# Supporting Information

# Copolymerization of $SO_2$ with propylene oxide mediated by organic ammonium salts: A comprehensive study of main-chain structure, living polymerization character and regio-selectivity

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## Contents

***1. General information.***

All the synthesis of compounds, involving air and/or water-sensitive were carried out in glove box or with the standard Schlenk techniques under dry nitrogen. Propylene oxide (PO) were distilled over calcium hydride under nitrogen. Sulfur dioxide ($SO_2$, 99.9%) was purchased from Dalian Guangming special gas products company and used as received.

**NMR** $^1H$ and $^{13}C$ NMR spectra were recorded on a Varian INOVA-400 MHz type spectrometer ($^1H$ NMR, 400 MHz and $^{13}C$ NMR, 101 MHz). Their peak frequencies were referenced versus an internal standard $CDCl_3$ shifts at 7.26 ppm for $^1H$ NMR and 77.2 ppm for $^{13}C$ NMR.

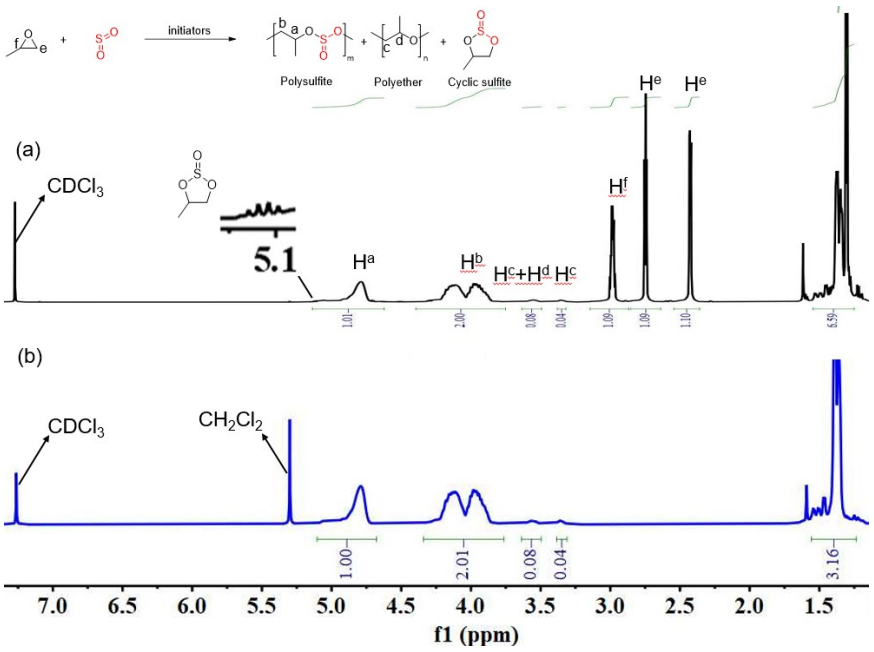
**Gel Permeation Chromatography** Molecular weights and molecular weight distributions of copolymers were measured by gel permeation chromatography (GPC) analysis at 30 ℃ and a flow rate of 1.0 mL/min, with THF as the eluent, on an Agilent 1260 instrument coupled with an Agilent RI detector and equipped with four PL gel columns. The sample concentration was about 0.1%, and the injection volume was 50 μL. The curve was calibrated using monodisperse polystyrene standards covering the molecular weight rage from 580 to 460000 Da.

**MALDI-TOF mass spectrum** MALDI-TOF mass spectrometric measurements were performed on a Waters MALDI micro MX mass spectrometer, equipped with a nitrogen laser delivering 3 ns laser pulses at 337 nm. Trans-2-[3-(4-tert-butylphenyl)-2-methyl2-propenylidene] malononitrile (DCTB) was used as a matrix. $CH_3COONa$ (Aldrich, 98%) was added for ion formation. The best results were obtained for samples prepared from methylene dichloride solution by mixing matrix (5.0 mg/mL), polymer (5.0 mg/mL), and salt (0.1 N solution) in a ratio of 3:1:1. A volume of 3 μL sample solution was deposited on the MALDI target and allowed to dry at room temperature for 2 h prior to the measurement.

***2. General procedure for the copolymerization of $SO_2$ with PO.***

In a 20 mL autoclave equipped with a magnetic stirrer, initiator (24.7 mg, 0.043 mmol, 1 equiv) and PO (500 mg, 8.62 mmol, 200 equiv) were added in an argon atmosphere. $SO_2$ (825.6 mg, 12.9 mmol, 300 equiv) was pumped into the autoclave. Undergoing an appropriate time at a certain reaction condition, a small amount of the resultant mixture was removed for $^1H$ NMR analysis. The crude polymer was dissolved in 10 mL $CH_2Cl_2$, then, the solution was precipitated with excess methanol. This process was repeated 2−3 times to completely remove the excess epoxide, and colorless transparent polymer was obtained by vacuum-drying.

### *3. $^1$H NMR of polymer and cyclic sulfite ester.*




$$\text{PO \% conversion} = \frac{H_a+H_b+H_c+H_d}{H_a+H_b+H_c+H_d+H_e+H_f}$$

$$\text{Selectivity for polymer over cyclic sulfite ester} = \frac{\text{Peak area of cyclic sulfite ester}}{H_a+H_b+H_c+H_d+\text{Peak area of cyclic sulfite ester}}$$

$$\text{Sulfite linkages of the polymer} = \frac{H_a+H_b}{H_a+H_b+H_c+H_d}$$

$$M^{\text{Theo}} = 122 \times \text{PO/Initiator} \times \text{PO conversion}$$

**Fig. S1.** $^1$H NMR spectrum of (a) crude polymer and (b) purified polymer from Table 1, entry 1.

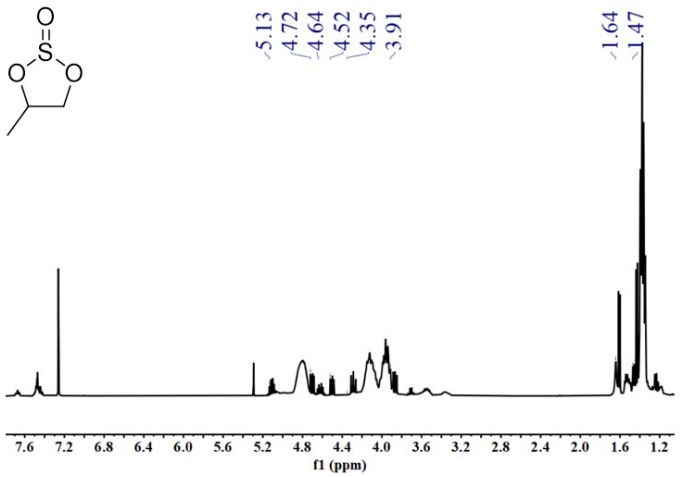



**Fig. S2.** $^1$H NMR spectrum of polymer with more cyclic sulfite ester resulted from the copolymerization at 60 °C (Table 1, entry 10). According to the reported literature,[3] chemical shift for obtained cyclic sulfite ester, major isomer: $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 5.13 (m, 1H), 4.74 (dd, 3$J$ = 8.4 and 6.0 Hz, 1H), 3.90 (dd, 3$J$ = 8.2 and 7.0 Hz, 1H), 1.47 (d, 3$J$ = 6.5Hz, 3H). Minor isomer: $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 4.64 (m, 1H), 4.53 (dd, 3$J$ = 8.9 and 6.2 Hz, 1H), 4.32 (m, 1H), 1.64 (d, 3$J$ = 6.5Hz, 3H).

*4. $^{13}C$ NMR of the purified polymer.*

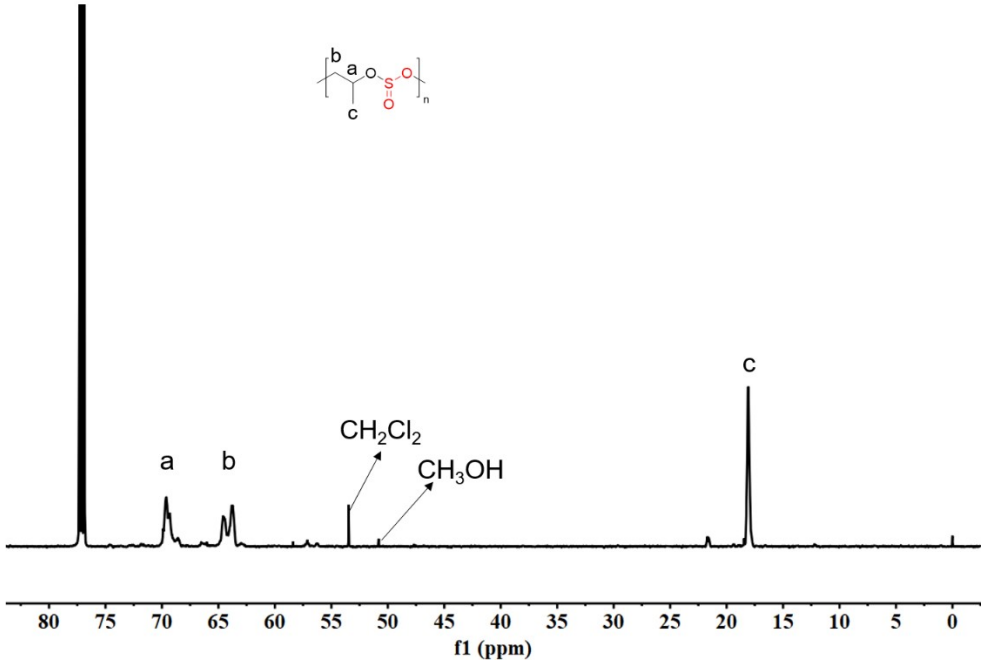



**Fig. S3.** $^{13}C$ NMR spectrum of purified polymer (entry 1, Table 1).

*5. $^{1}H$ DOSY NMR of the polymer.*

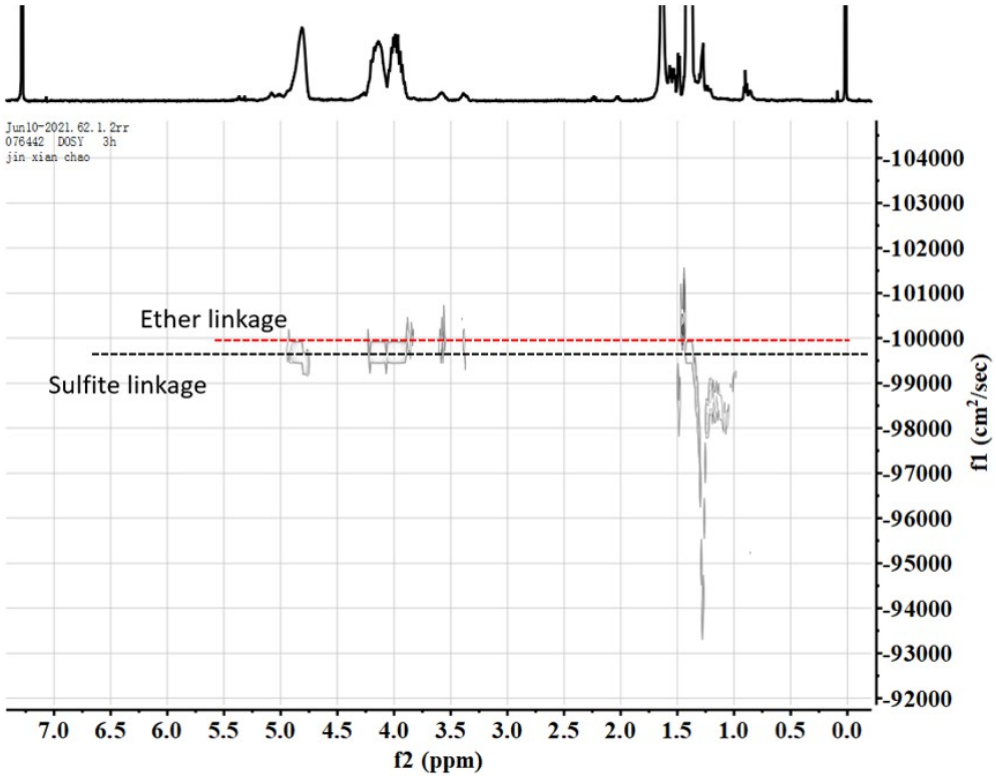



**Fig. S4.** $^{1}H$ DOSY NMR spectrum of the polymer (entry 1, Table 1).

*6. Typical GPC traces.*

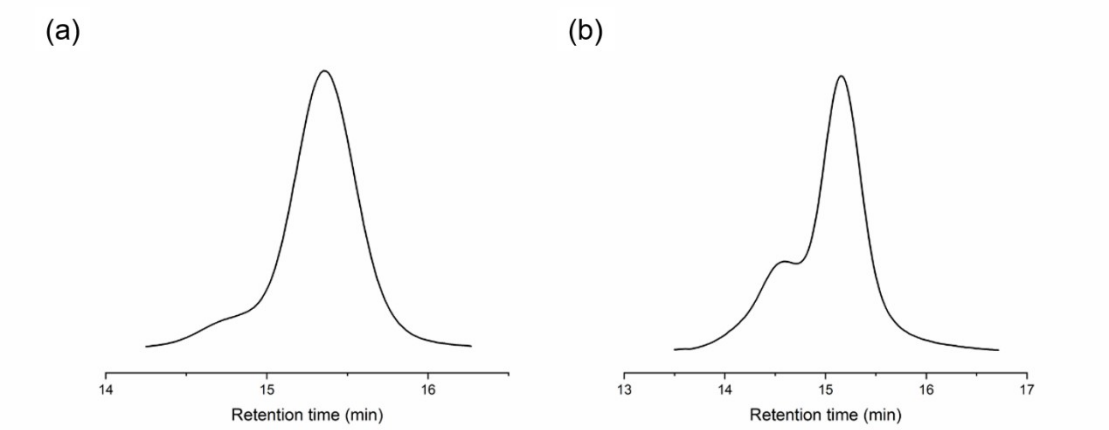



**Fig. S5.** GPC traces of poly(propylene sulfite) obtained from PO/$SO_2$ copolymerization at different temperatures: (a) 25 ℃ (Table 1, entry 1); (b) 40 ℃ (entry 8, Table 1).

*7. Structure of the chiral metal complex.*

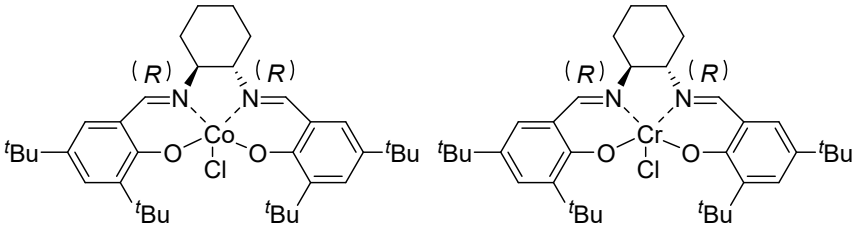



**Fig. S6.** Structure of the (*R*, *R*)-SalenCoCl and SalenCoCl Catalyst.

### *8. Study of living $SO_2$/PO copolymerization mediated by PPNCl.*

**Table S1.** Living $SO_2$/PO copolymerization mediated by PPNCl.[a]

| Entry | PO/$SO_2$/ Initiator/CTA | Time (h) | Conv.[b] (%) | Selectivity[b] (% Polymer) | Sulfite linkages[b] (%) | $M_n^{theo.}$[c] (kg/mol) | $M_n^{GPC}$[d] (kg/mol) | $Đ$[d] |
|---|---|---|---|---|---|---|---|---|
| 1 | 200/300/1/- | 4 | 43 | 99 | 96 | 10.5 | 6.1 | 1.12 |
| 2 | 200/300/1/- | 8 | 65 | 99 | 96 | 15.9 | 9.8 | 1.13 |
| 3 | 200/300/1/- | 12 | 80 | 99 | 96 | 19.5 | 12.6 | 1.12 |
| 4 | 200/300/1/- | 16 | 88 | 99 | 96 | 21.5 | 14.4 | 1.13 |
| 5 | 200/300/1/- | 24 | 97 | 98 | 92 | 23.7 | 16.7 | 1.14 |
| 6 | 200/300/1/1 | 4 | 44 | 99 | 96 | 5.4 | 3.8 | 1.08 |
| 7 | 200/300/1/1 | 8 | 66 | 99 | 96 | 8.1 | 6.1 | 1.10 |
| 8 | 200/300/1/1 | 12 | 79 | 99 | 95 | 9.6 | 7.8 | 1.09 |
| 9 | 200/300/1/1 | 16 | 86 | 99 | 95 | 10.5 | 8.5 | 1.10 |
| 10 | 200/300/1/1 | 24 | 97 | 98 | 94 | 11.8 | 10.3 | 1.10 |
| 11 | 200/300/1/4 | 12 | 79 | 99 | 96 | 4.2 | 2.7 | 1.10 |
| 12 | 200/300/1/3 | 12 | 79 | 99 | 96 | 4.8 | 2.9 | 1.11 |
| 13 | 200/300/1/2 | 12 | 79 | 99 | 96 | 6.0/2.3 | 4.1 | 1.12 |
| 14 | 200/300/1/1 | 12 | 82 | 99 | 96 | 9.6 | 6.6 | 1.12 |
| 15 | 200/300/1/0.8 | 12 | 82 | 99 | 96 | 10.9 | 7.5 | 1.11 |
| 16 | 200/300/4/- | 12 | >99 | 99 | 96 | 6.1 | 6.1 | 1.21 |
| 17[e] | 200/300/-/- | 24 | >99 | 96 | 95 | 24.4 | 15.8 | 1.35 |

[a]The copolymerization was performed in neat PO (1.5 g) with PPNCl as initiator in 10 mL autoclave. For entries 6 – 15, BnOH was added as chain transfer agent (CTA); [b]The conversion of PO, selectivity for the polymer over cyclic sulfite, and the sulfite linkage were determined by $^1$H NMR; [c]the theory molecular weight $M_n^{theo}$ was calculated as $M_n^{theo} = [122 \times 200 \times Conv.(PO)]/(1 + r)$, r = molar ratio of BnOH to PPNCl; [d]Determined by gel permeation chromatography (GPC) in tetrahydrofuran and calibrated with polystyrene. [e]chain extension of entry 16.

### *9. Copolymerization of $SO_2$ with optical pure epoxides.*

**Table S2.** Copolymerization of $SO_2$ with optical pure epoxides mediated by various initiators.[a]

| Entry | Epoxide Configuration | Initiator | $ee_p$[b] (%) | Regioselectivity[c] (Methylene%) | Regioselectivity[d] (Methine%) |
|---|---|---|---|---|---|
| 1 | (*S*)-PO | $Me_4NCl$ | 40 (*S*) | 70 | 30 |
| 2 | (*S*)-PO | $^nBu_4NCl$ | 43 (*S*) | 72 | 28 |
| 3 | (*S*)-PO | $^nBu_4NI$ | 44 (*S*) | 72 | 28 |
| 4 | (*S*)-PO | $Et_4NBr$ | 43 (*S*) | 71 | 29 |
| 5[e] | (*S*)-PO | SalenCoCl/PPNCl | 43 (*S*) | 72 | 28 |
| 6[f] | (*S*)-PO | SalenCrCl/PPNCl | 42 (*S*) | 71 | 29 |

[a]The copolymerization was performed in neat PO (1.5 g) with PPNCl as initiator in 10 mL autoclave. The selectivity for the polymer over cyclic sulfite, and the sulfite linkage were 99% and 1%, respectively as

determined by $^1$H NMR. [c]The regioselectiviry of the copolymerization was calculated as: Regioselectivity$_{(methylene)}$ = (0.5 + 0.5 × $ee_p$) × 100%; [d]Regioselectivity$_{(methine)}$ = 1 – Regioselectivity$_{(methylene)}$; [e](*R,R*)-SalenCoCl was added as catalyst; [f](*R,R*)-SalenCrCl was added as catalyst.

***10. Determination of the ee values of the poly(propylene sulfite) and the cyclic sulfite ester.***

A round-bottomed flask was charged with poly(propylene sulfite) or cyclic sulfite ester (50 mg), THF (5 mL), MeOH (1 mL) and NaOH (4 M, 1 mL). The resultant mixture was stirred at room temperature for 24 h. Then, it was concentrated to 4 mL by evaporation. The solution was exacted with ethyl acetate (5 mL × 3). The combined organic layers were dried over anhydrous $Na_2SO_4$ and concentrated by evaporation.[1]

The enantiomeric excess of the resultant propylene glycol derivative was determined by the same method according to the literature report.[2]

Propylene glycol derivative: Determined by GC analysis with a chiral GC column (Agilent HP-Chiral 19091G-B213, 30 m × 0.25 mm ID × 0.25 μm film). Injection temp. = 275 ℃; detection temp. = 275 ℃; Oven temperature 90 ℃. $t_S$ = 5.7 min, $t_R$ = 6.5 min.

$$ee = \frac{|[R] - [S]|}{|[R] + [S]|} \times 100\%$$

Regioselectivity for methylene = (0.5 + 0.5 × $ee_p$) × 100%

Regioselectivity for methine = 100% - Regio-selectivity for methylene

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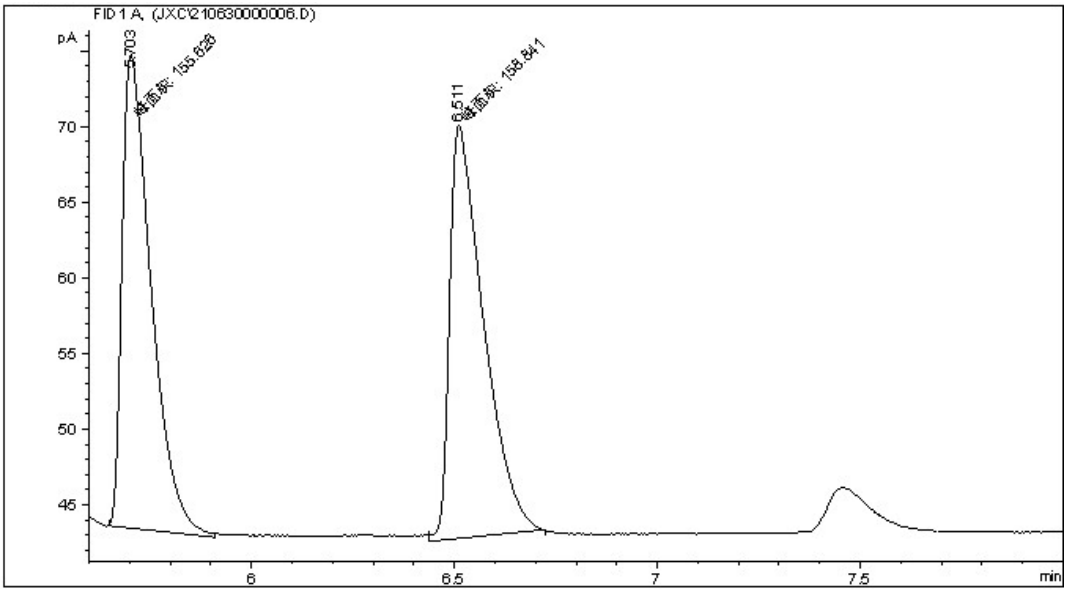


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面积百分比报告

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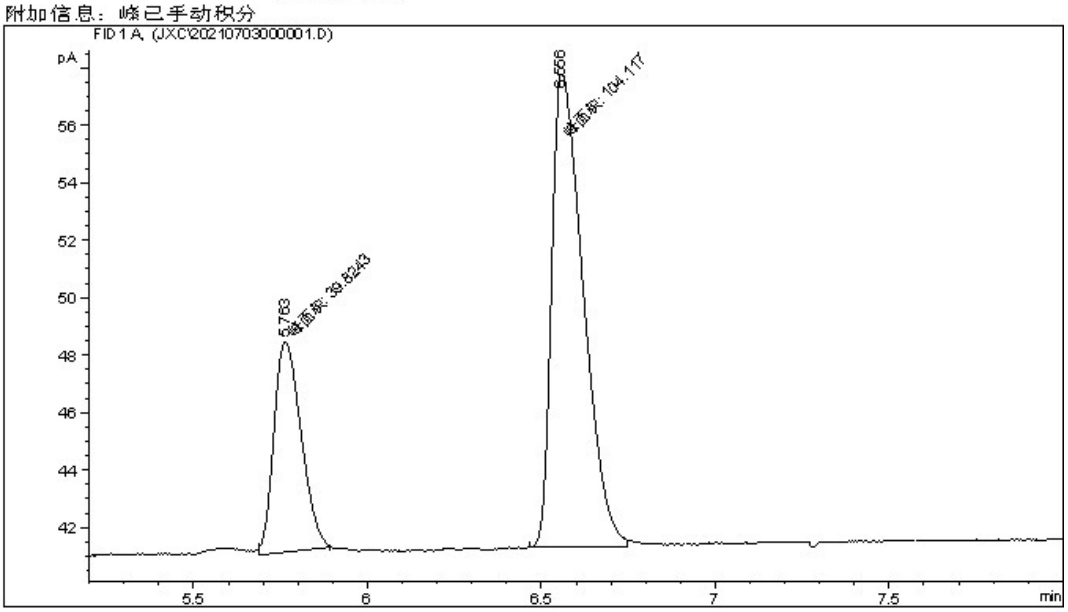


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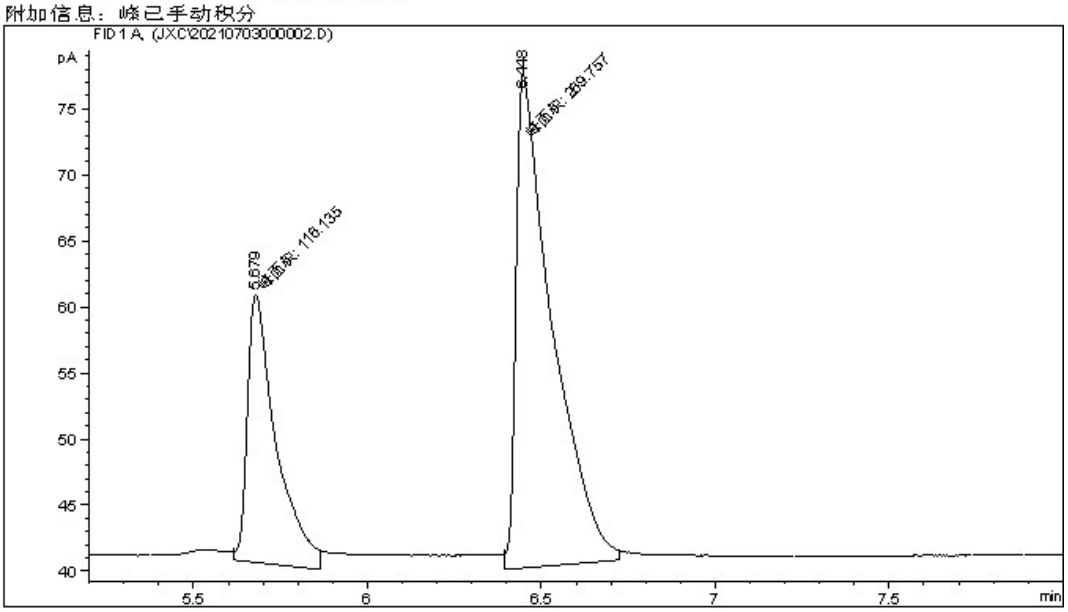


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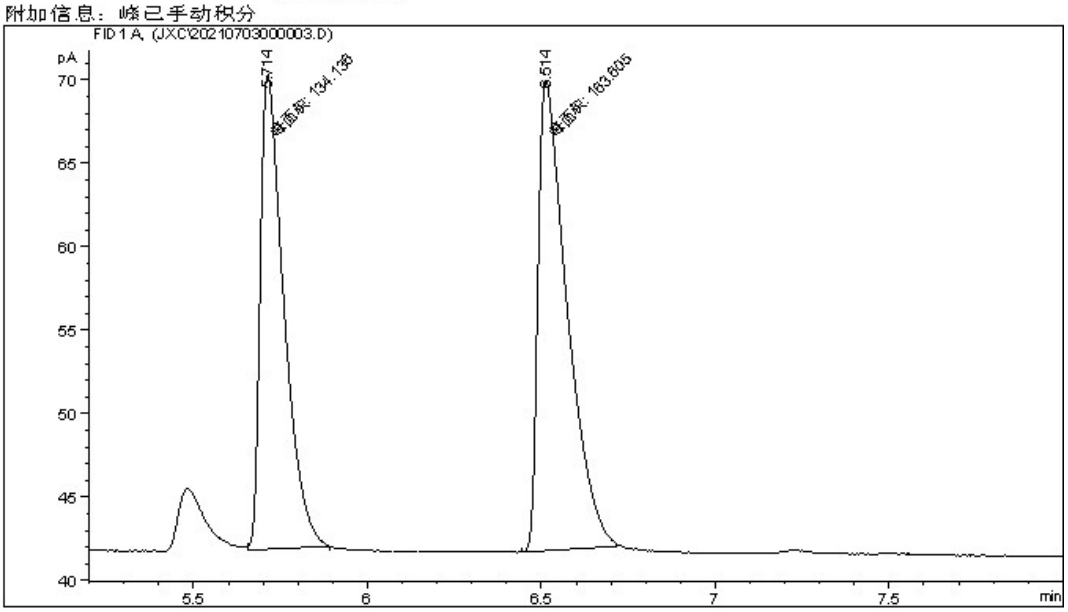


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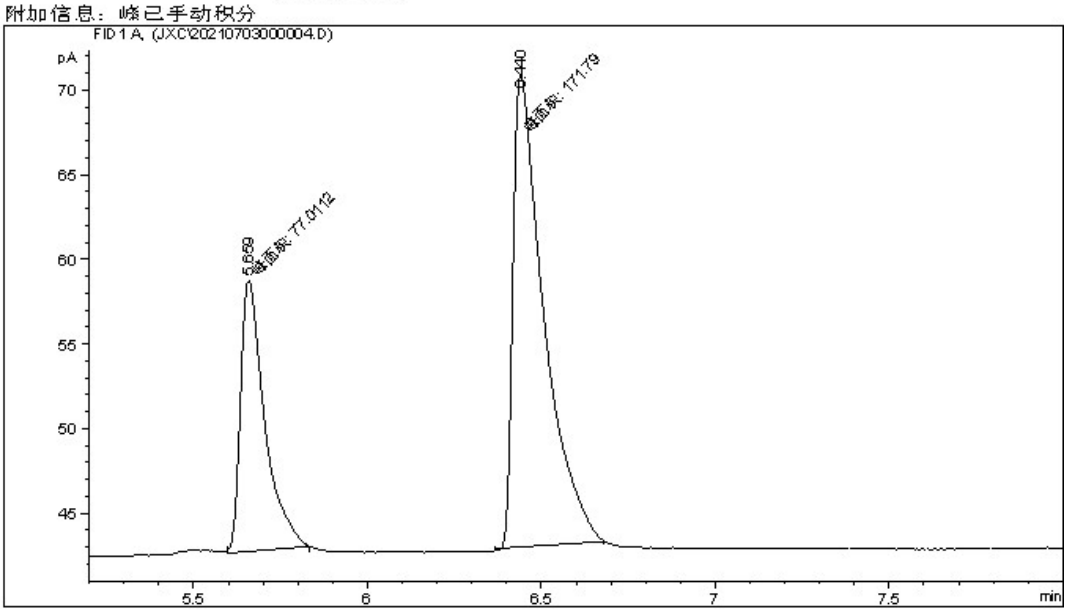


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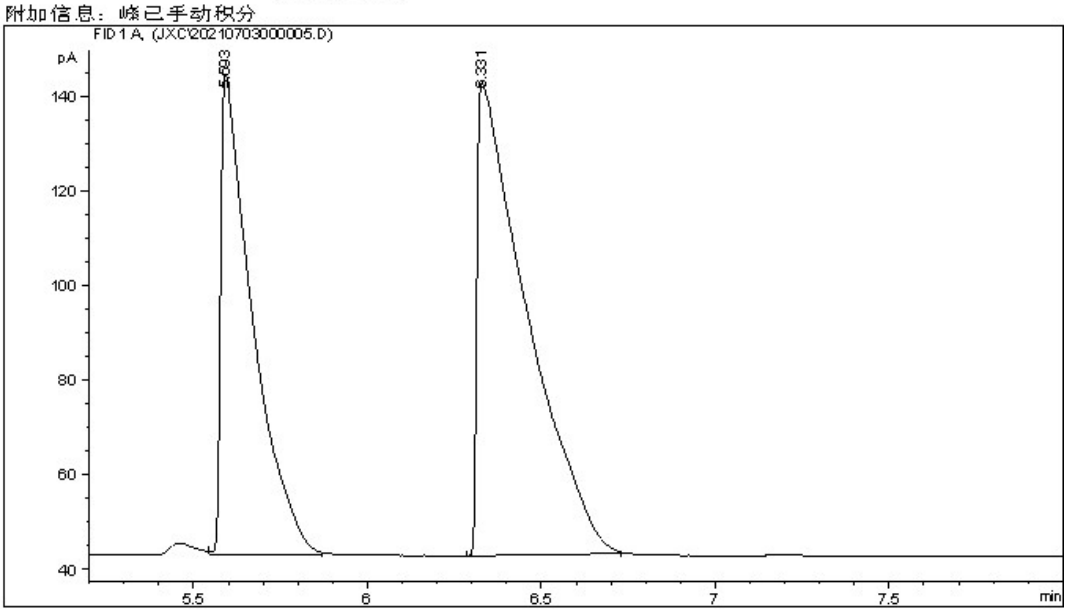


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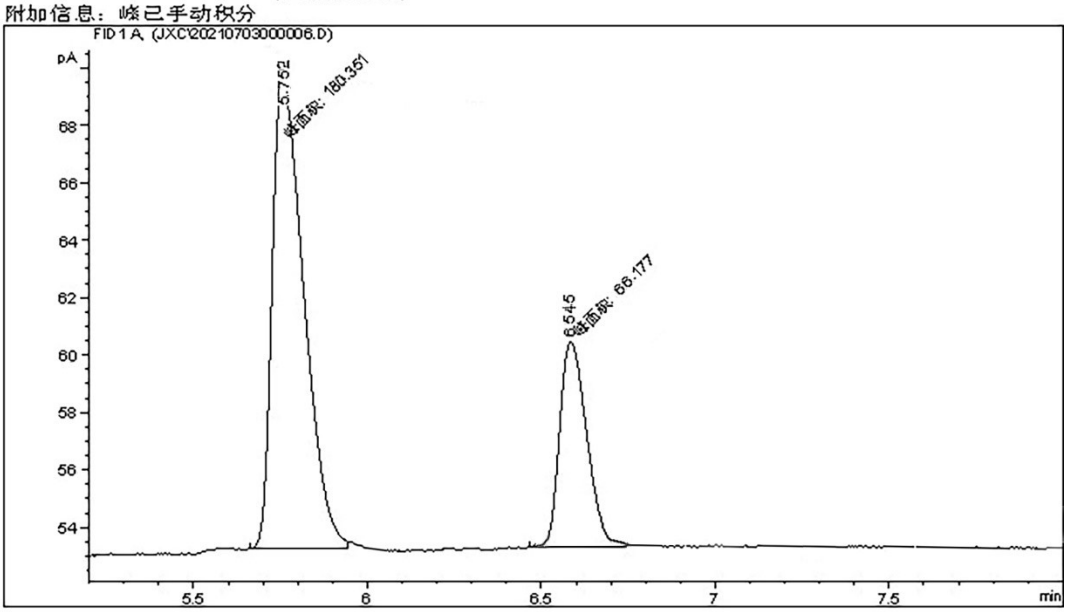


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内标使用乘积因子和稀释因子

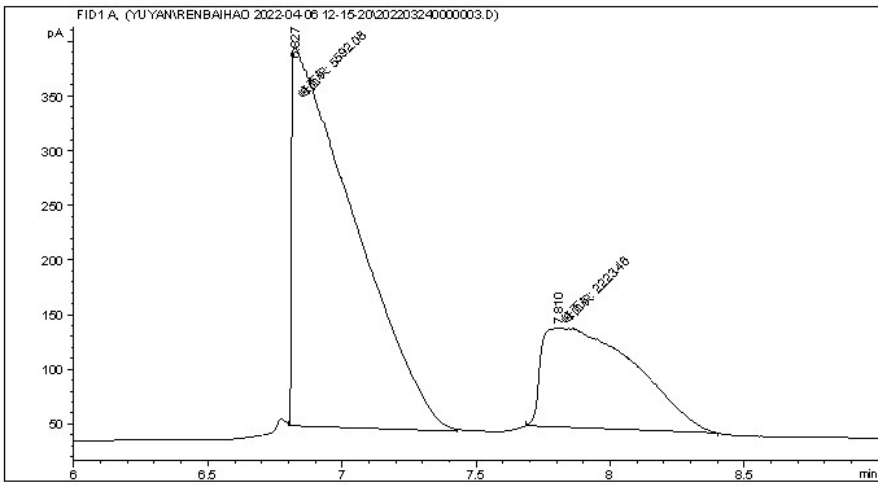
信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 5.752 | MM | 0.1184 | 180.35114 | 26.13211 | 73.15628 |
| 2 | 6.545 | MM | 0.0970 | 66.17744 | 14.51453 | 26.84372 |
| 总量 : | | | | 246.52858 | 40.64664 | |

*** 报告结束 ***

## *(S-PO- Salen Co/PPNCl-Copolymer-25 °C)*

数据文件: D:\CHEM32\1\DATA\YUYAN\RENBAIHAO 2022-04-06 12-15-20\202203240000003.D
样品名称: Salen Co/PPNCl

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面积百分比报告

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排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 6.827 | MM | 0.2692 | 5592.08008 | 346.22049 | 71.55082 |
| 2 | 7.810 | MM | 0.4080 | 2223.45581 | 90.81677 | 28.44918 |

总量 : 7815.53589 437.03726

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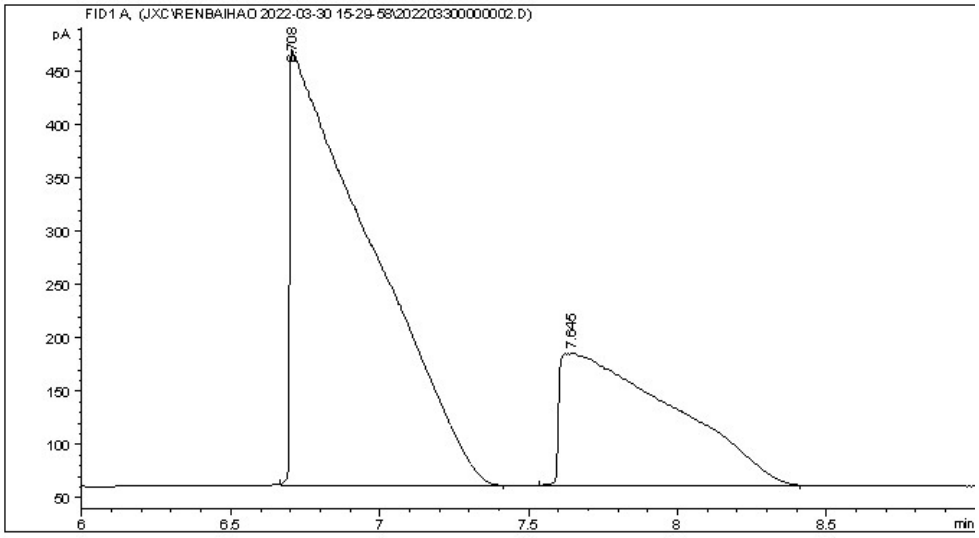
*** 报告结束 ***

## *(S-PO-Me$_4$NCl-Copolymer-25 $^o$C)*

数据文件: D:\CHEM32\1\DATA\JXC\RENBAIHAO 2022-03-30 15-29-58\202203300000002.D
样品名称: Me

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面积百分比报告

==========

排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 6.708 | BB | 0.2254 | 7711.57666 | 408.14249 | 70.12233 |
| 2 | 7.645 | BB | 0.3229 | 3285.74219 | 124.48630 | 29.87767 |
| 总量 : | | | | 1.09973e4 | 532.62878 | |

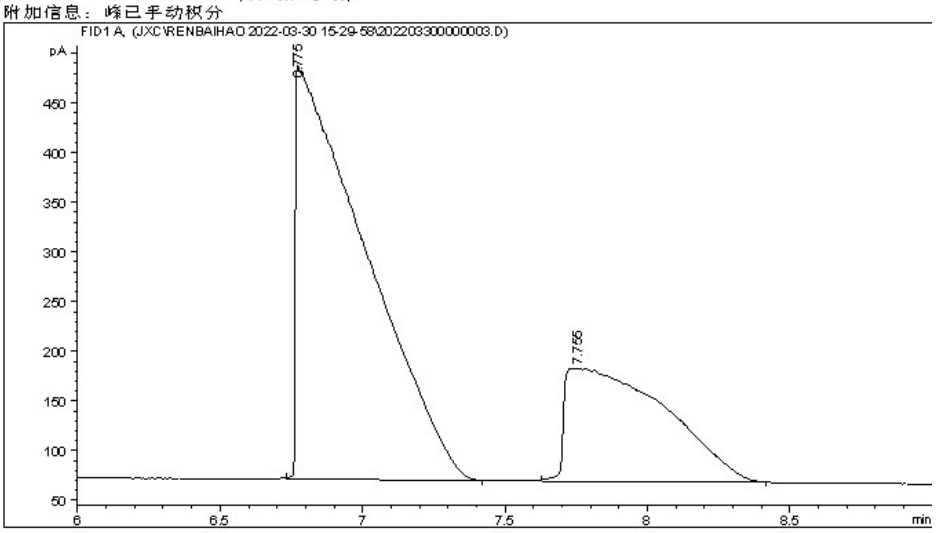
==========

*** 报告结束 ***

## *(S-PO-$^{n}Bu_4NCl$-Copolymer-25 $^{o}C$)*

数据文件: D:\CHEM32\1\DATA\JXC\RENBAIHA0 2022-03-30 15-29-58\202203300000003.D
样品名称: Bu

操作者 : LWJ 序列行 : 3
仪器 : 仪器 1 位置 : 样品瓶 103
进样日期 : 2022/3/30 16:14:13 进样次数 : 1
进样量 : 3 µl
采集方法 : D:\CHEM32\1\DATA\JXC\RENBAIHA0 2022-03-30 15-29-58\RENBAIHA0-C.M
最后修改 : 2022/3/30 15:25:45 : LWJ
分析方法 : D:\CHEM32\1\METHODS\RENBAIHA0-C.M
最后修改 : 2022/3/30 17:12:19 : LWJ
(调用后修改)
附加信息: 峰已手动积分




面积百分比报告

排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

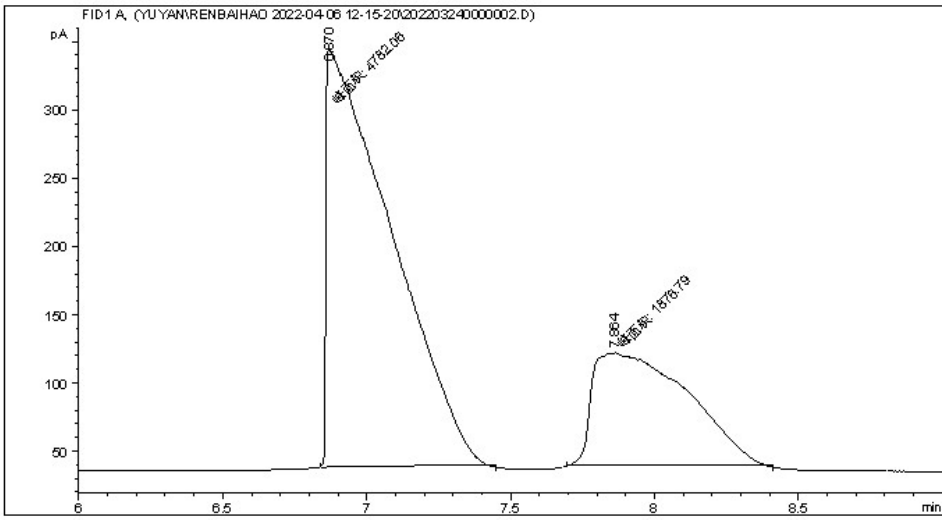
信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 6.775 | BB | 0.2041 | 7095.71436 | 415.75891 | 71.55958 |
| 2 | 7.755 | BB | 0.2962 | 2820.09937 | 113.75078 | 28.44042 |
| 总量 : | | | | 9915.81372 | 529.50969 | |

*** 报告结束 ***

## *(S-PO-$^{n}Bu_4NI$-Copolymer-25 $^{o}C$)*

数据文件: D:\CHEM32\1\DATA\YUYAN\RENBAIHAO 2022-04-06 12-15-20\2022032400000002.D
样品名称: tBu4NI

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面积百分比报告

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排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 6.870 | MM | 0.2602 | 4782.06006 | 306.27673 | 71.81510 |
| 2 | 7.864 | MM | 0.3803 | 1876.79028 | 82.25227 | 28.18490 |

总量 : 6658.85034 388.52901

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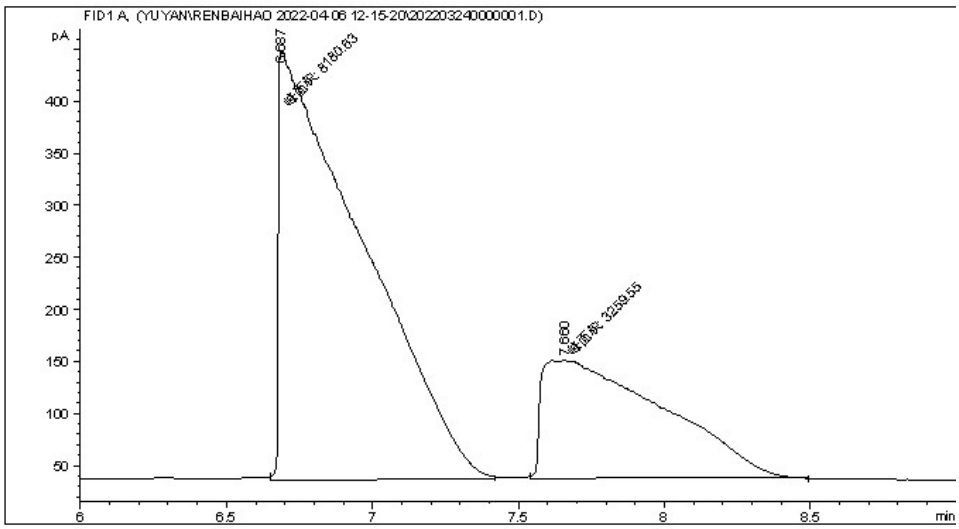
*** 报告结束 ***

## *(S-PO-Et$_4$NBr -Copolymer-25 $^o$C)*

数据文件: D:\CHEM32\1\DATA\YUYAN\RENBAIHAO 2022-04-06 12-15-20\202203240000001.D
样品名称: Et4NBr

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面积百分比报告

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排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 6.687 | MM | 0.3298 | 8180.62793 | 413.45367 | 71.50789 |
| 2 | 7.660 | MM | 0.4763 | 3259.54810 | 114.06113 | 28.49211 |

总量 : 1.14402e4 527.51481

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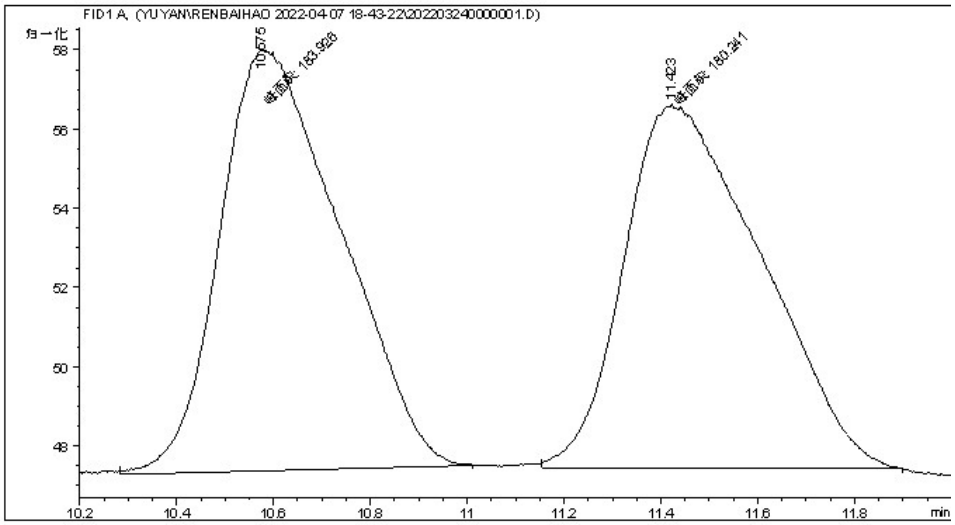
*** 报告结束 ***

## *(Rac-BO-PPNCl-Copolymer-25 °C)*

数据文件: D:\CHEM32\1\DATA\YUYAN\RENBAIHAO 2022-04-07 18-43-22\202203240000001.D
样品名称: rac-BO-07

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面积百分比报告

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排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 10.575 | MM | 0.2879 | 183.92645 | 10.64774 | 50.50604 |
| 2 | 11.423 | MM | 0.3278 | 180.24080 | 9.16286 | 49.49396 |

总量 : 364.16725 19.81061

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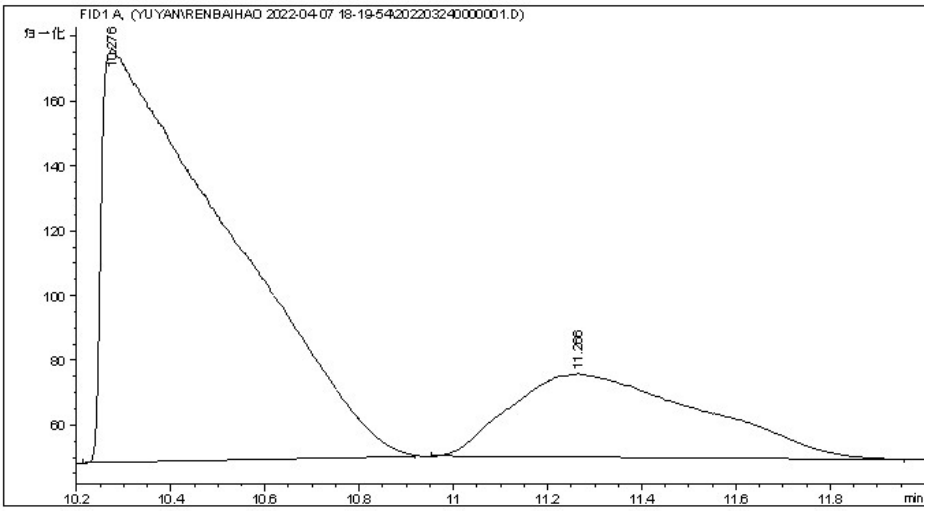
*** 报告结束 ***

## *(S-BO-PPNCl-Copolymer-25 °C)*

数据文件: D:\CHEM32\1\DATA\YUYAN\RENBAIHAO 2022-04-07 18-19-54\202203240000001.D
样品名称: s-BO-01

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面积百分比报告

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排序 : 信号
乘积因子: : 1.0000
稀释因子: : 1.0000
内标使用乘积因子和稀释因子

信号 1: FID1 A,

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [pA*s] | 峰高 [pA] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 10.276 | BB | 0.2268 | 2370.74683 | 127.54781 | 76.69980 |
| 2 | 11.266 | BB | 0.3329 | 720.19592 | 25.62450 | 23.30020 |
| 总量 : | | | | 3090.94275 | 153.17232 | |

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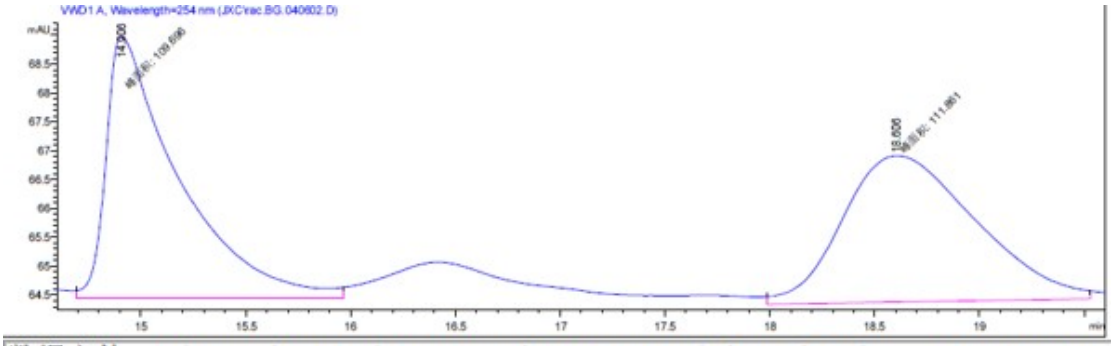
*** 报告结束 ***

*(Rac-BGE-PPNCl-Copolymer-25 °C)*




数据文件: C:\Users\Public\Documents\ChemStation\2\Data\JXC\rac.BG.040602.D
样品名称: rac.BG.01

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面积百分比报告

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排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 14.906 | MM | 0.4025 | 109.69575 | 4.54197 | 49.5115 |
| 2 | 18.606 | MM | 0.7355 | 111.86057 | 2.53483 | 50.4885 |
| 总量 : | | | | 221.55631 | 7.07680 | |

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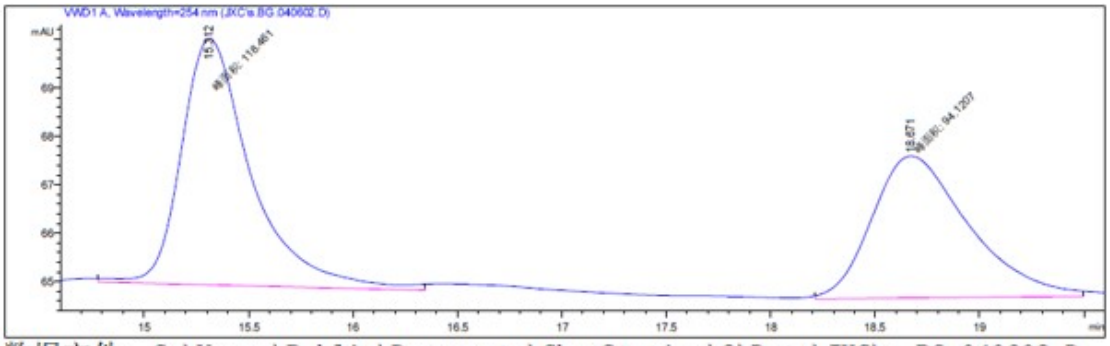
*** 报告结束 ***

*(S-BGE-PPNCl-Copolymer-25 °C)*




数据文件: C:\Users\Public\Documents\ChemStation\2\Data\JXC\s.BG.040602.D
样品名称: s.BG.01

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面积百分比报告

==========

排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 15.312 | MM | 0.3887 | 118.46051 | 5.07928 | 55.7248 |
| 2 | 18.671 | MM | 0.5360 | 94.12066 | 2.92672 | 44.2752 |
| 总量 : | | | | 212.58117 | 8.00600 | |

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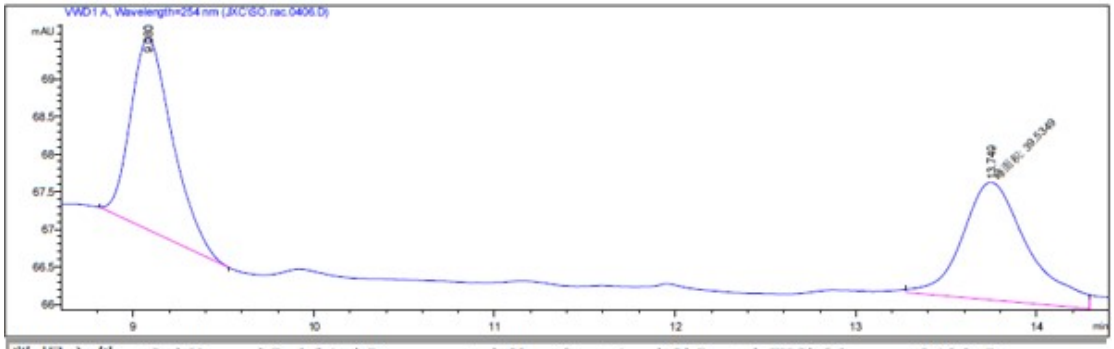
*** 报告结束 ***

***(Rac-SO-PPNCl-Copolymer-25 °C)***




数据文件: C:\Users\Public\Documents\ChemStation\2\Data\JXC\SO.rac.0406.D
样品名称: SO.rac

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面积百分比报告

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排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 9.080 | BB | 0.2455 | 41.40675 | 2.54952 | 51.1563 |
| 2 | 13.749 | MM | 0.4205 | 39.53486 | 1.56685 | 48.8437 |
| 总量 : | | | | 80.94161 | 4.11637 | |

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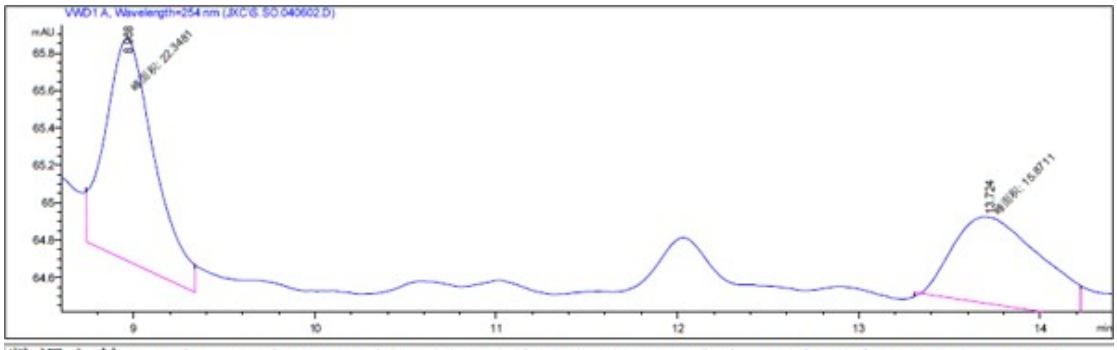
*** 报告结束 ***

***(S-SO-PPNCl-Copolymer-25 °C)***



数据文件：C:\Users\Public\Documents\ChemStation\2\Data\JXC\S.SO.040602.D
样品名称：S.SO.03

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面积百分比报告

==========

排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

| 峰 # | 保留时间 [min] | 类型 | 峰宽 [min] | 峰面积 [mAU*s] | 峰高 [mAU] | 峰面积 % |
|---|---|---|---|---|---|---|
| 1 | 8.968 | MM | 0.3141 | 22.34812 | 1.18568 | 58.4736 |
| 2 | 13.724 | MM | 0.5731 | 15.87105 | 4.61538e-1 | 41.5264 |
| 总量 : | | | | 38.21917 | 1.64722 | |

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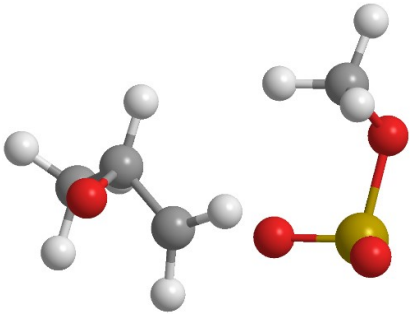
*** 报告结束 ***

***11. Computational details.***

All calculations were performed with Gaussian 16[4] suite of the programs. The DFT method of M06-2X was used for single point energy calculations, geometry optimizations and frequency analyses. The def2-SVP all election basis set was used for all atoms. Frequency calculations were performed to identify the geometrically optimized stationary points (no imaginary frequencies for minima and one imaginary frequency for transition-state structures), and to obtain the thermodynamic data. To improve the accuracy of the energy, the single point energy of each optimized structure was calculated with def2-TZVP for all atoms

and SMD solvation model with THF as a solvent was employed. The relative free energy was obtained by combining the single-point energy with Gibbs free energy correction.

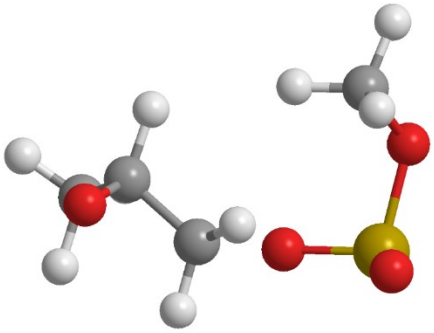
**PO-S-$CH_2$-R**



-1 1

| | | | |
|---|---|---|---|
| C | -1.35336 | -0.52122 | 0.68518 |
| C | -2.1909 | 0.46659 | 0.06594 |
| O | -2.7493 | -0.03909 | 1.25242 |
| H | -1.43977 | -1.59102 | 0.36033 |
| H | -0.51834 | -0.25406 | 1.37532 |
| H | -1.87222 | 1.51289 | 0.1231 |
| O | 0.27702 | -0.66889 | -0.82175 |
| S | 1.69958 | -0.70353 | -0.40658 |
| O | 2.12263 | 0.96564 | -0.52108 |
| O | 1.84238 | -0.98548 | 1.05639 |
| C | 1.45818 | 1.78915 | 0.38538 |
| H | 1.85038 | 2.81303 | 0.2676 |
| H | 0.3682 | 1.80926 | 0.20151 |
| H | 1.62506 | 1.4641 | 1.42659 |
| C | -2.90092 | 0.13514 | -1.2061 |
| H | -3.80321 | 0.75983 | -1.32729 |
| H | -2.22399 | 0.30675 | -2.05251 |
| H | -3.20997 | -0.92012 | -1.20128 |

**PO-S-$CH_2$-TS**

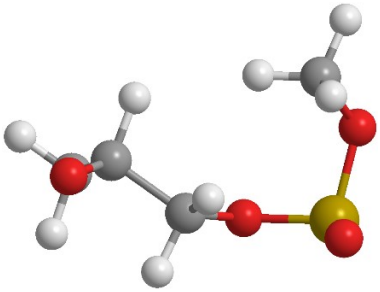


-1 1

| | | | |
|---|---|---|---|
| C | -1.12655800 | -0.54282300 | 0.49798400 |
| C | -2.19089600 | 0.40898500 | 0.13433500 |

| | | | |
|---|---|---|---|
| O | -2.83930200 | 0.01851400 | 1.25242000 |
| H | -1.41457000 | -1.58741600 | 0.40353000 |
| H | -0.51113800 | -0.28645800 | 1.35732400 |
| H | -1.82901800 | 1.47329200 | 0.11590000 |
| O | 0.19422300 | -0.65809000 | -0.75695100 |
| S | 1.69597500 | -0.69272600 | -0.39577700 |
| O | 2.10822500 | 0.94403800 | -0.52467700 |
| O | 1.84957800 | -0.99268400 | 1.04918600 |
| C | 1.45458300 | 1.79274900 | 0.38898100 |
| H | 1.86838400 | 2.80222500 | 0.25320100 |
| H | 0.36820400 | 1.82006000 | 0.20151000 |
| H | 1.62865500 | 1.46409600 | 1.42658900 |
| C | -2.89011800 | 0.13154400 | -1.19529600 |
| H | -3.78880900 | 0.76343200 | -1.28049000 |
| H | -2.22398600 | 0.31755000 | -2.05251200 |
| H | -3.21716900 | -0.92012000 | -1.20847700 |

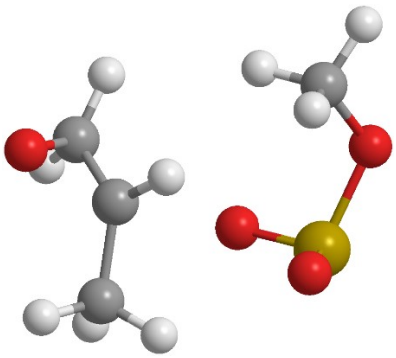
**PO-S-$CH_2$-P**



-1 1

| | | | |
|---|---|---|---|
| C | -0.89975800 | -0.56442300 | 0.31078400 |
| C | -2.19089600 | 0.35138500 | 0.20273500 |
| O | -2.92930200 | 0.07611400 | 1.25242000 |
| H | -1.38937000 | -1.58381600 | 0.44673000 |
| H | -0.50393800 | -0.31885800 | 1.33932400 |
| H | -1.78581800 | 1.43369200 | 0.10870000 |
| O | 0.11142300 | -0.64729000 | -0.69215100 |
| S | 1.69237500 | -0.68192600 | -0.38497700 |
| O | 2.09382500 | 0.92243800 | -0.52827700 |
| O | 1.85677800 | -0.99988400 | 1.04198600 |
| C | 1.45098300 | 1.79634900 | 0.39258100 |
| H | 1.88638400 | 2.79142500 | 0.23880100 |
| H | 0.36820400 | 1.83086000 | 0.20151000 |
| H | 1.63225500 | 1.46409600 | 1.42658900 |
| C | -2.87931800 | 0.12794400 | -1.18449600 |
| H | -3.77440900 | 0.76703200 | -1.23369000 |
| H | -2.22398600 | 0.32835000 | -2.05251200 |
| H | -3.22436900 | -0.92012000 | -1.21567700 |

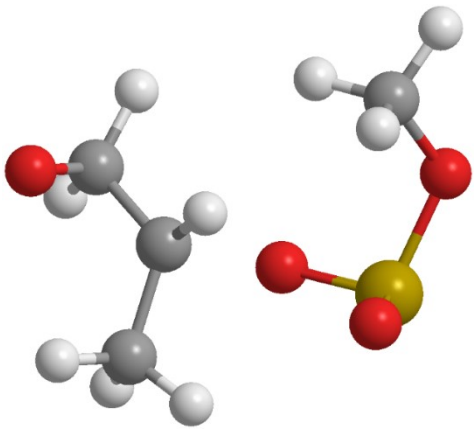
**PO-S-CH-R**



-1 1

| | | | |
|---|---|---|---|
| C | -1.61043700 | -0.00243200 | 0.26320400 |
| C | -2.20613700 | 0.94185200 | -0.64777900 |
| O | -2.96602900 | 0.78168500 | 0.53063600 |
| H | -0.83976500 | 0.37348200 | 0.98000000 |
| H | -1.74441400 | 1.91785300 | -0.79502900 |
| O | 0.23823500 | -0.39490200 | -1.01366500 |
| S | 1.52514500 | -0.72077300 | -0.36238200 |
| O | 2.25868500 | 0.83797400 | -0.27892600 |
| O | 1.33856000 | -1.08061800 | 1.08653200 |
| C | 1.55493200 | 1.76368000 | 0.48629200 |
| H | 2.15828800 | 2.68416400 | 0.55109300 |
| H | 0.57857300 | 2.01762800 | 0.03729200 |
| H | 1.37498400 | 1.38865900 | 1.51185700 |
| C | -1.83004800 | -1.50560400 | 0.20326400 |
| H | -1.98365300 | -1.85651700 | -0.82992900 |
| H | -0.94618700 | -2.02682900 | 0.61603300 |
| H | -2.73171200 | -1.75434400 | 0.81008000 |
| H | -2.66071000 | 0.55138900 | -1.56698600 |

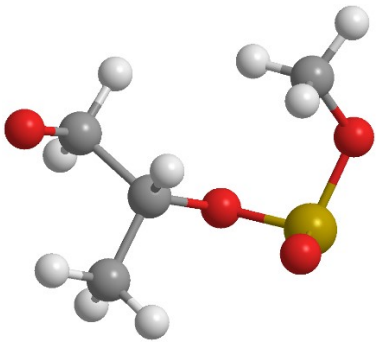
**PO-S-CH-TS**



-1 1

| | | | |
|---|---|---|---|
| C | -1.35963700 | -0.08163200 | 0.11360400 |
| C | -2.22373700 | 0.90225200 | -0.55537900 |
| O | -3.05402900 | 0.85648500 | 0.50863600 |
| H | -0.83096500 | 0.31188200 | 0.98000000 |
| H | -1.70481400 | 1.87385300 | -0.77302900 |
| O | 0.14583500 | -0.37290200 | -0.95646500 |
| S | 1.52074500 | -0.71197300 | -0.34918200 |
| O | 2.24108500 | 0.82037400 | -0.28772600 |
| O | 1.34736000 | -1.08941800 | 1.07773200 |
| C | 1.55053200 | 1.76808000 | 0.49069200 |
| H | 2.17588800 | 2.67096400 | 0.54229300 |
| H | 0.57857300 | 2.02642800 | 0.03729200 |
| H | 1.37938400 | 1.38865900 | 1.51185700 |
| C | -1.80364800 | -1.51440400 | 0.19446400 |
| H | -2.01885300 | -1.89171700 | -0.81672900 |
| H | -1.00778700 | -2.11922900 | 0.64683300 |
| H | -2.71411200 | -1.56074400 | 0.80128000 |
| H | -2.61231000 | 0.52938900 | -1.54058600 |

**PO-S-CH-P**

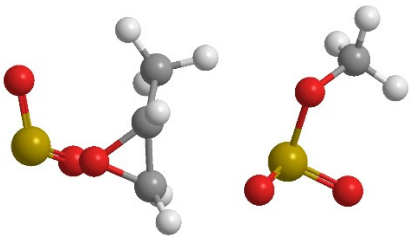


-1 1

| | | | |
|---|---|---|---|
| C | -1.10883700 | -0.16083200 | -0.03599600 |
| C | -2.24133700 | 0.86265200 | -0.46297900 |
| O | -3.14202900 | 0.93128500 | 0.48663600 |
| H | -0.82216500 | 0.25028200 | 0.98000000 |
| H | -1.66521400 | 1.82985300 | -0.75102900 |
| O | 0.05343500 | -0.35090200 | -0.89926500 |
| S | 1.51634500 | -0.70317300 | -0.33598200 |
| O | 2.22348500 | 0.80277400 | -0.29652600 |
| O | 1.35616000 | -1.09821800 | 1.06893200 |
| C | 1.54613200 | 1.77248000 | 0.49509200 |
| H | 2.19348800 | 2.65776400 | 0.53349300 |
| H | 0.57857300 | 2.03522800 | 0.03729200 |
| H | 1.38378400 | 1.38865900 | 1.51185700 |
| C | -1.77724800 | -1.52320400 | 0.18566400 |

| | | | |
|---|---|---|---|
| H | -2.05405300 | -1.92691700 | -0.80352900 |
| H | -1.06938700 | -2.21162900 | 0.67763300 |
| H | -2.69651200 | -1.36714400 | 0.79248000 |
| H | -2.56391000 | 0.50738900 | -1.51418600 |

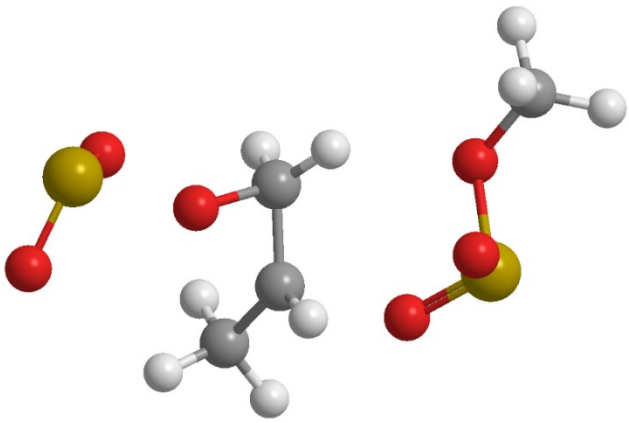
**$SO_2$-PO-S-$CH_2$-R**



-1 1

| | | | |
|---|---|---|---|
| C | -0.74335700 | -1.07498300 | 0.83160400 |
| C | -0.80528700 | 0.30956800 | 1.27063400 |
| O | -1.97321600 | -0.54393700 | 1.13983500 |
| H | -0.53813400 | -1.25906200 | -0.25888400 |
| H | -0.35108400 | -1.86012100 | 1.54208400 |
| H | -0.59394100 | 0.51660900 | 2.32096500 |
| S | -3.34944300 | -0.20962500 | -0.44069200 |
| O | -2.42787600 | -0.53463000 | -1.52450900 |
| O | -3.60813400 | 1.21345300 | -0.25264900 |
| C | -0.61208800 | 1.44469500 | 0.32582600 |
| H | -1.23494300 | 2.30846500 | 0.60613700 |
| H | 0.45634000 | 1.70028100 | 0.38445000 |
| H | -0.84507300 | 1.15574200 | -0.70658700 |
| O | 1.63436400 | -1.16325700 | 0.77813100 |
| S | 2.25725500 | -0.54818100 | -0.39438900 |
| O | 3.56688100 | -1.18575000 | -0.70541500 |
| O | 2.74074100 | 0.95899300 | 0.37961300 |
| C | 3.70366600 | 1.66067500 | -0.33008800 |
| H | 3.99019200 | 2.55611800 | 0.24382800 |
| H | 4.60483300 | 1.04355800 | -0.50910800 |
| H | 3.33913100 | 2.00420900 | -1.32268500 |

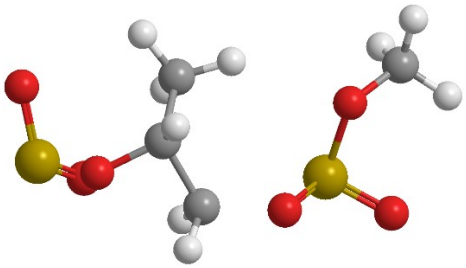
**$SO_2$-PO-S-$CH_2$-TS**



-1 1

| | | | |
|---|---|---|---|
| C | -0.24513700 | -0.87319500 | 0.21893300 |
| C | -0.29833700 | 0.58068500 | 0.24400100 |
| O | -1.44837900 | 0.24678500 | 0.99585600 |
| H | 0.16166400 | -1.33973600 | 1.11328700 |
| H | 0.48079100 | 1.08542800 | 0.82619600 |
| S | -3.21370800 | 0.69030700 | 0.21691500 |
| O | -3.85192200 | -0.62185300 | 0.37575700 |
| O | -2.79935900 | 1.00655300 | -1.16298000 |
| O | 1.58053500 | -1.31982600 | -0.68550500 |
| S | 2.78575300 | -0.66180800 | -0.05280700 |
| O | 2.57592300 | -0.42608300 | 1.40089700 |
| O | 2.56146400 | 0.91610300 | -0.72504100 |
| C | 3.36889400 | 1.88944600 | -0.13246400 |
| H | 3.15577800 | 2.85193000 | -0.62107000 |
| H | 3.17171700 | 1.98202800 | 0.94923300 |
| H | 4.44881000 | 1.67212000 | -0.26223500 |
| C | -1.03900200 | -1.68667600 | -0.75410100 |
| H | -1.39908600 | -1.05447000 | -1.57577800 |
| H | -0.39583400 | -2.48617200 | -1.13758000 |
| H | -1.91837300 | -2.10759800 | -0.25070700 |
| H | -0.52279700 | 1.06550000 | -0.71715700 |

**$SO_2$-PO-S-$CH_2$-P**

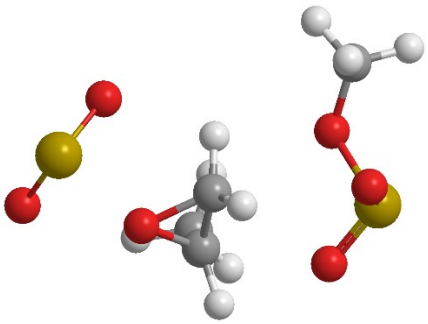


-1 1

| | | | |
|---|---|---|---|
| C | -0.14575700 | -1.08218300 | 0.77400400 |

| | | | |
|---|---|---|---|
| C | -0.89168700 | 0.18716800 | 1.20583400 |
| O | -2.16041600 | -0.42873700 | 1.13263500 |
| H | -0.52373400 | -1.33106200 | -0.26608400 |
| H | -0.40868400 | -1.91052100 | 1.50608400 |
| H | -0.65154100 | 0.45180900 | 2.25616500 |
| S | -3.31344300 | -0.20962500 | -0.39029200 |
| O | -2.41347600 | -0.53463000 | -1.52450900 |
| O | -3.61533400 | 1.22785300 | -0.27424900 |
| C | -0.62648800 | 1.41589500 | 0.32582600 |
| H | -1.28534300 | 2.23646500 | 0.62773700 |
| H | 0.42754000 | 1.71468100 | 0.42765000 |
| H | -0.85947300 | 1.17734200 | -0.72098700 |
| O | 1.46156400 | -1.14885700 | 0.79253100 |
| S | 2.25005500 | -0.51218100 | -0.42318900 |
| O | 3.52368100 | -1.20735000 | -0.65501500 |
| O | 2.72634100 | 0.91579300 | 0.37961300 |
| C | 3.69646600 | 1.64627500 | -0.33008800 |
| H | 3.94699200 | 2.52731800 | 0.27982800 |
| H | 4.60483300 | 1.05075800 | -0.49470800 |
| H | 3.31753100 | 1.99700900 | -1.30828500 |

**$SO_2$-PO-S-CH-R**

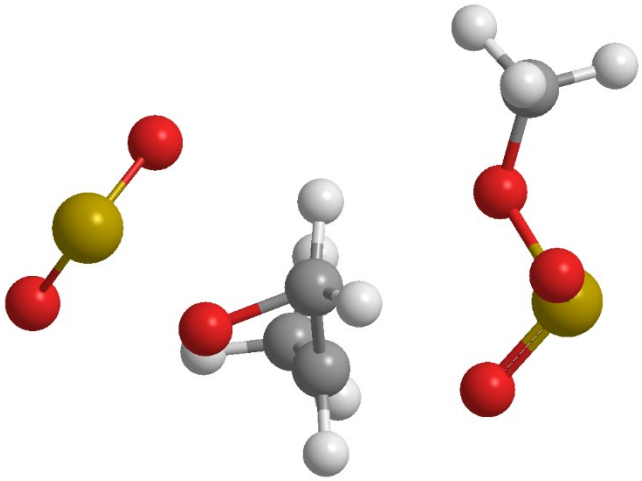


-1 1

| | | | |
|---|---|---|---|
| C | -0.44881200 | -1.21631900 | 0.01485900 |
| C | -0.23960700 | -0.20782500 | 1.04421700 |
| O | -1.54200100 | -0.80955700 | 0.92171100 |
| H | -0.11483100 | -2.25157200 | 0.28415400 |
| H | 0.30579300 | -0.43991200 | 1.95994400 |
| S | -3.06531600 | 0.48335100 | 0.36699700 |
| O | -3.73341400 | -0.43698100 | -0.54548500 |
| O | -2.23975400 | 1.51351900 | -0.26140400 |
| O | 1.91698700 | -1.50408000 | -0.48996200 |
| S | 2.81173100 | -0.42311300 | -0.04121000 |
| O | 2.66086600 | -0.09701400 | 1.41301000 |
| O | 1.96768700 | 0.92896900 | -0.78584400 |
| C | 2.34293200 | 2.17315200 | -0.30078300 |

| | | | |
|---|---|---|---|
| H | 1.67423900 | 2.93447000 | -0.73616500 |
| H | 2.26605000 | 2.22291800 | 0.80111300 |
| H | 3.38415100 | 2.44485000 | -0.57187000 |
| C | -0.58531700 | -0.90062000 | -1.46476600 |
| H | -0.25746900 | 0.12504300 | -1.66643100 |
| H | 0.05892100 | -1.58321400 | -2.03985100 |
| H | -1.64404500 | -1.02596200 | -1.75437100 |
| H | -0.20159300 | 0.82880400 | 0.69752200 |

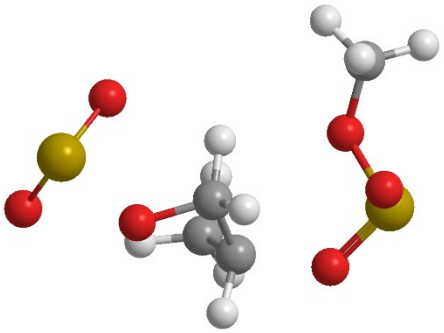
**$SO_2$-PO-S-CH-TS**



-1 1

| | | | |
|---|---|---|---|
| C | -0.21121200 | -1.23431900 | -0.05714100 |
| C | -0.29720700 | -0.24742500 | 1.01181700 |
| O | -1.61760100 | -0.75195700 | 0.97931100 |
| H | -0.15083100 | -2.27317200 | 0.25535400 |
| H | 0.25179300 | -0.44711200 | 1.93834400 |
| S | -3.05451600 | 0.47615100 | 0.38139700 |
| O | -3.72621400 | -0.44058100 | -0.54908500 |
| O | -2.23255400 | 1.51351900 | -0.26500400 |
| O | 1.82698700 | -1.48968000 | -0.47556200 |
| S | 2.79733100 | -0.41591300 | -0.03761000 |
| O | 2.67166600 | -0.10061400 | 1.40941000 |
| O | 1.98208700 | 0.91456900 | -0.78584400 |
| C | 2.34293200 | 2.17315200 | -0.29718300 |
| H | 1.65983900 | 2.91287000 | -0.73976500 |
| H | 2.25885000 | 2.21931800 | 0.80111300 |
| H | 3.38055100 | 2.44845000 | -0.57547000 |
| C | -0.56371700 | -0.90782000 | -1.47556600 |
| H | -0.27906900 | 0.12864300 | -1.69163100 |
| H | -0.00587900 | -1.58321400 | -2.13345100 |
| H | -1.64404500 | -1.02956200 | -1.62837100 |
| H | -0.21599300 | 0.79640400 | 0.67592200 |

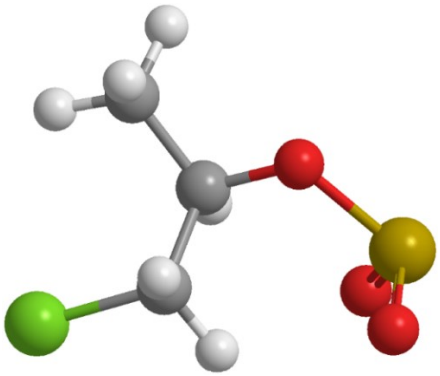
**$SO_2$-PO-S-CH-P**



-1 1

| | | | |
|---|---|---|---|
| C | 0.04618800 | -1.25381900 | -0.13514100 |
| C | -0.35960700 | -0.29032500 | 0.97671700 |
| O | -1.69950100 | -0.68955700 | 1.04171100 |
| H | -0.18983100 | -2.29657200 | 0.22415400 |
| H | 0.19329300 | -0.45491200 | 1.91494400 |
| S | -3.04281600 | 0.46835100 | 0.39699700 |
| O | -3.71841400 | -0.44448100 | -0.55298500 |
| O | -2.22475400 | 1.51351900 | -0.26890400 |
| O | 1.72948700 | -1.47408000 | -0.45996200 |
| S | 2.78173100 | -0.40811300 | -0.03371000 |
| O | 2.68336600 | -0.10451400 | 1.40551000 |
| O | 1.99768700 | 0.89896900 | -0.78584400 |
| C | 2.34293200 | 2.17315200 | -0.29328300 |
| H | 1.64423900 | 2.88947000 | -0.74366500 |
| H | 2.25105000 | 2.21541800 | 0.80111300 |
| H | 3.37665100 | 2.45235000 | -0.57937000 |
| C | -0.54031700 | -0.91562000 | -1.48726600 |
| H | -0.30246900 | 0.13254300 | -1.71893100 |
| H | -0.07607900 | -1.58321400 | -2.23485100 |
| H | -1.64404500 | -1.03346200 | -1.49187100 |
| H | -0.23159300 | 0.76130400 | 0.65252200 |

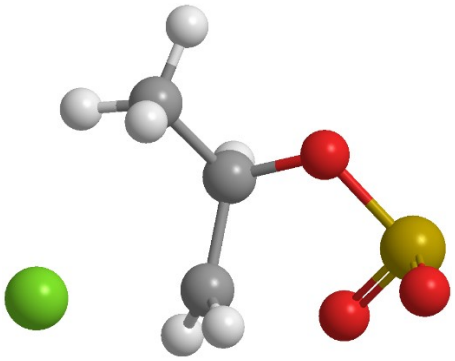
**Backbite-Path a-R**



-1 1

| | | | |
|---|---|---|---|
| C | -0.48205700 | 0.80673800 | -0.18391800 |
| C | -0.98794800 | -0.48047800 | 0.46868000 |
| H | -0.30449700 | -1.30179400 | 0.23066700 |
| S | 2.10335800 | -0.00480600 | -0.05555300 |
| O | 1.98429400 | -1.02368900 | 1.02286400 |
| O | 0.76136400 | 1.11201300 | 0.36748200 |
| O | 1.63279500 | -0.52693200 | -1.37214900 |
| H | -1.05352100 | -0.35952200 | 1.55739400 |
| Cl | -2.63740500 | -0.95207500 | -0.12456200 |
| C | -1.40294900 | 1.99611100 | 0.04865000 |
| H | -0.95774500 | 2.88993200 | -0.41041400 |
| H | -2.40016200 | 1.82098600 | -0.37890800 |
| H | -1.50229400 | 2.18220500 | 1.12965800 |
| H | -0.38951600 | 0.60500600 | -1.26803100 |

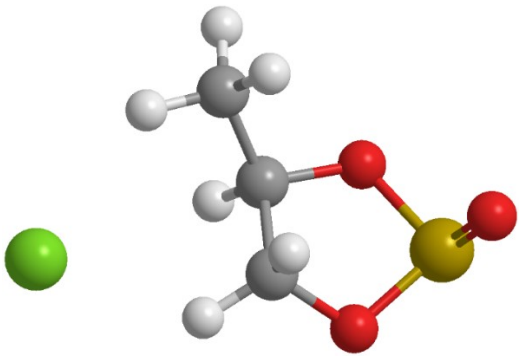
**Backbite-Path a-TS**



-1 1

| | | | |
|---|---|---|---|
| C | -0.32728600 | 0.86526000 | -0.49239600 |
| C | -0.61973100 | -0.62600800 | -0.34623300 |
| H | -0.95031200 | -1.22106800 | -1.18471600 |
| S | 2.09893800 | -0.07858200 | -0.10222100 |
| O | 2.25536900 | -0.64241900 | 1.25056300 |
| O | 0.93546000 | 1.15706000 | 0.09124900 |
| O | 1.19326600 | -0.96531600 | -0.97923200 |
| H | -0.41153200 | -1.11349900 | 0.60092400 |
| Cl | -2.87727900 | -0.73643400 | 0.24279400 |
| C | -1.30341900 | 1.83634200 | 0.14630400 |
| H | -0.88928400 | 2.85029400 | 0.04541600 |
| H | -2.28585000 | 1.75986300 | -0.32943800 |
| H | -1.42765400 | 1.59190000 | 1.20850000 |
| H | -0.27477300 | 1.06102000 | -1.57934300 |

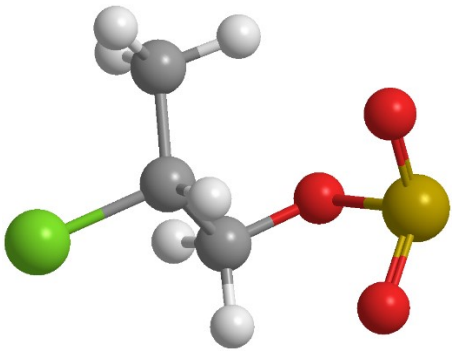
**Backbite-Path a-P**



-1 1

| | | | |
|---|---|---|---|
| C | -0.33279800 | 0.59449200 | -0.30550000 |
| C | -0.20263700 | -0.63660500 | 0.58685800 |
| H | -1.12885100 | -1.22359600 | 0.51912800 |
| S | 2.09021400 | -0.31577100 | -0.38368100 |
| O | 2.76229400 | 0.14220500 | 0.83340300 |
| O | 1.01076900 | 0.83123700 | -0.82120200 |
| O | 0.90637700 | -1.36963000 | 0.03850500 |
| H | 0.02479700 | -0.36150100 | 1.62990200 |
| Cl | -3.37670100 | -0.43816300 | -0.06608800 |
| C | -0.86104300 | 1.81262700 | 0.40882700 |
| H | -0.87655200 | 2.67788600 | -0.26862100 |
| H | -1.89192600 | 1.56122500 | 0.70297500 |
| H | -0.23376600 | 2.05124900 | 1.28140300 |
| H | -0.98985700 | 0.34227000 | -1.14915100 |

**Backbite-Path b-R**

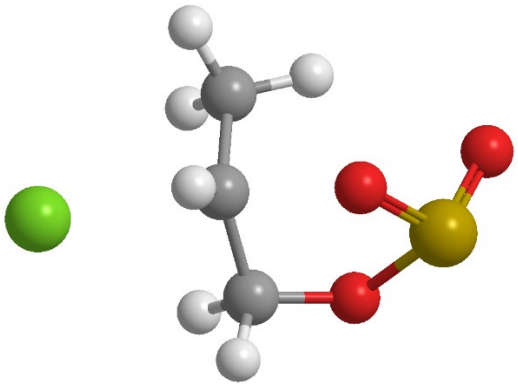


-1 1

| | | | |
|---|---|---|---|
| C | -0.36692200 | -0.54700400 | -0.97972300 |
| C | -1.07924100 | 0.21200000 | 0.14293000 |
| H | -0.54600500 | 0.02313200 | 1.08224200 |
| S | 2.09210300 | -0.09284400 | 0.00303400 |
| O | 1.76391500 | 1.10288300 | 0.83310700 |
| O | 0.85773200 | 0.03295500 | -1.28579200 |
| O | 1.68057000 | -1.36132900 | 0.67115000 |
| H | -1.00190900 | -0.51546900 | -1.88520900 |

| | | | |
|---|---|---|---|
| Cl | -2.73976900 | -0.52604300 | 0.34910600 |
| H | -0.25602000 | -1.59922600 | -0.66180800 |
| C | -1.19866000 | 1.69506600 | -0.11769800 |
| H | -1.74008600 | 2.19477200 | 0.69786800 |
| H | -0.17425200 | 2.08729100 | -0.17187400 |
| H | -1.72810500 | 1.88129200 | -1.06533600 |

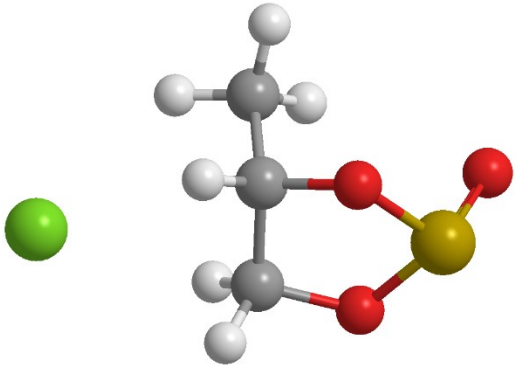
**Backbite-Path b-TS**



-1 1

| | | | |
|---|---|---|---|
| C | -0.40271300 | -1.09065400 | -0.23702900 |
| C | -0.78178100 | 0.24712600 | 0.37070800 |
| H | -1.13330400 | 0.30253200 | 1.39090300 |
| S | 2.04918200 | -0.27580000 | 0.25879900 |
| O | 2.60452400 | 0.75926600 | -0.63536700 |
| O | 0.91772300 | -1.09579400 | -0.73193500 |
| O | 0.99527000 | 0.30018800 | 1.22223600 |
| H | -1.06262200 | -1.27712500 | -1.09090400 |
| Cl | -3.11291700 | -0.09692200 | 0.02199800 |
| H | -0.56561400 | -1.88468600 | 0.51175700 |
| C | -0.68653200 | 1.48627800 | -0.48070100 |
| H | -1.17233600 | 2.33012000 | 0.02355000 |
| H | 0.36624900 | 1.71896000 | -0.68224400 |
| H | -1.21366700 | 1.30489300 | -1.42517600 |

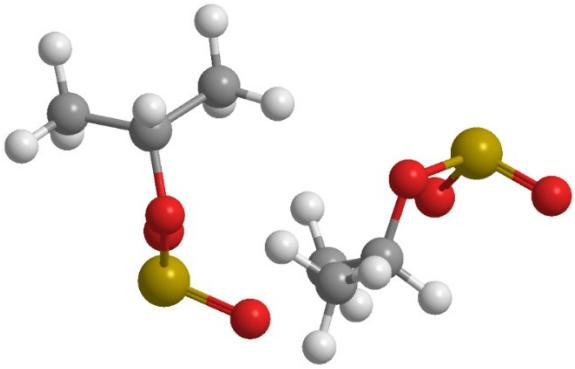
**Backbite-Path b-P**



-1 1

| | | | |
|---|---|---|---|
| C | -0.41800900 | -0.91267900 | -0.23190000 |
| C | -0.36303900 | 0.44448600 | 0.46342700 |
| H | -1.14456200 | 0.48969100 | 1.22752200 |
| S | 2.06713100 | -0.34805300 | 0.26106300 |
| O | 2.66117800 | 0.57977400 | -0.70169900 |
| O | 0.95431900 | -1.24698600 | -0.54488900 |
| O | 0.92441900 | 0.41748600 | 1.14425100 |
| H | -1.01254600 | -0.86896600 | -1.14853000 |
| Cl | -3.37038800 | -0.17318100 | -0.01177300 |
| H | -0.84664500 | -1.68338700 | 0.42113400 |
| C | -0.47642400 | 1.61712000 | -0.48725700 |
| H | -0.25799800 | 2.55675400 | 0.03978100 |
| H | 0.22818800 | 1.51004200 | -1.32482100 |
| H | -1.51842000 | 1.61303100 | -0.83887500 |

**Backbite-Path c-R**



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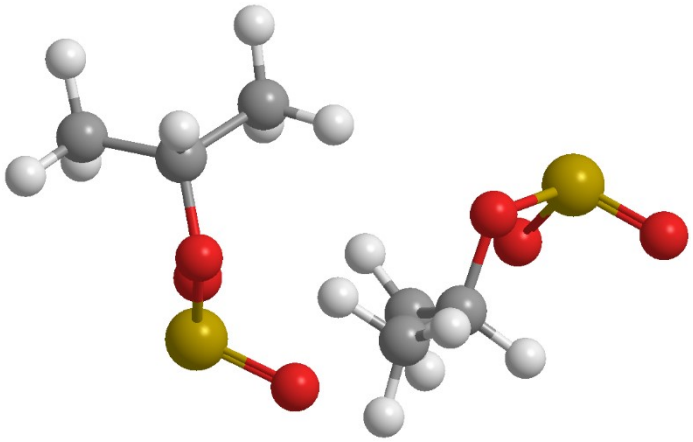
| | | | |
|---|---|---|---|
| C | 2.30572300 | 0.32744300 | -0.61687300 |
| C | 1.43979600 | 1.53596500 | -0.13358700 |
| C | 3.47734200 | 0.03131500 | 0.30830100 |
| H | 4.06050900 | 0.95469500 | 0.45305000 |
| H | 3.07989300 | -0.28281700 | 1.28318200 |
| S | 0.13896400 | -1.22612500 | 0.10818800 |
| O | 0.19102300 | 1.40269300 | -0.52252300 |
| O | 1.48884100 | -0.83893500 | -0.77529900 |
| O | 0.34087200 | -0.66240400 | 1.45470400 |
| H | 2.66207100 | 0.53039300 | -1.64224300 |
| H | 1.60689100 | 1.59566600 | 0.98893300 |
| O | -1.38622700 | -0.80666600 | -0.42933800 |
| C | -2.19897600 | 0.37117400 | -0.25480300 |
| H | -1.77595100 | 1.14879400 | -0.89962300 |
| C | -3.59532600 | -0.05118200 | -0.69394700 |
| H | -4.27654400 | 0.81141900 | -0.66571000 |
| H | -3.57850700 | -0.45110300 | -1.71977000 |

| | | | |
|---|---|---|---|
| H | -3.99037300 | -0.83395200 | -0.02709200 |
| C | -2.18938900 | 0.88269500 | 1.17800500 |
| H | -2.93017700 | 1.69329700 | 1.27853300 |
| H | -2.44624900 | 0.07544000 | 1.88584800 |
| H | -1.18541200 | 1.26281000 | 1.39119300 |
| H | 2.01514900 | 2.44947200 | -0.52411200 |
| H | 4.14898900 | -0.75167800 | -0.07932000 |

**Backbite-Path c-TS**



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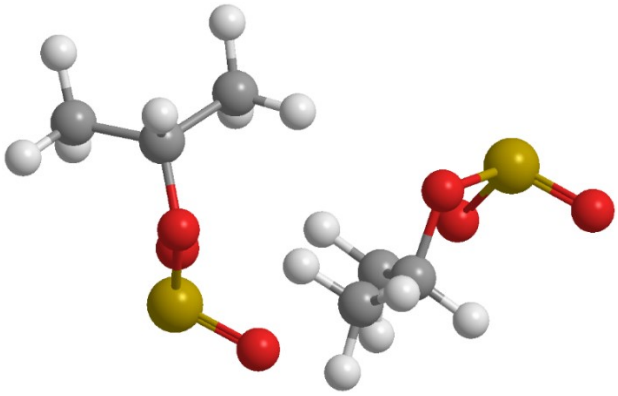
| | | | |
|---|---|---|---|
| C | 1.47379500 | -0.83471300 | 0.70664200 |
| C | 0.76491800 | -0.87038800 | -0.64371800 |
| H | 0.14072000 | -0.04359600 | -0.96210500 |
| S | 3.02137900 | 0.90205900 | -0.33686200 |
| O | 4.27323100 | 0.20389600 | 0.01576000 |
| O | 1.92451200 | 0.49631900 | 0.91532700 |
| O | 2.25475900 | 0.11738900 | -1.42173200 |
| S | -2.18775000 | -1.22159700 | -0.41152600 |
| O | -0.82681100 | -1.88410000 | -0.19470700 |
| O | -2.17019700 | -0.37574900 | -1.63363400 |
| O | -2.15188700 | -0.10279000 | 0.88890400 |
| C | -2.39935900 | 1.28748400 | 0.73412500 |
| H | -2.42619600 | 1.64760400 | 1.77775200 |
| C | -1.26409100 | 2.01557000 | 0.02077700 |
| H | -0.29448700 | 1.73176200 | 0.45810000 |
| H | -1.26178900 | 1.75938800 | -1.04725500 |
| H | -1.39034700 | 3.10464100 | 0.12825400 |
| C | -3.76756000 | 1.56384500 | 0.11331800 |
| H | -4.54742700 | 1.02330000 | 0.67045600 |
| H | -3.99291300 | 2.64051100 | 0.15207200 |
| H | -3.78124400 | 1.23088600 | -0.93251600 |
| H | 2.36170500 | -1.48527600 | 0.61201100 |
| C | 0.68589500 | -1.23949000 | 1.93734400 |

| | | | |
|---|---|---|---|
| H | 0.39925600 | -2.29549700 | 1.87631200 |
| H | 1.32659400 | -1.07012600 | 2.81397000 |
| H | -0.23350500 | -0.64766300 | 2.01613600 |
| H | 0.97113000 | -1.65689900 | -1.35922400 |

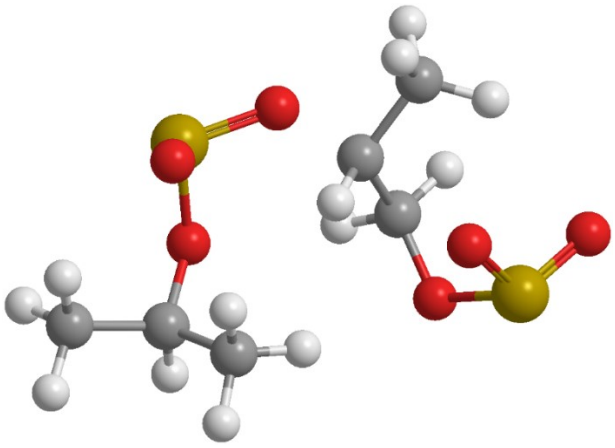
**Backbite-Path c-P**



-1 1

| | | | |
|---|---|---|---|
| C | 1.49079500 | -0.83131300 | 0.70324200 |
| C | 0.98251800 | -0.74118800 | -0.73211800 |
| H | 0.07272000 | -0.08099600 | -0.93150500 |
| S | 3.01457900 | 0.89865900 | -0.31646200 |
| O | 4.26983100 | 0.20729600 | 0.00216000 |
| O | 1.95171200 | 0.51331900 | 0.91532700 |
| O | 2.17655900 | 0.05618900 | -1.38773200 |
| S | -2.19795000 | -1.23859700 | -0.41492600 |
| O | -0.91181100 | -1.93170000 | -0.17770700 |
| O | -2.15999700 | -0.36894900 | -1.63363400 |
| O | -2.14508700 | -0.08579000 | 0.90250400 |
| C | -2.39935900 | 1.28408400 | 0.73752500 |
| H | -2.43299600 | 1.67140400 | 1.77775200 |
| C | -1.26749100 | 2.01897000 | 0.02077700 |
| H | -0.30128700 | 1.73516200 | 0.46150000 |
| H | -1.26518900 | 1.74918800 | -1.04385500 |
| H | -1.39034700 | 3.10804100 | 0.12145400 |
| C | -3.76756000 | 1.56384500 | 0.11331800 |
| H | -4.54742700 | 1.02330000 | 0.67045600 |
| H | -3.99631300 | 2.64051100 | 0.14527200 |
| H | -3.77444400 | 1.22068600 | -0.92911600 |
| H | 2.38550500 | -1.48187600 | 0.65621100 |
| C | 0.67909500 | -1.23269000 | 1.92034400 |
| H | 0.39245600 | -2.28529700 | 1.84231200 |
| H | 1.31639400 | -1.07012600 | 2.80037000 |
| H | -0.24710500 | -0.64766300 | 1.98553600 |
| H | 0.92013000 | -1.70449900 | -1.32862400 |

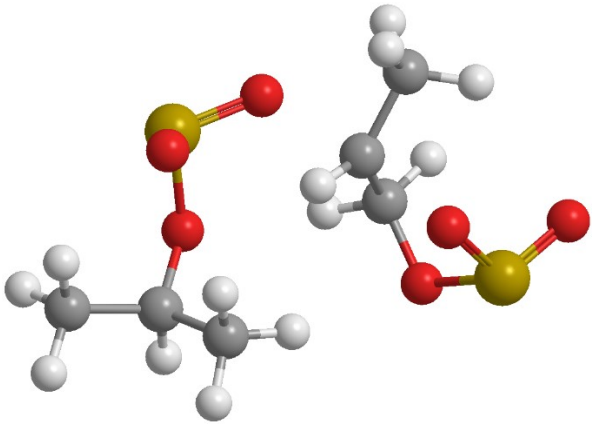
**Backbite-Path d-R**



-1 1

| | | | |
|---|---|---|---|
| C | 1.12496600 | 0.19246500 | -1.14274100 |
| C | 0.56943500 | 1.03201700 | 0.05667700 |
| H | 0.19491700 | 0.36373200 | 0.92695400 |
| H | 0.24839500 | 0.02685900 | -1.78329700 |
| S | 2.95917100 | -1.00092800 | 0.25138500 |
| O | 3.97666800 | -0.10720200 | -0.39104800 |
| O | 1.68824300 | -1.06873800 | -0.93545500 |
| O | 2.19939900 | -0.28066300 | 1.30130100 |
| S | -2.13826400 | 1.25304300 | -0.22064300 |
| O | -0.68166000 | 1.77227900 | -0.54905300 |
| O | -2.24021700 | 0.98195300 | 1.22570100 |
| O | -2.00472700 | -0.24393500 | -0.97622000 |
| C | -2.34342400 | -1.48329100 | -0.33386500 |
| H | -2.28195200 | -2.19704000 | -1.16902500 |
| C | -1.32567200 | -1.89442600 | 0.72407500 |
| H | -0.30244300 | -1.82061200 | 0.32507900 |
| H | -1.40862800 | -1.25525600 | 1.60795200 |
| H | -1.51444500 | -2.94082300 | 1.02180100 |
| C | -3.77991200 | -1.47170100 | 0.18268100 |
| H | -4.46932000 | -1.17309300 | -0.62143400 |
| H | -4.06160900 | -2.47489400 | 0.52943900 |
| H | -3.88219200 | -0.76983400 | 1.01895000 |
| H | 1.83526800 | 0.85106600 | -1.68497800 |
| C | 1.45073600 | 2.19656200 | 0.53018500 |
| H | 1.27832500 | 3.02737700 | -0.18179500 |
| H | 1.16383700 | 2.52649300 | 1.53388000 |
| H | 2.51290200 | 1.90088600 | 0.52272900 |

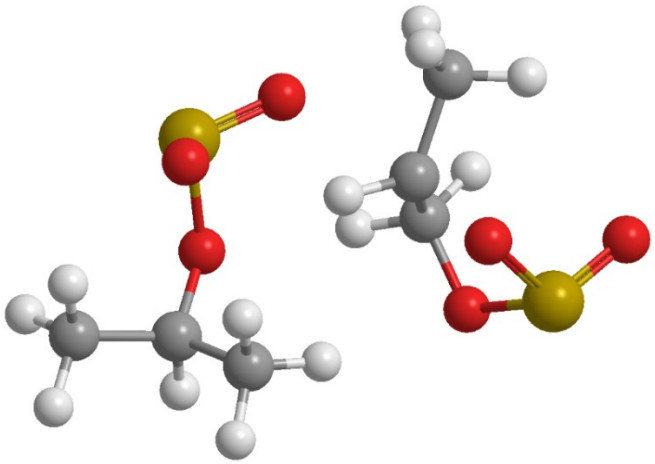
**Backbite-Path d-TS**



-1 1

| | | | |
|---|---|---|---|
| C | 1.13336600 | 0.18826500 | -1.11754100 |
| C | 0.78363500 | 0.89341700 | 0.19527700 |
| H | 0.09831700 | 0.42673200 | 0.89335400 |
| H | 0.20639500 | 0.03105900 | -1.67409700 |
| S | 2.95497100 | -0.99672800 | 0.23038500 |
| O | 3.97666800 | -0.11560200 | -0.38264800 |
| O | 1.71344300 | -1.08553800 | -0.93545500 |
| O | 2.11959900 | -0.21346300 | 1.24670100 |
| S | -2.15086400 | 1.26984300 | -0.22484300 |
| O | -0.77406000 | 1.82267900 | -0.59105300 |
| O | -2.22761700 | 0.97355300 | 1.22990100 |
| O | -1.99632700 | -0.26493500 | -0.98042000 |
| C | -2.34342400 | -1.48329100 | -0.33806500 |
| H | -2.29035200 | -2.21804000 | -1.16062500 |
| C | -1.32987200 | -1.89862600 | 0.72407500 |
| H | -0.30664300 | -1.82901200 | 0.32507900 |
| H | -1.41282800 | -1.24685600 | 1.60375200 |
| H | -1.51444500 | -2.94082300 | 1.03020100 |
| C | -3.77991200 | -1.47170200 | 0.18268100 |
| H | -4.46932000 | -1.17309400 | -0.62143400 |
| H | -4.06580900 | -2.47489500 | 0.53363900 |
| H | -3.87379200 | -0.76143500 | 1.01475000 |
| H | 1.81426800 | 0.84266600 | -1.68917800 |
| C | 1.46333600 | 2.19236200 | 0.53858500 |
| H | 1.18592500 | 2.95177700 | -0.20279500 |
| H | 1.15963700 | 2.53909300 | 1.53388000 |
| H | 2.54650200 | 2.02688600 | 0.51852900 |

**Backbite-Path d-P**



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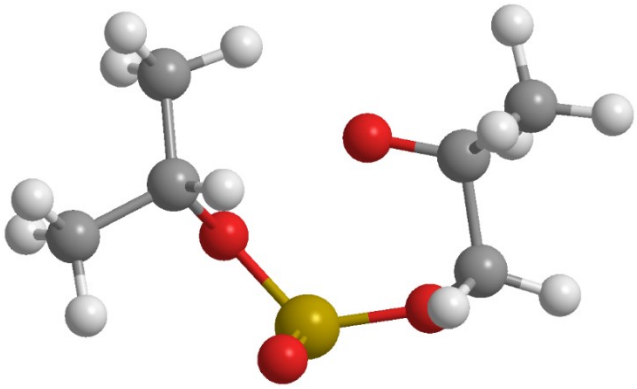
| | | | |
|---|---|---|---|
| C | 1.14176600 | 0.18406500 | -1.09234100 |
| C | 0.99783500 | 0.75481700 | 0.33387700 |
| H | 0.00171700 | 0.48973200 | 0.85975400 |
| H | 0.16439500 | 0.03525900 | -1.56489700 |
| S | 2.95077100 | -0.99252800 | 0.20938500 |
| O | 3.97666800 | -0.12400200 | -0.37424800 |
| O | 1.73864300 | -1.10233800 | -0.93545500 |
| O | 2.03979900 | -0.14626300 | 1.19210100 |
| S | -2.16346400 | 1.28664300 | -0.22904300 |
| O | -0.86646000 | 1.87307900 | -0.63305300 |
| O | -2.21501700 | 0.96515300 | 1.23410100 |
| O | -1.98792700 | -0.28593500 | -0.98462000 |
| C | -2.34342400 | -1.48329100 | -0.34226500 |
| H | -2.29875200 | -2.23904000 | -1.15222500 |
| C | -1.33407200 | -1.90282600 | 0.72407500 |
| H | -0.31084300 | -1.83741200 | 0.32507900 |
| H | -1.41702800 | -1.23845600 | 1.59955200 |
| H | -1.51444500 | -2.94082300 | 1.03860100 |
| C | -3.77991200 | -1.47170100 | 0.18268100 |
| H | -4.46932000 | -1.17309300 | -0.62143400 |
| H | -4.07000900 | -2.47489400 | 0.53783900 |
| H | -3.86539200 | -0.75303400 | 1.01055000 |
| H | 1.79326800 | 0.83426600 | -1.69337800 |
| C | 1.47593600 | 2.18816200 | 0.54698500 |
| H | 1.09352500 | 2.87617700 | -0.22379500 |
| H | 1.15543700 | 2.55169300 | 1.53388000 |
| H | 2.58010200 | 2.15288600 | 0.51432900 |

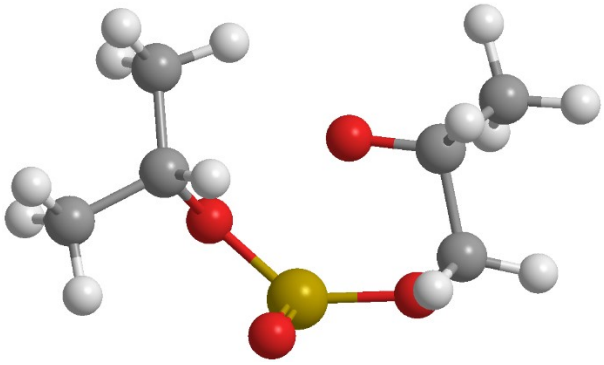
**Backbite-Path e-R**



-1 1

| | | | |
|---|---|---|---|
| C | 2.19986400 | -0.61177800 | 0.60312700 |
| C | 1.97186500 | 0.91790200 | 0.65018200 |
| C | 2.86776000 | 1.58233100 | -0.42660900 |
| H | 2.61376100 | 1.14744600 | -1.40698900 |
| H | 2.61866600 | 2.65531500 | -0.45491700 |
| S | -0.11933500 | -1.35204800 | -0.59086200 |
| O | 0.68192300 | 1.15866600 | 0.47587000 |
| O | 1.52049000 | -1.10944100 | -0.55463200 |
| O | -0.44780800 | -1.78531300 | 0.78559200 |
| H | 3.25114100 | -0.93386800 | 0.46994600 |
| H | 2.42577600 | 1.24085100 | 1.65724100 |
| O | -1.23200100 | -0.14272800 | -0.88928400 |
| C | -1.90034800 | 0.53832500 | 0.19012300 |
| H | -1.24160500 | 0.46823800 | 1.06605000 |
| C | -3.23757200 | -0.15446700 | 0.43102100 |
| H | -3.78149200 | 0.33719500 | 1.25256400 |
| H | -3.86638200 | -0.11343400 | -0.47446300 |
| H | -3.06725700 | -1.20653500 | 0.69894400 |
| C | -2.02548300 | 1.99830400 | -0.19129800 |
| H | -2.54084500 | 2.55530700 | 0.60959500 |
| H | -0.99759900 | 2.36914000 | -0.29881400 |
| H | -2.59643700 | 2.11496100 | -1.12781000 |
| H | 3.95462100 | 1.46636600 | -0.24161000 |
| H | 1.76987000 | -1.09648900 | 1.49180300 |

**Backbite-Path e-TS**



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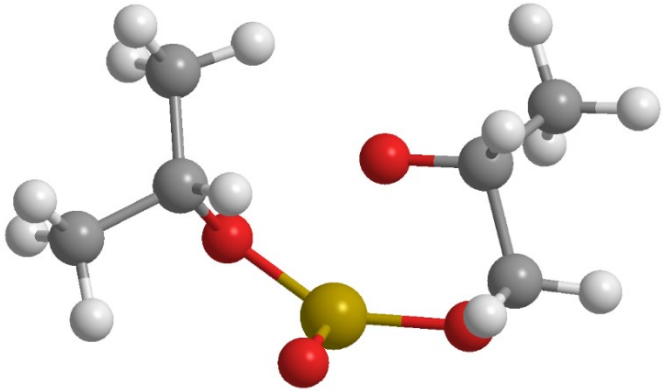
| | | | |
|---|---|---|---|
| C | 2.25836400 | -0.64687800 | 0.62262700 |
| C | 1.95626500 | 0.87500200 | 0.62678200 |
| C | 2.85216000 | 1.57453100 | -0.41880900 |
| H | 2.65666100 | 1.11234600 | -1.39918900 |
| H | 2.56796600 | 2.63581500 | -0.47831700 |
| S | -0.07253500 | -1.24284800 | -0.57526200 |
| O | 0.65852300 | 1.02606600 | 0.37447000 |
| O | 1.62579000 | -1.18744100 | -0.50783200 |
| O | -0.43220800 | -1.76191300 | 0.76219200 |
| H | 3.33304100 | -0.87926800 | 0.52844600 |
| H | 2.29707600 | 1.24085100 | 1.64164100 |
| O | -1.31390100 | -0.13492800 | -0.88148400 |
| C | -1.95104800 | 0.54222500 | 0.19402300 |
| H | -1.30010500 | 0.45263800 | 1.07385000 |
| C | -3.28827200 | -0.14276700 | 0.44662100 |
| H | -3.82829200 | 0.34109500 | 1.27596400 |
| H | -3.92098200 | -0.10173400 | -0.45496300 |
| H | -3.10625700 | -1.19483500 | 0.70674400 |
| C | -2.06058300 | 2.01000400 | -0.17569800 |
| H | -2.56034500 | 2.57870700 | 0.62519500 |
| H | -1.03269900 | 2.37304000 | -0.30271400 |
| H | -2.63543700 | 2.13446100 | -1.10831000 |
| H | 3.93122100 | 1.50146600 | -0.19091000 |
| H | 1.85177000 | -1.11598900 | 1.53470300 |

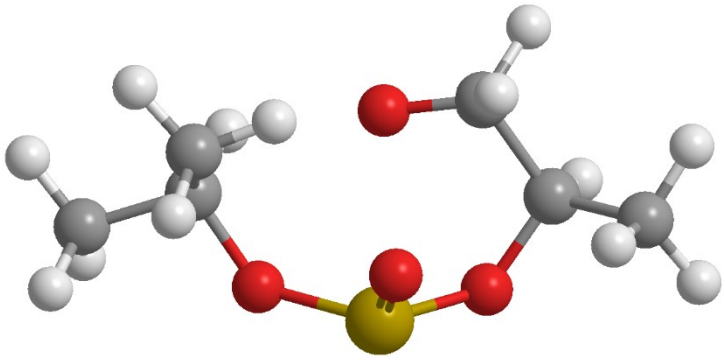
**Backbite-Path e-P**



-1 1

| | | | |
|---|---|---|---|
| C | 2.31686400 | -0.68197800 | 0.64212700 |
| C | 1.94066500 | 0.83210200 | 0.60338200 |
| C | 2.83656000 | 1.56673100 | -0.41100900 |
| H | 2.69956100 | 1.07724600 | -1.39138900 |
| H | 2.51726600 | 2.61631500 | -0.50171700 |
| S | -0.02573500 | -1.13364800 | -0.55966200 |
| O | 0.63512300 | 0.89346600 | 0.27307000 |
| O | 1.73109000 | -1.26544100 | -0.46103200 |
| O | -0.41660800 | -1.73851300 | 0.73879200 |
| H | 3.41494100 | -0.82466800 | 0.58694600 |
| H | 2.16837600 | 1.24085100 | 1.62604100 |
| O | -1.39580100 | -0.12712800 | -0.87368400 |
| C | -2.00174800 | 0.54612500 | 0.19792300 |
| H | -1.35860500 | 0.43703800 | 1.08165000 |
| C | -3.33897200 | -0.13106700 | 0.46222100 |
| H | -3.87509200 | 0.34499500 | 1.29936400 |
| H | -3.97558200 | -0.09003400 | -0.43546300 |
| H | -3.14525700 | -1.18313500 | 0.71454400 |
| C | -2.09568300 | 2.02170400 | -0.16009800 |
| H | -2.57984500 | 2.60210700 | 0.64079500 |
| H | -1.06779900 | 2.37694000 | -0.30661400 |
| H | -2.67443700 | 2.15396100 | -1.08881000 |
| H | 3.90782100 | 1.53656600 | -0.14021000 |
| H | 1.93367000 | -1.13548900 | 1.57760300 |

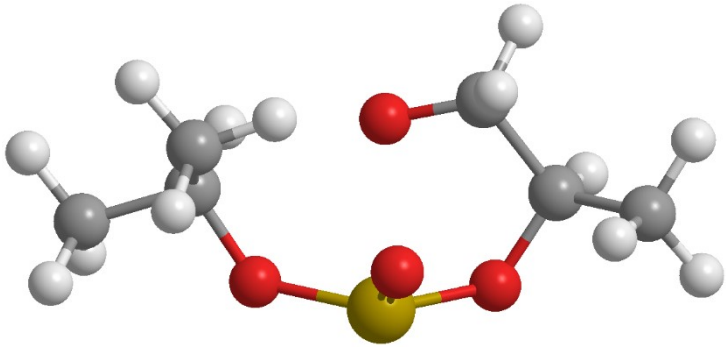
**Backbite-Path f-R**



-1 1

| | | | |
|---|---|---|---|
| C | 2.30572300 | 0.32744300 | -0.61687300 |
| C | 1.43979600 | 1.53596500 | -0.13358700 |
| C | 3.47734200 | 0.03131500 | 0.30830100 |
| H | 4.06050900 | 0.95469500 | 0.45305000 |
| H | 3.07989300 | -0.28281700 | 1.28318200 |
| S | 0.13896400 | -1.22612500 | 0.10818800 |
| O | 0.19102300 | 1.40269300 | -0.52252300 |
| O | 1.48884100 | -0.83893500 | -0.77529900 |
| O | 0.34087200 | -0.66240400 | 1.45470400 |
| H | 2.66207100 | 0.53039300 | -1.64224300 |
| H | 1.60689100 | 1.59566600 | 0.98893300 |
| O | -1.38622700 | -0.80666600 | -0.42933800 |
| C | -2.19897600 | 0.37117400 | -0.25480300 |
| H | -1.77595100 | 1.14879400 | -0.89962300 |
| C | -3.59532600 | -0.05118200 | -0.69394700 |
| H | -4.27654400 | 0.81141900 | -0.66571000 |
| H | -3.57850700 | -0.45110300 | -1.71977000 |
| H | -3.99037300 | -0.83395200 | -0.02709200 |
| C | -2.18938900 | 0.88269500 | 1.17800500 |
| H | -2.93017700 | 1.69329700 | 1.27853300 |
| H | -2.44624900 | 0.07544000 | 1.88584800 |
| H | -1.18541200 | 1.26281000 | 1.39119300 |
| H | 2.01514900 | 2.44947200 | -0.52411200 |
| H | 4.14898900 | -0.75167800 | -0.07932000 |

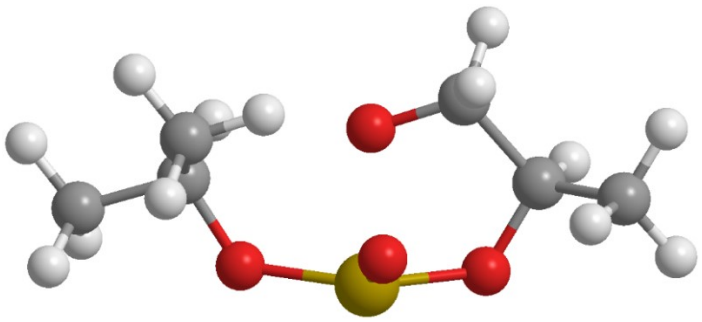
**Backbite-Path f-TS**



-1 1

| | | | |
|---|---|---|---|
| C | 2.36012300 | 0.32104300 | -0.62007300 |
| C | 1.43979600 | 1.49436500 | -0.13998700 |
| C | 3.51574200 | 0.06011500 | 0.33070100 |
| H | 4.09250900 | 0.98669500 | 0.48825000 |
| H | 3.09909300 | -0.26361700 | 1.29598200 |
| S | 0.13896400 | -1.14932500 | 0.06658800 |
| O | 0.19102300 | 1.25549300 | -0.50972300 |
| O | 1.58804100 | -0.84853500 | -0.76889900 |
| O | 0.34407200 | -0.67840400 | 1.44830400 |
| H | 2.73567100 | 0.55599300 | -1.63264300 |
| H | 1.59729100 | 1.59246600 | 0.97293300 |
| O | -1.45342700 | -0.80026600 | -0.40373800 |
| C | -2.24377600 | 0.37437400 | -0.24200300 |
| H | -1.83355100 | 1.14879400 | -0.89962300 |
| C | -3.64332600 | -0.03838200 | -0.68434700 |
| H | -4.32774400 | 0.82421900 | -0.65931000 |
| H | -3.61690700 | -0.44150300 | -1.70697000 |
| H | -4.03837300 | -0.82115200 | -0.01749200 |
| C | -2.22138900 | 0.89229500 | 1.18760500 |
| H | -2.94297700 | 1.71889700 | 1.29773300 |
| H | -2.48784900 | 0.08824000 | 1.89224800 |
| H | -1.20781200 | 1.24681000 | 1.40399300 |
| H | 1.90954900 | 2.42387200 | -0.57531200 |
| H | 4.19698900 | -0.71967800 | -0.04412000 |

**Backbite-Path f-P**



-1 1

| | | | |
|---|---|---|---|
| C | 2.43832300 | 0.31184300 | -0.62467300 |
| C | 1.43979600 | 1.43456500 | -0.14918700 |
| C | 3.57094200 | 0.10151500 | 0.36290100 |
| H | 4.13850900 | 1.03269500 | 0.53885000 |
| H | 3.12669300 | -0.23601700 | 1.31438200 |
| S | 0.13896400 | -1.03892500 | 0.00678800 |
| O | 0.19102300 | 1.04389300 | -0.49132300 |
| O | 1.73064100 | -0.86233500 | -0.75969900 |

| | | | |
|---|---|---|---|
| O | 0.34867200 | -0.70140400 | 1.43910400 |
| H | 2.84147100 | 0.59279300 | -1.61884300 |
| H | 1.58349100 | 1.58786600 | 0.94993300 |
| O | -1.55002700 | -0.79106600 | -0.36693800 |
| C | -2.30817600 | 0.37897400 | -0.22360300 |
| H | -1.91635100 | 1.14879400 | -0.89962300 |
| C | -3.71232600 | -0.01998200 | -0.67054700 |
| H | -4.40134400 | 0.84261900 | -0.65011000 |
| H | -3.67210700 | -0.42770300 | -1.68857000 |
| H | -4.10737300 | -0.80275200 | -0.00369200 |
| C | -2.26738900 | 0.90609500 | 1.20140500 |
| H | -2.96137700 | 1.75569700 | 1.32533300 |
| H | -2.54764900 | 0.10664000 | 1.90144800 |
| H | -1.24001200 | 1.22381000 | 1.42239300 |
| H | 1.75774900 | 2.38707200 | -0.64891200 |
| H | 4.26598900 | -0.67367800 | 0.00648000 |

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