

Supporting Information

Gradient Ioselective Ring-Opening Polymerization of Racemic Cyclic Diolide Driven by Chiral Phosphoric Acid Catalysis

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Materials

Toluene (TOL) was refluxed with sodium and distilled under nitrogen before use. Chloroform (CHCl₃) and benzyl alcohol (BnOH) were freshly distilled from CaH₂. All the Chiral Phosphoric Acids were purchased from DAICEL CHIRAL TECHNOLOGIES. All the other reagents and solvents were purchased from Energy Chemical and used as received without further purification unless otherwise stated.

Measurements

All room temperature ¹H NMR spectra and ¹³C NMR spectra were recorded on a Bruker AV-500 spectrometer and a Bruker AV-600 spectrometer, respectively. ¹H NMR chemical shifts were referenced as follows: δ7.26 ppm for chloroform-*d* (CDCl₃), δ2.50 ppm for dimethyl sulfoxide-*d*₆ (DMSO-*d*₆). ¹³C NMR chemical shifts were referenced as follows: δ77.16 ppm for chloroform-*d* (CDCl₃), δ39.52 ppm for dimethyl sulfoxide-*d*₆ (DMSO-*d*₆). ¹³C NMR peak fitting was implemented on software MestReNova-12.0.2.

MALDI-TOF Mass Spectrometry conditions were as follows. Instrument type: Bruker autoflex III smartbeam MALDI-TOF/TOF (Locality:Germany); Laser system: smartbeam laser with 355nm wavelength. Scan mode: linear; ionmode: positive; acceleration voltage: 20.00kV; ionextraction: 200ns; matrix: DCTB (2-[(2E)-3-(4-tert-butylphenyl)-2-Methylprop-2-enylidene]malononitrile); Ionized reagent : sodium trifluoroacetate.

Size exclusion chromatography (SEC) was conducted on a system composed of a Waters 2414 Refractive Index Detector equipped with a series of connected size exclusion columns (1000 Å and 10000 Å, Phenogel columns, 5 μm, 300 × 7.8 mm Phenomenex Torrance, CA, USA). The system was operated with DMF (containing 0.02 M LiBr) as the eluent at a flow rate of 1 mL/min at 50°C and calibrated with PMMA standards in the molecular weight range from 1860 to 3.3×10⁵ Da.

Optical rotation was performed on a Polarimeter 341 plus instrument at 20°C, using sodium lamp as the light source (λ = 589nm, 20W). The specific rotation [α]_D²⁰ were calculated as follows: [α]_D²⁰=(100×a)/(c×d), a, optical rotation; c, concentration in CHCl₃(1g/100ml); d, optical tube length (dm).

Synthesis of monomers and polymers

The *rac*-DL were synthesized according to the literature.^[1]

rac-DL: Recrystallized from EA/PE. ¹H NMR (500 MHz, CDCl₃): δ 5.35 - 5.23 (m, 2H), 2.71 - 2.52 (m, 4H), 1.44 (d, 6H); ¹³C NMR (CDCl₃, 125 MHz): δ 174.05, 74.69, 21.10.

General procedure for ROP of *rac*-DL monomers. Under N₂ atmosphere, Catalyst *R*-CPA5 (80 μL, 0.01 M in CHCl₃) and BnOH (8 μL, 1 M in CHCl₃) was added to a 5-mL Schlenk flask with *rac*-DL monomer (69 mg, 0.4 mmol) in TOL (400 μL). The solution was rapidly stirred at 60 °C. An aliquot was withdrawn to determine monomer conversion by ¹H NMR spectrum. And the polymer was precipitated into 50 mL CH₃OH. The product was isolated by centrifugation and dried under vacuum for 24 hours.

Poly(3-hydroxybutyrate) (P3HB): ¹H NMR (500 MHz, CDCl₃): δ 5.30 - 5.22 (m, 2H), 2.64 - 2.43 (m, 4H), 1.28 - 1.25 (d, 6H); ¹³C NMR (CDCl₃, 125 MHz): δ 169.37, 169.26, 67.92, 40.90, 19.88.

Table S1. Controlled ROP of *rac*-DL Mediated by *R*-CPA5^a

Entry	$[M]_0/[Cat.]_0$ /[BnOH] ₀	Time (h)	Conv. ^b (%)	$M_{n, SEC}^c$ (kg/mol)	$\bar{D} (M_w/M_n)^c$
1	50/1/1	24	26	2.2	1.07
2	50/1/1	36	40	2.9	1.06
3	50/1/1	42	46	3.1	1.06
4	50/1/1	48	50	3.5	1.06
5	50/1/1	60	60	4.5	1.05
6	50/1/1	66	62	4.7	1.06
7	50/1/1	72	66	4.9	1.06
8	50/1/1	84	72	5.4	1.05
9	50/1/1	90	74	5.7	1.05
10	50/1/1	96	79	6.1	1.06
11	50/1/1	108	84	6.6	1.05
12	50/1/1	120	87	6.9	1.05

[a] All ROPs were initiated using benzyl alcohol in dry toluene at 60 °C. [b] Monomer conversion measured by ¹H NMR. [c] Determined by SEC in DMF (0.02M LiBr) relative to PMMA standards.

Table S2. Controlled ROP of *rac*-DL Mediated by *S*-CPA5^a

Entry	$[M]_0/[Cat.]_0$ /[BnOH] ₀	Time (h)	Conv. ^b (%)	$M_{n, SEC}^c$ (kg/mol)	$\bar{D} (M_w/M_n)^c$
1	50/1/1	24	26	2.2	1.08
2	50/1/1	36	43	3.1	1.06
3	50/1/1	42	46	3.4	1.06
4	50/1/1	48	50	3.7	1.06
5	50/1/1	60	64	4.3	1.05
6	50/1/1	66	66	4.5	1.06
7	50/1/1	72	72	4.9	1.05
8	50/1/1	84	77	5.1	1.06
9	50/1/1	90	78	5.3	1.06
10	50/1/1	96	82	5.7	1.05
11	50/1/1	108	86	6.1	1.05
12	50/1/1	120	89	6.7	1.05

[a] All ROPs were initiated using benzyl alcohol in dry toluene at 60 °C. [b] Monomer conversion measured by ¹H NMR. [c] Determined by SEC in DMF (0.02M LiBr) relative to PMMA standards.

Table S3. Controlled ROP of *rac*-DL Mediated by *rac*-CPA5^a

Entry	[M] ₀ /[Cat.] ₀ /[BnOH] ₀	Time (h)	Conv. ^b (%)	<i>M</i> _{n, SEC} ^c (kg/mol)	<i>D</i> (<i>M</i> _w / <i>M</i> _n) ^c
1	50/1/1	24	32	2.8	1.07
2	50/1/1	36	49	3.6	1.06
3	50/1/1	42	52	4.0	1.06
4	50/1/1	48	59	4.5	1.05
5	50/1/1	60	67	4.9	1.04
6	50/1/1	66	70	5.2	1.06
7	50/1/1	72	77	5.7	1.05
8	50/1/1	84	81	6.2	1.04
9	50/1/1	90	85	6.4	1.04
10	50/1/1	96	87	6.6	1.05
11	50/1/1	108	90	7.0	1.05
12	50/1/1	120	91	7.1	1.05

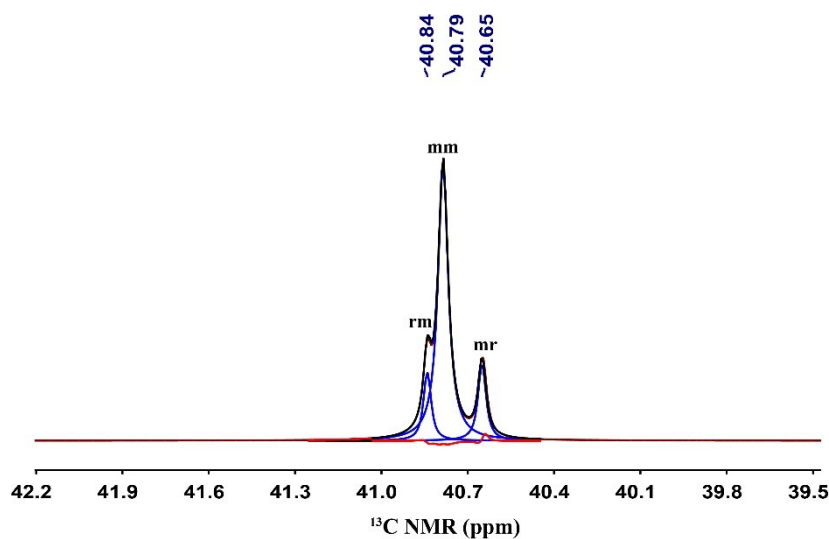
[a] All ROPs were initiated using benzyl alcohol in dry toluene at 60 °C. [b] Monomer conversion measured by ¹H NMR. [c] Determined by SEC in DMF (0.02M LiBr) relative to PMMA standards.

Statistical analyses for polymer samples

Table S4. Triads probabilities of ESC and CEC mechanisms based on non-Bernoullian and Bernoullian statistics [2].

triads	Probability of ESC (non-Bernoullian)	Probability of CEC (Bernoullian)
mm	$P_m^2 + (1 - P_m)^2$	P_m
mr	$P_m(1 - P_m)$	$(1 - P_m)/2$
rm	$P_m(1 - P_m)$	$(1 - P_m)/2$

Table S5. Analysis of microstructures of **P3HB**^a.



ppm	integration	Triads	$P_{m,ESC}$	$P_{m,CEC}$
40.84	0.143	rm	0.83	0.71
40.79	0.709	mm	0.82	0.71
40.65	0.148	mr	0.82	0.71

^a $M_n = 3.7$ kg/mol, $D = 1.05$. ^bThe tetrads in ¹³C NMR are assigned through comparing the observed integration value.

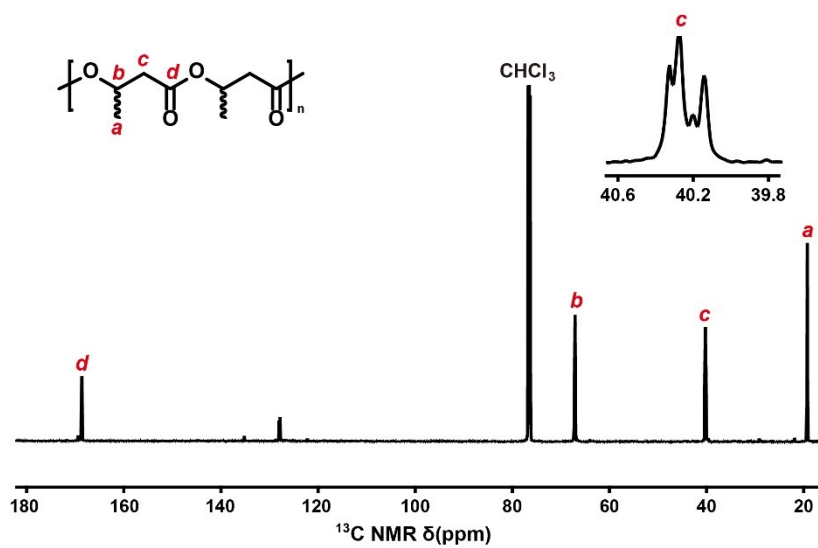


Figure S1. ^{13}C NMR spectrum (CDCl_3) of P3HB produced by *R*-CPA1 (entry 1).

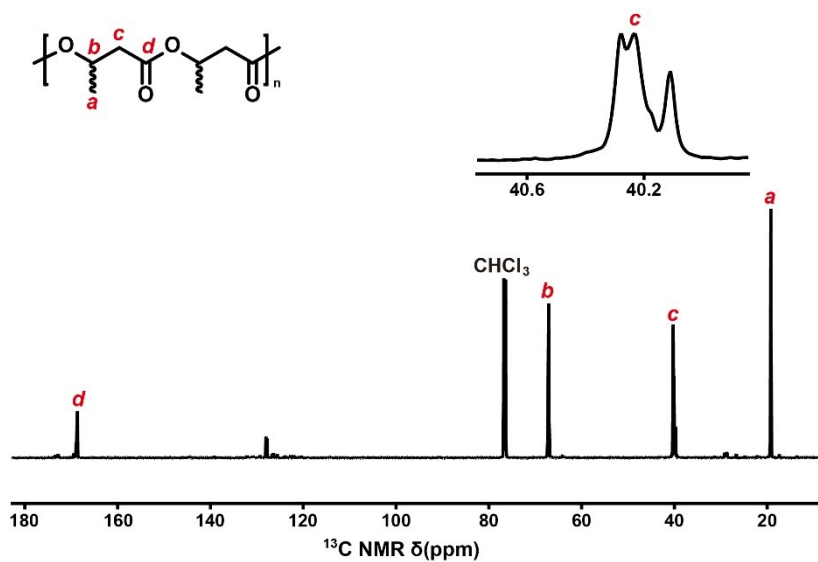


Figure S2. ^{13}C NMR spectrum (CDCl_3) of P3HB produced by *R*-CPA2 (entry 2).

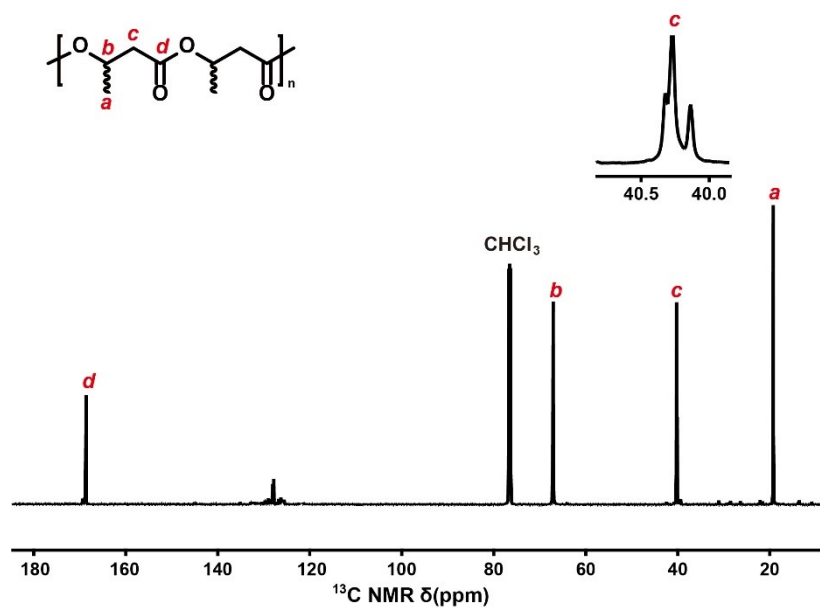


Figure S3. ^{13}C NMR spectrum (CDCl_3) of P3HB produced by R-CPA3 (entry 3).

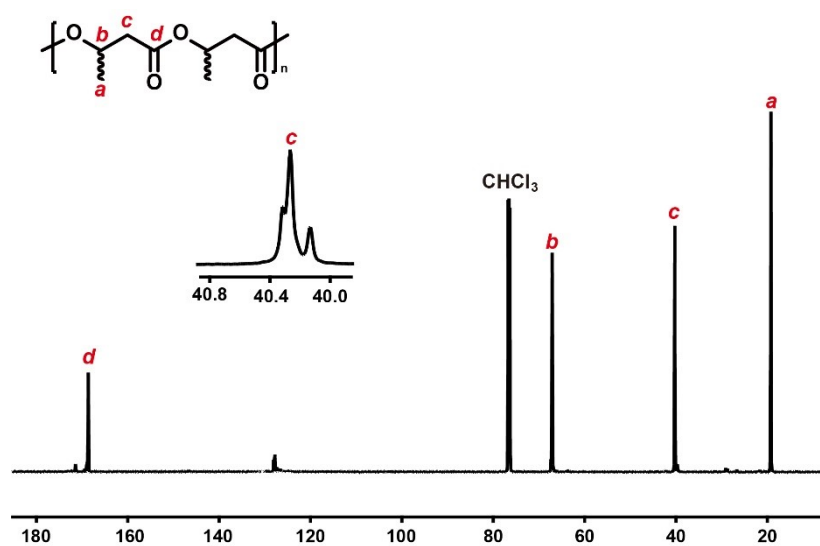


Figure S4. ^{13}C NMR spectrum (CDCl_3) of P3HB produced by R-CPA4 (entry 4).

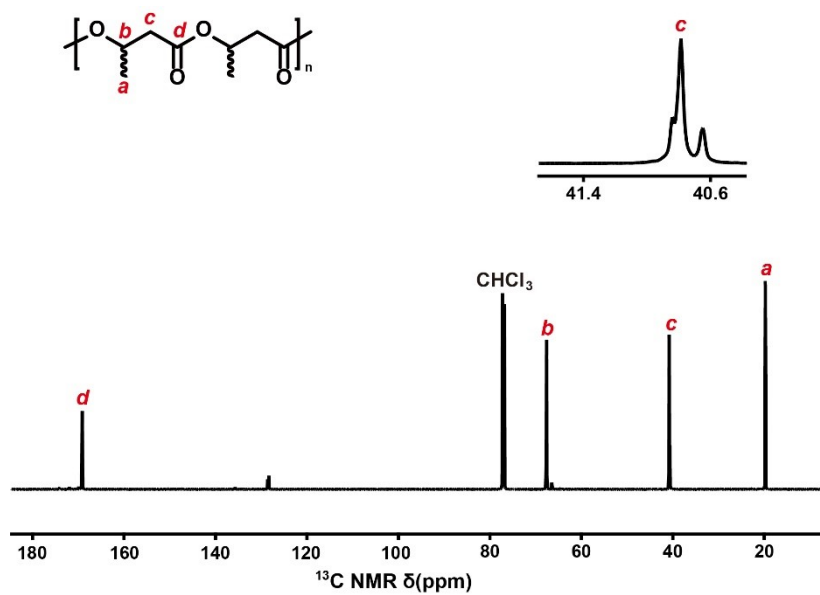


Figure S5. ^{13}C NMR spectrum (CDCl₃) of P3HB produced by *R*-CPA5 (entry 5).

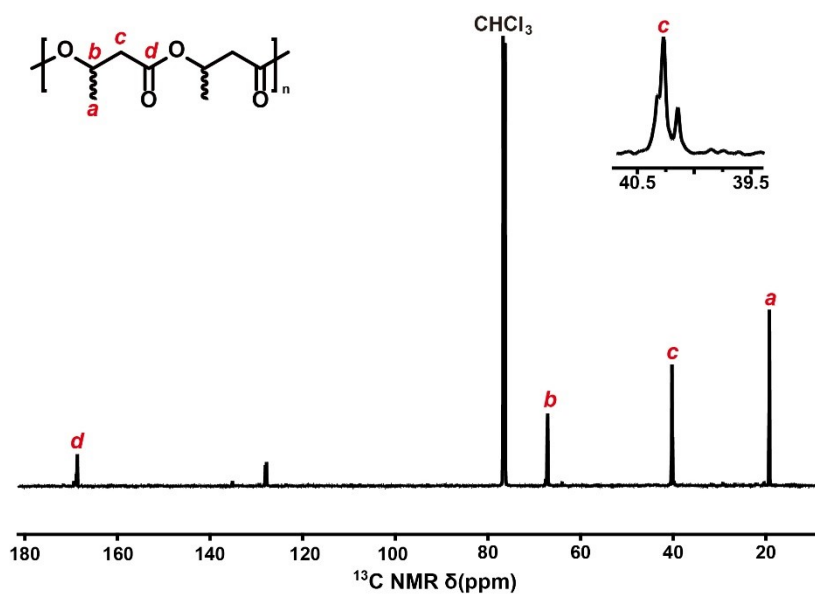


Figure S6. ^{13}C NMR spectrum (CDCl₃) of P3HB produced by *R*-CPA6 (entry 6).

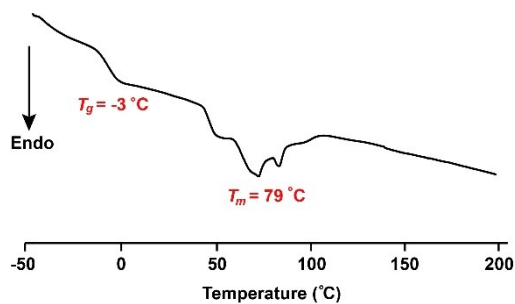


Figure S7. DSC thermograms (first heating scan) of P3HB using *R*-CPA5 as catalyst (Table 1, entry 10).

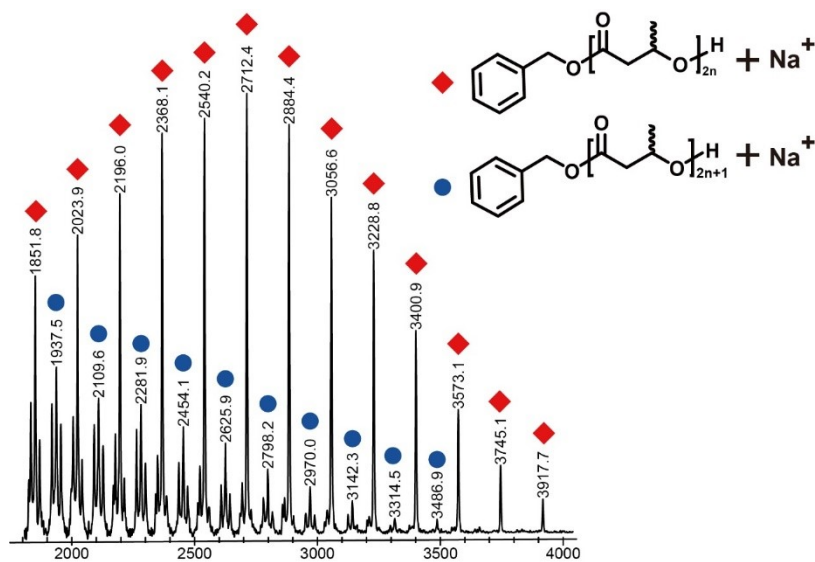


Figure S8. MALDI-TOF-MS of P3HB prepared by *R*-CPA1.

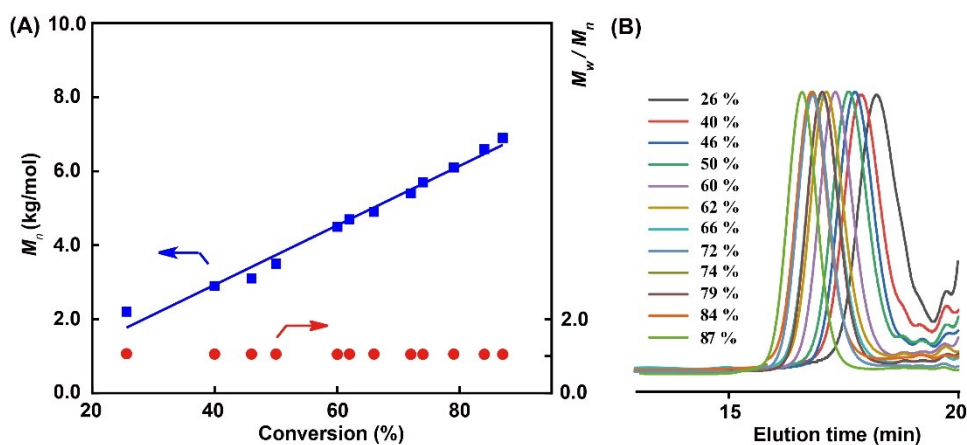


Figure S9. (A) Profiles of M_n and \bar{D} as a function of *rac*-DL conversions at the $[M]_0/[BnOH]_0/[R-CPA5]_0$ ratio of 50/1/1. (B) Overlay of SEC profiles at different *rac*-DL conversions.

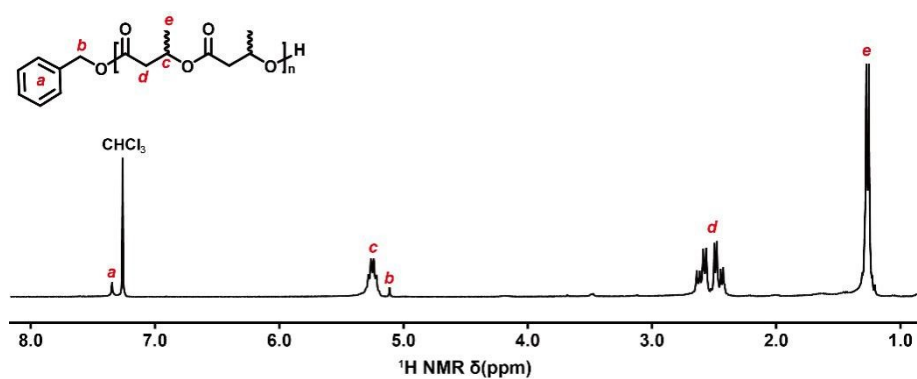


Figure S10. ^1H NMR spectrum of P3HB from *R*-CPA5/BnOH mediated ROP of *rac*-DL in CDCl_3 . The conversion of *rac*-DL was determined to be 50% and the polymerization condition is *rac*-DL/*R*-CPA5/BnOH = 50/1/1, 60 °C, and 48 h.

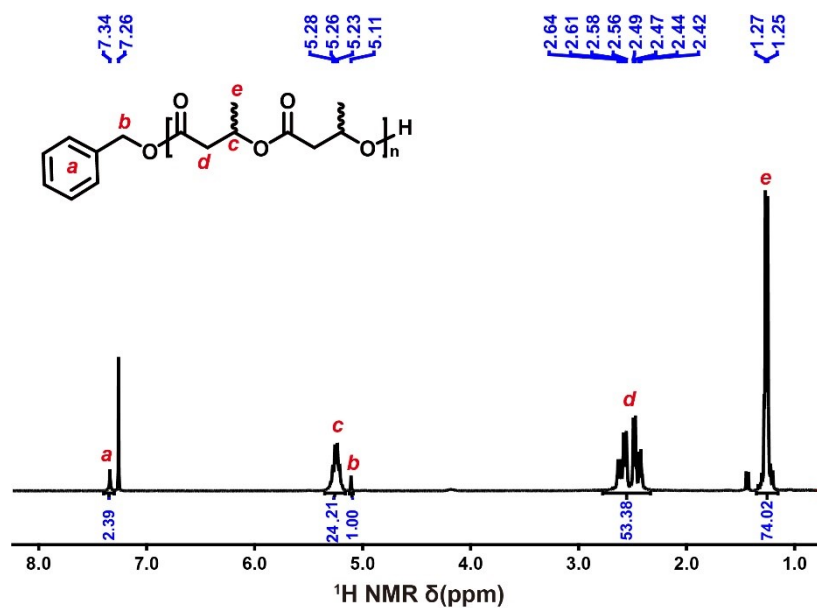


Figure S11. ^1H NMR spectrum of P3HB from *R*-CPA5/BnOH mediated ROP of *rac*-DL in CDCl_3 . The conversion of *rac*-DL was determined to be 90% and the polymerization condition is *rac*-DL/*R*-CPA5/BnOH = 50/1/1, 60 °C, and 132 h.

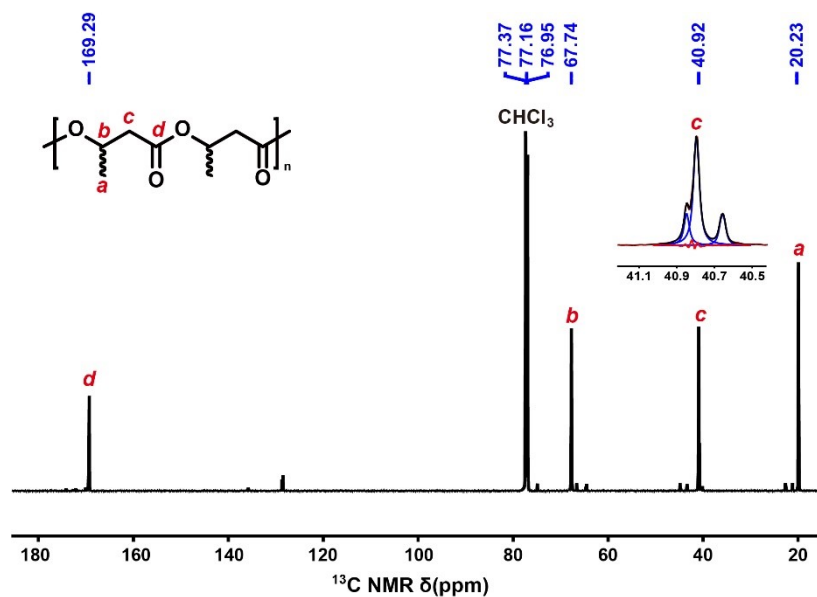


Figure S12. ^{13}C NMR spectrum of P3HB from *R*-CPA5/BnOH mediated ROP of *rac*-DL in CDCl_3 . The conversion of *rac*-DL was determined to be 90% and the polymerization condition is *rac*-DL/*R*-CPA5/BnOH = 50/1/1, 60 °C, and 132 h.

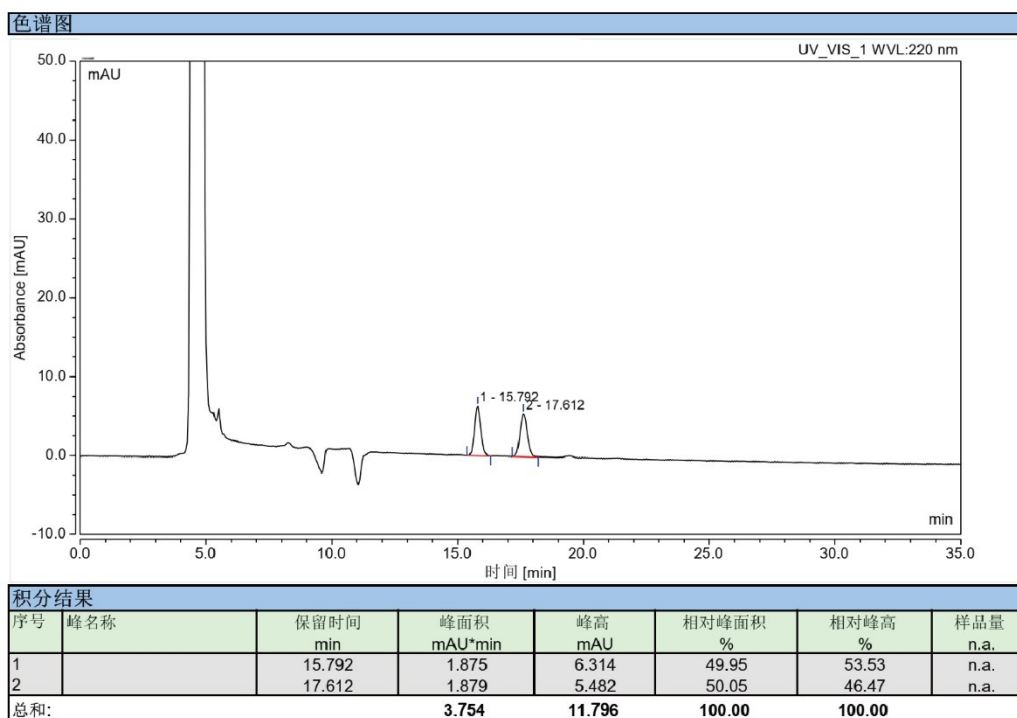


Figure S13. HPLC chromatogram of *rac*-DL separated by chiral column into enantiomers in 1:1 ratio.

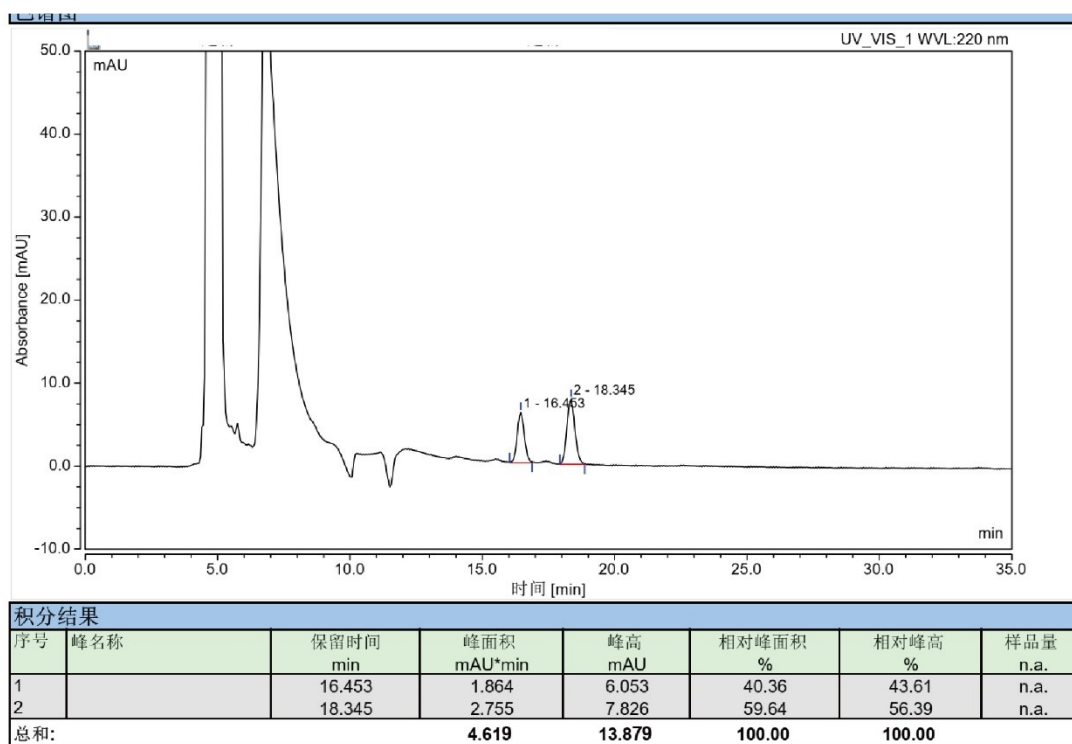


Figure S14. HPLC chromatogram of the unreacted monomer from the polymerization of *rac*-DL by *R*-CPA5 (Table 1, Entry 5). The stereoselectivity factor (s) was calculated from: $s = \ln[(1 - \text{conv.})(1 - ee)] / \ln[(1 - \text{conv.})(1 + ee)]$.

NMR spectra of synthesized compounds and polymers

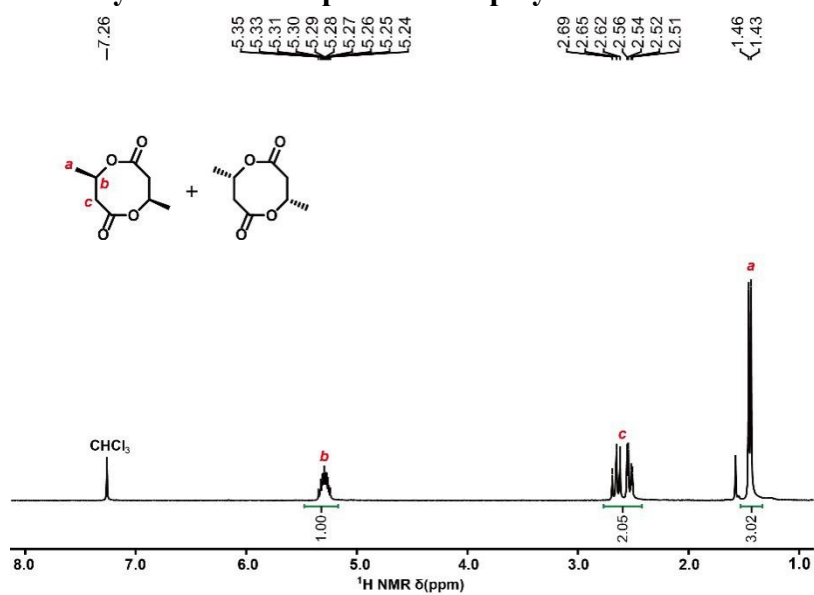


Figure S15: ^1H NMR spectrum of *rac*-DL in CDCl_3 .

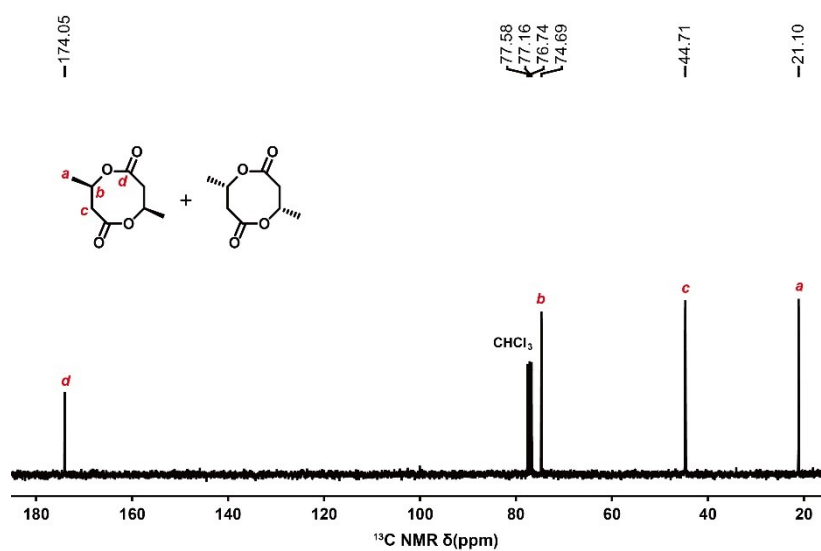


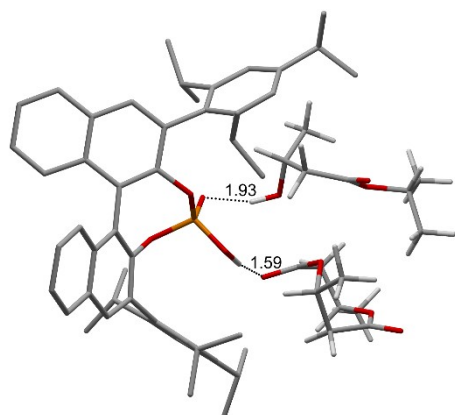
Figure S16: ^{13}C NMR spectrum of *rac*-DL in CDCl_3 .

Computational Methodology

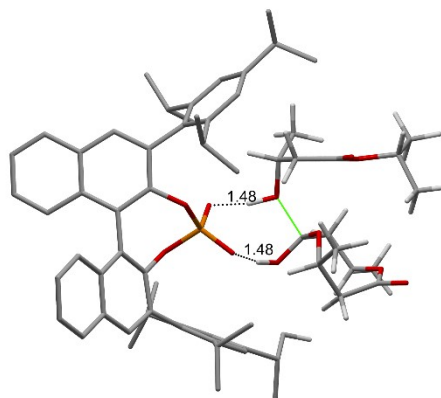
All the density functional theory (DFT) calculations were performed by Gaussian 09 program packages^[3] with empirical dispersion (D3)^[4-7] corrected B3LYP functional.^[8-9] Geometry optimizations were carried out in the gas phase with the 6-31G (d,p) basis set,^[10] and vibration analysis were conducted at 333.15 K. Normal modes of all the intermediates (INT) were verified by calculations of the vibrational frequencies and exhibited no imaginary frequencies. Only one imaginary frequency connecting to bond formation or bond breaking was attained for the transition states (TS), and intrinsic reaction coordinate (IRC)^[11-12] calculations were also conducted to ascertain the connectivity between the transition states and intermediates. The energy of each species was refined by a single-point calculation at the B3LYP /6-311+g(2d,p) level coupled with SMD model^[13] and solvation corrections in implicit toluene solvent, and a temperature $T = 333.15$ K was used. The energies reported in this method were the sum of electronic and thermal free energies in the unit of kcal/mol, and bond lengths were displayed in Å. All structures were visualized with CYLview.^[8]

Optimized structures

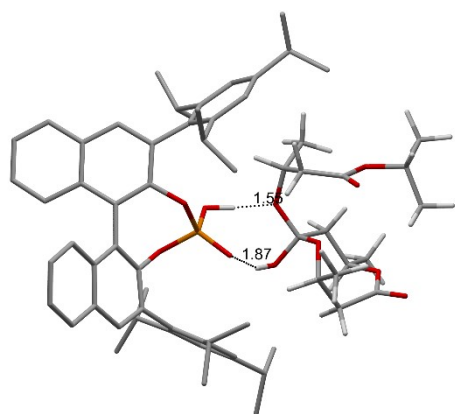
(A) *R*-Chain + (*R*, *R*)-DL



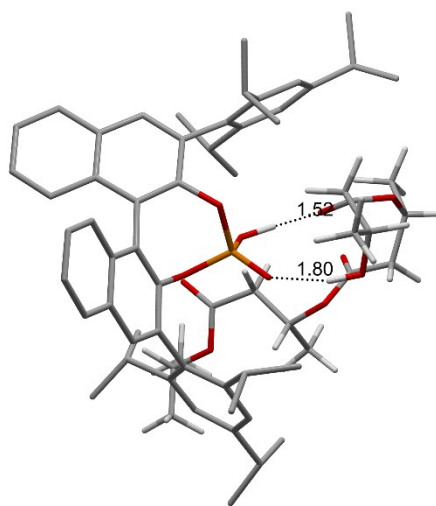
¹INT1 (-9.2)



¹TS1 (6.5)

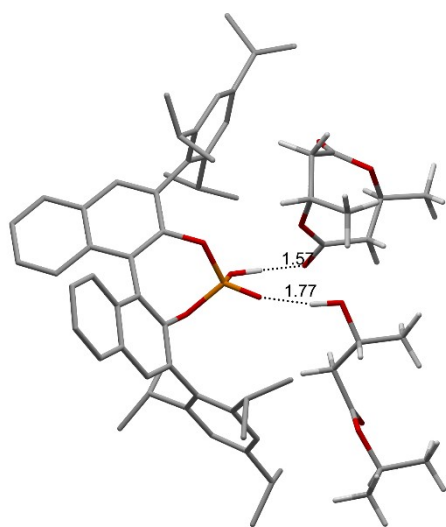


¹INT2 (2.3)

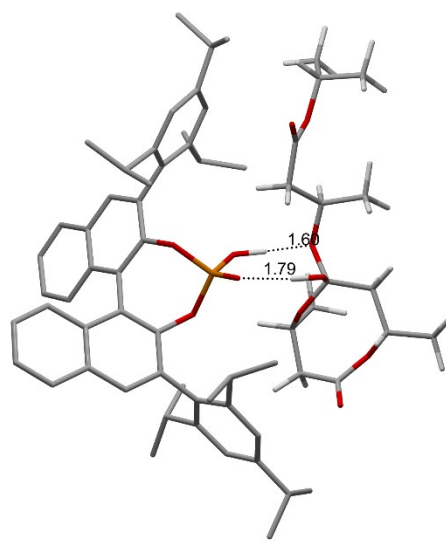


¹INT3 (-23.8)

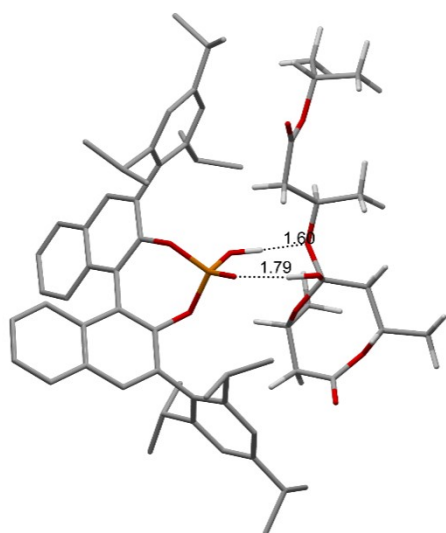
(B) R-Chain + (S, S)-DL



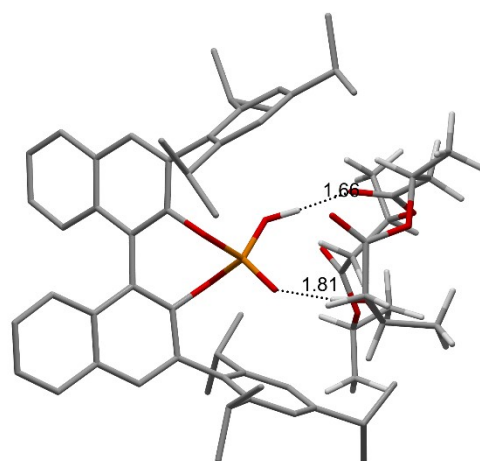
²INT1 (-11.1)



²TS1 (11.9)

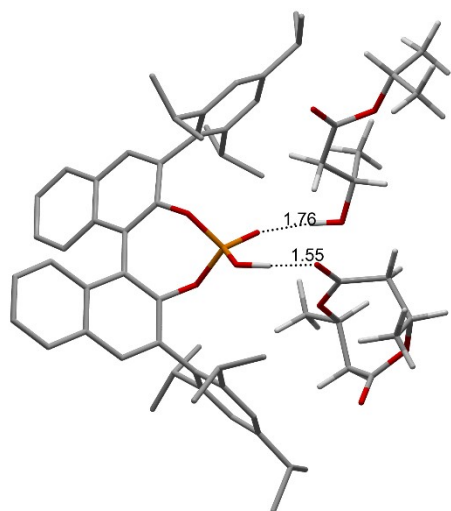


²INT2 (7.8)

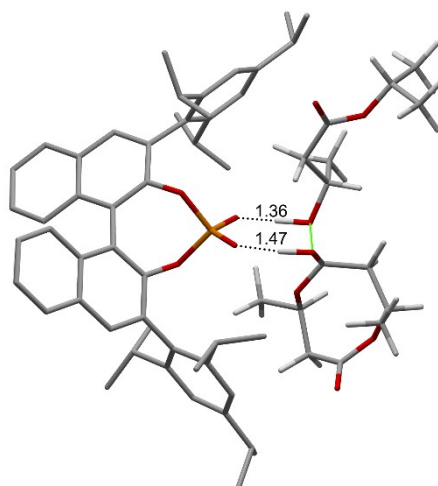


²INT3 (-24.3)

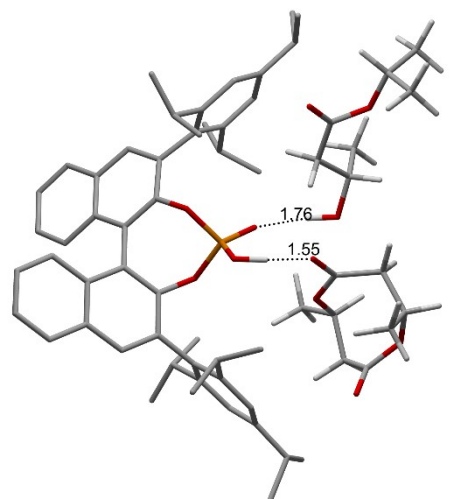
(C) S-Chain + (R, R)-DL



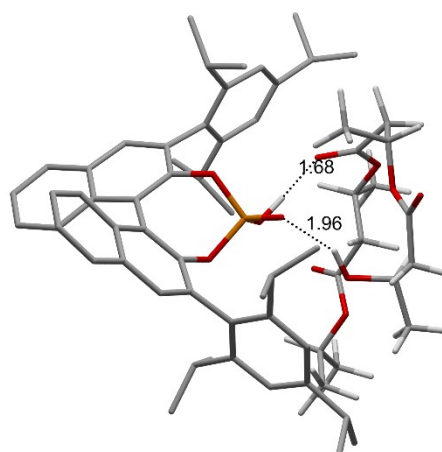
³INT1 (-10.0)



³TS1 (7.4)



³INT2 (3.6)



³INT3 (-19.2)

(D) S-Chain + (S, S)-DL

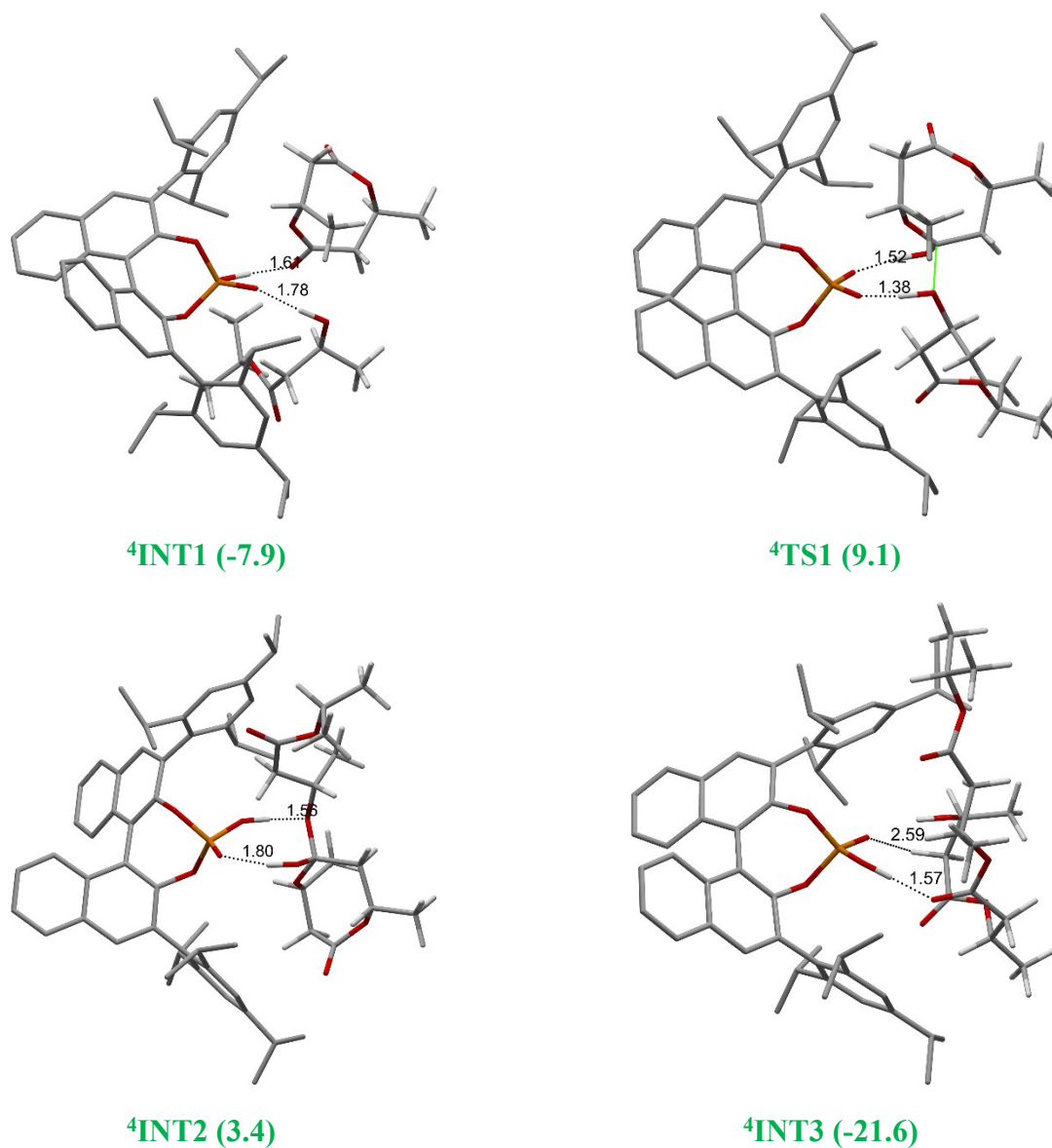


Figure S19. Optimized structures for all the transition states and intermediates. Select bond lengths are listed in Å. All energies are relative to the separated reactants in the unit of kcal/mol. In all cases, the following color-coding scheme applies: H = white, C = grey, O = red, P = brown. H-bonding interactions are indicated with black dotted lines. Breaking and forming bonds are indicated with green lines. (A) *R*-Chain + (*R, R*)-DL; (B) *R*-Chain + (*S, S*)-DL; (C) *S*-Chain + (*R, R*)-DL; (D) *S*-Chain + (*S, S*)-DL.

Coordinates
***R*-CPA5**

C	2.48943800	5.25026700	-2.57244900
C	3.24490100	4.17659500	-2.16297200
C	2.65854800	3.10448500	-1.43769600
C	0.51070300	4.27529000	-1.56349900
C	1.10577600	5.28959300	-2.27955500
H	4.47807200	1.94077800	-1.31298800
H	2.94714500	6.06012800	-3.13239400
H	4.30357100	4.12202300	-2.40180400
C	3.42080000	1.96746900	-1.06849200
H	-0.55142800	4.31506800	-1.35445500
H	0.50561800	6.12470800	-2.62815700
C	1.47560000	0.96972100	-0.10455800
C	2.85064900	0.87868700	-0.44490600
C	-0.71384100	2.13041300	0.15944000
C	-1.20746700	3.19788200	0.98794500
C	-1.57200000	1.08109700	-0.11547300
C	-0.38149700	4.24857900	1.47280300
C	-2.58863400	3.19193800	1.37367600
C	-2.91791000	1.00601300	0.33532800
C	-0.90207200	5.26138300	2.24710200
H	0.67402000	4.24512600	1.23115700
C	-3.09706300	4.26194400	2.15829400
C	-3.41340300	2.09214200	1.02225400
C	-2.27615800	5.28060400	2.58229100
H	-0.24918500	6.05017100	2.60847500
H	-4.14857500	4.24908400	2.43242000
H	-4.44738700	2.08725200	1.35182000
H	-2.67473000	6.08951000	3.18698800
O	-1.12194600	0.02851100	-0.91363600
O	0.92194800	-0.12876500	0.56587700
P	-0.10247700	-1.06350400	-0.27352500
C	-3.68767000	-0.26056100	0.12995400
C	-4.06994700	-0.66239800	-1.17052000
C	-4.59018800	-2.33158200	1.00933600
C	-4.97068200	-2.74906600	-0.26726600
H	-4.80128500	-2.98247100	1.85277900
C	3.63646300	-0.35365000	-0.12840500
C	4.00412800	-0.62779600	1.20769400
C	4.01005500	-1.23504200	-1.16605100
C	4.76328300	-1.76830200	1.47657000
C	4.78147400	-2.35731200	-0.84259700
C	5.16847200	-2.64394200	0.46582800
H	5.04667600	-1.97847100	2.50409900
H	5.08199800	-3.03644700	-1.63544500
C	-5.64354200	-4.09588000	-0.48176000
C	-4.77663300	-5.02223500	-1.35408800
C	-7.05437500	-3.93669300	-1.07641900
H	-5.74957900	-4.56909800	0.50332700
H	-3.78243500	-5.16029500	-0.91817000
H	-5.24566600	-6.00637800	-1.45885800
H	-4.64447200	-4.60600200	-2.35851900
H	-7.67975600	-3.29778000	-0.44539300
H	-7.01324400	-3.48440300	-2.07317100
H	-7.54496100	-4.91106400	-1.17331800
C	-3.83885500	0.21932500	-2.39366200
C	-5.18044200	0.74195500	-2.94170400
C	-3.03047700	-0.50158300	-3.48693800
H	-3.25852700	1.09162900	-2.08189100
H	-5.73279900	1.29404300	-2.17449400
H	-5.01331200	1.41103500	-3.79262300
H	-5.81617300	-0.08230000	-3.28311600
H	-2.07975000	-0.86849300	-3.09394600
H	-3.58374200	-1.35126200	-3.90156800

H	-2.81873400	0.18561000	-4.31304200
C	3.61411100	-0.99729600	-2.62148700
C	3.03765900	-2.25501800	-3.29492000
C	4.80701200	-0.44728900	-3.42650700
H	2.82333700	-0.24165100	-2.63552400
H	2.19797900	-2.64823500	-2.72016300
H	2.68102000	-2.00470200	-4.30019300
H	3.79325900	-3.04048200	-3.40596600
H	5.18801100	0.48564000	-2.99987000
H	5.63190100	-1.16867800	-3.43513800
H	4.51701000	-0.25301300	-4.46502500
C	3.60878400	0.28459500	2.36534100
C	4.84743900	0.87975500	3.05957300
C	2.69784100	-0.44343400	3.37064000
H	3.03784300	1.12556100	1.96158700
H	5.47481800	1.42390700	2.34633500
H	4.54792600	1.57382900	3.85261200
H	5.46366700	0.09813100	3.51660200
H	1.80557500	-0.83145300	2.87347100
H	3.21970400	-1.28283200	3.84304900
H	2.38095000	0.24116600	4.16541900
C	5.99569500	-3.88031200	0.78342500
C	5.22205200	-4.85746700	1.68711100
C	7.35429500	-3.51072100	1.40545000
H	6.19420000	-4.39353700	-0.16674700
H	4.26806000	-5.14154000	1.23287100
H	5.80523600	-5.76779000	1.86494100
H	5.00552700	-4.40386500	2.66050400
H	7.91688700	-2.83658900	0.75220400
H	7.22186700	-3.00721000	2.36930600
H	7.95950200	-4.40740900	1.57850100
C	0.68840600	2.08704200	-0.34414400
C	1.26714600	3.16371100	-1.10055300
C	-3.95614200	-1.10256300	1.24049600
C	-3.62372500	-0.70251100	2.67945900
C	-2.98689600	-1.82943600	3.51266600
C	-4.89282600	-0.18183400	3.38383800
H	-2.89872700	0.11447200	2.64549700
H	-2.07212300	-2.20724600	3.05116300
H	-2.72369100	-1.44681600	4.50415200
H	-3.67241900	-2.66965900	3.66392500
H	-5.34853300	0.64815000	2.83667400
H	-5.64280100	-0.97696300	3.46042100
H	-4.65935900	0.16362700	4.39664700
O	0.42647400	-1.96133900	-1.31208400
O	-0.86530800	-1.71740900	0.97745900
H	-1.74311900	-2.05789100	0.73310700
C	-4.70896300	-1.89306100	-1.33925400
H	-5.00296700	-2.19504600	-2.33994600

R-Chain

C	-0.23659200	2.49021000	4.02843300
C	-0.13963000	1.00779100	3.79272700
O	0.07951900	0.30981400	4.90984200
C	0.27442200	-1.15107400	4.82799000
O	-0.22152900	0.47747500	2.67181000
H	-0.14560800	2.70123500	5.11184600
H	-1.23546500	2.83455600	3.67875800
H	-0.24378800	-1.49908500	3.91088600
C	-0.37641600	-1.73119800	6.07847800
H	-1.45304500	-1.47136800	6.12911600
H	-0.28709200	-2.83638900	6.06967800
H	0.11654700	-1.35099100	6.99720300

C	1.76894400	-1.43198300	4.71943800
H	2.18911400	-0.97385900	3.80307600
H	2.31258700	-1.04083600	5.60455900
H	1.94326300	-2.52446300	4.65058900
O	0.70874357	2.96941712	1.79647414
H	1.22774652	3.59502050	1.28573316
C	2.21775355	2.79490366	3.70542048
H	2.16998160	2.64758509	4.76415325
H	2.48344920	1.87446558	3.22887084
H	2.95434212	3.53803267	3.48159789
C	0.84396900	3.26212500	3.18964900
H	0.73422307	4.32614391	3.21647403

S-Chain

C	-1.96732400	-0.51849500	-0.05762200
C	-1.39696500	0.75309800	-0.68982800
C	0.04806400	0.99706900	-0.29929600
O	0.80174600	-0.10027900	-0.54081700
C	2.19491100	-0.05218600	-0.11734500
C	-3.43547100	-0.73157100	-0.42380200
O	0.47988200	2.03453000	0.15292900
H	-1.36955900	-1.37146700	-0.41137800
H	-3.82421400	-1.63762300	0.05480100
H	-3.56377300	-0.84430600	-1.50554800
H	-4.03659200	0.11742200	-0.08388500
H	-1.45749100	0.67217100	-1.78120400
H	-1.97282700	1.62489000	-0.37087700
H	2.57735800	0.94782100	-0.34510300
C	2.91435000	-1.10609400	-0.94426900
H	2.80877000	-0.89962800	-2.01287900
H	3.97977700	-1.11672500	-0.69510300
H	2.50219100	-2.09981100	-0.74175900
C	2.26425400	-0.30090100	1.38502400
H	1.71383200	0.47439100	1.92145600
H	1.82797900	-1.27542500	1.62646400
H	3.30522100	-0.29021500	1.72353100
O	-1.80299600	-0.35458600	1.35331900
H	-2.05065700	-1.18433900	1.78087000

(R, R)-DL

O	-0.87648500	2.51847100	-0.15953600
C	-0.33602500	1.51085800	0.23066100
C	1.79310300	0.17209000	0.19584400
H	1.63846500	-0.06107500	1.25631800
C	-1.81149300	-0.52337800	0.22806700
H	-2.13947700	-1.36394200	0.84678300
C	0.21353600	-1.68100600	-0.17895400
O	0.09290200	-2.50266400	0.70016900
C	-2.96446200	0.05592200	-0.56932700
C	3.21178800	0.68670000	-0.01015900
H	-3.37663500	-0.70790900	-1.23342800
H	-3.75250000	0.39276400	0.11038700
H	-2.63506800	0.91031500	-1.16447200
H	3.94067700	-0.06526900	0.30510400
H	3.37802400	0.92101800	-1.06536600
H	3.36715900	1.59737900	0.57306800
C	1.52343200	-1.10381300	-0.64745800
H	2.32471600	-1.82392300	-0.46947400
H	1.48830400	-0.82361400	-1.70292200
C	-1.06748100	0.50568100	1.11568300
H	-1.78428400	1.06944300	1.71552600
H	-0.39689300	-0.02810600	1.79326800
O	0.93391400	1.26365500	-0.20106900

O	-0.82868900	-0.99888900	-0.73343100
(S, S)-DL			
O	0.87661600	2.51835900	-0.15976300
C	0.33608700	1.51087300	0.23062200
C	-1.79307400	0.17215100	0.19587400
H	-1.63840200	-0.06105700	1.25633400
C	1.81146700	-0.52339900	0.22817400
H	2.13938400	-1.36398200	0.84690600
C	-0.21361800	-1.68103300	-0.17899800
O	-0.09303100	-2.50287800	0.69995600
C	2.96447100	0.05578700	-0.56924300
C	-3.21176600	0.68678900	-0.01004500
H	3.37644900	-0.70804700	-1.23346700
H	3.75262200	0.39240900	0.11045500
H	2.63518300	0.91033000	-1.16424700
H	-3.94065200	-0.06519100	0.30521600
H	-3.37805100	0.92115600	-1.06523800
H	-3.36710500	1.59744600	0.57323300
C	-1.52346800	-1.10372400	-0.64749100
H	-2.32480700	-1.82379900	-0.46958100
H	-1.48829300	-0.82346000	-1.70294200
C	1.06753500	0.50577200	1.11572800
H	1.78439600	1.06958300	1.71545900
H	0.39694600	-0.02790700	1.79340400
O	-0.93388300	1.26373000	-0.20102300
O	0.82861400	-0.99880900	-0.73332700

R-Chain- (R, R)-DL

¹INT1			
C	-7.71203000	1.78167900	-1.46121700
C	-6.66573400	2.63249300	-1.19341600
C	-5.41349000	2.13103700	-0.74557400
C	-6.34843100	-0.12916900	-0.84843400
C	-7.54251200	0.38604300	-1.30005500
H	-4.44681800	4.06394000	-0.67928100
H	-8.66191200	2.17456800	-1.81082700
H	-6.77311800	3.70430300	-1.33657100
C	-4.31282500	2.99641900	-0.53280700
H	-6.23171900	-1.20032500	-0.73850400
H	-8.36035400	-0.28637500	-1.54097800
C	-2.93198200	1.12417500	0.01494500
C	-3.06045000	2.52127400	-0.20161700
C	-3.81138300	-1.19200100	0.35964900
C	-4.67099200	-1.82659800	1.32549800
C	-2.75570800	-1.93085600	-0.14286100
C	-5.67758300	-1.13006200	2.04844300
C	-4.49051300	-3.22274000	1.59780800
C	-2.48182700	-3.28231100	0.20691100
C	-6.49452000	-1.78640900	2.94213100
H	-5.79707000	-0.06482300	1.89600700
C	-5.36361000	-3.87356400	2.51061500
C	-3.39889700	-3.91745300	1.01562600
C	-6.35131900	-3.17555600	3.16533100
H	-7.25231200	-1.22943800	3.48488200
H	-5.22082000	-4.93477700	2.69620000
H	-3.24094000	-4.95947300	1.27867100
H	-7.00793200	-3.68228700	3.86600900
O	-1.91945300	-1.34859500	-1.09432300
O	-1.66180400	0.67041700	0.38668400
P	-0.82420600	-0.24159500	-0.65856500
C	-1.17215700	-3.88861100	-0.18097800
C	-0.84666100	-4.10496000	-1.53859300

C	1.07249600	-4.55097800	0.43844700
C	1.42591000	-4.73369000	-0.89917500
H	1.82266800	-4.73179900	1.20496800
C	-1.90291500	3.46329900	-0.08499500
C	-1.32925100	3.74421500	1.17792300
C	-1.44084800	4.14229200	-1.23630300
C	-0.35897500	4.74478600	1.26943400
C	-0.45609200	5.12859100	-1.08689700
C	0.08543200	5.46131400	0.15436300
H	0.06904700	4.96790900	2.24204000
H	-0.10473500	5.65772200	-1.96875100
C	2.83122600	-5.17894100	-1.27406100
C	3.36720500	-4.46637600	-2.52751200
C	2.89216800	-6.70907000	-1.44103200
H	3.48785700	-4.91491100	-0.43242800
H	3.21639900	-3.38630400	-2.45404800
H	4.43476600	-4.67465800	-2.66043500
H	2.85802700	-4.81431100	-3.43223300
H	2.56328000	-7.21929500	-0.53054800
H	2.23633700	-7.02830700	-2.25853800
H	3.91070400	-7.03938700	-1.67358600
C	-1.87131200	-3.93748300	-2.65643100
C	-2.27987900	-5.31535300	-3.21259500
C	-1.37648800	-3.00964000	-3.77984200
H	-2.77096000	-3.48435300	-2.23175800
H	-2.67828500	-5.95849900	-2.42124300
H	-3.04767000	-5.20708000	-3.98646900
H	-1.42156500	-5.82882100	-3.65980500
H	-1.07275800	-2.03773700	-3.38536600
H	-0.52552900	-3.44467000	-4.31517100
H	-2.17440800	-2.84866100	-4.51273500
C	-1.97575700	3.84991300	-2.63846900
C	-0.86749100	3.38171700	-3.59982500
C	-2.72695400	5.06736500	-3.20871800
H	-2.69233700	3.02845900	-2.56650900
H	-0.42996400	2.44171400	-3.25681300
H	-1.28568700	3.21481000	-4.59866000
H	-0.06936600	4.12543800	-3.69525400
H	-3.53999300	5.38206400	-2.54630600
H	-2.05606200	5.92362200	-3.33743800
H	-3.15733400	4.82971600	-4.18746500
C	-1.72764900	3.00752300	2.45402700
C	-2.29036100	3.97181600	3.51446100
C	-0.54437100	2.18996100	3.00972000
H	-2.52705700	2.30178200	2.21424300
H	-3.13833400	4.54042900	3.11939300
H	-2.63080700	3.41488000	4.39404100
H	-1.53399600	4.68902300	3.84991400
H	-0.21432900	1.44511800	2.28230800
H	0.31044800	2.83121600	3.24987800
H	-0.84034700	1.66539600	3.92496900
C	1.11081300	6.57714800	0.30108200
C	2.44397700	6.08299100	0.89391900
C	0.53582900	7.73540500	1.13852600
H	1.31739600	6.96587500	-0.70511200
H	2.92861300	5.35644800	0.23786800
H	3.13420900	6.92217200	1.03210600
H	2.30490800	5.59941300	1.86546500
H	-0.40195800	8.10420700	0.71153300
H	0.33100600	7.41106100	2.16454400
H	1.24474400	8.56901800	1.18659500
H	1.63282900	0.68175700	-2.09329200
C	-3.99239800	0.22893900	-0.05332200

C	-5.25401500	0.72343500	-0.53519100
C	-0.20714300	-4.13844600	0.82692800
C	-0.50555000	-4.00477400	2.32109700
C	0.45907100	-3.06106100	3.05666300
C	-0.53263000	-5.39527400	2.98364400
H	-1.49946000	-3.57083600	2.43792300
H	0.40495600	-2.05571200	2.63252700
H	0.18977200	-2.99829000	4.11645500
H	1.49593000	-3.41143500	3.00514800
H	-1.25558000	-6.05439300	2.49200800
H	0.44790800	-5.88027300	2.92382300
H	-0.80543700	-5.31536700	4.04158300
O	-0.26425100	0.39476100	-1.87519400
O	0.20261200	-0.88649900	0.35235500
H	1.02751300	-1.23886100	-0.11004200
C	0.44173800	-4.53175600	-1.86751900
H	0.68306600	-4.69530100	-2.91237200
O	6.31854600	-1.63733900	2.50124000
C	5.63390100	-1.88167200	1.53631600
C	5.55408200	-1.90474100	-0.98019900
H	5.00933900	-2.85299500	-0.92287700
C	3.22732200	-1.19159600	1.76894800
H	2.20853100	-1.55348200	1.65287400
C	3.36633500	-0.86976700	-0.58142100
O	2.39170600	-1.56375700	-0.86096200
C	3.35439600	-0.35138600	3.02322700
C	6.72140100	-2.05038700	-1.94607600
H	2.78515700	0.57454300	2.91752500
H	2.96292700	-0.91822600	3.87303100
H	4.39659300	-0.10024900	3.22608900
H	6.35751700	-2.32518500	-2.94003300
H	7.27050300	-1.10734000	-2.01905600
H	7.40716500	-2.82372900	-1.59206300
C	4.58971800	-0.77729000	-1.43147600
H	4.31569900	-0.92200000	-2.47671700
H	5.05774300	0.19895700	-1.29998400
C	4.20247100	-2.38892900	1.68066000
H	4.15809200	-2.96585800	2.60612100
H	3.89340100	-3.03607700	0.85674600
O	6.15569000	-1.61468500	0.30460400
O	3.55904800	-0.32956500	0.63477500
C	2.15107700	2.45087800	0.16054300
C	3.49586500	2.63093000	0.83008900
O	4.55575100	2.49021200	0.00885200
C	5.87203900	2.81704000	0.55394400
O	3.59642600	2.90315600	2.01298900
H	1.52528500	3.24625400	0.56832500
H	1.73254900	1.51847700	0.55302100
H	5.74654700	3.70502500	1.18239600
C	6.73660400	3.13438500	-0.65697400
H	6.30597700	3.95160200	-1.24220900
H	7.74105300	3.42555300	-0.33510200
H	6.82604600	2.25610700	-1.30495600
C	6.40826200	1.66788600	1.39477400
H	5.74037700	1.47149200	2.23278900
H	6.51246300	0.75718700	0.80190700
H	7.39322700	1.93048300	1.79412900
O	2.44842100	1.18252600	-1.91842100
C	2.69695100	3.57034400	-2.11634700
H	2.35643600	4.53967200	-1.74116600
H	3.78096400	3.50736400	-2.01508800
H	2.43952900	3.50454200	-3.17718700
C	2.00959300	2.43346500	-1.36785400

H	0.93392800	2.52228600	-1.54082300
¹ TS1			
C	-7.28435600	2.89723000	-1.56406500
C	-6.11236300	3.56883700	-1.30754000
C	-4.96791400	2.88073700	-0.82113200
C	-6.26806700	0.80815400	-0.86391300
C	-7.35339700	1.49970100	-1.35297400
H	-3.68703400	4.62188400	-0.81867000
H	-8.15059400	3.43115800	-1.94294300
H	-6.03560300	4.63756200	-1.48933200
C	-3.73773200	3.55445500	-0.62581600
H	-6.33481900	-0.26272100	-0.71689400
H	-8.26986200	0.96542600	-1.58505900
C	-2.69821800	1.49900700	0.03343500
C	-2.58995700	2.88742200	-0.25083800
C	-3.95515700	-0.63201900	0.39659500
C	-4.91393600	-1.11552500	1.35485900
C	-3.02559300	-1.53146100	-0.09436200
C	-5.80908600	-0.26363700	2.05766800
C	-4.95410000	-2.52013500	1.64238500
C	-2.97366800	-2.90820800	0.26418400
C	-6.72678800	-0.77500600	2.94835300
H	-5.76121200	0.80525400	1.89047600
C	-5.92578600	-3.01652500	2.55249600
C	-3.98145500	-3.38394500	1.07403100
C	-6.80051800	-2.16675200	3.18867700
H	-7.39626200	-0.10159200	3.47519700
H	-5.95097500	-4.08484500	2.75063300
H	-3.99203900	-4.43567600	1.34616900
H	-7.53409300	-2.55793200	3.88715600
O	-2.09689300	-1.08481400	-1.02583500
O	-1.53954400	0.86363100	0.46595900
P	-0.80787400	-0.24380400	-0.49548900
C	-1.77676300	-3.71299300	-0.12840500
C	-1.49313700	-3.96635000	-1.48885900
C	0.35403900	-4.69207400	0.47147100
C	0.67154300	-4.91333700	-0.86933200
H	1.07738600	-4.97782500	1.23190300
C	-1.29254400	3.63172300	-0.16301100
C	-0.70512800	3.91235800	1.09337700
C	-0.70684300	4.14533800	-1.34350900
C	0.40328000	4.76249000	1.14620500
C	0.41008700	4.98617300	-1.23313900
C	0.96746800	5.32975700	-0.00126300
H	0.84003800	4.98907800	2.11455100
H	0.84838200	5.39872300	-2.13832100
C	2.00226400	-5.54407900	-1.25147700
C	2.60082000	-4.94680000	-2.53624500
C	1.86815700	-7.07435300	-1.36695100
H	2.70315400	-5.33767500	-0.42973800
H	2.58086500	-3.85416400	-2.50370800
H	3.63464100	-5.28383800	-2.67099800
H	2.04144400	-5.26446800	-3.42240400
H	1.49541900	-7.50890700	-0.43442000
H	1.16137600	-7.33444900	-2.16271600
H	2.83253800	-7.53810000	-1.60308600
C	-2.48622100	-3.64059900	-2.60021900
C	-3.09322600	-4.93787500	-3.16853100
C	-1.86503400	-2.78209500	-3.71618400
H	-3.30840200	-3.06518600	-2.16676200
H	-3.57874800	-5.52437300	-2.38183000
H	-3.83945400	-4.71094600	-3.93794600

H	-2.32029100	-5.56649300	-3.62454800
H	-1.41947200	-1.87186500	-3.30967500
H	-1.09092000	-3.33199800	-4.26281700
H	-2.63405400	-2.49518100	-4.44168000
C	-1.25025600	3.82845200	-2.73661000
C	-0.18789700	3.17719700	-3.64115900
C	-1.84345900	5.08560600	-3.39909900
H	-2.05637600	3.09917500	-2.62871700
H	0.14004700	2.22469000	-3.22035200
H	-0.61220400	2.97781600	-4.63122000
H	0.68338800	3.82616600	-3.78121000
H	-2.63128800	5.52901700	-2.78219800
H	-1.07510200	5.85085300	-3.55536800
H	-2.27447600	4.83901100	-4.37531200
C	-1.24110400	3.33356900	2.39996100
C	-1.63892700	4.44048800	3.39346800
C	-0.22850800	2.35419000	3.02631500
H	-2.14768800	2.76492800	2.17880400
H	-2.36322600	5.12916800	2.94688200
H	-2.09021600	4.00237000	4.29001400
H	-0.77216000	5.02787200	3.71436100
H	-0.04649600	1.50982400	2.35755900
H	0.72856200	2.84488600	3.23577500
H	-0.61653700	1.95848200	3.97126300
C	2.13449100	6.30461500	0.09505400
C	3.40334500	5.66321300	0.68975800
C	1.73408400	7.55900600	0.89429400
H	2.37456600	6.62654800	-0.92708900
H	3.78575800	4.86040800	0.05291600
H	4.19722600	6.41060800	0.79260900
H	3.21713400	5.23688200	1.68092600
H	0.84275000	8.02960700	0.46837900
H	1.51243400	7.30601700	1.93658400
H	2.54597100	8.29418900	0.89472300
H	1.30968500	0.29472900	-1.61598600
C	-3.89564700	0.79412200	-0.03569700
C	-5.04916500	1.47513200	-0.55849300
C	-0.85080400	-4.10283300	0.87045000
C	-1.10813300	-3.92185700	2.36655600
C	-0.01145600	-3.11238000	3.07779400
C	-1.31714700	-5.29126100	3.04020400
H	-2.03150200	-3.35459500	2.49203900
H	0.05837300	-2.11424800	2.64120400
H	-0.24837600	-3.01110300	4.14255300
H	0.96827500	-3.59871100	3.00710900
H	-2.13255600	-5.84651500	2.56479200
H	-0.41446900	-5.90830800	2.97035200
H	-1.55942300	-5.16801100	4.10149700
O	-0.16522200	0.34772500	-1.73056300
O	0.08989000	-1.04275000	0.42814900
H	1.22164800	-1.64211500	-0.31448200
C	-0.28033800	-4.56930400	-1.82999100
H	-0.07095400	-4.75678200	-2.87770600
O	5.95238800	-2.37519500	2.30142200
C	5.20565900	-2.49258200	1.35825000
C	4.99408300	-2.41896700	-1.13418400
H	4.28736700	-3.24893300	-1.05394000
C	2.92154700	-1.49603800	1.69736200
H	1.86027600	-1.71690500	1.62856800
C	3.00679100	-0.95577800	-0.66754700
O	2.07175700	-1.85247000	-0.88062500
C	3.21174100	-0.74816400	2.98446400
C	6.05820000	-2.76170600	-2.16804900

H	2.70078200	0.21597000	2.99240700
H	2.84983200	-1.34571700	3.82610400
H	4.28096500	-0.57803900	3.11589000
H	5.59424500	-2.95941400	-3.13848200
H	6.76530700	-1.93396000	-2.27623300
H	6.61242200	-3.64916200	-1.85384000
C	4.24151600	-1.12991000	-1.51332200
H	3.93557400	-1.18235200	-2.55954400
H	4.89010100	-0.26481700	-1.36430900
C	3.72697900	-2.80257100	1.53164200
H	3.62970200	-3.39105300	2.44591600
H	3.30803500	-3.37829500	0.70599400
O	5.71044500	-2.26138900	0.11420900
O	3.28644500	-0.58882700	0.60406500
C	2.60173300	2.14545600	0.44146000
C	3.98223100	2.11781700	1.05842700
O	4.98240500	1.88901600	0.18508100
C	6.35385700	2.01548600	0.68367300
O	4.15393000	2.34607300	2.23932700
H	2.21929500	3.14394800	0.65851400
H	1.97357000	1.46977800	1.02343600
H	6.36568400	2.87043900	1.36719400
C	7.19935500	2.29945000	-0.54837100
H	6.84746800	3.19575100	-1.06694300
H	8.24348800	2.45068400	-0.25894600
H	7.15804800	1.45543500	-1.24509700
C	6.76454800	0.75301700	1.42477100
H	6.11818600	0.58951300	2.28675200
H	6.71140000	-0.12260500	0.77487200
H	7.79373200	0.85361100	1.78409400
O	2.31333800	0.48529300	-1.42517800
C	3.22392000	2.64881800	-2.04448000
H	3.18667000	3.72155300	-1.83345200
H	4.26050000	2.31917500	-2.00035500
H	2.83109500	2.48855100	-3.05151900
C	2.35030900	1.90760500	-1.04428400
H	1.31536600	2.22287600	-1.19759800

INT2

C	-7.11816400	3.15509500	-1.83662200
C	-5.91995800	3.77719900	-1.57624400
C	-4.82694600	3.05436800	-1.02622500
C	-6.23398300	1.05078800	-1.01389600
C	-7.26765500	1.77451200	-1.56437600
H	-3.46290800	4.73135600	-1.04102500
H	-7.94451000	3.71483300	-2.26400000
H	-5.78290200	4.83121200	-1.80234500
C	-3.57106000	3.67488300	-0.81614100
H	-6.36127400	-0.00694400	-0.81882600
H	-8.20528800	1.27901200	-1.79746600
C	-2.66188600	1.60129200	-0.04641000
C	-2.47074700	2.97010100	-0.37412700
C	-4.03019200	-0.44881100	0.36888500
C	-5.02101600	-0.84094900	1.33577000
C	-3.13949200	-1.41411500	-0.06045800
C	-5.89363400	0.08225700	1.97344400
C	-5.11366200	-2.22446000	1.70366900
C	-3.13878900	-2.76836000	0.36974500
C	-6.83929800	-0.34378700	2.87946200
H	-5.80640000	1.13704100	1.74436300
C	-6.11250100	-2.63158200	2.62871000
C	-4.16837700	-3.15577800	1.19916300
C	-6.96385700	-1.71542500	3.20094900

H	-7.49143900	0.38198300	3.35592900
H	-6.17771000	-3.68442100	2.88968000
H	-4.21931900	-4.18736800	1.53408300
H	-7.71861400	-2.03862800	3.91137900
O	-2.16659600	-1.04568100	-0.99616700
O	-1.54051300	0.92285500	0.44206800
P	-0.87041800	-0.27760700	-0.42107100
C	-1.97491600	-3.64184500	0.02480100
C	-1.73314900	-4.02260200	-1.31377800
C	0.11282800	-4.67630300	0.67447800
C	0.38313300	-5.04348800	-0.64418400
H	0.83601000	-4.93354800	1.44395400
C	-1.14297800	3.65093900	-0.23913700
C	-0.61584200	3.93844900	1.04187900
C	-0.45891200	4.08804800	-1.39710500
C	0.54982000	4.70441200	1.13620400
C	0.70539700	4.85294000	-1.24395400
C	1.22224600	5.18561200	0.00867900
H	0.94046600	4.93726400	2.12245900
H	1.22364600	5.20508300	-2.13173000
C	1.65585100	-5.80000200	-0.99203100
C	2.36118000	-5.22722300	-2.23399400
C	1.36782100	-7.30308900	-1.16518800
H	2.33945000	-5.68901800	-0.13960800
H	2.46683800	-4.14184000	-2.15924700
H	3.35248900	-5.67829800	-2.35337200
H	1.79589700	-5.44288900	-3.14721500
H	0.91458400	-7.72521700	-0.26293600
H	0.67249900	-7.46598600	-1.99626300
H	2.28873400	-7.85642200	-1.38013700
C	-2.72513500	-3.72392900	-2.43363800
C	-3.39562500	-5.02294900	-2.91982900
C	-2.07697500	-2.96126600	-3.60271700
H	-3.51711100	-3.08719200	-2.02904300
H	-3.89590700	-5.54089200	-2.09529700
H	-4.14109200	-4.80768600	-3.69327900
H	-2.65732800	-5.71063500	-3.34658600
H	-1.60029100	-2.04231700	-3.25451700
H	-1.32029100	-3.57024200	-4.10887400
H	-2.83517300	-2.69512300	-4.34727200
C	-0.94452000	3.76378100	-2.80916400
C	0.14979900	3.10486300	-3.66838200
C	-1.49492000	5.02140000	-3.50746200
H	-1.76065700	3.04106600	-2.72927200
H	0.51089400	2.18602700	-3.20330600
H	-0.25307400	2.84585800	-4.65315400
H	1.00335100	3.77201900	-3.82719200
H	-2.31307600	5.47171800	-2.93764700
H	-0.71263700	5.78018000	-3.61996800
H	-1.87171100	4.77520800	-4.50598100
C	-1.28071000	3.46130400	2.33010900
C	-1.68349300	4.64348700	3.23074600
C	-0.38262400	2.46134600	3.08303000
H	-2.20261500	2.93586200	2.06824800
H	-2.33462800	5.34267800	2.69635100
H	-2.21975600	4.28275500	4.11484100
H	-0.80840700	5.20134400	3.58034800
H	-0.17040200	1.58758400	2.46296300
H	0.57079400	2.91605300	3.37272100
H	-0.87923400	2.11709900	3.99656900
C	2.44691900	6.08227500	0.13999300
C	3.58087400	5.45267600	0.97095400
C	2.04453100	7.45131800	0.72191400

H	2.83501900	6.25294600	-0.87312300
H	3.95659200	4.53006800	0.52087300
H	4.42178300	6.14950600	1.05217700
H	3.25137400	5.21727700	1.98847400
H	1.26025600	7.92040300	0.11998700
H	1.66137000	7.34104900	1.74224800
H	2.90483500	8.12834100	0.75681200
H	0.75252600	0.25173100	-1.67875000
C	-3.88827400	0.95204600	-0.12295900
C	-4.99016900	1.66797400	-0.70590100
C	-1.04463300	-3.97860900	1.03765300
C	-1.25645800	-3.62875200	2.51018400
C	-0.04061300	-2.94601400	3.15870000
C	-1.66269700	-4.88866900	3.29904100
H	-2.08247400	-2.91751100	2.57859100
H	0.22026700	-2.03436400	2.61938600
H	-0.27082200	-2.68327300	4.19688700
H	0.83643600	-3.60172000	3.17970500
H	-2.55821200	-5.35583000	2.87654200
H	-0.86111200	-5.63537000	3.27768400
H	-1.86682100	-4.64173400	4.34663800
O	-0.26000200	0.29558500	-1.75500700
O	0.06854600	-1.05011400	0.43345900
H	1.36755900	-1.82351000	-0.66939600
C	-0.56397700	-4.72271700	-1.61924000
H	-0.38524700	-5.01659600	-2.64867300
O	6.16663200	-2.69743100	1.70389200
C	5.39830300	-2.68974300	0.76878600
C	5.06967900	-2.14827200	-1.64428400
H	4.40421000	-3.01303400	-1.70378300
C	3.06060500	-1.94824900	1.31971200
H	2.01813000	-2.25028100	1.20742300
C	2.99053300	-0.82079800	-0.87547500
O	2.17114900	-1.87131200	-1.23321700
C	3.29865400	-1.50113300	2.75286000
C	6.10236400	-2.23134000	-2.76227000
H	2.70115700	-0.61635400	2.97716900
H	3.01229200	-2.30667700	3.43502500
H	4.34818800	-1.25866700	2.92327000
H	5.60746600	-2.25708900	-3.73749400
H	6.76948500	-1.36452800	-2.72963200
H	6.70733900	-3.13419600	-2.64933000
C	4.25664600	-0.85305900	-1.72862500
H	3.94977700	-0.69292400	-2.76584700
H	4.89037700	-0.02060600	-1.41641500
C	3.95527700	-3.13736400	0.89762000
H	3.92564700	-3.89745800	1.68125000
H	3.56352800	-3.56968100	-0.02166800
O	5.84366400	-2.20265700	-0.41961500
O	3.32624800	-0.79480800	0.48981100
C	2.65696600	1.87443400	0.77737700
C	4.00796400	1.72156800	1.44134700
O	5.04824400	1.85604000	0.59312800
C	6.39235900	1.88778300	1.17070900
O	4.12696500	1.59590500	2.64222500
H	2.33266000	2.88702900	1.03404900
H	1.97205000	1.19967000	1.29077100
H	6.32582100	2.44943700	2.10787800
C	7.24280400	2.63541700	0.15491800
H	6.83702700	3.63308900	-0.03622300
H	8.26614500	2.73977900	0.52766600
H	7.27857000	2.08736400	-0.79240400
C	6.87272200	0.47207700	1.44517000

H	6.22781600	-0.02119900	2.17125900
H	6.87882100	-0.12798600	0.53250200
H	7.88896600	0.49534800	1.85166000
O	2.22295300	0.36587400	-1.19502900
C	3.38066700	2.47539500	-1.68001100
H	3.37350700	3.54022900	-1.43309900
H	4.40646600	2.12118800	-1.62224400
H	3.00997200	2.36345600	-2.70229700
C	2.44209300	1.73338200	-0.73304000
H	1.44609100	2.15774900	-0.89097900

¹INT3

C	-0.92544900	7.44554400	1.63855000
C	-1.87385800	6.45523900	1.74719700
C	-1.64312700	5.15921600	1.21221300
C	0.55363500	5.93576900	0.44910800
C	0.30456000	7.17568600	0.99371900
H	-3.52575600	4.34032500	1.89375600
H	-1.11160400	8.42957500	2.05804000
H	-2.81310800	6.64393500	2.26012300
C	-2.59545400	4.11986300	1.38067600
H	1.50147400	5.73921300	-0.03747200
H	1.06135200	7.95194500	0.93202200
C	-1.14375800	2.61779400	0.23567800
C	-2.35342300	2.83527300	0.94514800
C	0.98211200	3.24517300	-0.87912300
C	1.30766700	3.97786800	-2.07247800
C	1.76324400	2.14385100	-0.55952000
C	0.48849000	5.01823500	-2.59192100
C	2.49455900	3.62980700	-2.79590500
C	2.90144700	1.73536700	-1.30446500
C	0.85081800	5.70663500	-3.72783500
H	-0.43756000	5.26450700	-2.08764900
C	2.84910900	4.37257200	-3.95423200
C	3.27163000	2.52212500	-2.37364800
C	2.05015700	5.39442900	-4.41035600
H	0.20542800	6.49323700	-4.10711500
H	3.75858400	4.10263400	-4.48423600
H	4.17018200	2.27003100	-2.92790700
H	2.32661400	5.95031700	-5.30109500
O	1.46238300	1.40562700	0.58967800
O	-0.92289000	1.32098800	-0.24146200
P	0.14184400	0.44960600	0.59751000
C	3.67470400	0.50674600	-0.93154700
C	4.62667400	0.57190800	0.10803300
C	4.22775600	-1.82073900	-1.27378400
C	5.18360100	-1.78035200	-0.25612300
H	4.07282600	-2.75652300	-1.80185100
C	-3.28399800	1.68861900	1.18734800
C	-3.97966400	1.11340400	0.09986300
C	-3.42275600	1.14650000	2.48619800
C	-4.81452300	0.01946300	0.33700100
C	-4.29145800	0.06411500	2.66948100
C	-4.99420700	-0.51640700	1.61389900
H	-5.34391000	-0.42437900	-0.49962900
H	-4.41306800	-0.35143500	3.66544400
C	6.04359800	-3.00098000	0.04303900
C	6.09287900	-3.36214400	1.53712300
C	7.46498300	-2.79947700	-0.51695300
H	5.59371400	-3.85141000	-0.48651900
H	5.09464200	-3.56116400	1.93462500
H	6.70344600	-4.25850500	1.69147900
H	6.54353400	-2.55797800	2.12902500

H	7.43876000	-2.58214700	-1.58907900
H	7.95907500	-1.95826700	-0.01801900
H	8.07848600	-3.69360900	-0.36043800
C	4.87939600	1.85882000	0.88904600
C	6.35005600	2.30259800	0.79201800
C	4.42970600	1.72612500	2.35523200
H	4.27703300	2.65224700	0.43735700
H	6.66031100	2.41095200	-0.25205500
H	6.49292400	3.26547200	1.29419100
H	7.02222500	1.57965200	1.26638700
H	3.36198100	1.50378400	2.41526300
H	4.97685000	0.92569800	2.86632200
H	4.61497800	2.65770900	2.90101100
C	-2.67192500	1.70976900	3.69125800
C	-2.09621100	0.62166800	4.61509300
C	-3.57876000	2.65743600	4.50132200
H	-1.82387800	2.28872300	3.31478400
H	-1.49644500	-0.09917800	4.06044500
H	-1.45571700	1.08516600	5.37345100
H	-2.88470800	0.08032600	5.14925100
H	-3.95725900	3.48256400	3.89173200
H	-4.44483200	2.11355700	4.89517700
H	-3.03305500	3.08452700	5.35003100
C	-3.87053600	1.65228700	-1.32482600
C	-5.23559300	2.15477100	-1.83207000
C	-3.27704600	0.60563400	-2.28399100
H	-3.19816600	2.51474800	-1.31963000
H	-5.65407000	2.91055100	-1.15983100
H	-5.13501500	2.59828900	-2.82867400
H	-5.96016900	1.33619200	-1.90438300
H	-2.27674700	0.30284000	-1.97047600
H	-3.90242600	-0.28872500	-2.31561500
H	-3.20874700	1.00475400	-3.30153900
C	-5.91463500	-1.70642700	1.84260900
C	-5.34066900	-2.98604900	1.20665500
C	-7.34276000	-1.43656400	1.33630100
H	-5.97273600	-1.87131100	2.92653600
H	-4.35614100	-3.22110200	1.62231100
H	-6.00032600	-3.84237900	1.38642100
H	-5.22944500	-2.86893200	0.12303500
H	-7.75648200	-0.52788000	1.78407800
H	-7.36054800	-1.31076400	0.24820300
H	-8.00441500	-2.27423700	1.58216900
C	2.67277400	-1.57307500	2.44415400
C	0.53963900	-5.10881700	1.68581900
C	1.86559700	-1.62080400	3.77291500
H	2.47130300	-0.66359000	1.87981100
H	2.30936400	-2.40707400	4.39354200
H	0.22608700	-4.39574800	2.45230000
H	3.74567500	-1.60743200	2.64765100
H	0.18844900	-6.10191300	1.99198200
C	2.27505100	-2.75678700	1.61435700
O	1.60621700	-2.71281000	0.58188900
C	-0.18046400	-4.83411000	0.37641500
O	0.05765700	-5.42798600	-0.65753200
O	2.65150000	-3.90385200	2.15993400
O	0.52983200	-2.04773100	3.53885100
C	2.76634000	-5.55727800	0.34840300
H	3.84692400	-5.60475200	0.51126300
H	2.40522200	-6.53491400	0.02281200
H	2.54647400	-4.84336000	-0.44363700
C	1.92537700	-0.28146200	4.50414000
H	2.96002500	0.01065100	4.71357100

H	1.45642500	0.49711200	3.89609300
H	1.38097300	-0.35488600	5.44956800
O	-1.16940000	-3.93688000	0.54286100
H	0.10491900	-1.36837600	2.97863300
O	-3.73676000	-2.85024300	-2.62549800
C	-4.67285000	-2.54139700	-3.70294400
H	-4.32766000	-1.62364900	-4.18763600
C	-6.01959600	-2.32626400	-3.03065700
H	-5.97756400	-1.49370200	-2.32426000
H	-6.78144800	-2.10059800	-3.78271300
H	-6.32587300	-3.22495600	-2.48605500
C	-2.41623400	-2.70018100	-2.88883300
O	-1.98806300	-2.23872200	-3.92654200
C	-4.67628500	-3.68691300	-4.70867000
H	-3.68449600	-3.80797400	-5.14827500
H	-4.96985900	-4.62192800	-4.22053300
H	-5.38864000	-3.47801200	-5.51299500
C	-2.16953300	-3.75697500	-0.51774000
H	-2.82416800	-3.00029400	-0.08320500
C	-0.20096600	3.59206300	-0.03966400
C	-0.41439500	4.89756200	0.52067800
C	3.46354800	-0.70470600	-1.63256400
C	2.45567200	-0.81440400	-2.77727600
C	1.78176800	-2.19631600	-2.88095300
C	3.11592400	-0.47601600	-4.12929400
H	1.66648200	-0.08011900	-2.59138200
H	1.49007900	-2.58898800	-1.90679900
H	0.88325100	-2.12796300	-3.50181000
H	2.44769400	-2.93264400	-3.34564700
H	3.50784900	0.54271700	-4.15274200
H	3.94631500	-1.16246900	-4.32991000
H	2.38832000	-0.57688500	-4.94172000
C	-1.51259100	-3.17119500	-1.77011700
H	-0.91179800	-2.30488200	-1.48367600
H	-0.82414800	-3.89473300	-2.21083000
C	-2.94796200	-5.05439800	-0.71563300
H	-3.81786000	-4.86519100	-1.34455800
H	-2.32331000	-5.81644400	-1.18442600
H	-3.29320500	-5.42455600	0.25418600
C	2.08365300	-5.16312600	1.65144500
H	2.39712700	-5.85066000	2.44029400
O	-0.19926300	0.11532900	2.00141400
O	0.37829500	-0.72838000	-0.40977600
H	0.89341500	-1.50426500	0.00354500
C	5.36479200	-0.57348000	0.42390500
H	6.10447200	-0.51645600	1.21738800

**R-Chain- (S, S)-DL
2INT1**

C	-0.43140400	6.34718000	3.54804000
C	-1.49012400	5.69244600	2.96266300
C	-1.27532000	4.69268800	1.97604800
C	1.13607500	5.06990300	2.20834300
C	0.89375500	6.02302800	3.17214300
H	-3.37373300	4.25514900	1.67959300
H	-0.60823500	7.10503800	4.30527700
H	-2.51150000	5.92157700	3.25469000
C	-2.36056400	3.99065000	1.39152400
H	2.15482000	4.82660300	1.93024900
H	1.72730000	6.52800700	3.65108500
C	-0.82773400	2.66791900	0.12910600
C	-2.16743500	2.95834100	0.49725500
C	1.59879200	3.13931700	-0.05664100

C	2.30269900	4.21438400	-0.70210300
C	2.16482900	1.87020100	-0.06697600
C	1.72896800	5.49942300	-0.91459900
C	3.62433600	3.97957700	-1.19474000
C	3.49773400	1.63254900	-0.49879100
C	2.43804400	6.49640700	-1.54572900
H	0.71459200	5.68913500	-0.58692100
C	4.33661500	5.03377900	-1.82742400
C	4.19506400	2.69512800	-1.03875000
C	3.76005500	6.27011800	-1.99735000
H	1.97453500	7.46551100	-1.70438300
H	5.34374200	4.83734900	-2.18521100
H	5.22151200	2.53364900	-1.35466000
H	4.30870000	7.06849500	-2.48778200
O	1.44558900	0.78362700	0.44171200
O	-0.61914400	1.64176400	-0.79197000
P	0.04765400	0.27173300	-0.24130000
C	4.25430400	0.34827100	-0.32490400
C	5.03002700	0.16953700	0.84616600
C	5.32871800	-1.57346100	-1.32141700
C	6.15131700	-1.73325100	-0.20778800
H	5.43218900	-2.26661700	-2.14912900
C	-3.30282000	2.18237300	-0.08305100
C	-3.57775200	2.26714400	-1.46885400
C	-4.10842600	1.37306700	0.74907500
C	-4.65770300	1.55083200	-1.98873700
C	-5.17465200	0.67187200	0.17296300
C	-5.47031900	0.74508800	-1.18874800
H	-4.87378500	1.63202000	-3.04929200
H	-5.78363600	0.03370600	0.80393600
C	7.22299400	-2.81300600	-0.17858000
C	6.99790400	-3.83182400	0.95225500
C	8.62890000	-2.19146600	-0.08685900
H	7.15828300	-3.35948100	-1.12759000
H	6.04087900	-4.34306500	0.82650100
H	7.78911100	-4.58937700	0.95225800
H	7.00413400	-3.34547100	1.93410700
H	8.80201100	-1.48615100	-0.90553700
H	8.75696500	-1.64632700	0.85491100
H	9.40115600	-2.96721000	-0.13169300
C	4.83210700	1.06812600	2.06438500
C	6.12326200	1.34458300	2.84985300
C	3.74737900	0.47501800	2.98727000
H	4.46144200	2.03470200	1.70768900
H	6.92090400	1.70574600	2.19333100
H	5.93957900	2.10379000	3.61697700
H	6.48954500	0.44978600	3.36460900
H	2.79681900	0.36724600	2.45889900
H	4.05579300	-0.51292200	3.35028800
H	3.58207100	1.11830900	3.85871800
C	-3.88145000	1.24163500	2.25416500
C	-3.65651300	-0.21702800	2.68684800
C	-5.04727100	1.87553500	3.03630400
H	-2.97346200	1.78930000	2.51581400
H	-2.75848700	-0.61631400	2.21190900
H	-3.51751700	-0.27147200	3.77248700
H	-4.50610000	-0.85545200	2.42552600
H	-5.19653900	2.92296800	2.75374300
H	-5.98610300	1.34519000	2.84212800
H	-4.85633000	1.83584900	4.11436300
C	-2.77077100	3.14877500	-2.41937800
C	-3.63692700	4.29576100	-2.97369100
C	-2.13077800	2.33064900	-3.55547900

H	-1.95674000	3.61433600	-1.85859600
H	-4.05921600	4.89779700	-2.16258600
H	-3.03887700	4.95355900	-3.61395400
H	-4.46960200	3.91295900	-3.57344700
H	-1.50382700	1.53144100	-3.15419200
H	-2.89255900	1.88030000	-4.20109600
H	-1.50609100	2.97665700	-4.18216700
C	-6.68237900	0.02310200	-1.75798400
C	-6.39233300	-0.71445100	-3.07471500
C	-7.85574000	1.00821100	-1.92490900
H	-6.98479300	-0.72883600	-1.01989400
H	-5.56847100	-1.42200500	-2.96219200
H	-7.27465700	-1.27999800	-3.39177900
H	-6.14520200	-0.01385700	-3.87958500
H	-8.09787600	1.49945300	-0.97698400
H	-7.60054100	1.78967100	-2.64938700
H	-8.75206300	0.49136200	-2.28570400
C	3.35188300	-3.34057300	1.24568900
C	0.28881400	-4.97144700	-0.30314700
C	1.91050200	-2.83792500	1.48834400
H	3.98963300	-2.53389000	0.89452600
H	-0.11393000	-5.08508500	0.70271400
H	3.75716800	-3.72999000	2.18528100
H	-0.47613900	-5.28748200	-1.01453600
C	3.33727800	-4.41993900	0.19055100
O	3.90950500	-4.38657500	-0.87225300
C	0.50897200	-3.49796200	-0.58233800
O	0.03833400	-2.98857300	-1.59924500
O	2.47896100	-5.42257700	0.54906300
O	1.25147300	-2.68898400	0.17763500
O	-1.60279800	-3.05321200	1.08087000
H	-1.40902800	-2.09793300	0.97783600
O	-5.77435900	-2.57938800	0.71092800
C	-7.18244200	-2.95519000	0.73852400
H	-7.59083000	-2.79092500	-0.26320700
C	-7.84192900	-2.03033700	1.74938400
H	-7.75569400	-0.98541300	1.43951800
H	-8.90443200	-2.27415300	1.84317500
H	-7.37276200	-2.14006700	2.73205000
C	-5.06505000	-2.90338900	-0.40154900
O	-5.56069700	-3.41598900	-1.38348100
C	-7.29472400	-4.43194100	1.09903100
H	-6.79538000	-5.04279700	0.34363900
H	-6.83576200	-4.62029700	2.07504100
H	-8.34607300	-4.73257600	1.14611100
C	-2.99800500	-3.30302900	1.00165800
H	-3.50122500	-2.92935900	1.90298800
C	0.26774900	3.38840100	0.55996500
C	0.06486100	4.38611900	1.57242500
C	4.37500900	-0.55087300	-1.40110800
C	3.53056000	-0.39840000	-2.66051500
C	2.93563600	-1.73726600	-3.12654000
C	4.34001300	0.26791300	-3.78809200
H	2.68830600	0.25660700	-2.42194100
H	2.43793300	-2.25250200	-2.30435300
H	2.20023900	-1.56493100	-3.91864300
H	3.70286600	-2.40957100	-3.52408300
H	4.69167400	1.26064700	-3.49106300
H	5.21592000	-0.33792500	-4.04650800
H	3.72673800	0.38017200	-4.68882800
C	-3.60248100	-2.58085500	-0.22108400
H	-3.49076400	-1.49890800	-0.09232400
H	-3.06864600	-2.88286600	-1.12489200

C	-3.17952300	-4.81555200	0.93269900
H	-4.23651600	-5.08826400	0.99851700
H	-2.77890600	-5.20919900	-0.00662700
H	-2.64982700	-5.28946400	1.76429900
C	1.53952800	-5.85247700	-0.46655300
O	-0.74064500	-0.47212600	0.77438100
O	0.36519300	-0.41906400	-1.61078700
H	0.25153400	-1.42986600	-1.61997800
C	5.96441300	-0.86937700	0.87838500
H	6.57594300	-1.00188300	1.76494400
C	1.24167400	-7.32272800	-0.23116300
H	0.52118800	-7.68804900	-0.96867000
H	2.15977100	-7.90881900	-0.31743100
H	0.82395500	-7.47393200	0.76894100
H	1.99640900	-5.70402900	-1.44973200
C	1.12278700	-3.59214900	2.54959700
H	1.55308000	-3.32596400	3.52087500
H	0.07410100	-3.29389300	2.53265300
H	1.20123600	-4.67259200	2.43320700
H	1.96601800	-1.78901600	1.78358500

²TS1

C	-0.75433100	6.12198700	3.52409800
C	-1.79015500	5.32185600	3.10099800
C	-1.58802500	4.33615600	2.09779000
C	0.75994100	5.02858100	1.97578500
C	0.53419300	5.96445500	2.96027700
H	-3.63900400	3.64908500	2.07297400
H	-0.91918700	6.86815900	4.29558900
H	-2.78110300	5.42408500	3.53549700
C	-2.64415200	3.49593300	1.66467700
H	1.75174200	4.91339200	1.55465100
H	1.35358800	6.58528400	3.31027100
C	-1.14051800	2.33008800	0.21749800
C	-2.44729000	2.48044600	0.75062800
C	1.16108900	3.10916600	-0.28950200
C	1.63551800	4.23268400	-1.04899200
C	1.89643900	1.93318200	-0.30751400
C	0.86799400	5.41500900	-1.24068900
C	2.91893700	4.15178700	-1.67570200
C	3.21337000	1.86894200	-0.83734100
C	1.35569000	6.46174700	-1.99051300
H	-0.11922200	5.48268600	-0.80002500
C	3.39948600	5.25451100	-2.43132500
C	3.69108000	2.97703200	-1.50723400
C	2.63757800	6.38899800	-2.58560300
H	0.74741300	7.35027600	-2.13135100
H	4.38027200	5.17860600	-2.89323600
H	4.70265000	2.94999300	-1.90194700
H	3.01091100	7.22448400	-3.17013900
O	1.38113800	0.79161500	0.30196200
O	-0.92855900	1.30857700	-0.69911400
P	0.02768500	0.05140400	-0.28274300
C	4.16420200	0.74034700	-0.57885300
C	5.01705300	0.82890900	0.54740700
C	5.38289200	-1.19698300	-1.34479500
C	6.26753900	-1.10679800	-0.27036000
H	5.51402500	-2.00402700	-2.05672600
C	-3.59687000	1.64640200	0.28823400
C	-4.06382800	1.77397000	-1.04221100
C	-4.29456400	0.82490500	1.20293000
C	-5.25374400	1.13717400	-1.40389500
C	-5.48422000	0.21545400	0.78690300

C	-6.00269900	0.38544300	-0.49778100
H	-5.61727300	1.25778000	-2.41851900
H	-6.03821900	-0.39098500	1.49793100
C	7.43457100	-2.07395300	-0.14284800
C	7.46664400	-2.79047400	1.21761500
C	8.76803000	-1.35198700	-0.41351800
H	7.30130800	-2.84366100	-0.91234800
H	6.54014800	-3.34457600	1.38356900
H	8.29973800	-3.50072700	1.25705700
H	7.59956900	-2.08232700	2.04290900
H	8.76454600	-0.87362400	-1.39791800
H	8.94585900	-0.57150400	0.33504300
H	9.60875200	-2.05371300	-0.37462800
C	4.77918100	1.87282600	1.63643900
C	6.06783100	2.40160400	2.28447300
C	3.82140600	1.30762400	2.70599700
H	4.27953900	2.73027600	1.17490800
H	6.78063200	2.74893500	1.53012700
H	5.83595000	3.23999500	2.94947400
H	6.56533600	1.63780100	2.89178100
H	2.87211900	0.99697600	2.26216800
H	4.27210200	0.43608700	3.19608800
H	3.60974900	2.05784600	3.47618300
C	-3.80932400	0.58351700	2.63184500
C	-3.45729100	-0.89746500	2.86760600
C	-4.83111900	1.08626700	3.66777300
H	-2.88724700	1.15007600	2.78021400
H	-2.58735500	-1.17025100	2.26752200
H	-3.20445300	-1.06701200	3.92030700
H	-4.28691700	-1.56221800	2.60502100
H	-5.06931800	2.14317200	3.50992800
H	-5.76997300	0.52466300	3.61233000
H	-4.43595600	0.97374100	4.68319100
C	-3.35262800	2.61522300	-2.09983800
C	-4.25125700	3.75494400	-2.61517900
C	-2.84087400	1.73474300	-3.25486300
H	-2.48129000	3.08996400	-1.64485700
H	-4.59714800	4.38747700	-1.79112800
H	-3.69886400	4.38409500	-3.32154300
H	-5.13489100	3.37072800	-3.13562300
H	-2.16236500	0.96351300	-2.88373500
H	-3.66964300	1.24413800	-3.77698400
H	-2.29844100	2.34472400	-3.98558400
C	-7.38711300	-0.14125700	-0.84657500
C	-7.51490500	-0.65540200	-2.28926600
C	-8.44112300	0.94788800	-0.56056700
H	-7.59779200	-0.97763900	-0.16759100
H	-6.72316500	-1.36827600	-2.53189600
H	-8.48640500	-1.14109200	-2.43228700
H	-7.46052500	0.16810500	-3.00938900
H	-8.39311700	1.28121000	0.48083800
H	-8.26838400	1.82116100	-1.19924800
H	-9.45255600	0.57555200	-0.75887200
C	3.58464800	-2.64884100	1.56302600
C	0.79079500	-5.01638800	0.21222600
C	2.06755200	-2.39011500	1.69882500
H	4.08355200	-1.80298500	1.09361300
H	0.47544700	-5.22528900	1.23441700
H	4.02556200	-2.80030500	2.55450000
H	0.14490600	-5.56572100	-0.46979900
C	3.82522400	-3.86280100	0.69223300
O	4.57055800	-3.93422300	-0.25332300
C	0.60970400	-3.53211600	-0.10061800

O	0.34877900	-3.31291700	-1.38073200
O	3.00992300	-4.89465800	1.07065600
O	1.51113800	-2.63032800	0.35316200
O	-0.79786200	-3.07092800	0.77760700
H	-0.68674500	-1.96534000	0.86380800
O	-4.89426300	-3.08669100	0.14782700
C	-6.25745900	-3.55800400	-0.06603400
H	-6.74026200	-2.87209300	-0.76351900
C	-6.92795500	-3.50669900	1.29695400
H	-6.91558900	-2.49093900	1.69890500
H	-7.96815000	-3.83616700	1.21655300
H	-6.41001700	-4.16295000	2.00342600
C	-4.19716500	-2.65990400	-0.93390900
O	-4.66515800	-2.56129200	-2.04667600
C	-6.22726600	-4.95736300	-0.67066900
H	-5.70264800	-4.94678000	-1.62837000
H	-5.73151500	-5.65988800	0.00754800
H	-7.24831400	-5.31201900	-0.84242900
C	-2.17695500	-3.39871500	0.39827300
H	-2.72357800	-3.34149000	1.34279500
C	-0.10398700	3.20335100	0.48571600
C	-0.29140300	4.19497100	1.50611800
C	4.32353500	-0.29870300	-1.51443100
C	3.38683200	-0.42873600	-2.70928800
C	3.01240200	-1.88902000	-3.00779700
C	3.98730600	0.25055700	-3.95387600
H	2.45497600	0.08622300	-2.46016300
H	2.69154800	-2.40350600	-2.10083300
H	2.18990400	-1.92166700	-3.72891400
H	3.85185200	-2.44807700	-3.43558700
H	4.17055900	1.31445300	-3.77625700
H	4.94055500	-0.21653300	-4.22711800
H	3.30701700	0.16144700	-4.80800200
C	-2.76070900	-2.34844400	-0.56484900
H	-2.74774200	-1.35881500	-0.09749700
H	-2.17854700	-2.29161000	-1.48541300
C	-2.29519200	-4.81489100	-0.14826500
H	-3.35224900	-5.05249000	-0.27342900
H	-1.80464400	-4.90489300	-1.11987100
H	-1.87708100	-5.54375700	0.54823000
C	2.22988000	-5.51412500	0.02208500
O	-0.54558700	-0.65936300	0.94447400
O	0.24741000	-0.73468600	-1.54426600
H	0.36236700	-2.30559700	-1.54058500
C	6.05526000	-0.09843700	0.67548900
H	6.72042700	-0.03076800	1.52996400
C	2.34036400	-7.02342300	0.16620100
H	1.75275400	-7.52911800	-0.60592700
H	3.38500700	-7.32701900	0.06717400
H	1.97721200	-7.34321400	1.14807900
H	2.62716900	-5.19550200	-0.94656300
C	1.39822900	-3.10258400	2.86579000
H	1.80969300	-2.66957000	3.78340900
H	0.32195200	-2.93390900	2.86548100
H	1.60810700	-4.17152000	2.87323400
H	1.90530800	-1.31721200	1.81441600

²INT2

C	-0.62216400	6.10546900	3.58949700
C	-1.67098000	5.32305000	3.16544000
C	-1.49121900	4.35472800	2.14130100
C	0.86190100	5.02827200	2.00117300
C	0.65740400	5.94707400	3.00615800

H	-3.54919600	3.68801000	2.13286400
H	-0.76989900	6.83816500	4.37708900
H	-2.65490600	5.42584900	3.61520700
C	-2.56182900	3.53213500	1.70862000
H	1.84729400	4.91201700	1.56577900
H	1.48701100	6.55328000	3.35742500
C	-1.09003500	2.38637400	0.22064400
C	-2.38835400	2.53324200	0.77224000
C	1.22142700	3.13711100	-0.29511900
C	1.71713500	4.26080100	-1.04050700
C	1.93786900	1.95187200	-0.33303200
C	0.97482300	5.46195100	-1.21043800
C	2.99506700	4.15798900	-1.67628700
C	3.25046900	1.86039300	-0.86446400
C	1.48110000	6.50706700	-1.95009100
H	-0.00737700	5.54592500	-0.76128400
C	3.49448600	5.25969100	-2.42120700
C	3.74499900	2.96574200	-1.52669400
C	2.75675500	6.41256000	-2.55536000
H	0.89264700	7.41110800	-2.07491300
H	4.47016200	5.16850100	-2.89080700
H	4.75335700	2.92253200	-1.92778400
H	3.14476600	7.24689600	-3.13178900
O	1.39329300	0.80595100	0.26150600
O	-0.90455900	1.37142000	-0.71931600
P	0.05427000	0.11611900	-0.36506800
C	4.17240100	0.70851400	-0.60625300
C	5.02375900	0.77706800	0.52228500
C	5.32149500	-1.27729400	-1.35079800
C	6.20402700	-1.21072000	-0.27305900
H	5.42277300	-2.09735200	-2.05225700
C	-3.54825800	1.71805300	0.30041500
C	-4.03606700	1.89989000	-1.01615300
C	-4.22875900	0.85837800	1.19172400
C	-5.22808300	1.27285500	-1.38631500
C	-5.42242000	0.26149400	0.76858800
C	-5.95868500	0.47832500	-0.50144400
H	-5.60903100	1.43471400	-2.38896100
H	-5.96510900	-0.37277700	1.46330300
C	7.33054100	-2.22270800	-0.13232900
C	7.35172200	-2.90310600	1.24641700
C	8.68876900	-1.56449600	-0.44017900
H	7.15313900	-3.00667700	-0.87777300
H	6.40225900	-3.40571700	1.44255100
H	8.14950000	-3.65250500	1.29030900
H	7.53501000	-2.18180400	2.05043700
H	8.69224900	-1.11487200	-1.43811300
H	8.90797600	-0.77084200	0.28327800
H	9.50046300	-2.29898300	-0.39082800
C	4.81559500	1.83200000	1.60683900
C	6.11982800	2.33567500	2.24380000
C	3.85307800	1.29167900	2.68500300
H	4.33233100	2.69892400	1.14539400
H	6.83328700	2.66683700	1.48285600
H	5.91074900	3.17982800	2.90918500
H	6.60654900	1.56281400	2.84807100
H	2.89720700	0.99078500	2.24810900
H	4.29013900	0.41595600	3.17915500
H	3.65669700	2.05134300	3.45007200
C	-3.72855600	0.57465100	2.60744600
C	-3.45804900	-0.92444700	2.83304000
C	-4.70609600	1.12162300	3.66428700
H	-2.77436800	1.09021300	2.74243100

H	-2.64123000	-1.26193300	2.19340800
H	-3.16456900	-1.10579000	3.87286300
H	-4.33684000	-1.53952600	2.61593800
H	-4.88480300	2.19258100	3.52548300
H	-5.67610400	0.61573100	3.60846500
H	-4.30775200	0.97059200	4.67343400
C	-3.34289900	2.78885500	-2.04637100
C	-4.24802700	3.95399700	-2.48796000
C	-2.85636300	1.96477600	-3.25263400
H	-2.46105000	3.23946100	-1.58631100
H	-4.57262800	4.54857600	-1.62783900
H	-3.70993200	4.61359400	-3.17736000
H	-5.14469700	3.59575500	-3.00444800
H	-2.18176500	1.16754300	-2.93220000
H	-3.69686600	1.50918200	-3.78726500
H	-2.31843300	2.60625100	-3.95922700
C	-7.34178800	-0.04648600	-0.85734900
C	-7.45775500	-0.56735100	-2.29881600
C	-8.39569900	1.04587200	-0.58432800
H	-7.55807500	-0.87999900	-0.17671200
H	-6.67433000	-1.29411500	-2.52611500
H	-8.43432500	-1.03983400	-2.45149400
H	-7.38194300	0.25071400	-3.02319700
H	-8.35453100	1.38490200	0.45557700
H	-8.21811500	1.91551400	-1.22665800
H	-9.40613300	0.67371000	-0.78744500
C	3.46281700	-2.68208100	1.56975000
C	0.66565800	-5.10465800	0.29170600
C	1.93989000	-2.43406300	1.69112300
H	3.96037400	-1.83602600	1.09835100
H	0.38795800	-5.33063000	1.32290100
H	3.90319900	-2.82994900	2.56234700
H	0.02613000	-5.68935500	-0.36697100
C	3.70558900	-3.89750400	0.70163600
O	4.44835900	-3.96543800	-0.24789300
C	0.38605600	-3.61836000	-0.00992100
O	0.23142000	-3.48071700	-1.36508900
O	2.90678100	-4.93361800	1.09076100
O	1.39652500	-2.71659100	0.36118900
O	-0.80647100	-3.14578900	0.71487300
H	-0.62453500	-1.56259200	0.85482500
O	-4.90150900	-3.07760500	0.14232200
C	-6.28237200	-3.50769100	-0.04356700
H	-6.75643100	-2.81240200	-0.73829900
C	-6.92702300	-3.42593600	1.33046700
H	-6.88171400	-2.40756900	1.72349300
H	-7.97681400	-3.72834400	1.27129100
H	-6.41420000	-4.08957900	2.03368400
C	-4.20903200	-2.69206900	-0.95770100
O	-4.69568100	-2.58966900	-2.06254700
C	-6.30716200	-4.91237500	-0.63617300
H	-5.80224500	-4.92611500	-1.60426900
H	-5.81832200	-5.62326100	0.03814900
H	-7.34185800	-5.23718800	-0.78373700
C	-2.17435900	-3.49494500	0.33129000
H	-2.71096100	-3.42470600	1.28002600
C	-0.03812700	3.23929900	0.48891900
C	-0.20356500	4.21416000	1.52975600
C	4.29651300	-0.34313100	-1.53257100
C	3.35947500	-0.45382000	-2.72872600
C	2.91447100	-1.90055200	-2.99584800
C	3.99806200	0.17243100	-3.98205200
H	2.45337900	0.11317600	-2.49726700

H	2.55569200	-2.37573000	-2.08170600
H	2.10177800	-1.90911900	-3.72880300
H	3.73047500	-2.51065800	-3.39808200
H	4.23491800	1.22899000	-3.82147500
H	4.92779700	-0.34639000	-4.24205500
H	3.31824100	0.10256600	-4.83831900
C	-2.75461000	-2.43055800	-0.62168000
H	-2.70542100	-1.44099100	-0.15588500
H	-2.19338800	-2.39380300	-1.55556300
C	-2.35590600	-4.90734800	-0.21606800
H	-3.42361500	-5.09086200	-0.34689200
H	-1.86383300	-5.02433200	-1.18341700
H	-1.98259500	-5.65641500	0.48402300
C	2.10859400	-5.54959400	0.04913100
O	-0.55173300	-0.55786600	0.92745700
O	0.21111900	-0.72741100	-1.57623100
H	0.27617500	-2.51592100	-1.56833100
C	6.02696100	-0.18603400	0.66195600
H	6.68916800	-0.13671500	1.51988800
C	2.28124900	-7.05734800	0.14544000
H	1.69041900	-7.56361500	-0.62413300
H	3.33324600	-7.31843800	0.00844000
H	1.95887600	-7.41945400	1.12713700
H	2.46156600	-5.18830000	-0.92115900
C	1.28599900	-3.13129700	2.87994200
H	1.68760200	-2.67579200	3.79113000
H	0.20514200	-2.98886800	2.87445800
H	1.51503000	-4.19619600	2.90415500
H	1.78236200	-1.35849100	1.80669800

²INT3

C	-2.45960100	7.10836900	-1.90316700
C	-1.16853900	6.63564900	-1.87261200
C	-0.85937600	5.39081900	-1.26104700
C	-3.23338800	5.13902600	-0.71675700
C	-3.50188800	6.34104200	-1.33279100
H	1.22254400	5.41191100	-1.85123900
H	-2.68417700	8.05808100	-2.37920800
H	-0.36226300	7.19967400	-2.33389200
C	0.45262000	4.85500100	-1.32534000
H	-4.04503000	4.56018600	-0.29432500
H	-4.52554800	6.69931600	-1.38667800
C	-0.27540800	2.93232900	-0.10931200
C	0.75531500	3.61216800	-0.81413500
C	-2.58710700	2.56640000	0.72703000
C	-3.41325000	3.08393400	1.78322700
C	-2.74050800	1.23143400	0.38567300
C	-3.22684000	4.37601200	2.34636300
C	-4.45002100	2.25364700	2.32134400
C	-3.73060500	0.37251300	0.93432100
C	-4.04829700	4.83783100	3.35028300
H	-2.41963900	4.99896800	1.98049400
C	-5.29146200	2.76818300	3.34443400
C	-4.59599000	0.92192400	1.85603100
C	-5.10151900	4.03423100	3.84695000
H	-3.88202300	5.82597100	3.76870200
H	-6.08061000	2.13110400	3.73476100
H	-5.38509000	0.30457100	2.27370800
H	-5.74648800	4.41334300	4.63390500
O	-1.91770300	0.67514400	-0.59919900
O	0.07038600	1.72255600	0.50574200
P	-0.37294400	0.35791800	-0.24452900
C	-3.77716800	-1.06772800	0.53642800

C	-4.10027300	-1.42619000	-0.78991500
C	-3.45340600	-3.40643200	1.06415400
C	-3.77294500	-3.78307600	-0.24263000
H	-3.19282900	-4.18256900	1.77946400
C	2.05236500	2.91419100	-1.06516100
C	2.92950400	2.63501400	0.00603600
C	2.34502200	2.44198400	-2.36461500
C	4.06552500	1.85961500	-0.23319600
C	3.51087900	1.69055500	-2.55404200
C	4.37416200	1.37174300	-1.50703600
H	4.72483600	1.62346200	0.59475600
H	3.74863300	1.33057300	-3.55156600
C	-3.77379500	-5.25785100	-0.62399200
C	-3.67985400	-5.49982400	-2.13639400
C	-5.00781000	-5.96848000	-0.03407200
H	-2.88399400	-5.70728900	-0.15839500
H	-2.86206700	-4.92287400	-2.57720100
H	-3.51692000	-6.56226300	-2.34312600
H	-4.60771600	-5.20956100	-2.64155400
H	-5.05721700	-5.84520000	1.05209800
H	-5.92604600	-5.54821200	-0.45913400
H	-4.98839700	-7.04108800	-0.25807800
C	-4.46857200	-0.40154800	-1.85885200
C	-5.95241500	-0.53039900	-2.25164200
C	-3.55144100	-0.50643300	-3.09176400
H	-4.33985500	0.59986100	-1.44085500
H	-6.60424300	-0.40583100	-1.38062000
H	-6.22209500	0.22953800	-2.99350000
H	-6.16215200	-1.51310700	-2.68796200
H	-2.49961700	-0.47726400	-2.80281400
H	-3.71826500	-1.44253200	-3.63490000
H	-3.75446000	0.31927700	-3.78300100
C	1.45857200	2.73353500	-3.57404600
C	1.06213800	1.46464100	-4.34717300
C	2.13857500	3.75942200	-4.50042200
H	0.52808200	3.18146100	-3.21810800
H	0.54128300	0.77302100	-3.68408500
H	0.39753600	1.72346000	-5.17877700
H	1.93277300	0.95210600	-4.77091300
H	2.37358600	4.68570000	-3.96571000
H	3.07811600	3.36260700	-4.90079500
H	1.48902700	4.00808400	-5.34694800
C	2.69670200	3.21404400	1.39807500
C	3.75602700	4.28833200	1.71126100
C	2.66858200	2.13696900	2.49097300
H	1.72344200	3.71282300	1.40286400
H	3.75231000	5.07993100	0.95521100
H	3.56809800	4.74493600	2.68935500
H	4.76125200	3.85195500	1.73073500
H	1.92118500	1.37186800	2.26995700
H	3.64296800	1.65286100	2.58581700
H	2.42655400	2.57705700	3.46386000
C	5.62176600	0.53769500	-1.75348900
C	5.60490000	-0.76706000	-0.93788400
C	6.90172400	1.34821900	-1.47944000
H	5.62304700	0.26560900	-2.81763800
H	4.68431700	-1.32557500	-1.12367700
H	6.46345300	-1.39587900	-1.20202500
H	5.65609100	-0.56424500	0.13516900
H	6.93241500	2.26092000	-2.08300300
H	6.95867900	1.64229400	-0.42591300
H	7.79336600	0.75376400	-1.70799100
C	1.05360300	-2.32679500	-3.51039300

C	1.02264100	-5.31082500	-0.14872400
C	2.46336000	-2.10779100	-2.89931400
H	0.54848500	-1.37182600	-3.64643800
H	1.97674700	-5.70163100	-0.51119700
H	1.14942200	-2.80494000	-4.49320400
H	0.63068400	-6.03859400	0.57447200
C	0.12043400	-3.16224100	-2.66170300
O	-1.01708500	-2.85801800	-2.37319500
C	1.26702200	-4.03761000	0.63446600
O	0.43235300	-3.15652300	0.76714500
O	0.70992100	-4.32195300	-2.27663000
O	2.38886600	-1.88838100	-1.49359500
O	2.45899600	-4.08064400	1.22513500
H	1.81558900	-1.10752600	-1.36561600
O	4.92625400	-0.61852700	2.48437500
C	5.84639700	-0.01318900	3.44698400
H	5.25960000	0.64495900	4.09432500
C	6.84847000	0.78731100	2.63128000
H	6.35210900	1.58563500	2.07388000
H	7.58765800	1.24366600	3.29642400
H	7.37288800	0.14293500	1.91952900
C	3.70653100	-0.96966100	2.94629300
O	3.33287900	-0.75776100	4.08281300
C	6.48296900	-1.12086800	4.27786000
H	5.71612200	-1.66460800	4.83388600
H	7.02182500	-1.81941600	3.62973800
H	7.19187600	-0.69539100	4.99483200
C	2.81146100	-3.19188700	2.33349800
H	3.82738700	-3.53364800	2.55445600
C	-1.57374600	3.39623900	0.01559900
C	-1.90548600	4.63754900	-0.63265300
C	-3.45032200	-2.07281500	1.48088100
C	-3.12260600	-1.76134900	2.94072300
C	-1.83243300	-2.43936400	3.43074700
C	-4.30770600	-2.14195800	3.84926900
H	-2.96286100	-0.68453300	3.03420100
H	-0.98794200	-2.15312800	2.80481700
H	-1.61518200	-2.13401300	4.45996400
H	-1.91026700	-3.53174000	3.42192100
H	-5.22849800	-1.63555900	3.54385200
H	-4.49712600	-3.22037900	3.80571300
H	-4.10072800	-1.87581500	4.89179300
C	2.88871000	-1.71234800	1.90785600
H	3.33645700	-1.63675300	0.91576500
H	1.89274500	-1.26975800	1.88613200
C	1.90627100	-3.47167500	3.52666700
H	2.23233500	-2.87342400	4.37865000
H	0.87403100	-3.20454500	3.29843100
H	1.95126900	-4.53238700	3.78959600
C	0.03611500	-5.14638200	-1.29723200
O	0.37508600	-0.02388400	-1.46496100
O	-0.30946500	-0.63539100	0.98260300
H	-0.08328500	-1.57460600	0.75818300
C	-4.10404000	-2.77681900	-1.14634900
H	-4.34696500	-3.03548600	-2.16954100
C	-0.31638000	-6.47470400	-1.95189400
H	-0.85525900	-7.11836100	-1.24934600
H	-0.95459500	-6.30787900	-2.82106200
H	0.58864000	-6.99542200	-2.28045700
H	-0.85786300	-4.61919400	-0.95650800
H	2.87216800	-1.20955100	-3.39018000
C	3.43318900	-3.26061700	-3.13307300
H	3.54140200	-3.46245500	-4.20375800

H	4.41594600	-3.00554100	-2.72806200
H	3.07447500	-4.16552200	-2.64100500
S-Chain- (R, R)-DL			
³INT1			
C	-0.28267500	7.34893700	-1.92876500
C	0.85015800	6.59403100	-1.73482000
C	0.78756000	5.33972800	-1.06962200
C	-1.62547600	5.66641300	-0.80933000
C	-1.53322600	6.86955100	-1.47255500
H	2.88220200	4.87877600	-1.34499700
H	-0.22383900	8.30292100	-2.44398100
H	1.81340300	6.93718000	-2.10276500
C	1.93876500	4.52267900	-0.94274900
H	-2.59186700	5.31139600	-0.47349700
H	-2.43097800	7.45359400	-1.65192200
C	0.64406600	2.85728200	0.17255500
C	1.88594200	3.26559500	-0.37765500
C	-1.76170300	3.10486900	0.75801800
C	-2.50333100	3.87473900	1.71853300
C	-2.25138000	1.85518400	0.40742700
C	-2.00334600	5.07562600	2.29280400
C	-3.78609000	3.40293100	2.14462700
C	-3.53559500	1.38276800	0.78828800
C	-2.74570400	5.78421900	3.21061500
H	-1.01868700	5.42640100	2.00813700
C	-4.53422500	4.16712800	3.07993400
C	-4.28476800	2.18227900	1.62510200
C	-4.02936500	5.33519100	3.60166300
H	-2.33938400	6.69367800	3.64293100
H	-5.51059900	3.80085100	3.38569300
H	-5.28582800	1.86402600	1.89888900
H	-4.60626200	5.90746400	4.32185600
O	-1.49600700	1.02715400	-0.43080700
O	0.61290900	1.63446500	0.83898000
P	-0.12392700	0.36844100	0.14892400
C	-4.11397900	0.11792300	0.23397800
C	-4.61836200	0.11019900	-1.08375000
C	-4.89973800	-2.14720600	0.53650900
C	-5.44337100	-2.16779800	-0.75242000
H	-4.98741200	-3.04156600	1.14506600
C	3.07764600	2.36256400	-0.40630700
C	3.80096200	2.07395000	0.76732400
C	3.50797700	1.83530500	-1.64831500
C	4.98501600	1.33165000	0.66994000
C	4.69593400	1.10248500	-1.68916200
C	5.46898500	0.85467400	-0.54791600
H	5.52726200	1.11845300	1.58155600
H	5.02774100	0.70904700	-2.64510100
C	-6.22316200	-3.39767100	-1.20343400
C	-6.28081000	-3.58232200	-2.72598100
C	-7.64650800	-3.36288800	-0.61140900
H	-5.71019200	-4.26961400	-0.77603000
H	-5.28357800	-3.55794300	-3.17715600
H	-6.74280700	-4.54330400	-2.97329700
H	-6.88204400	-2.80079500	-3.20355700
H	-7.61685200	-3.28398100	0.47931000
H	-8.20004400	-2.49845300	-0.99532600
H	-8.20248300	-4.26945800	-0.87517700
C	-4.48988700	1.31625500	-2.01160300
C	-5.85859500	1.78793000	-2.53451000
C	-3.51641800	1.02694900	-3.16925100
H	-4.07017900	2.14647200	-1.43716700
H	-6.54383000	2.00046100	-1.70779400

H	-5.74500600	2.70077300	-3.12915900
H	-6.33027300	1.03465400	-3.17434400
H	-2.52298500	0.78028400	-2.78665600
H	-3.86943600	0.18825900	-3.78004000
H	-3.42470200	1.90197000	-3.82222100
C	2.72056400	2.04025100	-2.94235500
C	2.41656400	0.71328200	-3.66025500
C	3.44756100	3.01609000	-3.88578500
H	1.75570900	2.48447700	-2.68443800
H	1.89903300	0.02341500	-2.99146500
H	1.77503700	0.89742700	-4.52922800
H	3.32807800	0.22902200	-4.02699200
H	3.61070100	3.98800800	-3.41046800
H	4.42741600	2.62025300	-4.17538300
H	2.86557100	3.17803200	-4.79976100
C	3.35055100	2.54092600	2.14783700
C	4.40905000	3.43769400	2.81625000
C	2.98613600	1.34012200	3.04304300
H	2.44914600	3.14910300	2.02900000
H	4.66102100	4.29343700	2.18128400
H	4.03628000	3.81857500	3.77323200
H	5.33343900	2.88641100	3.01794300
H	2.15115700	0.78064900	2.61578900
H	3.82647500	0.64882800	3.15440600
H	2.68772900	1.68666600	4.03895000
C	6.76872600	0.05876400	-0.66578700
C	7.52931500	-0.08962500	0.65883600
C	7.70400200	0.66272600	-1.73216400
H	6.49162800	-0.95156000	-1.00210200
H	6.90922600	-0.53595100	1.43864000
H	8.41015400	-0.72447800	0.51625000
H	7.87825500	0.88460200	1.02004100
H	7.23201900	0.71983700	-2.71644900
H	8.00163100	1.67742400	-1.44561900
H	8.61203600	0.05821500	-1.83268800
C	-2.69762700	-4.23072400	-1.62179100
C	0.44045700	-4.96073400	0.20091800
C	-1.36743300	-3.47204100	-1.71111200
H	-3.51578300	-3.53113600	-1.46243100
H	-0.56734700	-4.11932000	-2.06966000
H	0.79581900	-5.06565000	-0.82407100
H	-2.86058700	-4.76340600	-2.56554600
H	1.29465100	-5.06563700	0.87260500
C	-2.68270000	-5.21593500	-0.47704900
O	-3.51175000	-5.28428000	0.39782800
C	-0.09141000	-3.56225900	0.42439800
O	0.22475000	-2.93297800	1.43556600
O	-1.58253900	-6.02751300	-0.55846600
O	-1.01622100	-3.01143700	-0.36172800
C	-1.15824700	-6.01446100	1.92098300
H	-1.91240700	-6.79043200	2.05813600
H	-0.33789900	-6.17794200	2.62680600
H	-1.61760900	-5.05204700	2.15109900
C	-1.48556000	-2.22334100	-2.56673900
H	-1.80913600	-2.50102800	-3.57499600
H	-2.22852200	-1.54655400	-2.13701300
H	-0.53123900	-1.70143100	-2.62398000
O	1.69900400	-2.76287700	-1.31778100
H	1.39325300	-1.83502600	-1.24797600
O	5.32156200	-3.16203600	0.63138800
C	6.50704900	-3.56412100	1.37731900
H	6.88681500	-2.68734100	1.90600100
C	7.50947900	-4.03568200	0.33630100

H	7.74513300	-3.22771000	-0.36207700
H	8.43588300	-4.35539000	0.82295500
H	7.10694600	-4.87967800	-0.23266500
C	4.53051200	-2.20171800	1.16350000
O	4.79079000	-1.61744700	2.19667200
C	6.10627600	-4.63501100	2.38408000
H	5.37575300	-4.23183300	3.08970600
H	5.66882500	-5.49728200	1.87051600
H	6.98128200	-4.97334800	2.94787900
C	-0.50988000	3.61985200	0.13730800
C	-0.47006500	4.87429500	-0.56402300
C	-4.23058600	-1.03229800	1.04640300
C	-3.66030600	-1.08050400	2.46077500
C	-2.91383800	-2.39577500	2.74079400
C	-4.76267200	-0.85717500	3.51275100
H	-2.92995400	-0.27149900	2.55382800
H	-2.20113400	-2.60881900	1.94542400
H	-2.36506200	-2.32491000	3.68532500
H	-3.59776800	-3.24756300	2.81624000
H	-5.25116500	0.11296200	3.38724900
H	-5.53231000	-1.63321600	3.43331700
H	-4.34406700	-0.89651600	4.52441900
C	3.28093700	-1.95586500	0.34643200
H	3.27462300	-0.89403800	0.07507900
H	2.44435600	-2.09985500	1.03727700
C	-0.59399300	-6.06522300	0.50528400
H	-0.09611500	-7.02673200	0.35026300
O	0.62406600	-0.28192900	-0.95738300
O	-0.48245600	-0.46923900	1.42132700
H	-0.22915900	-1.45435100	1.40844200
C	-5.26971500	-1.03804000	-1.55323300
H	-5.65743800	-1.03560700	-2.56633100
C	3.06378700	-2.83873200	-0.89593200
H	3.22429900	-3.88522600	-0.60962700
C	3.98994100	-2.49652400	-2.06105300
H	3.86870800	-1.44688200	-2.33850000
H	5.03486600	-2.67303300	-1.79631200
H	3.73342400	-3.11431000	-2.92637700

³TS1

C	-0.25275500	7.23521700	-2.04925200
C	0.88294800	6.48022700	-1.87286500
C	0.83732000	5.24427000	-1.17318300
C	-1.56326100	5.58799100	-0.84203600
C	-1.48894500	6.77286600	-1.53963700
H	2.91887700	4.76390000	-1.50578900
H	-0.20763300	8.17519400	-2.59102400
H	1.83496700	6.80898700	-2.28126200
C	1.98745100	4.42374500	-1.06333300
H	-2.51954200	5.24649300	-0.46597300
H	-2.39040500	7.35550000	-1.70476900
C	0.72326400	2.78866800	0.14233600
C	1.94541200	3.18275500	-0.46429400
C	-1.66194800	3.07524400	0.79160500
C	-2.37218000	3.87838300	1.74794700
C	-2.17496700	1.82538700	0.47419700
C	-1.83934700	5.08086900	2.28837900
C	-3.65705300	3.44202000	2.20344700
C	-3.47027000	1.39826300	0.87333300
C	-2.55121700	5.82213000	3.20458000
H	-0.85327900	5.40593500	1.97857900
C	-4.37318200	4.23865100	3.13652700
C	-4.19070000	2.22629300	1.70734900

C	-3.83614100	5.40610200	3.62695100
H	-2.11992200	6.73202000	3.61120400
H	-5.35157900	3.89847900	3.46536600
H	-5.19776800	1.93798200	1.99298500
H	-4.38890400	6.00350500	4.34575600
O	-1.44224600	0.96797400	-0.34614300
O	0.71443100	1.59257900	0.84615800
P	-0.07654900	0.28867600	0.26437700
C	-4.09525100	0.15383600	0.32432500
C	-4.68767300	0.19199700	-0.95519400
C	-4.85280900	-2.12230900	0.60086300
C	-5.47633200	-2.10211100	-0.65201000
H	-4.89679800	-3.03817500	1.18121500
C	3.13163400	2.27415500	-0.50357900
C	3.89782800	2.03799200	0.65413300
C	3.50629600	1.68224300	-1.73445700
C	5.05972000	1.26102700	0.55351600
C	4.66689600	0.90632400	-1.77711200
C	5.47454000	0.69509900	-0.65203500
H	5.63619200	1.09032000	1.45328200
H	4.95401300	0.45468100	-2.72230800
C	-6.26962400	-3.32476000	-1.09896300
C	-6.40928900	-3.46101900	-2.62136000
C	-7.65822600	-3.32474600	-0.42891900
H	-5.72500200	-4.20399000	-0.73047700
H	-5.43797100	-3.41251600	-3.12440400
H	-6.87599300	-4.41834200	-2.87433500
H	-7.04183200	-2.67075100	-3.04066700
H	-7.56861400	-3.28041100	0.66049700
H	-8.24044100	-2.45462100	-0.75312100
H	-8.21972300	-4.22858500	-0.69074600
C	-4.60607700	1.42970500	-1.84622300
C	-5.98456900	1.86563700	-2.37264800
C	-3.61031000	1.21212300	-3.00133600
H	-4.22366800	2.25697000	-1.24171100
H	-6.69278200	2.01182700	-1.55098100
H	-5.89897900	2.80841900	-2.92361400
H	-6.41343500	1.12533800	-3.05629800
H	-2.61021300	0.99778500	-2.61639400
H	-3.92393900	0.37266100	-3.63264100
H	-3.55104800	2.10539700	-3.63323500
C	2.70539100	1.89372200	-3.01955800
C	2.32872500	0.57683400	-3.71884900
C	3.46382700	2.82466500	-3.98433000
H	1.76556600	2.38385700	-2.75477100
H	1.75310400	-0.05893800	-3.04408800
H	1.71379200	0.78602400	-4.60119900
H	3.21155200	0.02659000	-4.06328700
H	3.68691100	3.78915000	-3.51849600
H	4.41616500	2.37676700	-4.28982700
H	2.87293500	3.01168400	-4.88773000
C	3.51675000	2.60994800	2.01602100
C	4.62661600	3.51882500	2.57605500
C	3.15343000	1.49039900	3.01012200
H	2.62913000	3.23572900	1.88676800
H	4.87591700	4.31984300	1.87234000
H	4.30406500	3.97721800	3.51708800
H	5.54298700	2.95515300	2.78092800
H	2.29314600	0.92141400	2.65100600
H	3.98226300	0.79128000	3.15213100
H	2.89313600	1.92051000	3.98385000
C	6.74250400	-0.14913800	-0.77754600
C	7.52752800	-0.29292900	0.53307000

C	7.67350700	0.39705500	-1.87846100
H	6.42274800	-1.15710200	-1.08403500
H	6.90662200	-0.67913800	1.34383300
H	8.37295100	-0.97450700	0.39233500
H	7.93247700	0.67393200	0.85270400
H	7.17881900	0.45174900	-2.85172100
H	8.01325400	1.40607000	-1.62055300
H	8.55705600	-0.24145600	-1.98731600
C	-2.73258500	-4.05447300	-1.73644400
C	0.53524100	-4.92110000	-0.06126100
C	-1.40385700	-3.29170200	-1.81948800
H	-3.54629400	-3.36646900	-1.51307600
H	-0.63033100	-3.91446800	-2.27216100
H	0.85210600	-5.09403900	-1.09074900
H	-2.93076900	-4.53404000	-2.70182500
H	1.39060600	-5.09342900	0.59549100
C	-2.68421300	-5.10048300	-0.64734000
O	-3.51607800	-5.25808100	0.21225500
C	0.13135500	-3.46150000	0.11844700
O	0.29070400	-3.03364100	1.34901600
O	-1.55494400	-5.86501700	-0.77201200
O	-1.00605900	-2.98951400	-0.43956900
C	-1.11031200	-5.84497000	1.70600100
H	-1.88602700	-6.59486400	1.86456200
H	-0.28656700	-6.02000800	2.40491600
H	-1.53135300	-4.86433000	1.92098600
C	-1.56057400	-1.97359200	-2.55794800
H	-1.97335300	-2.15921500	-3.55486700
H	-2.25061700	-1.32592600	-2.01162000
H	-0.60823100	-1.45345800	-2.65359500
O	1.31314900	-2.64337000	-0.88047800
H	1.01243400	-1.60078500	-0.90858500
O	5.06298300	-3.11768300	0.75854600
C	6.24867500	-3.61582300	1.44871600
H	6.72533800	-2.77061300	1.94919500
C	7.15357100	-4.17506300	0.36322100
H	7.42181800	-3.39385500	-0.35334600
H	8.07278300	-4.56908100	0.80677600
H	6.65416400	-4.98614400	-0.17622700
C	4.37700200	-2.09819000	1.32715900
O	4.73860600	-1.52610200	2.33366800
C	5.80911600	-4.64393000	2.48305100
H	5.14931300	-4.17903700	3.21963100
H	5.27863400	-5.47057100	1.99929500
H	6.67964300	-5.05013700	3.00728400
C	-0.42464600	3.56202300	0.12340300
C	-0.40333100	4.79700400	-0.61324600
C	-4.15495800	-1.02185100	1.10352300
C	-3.48852500	-1.10107900	2.47296500
C	-2.79753900	-2.45342800	2.70502300
C	-4.49691600	-0.81106900	3.60007300
H	-2.70577600	-0.33785100	2.50515800
H	-2.18251500	-2.71502200	1.84513600
H	-2.15331900	-2.40100500	3.58831000
H	-3.51850400	-3.26223100	2.86621100
H	-4.92993600	0.18847200	3.50724500
H	-5.31730600	-1.53758800	3.57822200
H	-4.00949000	-0.87818000	4.57902900
C	3.10418100	-1.76543000	0.57493400
H	3.20264800	-0.74801600	0.18405100
H	2.31578000	-1.73189200	1.32871700
C	-0.56482400	-5.94375900	0.28669800
H	-0.12102600	-6.93456200	0.14624700

O	0.65691400	-0.28809700	-0.93735700
O	-0.33247300	-0.60627800	1.44982300
H	-0.03211300	-2.04804100	1.43278900
C	-5.36233800	-0.94376500	-1.42230600
H	-5.81259800	-0.91091300	-2.40852400
C	2.72882800	-2.75159700	-0.54226100
H	2.87225400	-3.77105500	-0.18128800
C	3.51187200	-2.55647100	-1.83275600
H	3.37408900	-1.54127300	-2.20719500
H	4.57498700	-2.71851000	-1.64573000
H	3.17060500	-3.26444700	-2.59290500

³INT2

C	-0.62216400	6.10546900	3.58949700
C	-1.67098000	5.32305000	3.16544000
C	-1.49121900	4.35472800	2.14130100
C	0.86190100	5.02827200	2.00117300
C	0.65740400	5.94707400	3.00615800
H	-3.54919600	3.68801000	2.13286400
H	-0.76989900	6.83816500	4.37708900
H	-2.65490600	5.42584900	3.61520700
C	-2.56182900	3.53213500	1.70862000
H	1.84729400	4.91201700	1.56577900
H	1.48701100	6.55328000	3.35742500
C	-1.09003500	2.38637400	0.22064400
C	-2.38835400	2.53324200	0.77224000
C	1.22142700	3.13711100	-0.29511900
C	1.71713500	4.26080100	-1.04050700
C	1.93786900	1.95187200	-0.33303200
C	0.97482300	5.46195100	-1.21043800
C	2.99506700	4.15798900	-1.67628700
C	3.25046900	1.86039300	-0.86446400
C	1.48110000	6.50706700	-1.95009100
H	-0.00737700	5.54592500	-0.76128400
C	3.49448600	5.25969100	-2.42120700
C	3.74499900	2.96574200	-1.52669400
C	2.75675500	6.41256000	-2.55536000
H	0.89264700	7.41110800	-2.07491300
H	4.47016200	5.16850100	-2.89080700
H	4.75335700	2.92253200	-1.92778400
H	3.14476600	7.24689600	-3.13178900
O	1.39329300	0.80595100	0.26150600
O	-0.90455900	1.37142000	-0.71931600
P	0.05427000	0.11611900	-0.36506800
C	4.17240100	0.70851400	-0.60625300
C	5.02375900	0.77706800	0.52228500
C	5.32149500	-1.27729400	-1.35079800
C	6.20402700	-1.21072000	-0.27305900
H	5.42277300	-2.09735200	-2.05225700
C	-3.54825800	1.71805300	0.30041500
C	-4.03606700	1.89989000	-1.01615300
C	-4.22875900	0.85837800	1.19172400
C	-5.22808300	1.27285500	-1.38631500
C	-5.42242000	0.26149400	0.76858800
C	-5.95868500	0.47832500	-0.50144400
H	-5.60903100	1.43471400	-2.38896100
H	-5.96510900	-0.37277700	1.46330300
C	7.33054100	-2.22270800	-0.13232900
C	7.35172200	-2.90310600	1.24641700
C	8.68876900	-1.56449600	-0.44017900
H	7.15313900	-3.00667700	-0.87777300
H	6.40225900	-3.40571700	1.44255100
H	8.14950000	-3.65250500	1.29030900

H	7.53501000	-2.18180400	2.05043700
H	8.69224900	-1.11487200	-1.43811300
H	8.90797600	-0.77084200	0.28327800
H	9.50046300	-2.29898300	-0.39082800
C	4.81559500	1.83200000	1.60683900
C	6.11982800	2.33567500	2.24380000
C	3.85307800	1.29167900	2.68500300
H	4.33233100	2.69892400	1.14539400
H	6.83328700	2.66683700	1.48285600
H	5.91074900	3.17982800	2.90918500
H	6.60654900	1.56281400	2.84807100
H	2.89720700	0.99078500	2.24810900
H	4.29013900	0.41595600	3.17915500
H	3.65669700	2.05134300	3.45007200
C	-3.72855600	0.57465100	2.60744600
C	-3.45804900	-0.92444700	2.83304000
C	-4.70609600	1.12162300	3.66428700
H	-2.77436800	1.09021300	2.74243100
H	-2.64123000	-1.26193300	2.19340800
H	-3.16456900	-1.10579000	3.87286300
H	-4.33684000	-1.53952600	2.61593800
H	-4.88480300	2.19258100	3.52548300
H	-5.67610400	0.61573100	3.60846500
H	-4.30775200	0.97059200	4.67343400
C	-3.34289900	2.78885500	-2.04637100
C	-4.24802700	3.95399700	-2.48796000
C	-2.85636300	1.96477600	-3.25263400
H	-2.46105000	3.23946100	-1.58631100
H	-4.57262800	4.54857600	-1.62783900
H	-3.70993200	4.61359400	-3.17736000
H	-5.14469700	3.59575500	-3.00444800
H	-2.18176500	1.16754300	-2.93220000
H	-3.69686600	1.50918200	-3.78726500
H	-2.31843300	2.60625100	-3.95922700
C	-7.34178800	-0.04648600	-0.85734900
C	-7.45775500	-0.56735100	-2.29881600
C	-8.39569900	1.04587200	-0.58432800
H	-7.55807500	-0.87999900	-0.17671200
H	-6.67433000	-1.29411500	-2.52611500
H	-8.43432500	-1.03983400	-2.45149400
H	-7.38194300	0.25071400	-3.02319700
H	-8.35453100	1.38490200	0.45557700
H	-8.21811500	1.91551400	-1.22665800
H	-9.40613300	0.67371000	-0.78744500
C	3.46281700	-2.68208100	1.56975000
C	0.66565800	-5.10465800	0.29170600
C	1.93989000	-2.43406300	1.69112300
H	3.96037400	-1.83602600	1.09835100
H	0.38795800	-5.33063000	1.32290100
H	3.90319900	-2.82994900	2.56234700
H	0.02613000	-5.68935500	-0.36697100
C	3.70558900	-3.89750400	0.70163600
O	4.44835900	-3.96543800	-0.24789300
C	0.38605600	-3.61836000	-0.00992100
O	0.23142000	-3.48071700	-1.36508900
O	2.90678100	-4.93361800	1.09076100
O	1.39652500	-2.71659100	0.36118900
O	-0.80647100	-3.14578900	0.71487300
H	-0.62453500	-1.56259200	0.85482500
O	-4.90150900	-3.07760500	0.14232200
C	-6.28237200	-3.50769100	-0.04356700
H	-6.75643100	-2.81240200	-0.73829900
C	-6.92702300	-3.42593600	1.33046700

H	-6.88171400	-2.40756900	1.72349300
H	-7.97681400	-3.72834400	1.27129100
H	-6.41420000	-4.08957900	2.03368400
C	-4.20903200	-2.69206900	-0.95770100
O	-4.69568100	-2.58966900	-2.06254700
C	-6.30716200	-4.91237500	-0.63617300
H	-5.80224500	-4.92611500	-1.60426900
H	-5.81832200	-5.62326100	0.03814900
H	-7.34185800	-5.23718800	-0.78373700
C	-2.17435900	-3.49494500	0.33129000
H	-2.71096100	-3.42470600	1.28002600
C	-0.03812700	3.23929900	0.48891900
C	-0.20356500	4.21416000	1.52975600
C	4.29651300	-0.34313100	-1.53257100
C	3.35947500	-0.45382000	-2.72872600
C	2.91447100	-1.90055200	-2.99584800
C	3.99806200	0.17243100	-3.98205200
H	2.45337900	0.11317600	-2.49726700
H	2.55569200	-2.37573000	-2.08170600
H	2.10177800	-1.90911900	-3.72880300
H	3.73047500	-2.51065800	-3.39808200
H	4.23491800	1.22899000	-3.82147500
H	4.92779700	-0.34639000	-4.24205500
H	3.31824100	0.10256600	-4.83831900
C	-2.75461000	-2.43055800	-0.62168000
H	-2.70542100	-1.44099100	-0.15588500
H	-2.19338800	-2.39380300	-1.55556300
C	-2.35590600	-4.90734800	-0.21606800
H	-3.42361500	-5.09086200	-0.34689200
H	-1.86383300	-5.02433200	-1.18341700
H	-1.98259500	-5.65641500	0.48402300
C	2.10859400	-5.54959400	0.04913100
O	-0.55173300	-0.55786600	0.92745700
O	0.21111900	-0.72741100	-1.57623100
H	0.27617500	-2.51592100	-1.56833100
C	6.02696100	-0.18603400	0.66195600
H	6.68916800	-0.13671500	1.51988800
C	2.28124900	-7.05734800	0.14544000
H	1.69041900	-7.56361500	-0.62413300
H	3.33324600	-7.31843800	0.00844000
H	1.95887600	-7.41945400	1.12713700
H	2.46156600	-5.18830000	-0.92115900
C	1.28599900	-3.13129700	2.87994200
H	1.68760200	-2.67579200	3.79113000
H	0.20514200	-2.98886800	2.87445800
H	1.51503000	-4.19619600	2.90415500
H	1.78236200	-1.35849100	1.80669800

³INT3

C	1.81287700	7.05992100	-2.12907400
C	2.67497600	6.04366600	-1.78992200
C	2.20287300	4.87163500	-1.13932900
C	-0.05337800	5.82484200	-1.19305700
C	0.43325000	6.93931500	-1.83855900
H	4.12513400	3.88229000	-1.11676700
H	2.18399600	7.94742000	-2.63265600
H	3.73260300	6.11231000	-2.02988100
C	3.07565300	3.79126900	-0.85552400
H	-1.11293600	5.74261000	-0.98348200
H	-0.24953800	7.73076900	-2.13273000
C	1.25339600	2.55270900	0.05875800
C	2.62272700	2.60895700	-0.30894000
C	-1.04510800	3.44494900	0.37469100

C	-1.64164400	4.39948100	1.26900600
C	-1.78712900	2.32777000	0.02202100
C	-0.92464100	5.49241800	1.82992400
C	-3.01447800	4.23130000	1.64294900
C	-3.11964000	2.09407900	0.45751600
C	-1.54436600	6.39349800	2.66638600
H	0.12648000	5.61055100	1.59806300
C	-3.62876500	5.18932300	2.49411700
C	-3.72020900	3.08183900	1.20902900
C	-2.91416400	6.25331100	2.99196700
H	-0.97360200	7.21684700	3.08530100
H	-4.67379300	5.05214300	2.75880300
H	-4.74902600	2.94749500	1.52811200
H	-3.39158600	6.97562100	3.64716300
O	-1.22588500	1.38651400	-0.84539000
O	0.80533800	1.36869600	0.66376700
P	-0.05091700	0.39895000	-0.30589400
C	-3.81412300	0.79668500	0.18290800
C	-4.28302600	0.49122700	-1.11267800
C	-4.69598300	-1.31135500	0.97849900
C	-5.17551500	-1.63188600	-0.29218400
H	-4.87799600	-2.00524300	1.79509600
C	3.52550500	1.42979400	-0.13235200
C	3.91070500	1.01883300	1.16063500
C	4.01306200	0.74387500	-1.27105800
C	4.81945900	-0.03752900	1.29590100
C	4.91918600	-0.30125400	-1.07882000
C	5.35244800	-0.69833600	0.18923800
H	5.12382200	-0.33372100	2.29406100
H	5.31693500	-0.81892700	-1.94855100
C	-5.99823200	-2.89359700	-0.51604900
C	-5.42874900	-3.79914400	-1.62100300
C	-7.46704200	-2.53191200	-0.80914500
H	-5.97890900	-3.46627000	0.42125000
H	-4.42879400	-4.15622100	-1.36453700
H	-6.06969500	-4.67495300	-1.76920600
H	-5.37085600	-3.26911000	-2.57819800
H	-7.88572300	-1.91166600	-0.01092300
H	-7.54855300	-1.96909900	-1.74551900
H	-8.08083800	-3.43441600	-0.90377200
C	-4.14376100	1.47512600	-2.26961800
C	-5.52508200	1.95430100	-2.75365000
C	-3.31342800	0.89082800	-3.42237100
H	-3.61083300	2.35713000	-1.90313900
H	-6.09899400	2.39619700	-1.93282600
H	-5.41576000	2.70815500	-3.54087500
H	-6.11369000	1.12666300	-3.16414000
H	-2.31571000	0.62429700	-3.07361500
H	-3.78341600	-0.00748500	-3.83845600
H	-3.21416400	1.62057300	-4.23338400
C	3.61327800	1.12414700	-2.69634300
C	3.14474500	-0.08096500	-3.52885700
C	4.76793100	1.85442600	-3.40892300
H	2.76561200	1.81158500	-2.63770900
H	2.32138800	-0.58842800	-3.02867700
H	2.79044000	0.25467300	-4.50927700
H	3.95116600	-0.79904700	-3.71044400
H	5.08180300	2.74911000	-2.86272700
H	5.64213100	1.19994200	-3.49974700
H	4.46885200	2.15895700	-4.41786600
C	3.40343200	1.71732100	2.41927400
C	4.55398000	2.39844100	3.18315500
C	2.62042800	0.75585100	3.33114000

H	2.71313200	2.50936000	2.11860000
H	5.08276900	3.11203100	2.54316500
H	4.17022600	2.93894300	4.05551700
H	5.28513500	1.66515000	3.54028900
H	1.81384000	0.26640500	2.77952900
H	3.27557400	-0.01716900	3.74448800
H	2.18070200	1.30234700	4.17281300
C	6.44110500	-1.75814400	0.30304600
C	6.46521400	-2.50299900	1.64386400
C	7.81722800	-1.12254000	0.01620000
H	6.25397500	-2.49929100	-0.48678600
H	5.48873900	-2.92903700	1.88537400
H	7.19639300	-3.31710500	1.61100400
H	6.75670000	-1.83870300	2.46485400
H	7.83069800	-0.63297300	-0.96215600
H	8.04991500	-0.36410500	0.77209400
H	8.61042600	-1.87837300	0.03497100
C	2.79277500	-3.59478600	-2.35692600
C	-1.88755200	-3.62586700	-2.90027500
C	2.34225500	-3.73240200	-0.89925500
H	3.51454000	-2.77587900	-2.44026500
H	1.48986900	-4.42906900	-0.87738500
H	-1.89522500	-4.71676500	-2.93284600
H	3.30834100	-4.50330600	-2.68990600
H	-2.80696100	-3.26103200	-3.36971400
C	1.69862000	-3.34003600	-3.37897800
O	1.89402700	-3.19005000	-4.56504000
C	-1.90898100	-3.19174700	-1.44991400
O	-1.84171000	-2.02662300	-1.08877900
O	0.46751300	-3.32243300	-2.81171500
O	1.97096300	-2.48152400	-0.33387800
C	-0.75890500	-1.59917300	-4.03668100
H	0.11014300	-1.32422700	-4.63644800
H	-1.66406000	-1.41018600	-4.62163500
H	-0.77329300	-0.98971900	-3.13585300
C	3.44759400	-4.29126700	-0.01269300
H	3.74615500	-5.29444600	-0.33433100
H	4.31812600	-3.63188600	-0.04432000
H	3.08827900	-4.33919500	1.01762300
O	-2.02263200	-4.23082100	-0.61983900
H	1.47518200	-1.93185600	-0.96623700
O	1.22139000	-3.76265100	2.76500700
C	1.78130200	-3.24000700	4.00719700
H	1.22041100	-2.33329300	4.25776700
C	3.22534100	-2.90357200	3.67087000
H	3.26845600	-2.24692300	2.79889100
H	3.70498600	-2.40439900	4.51834300
H	3.78758500	-3.81591000	3.44726000
C	-0.10950300	-3.69852800	2.59561000
O	-0.90168600	-3.38975200	3.46482900
C	1.62977400	-4.26898900	5.12011400
H	0.57390900	-4.46886000	5.31151000
H	2.12859000	-5.20293400	4.84132600
H	2.08833000	-3.89479400	6.04108900
C	0.35355100	3.59165700	-0.11800800
C	0.81408100	4.76819200	-0.80210200
C	-4.01878000	-0.11463100	1.24587700
C	-3.59633000	0.18481200	2.68416200
C	-2.80472200	-0.95850100	3.33421900
C	-4.83059200	0.54149100	3.53625500
H	-2.93850500	1.05721900	2.67194200
H	-1.89129100	-1.17411500	2.78279300
H	-2.51608100	-0.68441400	4.35447300

H	-3.38228600	-1.88516700	3.40408300
H	-5.38719100	1.38285200	3.11228300
H	-5.51711900	-0.31009000	3.59986200
H	-4.53061000	0.80947500	4.55509000
C	-0.44912700	-4.02720400	1.16175100
H	-0.03727900	-5.01284800	0.91865700
H	0.10614400	-3.30480300	0.55307000
C	-0.67738500	-3.07393000	-3.67534200
H	-0.54437300	-3.67149500	-4.58295800
O	0.65684300	-0.22199000	-1.44872200
O	-0.69573500	-0.56908000	0.77087000
H	-1.24545300	-1.22928500	0.26979000
C	-4.94983000	-0.71837900	-1.32501500
H	-5.32636800	-0.93927900	-2.32002400
C	-2.76932800	-5.07022200	1.49029300
H	-3.81233700	-4.99922000	1.16943000
H	-2.39096600	-6.06478600	1.23464700
H	-2.71897100	-4.93381100	2.57249000
C	-1.93660600	-3.99031500	0.82688500
H	-2.36438800	-3.00876400	1.04163500

**S-Chain- (S, S)-DL
4INT1**

C	2.24473500	6.26134900	-3.05188900
C	3.06003600	5.17816600	-2.82177900
C	2.64827700	4.12518400	-1.96105600
C	0.55315700	5.33426500	-1.57990500
C	0.97404900	6.32963400	-2.43299000
H	4.43071400	2.93591300	-2.24516200
H	2.56607300	7.05732400	-3.71679000
H	4.02922900	5.10165600	-3.30726100
C	3.45829400	2.97928500	-1.76493800
H	-0.42473700	5.39909500	-1.11884400
H	0.32182200	7.17369700	-2.63632900
C	1.79917200	2.03014400	-0.33494600
C	3.04593400	1.90623500	-1.00260600
C	-0.25879300	3.23119500	0.38951200
C	-0.51231800	4.32612900	1.28361800
C	-1.22386000	2.24325900	0.27031100
C	0.47611300	5.29177200	1.61903800
C	-1.80539600	4.44136900	1.88589100
C	-2.52571200	2.35411400	0.82681400
C	0.18917600	6.32752100	2.47937400
H	1.46944200	5.19924200	1.19659200
C	-2.07438200	5.53188400	2.75601100
C	-2.79248100	3.46680100	1.59748300
C	-1.10078100	6.45865700	3.04669000
H	0.96190000	7.04838700	2.72899400
H	-3.06396100	5.61113900	3.19800200
H	-3.79376600	3.59993700	1.99511300
H	-1.31419500	7.28427000	3.71880700
O	-0.94857200	1.11419100	-0.51047400
O	1.39691500	0.98143000	0.50023200
P	0.17271900	0.04535900	-0.00146600
C	-3.62762000	1.38971500	0.51033000
C	-4.34469300	1.54625100	-0.69419800
C	-5.14478300	-0.36949900	1.17038300
C	-5.90147400	-0.20606000	0.00607900
H	-5.45565500	-1.12842300	1.88156700
C	3.92468100	0.70151200	-0.86958800
C	4.71984700	0.54384600	0.28294000
C	4.01711400	-0.22779900	-1.93207700
C	5.62622700	-0.52107200	0.34213500

C	4.95470300	-1.25890700	-1.83292900
C	5.77135000	-1.42487000	-0.70988400
H	6.22236100	-0.64760200	1.23917700
H	5.03499200	-1.97903400	-2.64221600
C	-7.17491400	-1.02205200	-0.17027200
C	-7.57844900	-1.26026600	-1.63093200
C	-8.32934000	-0.35654000	0.60604300
H	-6.98117900	-2.00352100	0.27608900
H	-6.76833700	-1.72464600	-2.19982000
H	-8.44480400	-1.92773600	-1.67651000
H	-7.86076700	-0.32851200	-2.13379300
H	-8.07210600	-0.22665400	1.66176700
H	-8.55056900	0.63409400	0.19237400
H	-9.24096200	-0.96161600	0.54671500
C	-3.92340300	2.55436200	-1.76078000
C	-5.08508300	3.45328900	-2.21830600
C	-3.26802400	1.83779100	-2.95705300
H	-3.16709600	3.21390800	-1.32602300
H	-5.55741900	3.95115900	-1.36578100
H	-4.71980600	4.22334300	-2.90611300
H	-5.85903600	2.88545900	-2.74513900
H	-2.37690000	1.29107600	-2.63718400
H	-3.96681900	1.12876500	-3.41644200
H	-2.96661200	2.55852500	-3.72520200
C	3.11453900	-0.13647600	-3.16109000
C	2.63252900	-1.51466000	-3.64927900
C	3.80742800	0.61003900	-4.31738900
H	2.22427400	0.42987900	-2.87020300
H	2.27979600	-2.13879700	-2.82764400
H	1.81411800	-1.38731400	-4.36593100
H	3.43041100	-2.05968900	-4.16674300
H	4.06465000	1.63676900	-4.04734800
H	4.73158000	0.09532800	-4.60386900
H	3.15456200	0.64668200	-5.19667100
C	4.60408300	1.48150700	1.47958700
C	5.94942700	2.13944400	1.83253300
C	4.00514000	0.73728300	2.68525600
H	3.91453400	2.28927600	1.21798600
H	6.36152600	2.67998200	0.97431600
H	5.82240200	2.84992400	2.65658500
H	6.69051900	1.39743300	2.14758500
H	3.03365300	0.30625100	2.43289900
H	4.66022700	-0.07838400	3.00857300
H	3.87341300	1.41728800	3.53464100
C	6.77677900	-2.56810600	-0.66959300
C	7.02330500	-3.13073400	0.73912700
C	8.10138800	-2.13040100	-1.32556700
H	6.35820200	-3.37968200	-1.28138100
H	6.09127500	-3.38594700	1.25227400
H	7.64319100	-4.03138800	0.67832700
H	7.56432200	-2.41213000	1.36517400
H	7.93989800	-1.77803700	-2.34926200
H	8.55414000	-1.31021600	-0.75700600
H	8.81699500	-2.95961900	-1.35464200
C	-3.85484400	-2.23507000	-2.24413000
C	-1.55210200	-4.71858200	-0.48223200
C	-2.33366400	-2.01706400	-2.06507000
H	-4.41014100	-1.37207300	-1.88113600
H	-0.93700600	-4.77209000	-1.38226800
H	-4.07165500	-2.39043200	-3.30587800
H	-1.05077600	-5.30382400	0.29100200
C	-4.26750200	-3.43839100	-1.43232700
O	-5.03711000	-3.44309400	-0.50241700

C	-1.52856800	-3.28854800	0.02443000
O	-1.07522300	-3.04755500	1.14525100
O	-3.53932500	-4.53060300	-1.81396800
O	-2.00783600	-2.23995500	-0.64201700
O	1.27600000	-3.51958000	-1.10277300
H	1.02441700	-2.57454900	-1.07164800
O	2.05955900	-2.26066800	2.66938400
C	1.84272700	-2.49161100	4.09171300
H	2.10872800	-3.53540900	4.29317500
C	0.35342100	-2.25866600	4.29972800
H	-0.23393100	-2.92713300	3.66540300
H	0.08460600	-2.43203600	5.34648200
H	0.09568300	-1.22924300	4.03411900
C	3.10570900	-2.87125900	2.07111300
O	3.99046700	-3.45060800	2.67203700
C	2.72719200	-1.57610300	4.92712500
H	3.77929100	-1.76010200	4.70307800
H	2.49473400	-0.52742800	4.72364500
H	2.55739200	-1.76893300	5.99159200
C	0.99476400	3.15364700	-0.40872100
C	1.38127400	4.21240400	-1.30009300
C	-4.01871200	0.40843200	1.44882900
C	-3.26779600	0.21775500	2.76422000
C	-3.14470100	-1.25841400	3.17560300
C	-3.93249100	1.02107900	3.89938400
H	-2.25214100	0.60118500	2.62546400
H	-2.77163200	-1.87468700	2.35688000
H	-2.45178200	-1.35441200	4.01707400
H	-4.10649900	-1.67073400	3.49944500
H	-3.94744300	2.09227300	3.68520400
H	-4.96747800	0.69177400	4.04530600
H	-3.39294400	0.87308600	4.84141500
C	2.93716800	-2.81852800	0.57412500
H	3.88920100	-3.02543600	0.09018300
H	2.61787400	-1.81552300	0.28321500
C	-2.94681100	-5.31139700	-0.74857300
O	0.49766800	-0.87972000	-1.11796200
O	-0.29749200	-0.55519600	1.37040300
H	-0.62829400	-1.50745400	1.32022900
C	-5.47270700	0.74603600	-0.92036200
H	-6.02717500	0.87860100	-1.84328800
C	-2.87396100	-6.75467400	-1.21586600
H	-2.41645800	-7.38214500	-0.44550600
H	-3.87825500	-7.13132200	-1.42395200
H	-2.27566600	-6.83209300	-2.12874100
H	-3.58101800	-5.22548400	0.13904600
C	-1.44259100	-2.74047700	-3.06268500
H	-1.56856500	-2.24184600	-4.02933000
H	-0.39585700	-2.65484600	-2.77493600
H	-1.71544300	-3.78729000	-3.18675700
H	-2.12728300	-0.94916200	-2.13612400
C	2.46164400	-5.25175300	0.02215200
H	1.68212500	-5.98536500	-0.20584700
H	3.19619900	-5.26775000	-0.78930000
H	2.96106700	-5.54074100	0.95170900
C	1.86674400	-3.85669900	0.15037100
H	1.08842000	-3.86378700	0.92417400

⁴TS1

C	-0.35325500	6.93595000	-2.55954200
C	0.79505500	6.20076000	-2.37966600
C	0.79647700	5.03466600	-1.56772800
C	-1.58405000	5.40855400	-1.13154200

C	-1.55581000	6.52434000	-1.93801500
H	2.86839000	4.54619800	-1.94307500
H	-0.34390100	7.82200700	-3.18720900
H	1.72059900	6.49199700	-2.86936400
C	1.95990600	4.23522100	-1.43680100
H	-2.51404200	5.10371800	-0.66762200
H	-2.46735300	7.09142600	-2.10203300
C	0.77037200	2.71375000	-0.02812600
C	1.96235000	3.05698200	-0.72074300
C	-1.57419800	3.04845000	0.72355500
C	-2.21026700	3.92832500	1.66340100
C	-2.10869800	1.77959000	0.54032500
C	-1.64099000	5.16919500	2.06208000
C	-3.45357300	3.53364700	2.25204800
C	-3.37552500	1.39799600	1.05844900
C	-2.28028800	5.98192900	2.97103600
H	-0.68419100	5.46687100	1.64994000
C	-4.09529200	4.40211700	3.17516200
C	-4.02412700	2.28886400	1.88831700
C	-3.52506700	5.60303600	3.52772600
H	-1.82187700	6.92047800	3.26816000
H	-5.04331200	4.09152300	3.60635000
H	-5.00766000	2.02903900	2.26866400
H	-4.02043100	6.25642600	4.23964800
O	-1.43839000	0.85783900	-0.25968400
O	0.78585200	1.57696100	0.76969700
P	0.00507800	0.24327300	0.24204400
C	-4.08923100	0.14989900	0.63433200
C	-4.87997800	0.18638400	-0.53682200
C	-4.92231700	-2.06538200	1.11682500
C	-5.75404100	-2.03479600	-0.00317600
H	-4.92260000	-2.95575100	1.73560300
C	3.17098200	2.17631700	-0.69127600
C	3.96297600	2.09299700	0.47118200
C	3.54014500	1.45731200	-1.85490300
C	5.13418000	1.32259400	0.44469100
C	4.72200000	0.71446300	-1.83090400
C	5.54136000	0.63564200	-0.69773100
H	5.72315000	1.25521300	1.35064200
H	5.01970800	0.17423600	-2.72573900
C	-6.71208800	-3.18289100	-0.28530100
C	-6.58983600	-3.73723900	-1.71411100
C	-8.16160700	-2.75270900	0.01080600
H	-6.45069500	-3.99668700	0.40145000
H	-5.58091800	-4.11145400	-1.90056100
H	-7.29007600	-4.56626600	-1.86330500
H	-6.81998300	-2.97423500	-2.46569700
H	-8.26310500	-2.39328200	1.03953300
H	-8.46859000	-1.94000800	-0.65731300
H	-8.85605200	-3.58819600	-0.13238900
C	-4.81905500	1.36573400	-1.50404300
C	-6.19960000	1.81054000	-2.01337300
C	-3.87408500	1.03543400	-2.67717500
H	-4.38796600	2.21804600	-0.97073900
H	-6.88321800	2.01019500	-1.18232500
H	-6.10495600	2.72574200	-2.60732400
H	-6.66368800	1.05467100	-2.65581200
H	-2.87067700	0.79936800	-2.31252300
H	-4.25042200	0.17294400	-3.24038900
H	-3.79740800	1.88317900	-3.36727400
C	2.70742800	1.49236700	-3.13593000
C	2.45648600	0.09583700	-3.73067600
C	3.36399500	2.40696700	-4.18782300

H	1.72765900	1.90765600	-2.88705000
H	1.98170500	-0.55429900	-2.99602500
H	1.78993100	0.17509300	-4.59651300
H	3.38184100	-0.37715800	-4.07777700
H	3.49533800	3.42546600	-3.81246000
H	4.35327400	2.02630100	-4.46640300
H	2.75231500	2.45637200	-5.09551400
C	3.59909900	2.82883400	1.75739500
C	4.70847100	3.81284000	2.17305100
C	3.26607300	1.84636100	2.89534200
H	2.70301500	3.42588900	1.56616700
H	4.93400100	4.51973600	1.36775700
H	4.39904800	4.38459500	3.05463900
H	5.63551300	3.28857100	2.42835000
H	2.42116400	1.21119700	2.62113500
H	4.11205300	1.19329500	3.12379900
H	2.99861100	2.39934700	3.80298300
C	6.82535100	-0.18629400	-0.76792100
C	7.51125200	-0.40261100	0.58703200
C	7.81787200	0.44287700	-1.76682200
H	6.54580900	-1.17558000	-1.16114500
H	6.82123400	-0.79949700	1.33465300
H	8.34891000	-1.09941900	0.47816100
H	7.91681500	0.53788600	0.97691700
H	7.37657800	0.55849100	-2.76087900
H	8.12323900	1.43647300	-1.42063800
H	8.71729800	-0.17534200	-1.86350600
C	-2.90053200	-3.13532100	-1.92883100
C	0.31227100	-4.83296700	-0.52992000
C	-1.48748600	-2.50953200	-1.97612400
H	-3.61797100	-2.44899200	-1.48076200
H	0.69382200	-4.88148700	-1.54924600
H	-3.23330200	-3.37424200	-2.94464700
H	1.07512500	-5.22447800	0.14641700
C	-2.86937400	-4.38742100	-1.07725100
O	-3.58381400	-4.63372800	-0.13760100
C	0.07229400	-3.38467800	-0.12911200
O	0.24102500	-3.16592600	1.15443500
O	-1.84103500	-5.20408800	-1.46791500
O	-0.95035100	-2.66741300	-0.61131000
O	1.47883900	-2.58169700	-0.93427900
H	1.17751300	-1.55158500	-0.96984800
O	4.80218500	-3.18900400	1.41849500
C	5.89124500	-3.60216800	2.29774300
H	6.48852400	-2.71605000	2.52795900
C	6.70676100	-4.60340900	1.49597300
H	7.09061300	-4.14275000	0.58129200
H	7.55550800	-4.95708100	2.08885300
H	6.09379900	-5.46715200	1.21958600
C	4.25164500	-1.97122700	1.63037800
O	4.64178900	-1.20134100	2.48277700
C	5.29936900	-4.16936800	3.58149400
H	4.71620000	-3.40342100	4.09744500
H	4.65083300	-5.02261300	3.35837300
H	6.09834700	-4.50550200	4.24968600
C	-0.38254500	3.47701200	-0.05895100
C	-0.40924400	4.64074000	-0.90156500
C	-4.08055100	-0.99877300	1.45027200
C	-3.18984500	-1.08400200	2.68466400
C	-2.57567400	-2.48171900	2.86776900
C	-3.95305700	-0.66110900	3.95372800
H	-2.35688200	-0.39013500	2.54034500
H	-2.16569000	-2.85826300	1.92963300

H	-1.76770300	-2.44067300	3.60491800
H	-3.31331400	-3.20798900	3.22667400
H	-4.30943900	0.37005400	3.88260700
H	-4.82173900	-1.30984100	4.11528800
H	-3.30533600	-0.73455600	4.83436800
C	3.08609800	-1.68756800	0.70510600
H	3.27392000	-0.72219700	0.22600300
H	2.22034500	-1.54098500	1.35555800
C	-0.95841100	-5.69326400	-0.42947200
O	0.65313100	-0.28090800	-1.02929500
O	-0.11066600	-0.66590300	1.44009500
H	0.01592200	-2.17592800	1.34850800
C	-5.69941300	-0.90875800	-0.83039800
H	-6.31844600	-0.87757800	-1.72165300
C	-0.68459900	-7.16549700	-0.68548100
H	-0.00531200	-7.56735700	0.07224600
H	-1.62081200	-7.72729600	-0.65058600
H	-0.23136900	-7.30599900	-1.67176700
H	-1.44740100	-5.55739700	0.54014800
C	-0.61282500	-2.99066300	-3.12452900
H	-1.05631900	-2.60357800	-4.04762700
H	0.39911500	-2.59579600	-3.04376900
H	-0.58498900	-4.07770300	-3.19364500
H	-1.57830700	-1.42401600	-2.04215200
C	3.80233300	-2.83446000	-1.47176900
H	3.52895000	-3.62006300	-2.18160500
H	3.82926500	-1.87867500	-1.99882700
H	4.79718900	-3.04578600	-1.07428800
C	2.79000500	-2.77599600	-0.33471300
H	2.74666400	-3.74100600	0.17488700

⁴INT2

C	-0.76038400	6.89718300	-2.64452200
C	0.42303900	6.22388400	-2.45128100
C	0.48222800	5.07546500	-1.61650400
C	-1.91457800	5.33924200	-1.18588900
C	-1.94130000	6.43853000	-2.01468900
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C	1.84426200	-3.02476700	2.26575600
H	1.20991800	-2.15551800	2.09609500

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