TS8-9

O	-4.53484900	-3.09373100	5.33455400
C	-4.49790200	-3.84241000	4.10247300
O	-3.07469900	-3.89424600	3.82004900
O	-5.10094700	-4.91187400	4.00431800
C	-3.09491200	0.93216200	3.35818100
C	-2.40304300	-0.25549900	3.56829000
C	-3.06203400	-1.47854900	3.45198100
C	-4.41493500	-1.49247800	3.11229900

C	-5.11733800	-0.31066400	2.90489000
C	-4.45123400	0.90438700	3.03142400
N	-5.00569900	-2.78728000	2.98022800
C	-2.34079400	-2.76065500	3.68199000
N	-1.07175200	-2.78129400	3.68639600
C	-5.76332200	-2.65678300	5.74288900
C	-5.85775300	-1.30369000	6.07745000
C	-6.87778600	-3.49436200	5.83956500
C	-7.07697800	-0.80356200	6.51116600
C	-8.08739400	-2.95651700	6.27169300
C	-8.20468600	-1.61141400	6.61200100
H	-2.58118200	1.88247100	3.45894200
H	-1.35104300	-0.26455400	3.83276000
H	-6.17626600	-0.34510300	2.66393000
H	-4.99557500	1.83142900	2.88292300
H	-6.02588800	-2.77212400	3.03118800
H	-6.77182200	-4.53816600	5.57440800
H	-9.14506400	-1.19360400	6.95302000
N	-2.87764900	-5.23543200	-0.57492200
N	-3.86646800	-3.62088200	0.81206200
C	-3.07277900	-2.55041800	0.21521400
C	-2.68390200	-2.88387800	-1.21733000
C	-2.02189900	-4.25270900	-1.23794000
C	-3.71623400	-4.85102700	0.42256700
C	-2.61360200	-6.64583300	-0.86483900
C	-1.89569300	-7.40156000	0.25817000
C	-4.49490300	-5.91846900	1.14750800
C	-2.83820400	-7.87969300	1.36347100
C	-3.60278100	-6.76454300	2.07407100
H	-3.66062800	-1.62787100	0.25797800
H	-2.17541100	-2.38443800	0.82770800
H	-3.57929200	-2.90497600	-1.84784900
H	-2.00083700	-2.13234600	-1.62208400
H	-1.04015200	-4.21314100	-0.74514700
H	-1.86298100	-4.58582300	-2.26806200
H	-3.55164200	-7.15443600	-1.11911800
H	-2.00014800	-6.65496200	-1.76928400
H	-1.11341900	-6.75236900	0.67259400
H	-1.39013800	-8.26892900	-0.18210400
H	-5.01887800	-6.55737400	0.42536900
H	-5.23794400	-5.41883400	1.76937900
H	-3.55919200	-8.58210600	0.92032100
H	-2.26471100	-8.45098000	2.10169300
H	-4.24807200	-7.19021200	2.84681600

H	-2.92076800	-6.09149400	2.60546300
H	-4.98266200	-0.66903400	5.98525400
H	-8.95698400	-3.60140000	6.35327800
Cl	-7.19876900	0.89338600	6.91476100
H	-0.75487000	-3.73594300	3.87387900
H	-4.60380100	-3.25984300	1.95424600

Int9

O	-6.06306000	-1.48692400	3.66775800
C	-5.33449500	-2.19621900	2.69116200
O	-4.36517200	-3.01309000	3.33729500
O	-6.14335300	-2.97379600	1.95556900
C	-1.59825200	0.92291600	3.78923400
C	-1.96039800	-0.34004700	4.23331700
C	-2.98330900	-1.04501000	3.59793500
C	-3.65735600	-0.47509200	2.51060900
C	-3.28915700	0.79591700	2.06042800
C	-2.26678500	1.48409900	2.69832700
N	-4.65625300	-1.21948700	1.87948100
C	-3.34627100	-2.40581200	4.03364000
N	-2.72407000	-3.02329200	4.94683900
C	-6.70944100	-2.14701300	4.68080500
C	-7.17447500	-1.31156200	5.69746000
C	-6.92006900	-3.52496700	4.74406200
C	-7.85245100	-1.86865200	6.77024500
C	-7.59869500	-4.04986200	5.84049500
C	-8.07422000	-3.23807100	6.86461700
H	-0.80392400	1.47032700	4.28476900
H	-1.46456200	-0.81318700	5.07453500
H	-3.81215600	1.23663800	1.21614400
H	-1.99197900	2.47323500	2.34446500
H	-5.32830700	-0.67210400	1.35191100
H	-6.57365400	-4.16517300	3.94521000
H	-8.60508900	-3.64896600	7.71533500
N	-2.97198200	-5.71005900	-0.40640100
N	-4.52137500	-4.04189900	0.20502800
C	-4.17726400	-3.23033400	-0.95183800
C	-3.62095900	-4.06877900	-2.09523900
C	-2.50099700	-4.95062500	-1.56109000
C	-3.91944700	-5.16425500	0.41434000
C	-2.23796000	-6.92192000	-0.05287100
C	-1.30220300	-6.77795400	1.15228800
C	-4.26278100	-5.90131700	1.68749700
C	-2.02512200	-6.90487700	2.49303800

C	-3.12087500	-5.86408900	2.71907500
H	-5.07835700	-2.69379600	-1.26659200
H	-3.45006500	-2.46843000	-0.64087600
H	-4.41354300	-4.70510500	-2.50352200
H	-3.24535900	-3.43541100	-2.90393500
H	-1.62899200	-4.33856000	-1.28736300
H	-2.17688900	-5.66268500	-2.32635700
H	-2.94211500	-7.74568500	0.12086600
H	-1.65893200	-7.19333700	-0.93943700
H	-0.78594200	-5.81173500	1.08416300
H	-0.53299800	-7.55633800	1.08798800
H	-4.54454700	-6.93947500	1.47055400
H	-5.13936600	-5.39860200	2.09977500
H	-2.46836700	-7.90915700	2.55521500
H	-1.29347200	-6.83650700	3.30539700
H	-3.56011500	-6.02468700	3.71037800
H	-2.68973300	-4.85632900	2.73355600
H	-6.99511100	-0.24478800	5.63382300
H	-7.76558300	-5.12132600	5.89251400
Cl	-8.43619500	-0.81774500	8.03785500
H	-3.15816500	-3.93664800	5.09841100
H	-5.54663700	-3.42288900	1.23757400

TS9-10

O	-8.69652200	-3.25131700	0.02252400
C	-7.92872400	-2.40507200	-0.83963500
O	-6.63968800	-1.97618900	0.40803500
O	-7.34159000	-2.87065700	-1.80133900
C	-9.93504000	0.78221900	2.57580900
C	-8.74462600	0.06780500	2.59489000
C	-8.27644500	-0.58941000	1.45709200
C	-9.03113300	-0.52973800	0.27227600
C	-10.22052900	0.20623300	0.24921200
C	-10.66609900	0.85773300	1.39055500
N	-8.56015600	-1.14605900	-0.88561400
C	-6.94231200	-1.25949900	1.47520200
N	-6.16707400	-1.06866700	2.48669000
C	-8.33106100	-4.54997000	0.16473900
C	-8.24720900	-5.03425900	1.47260000
C	-8.12993100	-5.41335200	-0.91876100
C	-7.94066200	-6.37345000	1.67711100
C	-7.83031200	-6.75002600	-0.67617400
C	-7.71652400	-7.24826600	0.62102200

H	-10.28568000	1.28624600	3.47053200
H	-8.13036500	0.01682200	3.48778500
H	-10.79621900	0.25225500	-0.67188200
H	-11.59411600	1.42112200	1.35526800
H	-9.07480900	-0.99365500	-1.74237400
H	-8.21800200	-5.02547000	-1.92420400
H	-7.49129900	-8.29158100	0.81228900
N	-4.16274300	-6.00384400	1.05495900
N	-5.03154100	-4.07991400	0.10286700
C	-4.63945000	-4.40896800	-1.26399800
C	-4.42408200	-5.90865200	-1.38414900
C	-3.57410900	-6.41151600	-0.22461800
C	-4.83122000	-4.84879000	1.14329300
C	-3.87638500	-6.81291600	2.24548400
C	-2.86312300	-6.17216400	3.19887300
C	-5.29343700	-4.35067400	2.48294100
C	-3.45920800	-5.09583300	4.10903000
C	-4.11256500	-3.92437500	3.37405700
H	-5.44733500	-4.05153300	-1.90788300
H	-3.72502000	-3.85662100	-1.51008000
H	-5.39264600	-6.41531000	-1.35806200
H	-3.93427300	-6.14728500	-2.33152500
H	-2.54761200	-6.02614300	-0.29287900
H	-3.52377800	-7.50319200	-0.23312200
H	-4.81590400	-7.03622500	2.76558100
H	-3.48773900	-7.76365100	1.87411300
H	-2.03634900	-5.76010700	2.60534800
H	-2.43857500	-6.96600600	3.82378100
H	-5.87425300	-5.13010800	2.98585600
H	-5.96538000	-3.50723200	2.31282300
H	-4.21567400	-5.56508400	4.75326000
H	-2.67592000	-4.71644700	4.77381900
H	-4.49761600	-3.20565500	4.10420900
H	-3.36920500	-3.38695300	2.77018500
H	-8.42991600	-4.35547400	2.29942500
H	-7.69296300	-7.42563000	-1.51624400
Cl	-7.82751700	-6.97841700	3.32020400
H	-5.26824700	-1.51928200	2.29267900
H	-5.60118700	-3.20383400	0.24632800
Int10			
O	-9.49235300	-3.80723800	1.19556200
C	-8.84178700	-3.64457800	0.00081300
O	-5.88458100	-1.55893400	-0.71452900

O	-8.66885100	-4.53262700	-0.80038000
C	-8.32951900	0.69255900	2.73621200
C	-7.15876500	0.31997500	2.09266300
C	-7.14790200	-0.69459200	1.12989600
C	-8.35717500	-1.34092300	0.81940900
C	-9.53650200	-0.95838400	1.46289500
C	-9.52276400	0.04558900	2.42033300
N	-8.40326100	-2.36665700	-0.16058800
C	-5.82635800	-1.06929700	0.53927600
N	-4.77156300	-0.90181600	1.23572100
C	-9.72875300	-5.10237900	1.62209000
C	-9.21822800	-5.43340600	2.87194400
C	-10.47319700	-6.00786700	0.87429700
C	-9.45659500	-6.70980000	3.36650900
C	-10.69805000	-7.27631900	1.39924200
C	-10.19307300	-7.64184700	2.64490700
H	-8.31364000	1.48398300	3.47837800
H	-6.21253100	0.79448200	2.32829800
H	-10.45961100	-1.46207900	1.19981000
H	-10.44843900	0.33031900	2.91068800
H	-7.74177700	-2.26921400	-0.92404000
H	-10.84650400	-5.72314900	-0.10096700
H	-10.36522300	-8.63106800	3.05345200
N	-3.28387800	-5.31503500	0.28179700
N	-3.86886000	-3.28853800	-0.78539900
C	-2.47002400	-2.99199200	-1.06485700
C	-1.61826100	-4.25229300	-1.14602600
C	-1.85351000	-5.08801300	0.10317200
C	-4.17539200	-4.37941000	-0.15618400
C	-3.68436700	-6.40979900	1.16613000
C	-4.19298800	-5.96955400	2.54523900
C	-5.63250400	-4.61398100	0.15543900
C	-5.65607600	-5.52075800	2.55315000
C	-5.95169800	-4.33478100	1.63564600
H	-2.42229600	-2.43330800	-2.00456900
H	-2.07259800	-2.32789500	-0.28260200
H	-1.91029600	-4.83386700	-2.02698200
H	-0.55696100	-4.00542500	-1.23937900
H	-1.43091500	-4.58735200	0.98698500
H	-1.36355700	-6.06239800	0.01050200
H	-4.43863600	-7.03324400	0.67063400
H	-2.79625300	-7.03561800	1.28723500
H	-3.54481400	-5.16471200	2.91608900
H	-4.07946600	-6.81364500	3.23525000

H	-5.93293300	-5.63356700	-0.11137700
H	-6.20288700	-3.94846900	-0.48918300
H	-6.28848800	-6.36790200	2.25012900
H	-5.94785300	-5.27111200	3.58000700
H	-7.01359900	-4.07896100	1.72246600
H	-5.39763100	-3.44553500	1.96330100
H	-8.65054800	-4.70209700	3.43688400
H	-11.27412100	-7.99599700	0.82689900
Cl	-8.80056600	-7.14582600	4.92328500
H	-3.95008900	-1.17779600	0.69304100
H	-5.06203700	-2.14989200	-0.87840600

TS10-11

O	-9.13855500	-3.96978600	1.16496300
C	-8.49425300	-3.36014800	0.12899100
O	-5.76584800	-1.05848500	1.65609600
O	-8.02731900	-3.93048500	-0.82586400
C	-9.56600400	0.41994000	3.55124300
C	-8.33700900	0.58602500	2.92090000
C	-7.96117100	-0.25394200	1.87759100
C	-8.84286800	-1.24582700	1.43644300
C	-10.08351200	-1.40291400	2.05234800
C	-10.43154100	-0.58151700	3.11847600
N	-8.46249700	-2.00863800	0.30516000
C	-6.62287800	-0.12749300	1.21862700
N	-6.42945600	0.76845200	0.33191400
C	-9.24038400	-5.34736800	1.19887000
C	-8.17714600	-6.18627500	0.87743400
C	-10.44964400	-5.85313300	1.66221000
C	-8.36513100	-7.55471500	1.02639200
C	-10.60269700	-7.22743400	1.80430400
C	-9.56201800	-8.09383300	1.48505000
H	-9.84884100	1.06969000	4.37306900
H	-7.65113700	1.36491000	3.24095700
H	-10.76746200	-2.15960100	1.68671700
H	-11.39618700	-0.71285000	3.59878500
H	-7.89098000	-1.53723600	-0.38645800
H	-11.24836300	-5.16235600	1.90912900
H	-9.66943000	-9.16751100	1.58803200
N	-1.46058600	0.87621600	0.63242000
N	-3.37922400	-0.49580300	0.51637700
C	-2.81092000	-1.25205600	-0.59227200
C	-1.28840600	-1.24729500	-0.56464300
C	-0.80097400	0.19116300	-0.47636800

C	-2.70513900	0.48070200	1.03228900
C	-0.83999000	2.10542600	1.12036800
C	-1.58187100	3.39144000	0.73840200
C	-3.36497900	1.26342800	2.14539900
C	-2.75573900	3.71679600	1.66217300
C	-3.85234700	2.65317900	1.69588600
H	-3.19749800	-2.27392800	-0.53780500
H	-3.17112900	-0.82890400	-1.54030400
H	-0.93843500	-1.80110900	0.31327600
H	-0.87431900	-1.72817700	-1.45529500
H	-0.99276900	0.72163000	-1.42094500
H	0.27870100	0.21875500	-0.29687100
H	-0.71331800	2.05667200	2.20982900
H	0.16621700	2.12351400	0.69347400
H	-1.92283500	3.30381600	-0.30148900
H	-0.86758200	4.22236000	0.77054700
H	-2.67888800	1.36479600	2.99572500
H	-4.21231100	0.66420500	2.48391700
H	-2.36554700	3.85544100	2.68066300
H	-3.19354700	4.67577200	1.36413900
H	-4.64029800	2.97725600	2.38364200
H	-4.33018200	2.56714900	0.71255800
H	-7.24220400	-5.78801000	0.50763500
H	-11.54327900	-7.62877300	2.16724400
Cl	-7.04720800	-8.62911700	0.62939300
H	-5.47173100	0.68992600	-0.02593500
H	-4.86797800	-0.92707000	1.20603100

Int11

O	-8.39062100	-3.27993700	1.26568000
C	-7.12695500	-3.48107300	0.77137300
O	-4.68522300	0.95749600	1.19810500
O	-6.89425400	-4.06669100	-0.25966400
C	-6.81424400	-0.02608900	4.56151400
C	-5.95264100	0.23524800	3.50537600
C	-5.72172100	-0.71532500	2.50623900
C	-6.39339300	-1.95248000	2.57454300
C	-7.25850500	-2.21019600	3.64005100
C	-7.47038400	-1.25347500	4.62330200
N	-6.17590600	-2.93494500	1.57913200
C	-4.80732000	-0.36080100	1.38198700
N	-4.23745000	-1.27226200	0.68567300
C	-9.46029200	-3.53520000	0.42888500
C	-10.37416200	-2.49729800	0.28190500

C	-9.64591300	-4.76408400	-0.19657400
C	-11.48599200	-2.70408400	-0.52476800
C	-10.76943500	-4.93830600	-0.99822600
C	-11.69768300	-3.91493300	-1.17351400
H	-6.97524000	0.72255900	5.33019700
H	-5.44526000	1.19034000	3.42813200
H	-7.75845800	-3.17064000	3.68382500
H	-8.14512300	-1.47295000	5.44496100
H	-8.91258200	-5.54967100	-0.07107200
H	-12.57266400	-4.04955200	-1.79905100
N	-5.84078800	0.67833700	-3.36705100
N	-4.55866100	1.14265700	-1.43873200
C	-3.35668100	1.33199800	-2.24016600
C	-3.67582000	1.76305300	-3.66533800
C	-4.68876300	0.79430400	-4.25592800
C	-5.67483400	0.83442100	-2.02152200
C	-7.07544900	0.14313400	-3.94337700
C	-7.38976500	-1.30695000	-3.55655500
C	-6.88239000	0.59533200	-1.14455300
C	-8.06441800	-1.44822500	-2.19179000
C	-7.23766300	-0.89983500	-1.03058500
H	-2.73099600	2.07879900	-1.74188100
H	-2.77853400	0.39633000	-2.25601700
H	-4.10587100	2.77034000	-3.65467000
H	-2.77318900	1.78647200	-4.28234400
H	-4.22965600	-0.19208100	-4.41835800
H	-5.04394800	1.15588800	-5.22594600
H	-7.92078700	0.79172600	-3.68167100
H	-6.95396700	0.21721900	-5.02721000
H	-6.45916800	-1.88857500	-3.58251000
H	-8.05007800	-1.72940900	-4.32268200
H	-7.74250700	1.16018700	-1.52455000
H	-6.64169100	0.99857100	-0.15982800
H	-9.03439200	-0.92970200	-2.22054400
H	-8.27637600	-2.50645900	-2.00208200
H	-7.79729600	-1.04229400	-0.09676600
H	-6.31200000	-1.47824300	-0.92612100
H	-10.20674700	-1.55356600	0.78895600
H	-10.92504800	-5.88894300	-1.49775400
Cl	-12.63155300	-1.40441300	-0.73329300
H	-3.66037500	-0.85839600	-0.04796700
H	-4.49956100	1.12549700	0.20387500
H	-5.27842100	-2.83111800	1.09560000

TS11-12

O	-8.08324900	-1.21033200	-0.64725400
C	-7.00842500	-2.14689000	-0.57345700
O	-4.72794300	0.66456900	1.25118900
O	-6.69891500	-2.82708100	-1.53159100
C	-7.18358800	-0.58519600	4.34358500
C	-6.47017000	-0.08691300	3.26587800
C	-6.42826500	-0.77690900	2.05086800
C	-7.12450100	-1.99614000	1.90498800
C	-7.82394200	-2.50201800	3.01164000
C	-7.85085300	-1.80582800	4.20853200
N	-7.05037900	-2.72024200	0.73398300
C	-5.57744700	-0.29785700	0.95350900
N	-5.68189400	-0.86620200	-0.19976700
C	-8.18624900	-0.37285200	-1.70866800
C	-9.18350600	0.60176300	-1.58004100
C	-7.38964600	-0.40882200	-2.86048900
C	-9.37918400	1.51375200	-2.60381100
C	-7.61510600	0.52772600	-3.86690300
C	-8.60775500	1.49723800	-3.76194700
H	-7.21512500	-0.04136900	5.28117700
H	-5.91505400	0.84161800	3.34531700
H	-8.35577100	-3.44397300	2.91073700
H	-8.40683900	-2.21537000	5.04673700
H	-6.64845500	-1.18701200	-2.97561900
H	-8.78722200	2.21805400	-4.55219800
N	-3.81903200	3.16845500	-2.65878800
N	-3.69467200	1.52001700	-0.97961000
C	-2.69586700	0.76810500	-1.72965000
C	-1.89507200	1.66333300	-2.66481900
C	-2.86209000	2.47227800	-3.51595100
C	-4.17805600	2.62127000	-1.46607700
C	-4.52401800	4.31403800	-3.23590600
C	-5.99006800	4.04800800	-3.59497400
C	-5.24521900	3.32236000	-0.65917400
C	-6.93824600	4.15299800	-2.40163300
C	-6.64527500	3.15869000	-1.27957700
H	-2.03991300	0.26746800	-1.01119200
H	-3.19068500	-0.02381400	-2.31127400
H	-1.27494600	2.34704000	-2.07538800
H	-1.23448400	1.07276800	-3.30535600
H	-3.39206100	1.81914000	-4.22453200
H	-2.32192300	3.22382500	-4.09950200
H	-4.45459200	5.17346700	-2.55709400

H	-3.96644700	4.58483700	-4.13600800
H	-6.06825300	3.05273400	-4.05208400
H	-6.29253100	4.77695300	-4.35593200
H	-4.99968200	4.38576500	-0.54869000
H	-5.22739100	2.87973500	0.33776100
H	-6.87723100	5.17341600	-1.99573000
H	-7.96917500	4.01542600	-2.74320100
H	-7.39261500	3.28743300	-0.48962700
H	-6.75441800	2.12851700	-1.64373200
H	-9.78424100	0.62687800	-0.67825300
H	-7.00797500	0.48746500	-4.76715800
Cl	-10.61429300	2.73898300	-2.42026400
H	-5.05255100	-0.55190100	-0.93359900
H	-7.42749700	-3.65856800	0.73062200
H	-4.24652800	0.99749400	0.38787200

Int12

O	-6.20558000	-4.42317800	3.52755600
C	-4.52759100	-1.66181600	0.69093500
O	-4.82473800	-2.08974300	-0.40879700
C	-4.34520400	1.08649400	4.94557100
C	-4.02860600	-0.22901400	4.64910300
C	-4.10983900	-0.69236400	3.33554200
C	-4.52289700	0.16832200	2.31325600
C	-4.82806300	1.50109100	2.60530000
C	-4.73989700	1.94663900	3.91549900
N	-4.64386300	-0.33036900	1.02292900
C	-3.82489000	-2.10630100	3.02927600
C	-6.66951300	-3.16348600	3.55742900
C	-6.74479800	-2.52958500	4.80397100
C	-7.07088800	-2.47119300	2.40684900
C	-7.21237000	-1.22677700	4.87278500
C	-7.53094300	-1.16225100	2.51117400
C	-7.60748600	-0.51723300	3.74275800
H	-4.30092900	1.44356100	5.96823200
H	-3.73295700	-0.93589700	5.41810500
H	-5.14655900	2.16919500	1.81013600
H	-4.99017800	2.97881300	4.14069200
H	-5.02875700	0.25133600	0.29069200
H	-7.00288900	-2.95757200	1.43646100
H	-7.95537900	0.50523300	3.83041000
N	-3.62421900	-7.04850100	0.55232800

N	-5.01273400	-5.24791700	1.19185700
C	-5.69419700	-5.26730600	-0.10030200
C	-5.64221000	-6.63924300	-0.75824100
C	-4.19862600	-7.11587900	-0.78948400
C	-4.05922400	-6.09826600	1.42783700
C	-2.43637000	-7.85973600	0.81124100
C	-1.12219500	-7.07175000	0.84958300
C	-3.34716300	-5.98266800	2.75569200
C	-0.86404900	-6.39036100	2.19384000
C	-1.93517300	-5.38515400	2.61463500
H	-6.73413000	-4.96513300	0.06539700
H	-5.24821100	-4.50100600	-0.74596900
H	-6.24100900	-7.35092300	-0.17942300
H	-6.04684400	-6.60356100	-1.77363200
H	-3.60717500	-6.50585600	-1.48768100
H	-4.14333300	-8.15491500	-1.12890500
H	-2.56348600	-8.41849700	1.74677900
H	-2.39819000	-8.60186900	0.00965000
H	-1.13353600	-6.33209100	0.03834200
H	-0.29903800	-7.76409800	0.63770200
H	-3.29493000	-6.96129800	3.24885200
H	-3.94890300	-5.32370100	3.38430300
H	-0.78825100	-7.16863600	2.96675100
H	0.11008000	-5.88973300	2.16273300
H	-1.66405000	-4.94226500	3.57686300
H	-1.96917800	-4.54966300	1.90238800
H	-6.41373000	-3.06199000	5.68786900
H	-7.83273200	-0.63289000	1.61144100
Cl	-7.28018700	-0.43949500	6.43451500
N	-4.02535700	-2.46317100	1.69954700
O	-3.45471300	-2.92585900	3.84764100
H	-4.09832900	-3.46909100	1.50858400
H	-5.88111300	-4.67629400	2.61699100

For other ILs

[HDBU⁺][Im⁻]-Int1

0 1

C	1.02162900	-1.78353500	2.23649400
O	-0.05622400	-2.00596600	1.64894500
O	1.28831700	-1.50757300	3.40594600
C	-3.74817300	-0.43608600	0.25954100
C	-2.91150700	-1.45871100	0.67651700
C	-3.28771800	-2.79092500	0.45734900

C	-4.50228100	-3.12082500	-0.18339200
C	-5.32971000	-2.06599000	-0.59413700
C	-4.95386300	-0.75020600	-0.37321200
N	-4.83883300	-4.43367600	-0.44425100
C	-2.45681400	-3.87136500	0.89890800
N	-1.86476900	-4.81038200	1.23827000
H	-3.46604300	0.59757500	0.42368300
H	-1.96222000	-1.26853700	1.16986200
H	-6.26609200	-2.29513000	-1.09499500
H	-5.61451700	0.04661100	-0.70212800
H	-4.36177900	-5.14250100	0.09815200
H	-5.82120400	-4.62156300	-0.58437300
N	2.49724500	-5.33105500	3.34943500
N	0.41960300	-4.32491700	3.26418900
C	0.35648200	-3.99691700	4.68662600
C	1.76818600	-3.95636400	5.24735700
C	2.53889500	-5.19398900	4.80975500
C	1.45660400	-4.86684300	2.66131600
C	3.60029400	-6.02835700	2.67470200
C	3.20074300	-7.38420100	2.08412700
C	1.39990300	-5.01771500	1.17037900
C	2.48014100	-7.29571600	0.73674200
C	1.18538900	-6.48267200	0.75393500
H	-0.10471400	-3.01113700	4.75866900
H	-0.26601900	-4.74033300	5.19696600
H	2.25293600	-3.05501100	4.86223200
H	1.74199600	-3.90613900	6.33846600
H	2.13056600	-6.10312000	5.27101400
H	3.58890200	-5.11175700	5.10074900
H	4.02060700	-5.36521000	1.90832200
H	4.37104800	-6.16980100	3.43515600
H	2.58073700	-7.91488200	2.81848100
H	4.11472100	-7.97494700	1.95615600
H	2.32608200	-4.62498700	0.73302100
H	0.58194100	-4.38898500	0.81388700
H	3.16423600	-6.84333400	0.00620900
H	2.26885300	-8.30991800	0.38092900
H	0.75211700	-6.47952700	-0.25037500
H	0.43698700	-6.94297500	1.41035500
H	-0.25183800	-3.86165800	2.64736200
N	2.20972900	-2.00334700	1.37256900
C	3.48586500	-2.25991200	1.81090700
C	2.21602500	-2.18401700	0.02382000
C	4.20000300	-2.59193800	0.68834500

H	3.74242600	-2.15420400	2.85339400
H	1.31303800	-2.05847800	-0.55652300
H	5.24969000	-2.84363100	0.61420100
N	3.39666500	-2.53885200	-0.43111000

[HDBU⁺][Im⁻]-TS1-2

0 1

C	0.13575900	-1.80800700	2.31839000
O	-1.11087800	-1.57062600	2.01841500
O	0.65457200	-1.67225300	3.40210900
C	-3.90582700	-0.12601100	-0.55617000
C	-2.98603700	-0.71410500	0.29747100
C	-2.97204500	-2.09746900	0.52366700
C	-3.91614100	-2.92027200	-0.14676300
C	-4.84649800	-2.30285200	-1.00429600
C	-4.84185700	-0.93466200	-1.20409200
N	-3.91209000	-4.28586300	-0.01599600
C	-2.02022700	-2.74386000	1.44592200
N	-1.86380500	-3.89213800	1.82292700
H	-3.89847600	0.94710800	-0.71171500
H	-2.26186300	-0.10165500	0.81984100
H	-5.56934000	-2.93013000	-1.51971800
H	-5.57415900	-0.49280600	-1.87377500
H	-3.37041100	-4.65052000	0.76324400
H	-4.76975600	-4.76317700	-0.25027100
N	2.33154200	-5.46423100	3.02118800
N	0.11444700	-4.76322500	3.21481800
C	0.23498400	-4.43012600	4.62860600
C	1.68602300	-4.16947500	5.00417600
C	2.56755800	-5.28339700	4.45527900
C	1.10969700	-5.22323200	2.50906500
C	3.42382700	-5.98286500	2.19155100
C	3.24181300	-7.44340300	1.76920600
C	0.84126100	-5.55468900	1.06376700
C	2.29308100	-7.62390800	0.58401700
C	0.88371000	-7.07255700	0.80451800
H	-0.37183800	-3.53840400	4.80554400
H	-0.18324000	-5.25327600	5.22109600
H	1.98971600	-3.20910400	4.57923100
H	1.79711800	-4.11340700	6.09037400
H	2.37643400	-6.22885000	4.98160100
H	3.62358500	-5.03598800	4.59137100
H	3.55181900	-5.33221700	1.31668800
H	4.33036200	-5.88333300	2.79295600

H	2.88865600	-8.01744700	2.63586800
H	4.22471400	-7.84658600	1.50025600
H	1.56630400	-5.04152200	0.42300200
H	-0.14601300	-5.15775800	0.81818100
H	2.72950800	-7.12180600	-0.29016800
H	2.23008100	-8.68858700	0.33341100
H	0.28528800	-7.27579300	-0.08892900
H	0.39227400	-7.59821000	1.63336300
H	-0.84530600	-4.37429000	2.62003800
N	0.94539000	-2.22069600	1.21193200
C	2.26853700	-2.56844900	1.31021500
C	0.61603700	-2.28640600	-0.12992000
H	2.77229500	-2.57565100	2.26647700
C	1.75849400	-2.68328800	-0.76007700
H	-0.37251400	-2.03659200	-0.48505100
H	1.90977200	-2.84910500	-1.81700200
N	2.78711600	-2.86507700	0.14884500

[HDBU⁺][Im⁻]-Int6

0 1

C	-4.96695000	-1.48194100	0.91197600
O	-5.47243200	-1.94316700	-0.09251700
C	-3.82696500	1.21471400	5.05776400
C	-3.32420500	0.04269500	4.51765200
C	-3.84502700	-0.46061500	3.32461100
C	-4.88584700	0.21057200	2.67264400
C	-5.40350900	1.38839500	3.22151700
C	-4.87229100	1.87800100	4.40413400
N	-5.39146600	-0.31014400	1.49285900
C	-3.37626400	-1.75371600	2.79403100
C	-6.38519700	-2.71041900	3.78599400
C	-7.63936800	-2.58129500	1.99220500
C	-7.32304000	-1.71902700	3.91553200
H	-3.42254300	1.61209600	5.98213200
H	-2.52881500	-0.51737000	4.99897500
H	-6.22178100	1.89932100	2.72338100
H	-5.27951700	2.79111100	4.82732300
H	-6.25548500	0.05651600	1.11300900
H	-7.99317300	-2.79348900	0.99288400
N	-3.71426700	-7.06527300	0.77262900
N	-4.68809700	-4.91765800	0.96628700
C	-5.31002000	-5.05217200	-0.34791200
C	-5.56810900	-6.50701100	-0.71593900
C	-4.27622900	-7.29374000	-0.55621800

C	-3.95143800	-5.88294800	1.41572100
C	-2.72003600	-8.02445400	1.24663100
C	-1.27385400	-7.51780700	1.20357100
C	-3.25541100	-5.65409200	2.73768200
C	-0.90181200	-6.64905600	2.40563200
C	-1.74875200	-5.38832100	2.57161800
H	-6.23755700	-4.47201000	-0.34517600
H	-4.66725700	-4.57197200	-1.09728500
H	-6.32801200	-6.92667000	-0.04732000
H	-5.93609200	-6.59646900	-1.74201700
H	-3.55166200	-7.00408100	-1.33171200
H	-4.46289500	-8.36709300	-0.66472100
H	-2.96959700	-8.35052700	2.26442900
H	-2.82142000	-8.90488100	0.60663100
H	-1.12449300	-6.96475900	0.26698700
H	-0.60453200	-8.38545500	1.17148300
H	-3.42048300	-6.49856400	3.41857500
H	-3.71747600	-4.76970400	3.18159200
H	-0.99710200	-7.25985400	3.31498000
H	0.15420100	-6.36618700	2.33310400
H	-1.40757700	-4.83113500	3.44793400
H	-1.60342100	-4.71360500	1.71792300
H	-5.59867400	-3.05996900	4.43869400
N	-3.91230700	-2.10386600	1.56637100
O	-2.59098300	-2.48624400	3.37196900
H	-3.78381700	-3.07615200	1.26516100
H	-7.47484900	-1.05295400	4.75356000
N	-6.60509800	-3.26303400	2.54829900
H	-5.99362500	-3.94251200	2.07649700
N	-8.10251400	-1.64073400	2.78655600

[HDBU⁺][TFE⁻]-Int1

0 1

O	-0.11787400	0.87882900	-0.93809300
C	-0.02718800	-0.55171900	-1.16644800
O	0.57537100	-1.10840700	-0.23891800
O	-0.60616700	-0.98326800	-2.16651800
C	3.96265800	1.46355500	-0.12605400
C	2.97639800	0.68114300	0.45186000
C	3.30936900	-0.19499000	1.49481400
C	4.63259200	-0.29510400	1.97925600
C	5.61144100	0.50543700	1.37474400
C	5.27589900	1.36547400	0.34060400
N	4.94519800	-1.11275700	3.04931300

C	2.32362400	-1.02746300	2.11600300
N	1.62065900	-1.73500400	2.70853800
H	3.70804400	2.13570800	-0.93613700
H	1.94831900	0.71404100	0.10681900
H	6.63514500	0.44674500	1.73384400
H	6.05541500	1.97204100	-0.11129600
H	4.29068200	-1.85700600	3.25475200
H	5.91165600	-1.39992700	3.11319900
N	-2.35779000	-1.84147400	0.08625100
N	-0.91655000	-2.77251500	1.63742300
C	-0.78458000	-4.03799800	0.91868200
C	-1.01498700	-3.80126900	-0.56563400
C	-2.31551900	-3.04200100	-0.76827300
C	-1.57443000	-1.73181700	1.14578300
C	-3.15113500	-0.70003300	-0.39766200
C	-4.27782300	-0.29201500	0.55309600
C	-1.46997600	-0.43417100	1.89548800
C	-3.81766100	0.58958000	1.71447700
C	-2.77173900	-0.05576400	2.62271400
H	0.22334200	-4.41237900	1.10901400
H	-1.50222600	-4.76015400	1.32595800
H	-0.20163300	-3.19235500	-0.96779200
H	-1.06484600	-4.75374200	-1.09938100
H	-3.19431500	-3.66221000	-0.54911900
H	-2.36105900	-2.68787200	-1.79874400
H	-2.48008900	0.14084900	-0.60598600
H	-3.56207000	-1.01561100	-1.35724400
H	-4.77268200	-1.19687200	0.92861800
H	-5.02459800	0.25818200	-0.03024500
H	-1.16219300	0.34422100	1.18727100
H	-0.65245300	-0.54200600	2.61137200
H	-3.39658400	1.51660600	1.30238000
H	-4.68735900	0.87965200	2.31408900
H	-2.51652400	0.64784300	3.42118300
H	-3.18951500	-0.94489600	3.11255800
H	-0.15519600	-2.53017200	2.27157900
C	-0.36531600	1.66695700	-2.06520500
H	-1.01666000	2.50583600	-1.79872100
H	-0.81408200	1.07633300	-2.86837700
C	0.95001500	2.23571200	-2.54687900
F	1.83301500	1.26816600	-2.81921600
F	0.78101500	2.97220900	-3.65615100
F	1.51409400	3.03050400	-1.61950700

[HDBU⁺][TFE⁻]-TS1-2

0 1

O	0.67555000	0.36174300	-0.96902300
C	0.83314100	-0.89028300	-1.52156400
O	1.75074800	-1.57970200	-0.93574900
O	0.13712300	-1.24071700	-2.45486800
C	5.35456500	0.43233600	-0.85664300
C	4.11799100	-0.18754500	-0.76926800
C	3.51755000	-0.44918100	0.46762900
C	4.17732400	-0.05462500	1.66098900
C	5.43711000	0.56204400	1.55252500
C	6.01414300	0.79944000	0.31781500
N	3.59984400	-0.21946800	2.89665000
C	2.22365100	-1.12424100	0.60673100
N	1.49099400	-1.46620900	1.50875300
H	5.80138300	0.62415700	-1.82588300
H	3.59910300	-0.49158600	-1.66930500
H	5.94674100	0.86325400	2.46429600
H	6.98714400	1.28016600	0.26968800
H	2.79198400	-0.83458800	2.93011900
H	4.22696500	-0.24221300	3.68681000
N	-2.88508900	-1.58577000	-0.17453800
N	-0.75929600	-2.26620900	0.48256500
C	-0.77454000	-3.49709800	-0.30104900
C	-1.83337500	-3.43474900	-1.39326900
C	-3.13090700	-2.87612000	-0.82614600
C	-1.72416900	-1.39190100	0.47859200
C	-4.01268600	-0.66340400	-0.02938600
C	-4.62263000	-0.63657800	1.37595800
C	-1.53210000	-0.14633000	1.30637200
C	-3.84947700	0.24062900	2.36223900
C	-2.39228800	-0.16782700	2.58295600
H	0.22480700	-3.60260000	-0.73367800
H	-0.94831300	-4.33955500	0.37874300
H	-1.47556400	-2.78474900	-2.19476500
H	-2.01211700	-4.43210700	-1.80367800
H	-3.57974900	-3.57084700	-0.10186500
H	-3.85649200	-2.71064400	-1.62636700
H	-3.70359600	0.34570700	-0.32823100
H	-4.76061700	-0.98739800	-0.75627900
H	-4.69198700	-1.66709800	1.74787800
H	-5.64815200	-0.25877800	1.29679800
H	-1.77360300	0.73861500	0.70556800
H	-0.47102400	-0.08783200	1.55912500
H	-3.87083500	1.27631700	1.99497800

H	-4.37170400	0.24343400	3.32497700
H	-1.93954300	0.51914100	3.30431300
H	-2.33862700	-1.16775900	3.03144200
H	0.23134500	-1.97790900	0.99742600
C	-0.25815900	1.17097200	-1.63707600
H	-0.37780200	2.06176000	-1.01906300
H	-1.21456900	0.65482200	-1.76932300
C	0.23542200	1.61428000	-3.02378500
F	-0.48095300	1.07772700	-4.01350300
F	0.11858500	2.94984200	-3.14256100
F	1.51669500	1.30100200	-3.21566200

[HDBU⁺][TFE⁻]-Int6

0 1

O	-3.85107200	-3.25098900	5.75420600
C	-4.24548400	-1.91581500	7.99132800
O	-2.66350500	-4.79477200	9.38637000
O	-5.35992200	-1.56345300	7.67438500
C	0.77642800	-2.41852200	8.58194000
C	-0.30472900	-3.24056500	8.86189400
C	-1.60464000	-2.81137900	8.58932300
C	-1.82663300	-1.55077600	8.02012600
C	-0.73407900	-0.72342500	7.72660000
C	0.55033600	-1.15888100	8.01252500
N	-3.12405100	-1.13869400	7.78131800
C	-2.75638100	-3.67802000	8.91179500
N	-3.98984600	-3.10174700	8.66679800
H	1.78668600	-2.74183900	8.80968200
H	-0.17776600	-4.22508400	9.30151900
H	-0.90378900	0.25540000	7.28776600
H	1.39031800	-0.50718000	7.79159600
H	-3.29844200	-0.29766600	7.24786000
N	0.17774600	-5.62729300	6.47581000
N	-2.13391000	-5.25310600	6.16331600
C	-2.48420100	-6.52383600	6.78725500
C	-1.36562300	-7.10086800	7.64541000
C	-0.04791100	-7.00760100	6.89172500
C	-0.90121800	-4.89098900	6.05519600
C	1.54567500	-5.23345000	6.16535500
C	1.90625000	-5.28192700	4.67511800
C	-0.62173000	-3.57570600	5.36381900
C	1.45628100	-4.03869200	3.90740100
C	-0.04890700	-3.77169700	3.94820200

H	-3.37466900	-6.35734100	7.40034300
H	-2.77167100	-7.22651200	5.99359500
H	-1.29618000	-6.52205300	8.57059400
H	-1.57689300	-8.14201700	7.90745600
H	-0.05322100	-7.67635600	6.01667500
H	0.78673800	-7.30989400	7.53200000
H	1.73597600	-4.22773200	6.56248700
H	2.19220900	-5.91551000	6.72491900
H	1.46507900	-6.18614200	4.23535000
H	2.99406500	-5.38146400	4.58082700
H	0.05792600	-2.96094800	5.96634900
H	-1.57427000	-3.04551000	5.30624100
H	1.97657200	-3.16641000	4.32858400
H	1.78128200	-4.11984500	2.86390900
H	-0.25637100	-2.86791500	3.36534200
H	-0.59213600	-4.58928200	3.45678100
H	-4.79510500	-3.71125500	8.75683600
H	-3.30388700	-4.09870900	5.79506000
C	-5.09796300	-3.45505800	5.17547500
H	-5.71595000	-2.57172100	5.36113500
H	-5.05304300	-3.63969000	4.09140900
C	-5.81625100	-4.64207700	5.77774100
F	-7.03179500	-4.79344500	5.23516700
F	-5.97944200	-4.53175000	7.10736200
F	-5.13424900	-5.78277600	5.56612600

[HDBU⁺][2-Br-PhO⁻]-Int1

0 1

O	0.21327400	-2.88653000	0.48556800
C	0.82670200	-2.76845400	1.80691400
O	0.04515400	-2.27806400	2.62040000
O	1.97882700	-3.21073200	1.90874400
C	-2.67426700	-0.27884000	-0.14345500
C	-2.29915200	-1.23637300	0.78477800
C	-2.94249700	-2.47881200	0.78903400
C	-3.94997100	-2.79552900	-0.14537200
C	-4.30915900	-1.81157900	-1.07517800
C	-3.68068300	-0.57550100	-1.06624400
N	-4.51265600	-4.05950500	-0.18514600
C	-2.59660100	-3.48457600	1.74558400
N	-2.44744600	-4.35007500	2.50302600
C	0.93556900	-3.33981100	-0.56343800
C	0.35417500	-4.27431000	-1.43115700
C	2.23247200	-2.89648100	-0.85174600

C	1.03311100	-4.75448300	-2.54647700
C	2.91459900	-3.37695500	-1.96194200
C	2.32185800	-4.30766700	-2.81385000
H	-2.18214500	0.68693600	-0.15927000
H	-1.49841200	-1.08039000	1.50110700
H	-5.07718000	-2.03443900	-1.81047100
H	-3.97715300	0.16943400	-1.79897900
H	-4.44881000	-4.60225900	0.66762400
H	-5.41900200	-4.11984700	-0.62821900
H	2.69164400	-2.18738500	-0.17516700
N	2.25531000	-5.73933100	3.32888200
N	0.10469300	-5.03587600	3.79568500
C	0.43609500	-4.24911200	4.98484800
C	1.92454700	-3.95031300	4.98186200
C	2.68277700	-5.22802600	4.64014300
C	0.98754800	-5.56444200	2.97042200
C	3.27320800	-6.03401900	2.30622600
C	3.22046000	-7.46254500	1.76004400
C	0.50092100	-5.96018700	1.60909500
C	2.14123300	-7.69275900	0.70374800
C	0.72135900	-7.41925700	1.19528700
H	-0.14055100	-3.32516900	4.90978600
H	0.13287500	-4.80540900	5.87887100
H	2.13284200	-3.19980900	4.21437300
H	2.23688800	-3.58069300	5.96173100
H	2.50948000	-6.00330700	5.39761100
H	3.75576500	-5.04071000	4.58813100
H	3.18274900	-5.28338200	1.51035900
H	4.23638400	-5.87380000	2.79311600
H	3.08942200	-8.15667700	2.59992400
H	4.19901800	-7.68084800	1.31730800
H	1.01980500	-5.30235500	0.90222900
H	-0.55771500	-5.70126100	1.54768300
H	2.34012200	-7.03654800	-0.15532700
H	2.21028600	-8.72299500	0.33750400
H	0.02028800	-7.61638900	0.37722200
H	0.45834300	-8.09612200	2.01797500
H	-0.83200300	-4.89285300	3.41248200
H	3.91877300	-3.01733400	-2.16450500
H	0.54311100	-5.47368100	-3.19395400
H	2.85400500	-4.68127500	-3.68251400
Br	-1.39715800	-4.90500900	-1.08049100

[HDBU⁺][2-Br-PhO⁻]-TS1-2

0 1

O	0.84100600	0.53696900	-1.02208900
C	0.41922500	-0.74732100	-1.29222100
O	1.28516600	-1.61647400	-0.87267700
O	-0.62875000	-0.98381300	-1.85668800
C	5.02958900	0.15595500	-1.34682700
C	3.83311800	-0.48999300	-1.07837400
C	3.31151400	-0.54982200	0.21718100
C	4.01028300	0.06990000	1.28268800
C	5.21708800	0.72763400	0.99127500
C	5.71881400	0.76720000	-0.29826600
N	3.50427000	0.09493200	2.56776200
C	2.06555500	-1.25680200	0.53430500
N	1.52978400	-1.64100800	1.55480000
C	-0.04137300	1.58584100	-1.04444900
C	-0.03907700	2.42551400	0.07435800
C	-0.89371000	1.84929000	-2.11261100
C	-0.89295300	3.51989600	0.13051200
C	-1.75179100	2.94459000	-2.04920300
C	-1.75398600	3.77778100	-0.93370100
H	5.42002700	0.18719000	-2.35811300
H	3.27998600	-0.97175100	-1.87576200
H	5.75094500	1.21600100	1.80257700
H	6.65623300	1.28193200	-0.48836200
H	2.80913100	-0.62259500	2.76025200
H	4.18954600	0.24030700	3.29614400
H	-0.88494100	1.18432700	-2.96647400
H	-2.42160400	4.63198400	-0.88849400
N	-2.75726200	-2.15463900	-0.03771600
N	-0.77701700	-2.63890800	1.09833200
C	-0.74371100	-3.99476400	0.57623700
C	-1.33632500	-4.01963100	-0.82522600
C	-2.73355500	-3.41863100	-0.78872300
C	-1.71428400	-1.80762000	0.73752500
C	-3.76336300	-1.16809900	-0.44230500
C	-4.61580900	-0.62075100	0.70682100
C	-1.58523500	-0.38762800	1.21623000
C	-3.95630200	0.48827000	1.52609900
C	-2.65893500	0.06888900	2.21304800
H	0.30387100	-4.30971900	0.57019700
H	-1.29449600	-4.66457400	1.24958000
H	-0.70341600	-3.41608900	-1.48117900
H	-1.38842100	-5.03980300	-1.21521900
H	-3.45502500	-4.11568500	-0.34279200

H	-3.06249400	-3.19710400	-1.80818200
H	-3.27867800	-0.35573200	-1.00288800
H	-4.42056400	-1.68886000	-1.14220000
H	-4.89819400	-1.45911500	1.35627700
H	-5.54294400	-0.22952800	0.27224900
H	-1.61991000	0.26852600	0.33888300
H	-0.59239800	-0.28509300	1.66064200
H	-3.73578800	1.33488200	0.86001600
H	-4.66897200	0.85329500	2.27402400
H	-2.25226600	0.92497700	2.76194600
H	-2.84662500	-0.72302100	2.94878900
H	-2.41777900	3.14731500	-2.88166700
H	0.30524400	-2.17759400	1.41585400
H	-0.87980500	4.15717300	1.00796200
Br	1.10304700	2.00381100	1.51312800

[HDBU⁺][2-Br-PhO⁻]-Int6

0 1

O	-5.97268800	-4.16709600	3.43361000
C	-4.70169700	-1.61284500	0.87969300
O	-5.11122400	-2.02919200	-0.18755700
C	-4.08646800	1.01575500	5.17098200
C	-3.69216500	-0.25027800	4.76971600
C	-3.95541200	-0.68565200	3.46999000
C	-4.61918600	0.15303100	2.56814900
C	-5.00394500	1.43748200	2.96605700
C	-4.73940200	1.85492700	4.26094500
N	-4.88626700	-0.31026400	1.28758900
C	-3.61586000	-2.06417900	3.06894700
C	-6.62689600	-2.99986700	3.37932700
C	-6.64887200	-2.17909100	4.51787000
C	-7.29035900	-2.54546200	2.23264600
C	-7.30549300	-0.95687900	4.51776100
C	-7.94383900	-1.31736100	2.22760100
C	-7.95761800	-0.51777600	3.36774600
H	-3.89049300	1.35636500	6.18170700
H	-3.19965700	-0.94118000	5.44554500
H	-5.51905700	2.08752200	2.26465300
H	-5.04928100	2.84876600	4.56959600
H	-5.47252600	0.23635700	0.67096100
H	-7.26224700	-3.15936600	1.33650500
H	-8.46552500	0.44099800	3.36766700
N	-3.62261500	-7.08558800	0.57018000
N	-4.91411200	-5.18908000	1.13083700

C	-5.57354000	-5.21724100	-0.17170700
C	-5.61619100	-6.61999600	-0.76089400
C	-4.20893200	-7.19463500	-0.76363500
C	-4.00776700	-6.07870000	1.40555800
C	-2.48361000	-7.95256600	0.86606600
C	-1.12628500	-7.24138500	0.86957400
C	-3.28719100	-5.94845100	2.72785400
C	-0.82983200	-6.51583600	2.18197900
C	-1.84427500	-5.43709800	2.55795600
H	-6.58754200	-4.82393400	-0.04785100
H	-5.06026500	-4.52047600	-0.84495400
H	-6.26307000	-7.25813500	-0.14887800
H	-6.01730100	-6.60817400	-1.77828000
H	-3.58076300	-6.67076000	-1.49881300
H	-4.22647100	-8.25376300	-1.03957900
H	-2.64081100	-8.46092900	1.82543100
H	-2.49031200	-8.73051800	0.09824800
H	-1.09652900	-6.53988900	0.02553700
H	-0.34463600	-7.98891600	0.69036400
H	-3.28759100	-6.90701200	3.26143100
H	-3.84493300	-5.23180600	3.33435700
H	-0.79459900	-7.26200700	2.98874000
H	0.16960400	-6.06975400	2.12993000
H	-1.54708100	-4.96594500	3.49815000
H	-1.83670900	-4.63282500	1.80961400
H	-8.44376500	-0.98878100	1.32099200
N	-3.99499300	-2.39838000	1.77193900
O	-3.06100200	-2.87033300	3.78892500
H	-3.99542600	-3.39509700	1.53219300
H	-5.73127400	-4.50923600	2.52327800
H	-7.28021400	-0.34713000	5.41473300
Br	-5.69969100	-2.73459900	6.04835600

[HDBU⁺][2,4-Cl-PhO⁻]-Int1

0 1

O	0.19285100	-2.94449600	0.44750400
C	0.83008000	-2.81002100	1.75842300
O	0.06266100	-2.30867900	2.57740700
O	1.98300900	-3.25141600	1.84538800
C	-2.69686200	-0.15970900	-0.00658400
C	-2.29369700	-1.18345200	0.83441400
C	-2.94540500	-2.42095100	0.77493100
C	-3.99096200	-2.66468900	-0.14034200
C	-4.37915000	-1.61235100	-0.98120400

C	-3.74171500	-0.38375800	-0.90762300
N	-4.56745800	-3.91547000	-0.24681600
C	-2.57701500	-3.49364000	1.64617800
N	-2.41096300	-4.42105500	2.32248500
C	0.89520900	-3.39667400	-0.61170300
C	0.26396700	-4.27515400	-1.50536400
C	2.21094600	-3.00941600	-0.89753400
C	0.91294200	-4.76100400	-2.63593800
C	2.87291300	-3.49029300	-2.01907900
C	2.22064000	-4.36686700	-2.87930700
H	-2.19915500	0.80267200	0.02885900
H	-1.46802200	-1.08097600	1.53186300
H	-5.17789800	-1.77698000	-1.69885000
H	-4.06169500	0.41400900	-1.57158500
H	-4.46027400	-4.53293800	0.54802100
H	-5.48749000	-3.94601600	-0.66273500
H	2.70972200	-2.34018600	-0.20957100
N	2.27760200	-5.70276600	3.33020500
N	0.07885000	-5.09231600	3.69400500
C	0.32293200	-4.29930200	4.89943300
C	1.78975200	-3.91185800	4.94706100
C	2.63834400	-5.14024900	4.64088000
C	1.01948100	-5.59289100	2.91747600
C	3.34696000	-6.00242200	2.36371600
C	3.37803900	-7.45919800	1.89753900
C	0.60748500	-6.06604700	1.55374000
C	2.33868900	-7.80092200	0.83142100
C	0.89593000	-7.54624500	1.26432600
H	-0.30585900	-3.41112900	4.81562400
H	0.02558700	-4.88254800	5.77822500
H	1.97759400	-3.14952100	4.18626600
H	2.04437500	-3.52189700	5.93570500
H	2.50539500	-5.91342100	5.40851400
H	3.69615400	-4.87721300	4.60631300
H	3.25553300	-5.29998000	1.52577900
H	4.28240200	-5.77095900	2.87517700
H	3.25704800	-8.11077200	2.77222300
H	4.37694600	-7.65476400	1.49142400
H	1.13846700	-5.43504400	0.83052900
H	-0.45650700	-5.84612300	1.43346700
H	2.54079700	-7.20113800	-0.06687500
H	2.45339300	-8.85101200	0.54149500
H	0.22411700	-7.85680800	0.45804000
H	0.64327800	-8.15825300	2.13954900

H	-0.84654500	-4.99246100	3.27097400
H	3.89142100	-3.18336600	-2.22979900
H	0.39823500	-5.43567900	-3.31020600
Cl	-1.37617900	-4.77552100	-1.20782400
Cl	3.05089200	-4.98178900	-4.28792700

[HDBU⁺][2,4-Cl-PhO⁻]-TS1-2

0 1

O	1.07585700	0.33166800	-1.29886000
C	1.09716200	-0.98601900	-1.72723900
O	1.97290700	-1.66364600	-1.06450500
O	0.38663500	-1.39410800	-2.61915000
C	5.78473900	-0.12827500	-0.73137900
C	4.50701400	-0.66527600	-0.71247400
C	3.66991600	-0.51681700	0.39866300
C	4.12840900	0.20793600	1.52814600
C	5.42625700	0.74747000	1.48988700
C	6.23875700	0.58034200	0.38228300
N	3.31977600	0.43664900	2.61826600
C	2.32712700	-1.09990300	0.46625500
N	1.47854900	-1.27572100	1.31367600
C	-0.02502200	1.12678900	-1.36218000
C	0.00087200	2.23105900	-0.49341000
C	-1.14357700	0.92534300	-2.17266400
C	-1.06940500	3.11279100	-0.42649100
C	-2.22702900	1.79804000	-2.09367500
C	-2.18560700	2.87923500	-1.22306700
H	6.41935500	-0.25842300	-1.60100200
H	4.13683700	-1.22471400	-1.56238900
H	5.77956000	1.31072600	2.34988400
H	7.23674200	1.00930100	0.38605100
H	2.50931000	-0.17159400	2.69255200
H	3.79424300	0.65425400	3.48250500
H	-1.15361500	0.08984100	-2.85755500
N	-2.96175800	-1.56581400	-0.22037900
N	-0.75363800	-2.09497300	0.31654300
C	-0.75705800	-3.34065800	-0.44299800
C	-1.83776000	-3.31884400	-1.51351200
C	-3.15210200	-2.84354800	-0.91126500
C	-1.78473700	-1.30124100	0.37982600
C	-4.13136800	-0.70411700	-0.03524300
C	-4.70972100	-0.72987300	1.38315100
C	-1.65967000	-0.06586500	1.23246800
C	-3.95345500	0.16466000	2.36637100

C	-2.47277100	-0.17887900	2.53507200
H	0.23443000	-3.44665300	-0.89215200
H	-0.90819700	-4.17372200	0.25465500
H	-1.52782300	-2.63738400	-2.30929200
H	-1.96840400	-4.31520100	-1.94414400
H	-3.55560000	-3.58549100	-0.20771800
H	-3.89787500	-2.68985900	-1.69586200
H	-3.87804000	0.32320800	-0.32622700
H	-4.87978200	-1.05704000	-0.74865300
H	-4.72409600	-1.76854800	1.73857400
H	-5.75248300	-0.39680800	1.33303400
H	-1.98825900	0.81059500	0.66277300
H	-0.59752500	0.06722200	1.45672900
H	-4.03198900	1.20467300	2.01917400
H	-4.44792000	0.12364800	3.34294600
H	-2.03362500	0.50841000	3.26457300
H	-2.35643300	-1.18845400	2.94914000
H	-3.09773800	1.64219300	-2.72174600
H	0.27203800	-1.75853000	0.83003500
H	-1.03718800	3.95336300	0.25711200
Cl	1.34644400	2.43596100	0.57489400
Cl	-3.55452800	3.95515600	-1.11181600

[HDBU⁺][2,4-Cl-PhO⁻]-Int6

0 1

O	-5.99210200	-4.19584800	3.52705000
C	-4.59099500	-1.61282900	0.78999700
O	-4.95804800	-2.02248900	-0.29547000
C	-4.24837100	0.95790000	5.14212100
C	-3.82401600	-0.30072200	4.74937000
C	-3.99302300	-0.71475800	3.42706900
C	-4.58673200	0.13988400	2.49204400
C	-5.00337000	1.41621400	2.88277200
C	-4.83960400	1.80991700	4.20152400
N	-4.76134100	-0.30543000	1.18754700
C	-3.63242700	-2.08904300	3.03366700
C	-6.59444400	-3.00665000	3.45152100
C	-6.70006500	-2.22015100	4.61180000
C	-7.12402800	-2.48632800	2.26351300
C	-7.29479400	-0.96598400	4.58923200
C	-7.72192400	-1.23209400	2.22586400
C	-7.80171000	-0.47874200	3.39017600
H	-4.12970300	1.28043400	6.17070300
H	-3.37728700	-1.00255300	5.44617400

H	-5.47928900	2.07463100	2.16195100
H	-5.18539300	2.79342600	4.50414300
H	-5.28433300	0.26217100	0.53357300
H	-7.03324800	-3.06780200	1.34999500
N	-3.63398700	-7.06110400	0.57624100
N	-4.96348600	-5.22022600	1.22441000
C	-5.68695200	-5.24748800	-0.04477000
C	-5.67139000	-6.62506800	-0.69229300
C	-4.23715600	-7.12535000	-0.75279600
C	-4.02191800	-6.08801600	1.44834500
C	-2.47933600	-7.92135000	0.82891200
C	-1.12932100	-7.19680100	0.81733200
C	-3.26543000	-5.96742200	2.75115800
C	-0.81395700	-6.49311000	2.13704500
C	-1.83389900	-5.43452600	2.55320200
H	-6.71956100	-4.93780300	0.15026100
H	-5.25870000	-4.48912100	-0.71148100
H	-6.26737600	-7.32266500	-0.09386600
H	-6.09989900	-6.58991700	-1.69780700
H	-3.65092500	-6.52823300	-1.46626600
H	-4.20641300	-8.16629600	-1.08852500
H	-2.61097200	-8.44921700	1.78143000
H	-2.49581300	-8.68466700	0.04681200
H	-1.12341600	-6.47939400	-0.01367600
H	-0.34437900	-7.93293300	0.60818800
H	-3.23975200	-6.93433400	3.26894300
H	-3.81655900	-5.26751300	3.38219500
H	-0.75256900	-7.25364300	2.92864300
H	0.17832900	-6.03302600	2.07289100
H	-1.52022100	-4.97303100	3.49300300
H	-1.85350500	-4.61971900	1.81673400
H	-8.11783800	-0.84220300	1.29392200
N	-3.95203400	-2.41530900	1.71806000
O	-3.12065700	-2.90395400	3.77518100
H	-3.96424000	-3.41274100	1.48674900
H	-5.71744200	-4.53959900	2.62219400
H	-7.34177100	-0.37245200	5.49512800
Cl	-8.53046600	1.10971500	3.35014200
Cl	-6.01747300	-2.81198500	6.09262800

[HDBU⁺][2-Cl-PhO⁻]-Int1

0 1

O	0.19848100	-2.94883100	0.45235900
C	0.82614200	-2.81201400	1.76132600

O	0.05534700	-2.30835500	2.57796900
O	1.97892300	-3.25325200	1.86103300
C	-2.68802700	-0.16428100	-0.01787000
C	-2.28363000	-1.18656100	0.82451000
C	-2.94102700	-2.42131300	0.77409000
C	-3.99308200	-2.66418800	-0.13404300
C	-4.38258200	-1.61325100	-0.97609300
C	-3.73969100	-0.38702400	-0.91112900
N	-4.57645700	-3.91221000	-0.23197400
C	-2.57546400	-3.49185300	1.64946100
N	-2.41737400	-4.41765300	2.32995200
C	0.90467400	-3.40709400	-0.60564400
C	0.27411600	-4.29023100	-1.49479600
C	2.22042600	-3.01933600	-0.88990500
C	0.92856600	-4.77758800	-2.62168400
C	2.87656100	-3.50976600	-2.01189700
C	2.23850900	-4.39222500	-2.88127900
H	-2.18578600	0.79599900	0.01061700
H	-1.45327800	-1.08551400	1.51670600
H	-5.18639300	-1.77754500	-1.68818800
H	-4.06068700	0.40967700	-1.57596100
H	-4.45916600	-4.53109300	0.56023200
H	-5.50161400	-3.93991800	-0.63627400
H	2.71456300	-2.34613900	-0.20219700
N	2.27062500	-5.70731600	3.33148400
N	0.07339500	-5.09298800	3.69846500
C	0.31993000	-4.29487200	4.90026800
C	1.78901800	-3.91644700	4.95001200
C	2.62926300	-5.15115500	4.64532900
C	1.01201700	-5.59390100	2.91978300
C	3.33974800	-5.98792400	2.35863700
C	3.38087600	-7.43903300	1.87614500
C	0.59790800	-6.06290600	1.55567100
C	2.33992700	-7.77621100	0.81016600
C	0.89743000	-7.53800100	1.25322300
H	-0.30258400	-3.40298000	4.80908000
H	0.01636100	-4.87163600	5.78125200
H	1.98285000	-3.15646800	4.18831700
H	2.04444900	-3.52774100	5.93899600
H	2.48454500	-5.92505100	5.41019700
H	3.68967000	-4.89811300	4.61783800
H	3.23996200	-5.27663600	1.52913200
H	4.27476100	-5.75497600	2.87031200
H	3.26824700	-8.10187800	2.74349700

H	4.37993500	-7.62183600	1.46421000
H	1.12017200	-5.42290200	0.83407500
H	-0.46812700	-5.85079900	1.44046500
H	2.53236100	-7.16304800	-0.08127300
H	2.46161600	-8.82199000	0.50721700
H	0.22399600	-7.84683900	0.44759900
H	0.65512400	-8.16011200	2.12432200
H	-0.85217900	-4.99150100	3.27606500
H	3.89614200	-3.19351500	-2.20980800
H	0.39928000	-5.45408300	-3.28443200
H	2.75037200	-4.77287800	-3.75897800
Cl	-1.36978100	-4.78902500	-1.19285900

[HDBU⁺][2-Cl-PhO⁻]-TS1-2

0 1

O	1.03256300	0.31974600	-1.24117400
C	1.06274900	-0.98510500	-1.69493500
O	1.94612600	-1.66921700	-1.04640300
O	0.35360300	-1.38723500	-2.59145200
C	5.75106200	-0.10695600	-0.75476400
C	4.47817000	-0.65532900	-0.72162500
C	3.65620800	-0.52364400	0.40248600
C	4.12490400	0.19617800	1.53091900
C	5.41730300	0.74725700	1.47853400
C	6.21523000	0.59630800	0.35789900
N	3.32990800	0.40823400	2.63439100
C	2.31951500	-1.12014800	0.48542500
N	1.48746800	-1.31391000	1.34503500
C	-0.05045500	1.14014300	-1.33607100
C	-0.01640500	2.24618200	-0.47008000
C	-1.15566000	0.95854400	-2.16964600
C	-1.06532400	3.15496700	-0.43895900
C	-2.21107900	1.86911600	-2.11841800
C	-2.17394300	2.96458700	-1.26144000
H	6.37385200	-0.22422100	-1.63477300
H	4.10004200	-1.21090500	-1.57059400
H	5.77796200	1.30689200	2.33789400
H	7.20945000	1.03400700	0.35082000
H	2.52472000	-0.20682600	2.71233000
H	3.81468000	0.61992100	3.49430700
H	-1.17021800	0.11717400	-2.84700500
H	-2.99363500	3.67509000	-1.23585200
N	-2.94713200	-1.58701700	-0.21655100
N	-0.74840500	-2.12663100	0.33991900

C	-0.74796300	-3.37292900	-0.41856000
C	-1.82707300	-3.35502500	-1.49085000
C	-3.14072900	-2.87123500	-0.89381700
C	-1.77294100	-1.32341500	0.38866300
C	-4.10918700	-0.71233500	-0.05177100
C	-4.70249600	-0.72293400	1.36091600
C	-1.64590600	-0.08332000	1.23407400
C	-3.94650400	0.16768300	2.34826300
C	-2.46987800	-0.18659800	2.53064500
H	0.24463600	-3.47465000	-0.86640900
H	-0.89693600	-4.20567800	0.27985200
H	-1.51425900	-2.67909300	-2.29005000
H	-1.96006500	-4.35421900	-1.91421400
H	-3.54578400	-3.60500100	-0.18248500
H	-3.88592900	-2.72390300	-1.68010800
H	-3.83982300	0.30882300	-0.34891000
H	-4.85369700	-1.06351600	-0.77021900
H	-4.73222300	-1.75940500	1.72171900
H	-5.74131900	-0.37911100	1.29898400
H	-1.96379100	0.79272000	0.65740700
H	-0.58444300	0.04481000	1.46507100
H	-4.01224300	1.20729400	1.99752700
H	-4.45011700	0.13400300	3.32052500
H	-2.03186900	0.49983300	3.26163300
H	-2.36513600	-1.19556600	2.94927000
H	-3.06404700	1.71991100	-2.77380100
H	0.26741200	-1.79658500	0.85437600
H	-1.00935000	3.99616100	0.24370800
Cl	1.31111400	2.41553900	0.63221900

[HDBU⁺][2-Cl-PhO⁻]-Int6

0 1

O	-6.02756400	-4.24466200	3.52176400
C	-4.62353900	-1.61689500	0.78759400
O	-4.99119600	-2.02535900	-0.29790100
C	-4.21964800	0.99778300	5.11043000
C	-3.84717100	-0.28288500	4.73679900
C	-4.02505000	-0.70728800	3.41921900
C	-4.58616100	0.15412000	2.47139900
C	-4.95176100	1.45239300	2.84324900
C	-4.76906100	1.86070500	4.15493900
N	-4.77179000	-0.30217800	1.17347400
C	-3.69119200	-2.09288300	3.03962700
C	-6.61929300	-3.04532500	3.46692300

C	-6.70797400	-2.27420900	4.63700000
C	-7.15015900	-2.50691000	2.28725500
C	-7.29632800	-1.01630400	4.62904400
C	-7.73861700	-1.24706600	2.27789400
C	-7.81552800	-0.49454600	3.44707200
H	-4.08879800	1.33056200	6.13424500
H	-3.42985600	-0.99225700	5.44427500
H	-5.38701700	2.12202000	2.10690600
H	-5.06259600	2.86621800	4.44083100
H	-5.28043900	0.26806100	0.51097400
H	-7.06839700	-3.08288800	1.36874300
H	-8.26803400	0.49144300	3.44453900
N	-3.62595100	-7.07091000	0.57026100
N	-4.95986700	-5.22356400	1.19260700
C	-5.65794700	-5.25069600	-0.09034200
C	-5.64761500	-6.63460000	-0.72438600
C	-4.21724600	-7.14809200	-0.76330800
C	-4.02419100	-6.09259300	1.43288300
C	-2.46384700	-7.91721700	0.83399600
C	-1.12248300	-7.17608300	0.83433600
C	-3.28661900	-5.96917900	2.74610400
C	-0.82489700	-6.46955200	2.15693800
C	-1.85855100	-5.42149100	2.56624000
H	-6.68870100	-4.92178400	0.08020600
H	-5.20498900	-4.50549500	-0.75549300
H	-6.25708500	-7.32045300	-0.12586600
H	-6.06372000	-6.60641800	-1.73538600
H	-3.61891300	-6.56626100	-1.47955900
H	-4.19225200	-8.19404000	-1.08440500
H	-2.59734500	-8.44686400	1.78532500
H	-2.46362800	-8.68056700	0.05163500
H	-1.11884600	-6.45790900	0.00392500
H	-0.32691100	-7.90237100	0.63074200
H	-3.25750800	-6.93728600	3.26139900
H	-3.85282200	-5.27652600	3.37182000
H	-0.76228700	-7.23011000	2.94845300
H	0.16351700	-6.00003400	2.10071300
H	-1.55899900	-4.96106300	3.51125100
H	-1.87904100	-4.60413800	1.83259500
H	-8.13397600	-0.85562700	1.34479900
N	-4.00170500	-2.42278300	1.72322000
O	-3.19854400	-2.90950500	3.79197800
H	-4.03263600	-3.42315800	1.49969200
H	-5.75996300	-4.56825600	2.61283400

Cl	-6.01494000	-2.89283500	6.10630900
H	-7.32665900	-0.44736600	5.55244400

[HDBU⁺][2-F-PhO⁻]-Int1

0 1

O	0.17559900	-2.84455200	0.54989000
C	0.86149000	-2.75256900	1.82834400
O	0.13165700	-2.25343100	2.68582200
O	2.01128100	-3.21155300	1.86973600
C	-2.67900400	-0.07086800	0.13378800
C	-2.27012200	-1.16446400	0.87807500
C	-2.88202600	-2.40736400	0.67121700
C	-3.89176300	-2.58494900	-0.29720700
C	-4.28769700	-1.46054900	-1.03713200
C	-3.69113800	-0.22934400	-0.81780700
N	-4.43830900	-3.82703500	-0.54507300
C	-2.51682500	-3.53675700	1.46894600
N	-2.34317700	-4.49205400	2.10272800
C	0.77983100	-3.39634800	-0.52722700
C	0.01265300	-4.27815700	-1.29679200
C	2.08900600	-3.14110500	-0.93911400
C	0.50642700	-4.89996800	-2.42905100
C	2.60063900	-3.76462500	-2.07647400
C	1.81862000	-4.64132800	-2.82332200
H	-2.21238900	0.89599900	0.28404500
H	-1.47148900	-1.11003600	1.61293100
H	-5.05993000	-1.57272300	-1.79298200
H	-4.01687700	0.62378500	-1.40598200
H	-4.28359100	-4.54120600	0.15465000
H	-5.36632300	-3.83648400	-0.94271000
H	2.69586200	-2.47475700	-0.34011500
N	2.31731800	-5.67452200	3.34929600
N	0.08337800	-5.13177000	3.58869600
C	0.23059800	-4.38591100	4.83902100
C	1.67683800	-3.94841400	4.98297200
C	2.58929500	-5.13244400	4.68954400
C	1.08475600	-5.58362000	2.86063200
C	3.44823000	-5.93773900	2.44561000
C	3.53522200	-7.38759900	1.96330700
C	0.78024400	-6.03166000	1.46160900
C	2.56727000	-7.73936900	0.83446600
C	1.09648500	-7.50799200	1.17840300
H	-0.42412600	-3.51667000	4.75884100
H	-0.09096700	-5.01883000	5.67406500

H	1.87317500	-3.15317800	4.25889500
H	1.86022100	-3.58161600	5.99604200
H	2.45451000	-5.93050300	5.43103900
H	3.63511400	-4.82343400	4.71267000
H	3.39459700	-5.22363400	1.61420900
H	4.34668300	-5.69830500	3.01641000
H	3.37666600	-8.05163900	2.82254600
H	4.55991600	-7.55943300	1.61450800
H	1.37125100	-5.39203000	0.79632700
H	-0.26958400	-5.80378400	1.25508000
H	2.81254800	-7.13075400	-0.04688800
H	2.71678200	-8.78609000	0.54764800
H	0.48202000	-7.81959300	0.32814100
H	0.79638000	-8.13150900	2.03016600
H	-0.81685700	-5.04360500	3.11164900
H	3.62135400	-3.55551400	-2.38113400
H	-0.14161400	-5.57397200	-2.97910400
H	2.22056100	-5.12103600	-3.70965600
F	-1.23975400	-4.55497600	-0.88871100

[HDBU⁺][2-F-PhO⁻]-TS1-2

0 1

O	0.89451200	0.40330100	-1.20004900
C	1.06431700	-0.87335300	-1.70085100
O	1.99488700	-1.49913800	-1.06370000
O	0.41132400	-1.30485900	-2.62759800
C	5.80842200	-0.00455900	-0.68203000
C	4.50244300	-0.46856500	-0.69553200
C	3.72555100	-0.49962100	0.46790600
C	4.28050400	-0.03776700	1.69056500
C	5.60932800	0.42470500	1.68515900
C	6.35765300	0.44021300	0.52194000
N	3.54501500	0.00605300	2.84848400
C	2.35319500	-1.01190800	0.50441300
N	1.50225100	-1.20941300	1.34227300
C	-0.21698900	1.16110500	-1.43107500
C	-0.20191500	2.38697600	-0.75060500
C	-1.34789000	0.82823200	-2.17638700
C	-1.27403100	3.25729400	-0.77982700
C	-2.43523200	1.70671200	-2.20602300
C	-2.41074700	2.91046100	-1.51141800
H	6.39289400	0.00863600	-1.59536200
H	4.06251800	-0.83227200	-1.61498500
H	6.03688900	0.78271200	2.61829200

H	7.38043900	0.80507000	0.55329600
H	2.67517100	-0.51819400	2.84388700
H	4.06381800	0.03203200	3.71322100
H	-1.36465700	-0.09775200	-2.73108900
H	-3.25855300	3.58652600	-1.54612600
N	-2.95049500	-1.54817900	-0.19863700
N	-0.72533500	-2.01756400	0.30385300
C	-0.70574000	-3.27093600	-0.44158200
C	-1.79422000	-3.27571300	-1.50370600
C	-3.11492200	-2.82772800	-0.89326400
C	-1.77170000	-1.24413700	0.37492600
C	-4.14185700	-0.72502500	0.01719400
C	-4.67017200	-0.76170800	1.45531300
C	-1.65629900	0.00741100	1.20572100
C	-3.91704400	0.16564800	2.41106800
C	-2.41929500	-0.11847600	2.53665200
H	0.28517100	-3.35830100	-0.89631200
H	-0.83549000	-4.10090400	0.26389700
H	-1.50147500	-2.59173300	-2.30417500
H	-1.90720700	-4.27577600	-1.93051700
H	-3.49997700	-3.58013800	-0.19050400
H	-3.86719300	-2.68678300	-1.67427300
H	-3.93144300	0.30629100	-0.29222000
H	-4.90103900	-1.11110700	-0.66722000
H	-4.63452500	-1.79803600	1.81603100
H	-5.72596000	-0.46826700	1.43911100
H	-2.03410700	0.86427700	0.63564500
H	-0.59081900	0.17715900	1.38607200
H	-4.04552400	1.19995100	2.06250800
H	-4.38013100	0.11111600	3.40229600
H	-1.98407900	0.59474300	3.24315300
H	-2.25049100	-1.11694600	2.95931100
H	-3.30651700	1.43805800	-2.79583300
H	0.26913400	-1.67816700	0.81627800
H	-1.20216500	4.18655100	-0.22536700
F	0.87640000	2.69172300	-0.02537700

[HDBU⁺][2-F-PhO⁻]-Int6

0 1

O	-5.86358600	-4.03405500	3.44537100
C	-4.69072000	-1.59335400	0.87086100
O	-5.10919000	-2.00508200	-0.19433500
C	-4.12765100	0.94723000	5.21855100
C	-3.69502600	-0.29405400	4.78166000

C	-3.93918300	-0.69819500	3.46869700
C	-4.64015600	0.13860800	2.59355300
C	-5.06333100	1.39913300	3.02701200
C	-4.80666200	1.79070500	4.33138400
N	-4.90915700	-0.30436000	1.30649600
C	-3.54088600	-2.04838600	3.02665500
C	-6.59025500	-2.90817700	3.34922600
C	-6.62684100	-2.05663600	4.46426800
C	-7.30177100	-2.51749500	2.21367700
C	-7.33906700	-0.87472400	4.46573700
C	-8.01886600	-1.31988800	2.19941100
C	-8.04462100	-0.49796700	3.32037900
H	-3.94358800	1.26477400	6.23901200
H	-3.17856600	-0.98839400	5.43608800
H	-5.60597800	2.04866700	2.34629600
H	-5.14629600	2.76593900	4.66696900
H	-5.54167000	0.22521300	0.72123400
H	-7.26513400	-3.14949600	1.33070200
H	-8.60283300	0.43243800	3.31224800
N	-3.62949900	-7.09672500	0.58694800
N	-4.86713800	-5.15955700	1.13416100
C	-5.54317700	-5.19148300	-0.15989100
C	-5.62306200	-6.60016800	-0.73110300
C	-4.22920100	-7.20644700	-0.74046900
C	-3.98040100	-6.06713500	1.41103500
C	-2.50860500	-7.98632700	0.88355600
C	-1.13428400	-7.30878400	0.86176900
C	-3.24189300	-5.93574800	2.72324600
C	-0.80558200	-6.57251300	2.16047500
C	-1.78858700	-5.46346700	2.53162900
H	-6.54665400	-4.77429900	-0.02995700
H	-5.02428700	-4.51452100	-0.84902600
H	-6.27759500	-7.21629700	-0.10481400
H	-6.03440400	-6.59161200	-1.74445700
H	-3.59633800	-6.70428300	-1.48683200
H	-4.27285000	-8.26766900	-1.00534000
H	-2.66713400	-8.47621600	1.85230900
H	-2.54281900	-8.77558800	0.12805900
H	-1.09705500	-6.61988400	0.00769600
H	-0.37302200	-8.07756700	0.68461500
H	-3.26116500	-6.88547000	3.27215200
H	-3.77583000	-5.19571400	3.32272900
H	-0.78014700	-7.30803200	2.97736100
H	0.20403600	-6.15238100	2.09159000

H	-1.46925200	-4.98683200	3.46175200
H	-1.76917700	-4.66966600	1.77260100
H	-8.55976500	-1.03856900	1.30084000
N	-3.93512600	-2.36907600	1.73160400
O	-2.92560400	-2.84021200	3.71219300
H	-3.90813100	-3.36060900	1.47500100
H	-5.64648800	-4.41344200	2.54693700
H	-7.30592100	-0.25208200	5.35368700
F	-5.90196400	-2.39904000	5.53880000

[HDBU⁺][4-Cl-PhO⁻]-Int1

0 1

O	0.21585200	-2.67065800	0.44162500
C	0.81175800	-2.71600000	1.76112700
O	0.06144500	-2.23032800	2.61095100
O	1.93104700	-3.24177200	1.84824600
C	-2.79694000	0.04667900	0.27447800
C	-2.32359300	-1.08631900	0.91453800
C	-2.91168900	-2.32752400	0.63796800
C	-3.96512300	-2.45974100	-0.29154500
C	-4.42281300	-1.29698100	-0.92686700
C	-3.84616900	-0.06907300	-0.64188600
N	-4.48303500	-3.70165700	-0.61158300
C	-2.46892200	-3.51595600	1.29984600
N	-2.23001900	-4.54169500	1.78567900
C	0.75961100	-3.38639900	-0.57681000
C	-0.11291400	-4.17153400	-1.33587800
C	2.12069400	-3.35757400	-0.90089300
C	0.36629300	-4.95639200	-2.37925300
C	2.60360500	-4.14911500	-1.93825400
C	1.72699800	-4.95078500	-2.66259700
H	-2.34967400	1.01300200	0.47747200
H	-1.49355000	-1.06588800	1.61563000
H	-5.22858600	-1.37320400	-1.65147200
H	-4.21969800	0.81595100	-1.14870100
H	-4.34929300	-4.43481400	0.07368400
H	-5.40814100	-3.69903100	-1.01797200
H	2.78979300	-2.74123400	-0.31582400
N	2.34578900	-5.65621400	3.33769900
N	0.08368700	-5.20225800	3.46720100
C	0.14056500	-4.43221500	4.71153200
C	1.56318100	-3.95132000	4.93155800
C	2.52444600	-5.10851900	4.69133300
C	1.13558500	-5.62373500	2.79161400

C	3.52865200	-5.85296800	2.48407200
C	3.73186700	-7.29808000	2.02543500
C	0.90920700	-6.12073700	1.39311500
C	2.83144500	-7.71957300	0.86553700
C	1.33738700	-7.57650300	1.15215600
H	-0.53023700	-3.58152900	4.58068400
H	-0.21049000	-5.06245600	5.53661500
H	1.77339000	-3.15129500	4.21746600
H	1.67940700	-3.57862400	5.95237300
H	2.36691800	-5.91185700	5.42253400
H	3.55870000	-4.77322900	4.77725300
H	3.45815500	-5.15634400	1.63944300
H	4.38473700	-5.54244700	3.08488500
H	3.58408200	-7.96300900	2.88587000
H	4.77816000	-7.40500800	1.71732000
H	1.45901900	-5.44877200	0.72373000
H	-0.15034100	-5.98303800	1.16095800
H	3.07239600	-7.10671900	-0.01396600
H	3.05411300	-8.75780300	0.59661200
H	0.77784800	-7.94319500	0.28613400
H	1.04720700	-8.20333700	2.00510300
H	-1.16944500	-4.17048100	-1.08437600
H	-0.79198300	-5.15384500	2.94487100
H	3.65885200	-4.14049800	-2.19093200
H	-0.30756300	-5.57279500	-2.96457300
Cl	2.34514100	-5.95867900	-3.95356700

[HDBU⁺][4-Cl-PhO⁻]-TS1-2

0 1

O	1.00595600	0.38935200	-1.29621100
C	1.11087300	-0.91582800	-1.73310400
O	2.01568000	-1.55533200	-1.06756500
O	0.43883200	-1.36208300	-2.63807400
C	5.82046200	-0.03212600	-0.68366800
C	4.52194900	-0.51719300	-0.70156800
C	3.71692300	-0.49534100	0.44295600
C	4.23528700	0.04367400	1.64956800
C	5.55610000	0.52755300	1.64946100
C	6.33320200	0.48928500	0.50535900
N	3.46779700	0.14486200	2.78555800
C	2.34947600	-1.02685700	0.47121400
N	1.48992400	-1.19811600	1.30904200
C	-0.12511400	1.14672500	-1.43716600
C	-0.08026300	2.34900400	-0.72457600

C	-1.27091400	0.80096700	-2.15697200
C	-1.18367800	3.18845500	-0.68677900
C	-2.37907800	1.64687100	-2.11262800
C	-2.33961700	2.82042400	-1.37127000
H	6.42717400	-0.06196000	-1.58201100
H	4.11057200	-0.93919500	-1.60953300
H	5.95528400	0.94435200	2.57071700
H	7.34944500	0.87158000	0.54021100
H	2.61814900	-0.41299100	2.78989600
H	3.97054100	0.21476200	3.65795600
H	-1.29325100	-0.10353900	-2.74598000
N	-2.97188700	-1.53871100	-0.20319100
N	-0.74830700	-2.02632600	0.29103800
C	-0.73829900	-3.27428900	-0.46386500
C	-1.82677500	-3.26176300	-1.52577300
C	-3.14457900	-2.80987700	-0.91194300
C	-1.79194200	-1.24883000	0.37412800
C	-4.15678000	-0.70371300	0.00887400
C	-4.69914500	-0.74095500	1.44099600
C	-1.66752700	-0.00885400	1.22017900
C	-3.94307200	0.17778800	2.40176900
C	-2.45133200	-0.12952500	2.53976300
H	0.25153100	-3.36732000	-0.91934800
H	-0.87597300	-4.10806700	0.23555400
H	-1.52919400	-2.57369400	-2.32084900
H	-1.94678500	-4.25714200	-1.96144900
H	-3.53609800	-3.56628500	-0.21735500
H	-3.89497800	-2.65543200	-1.69207500
H	-3.93320600	0.32861900	-0.28817400
H	-4.91344500	-1.07493800	-0.68628900
H	-4.67723100	-1.77823200	1.80006400
H	-5.75118900	-0.43569800	1.41513400
H	-2.01448900	0.86239700	0.65217300
H	-0.60280400	0.13449500	1.42195700
H	-4.05462300	1.21312900	2.05012500
H	-4.41438600	0.13104200	3.38946100
H	-2.01276300	0.57320400	3.25477400
H	-2.30247700	-1.13261500	2.95922000
H	-3.27643500	1.39076900	-2.66702400
H	0.24664600	-1.68901200	0.79131500
H	-1.15591900	4.11435700	-0.12285700
H	0.82715400	2.58879000	-0.18035500
Cl	-3.75392200	3.84324900	-1.29789700

[HDBU⁺][4-Cl-PhO⁻]-Int6

0 1

O	-6.08305600	-4.28343900	3.52783100
C	-4.60295100	-1.63301900	0.77607600
O	-4.95676500	-2.05264100	-0.30983300
C	-4.22026800	1.03337100	5.06864500
C	-3.84774800	-0.25180900	4.71292100
C	-4.02334000	-0.69618000	3.40175600
C	-4.57535400	0.15594900	2.44005700
C	-4.94823600	1.45642500	2.79456800
C	-4.77500500	1.88057600	4.10205000
N	-4.75124900	-0.31477200	1.14565900
C	-3.70928000	-2.09213900	3.04663900
C	-6.64055000	-3.06079900	3.48918400
C	-6.73083300	-2.33875500	4.68576100
C	-7.12436600	-2.48423700	2.30811800
C	-7.27775000	-1.06270900	4.70198800
C	-7.67228400	-1.20537600	2.32219800
C	-7.74313200	-0.49984600	3.51721000
H	-4.09189600	1.38082700	6.08795000
H	-3.43134200	-0.95105200	5.43110300
H	-5.39622400	2.11179300	2.05342000
H	-5.08570200	2.88390900	4.37596500
H	-5.24164600	0.25462200	0.46855300
H	-7.04523900	-3.02810300	1.36995600
N	-3.62766600	-7.07015500	0.56558900
N	-4.96738700	-5.22582300	1.18658700
C	-5.65973200	-5.25228900	-0.09953100
C	-5.64771000	-6.63658200	-0.73288700
C	-4.21689500	-7.14930400	-0.76890300
C	-4.03120300	-6.09338800	1.42775600
C	-2.45865500	-7.90694200	0.82840500
C	-1.12383000	-7.15378400	0.83471800
C	-3.29957300	-5.97014400	2.74433200
C	-0.83351800	-6.45098900	2.16106600
C	-1.87486100	-5.41154900	2.57308100
H	-6.69059900	-4.92129700	0.06660000
H	-5.20205800	-4.50833800	-0.76261300
H	-6.25815200	-7.32252800	-0.13543100
H	-6.06160900	-6.60914500	-1.74480000
H	-3.61779400	-6.56793700	-1.48488100
H	-4.19062100	-8.19571400	-1.08859300
H	-2.58915400	-8.44213600	1.77715100
H	-2.44967900	-8.66683800	0.04273900

H	-1.12518100	-6.43162600	0.00778900
H	-0.32151800	-7.87196600	0.62894700
H	-3.26562300	-6.93985000	3.25642000
H	-3.87528000	-5.28365800	3.36815400
H	-0.76726500	-7.21465400	2.94932000
H	0.15183600	-5.97468000	2.10869100
H	-1.58095700	-4.95452100	3.52165100
H	-1.89819600	-4.59049900	1.84370300
H	-8.04011000	-0.75844000	1.40383100
N	-4.00165200	-2.43406500	1.73067800
O	-3.24832100	-2.90895600	3.82058100
H	-4.04602900	-3.43693700	1.51845300
H	-5.79886800	-4.59017200	2.62139800
H	-7.33018800	-0.49624500	5.62575500
H	-6.33625000	-2.79095000	5.58947100
Cl	-8.42379300	1.11359200	3.52916500

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