Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Cationic Ring-Opening Polymerization of *N*-benzylaziridines to Polyamines via Organic Boron

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I. Experimental section

Nuclear magnetic resonance (NMR). ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on a Varian INOVA-400 MHz type spectrometer (^{1}H NMR, 400 MHz; ^{13}C NMR, 100 MHz; ^{19}F NMR, 376 MHz; and ^{31}P NMR, 162 MHz). The peak frequencies were referenced versus an internal standard TMS shift at 0.00 ppm for ^{1}H NMR and an internal standard $CHCl_3$ shift at 77.16 ppm for ^{13}C NMR.

Gel permeation chromatography (GPC). Molecular weights and molecular weight distributions of polyamines were measured by GPC analysis at 30 ℃ and a flow rate of 1.0 mL/min, with THF as the eluent and polystyrene as the standards, on an Agilent 1260 instrument coupled with an Agilent RI detector and equipped with two PL gel columns. The sample concentration was about 2 mg/mL, and the injection volume was 100 μL.

Gas chromatography-mass spectrometry (GC-MS). An Agilent 7890B-5977B instrument equipped with HP-5ms capillary chromatographic column (30 m*0.25 mm*0.25 μm) was employed for GC-MS experiments. The inlet temperature was set to 250 ℃ and the heating program was set to 30 ℃ (2 min), and then, the temperature was increased to 300 ℃ at a rate of 10 ℃/min.

Electrospray ionization mass spectrometry (ESI-MS). On-line monitoring of the polymerization by ESI-MS was carried out on the Waters Xevo G2-XS QTof instrument equipped with an orthogonal electrospray source (Z-spray) and referenced against the leucine enkephalin (LE), lock mass of m/z = 556.2771 for positive mode and m/z = 554.2620 for negative mode.

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS). MALDI-TOF mass spectrometry was performed on a Bruker ultrafleXetreme MALDI TOF/TOF mass spectrometer. Trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) was used as a matrix. Silver acetate (Aldrich, 99.95%) was added for ion formation.

General procedure for the CROP of *N*-benzylaziridines. In a glovebox, tris(pentafluorophenyl)boron (BCF) was measured (5.1 mg, 0.01 mmol) into a flame-dried 10 mL flask equipped with a magnetic stirrer. 1 mL dichloromethane (DCM) was added via syringe and the monomer was added subsequently. The vial was removed from the glovebox, and placed in an aluminum heat block preheated to 25 °C. After the reaction finished, the vial was removed from the heat block, the mixture was dissolved in DCM, and a small aliquot was analyzed by ^{1}H NMR for conversion. Then the mixture was then dissolved in DCM and precipitated into an excess of methyl alcohol. This process was repeated three times and resultant polyamines were obtained by vacuum-drying.

II. Results

We also have investigated the effect of solvent on the CROP. By changing solvent polarity from polar DCM (dielectric constant, ε = 8.93) to relatively nonpolar toluene (Tol, ε = 2.37), the BMA conversion decreased noticeably and the resultant polymer has a reduction in M_n (4.2 kg/mol) and a high $Đ$ of 2.44 (Table S1, entry 1 and 2). This is attributed to the propagating species are more stable and less reactive in nonpolar solvent, so there is a significant improvement in conversion and molecular weight of product with the increase in solvent polarity. However, by using polar tetrahydrofuran (THF) (ε = 7.43) as the solvent, BMA converted to 97%, yielding the PBMA with M_n of 8.3 kg/mol and a high $Đ$ of 2.23 (Table S1, entry 3). It is speculated that there is an interaction between cyclic ethers and BCF. While in the case of *N*,*N*-dimethylformamide (DMF), an electron-donor solvent, the CROP did not occur (Table S1, entry 4).

Table S1 Effect of solvent on the CROP of BMA.[a]

Entry	Solvent	Time [h]	Conv.[b] [%]	M_n[c] [kg mol^{-1}]	$Đ$[c]
1	DCM	8	99	14.5	1.81
2	Tol	24	53	4.2	2.44
3	THF	12	97	8.3	2.23
4	DMF	12	N.R.[d]	--	--

[a]Reactions carried out with a BMA/BCF ratio of 100/1 under 25 °C; [b]Obtained by ^{1}H NMR spectroscopy; [c]Determined by gel permeation chromatography in THF, calibrated with polystryene standards.

Table S2 Lewis acidity of boron compounds evaluating by Guttmann-Beckett method.[1]

Boron compounds	^{31}P ppm[a]	$\Delta\delta$ ppm[a]
Et_3PO	45.75	0.00
TEB	48.61	2.86
TPB	56.64	10.89
$BF_3.Et_2O$	76.49	30.74
BCF	75.83	30.08

[a]The boron compound and the triethylphosphine oxide (Et_3PO) were placed together in 1:1 mole ratio in a small glass vial and dissolved in the minimum amount of C_6D_6. The solution was placed in an NMR tube, and the ^{31}P NMR chemical shift was recorded at room temperature.

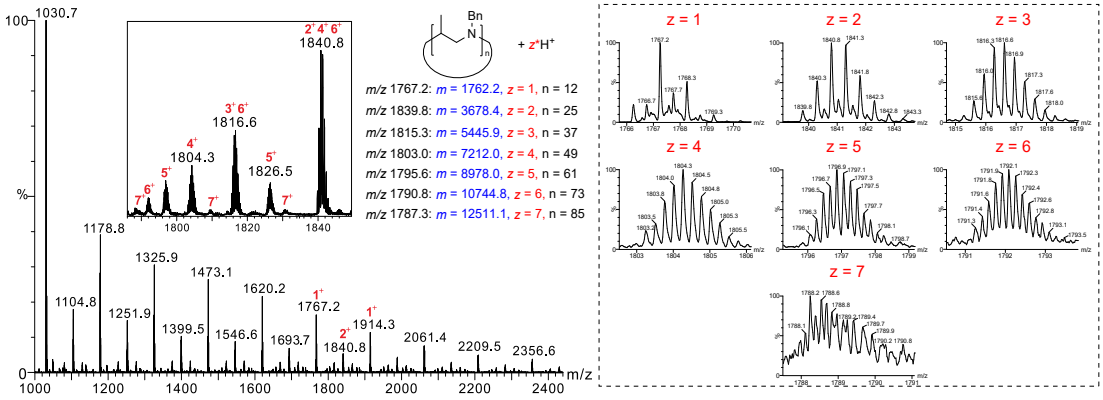


Fig. S1 ESI-MS spectra of the cyclic poly(1-benzyl-2-methylaziridine) (PBMA). Insets identifying the multiple charged ions (z = 1–7) are also shown.

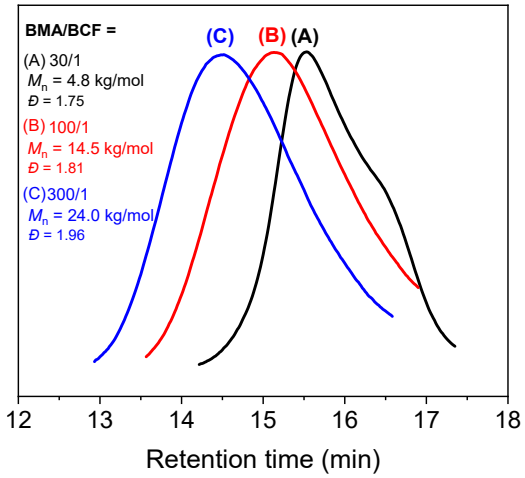


Fig. S2 GPC traces of PBMAs reacted under 25 °C in DCM at different BMA/BCF ratios: (A) 30/1, (B) 100/1 and (C) 300/1.

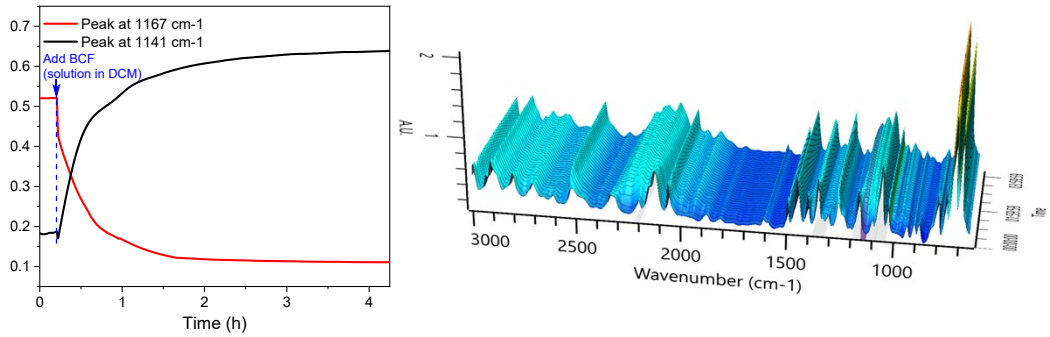


Fig. S3 *In situ* FTIR traces of the BCF-initiated CROP of BMA, 1141 cm^{-1} and 1167 cm^{-1} correspond to polymer and monomer, respectively (left), and three-dimensional stack plot of the infrared spectrum (right).

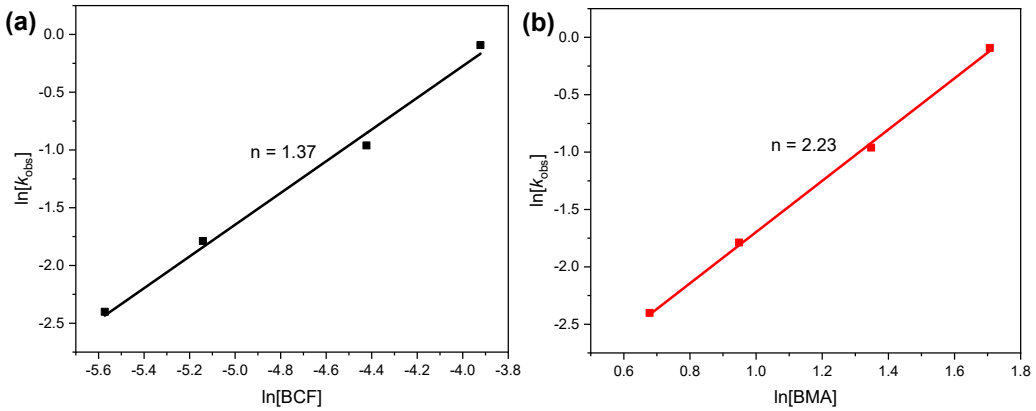


Fig. S4 Reaction kinetic analysis to determine order in (a) BCF (approximate first order) and (b) BMA (second order).

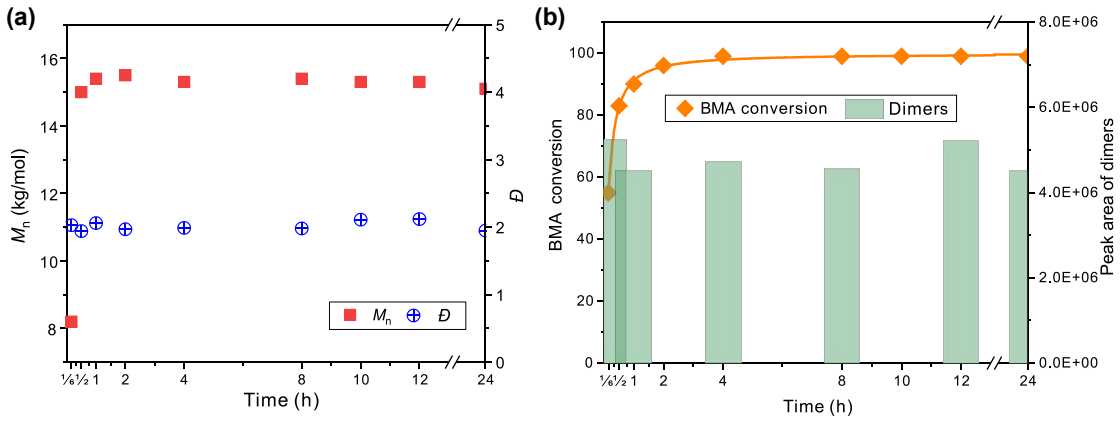


Fig. S5 The relationship of reaction time versus (a) M_ns and $Đ$s of the resulting polyamines and (b) BMA conversion and the peak area of dimers. The polymerization was conducted at 25 °C in DCM with a BMA/BCF ratio of 100/1.

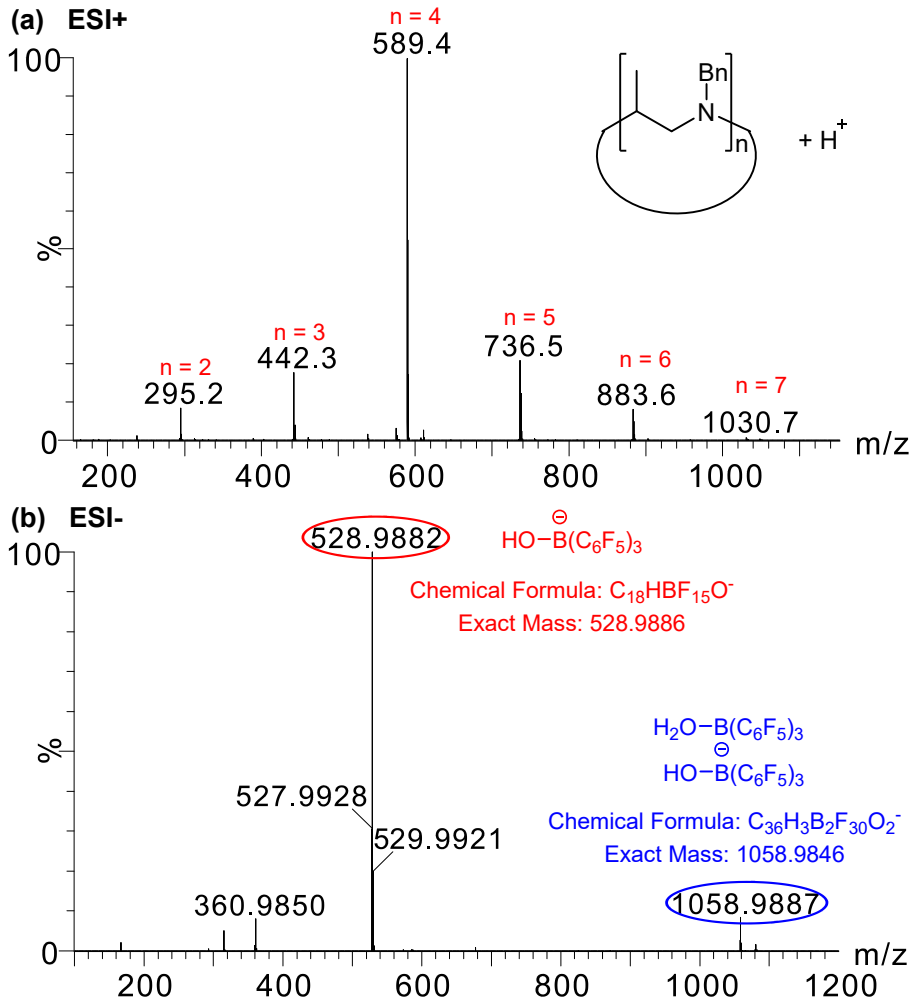


Fig. S6 ESI-MS spectra of on-line monitoring of the polymerization progress (a) in the positive mode and (b) in the negative mode (BMA/BCF = 10/1).

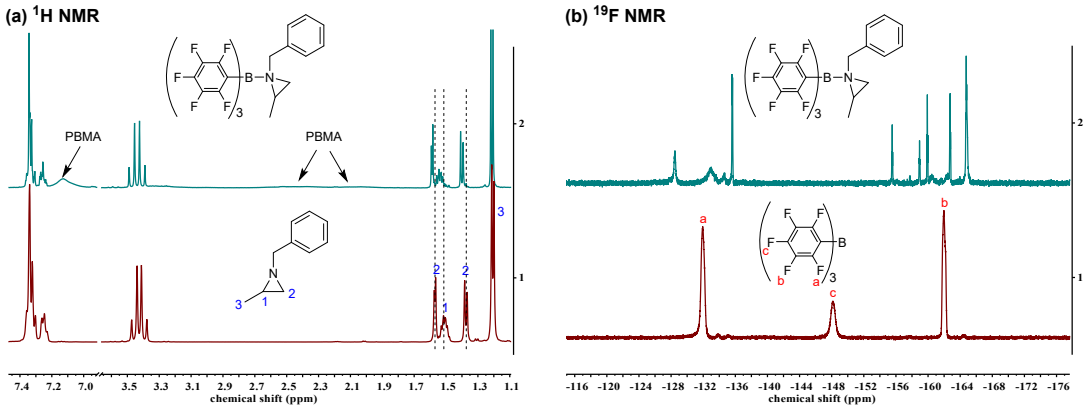


Fig. S7 (a) ^{1}H NMR spectra of BMA and BCF/BMA (mole ratio of 1/1) and (b) ^{19}F NMR spectra of BCF and BCF/BMA (mole ratio of 1/1).

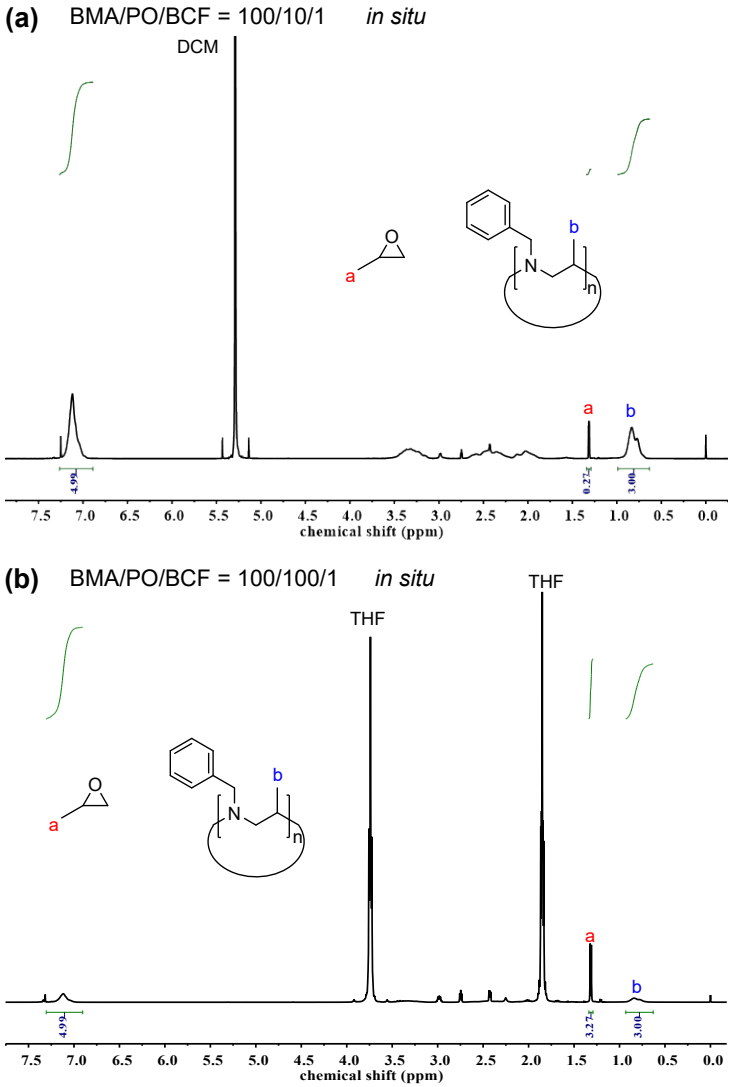


Fig. S8 *In situ* ^{1}H NMR spectra of reaction mixture with different feed ratios: (a) BMA/PO/BCF ratio of 100/10/1 in DCM and (b) BMA /PO/BCF ratio of 100/100/1 in THF.

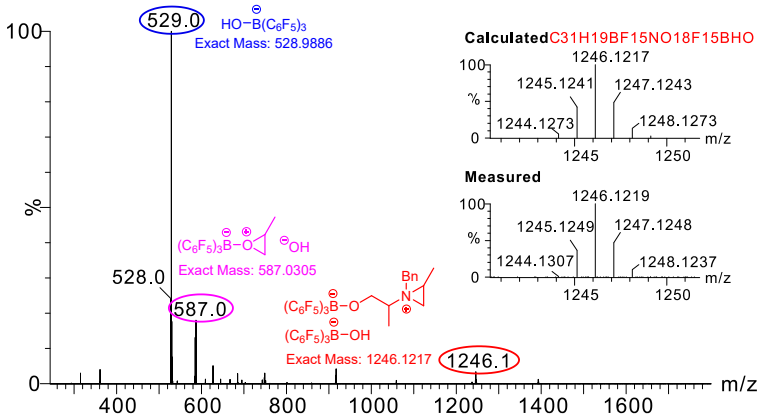


Fig. S9 ESI-MS spectrum of the reaction mixtures at the beginning of the polymerization under BMA/PO/BCF = 10/1/1 in the negative mode. Inset identifying high resolution mass spectrum of $[BCF + PO + BMA + (BCF + OH)]^{-}$ is also shown.

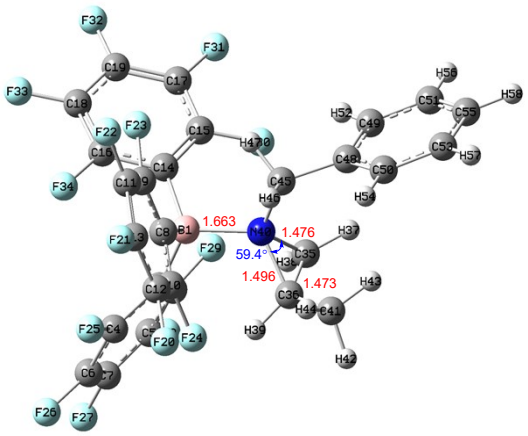


Fig. S10 Key optimized structure (bond length/Å) for the **IN-0**. Atoms C, N, B, F and H are shown in gray, blue, pink, cyan and white, respectively.

Table S3 Atomic charge analysis of **IN-0** calculated by three methods.

	B(1)	**N(40)**	**-CH$_2$(35)**	**-CH(36)**
Mulliken	0.427103	-0.494326	-0.234471	-0.015844
NPA	0.62128	-0.47501	-0.24183	-0.05378
RESP	2.497258	-0.531030	-0.255555	0.177965

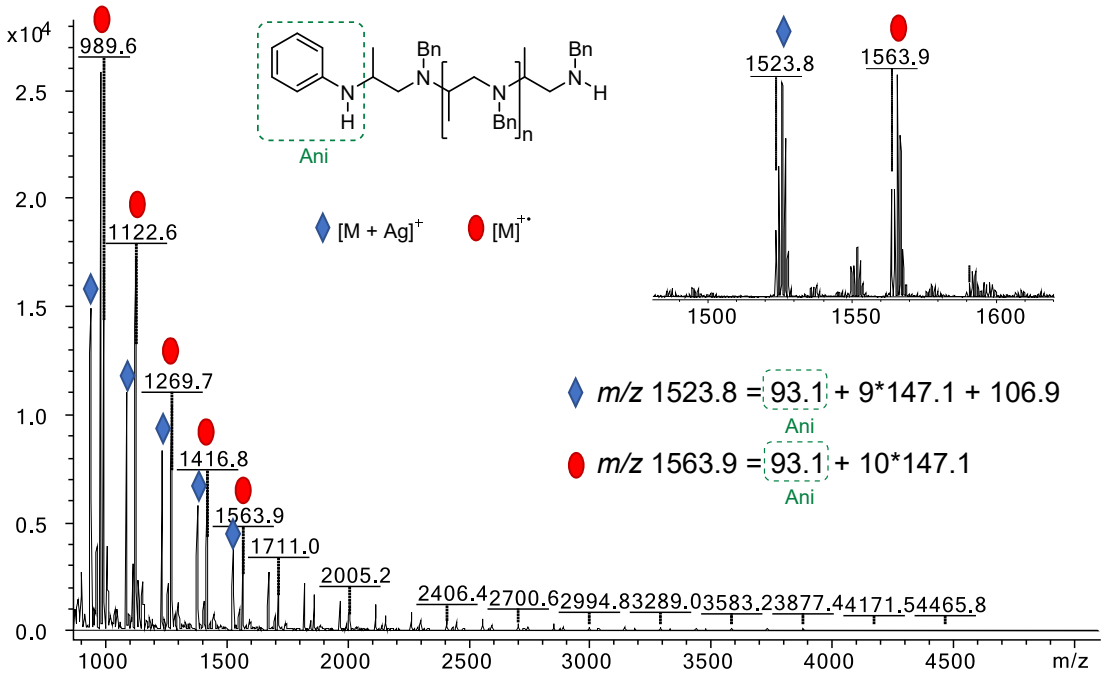


Fig. S11 MALDI-TOF MS spectra of the linear PBMA produced by the BMA/Ani/BCF ratio of 100/10/1.

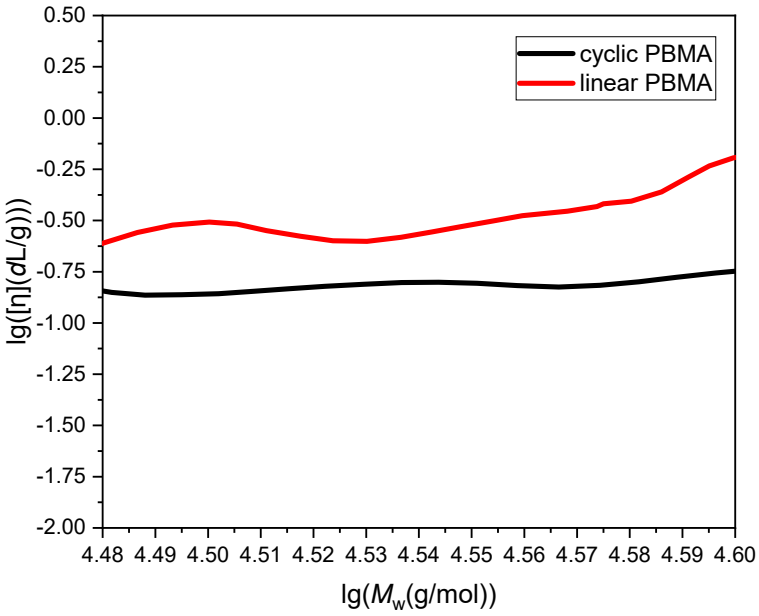


Fig.12 Double-logarithm (Mark–Houwink) plots of intrinsic viscosity [η] versus weight-average molecular weight (M_w) of the linear PBMA (21.0 kg/mol in GPC triple analysis) and cyclic PBMA (25.7 kg/mol in GPC triple analysis).

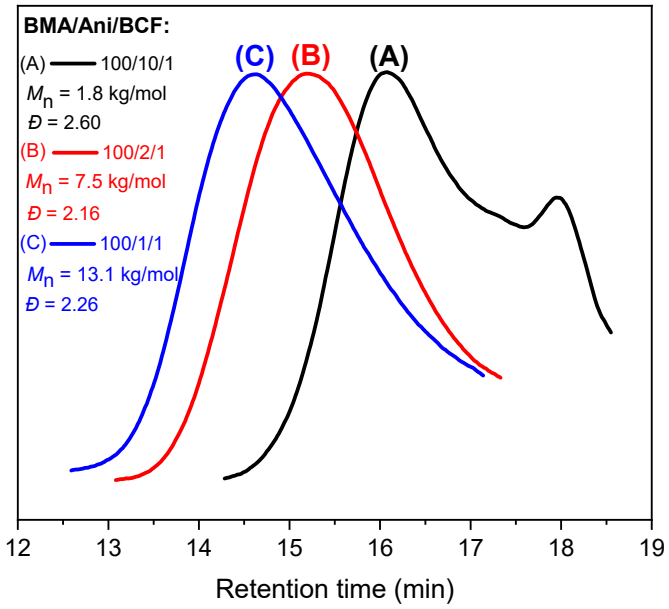
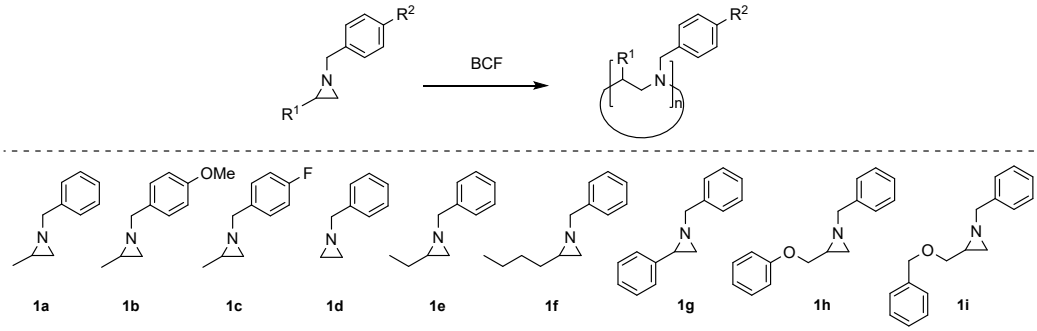


Fig. S13 GPC traces of linear PBMAs reacted under different BMA/Ani/BCF ratios: (A) 100/10/1, (B) 100/2/1 and (C) 100/1/1.

Table S4 Results for CROP of several *N*-benzylaziridines.[a]



Entry	Monomer	Conv.[b] [%]	M_n[c] [kg mol^{-1}]	$Đ$[c]
1	**1a**	99	17.4	1.96
2	**1b**	96	8.2	1.99
3	**1c**	80	10.7	2.26
4	**1d**	60	3.8	1.58
5	**1e**	86	10.1	2.14
6	**1f**	94	30.7	1.97
7	**1g**	76	7.8	2.09
8	**1h**	85	4.5	2.17
9	**1i**	68	5.8	1.95

[a]Reactions carried out with a monomer/BCF ratio of 100/1 under 25 °C in DCM for 12 h; [b]Obtained by ^{1}H NMR spectroscopy; [c]Determined by gel permeation chromatography in THF, calibrated with polystryene standards.

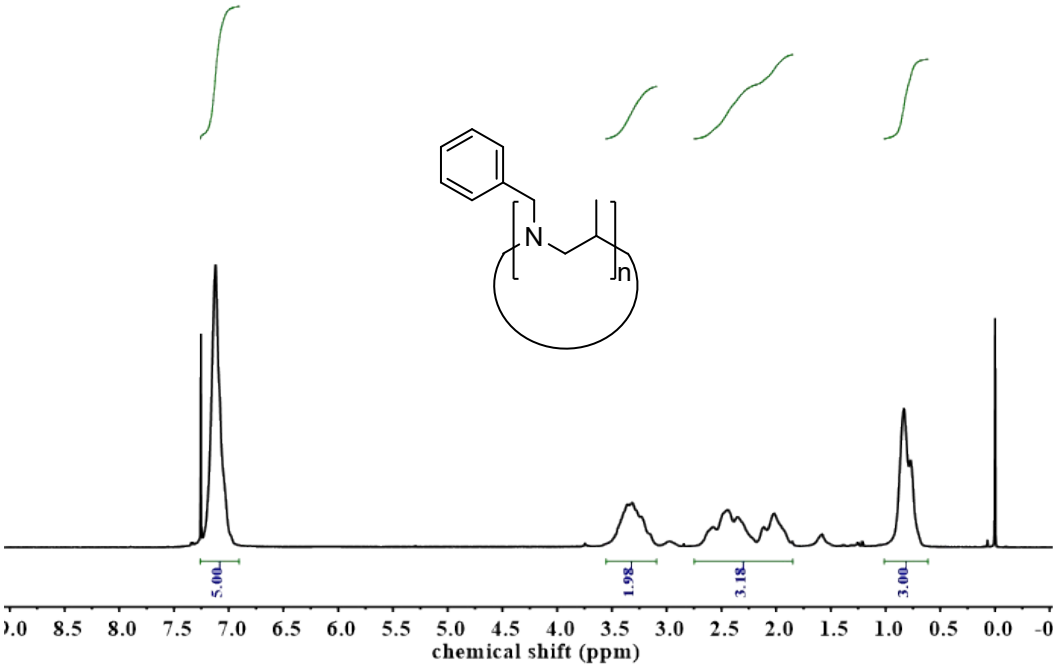


Fig. S14 ^{1}H NMR spectrum of poly(1-benzyl-2-methylaziridine) in $CDCl_3$.

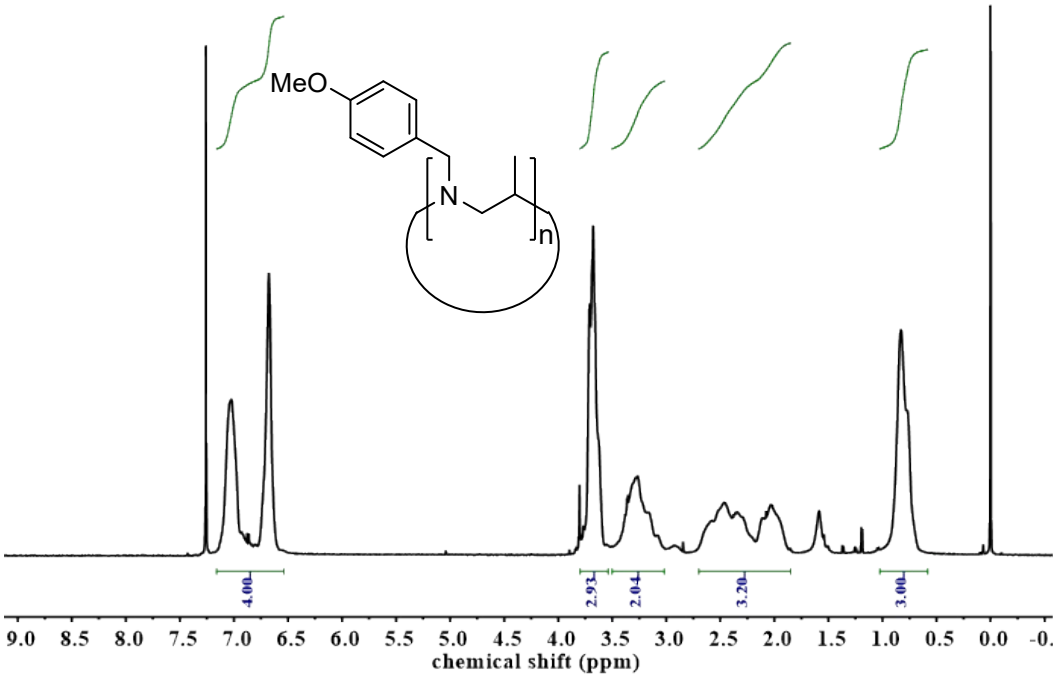


Fig. S15 ^{1}H NMR spectrum of poly(1-(4-methoxybenzyl)-2-methylaziridine) in $CDCl_3$.

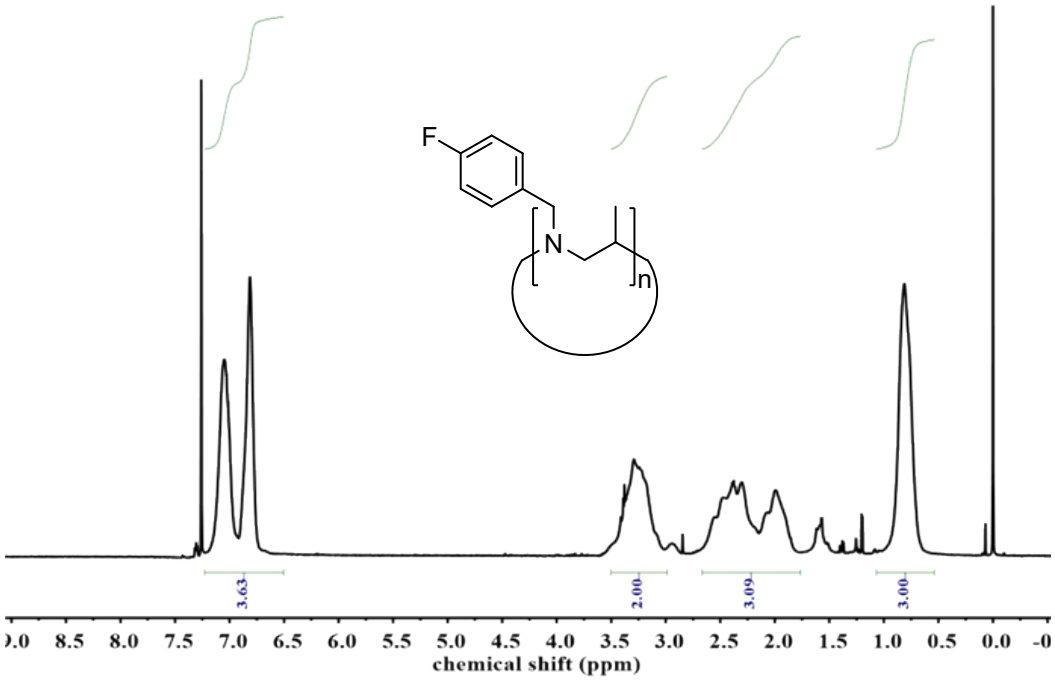


Fig. S16 ^{1}H NMR spectrum of poly(1-(4-fluorobenzyl)-2-methylaziridine) in $CDCl_3$.

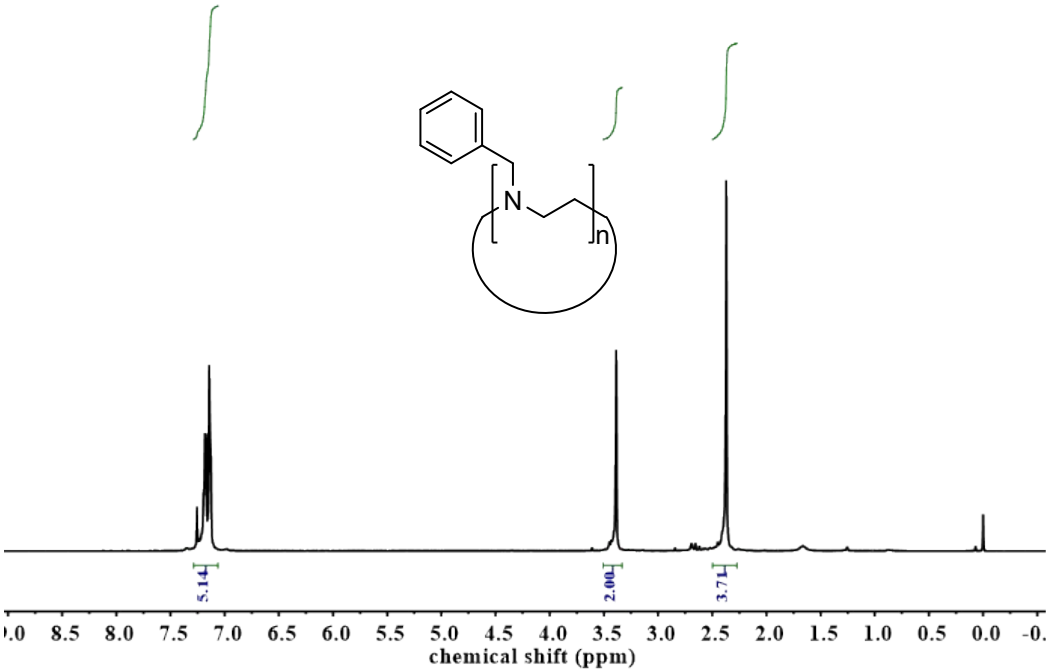


Fig. S17 ^{1}H NMR spectrum of poly(1-benzylaziridine) in $CDCl_3$.

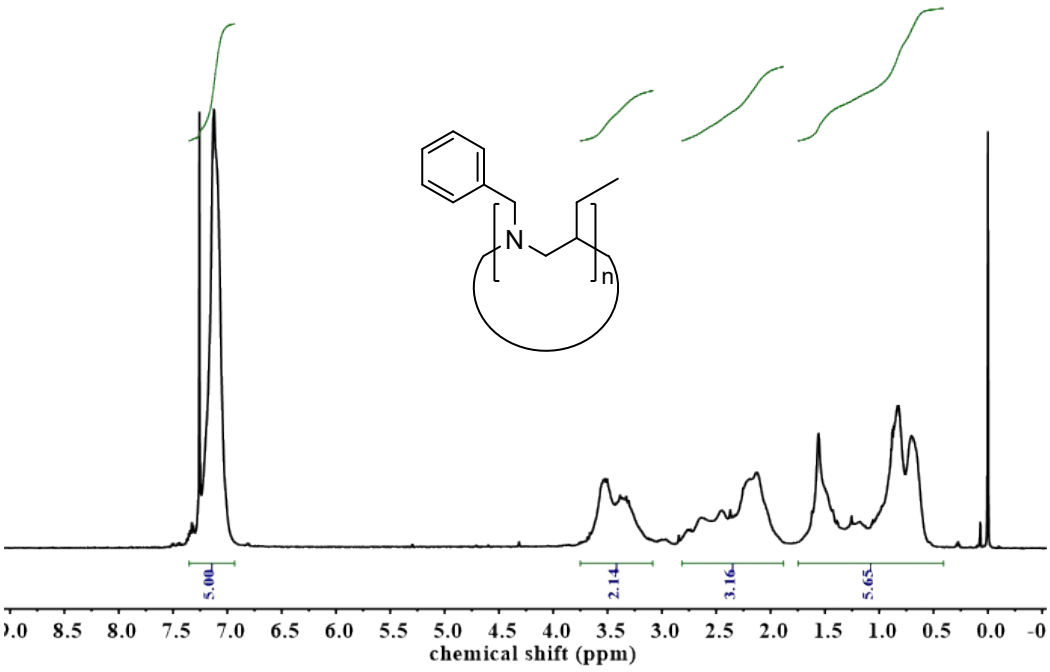


Fig. S18 ^{1}H NMR spectrum of poly(2-ethyl-1-(benzyl)aziridine) in $CDCl_3$.

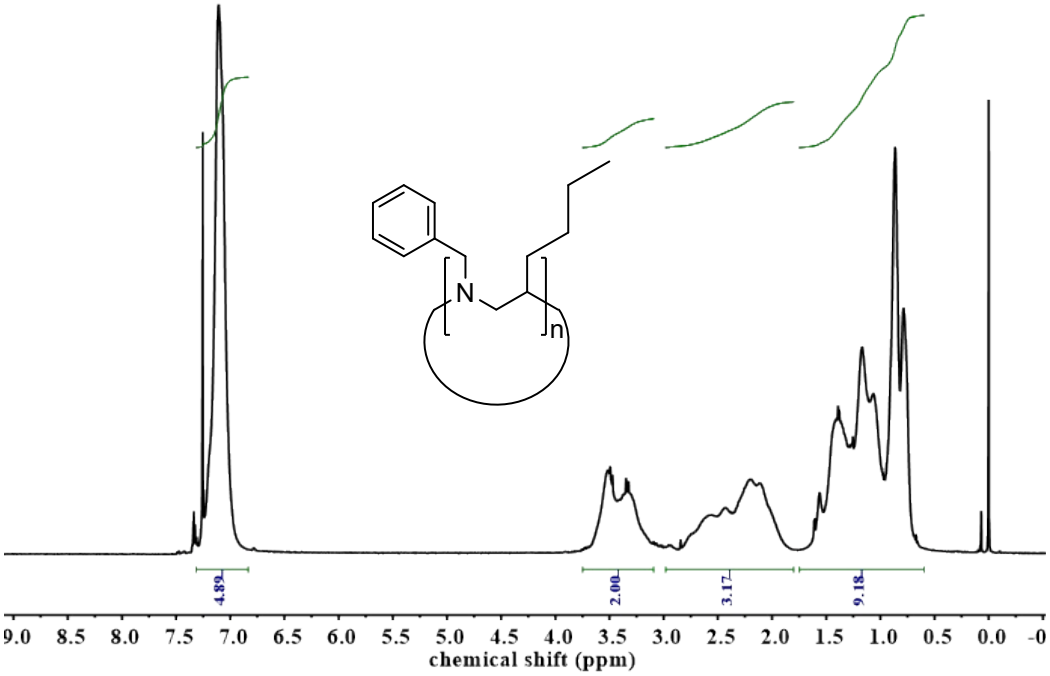


Fig. S19 ^{1}H NMR spectrum of poly(2-butyl-1-(benzyl)aziridine) in $CDCl_3$.

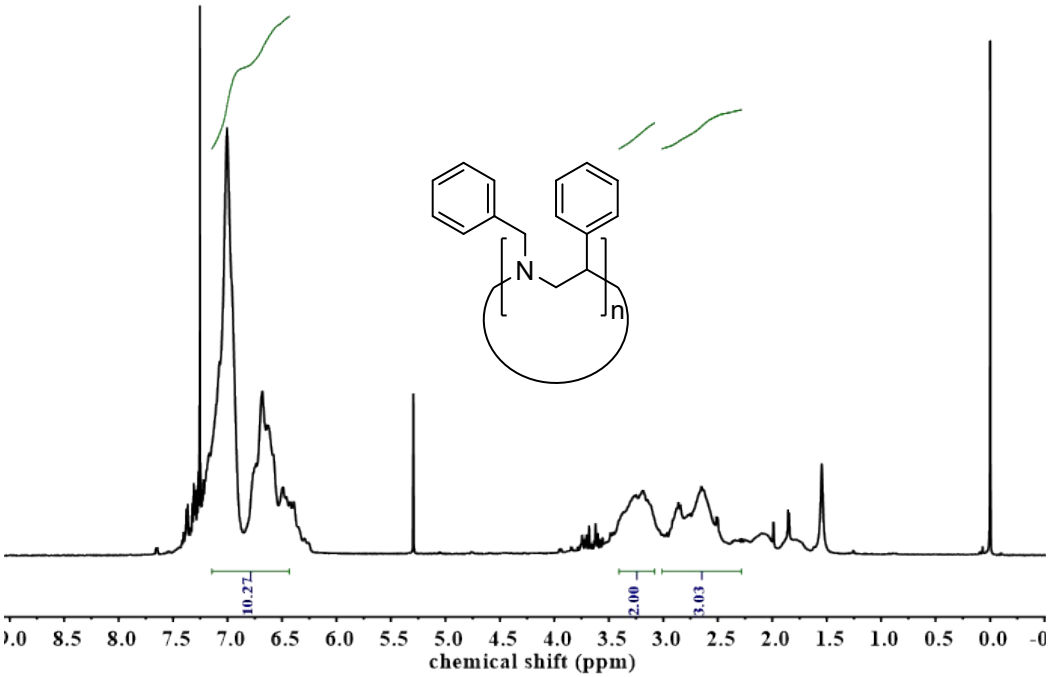


Fig. S20 ^{1}H NMR spectrum of poly(1-benzyl-2-phenylaziridine) in $CDCl_3$.

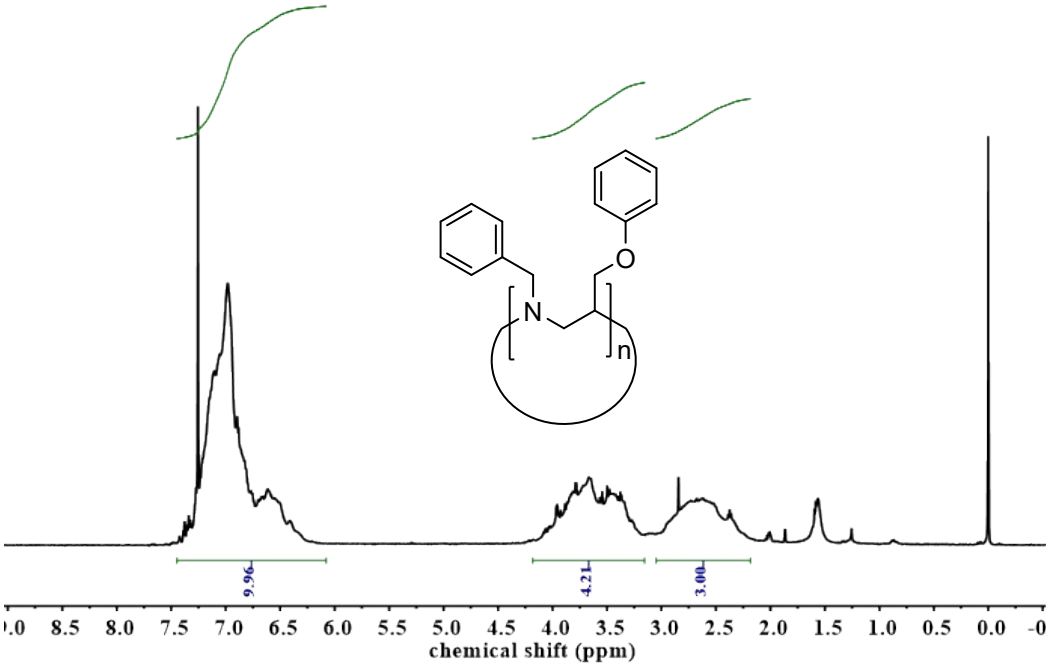


Fig. S21 ^{1}H NMR spectrum of poly(2-(phenoxymethyl)-1-(benzyl)aziridine) in $CDCl_3$.

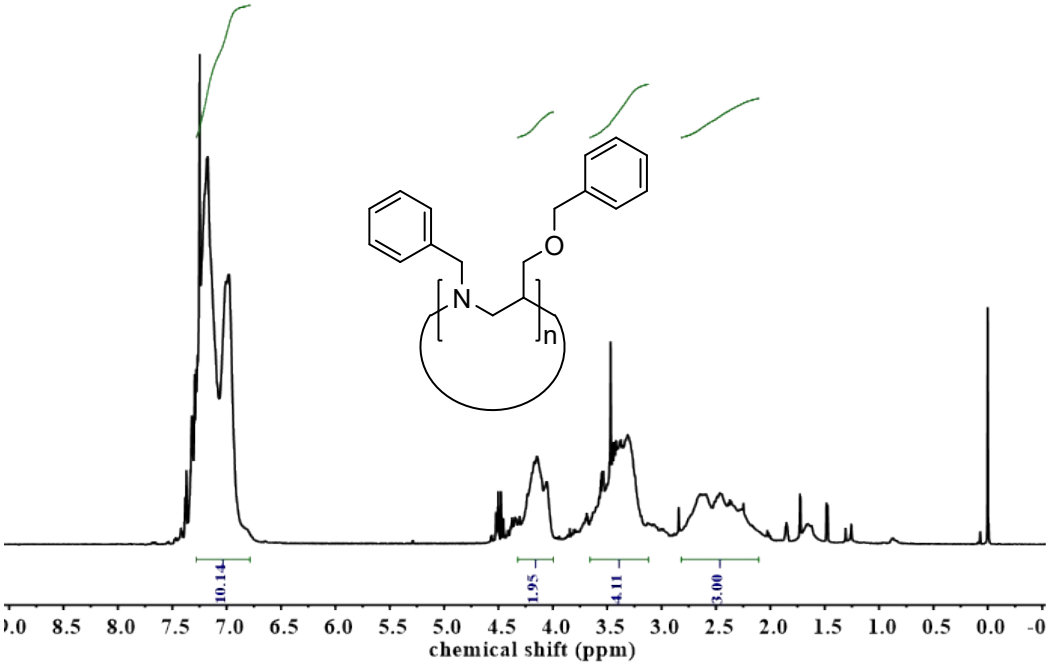


Fig. S22 ^{1}H NMR spectrum of poly(2-[(phenylmethoxy)methyl]-1-(benzyl)aziridine) in $CDCl_3$.

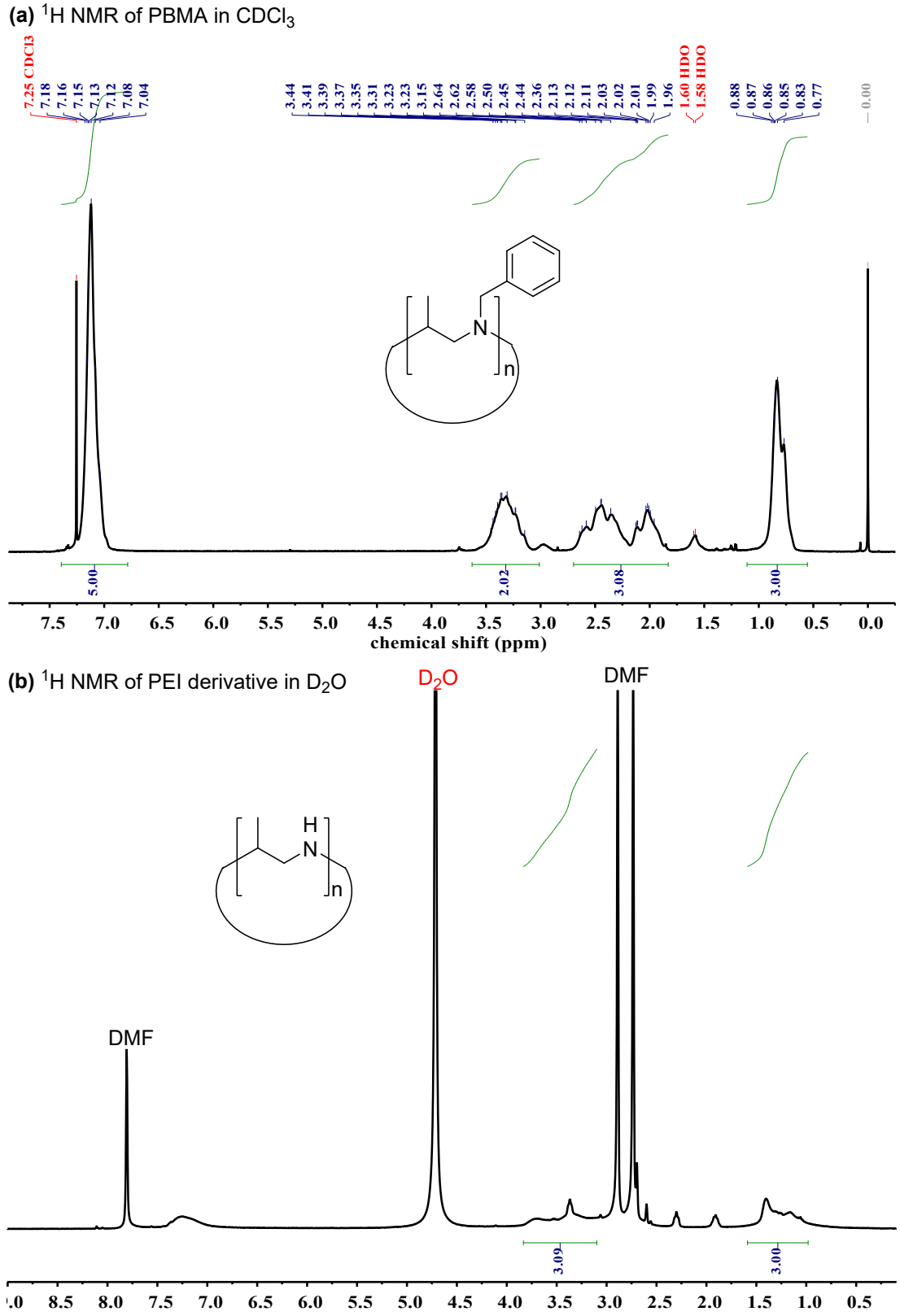


Fig. S23 ^{1}H NMR spectra of (a) PBMA in $CDCl_3$ and (b) PEI derivative in D_2O.

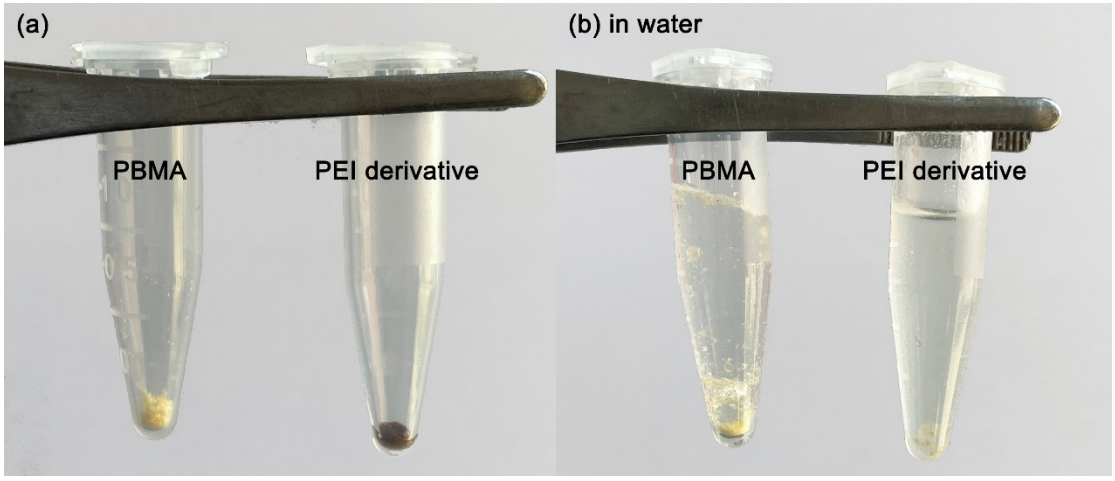
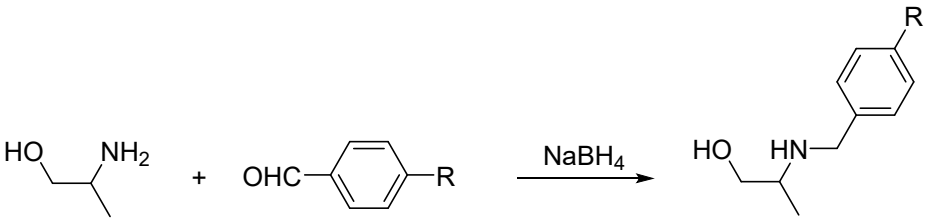


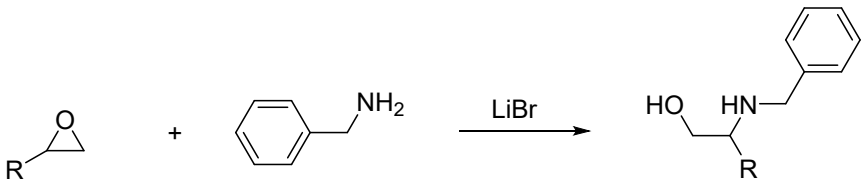
Fig. S24 Appearance properties before/after debenzylation: (a) PBMA/PEI derivative and (b) PBMA: unsoluble in water/PEI derivative: water-soluble.

III. Synthesis of *N*-benzylaziridines



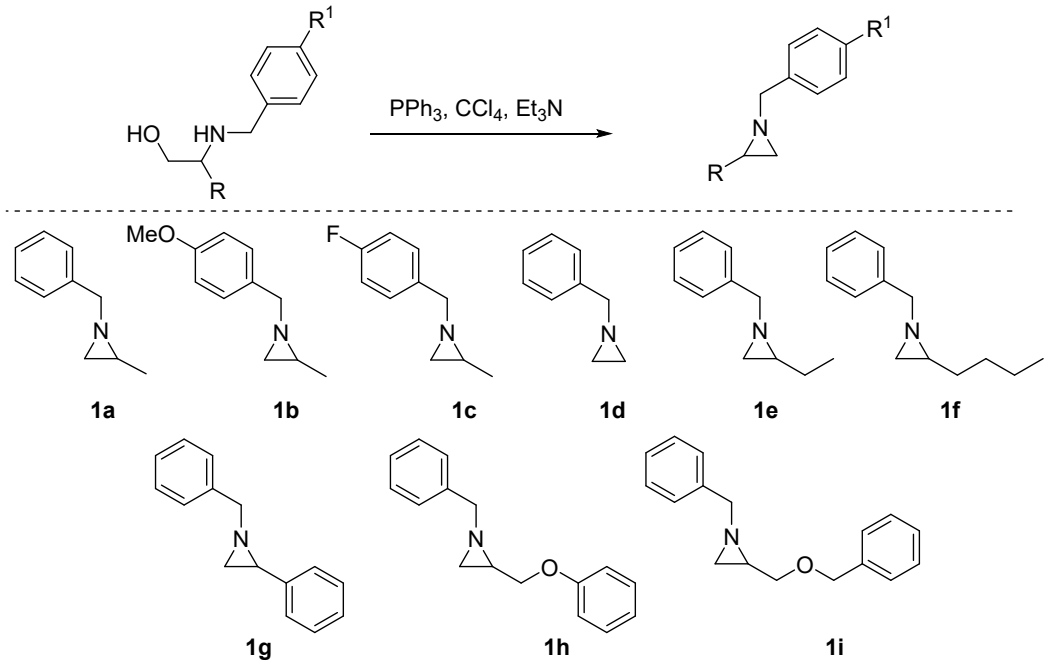
P1a: R = H
P1b: R = OCH_3
P1c: R = F

General synthesis method (**P1a-P1c**): 2-amino-1-propanol (37.5 g, 0.5 mol) and 4-substituted benzaldehyde (0.6 mol) were added to a 250 mL three-necked flask with a magnetic stirring bar, and reacted at 120 °C for 6 h under an atmosphere of nitrogen. After the reaction mixture returned to room temperature, 100 mL of methanol was added and stirred until the reaction system was homogeneous. The system was placed in an ice bath, $NaBH_4$ (22.8 g, 0.6 mol) was slowly added to the reaction mixture, and methanol was removed under vacuum when no bubbles were formed. 250 mL of ethyl acetate was added to the system, followed by 3 mol/L hydrochloric acid to adjust the system to pH = 5–6, and then separated the liquid to collect the aqueous phase. Then 3 mol/L sodium hydroxide aqueous solution was added to adjust the pH to 11–12, and extracted with ethyl acetate for 3 times. The combined organics were dried over anhydrous Na_2SO_4 and the solvent was removed under vacuum. The compound was used in the following reactions without further purification.



P1e: $R^1 = CH_2CH_3$, $R^2 = H$
P1f: $R^1 = (CH_2)_3CH_3$, $R^2 = H$
P1g: $R^1 = Ph$, $R^2 = H$
P1h: $R^1 = CH_2OPh$, $R^2 = H$
P1i: $R^1 = CH_2OBn$, $R^2 = H$

General synthesis method (**P1e**-**P1i**)[2]: epoxide (0.1 mol), benzylamine (10.7 g, 0.1 mol) and lithium bromide (4.35 g, 0.05 mol) were measured into a 250 mL three-necked flask with a magnetic stirring bar flask under an atmosphere of nitrogen. The solution was stirred at room temperature, during the process the solution gradually solidified. The crude product was purified using column chromatography (silica gel, dichloride methane/methanol = 20/1).



General synthesis method (**1a**-**1i**)[3]: amino alcohol (**P1a**-**P1i**) (0.1 mol), triphenylphosphine (30.0 g, 0.114 mol), carbon tetrachloride (9.7 mL, 0.1 mol), and triethylamine (13.9 mL, 0.1 mol) were measured into a 250 mL round-bottom flask placed in an ice bath, followed by the addition of 80 mL acetonitrile to form a solution. Acetonitrile was removed by vacuum, then 500 mL n-hexane was poured into the yellow solid. The system was stirred vigorously for 30 min, then the white powder was filtered and the n-hexane solution was collected. After the removal of n-hexane by vacuum, crude product was obtained. The purified *N*-benzylaziridines were obtained from the crude product by distillation (colorless liquid).

1-benzyl-2-methylaziridine (**1a**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.22 (m, 5H), 3.53–3.39 (m,

2H), 1.61 (d, 1H), 1.59–1.51 (m, 1H), 1.41 (d, 1H), 1.24 (d, 3H).

1-(4-methoxybenzyl)-2-methylaziridine (**1b**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25 (d, 2H), 6.36 (d, 2H), 3.80 (s, 3H), 3.35 (s, 2H), 1.55 (d, 1H), 1.52–1.45 (m, 1H), 1.37 (d, 1H), 1.19 (d, 3H).

1-(4-fluorobenzyl)-2-methylaziridine (**1c**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26–7.34 (m, 2H), 7.05-6.97 (m, 2H), 3.43–3.33 (m, 2H), 1.56 (d, 1H), 1.55–1.47 (m, 1H), 1.37 (d, 1H), 1.19 (d, 3H).

1-benzylaziridine (**1d**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, 4H), 7.30 (t, 1H), 3.41 (s, 2H), 1.90–1.81 (m, 2H), 1.30 (d, 2H).

2-ethyl-1-(benzyl)aziridine (**1e**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43–7.26 (m, 4H), 7.26–7.17 (m, 1H), 3.39 (dd, 2H), 1.59 (d, 1H), 1.48–1.31 (m, 4H), 0.87 (t, 3H).

2-butyl-1-(benzyl)aziridine (**1f**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40–7.27 (m, 4H), 7.26–7.16 (m, 1H), 3.55–3.25 (dd, 2H), 1.60 (d, 1H), 1.49–1.17 (m, 8H), 0.90–0.77 (m, 3H).

1-benzyl-2-phenylaziridine (**1g**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42–7.13 (m, 10H), 3.74–3.56 (dd, 2H), 2.49 (dd, 1H), 1.97 (d, 1H), 1.83 (d, 1H).

2-(phenoxymethyl)-1-(benzyl)aziridine (**1h**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (dt, 4H), 7.29–7.21 (m, 3H), 6.91 (dd, 3H), 3.95 (d, 2H), 3.50 (q, 2H), 1.98 (dd, 1H), 1.85 (d, 1H), 1.56 (d, 1H).

2-[(phenylmethoxy)methyl]-1-(benzyl)aziridine (**1i**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (d, 2H), 7.34–7.20 (m, 8H), 4.52–4.44 (dd, 2H), 3.54 (dd, 1H), 3.47–3.40 (m, 3H), 1.87–1.80 (m, 1H), 1.71 (d, 1H), 1.46 (d, 1H).

IV. Computational details

Computations were performed using the Gaussian 16 suite of the programs[4] and Multiwfn[5] software package. Atomic charge analysis was calculated by three methods: Mulliken, natural population analysis (NPA) and restrained electro static potential (RESP). Optimized structures were obtained using the M062X functional with the 6-31G(d) basis sets. Single-point calculation and vibration analysis were performed using the M062X functional with the triple-zeta, diffuse, polarized 6-311G+(d,p) basis set. The SMD solvent model (DCM) was used. The relative free energy was obtained by combining the single-point energy with Gibbs free energy correction.

BCF
Charge = 0 Multiplicity = 1
B 0.00008 -0.00006 0.00013
C 0.26302 1.54543 -0.00002
C -0.59491 2.44873 0.63593
C 1.37145 2.11429 -0.63585
C -0.37408 3.81704 0.65444
C 1.61575 3.47858 -0.65366
C 0.73743 4.33299 0.0005
C 1.20703 -1.00061 0.00016
C 1.14501 -2.24502 -0.63546
C 2.41866 -0.70957 0.63552
C 2.20419 -3.13891 -0.65407
C 3.49315 -1.58507 0.65316
C 3.38377 -2.80565 -0.00068
C -1.46988 -0.54482 -0.00004
C -1.82394 -1.73851 0.63724
C -2.51619 0.13001 -0.63729

C -3.1194 -2.2311 0.65554
C -3.81984 -0.3405 -0.65588
C -4.12148 -1.52735 -0.00026
F 0.03919 -2.61857 -1.28117
F 2.10166 -4.30424 -1.28408
F 4.40252 -3.65039 -0.00094
F 4.61962 -1.26886 1.28276
F 2.58107 0.44555 1.28252
F -0.90479 -2.45589 1.28514
F -3.40898 -3.36325 1.28776
F -5.36244 -1.98724 -0.00055
F -4.77709 0.32971 -1.28816
F -2.28616 1.27326 -1.28486
F 2.24738 1.34383 -1.28277
F 2.67584 3.97306 -1.28378
F 0.95945 5.63764 0.00059
F -1.21077 4.63413 1.28512
F -1.67637 2.01132 1.2828

BMA

Charge = 0 Multiplicity = 1
C -3.15529 0.13826 -0.45742
C -2.2902 0.40258 0.72557
H -3.37394 -0.90885 -0.67139
H -3.92923 0.83831 -0.75978
C -0.83032 -0.38872 -1.1459
H -0.81626 -0.26993 -2.23678
H -1.12622 -1.43263 -0.9524
C 0.55437 -0.1534 -0.58413
C 0.97068 1.12993 -0.22342
C 1.44048 -1.2203 -0.42874
C 2.25273 1.33908 0.27729
H 0.27537 1.95627 -0.33415
C 2.72484 -1.01189 0.0663
H 1.11921 -2.22507 -0.69457
C 3.13448 0.2705 0.42172
H 2.56449 2.34122 0.55657
H 3.40223 -1.85261 0.18254
H 4.13347 0.43541 0.81359
N -1.78508 0.58257 -0.63
H -2.42762 1.35256 1.23989
C -1.83059 -0.72107 1.62633
H -0.83231 -0.51667 2.02559
H -2.52182 -0.82359 2.46824
H -1.79902 -1.68225 1.10702

IN-0

Charge = 0 Multiplicity = 1
B 0.19778 0.09698 -0.14094
C 1.63872 0.29599 -0.91826
C 2.24528 -0.77796 -1.57928
C 2.4712 1.41454 -0.80635
C 3.49721 -0.73761 -2.17498
C 3.73532 1.49875 -1.38389
C 4.25217 0.42147 -2.08279
C -0.35876 1.45056 0.62404
C -0.87978 1.46984 1.91717
C -0.4806 2.66922 -0.04497
C -1.42569 2.59973 2.51923
C -1.02202 3.81979 0.50822
C -1.49695 3.78747 1.8114
C 0.46613 -1.16422 0.86273
C 0.08474 -2.4816 0.66705
C 1.30325 -0.96102 1.95907
C 0.44637 -3.5274 1.50901
C 1.69588 -1.9669 2.8267
C 1.25875 -3.26688 2.59979
F -1.09517 4.94464 -0.20118
F -2.02534 4.87388 2.36297
F -1.90444 2.53556 3.75947
F -0.93659 0.35639 2.66179
F -0.06042 2.79218 -1.31834
F 2.12324 2.48788 -0.09196
F 4.459 2.60671 -1.24724
F 5.45567 0.48909 -2.63852
F 3.98258 -1.80468 -2.80584
F 1.6248 -1.97301 -1.65031
F -0.66955 -2.8221 -0.39907
F 0.03129 -4.76945 1.26217
F 1.62285 -4.24885 3.41791
F 2.48626 -1.7056 3.86517
F 1.75947 0.27397 2.20968
C -0.9788 -0.9781 -2.44352
C -1.03589 0.49341 -2.48991
H -1.87899 -1.53198 -2.68528
H -0.05065 -1.49987 -2.6121
H -0.08073 0.98782 -2.61881
N -1.06517 -0.22147 -1.17555
C -2.21723 1.29037 -2.97259
H -1.97175 1.70068 -3.95567

H -3.11971 0.68732 -3.07084
H -2.41215 2.13712 -2.30636
C -2.3629 -0.28279 -0.40066
H -2.63566 0.75221 -0.1861
H -2.09282 -0.75054 0.55096
C -3.56076 -0.9958 -0.98744
C -3.61529 -2.3902 -1.09289
C -4.6977 -0.25468 -1.32219
C -4.76542 -3.01807 -1.5615
H -2.75863 -2.98591 -0.79838
C -5.85202 -0.88137 -1.78261
H -4.68007 0.82749 -1.21523
C -5.88486 -2.2667 -1.91105
H -4.78977 -4.10027 -1.64074
H -6.72443 -0.28717 -2.03503
H -6.78234 -2.76 -2.27048

IN-1

Charge = 0 Multiplicity = 1
B 0.77232 0.03438 -0.3668
C -0.75988 -0.31034 -0.87669
C -1.26138 -1.61155 -0.78645
C -1.59377 0.54474 -1.60576
C -2.50721 -2.01511 -1.24048
C -2.83451 0.17194 -2.11492
C -3.32382 -1.102 -1.88617
C 1.21161 1.61087 -0.58976
C 2.41456 2.04054 -1.14702
C 0.42259 2.65036 -0.10066
C 2.78037 3.37867 -1.26612
C 0.73882 3.99591 -0.19598
C 1.93553 4.368 -0.79111
C 1.71104 -1.02303 -1.18799
C 2.28314 -2.18921 -0.70668
C 1.83897 -0.84294 -2.56495
C 2.97718 -3.09753 -1.49894
C 2.51655 -1.71673 -3.39902
C 3.09556 -2.85857 -2.85749
F -0.09378 4.922 0.28032
F 2.27061 5.64965 -0.89018
F 3.94884 3.71018 -1.81133
F 3.33759 1.16581 -1.57096
F -0.74693 2.37881 0.50942
F -1.23351 1.79475 -1.91339
F -3.54351 1.03106 -2.84295
F -4.53106 -1.45816 -2.31223
F -2.91292 -3.27496 -1.06251
F -0.51693 -2.60125 -0.24772
F 2.17579 -2.51669 0.59798
F 3.50976 -4.19518 -0.96175
F 3.75037 -3.71304 -3.63746
F 2.61449 -1.47999 -4.70541
F 1.28764 0.23828 -3.13414
C 0.32191 -1.16777 2.11935
C -0.23332 0.1899 2.11425
H 0.92798 -1.47337 2.96498
H -0.1747 -1.96395 1.5899
H -1.11037 0.31154 1.49103
N 0.96577 -0.13221 1.27212
C -0.16057 1.13594 3.27855
H -1.13546 1.10617 3.77599
H 0.59901 0.85502 4.00847
H 0.012 2.16306 2.94159
C 2.33158 0.36406 1.68482
H 2.27369 1.45434 1.68256
H 2.99225 0.0723 0.86201
C 2.93812 -0.09248 2.99301
C 3.42515 -1.39276 3.16683
C 3.13001 0.83634 4.01947
C 4.0503 -1.75983 4.35463
H 3.31983 -2.11671 2.36643
C 3.76188 0.47351 5.20563
H 2.78388 1.85863 3.88544
C 4.21717 -0.83009 5.37837
H 4.41911 -2.77362 4.47456
H 3.90181 1.21071 5.98982
H 4.71009 -1.11794 6.30156
C -2.96982 -2.32073 3.37994
C -3.21756 -2.47836 1.92164
H -3.82169 -2.48933 4.03939
H -2.00109 -2.55309 3.81598
C -4.17561 -0.27501 2.68186
H -3.96395 0.34311 3.56277
H -5.10282 -0.8259 2.89838
C -4.38094 0.61424 1.47903
C -5.4327 0.39415 0.58824
C -3.52163 1.69076 1.25042
C -5.63363 1.24437 -0.49713
H -6.11105 -0.4392 0.75601

C -3.71376 2.54283 0.16638
H -2.70453 1.87659 1.94396
C -4.78209 2.32736 -0.70123
H -6.45591 1.06177 -1.1821
H -3.02855 3.36879 0.00356
H -4.9366 2.98801 -1.54788
N -3.0189 -1.15546 2.50989
H -2.37364 -2.79335 1.31101
C -4.54976 -2.96296 1.39612
H -4.79724 -2.48249 0.44409
H -4.49374 -4.04029 1.21748
H -5.36681 -2.78519 2.09959

TS-1

Charge = 0 Multiplicity = 1
B -0.8841 -0.35558 0.00466
C 0.55176 -1.07297 -0.45603
C 1.10054 -0.8464 -1.72193
C 1.28565 -2.00161 0.28757
C 2.32951 -1.32527 -2.1529
C 2.49263 -2.55689 -0.12962
C 3.05203 -2.18158 -1.33752
C -1.33282 -0.77109 1.54408
C -2.59367 -1.20412 1.9417
C -0.47112 -0.51046 2.60794
C -2.96009 -1.40961 3.27045
C -0.78508 -0.69431 3.94393
C -2.05058 -1.15468 4.2816
C -1.94543 -0.88618 -1.13594
C -2.45496 -0.14588 -2.19011
C -2.27594 -2.2396 -1.16776
C -3.27303 -0.6746 -3.18369
C -3.08404 -2.81717 -2.13322
C -3.59149 -2.02158 -3.15391
F 0.10908 -0.43172 4.89958
F -2.38321 -1.3373 5.55663
F -4.18891 -1.82559 3.57374
F -3.57405 -1.40962 1.05078
F 0.77741 -0.04984 2.36729
F 0.8721 -2.44598 1.4789
F 3.12555 -3.43219 0.65145
F 4.23409 -2.65364 -1.72276
F 2.81016 -0.96581 -3.34842
F 0.44301 -0.1089 -2.64422
F -2.15637 1.16468 -2.32358
F -3.73526 0.10105 -4.16653
F -4.36826 -2.55198 -4.09578
F -3.37323 -4.11777 -2.10147
F -1.79821 -3.049 -0.21019
C 0.02324 2.04915 -0.78026
C 1.05017 1.9116 0.26931
H -0.35973 3.06541 -0.87883
H 0.19877 1.62725 -1.7603
H 1.4747 0.92783 0.40219
N -0.80343 1.22838 0.08683
C 1.04233 2.8481 1.44341
H 2.00027 2.83372 1.96509
H 0.81528 3.87265 1.13388
H 0.28758 2.52589 2.16671
C -1.96974 1.85401 0.75188
H -1.86391 1.73634 1.83897
H -2.85244 1.26325 0.46653
C -2.26074 3.31136 0.46523
C -2.83473 3.71324 -0.74672
C -2.01388 4.28222 1.43852
C -3.12736 5.05247 -0.9834
H -3.04985 2.96845 -1.50547
C -2.30928 5.6241 1.20665
H -1.59723 3.98231 2.39702
C -2.8623 6.01321 -0.00905
H -3.57417 5.34536 -1.92855
H -2.11491 6.3612 1.97973
H -3.0967 7.05703 -0.19344
C 2.70018 3.55574 -1.57016
C 2.93671 2.16028 -2.03042
H 3.53176 4.25401 -1.64596
H 1.71208 4.00381 -1.62888
C 4.06917 2.44585 0.22508
H 3.87914 3.08328 1.09458
H 4.90421 2.9016 -0.32081
C 4.43858 1.04381 0.65354
C 5.5186 0.38591 0.06187
C 3.72158 0.38744 1.65839
C 5.86597 -0.90561 0.45147
H 6.10208 0.89114 -0.70341
C 4.05882 -0.90569 2.04412
H 2.89487 0.88395 2.1564
C 5.13582 -1.55428 1.44254
H 6.70607 -1.404 -0.02144

H 3.46688 -1.40922 2.80273
H 5.39382 -2.56587 1.73656
N 2.84611 2.4776 -0.59926
H 2.07794 1.59804 -2.38509
C 4.22529 1.75709 -2.70566
H 4.4667 0.71205 -2.49902
H 4.08976 1.86075 -3.78579
H 5.06979 2.38617 -2.41429

IN-2

Charge = 0 Multiplicity = 1
B -0.89779 0.42479 0.06544
C 0.57446 0.97145 -0.50821
C 1.40075 1.75016 0.30485
C 1.06043 0.8523 -1.8121
C 2.64603 2.24032 -0.05987
C 2.2841 1.36589 -2.23745
C 3.10888 2.03204 -1.34953
C -1.68884 -0.51695 -1.05202
C -3.03415 -0.44899 -1.39174
C -1.04074 -1.64273 -1.55495
C -3.68188 -1.38918 -2.19333
C -1.62942 -2.60077 -2.36147
C -2.97436 -2.47201 -2.68694
C -1.67394 1.85632 0.36856
C -1.81204 2.44295 1.6191
C -2.10493 2.64893 -0.69255
C -2.38612 3.69455 1.82249
C -2.68303 3.89952 -0.5436
C -2.82868 4.42662 0.73345
F -0.92786 -3.64207 -2.81899
F -3.56982 -3.37814 -3.4607
F -4.9768 -1.25646 -2.48101
F -3.82062 0.52826 -0.91399
F 0.26346 -1.85468 -1.26089
F 0.37389 0.22542 -2.7722
F 2.68232 1.18285 -3.49768
F 4.30431 2.48154 -1.72704
F 3.39363 2.91576 0.82538
F 1.01357 2.08867 1.55541
F -1.36447 1.82861 2.73294
F -2.496 4.2011 3.05367
F -3.37648 5.629 0.90606
F -3.08659 4.60476 -1.60181
F -1.95529 2.19811 -1.94898
C 0.31203 -0.65672 2.17747
C 1.44652 -1.42159 1.45341
H 0.00508 -1.27936 3.02921
H 0.62495 0.30357 2.59911
H 1.52432 -1.03707 0.43885
N -0.80742 -0.53652 1.28073
C 1.11616 -2.90791 1.45246
H 1.70935 -3.49987 0.75244
H 1.21627 -3.33441 2.4585
H 0.06922 -2.99576 1.15243
C -2.08615 -0.83567 1.93068
H -2.89039 -0.48411 1.27611
H -2.19483 -0.28234 2.87521
C -2.26797 -2.31637 2.19804
C -2.04684 -2.85346 3.46716
C -2.60308 -3.18751 1.15514
C -2.11934 -4.22919 3.68833
H -1.82419 -2.18246 4.29499
C -2.68075 -4.55882 1.36957
H -2.80512 -2.77834 0.1689
C -2.428 -5.08565 2.63704
H -1.94311 -4.62855 4.68299
H -2.94382 -5.21905 0.54837
H -2.48758 -6.15679 2.8041
C 2.9374 -1.09876 3.51247
C 3.20104 0.0994 2.67741
H 3.78227 -1.62464 3.94698
H 1.99214 -1.20102 4.03316
C 3.92851 -1.97036 1.33762
H 3.62925 -3.01832 1.37954
H 4.83127 -1.86253 1.93974
C 4.18571 -1.50863 -0.07695
C 5.33069 -0.75833 -0.36026
C 3.33823 -1.86973 -1.13023
C 5.6093 -0.34887 -1.66099
H 6.02242 -0.5047 0.43856
C 3.61135 -1.45404 -2.429
H 2.45523 -2.47343 -0.95126
C 4.74572 -0.69126 -2.69709
H 6.49766 0.24063 -1.86203
H 2.92109 -1.71091 -3.22651
H 4.94733 -0.35542 -3.70856
N 2.84015 -1.20572 2.04244
H 2.4013 0.82331 2.58677

C 4.57675 0.6974 2.53828
H 4.72809 1.11353 1.54185
H 4.63457 1.52324 3.25262
H 5.3791 -0.00399 2.77553

IN-3

Charge = 0 Multiplicity = 1
C -3.52884 0.49147 0.09013
C -3.68208 0.1528 -1.33376
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H -3.09006 -0.22481 0.78072
H -3.29592 -0.8111 -1.65117
N -2.55943 1.04422 -0.89939
C -4.7896 0.71536 -2.17662
H -5.60891 -0.0067 -2.14976
H -5.16736 1.66216 -1.78366
H -4.46982 0.84625 -3.21515
C -2.57125 2.49165 -1.30592
H -2.87016 2.52862 -2.35649
H -1.53191 2.82 -1.24823
C -3.43664 3.40433 -0.47389
C -3.21764 3.54664 0.90025
C -4.42692 4.1714 -1.08729
C -3.98682 4.43232 1.6459
H -2.45206 2.95046 1.39198
C -5.19131 5.06749 -0.34288
H -4.59621 4.0741 -2.1572
C -4.97412 5.19651 1.02487
H -3.80964 4.53247 2.71203
H -5.95462 5.66229 -0.83388
H -5.56927 5.8923 1.60739
C -7.56079 -0.6612 0.81831
C -6.41494 -1.15863 1.62603
H -8.43328 -1.31364 0.77349
H -7.77767 0.40004 0.73142
C -6.41169 -2.35609 -0.60978
H -7.05499 -2.16575 -1.47642
H -6.87203 -3.18363 -0.04937
C -5.02997 -2.74384 -1.08506
C -3.98378 -2.87432 -0.1671
C -4.7549 -2.91015 -2.44262
C -2.68787 -3.14137 -0.5954
H -4.17793 -2.71569 0.88984
C -3.45732 -3.18381 -2.87829
H -5.55938 -2.81012 -3.16797
C -2.41674 -3.29 -1.95768
H -1.87706 -3.21923 0.12281
H -3.25904 -3.30595 -3.93892
H -1.4029 -3.49196 -2.28548
N -6.34476 -1.11552 0.16584
H -5.75927 -0.42192 2.09019
C -6.55764 -2.43847 2.4185
H -5.6272 -3.01664 2.44028
H -6.81893 -2.19029 3.45186
H -7.34911 -3.08374 2.03012
C -1.19452 0.38372 -0.92739
H -1.35159 -0.60274 -0.48678
C -0.7396 0.25433 -2.37124
H -0.69453 1.23315 -2.86305
H 0.27523 -0.14896 -2.39054
H -1.39079 -0.41057 -2.94871
C -0.20261 1.16687 -0.04033
H -0.79431 1.76281 0.67072
H 0.31998 1.89436 -0.67895
N 0.73136 0.34282 0.69681
C 0.50313 0.49956 2.12435
H 0.56932 1.5562 2.4409
H 1.28194 -0.02772 2.67751
C -0.8471 -0.04187 2.56114
C -1.77123 0.76799 3.22291
C -1.18052 -1.38085 2.3199
C -2.99706 0.25837 3.65693
H -1.5145 1.80703 3.42321
C -2.38877 -1.90072 2.77484
H -0.46686 -2.00241 1.78752
C -3.30287 -1.08283 3.44539
H -3.6995 0.90304 4.17809
H -2.61344 -2.95408 2.62283
H -4.23721 -1.4952 3.81606
B 2.16955 0.16214 0.12479
C 2.63453 1.63654 -0.47414
C 2.81941 2.6822 0.4274
C 2.6712 2.02213 -1.8073
C 3.06224 3.99633 0.06079
C 2.90796 3.32838 -2.22977
C 3.10843 4.32338 -1.28865
C 2.30215 -1.04601 -1.01801
C 1.42627 -2.10488 -1.22055
C 3.50393 -1.16839 -1.7194

C 1.68744 -3.17371 -2.07394
C 3.80885 -2.20923 -2.5824
C 2.88416 -3.22913 -2.76488
C 3.23449 -0.41848 1.25396
C 4.51201 0.06755 1.52356
C 2.94134 -1.62066 1.89748
C 5.39988 -0.55156 2.4003
C 3.78784 -2.27112 2.78202
C 5.0381 -1.72668 3.03689
F 0.78309 -4.15142 -2.23454
F 0.22193 -2.16185 -0.60888
F 3.14574 -4.24358 -3.58739
F 4.97447 -2.2495 -3.22782
F 4.45425 -0.2362 -1.55994
F 2.43264 1.13702 -2.79483
F 2.9179 3.63154 -3.53063
F 3.32675 5.58178 -1.66994
F 3.23907 4.94818 0.97973
F 2.76134 2.43378 1.74775
F 1.75754 -2.22329 1.667
F 4.98229 1.17601 0.93946
F 6.6043 -0.02436 2.62365
F 5.87734 -2.32844 3.87782
F 3.42152 -3.41138 3.37139

TS-2

Charge = 0 Multiplicity = 1
C -3.63426 0.72382 0.04657
C -4.37731 -0.01956 -0.97541
H -4.10048 1.63436 0.42776
H -3.19347 0.12974 0.84588
H -3.94276 -0.96692 -1.26501
N -2.69332 0.97682 -1.04073
C -5.30843 0.64406 -1.94613
H -6.17962 0.0069 -2.11704
H -5.64528 1.62051 -1.58563
H -4.8179 0.77795 -2.91565
C -2.70344 2.23287 -1.79783
H -3.32532 2.14295 -2.69943
H -1.68088 2.3894 -2.15425
C -3.14888 3.4364 -1.00258
C -2.43919 3.82382 0.13711
C -4.26162 4.1786 -1.39521
C -2.83956 4.93312 0.87261
H -1.56915 3.24623 0.44095
C -4.66372 5.29437 -0.66189
H -4.80936 3.89081 -2.29023
C -3.95501 5.67051 0.47434
H -2.27557 5.23042 1.75167
H -5.52748 5.86891 -0.98134
H -4.2647 6.53921 1.04656
C -7.01061 -0.46237 0.56466
C -5.95728 -0.85833 1.53567
H -7.93252 -1.04148 0.56025
H -7.11039 0.57249 0.24619
C -5.94944 -2.5198 -0.41276
H -6.53441 -2.45612 -1.33724
H -6.5257 -3.1388 0.28674
C -4.59834 -3.13131 -0.70783
C -3.54527 -3.00704 0.20413
C -4.36297 -3.74878 -1.93546
C -2.27368 -3.46849 -0.11913
H -3.70368 -2.4921 1.14851
C -3.09249 -4.2281 -2.25322
H -5.17257 -3.83994 -2.65599
C -2.04212 -4.07561 -1.35391
H -1.44869 -3.3323 0.57396
H -2.91902 -4.69644 -3.21694
H -1.0416 -4.39882 -1.61607
N -5.80998 -1.1473 0.10467
H -5.27182 -0.0803 1.86618
C -6.19616 -1.93929 2.56044
H -5.28953 -2.52593 2.74033
H -6.48265 -1.46729 3.50441
H -7.00311 -2.6184 2.2762
C -1.53808 0.05244 -1.21381
H -1.69761 -0.77084 -0.5108
C -1.55249 -0.4934 -2.64359
H -1.38013 0.3102 -3.36974
H -0.75871 -1.23198 -2.76557
H -2.50457 -0.97975 -2.88419
C -0.15538 0.69632 -0.88319
H -0.26489 1.79746 -0.84701
H 0.48193 0.50053 -1.75199
N 0.54195 0.22223 0.30159
C 0.20644 0.98428 1.48743
H 0.17746 2.07613 1.29012
H 1.00791 0.8455 2.22016
C -1.07758 0.5835 2.18747

C -1.90616 1.53698 2.7826
C -1.38958 -0.77121 2.35011
C -3.02688 1.15487 3.52049
H -1.66247 2.59225 2.68444
C -2.49395 -1.15852 3.10499
H -0.72787 -1.50078 1.89432
C -3.31996 -0.19629 3.6909
H -3.65632 1.91213 3.97933
H -2.69506 -2.21626 3.26156
H -4.17074 -0.49947 4.2958
B 2.07287 0.07266 0.04396
C 2.61868 1.57874 -0.42922
C 2.80812 2.61238 0.4868
C 2.7252 1.98692 -1.7558
C 3.09912 3.9251 0.14032
C 3.01216 3.28748 -2.15653
C 3.2042 4.26878 -1.19878
C 2.38115 -1.09082 -1.08802
C 1.52836 -2.1258 -1.44963
C 3.65679 -1.18258 -1.64545
C 1.87985 -3.13758 -2.33893
C 4.05518 -2.17534 -2.52733
C 3.15165 -3.16852 -2.88167
C 2.86452 -0.53344 1.36042
C 4.10282 -0.1105 1.84195
C 2.37357 -1.67854 1.98859
C 4.75912 -0.71357 2.91111
C 2.98942 -2.30903 3.0606
C 4.19631 -1.81627 3.53232
F 0.99538 -4.09199 -2.66876
F 0.26845 -2.21148 -0.97083
F 3.50338 -4.13518 -3.72888
F 5.28947 -2.19401 -3.03135
F 4.5799 -0.26529 -1.32622
F 2.52426 1.11682 -2.76629
F 3.0914 3.59897 -3.45316
F 3.47172 5.52463 -1.55768
F 3.2696 4.85861 1.08012
F 2.71673 2.37821 1.80936
F 1.25182 -2.27455 1.53813
F 4.75766 0.91224 1.28067
F 5.93439 -0.24608 3.33471
F 4.81296 -2.40595 4.55571
F 2.447 -3.39467 3.61938

IN-4

Charge = 0 Multiplicity = 1
C -3.6977 0.53424 -0.04774
C -4.60024 -0.39842 -0.88473
H -4.29488 1.34061 0.40151
H -3.26761 -0.05866 0.76666
H -3.94137 -1.09523 -1.40036
N -2.58631 1.11924 -0.75684
C -5.50777 0.29707 -1.89187
H -6.30819 -0.36281 -2.24537
H -5.95284 1.20826 -1.47893
H -4.91862 0.58686 -2.76411
C -2.85865 2.24571 -1.64021
H -3.41668 1.97915 -2.55404
H -1.88602 2.61471 -1.98558
C -3.57865 3.36673 -0.92748
C -3.01368 3.92047 0.22452
C -4.79344 3.86753 -1.39236
C -3.65653 4.94875 0.9031
H -2.0601 3.53065 0.57081
C -5.44149 4.9018 -0.71607
H -5.2286 3.45622 -2.30123
C -4.87645 5.44002 0.43516
H -3.20314 5.37702 1.79217
H -6.38369 5.2883 -1.09292
H -5.37697 6.24617 0.96247
C -6.69314 -0.76972 0.57105
C -5.58441 -1.14109 1.47449
H -7.55685 -1.42438 0.49737
H -6.86612 0.2741 0.33499
C -5.53671 -2.71421 -0.5743
H -6.07454 -2.62484 -1.52379
H -6.15776 -3.304 0.10312
C -4.17416 -3.32619 -0.79674
C -3.10855 -3.09134 0.07754
C -3.96414 -4.09715 -1.93943
C -1.84672 -3.60469 -0.20001
H -3.2293 -2.45035 0.94741
C -2.70373 -4.62808 -2.2055
H -4.78244 -4.26989 -2.63461
C -1.63997 -4.37041 -1.34637
H -1.01117 -3.37275 0.45277
H -2.54755 -5.21531 -3.10452
H -0.64436 -4.72781 -1.58256

N -5.45381 -1.32808 -0.0126
H -4.95531 -0.3331 1.83354
C -5.66594 -2.32853 2.39798
H -4.71842 -2.86996 2.44388
H -5.87682 -1.94214 3.39856
H -6.46968 -3.0193 2.13623
C -1.57226 0.16029 -1.2444
H -1.66258 -0.7334 -0.61597
C -1.75747 -0.24925 -2.71476
H -1.4655 0.56466 -3.38853
H -1.11436 -1.10694 -2.92743
H -2.78747 -0.53024 -2.96475
C -0.13853 0.69382 -1.04119
H -0.1598 1.7976 -1.14783
H 0.47042 0.33194 -1.8755
N 0.51911 0.30453 0.19512
C 0.08233 1.0967 1.32792
H -0.09858 2.15435 1.04957
H 0.89105 1.11991 2.06565
C -1.13069 0.58376 2.08396
C -2.01295 1.46861 2.7093
C -1.31316 -0.78794 2.28495
C -3.04405 1.00459 3.52451
H -1.87953 2.53865 2.57359
C -2.32791 -1.2584 3.11782
H -0.62002 -1.46672 1.79961
C -3.19684 -0.36417 3.74571
H -3.70854 1.71378 4.01061
H -2.41495 -2.32719 3.30562
H -3.9643 -0.72669 4.42549
B 2.05827 0.19587 0.01391
C 2.59917 1.69788 -0.475
C 2.70635 2.77507 0.40347
C 2.77399 2.05223 -1.81052
C 2.99277 4.07769 0.01736
C 3.05961 3.34089 -2.24943
C 3.17381 4.36623 -1.32631
C 2.47271 -0.98367 -1.07299
C 1.66625 -2.01631 -1.53166
C 3.80505 -1.08201 -1.47511
C 2.12104 -3.04362 -2.35358
C 4.30502 -2.08555 -2.29049
C 3.44923 -3.08414 -2.73655
C 2.78077 -0.37532 1.38554
C 3.94097 0.10906 1.98739
C 2.30249 -1.55923 1.94939
C 4.51672 -0.46497 3.118
C 2.83865 -2.16288 3.07759
C 3.95724 -1.60264 3.67546
F 1.2801 -4.00564 -2.76785
F 0.35477 -2.0898 -1.21798
F 3.89999 -4.06487 -3.51956
F 5.59151 -2.11138 -2.64231
F 4.68463 -0.16061 -1.05706
F 2.65173 1.13803 -2.79287
F 3.21155 3.59903 -3.55157
F 3.43995 5.61146 -1.72277
F 3.08583 5.05465 0.92387
F 2.53149 2.60222 1.72738
F 1.28397 -2.22881 1.36841
F 4.59966 1.1613 1.49038
F 5.61574 0.06213 3.66043
F 4.49738 -2.16441 4.75688
F 2.31056 -3.28833 3.56935

IN-5

Charge = 0 Multiplicity = 1
C 4.77182 -0.15294 0.51232
C 5.62629 0.81293 -0.20789
H 5.23756 -1.00515 1.00482
H 3.80107 0.16493 0.8779
N 4.83427 -0.22977 -0.96792
C 5.37017 -1.49284 -1.59113
H 5.13293 -1.42234 -2.65338
H 4.78079 -2.30098 -1.15327
C 6.83686 -1.76356 -1.42011
C 7.29532 -2.53109 -0.3479
C 7.75093 -1.25947 -2.34704
C 8.65994 -2.75215 -0.17935
H 6.58122 -2.94888 0.35824
C 9.11345 -1.48081 -2.18125
H 7.39086 -0.67961 -3.19455
C 9.5693 -2.21958 -1.09023
H 9.01239 -3.34485 0.65864
H 9.8196 -1.08265 -2.90267
H 10.63265 -2.39295 -0.95958
C 3.29187 2.08387 2.76363
C 1.93415 1.9368 2.1792
H 3.44465 2.90882 3.45918

H 3.92011 1.21308 2.94594
C 3.06503 3.85034 1.00374
H 3.13719 4.50436 1.88412
H 2.12617 4.08995 0.4919
C 4.22897 4.09014 0.0748
C 5.51484 4.28667 0.5848
C 4.05604 4.00866 -1.30912
C 6.61025 4.38477 -0.27017
H 5.65501 4.3596 1.661
C 5.14958 4.10748 -2.16813
H 3.05518 3.86599 -1.71281
C 6.43091 4.28657 -1.64955
H 7.60412 4.54348 0.1383
H 4.9993 4.05586 -3.24276
H 7.28291 4.37127 -2.31707
N 3.05027 2.42584 1.36554
H 1.6335 0.93374 1.87805
C 0.79043 2.83837 2.57065
H 0.17674 2.34142 3.3241
H 1.14104 3.79165 2.97614
H 0.14645 3.03874 1.70651
C 3.62957 0.34207 -1.68602
H 3.34738 1.20152 -1.07298
C 4.03778 0.81506 -3.07388
H 4.12131 -0.00372 -3.79533
H 3.267 1.49616 -3.44663
H 4.98436 1.36504 -3.04117
C 2.44282 -0.63832 -1.68363
H 2.80479 -1.66214 -1.83801
H 1.82975 -0.41158 -2.56846
N 1.66315 -0.57026 -0.45372
C 1.34424 -1.88684 0.1139
H 1.0679 -2.62054 -0.65979
H 0.46501 -1.75691 0.74743
C 2.46332 -2.44392 0.96229
C 3.27525 -3.48103 0.50335
C 2.69036 -1.93237 2.24675
C 4.31667 -3.97948 1.29012
H 3.07013 -3.9269 -0.46884
C 3.72687 -2.42198 3.03356
H 2.03707 -1.15508 2.63938
C 4.55206 -3.44172 2.55249
H 4.92544 -4.80196 0.92411
H 3.87903 -2.02558 4.03293
H 5.35024 -3.83627 3.17405
C 0.45605 0.29353 -0.53832
H 0.13134 0.43205 0.49349
C -0.74425 -0.32616 -1.28808
H -0.55191 -0.31407 -2.37213
H -0.83335 -1.3868 -1.02563
C 0.78525 1.68507 -1.06821
H -0.10256 2.31769 -0.97649
H 1.59341 2.13702 -0.48732
H 1.07006 1.67262 -2.12985
N -1.98047 0.36995 -0.95921
C -2.37416 1.32778 -1.98495
H -1.4868 1.55828 -2.59116
H -3.10073 0.91334 -2.69559
C -2.9119 2.65507 -1.47651
C -2.60433 3.13976 -0.20414
C -3.75612 3.4095 -2.29447
C -3.14032 4.34415 0.24531
H -1.99736 2.52059 0.44852
C -4.28888 4.61684 -1.85151
H -4.03018 3.02322 -3.2737
C -3.98551 5.0877 -0.5759
H -2.91438 4.6924 1.24972
H -4.96227 5.17778 -2.49295
H -4.4183 6.01734 -0.2188
B -3.04395 -0.46358 -0.19041
C -2.22034 -1.19597 1.07926
C -1.48947 -0.41773 1.98053
C -2.07042 -2.5654 1.2994
C -0.67179 -0.92248 2.97959
C -1.27804 -3.12112 2.30781
C -0.56356 -2.29434 3.15438
C -4.27643 0.51338 0.37039
C -4.51591 0.89936 1.6891
C -5.17586 1.08107 -0.53387
C -5.45672 1.8532 2.06361
C -6.11993 2.04669 -0.21305
C -6.25652 2.44913 1.10427
C -3.81323 -1.62173 -1.10957
C -3.58505 -1.92115 -2.444
C -4.86428 -2.33614 -0.53675
C -4.34131 -2.83749 -3.17152
C -5.64548 -3.25744 -1.21406
C -5.38178 -3.50823 -2.55472

F -1.18605 -4.44567 2.43991
F -2.65657 -3.47873 0.51475
F 0.24033 -2.79272 4.09492
F 0.06458 -0.10132 3.75022
F -1.511 0.9251 1.90458
F -5.14105 0.74973 -1.83789
F -6.88534 2.58947 -1.16229
F -7.15339 3.37442 1.44519
F -5.60368 2.18834 3.34958
F -3.84453 0.36353 2.72318
F -5.13098 -2.17117 0.76998
F -2.59164 -1.33195 -3.14263
F -6.63376 -3.91302 -0.59972
F -4.0667 -3.07493 -4.45912
F -6.11558 -4.3921 -3.23343
H 5.15793 1.77947 -0.37826
C 7.12535 0.89913 -0.09981
H 7.60224 -0.01566 0.24796
H 7.57688 1.21279 -1.04373
H 7.31159 1.69124 0.63228

TS-3

Charge = 0 Multiplicity = 1
C 4.25962 -0.64222 -0.59978
C 4.80136 0.51102 -1.31576
H 4.96292 -1.14729 0.06502
H 3.26578 -0.56981 -0.17301
N 4.26513 -1.21401 -1.95803
C 5.00643 -2.49079 -2.08741
H 4.82295 -2.87272 -3.09256
H 4.59277 -3.20595 -1.36389
C 6.49225 -2.34246 -1.87964
C 7.07189 -2.59154 -0.63498
C 7.30308 -1.92747 -2.9386
C 8.43775 -2.39009 -0.44072
H 6.44939 -2.94575 0.18468
C 8.66569 -1.72735 -2.74917
H 6.85588 -1.7498 -3.91482
C 9.2335 -1.94994 -1.4947
H 8.87994 -2.58416 0.53142
H 9.287 -1.40211 -3.57761
H 10.29703 -1.79382 -1.34488
C 3.67774 1.71444 1.5171
C 2.72304 1.97669 0.41643
H 3.76872 2.47155 2.29446
H 3.89181 0.69687 1.83482
C 4.78305 3.40419 0.05774
H 4.13248 4.18384 0.47474
H 4.86957 3.61992 -1.01655
C 6.14478 3.50735 0.71687
C 6.76022 2.43054 1.35493
C 6.80431 4.73969 0.68503
C 8.01173 2.5837 1.95038
H 6.2643 1.4648 1.38541
C 8.05221 4.8932 1.27644
H 6.33059 5.5873 0.19449
C 8.66056 3.81261 1.91362
H 8.47698 1.73704 2.44569
H 8.54939 5.8575 1.24411
H 9.63331 3.93145 2.37983
N 4.179 2.08184 0.19112
H 2.29959 1.09948 -0.07418
C 1.79637 3.16738 0.41226
H 0.80734 2.82608 0.72797
H 2.1121 3.95053 1.10547
H 1.70352 3.59575 -0.59122
C 2.96254 -1.12396 -2.67678
H 2.68936 -0.07013 -2.62858
C 3.12068 -1.49108 -4.14926
H 3.13224 -2.57345 -4.3111
H 2.26884 -1.0921 -4.70653
H 4.03564 -1.06071 -4.56804
C 1.81258 -1.91141 -2.01645
H 2.1907 -2.90178 -1.73401
H 1.03873 -2.09017 -2.78016
N 1.26503 -1.24805 -0.83438
C 0.96512 -2.18798 0.25976
H 0.46175 -3.09694 -0.1043
H 0.26662 -1.68724 0.93552
C 2.20321 -2.56505 1.0411
C 2.92796 -3.72287 0.75618
C 2.6619 -1.72198 2.05952
C 4.10587 -4.01863 1.44532
H 2.55692 -4.41462 0.00232
C 3.82948 -2.01533 2.75689
H 2.09618 -0.82498 2.30364
C 4.56257 -3.16139 2.44343
H 4.65274 -4.92909 1.21618
H 4.15814 -1.36049 3.55909

H 5.46736 -3.39904 2.99498
C 0.13343 -0.31302 -1.07228
H 0.0667 0.27239 -0.15355
C -1.24237 -0.991 -1.27274
H -1.26209 -1.48613 -2.25544
H -1.36006 -1.80034 -0.54342
C 0.40023 0.6878 -2.19223
H -0.44698 1.37615 -2.24347
H 1.29845 1.29014 -2.01001
H 0.49611 0.20454 -3.17348
N -2.33589 -0.0381 -1.13421
C -2.87874 0.38173 -2.42136
H -2.11837 0.18431 -3.19025
H -3.74978 -0.21302 -2.72655
C -3.24696 1.8515 -2.54147
C -2.67936 2.83251 -1.72677
C -4.1994 2.2365 -3.48827
C -3.06711 4.16506 -1.84643
H -1.98163 2.52329 -0.95528
C -4.58506 3.56769 -3.61501
H -4.67238 1.47476 -4.10399
C -4.02214 4.53861 -2.7896
H -2.63735 4.9121 -1.18452
H -5.34418 3.8435 -4.34107
H -4.33767 5.57454 -2.86947
B -3.2793 -0.26468 0.08206
C -2.27037 -0.45339 1.41251
C -1.29791 0.51018 1.68922
C -2.19007 -1.56355 2.25427
C -0.30903 0.38229 2.65129
C -1.23951 -1.71817 3.26719
C -0.28314 -0.74044 3.46493
C -4.31137 1.03107 0.28231
C -4.24238 2.01905 1.2639
C -5.34936 1.23866 -0.62787
C -5.03513 3.16195 1.27671
C -6.15628 2.36735 -0.66589
C -5.99163 3.35056 0.29448
C -4.28541 -1.58681 -0.05815
C -4.3369 -2.49602 -1.10391
C -5.2594 -1.78807 0.91907
C -5.28273 -3.51456 -1.19862
C -6.22019 -2.78425 0.87393
C -6.23451 -3.65845 -0.20563
F -1.2337 -2.81524 4.02548
F -3.01383 -2.61107 2.13094
F 0.67543 -0.88357 4.3837
F 0.66893 1.30062 2.76412
F -1.23398 1.64881 0.97238
F -5.60009 0.34329 -1.60081
F -7.07629 2.51219 -1.62175
F -6.74928 4.44715 0.28466
F -4.88602 4.07625 2.24098
F -3.38542 1.93982 2.29709
F -5.26147 -1.00462 2.01086
F -3.45445 -2.45355 -2.1245
F -7.11928 -2.92437 1.85153
F -5.27491 -4.35416 -2.23981
F -7.14644 -4.62964 -0.27594
H 4.09638 1.07483 -1.91713
C 6.25132 0.81276 -1.51299
H 6.89674 0.22402 -0.85807
H 6.53233 0.62437 -2.55141
H 6.42019 1.87421 -1.31562

IN-6

Charge = 0 Multiplicity = 1

C 4.43453 -0.53088 -0.72997
C 4.60079 0.96306 -1.05383
H 5.32819 -0.85672 -0.184
H 3.56829 -0.74368 -0.10046
N 4.37402 -1.28004 -1.98291
C 4.94611 -2.62009 -1.81913
H 4.72029 -3.19473 -2.72189
H 4.5077 -3.16213 -0.96652
C 6.44717 -2.54486 -1.64594
C 7.05799 -2.9431 -0.45783
C 7.24131 -2.04179 -2.68048
C 8.44099 -2.84433 -0.30299
H 6.441 -3.32675 0.3527
C 8.6196 -1.94249 -2.53119
H 6.76269 -1.72522 -3.60482
C 9.22309 -2.34413 -1.33868
H 8.90506 -3.15908 0.62683
H 9.2272 -1.55702 -3.34436
H 10.29972 -2.26902 -1.22173
C 3.96535 1.38448 1.46674
C 2.75113 1.56004 0.64666
H 4.20159 2.13953 2.21141

H 4.35233 0.38701 1.6519
C 4.46974 3.30466 -0.11879
H 3.68625 3.90031 0.35031
H 4.40357 3.49109 -1.19531
C 5.81438 3.74849 0.42353
C 6.66923 2.9554 1.18721
C 6.17989 5.07041 0.15175
C 7.86961 3.4761 1.66893
H 6.42532 1.92021 1.40328
C 7.37603 5.58907 0.63144
H 5.51971 5.6993 -0.44151
C 8.2259 4.79117 1.39504
H 8.52592 2.8442 2.25841
H 7.64411 6.61671 0.4089
H 9.16051 5.19339 1.77157
N 4.11993 1.87361 0.07062
H 2.35033 0.65328 0.19037
C 1.74116 2.65203 0.87305
H 0.87001 2.19768 1.34952
H 2.10068 3.44128 1.53719
H 1.40513 3.08438 -0.0748
C 3.06023 -1.22688 -2.65486
H 2.8252 -0.16454 -2.74633
C 3.16577 -1.77524 -4.0794
H 3.14612 -2.86973 -4.10524
H 2.31716 -1.42551 -4.67432
H 4.08946 -1.43114 -4.55289
C 1.88224 -1.91224 -1.92772
H 2.22732 -2.9056 -1.61305
H 1.07875 -2.09337 -2.65986
N 1.36107 -1.20796 -0.74664
C 0.99163 -2.15196 0.325
H 0.50188 -3.05242 -0.0764
H 0.2586 -1.65394 0.96204
C 2.17348 -2.55099 1.17723
C 2.84409 -3.75814 0.98352
C 2.62142 -1.69197 2.18832
C 3.96463 -4.08651 1.74787
H 2.48048 -4.4553 0.23145
C 3.73516 -2.0159 2.9571
H 2.07444 -0.77139 2.38891
C 4.41936 -3.21078 2.72916
H 4.47249 -5.03252 1.58355
H 4.05376 -1.35147 3.75602
H 5.28258 -3.46966 3.33464
C 0.25217 -0.25196 -1.00119
H 0.12517 0.28764 -0.05642
C -1.12586 -0.88556 -1.31091
H -1.1256 -1.28121 -2.33719
H -1.27704 -1.75903 -0.66707
C 0.60967 0.79207 -2.05459
H -0.17415 1.55412 -2.07944
H 1.55991 1.29502 -1.83164
H 0.68519 0.35469 -3.05795
N -2.20595 0.07219 -1.10969
C -2.65743 0.6764 -2.35802
H -1.8694 0.53472 -3.11045
H -3.53772 0.17332 -2.77706
C -2.9477 2.16718 -2.30036
C -2.37894 2.99734 -1.33296
C -3.82911 2.72715 -3.22839
C -2.6986 4.35224 -1.28414
H -1.7388 2.54681 -0.58122
C -4.14517 4.0819 -3.18759
H -4.30409 2.0821 -3.96412
C -3.58361 4.90051 -2.21
H -2.273 4.97892 -0.50478
H -4.85101 4.49371 -3.90287
H -3.84759 5.95259 -2.15975
B -3.22654 -0.27781 0.0106
C -2.30397 -0.67322 1.35802
C -1.36257 0.23259 1.84862
C -2.27456 -1.89865 2.02432
C -0.47055 -0.03136 2.87497
C -1.40755 -2.20493 3.07719
C -0.48829 -1.26589 3.50605
C -4.23255 1.01945 0.32746
C -4.21222 1.8551 1.44418
C -5.19392 1.39577 -0.61264
C -4.96029 3.0221 1.55978
C -5.95311 2.55637 -0.55079
C -5.82711 3.39097 0.54609
C -4.26201 -1.53045 -0.35172
C -4.28928 -2.2889 -1.51198
C -5.28047 -1.83207 0.55088
C -5.25461 -3.25675 -1.78073
C -6.26217 -2.78442 0.33402
C -6.25102 -3.50473 -0.85377

F -1.44531 -3.40683 3.65284
F -3.06933 -2.91573 1.67189
F 0.38556 -1.53946 4.47516
F 0.46494 0.87489 3.22513
F -1.24367 1.46212 1.30812
F -5.41076 0.64935 -1.7111
F -6.79104 2.87213 -1.54033
F -6.54024 4.51348 0.63518
F -4.85679 3.78446 2.65355
F -3.45385 1.58934 2.52282
F -5.30961 -1.20169 1.73779
F -3.36124 -2.13509 -2.47934
F -7.20503 -3.02796 1.24783
F -5.22292 -3.94853 -2.92456
F -7.18205 -4.43017 -1.09045
H 3.92649 1.23324 -1.87334
C 6.03584 1.23464 -1.4818
H 6.74984 0.99173 -0.69089
H 6.22494 0.55425 -2.31625
H 6.21193 2.25841 -1.8187

IN-C1

Charge = 0 Multiplicity = 1
B -1.18201 -0.1184 0.00536
C -2.20328 -0.1444 1.32368
C -1.87962 -0.10868 2.67211
C -3.5739 -0.08521 1.07077
C -2.81892 -0.0252 3.6965
C -4.54942 0.00096 2.0501
C -4.16526 0.03411 3.38478
C -1.56473 1.33107 -0.74979
C -1.98051 1.48112 -2.07873
C -1.63205 2.5378 -0.04011
C -2.27782 2.70095 -2.67941
C -1.9185 3.77878 -0.59553
C -2.23342 3.86836 -1.93952
C -1.45039 -1.43514 -0.977
C -0.7209 -1.56463 -2.15836
C -2.19327 -2.56961 -0.6606
C -0.6943 -2.69722 -2.95528
C -2.21929 -3.72588 -1.44003
C -1.45974 -3.79715 -2.59393
F -1.92472 4.874 0.16666
F -2.5184 5.04241 -2.49782
F -2.63813 2.74463 -3.96325
F -2.17963 0.43332 -2.88954
F -1.45922 2.5826 1.29772
F -4.00434 -0.1403 -0.19956
F -5.84367 0.04674 1.73259
F -5.0806 0.11508 4.34934
F -2.42687 0.00109 4.97387
F -0.59263 -0.15324 3.09926
F 0.05835 -0.55246 -2.59106
F 0.07636 -2.74595 -4.04632
F -1.45104 -4.90226 -3.33754
F -2.94739 -4.77741 -1.06081
F -2.91153 -2.65116 0.46903
C 0.61705 -1.55634 0.9545
C 1.92412 -1.83175 1.71059
H 0.52206 -2.30902 0.16776
H -0.13692 -1.84858 1.70673
H 1.97482 -1.16016 2.56897
N 0.34234 -0.24026 0.39002
C 1.91676 -3.25626 2.25556
H 1.72569 -3.99587 1.47124
H 2.85566 -3.50286 2.76073
H 1.11034 -3.33942 2.98707
C 0.93215 0.90012 1.07831
C 1.86374 1.76264 0.23938
C 1.99573 1.60706 -1.14048
C 2.57619 2.79295 0.86845
C 2.82887 2.45603 -1.8728
H 1.40257 0.84663 -1.63514
C 3.40244 3.64372 0.14114
H 2.46478 2.93752 1.94239
C 3.53512 3.47469 -1.23772
H 2.90824 2.33063 -2.9489
H 3.94033 4.43956 0.64763
H 4.17208 4.14107 -1.81155
C 3.49402 -1.6639 -0.49361
C 4.09 -2.63894 0.43943
H 4.13463 -0.85744 -0.83498
H 5.13799 -2.58023 0.71103
H 3.63338 -3.61984 0.49036
N 3.25275 -1.54051 0.98289
C 2.41532 -2.06374 -1.4551
H 2.87814 -2.17178 -2.44025
H 1.95689 -3.02 -1.19256
H 1.65587 -1.28711 -1.5084

H 0.16536 1.5576 1.48334
C 4.03914 -0.47511 1.73279
H 3.40485 0.40997 1.73434
H 4.1223 -0.86734 2.75083
C 5.39625 -0.12627 1.18967
C 5.51594 0.84645 0.19189
C 6.54958 -0.71343 1.71849
C 6.77179 1.20529 -0.28692
H 4.62382 1.32648 -0.20322
C 7.80566 -0.35227 1.24023
H 6.46424 -1.44449 2.52014
C 7.91616 0.60532 0.23423
H 6.85134 1.96365 -1.0593
H 8.69607 -0.80972 1.65898
H 8.89582 0.89115 -0.13528
H 1.47099 0.59545 1.98173

TS-C

Charge = 0 Multiplicity = 1
B -1.05319 -0.20133 0.03329
C -1.73058 -0.77106 1.44747
C -1.15056 -0.93232 2.69795
C -3.0957 -1.06203 1.41816
C -1.84746 -1.33534 3.83405
C -3.8356 -1.46542 2.51751
C -3.20207 -1.60116 3.74626
C -1.93124 1.20691 -0.22189
C -2.84248 1.4137 -1.2667
C -1.96739 2.24818 0.71436
C -3.57039 2.5839 -1.45941
C -2.67207 3.43626 0.56477
C -3.47494 3.61874 -0.54669
C -1.26541 -1.29863 -1.19589
C -1.01256 -0.9296 -2.5135
C -1.52669 -2.65689 -1.04009
C -1.00742 -1.79891 -3.59376
C -1.54747 -3.57112 -2.09162
C -1.28298 -3.1423 -3.38122
F -2.60516 4.38101 1.50387
F -4.16656 4.74287 -0.71366
F -4.38841 2.6976 -2.5068
F -3.13177 0.46074 -2.16302
F -1.32978 2.15528 1.89624
F -3.7582 -0.9742 0.25351
F -5.13769 -1.72904 2.41066
F -3.88735 -1.9883 4.82017
F -1.21477 -1.46898 5.00225
F 0.17186 -0.71909 2.90183
F -0.74074 0.3568 -2.81562
F -0.71652 -1.35726 -4.82053
F -1.27553 -4.00306 -4.39651
F -1.79072 -4.86119 -1.86021
F -1.72478 -3.19458 0.17349
C 1.09939 -1.39959 0.34652
C 2.47833 -1.51375 1.00232
H 1.14549 -1.93132 -0.62007
H 0.44011 -2.02414 0.96637
H 2.40794 -1.11177 2.0159
N 0.53617 -0.06177 0.11958
C 2.87266 -2.98869 1.1121
H 2.97295 -3.4569 0.12705
H 3.81921 -3.10104 1.64713
H 2.10382 -3.53823 1.66224
C 1.06115 1.0183 0.95772
C 1.36511 2.31013 0.22023
C 0.87904 2.59528 -1.05835
C 2.17382 3.26315 0.85186
C 1.20491 3.79433 -1.69125
H 0.2375 1.87189 -1.5488
C 2.50145 4.4607 0.22239
H 2.54438 3.06243 1.85618
C 2.01912 4.72912 -1.05696
H 0.81103 4.00087 -2.68226
H 3.12933 5.18541 0.73208
H 2.2694 5.6627 -1.551
C 2.92115 0.08597 -1.63833
C 3.8322 -0.90867 -1.05841
H 2.99431 1.10818 -1.27087
H 4.89441 -0.70667 -1.26138
H 3.60254 -1.92456 -1.39706
N 3.52261 -0.72248 0.33742
C 2.04082 -0.23382 -2.75455
H 2.71729 -0.50509 -3.58699
H 1.46046 -1.14527 -2.55773
H 1.37993 0.57603 -3.04341
H 0.39518 1.24681 1.78661
C 4.33746 0.24547 1.05764
H 4.07368 1.27728 0.7691
H 4.08419 0.14787 2.11887

C 5.82481 0.04568 0.85369
C 6.62256 1.10534 0.42281
C 6.41462 -1.19965 1.08777
C 7.99394 0.93179 0.2448
H 6.16706 2.07442 0.23157
C 7.78129 -1.37727 0.90533
H 5.79459 -2.0309 1.41417
C 8.57431 -0.30956 0.48548
H 8.60558 1.76514 -0.086
H 8.23057 -2.34718 1.09409
H 9.64161 -0.44792 0.34532
H 1.98606 0.71794 1.44671

IN-C2

Charge = 0 Multiplicity = 1
B 2.26729 -0.60076 0.19448
C 2.35316 -1.42789 -1.14364
C 1.37765 -2.34183 -1.54369
C 3.41009 -1.24633 -2.03746
C 1.43208 -3.03261 -2.74359
C 3.51221 -1.93373 -3.23804
C 2.5124 -2.82917 -3.59325
C 2.64915 0.91529 0.13837
C 3.26043 1.58359 1.20228
C 2.38181 1.69481 -0.99289
C 3.56197 2.93509 1.16956
C 2.68373 3.04475 -1.06848
C 3.26173 3.66886 0.02798
C 1.73083 -1.27603 1.50208
C 1.07299 -0.54957 2.50442
C 1.72522 -2.66795 1.67796
C 0.41131 -1.14638 3.56719
C 1.09262 -3.29703 2.73698
C 0.41969 -2.52827 3.68086
F 2.42246 3.74332 -2.16792
F 3.53084 4.96471 -0.01569
F 4.13634 3.53321 2.20942
F 3.59138 0.91306 2.30713
F 1.77855 1.15755 -2.05742
F 4.39318 -0.3906 -1.74866
F 4.54709 -1.73887 -4.04837
F 2.58622 -3.48712 -4.74036
F 0.46794 -3.88101 -3.08608
F 0.30908 -2.57246 -0.76907
F 1.0254 0.77691 2.46468
F -0.24199 -0.40917 4.45903
F -0.20535 -3.11682 4.6878
F 1.12054 -4.61994 2.86004
F 2.35241 -3.46191 0.80959
C -1.85437 -1.19173 1.14569
C -2.86344 -1.69534 0.0944
H -2.1968 -1.47626 2.15083
H -0.89436 -1.6909 0.98714
H -2.36343 -1.68695 -0.88275
N -1.66232 0.2543 1.1271
C -3.28751 -3.12801 0.40372
H -3.82535 -3.16358 1.35777
H -3.9552 -3.50626 -0.37507
H -2.41653 -3.79037 0.47106
C -1.0192 0.69258 -0.10509
C -0.70463 2.17144 -0.16532
C -0.32733 2.89801 0.968
C -0.73751 2.82447 -1.40031
C 0.02194 4.24157 0.8618
H -0.31301 2.40212 1.93026
C -0.38552 4.16751 -1.50885
H -1.03305 2.27002 -2.28816
C 0.00186 4.88029 -0.37716
H 0.31426 4.79211 1.75156
H -0.4049 4.65365 -2.47919
H 0.28403 5.92546 -0.459
C -2.93326 0.94446 1.46205
C -4.15791 0.03434 1.20319
H -3.00897 1.82925 0.8197
H -5.06092 0.64655 1.1082
H -4.31599 -0.61407 2.0759
N -4.03352 -0.80524 0.02395
C -2.92322 1.38842 2.92199
H -3.90224 1.78234 3.21666
H -2.68564 0.53739 3.5699
H -2.17275 2.16272 3.09595
H -0.07316 0.12817 -0.18275
C -4.2475 -0.09544 -1.22587
H -3.6326 0.81869 -1.32876
H -3.94491 -0.7668 -2.03954
C -5.70115 0.28776 -1.42477
C -6.03834 1.51142 -2.00153
C -6.7219 -0.59308 -1.05927
C -7.37158 1.84763 -2.22781

H -5.2493 2.209 -2.27387
C -8.0536 -0.2587 -1.2803
H -6.45191 -1.53344 -0.58719
C -8.3827 0.96202 -1.86824
H -7.619 2.80471 -2.67709
H -8.83904 -0.95105 -0.99184
H -9.42273 1.22294 -2.03847
H -1.58182 0.42581 -1.01569

TS-D

Charge = 0 Multiplicity = 1
C 3.01624 -0.26061 -0.86522
C 3.58066 -0.00946 0.56041
H 3.55007 -1.13476 -1.26675
H 1.9687 -0.56706 -0.78293
N 3.06391 0.88476 -1.76289
C 4.33502 1.08044 -2.488
H 4.35483 2.1117 -2.85576
H 4.35257 0.42456 -3.3731
C 5.57774 0.81301 -1.67835
C 6.13989 -0.46697 -1.65036
C 6.18153 1.8316 -0.94119
C 7.25645 -0.73263 -0.86371
H 5.68754 -1.26514 -2.2358
C 7.30934 1.57399 -0.16386
H 5.7652 2.83609 -0.97739
C 7.84123 0.28715 -0.11415
H 7.67377 -1.73447 -0.84115
H 7.77413 2.37755 0.40037
H 8.7181 0.08377 0.49277
C 1.95758 1.86683 1.01811
C 2.27711 2.58581 -0.22734
H 1.71936 2.46477 1.9002
H 1.20662 1.08064 0.89054
C 4.2588 1.93747 1.9752
H 3.88786 2.93162 2.23767
H 5.23158 2.05258 1.48596
C 4.41394 1.11065 3.23247
C 5.58326 0.38131 3.44188
C 3.37072 1.02131 4.15877
C 5.71081 -0.43823 4.56149
H 6.38861 0.44393 2.71242
C 3.49547 0.19951 5.27303
H 2.44721 1.57413 4.00081
C 4.66531 -0.53246 5.47539
H 6.62311 -1.00573 4.71649
H 2.6786 0.12748 5.98385
H 4.75971 -1.17435 6.34549
N 3.32107 1.3504 1.00934
H 1.63533 2.4262 -1.07792
C 3.08008 3.83576 -0.30183
H 3.56529 3.91624 -1.27912
H 2.37728 4.67803 -0.22859
H 3.8284 3.94713 0.48065
C 1.89792 0.90613 -2.6847
H 1.01467 0.92602 -2.03041
C 1.88325 2.15436 -3.56527
H 2.60314 2.07965 -4.38687
H 0.88404 2.2636 -4.00064
H 2.09308 3.07285 -3.00734
C 1.76089 -0.38192 -3.53065
H 2.71881 -0.91362 -3.54192
H 1.54379 -0.11497 -4.58147
N 0.74972 -1.27033 -2.97669
C 0.95473 -2.65528 -3.40199
H 1.05076 -2.74804 -4.49852
H 0.06583 -3.22564 -3.10893
C 2.16904 -3.25449 -2.73276
C 3.36881 -3.44655 -3.41821
C 2.1059 -3.58234 -1.37785
C 4.49223 -3.94812 -2.75856
H 3.42287 -3.20457 -4.47784
C 3.21507 -4.10068 -0.71849
H 1.17903 -3.40877 -0.83992
C 4.41667 -4.27491 -1.40696
H 5.41971 -4.09516 -3.30485
H 3.13805 -4.36608 0.33164
H 5.28493 -4.67768 -0.89408
C -0.61669 -0.77022 -3.25432
H -0.53578 0.32007 -3.21492
C -1.62179 -1.18923 -2.15121
H -2.49769 -1.64594 -2.63711
H -1.1533 -1.97136 -1.55099
C -1.12459 -1.12812 -4.65751
H -2.04933 -0.58154 -4.86685
H -0.39884 -0.86962 -5.43702
H -1.35395 -2.1952 -4.74457
N -2.01752 -0.07379 -1.28896
C -2.6154 0.98856 -2.09557

H -2.93501 0.59728 -3.07198
H -3.54227 1.33759 -1.63021
C -1.79082 2.24293 -2.35144
C -0.95768 2.80858 -1.38206
C -1.96148 2.93756 -3.55438
C -0.3757 4.05911 -1.58514
H -0.79319 2.26633 -0.45415
C -1.35288 4.17127 -3.77508
H -2.59972 2.50773 -4.32386
C -0.56729 4.74831 -2.78054
H 0.20588 4.5141 -0.78595
H -1.50595 4.68864 -4.71761
H -0.11682 5.72446 -2.93222
B -2.72828 -0.34279 0.06924
C -2.14149 -1.72735 0.79842
C -0.77554 -2.02494 0.82853
C -2.91569 -2.69087 1.4518
C -0.22067 -3.12926 1.45657
C -2.40059 -3.82163 2.08691
C -1.04033 -4.04754 2.09336
C -2.41451 1.02529 1.03385
C -1.34739 1.16749 1.92329
C -3.15623 2.20719 0.90955
C -1.01 2.35123 2.57347
C -2.85526 3.41398 1.53334
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C -6.53213 -0.76483 -1.20478
C -6.56958 -0.23852 1.12071
C -7.25616 -0.50796 -0.05666
F -3.22084 -4.68617 2.68373
F -4.24957 -2.62167 1.525
F -0.51928 -5.11552 2.69331
F 1.10592 -3.33903 1.46012
F 0.11136 -1.2053 0.22458
F -4.2486 2.27638 0.12951
F -3.61011 4.49109 1.32392
F -1.43289 4.63949 2.97524
F 0.05053 2.3931 3.40245
F -0.51966 0.14763 2.23166
F -4.59477 -0.00975 2.29638
F -4.54134 -1.0156 -2.33674
F -7.24995 -0.01216 2.2472
F -7.16657 -1.03763 -2.34873
F -8.58872 -0.5278 -0.07273
H 4.6722 -0.0933 0.53858
C 3.00474 -1.09083 1.47705
H 1.95594 -0.88846 1.71204
H 3.04093 -2.04757 0.95057
H 3.56548 -1.1815 2.40809

IN-D

Charge = 0 Multiplicity = 1

C -2.76638 -0.30276 0.42817
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C -4.29449 -0.5051 2.46346
H -4.57581 0.18528 3.25261
H -4.10449 -1.46651 2.93961
C -5.43537 -0.66937 1.4958
C -5.59318 -1.86113 0.78323
C -6.37888 0.34815 1.34205
C -6.65929 -2.0154 -0.09867
H -4.87979 -2.67731 0.89713
C -7.44591 0.19436 0.46346
H -6.26664 1.27348 1.90035
C -7.58206 -0.98622 -0.26523
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H -8.17197 0.99346 0.34979
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H -1.83128 2.24619 0.26281
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H -5.72858 2.23977 -0.71072
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C -5.0076 3.27836 -2.95961
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H -0.91071 -1.14367 4.51395
H -1.58296 0.46206 4.36489
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H -0.26505 -4.44134 0.31209
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C -3.41975 -5.06322 0.26983
C -2.42889 -3.35928 -1.11045
C -4.51767 -5.12107 -0.59132
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C -3.52196 -3.40822 -1.96822
H -1.61081 -2.67201 -1.29579
C -4.5672 -4.29774 -1.71297
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H -5.41296 -4.353 -2.3924
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H 0.44776 -1.80711 2.66434
C 1.55017 -2.34901 0.92157
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H 1.13636 -2.59775 -0.05749
C 0.89137 -3.86631 2.87302
H 1.80762 -3.61974 3.4183
H 0.12072 -4.11919 3.61099
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N 1.95794 -0.94416 0.94507
C 2.56945 -0.6279 2.23699
H 2.89225 -1.55037 2.74237
H 3.49708 -0.06637 2.08187
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C 0.98191 1.28623 2.88557
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H 0.80636 1.48172 1.83151
C 1.39179 0.76714 5.58572
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B 2.68443 -0.29943 -0.27685
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C 0.19437 -1.5467 -3.16798
C 2.36982 -1.55514 -4.10484
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C 1.68687 4.09225 0.50213
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C 5.06632 -1.46008 0.40841
C 5.17345 0.41697 -0.95739
C 6.45771 -1.54836 0.43397
C 6.55579 0.37599 -0.96909
C 7.21182 -0.6218 -0.25884
F 3.19638 -1.7639 -5.12957
F 4.20357 -0.98028 -2.89439
F 0.50708 -2.17133 -5.42204
F -1.12866 -1.74563 -3.29779
F -0.1607 -0.977 -0.97132
F 4.28537 1.7738 1.28026
F 3.62896 4.22828 1.81784
F 1.34843 5.34652 0.79962
F -0.22502 3.84516 -0.8578
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F 4.4407 -2.41901 1.12136

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F 7.06002 -2.52297 1.12221
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H -3.48476 1.04946 -2.63875

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