**Supporting Information:**

# New mechanism for internal nucleophilic substitution reactions.

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**Table S1**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of all species involved in the decomposition of ethyl chlorosulfite **2a** in gas phase, dichloromethane and acetonitrile.

| | Gas phase[a] | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2a** | -1088.020931 | 0.0 | 0.082346 | 89.333 | -1087.938585 | 0.0 |
| **TS2a** | -1087.941108 | 50.1 | 0.078445 | 92.913 | -1087.862663 | 46.6 |
| **3a** | -1088.024566 | -2.3 | 0.080806 | 97.010 | -1087.943760 | -5.5 |
| **TS3a** | -1087.955518 | 41.0 | 0.075328 | 88.774 | -1087.880190 | 36.8 |
| **IN2a** | -1087.992290 | 18.0 | 0.077026 | 112.160 | -1087.915264 | 7.8 |
| **TS4a** | -1087.938080 | 52.0 | 0.073716 | 93.944 | -1087.864364 | 45.2 |
| **$RSO_2^+$** | -627.509032 | | 0.078874 | 81.433 | -627.430158 | |
| **$R^+$** | -78.869024 | | 0.062424 | 56.308 | -78.806600 | |
| **$Cl^-$** | -460.252233 | | 0.002360 | 36.586 | -460.249873 | |
| **$SO_2Cl^-$** | -1008.883169 | | 0.013385 | 73.399 | -1008.869784 | |
| **$RSO_2^+$+$Cl^-$** | -1087.761265 | 162.9 | | | | |
| **$R^+$+$SO_2Cl^-$** | -1087.752193 | 168.6 | | | | |
| | Dichloromethane (DCM)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2a** | -1088.026460 | 0.0 | 0.082139 | 89.857 | -1087.944321 | 0.0 |
| **TS2a** | -1087.957277 | 43.4 | 0.077788 | 94.237 | -1087.879489 | 39.4 |
| **3a** | -1088.029830 | -2.1 | 0.080622 | 99.156 | -1087.949208 | -5.8 |
| **TS3a** | -1087.967390 | 37.1 | 0.075516 | 91.505 | -1087.891874 | 32.4 |
| **IN2a** | -1087.997742 | 18.0 | 0.076764 | 115.479 | -1087.920978 | 7.0 |
| **TS4a** | -1087.955673 | 44.4 | 0.075019 | 95.605 | -1087.880654 | 38.2 |
| **$RSO_2^+$** | -627.590906 | | 0.079196 | 78.850 | -627.511710 | |
| **$R^+$** | -78.960780 | | 0.062827 | 56.257 | -78.897953 | |
| **$Cl^-$** | -460.357643 | | 0.002360 | 36.586 | -460.355283 | |
| **$SO_2Cl^-$** | -1008.964782 | | 0.013352 | 74.008 | -1008.951430 | |
| **$RSO_2^+$---$Cl^-$** [c] | -1087.959508 | 42.0 | 0.079037 | 87.604 | -1087.880471 | 40.7 |
| | Acetonitrile ($CH_3CN$)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2a** | -1088.027349 | 0.0 | 0.082102 | 89.948 | -1087.945247 | 0.0 |
| **TS2a** | -1087.960197 | 42.1 | 0.077655 | 94.607 | -1087.882542 | 38.0 |
| **3a** | -1088.030646 | -2.1 | 0.080588 | 99.904 | -1087.950058 | -6.0 |
| **TS3a** | -1087.969466 | 36.3 | 0.075547 | 92.035 | -1087.893919 | 31.6 |
| **IN2a** | -1087.998618 | 18.0 | 0.076692 | 120.219 | -1087.921926 | 5.6 |
| **TS4a** | -1087.958740 | 43.1 | 0.075145 | 96.214 | -1087.883595 | 36.8 |
| **$RSO_2^+$** | -627.599125 | | 0.079202 | 79.043 | -627.519923 | |
| **$R^+$** | -78.969499 | | 0.062686 | 56.297 | -78.906813 | |
| **$Cl^-$** | -460.367610 | | 0.002360 | 36.586 | -460.365250 | |
| **$SO_2Cl^-$** | -1008.972986 | | 0.013334 | 74.188 | -1008.959652 | |
| **$RSO_2^+$---$Cl^-$** [c] | -1087.969158 | 36.5 | 0.079017 | 86.561 | -1087.890141 | 35.6 |

[a] Structures fully optimized. [b] Relative to **2a**. [c] The distance $RSO2^+$---$Cl^-$ fixed to 6Å

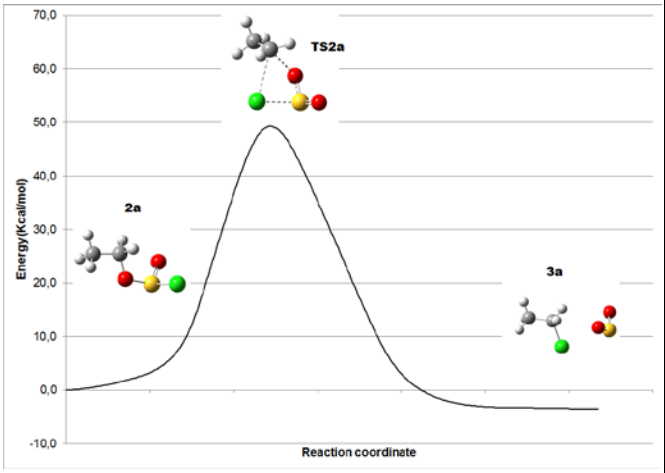



**Figure S1a-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS2a** in **gas-phase**

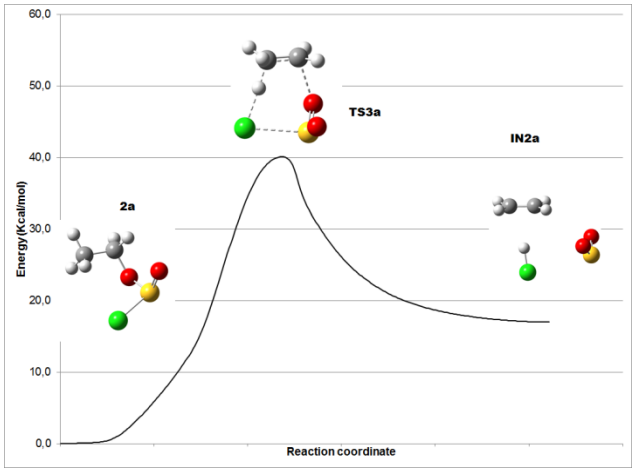



**Figure S2a-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3a** in **gas-phase**

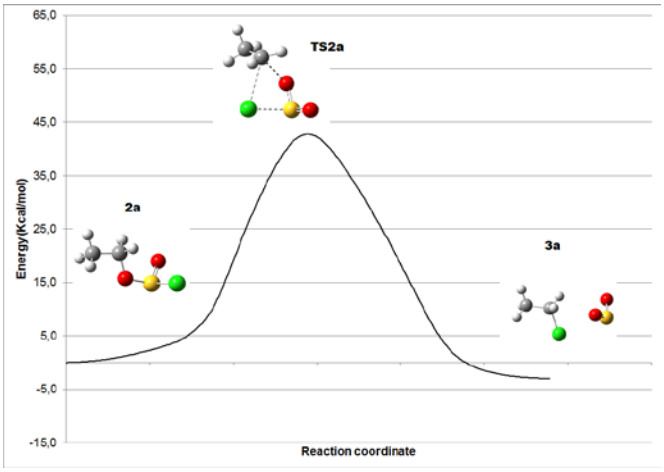



**Figure S1a-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS2a** in **DCM**

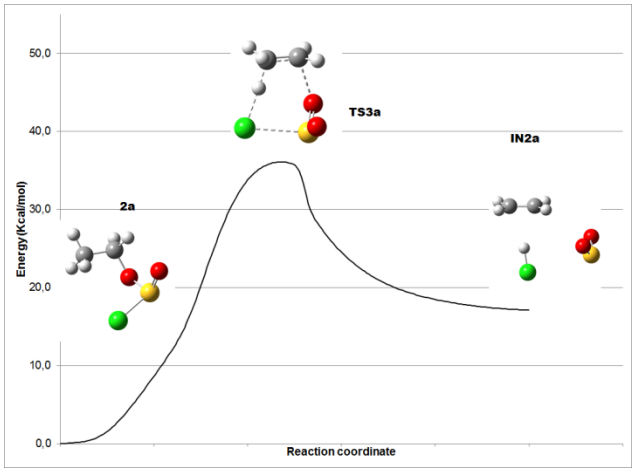



**Figure S2a-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3a** in **DCM**

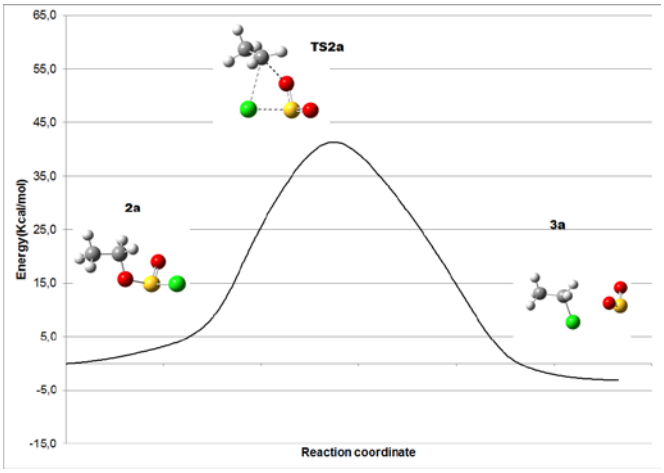



**Figure S1a-3**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS2a** in **acetonitrile**

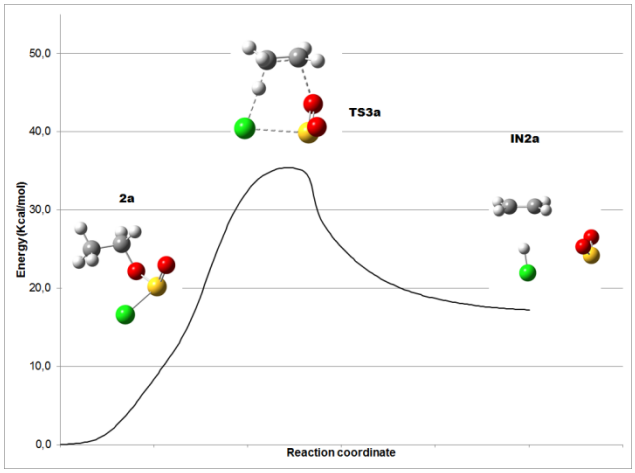



**Figure S2a-3**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3a** in **acetonitrile**

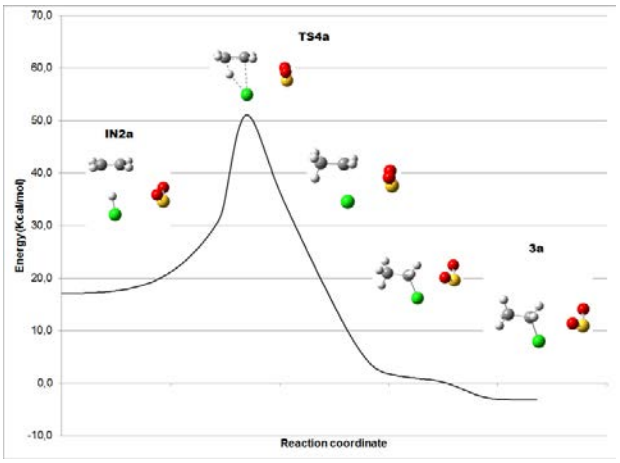



**Figure S3a-1**. Energy profile (IRC, $\Delta E$) corresponding to the transition state **TS4a** in **gas-phase**

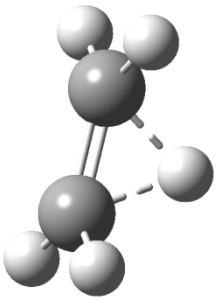


**Figure S4a**. $CH_3CH_2^+$.

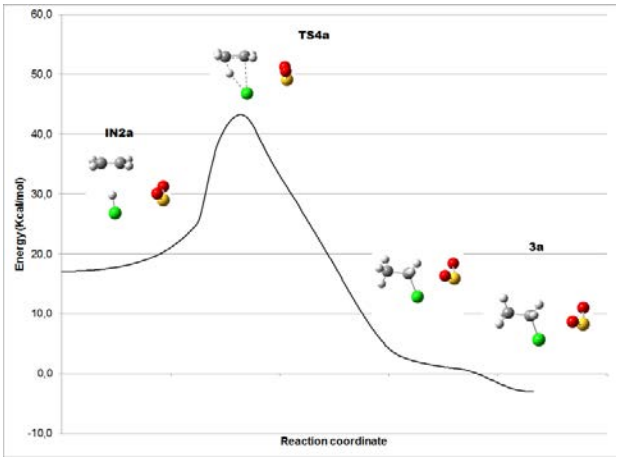



**Figure S3a-2**. Energy profile (IRC, $\Delta E$) corresponding to the transition state **TS4a** in **DCM**

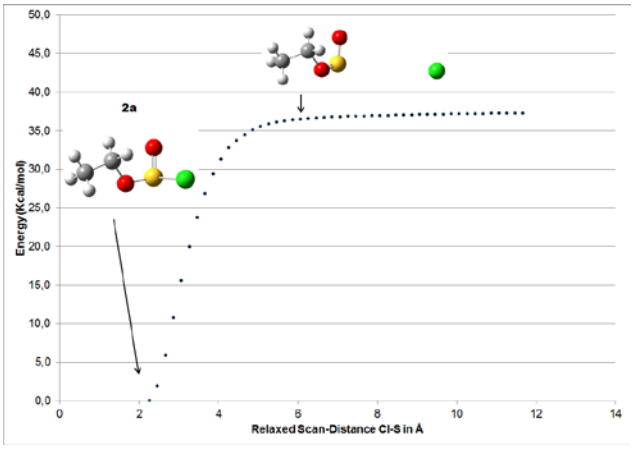



**Figure S5a**. Energy profile (Relaxed Scan, $\Delta E$) corresponding to the ionization of **2a** in **acetonitrile**

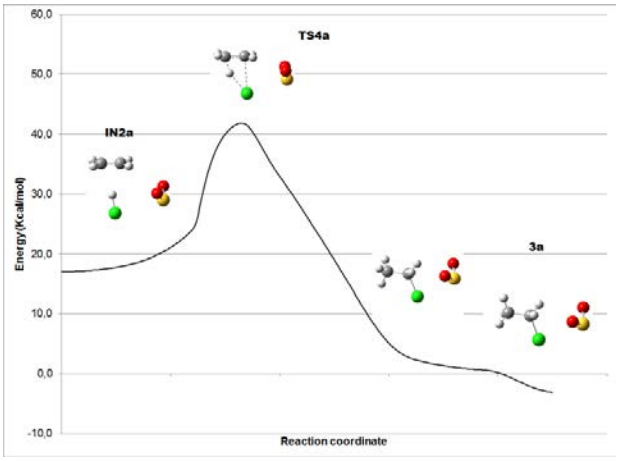
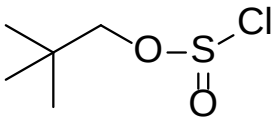
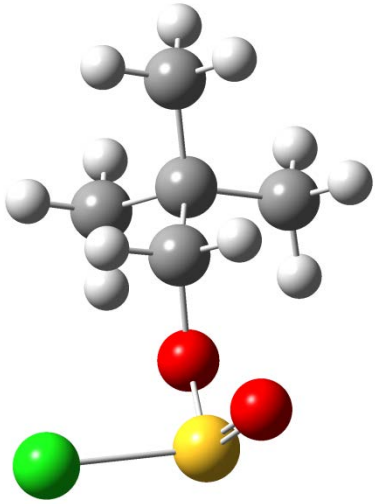
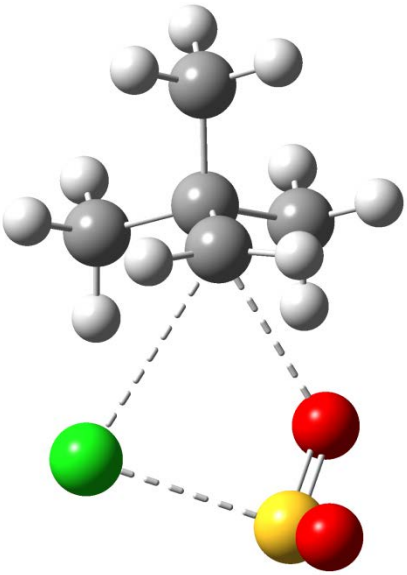



**Figure S3a-3**. Energy profile (IRC, $\Delta E$) corresponding to the transition state **TS4a** in **acetonitrile**

**Table S2**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of neopentyl chlorosulfite **2a1** and **TS2a1** in acetonitrile.



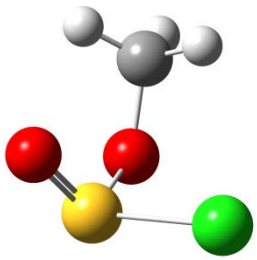

**2a1**

| | Acetonitrile ($CH_3CN$)[a] | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | Δ*E* [a] | Thermal correction to *H* | *S* | *H* | Δ*G* [a] |
| **2a1** | -1205.977772 | 0.0 | 0.167163 | 110,274 | -1205,810609 | 0.0 |
| **TS2a1** | -1205,910704 | 42,1 | 0,162851 | 109,966 | -1205,747853 | 39,5 |
| |  | | |  | | |
| | **2a1** | | | **TS2a1** | | |

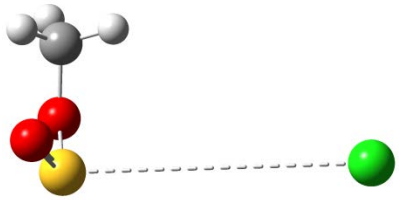
[a] Relative to **2a1**

**Table S3**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of chlorine exchange in metyl chlorosulfite (in acetonitrile).

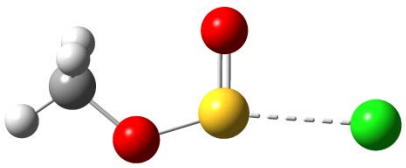
| | Acetonitrile ($CH_3CN$)[a] | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | Δ*E* | Thermal correction to *H* | *S* | *H* | Δ*G* |
| **$MeSO_2Cl$** | -1048.704603 | 0.0 | 0.053533 | 82.078 | -1048.651070 | 0.0 |
| **$MeSO_2$---Cl** [d] | | | | | | 35.6 [a] |
| **TS-I** | -1048.663568 | 25.7 [a] | 0.052179 | 82.304 | -1048.611389 | 24.8 [a] |
| **2 $MeSO_2Cl$** | -2097.409878 | 0.0 | 0.107995 | 139.298 | -2097.301883 | 0.0 |
| **TS-II** | -2097.375074 | 21.8 [b] | 0.107844 | 135.606 | -2097.267230 | 22.8 [b] |
| **3 $MeSO_2Cl$** | -3146.114958 | 0.0 | 0.162492 | 193.784 | -3145.952466 | 0.0 |
| **TS-III** | -3146.094899 | 12.6 [c] | 0.162402 | 179.328 | -3145.932497 | 16.8 [c] |



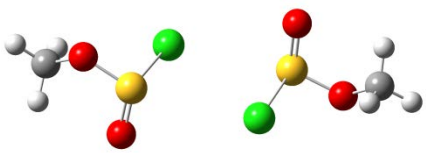
**$MeSO_2Cl$**



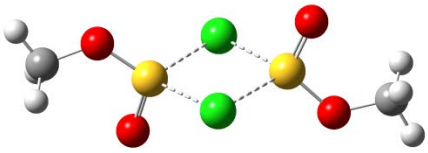
**$MeSO_2$---Cl**



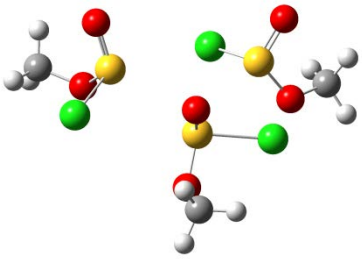
**TS-I**



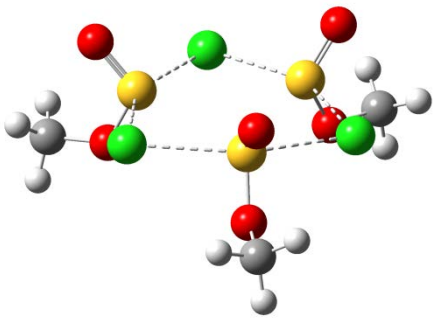
**2 $MeSO_2Cl$**



**TS-II**



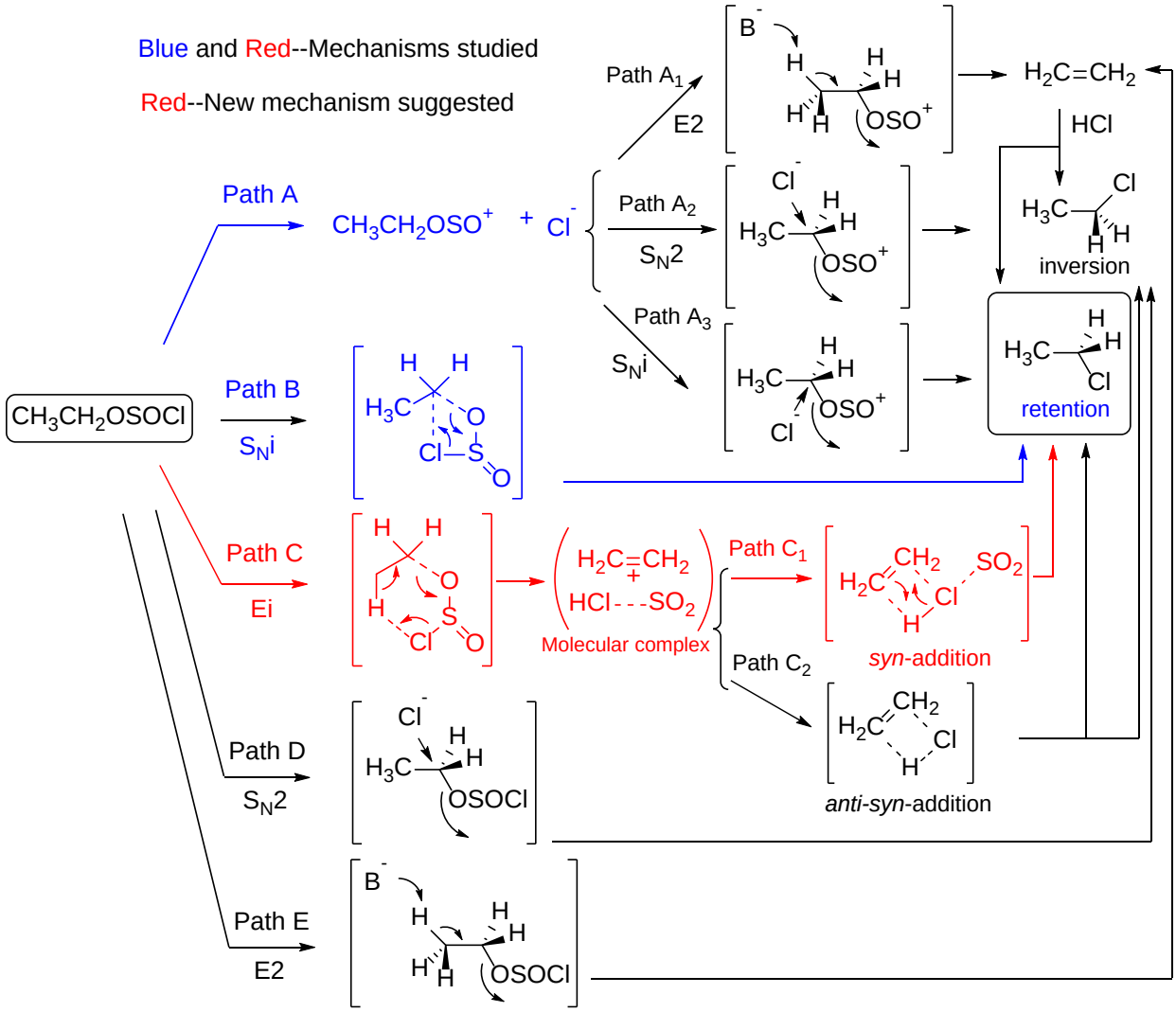
**3 $MeSO_2Cl$**



**TS-III**

[a] Relative to **$MeSO_2Cl$**. [b] Relative to **2 $MeSO_2Cl$**. [c] Relative to **3 $MeSO_2Cl$**. [d] The distance MeSO2---Cl fixed to 6Å

**Scheme S1a.** Global mechanistic pathways for the conversion of primary alkanenesulfonyl chlorides into chloroalkanes or alkenes.




The routes paths D and E (Scheme **S1a**) correspond to the classical mechanisms $S_N2$ and E2, typical of primary substrates with good leaving groups, which lead to a chloroalkane or an olefin, respectively. The olefin can suffer a non-selective addition by HCl to give the chloroalkane. These mechanisms can compete, depending on the reaction conditions and used solvent, with the routes path A-C herein studied.

According to our results, to obtain the chloroalkane with retention of configuration, it is preferred the mechanism suggested by us (path C and path $C_1$) over the one suggested by the literature (path B). However, this mechanism can lead to chloroalkanes with inversion of configuration through the path $C_2$. Finally, the calculations suggest the formation of the ions $CH_3CH_2OSO^+$ and $Cl^-$ in polar solvents such as $CH_3CN$ (path A). These ions can suffer either an E2 elimination reaction to give the corresponding olefin (path $A_1$) or a $S_N2$ substitution (path $A_2$) and $S_Ni$ (path $A_3$) to give the chloroalkanes with inversion and retention of configuration, respectively.

**Table S4**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of all species involved in the decomposition of isopropyl chlorosulfite **2b** in gas phase, dichloromethane and acetonitrile.

| | Gas phase[a] | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2b** | -1127.337552 | 0.0 | 0.110553 | 93.744 | -1127.226999 | 0.0 |
| **TS2b** | -1127.276036 | 38.6 | 0.106385 | 98.910 | -1127.169651 | 34.4 |
| **3b** | -1127.345876 | -5.2 | 0.110081 | 107.040 | -1127.235795 | -9.5 |
| **TS3b** | -1127.285978 | 32.4 | 0.104440 | 97.152 | -1127.181538 | 27.5 |
| **IN2b** | -1127.316770 | 13.0 | 0.105672 | 116.924 | -1127.211098 | 3.1 |
| **TS4b** | -1127.276825 | 38.1 | 0.102393 | 92.483 | -1127.174432 | 33.4 |
| $RSO_2^+$ | -666.836156 | | 0.106830 | 87.484 | -666.729326 | |
| $R^+$ | -118.222525 | | 0.090683 | 67.629 | -118.131842 | |
| $RSO_2^+ + Cl^-$ [c] | -1127.088390 | 156.4 | | | | |
| $R^+ + SO_2Cl^-$ [c] | -1127.105694 | 145.5 | | | | |
| | Dichloromethane (DCM)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2b** | -1127.343215 | 0.0 | 0.110291 | 94.788 | -1127.232924 | 0.0 |
| **IN1b** [d] | -1127.300683 | 26.7 | 0.105036 | 103.133 | -1127.195647 | 20,9 |
| **TS2b** [e] | -1127.296566 | 29.3 | 0.104812 | 99.768 | -1127.191754 | 24.3 |
| **3b** | -1127.350979 | -4.9 | 0.109846 | 110.808 | -1127.241133 | -9.9 |
| **TS3b** | -1127.302057 | 25.8 | 0.104632 | 103.582 | -1127.197425 | 19.7 |
| **IN2b** | -1127.321988 | 13.3 | 0.105296 | 120.063 | -1127.216692 | 2.7 |
| **TS4b** | -1127.297185 | 28.9 | 0.103830 | 99.395 | -1127.193355 | 23.5 |
| $RSO_2^+$ | -666.912882 | | 0.107159 | 86.169 | -666.805723 | |
| $R^+$ | -118.305644 | | 0.090741 | 66.798 | -118.214903 | |
| | Acetonitrile ($CH_3CN$)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2b** | -1127.344181 | 0.0 | 0.110254 | 94.859 | -1127.233927 | 0.0 |
| **IN1b** [d] | -1127.303741 | 25.4 | 0.105076 | 103.243 | -1127.198665 | 19.6 |
| **TS2b** [e] | -1127.300207 | 27.6 | 0.104755 | 100.142 | -1127.195452 | 22.6 |
| **3b** | -1127.351776 | -4.8 | 0.108858 | 103.772 | -1127.242918 | -8.3 |
| **TS3b** | -1127.305090 | 24.5 | 0.104669 | 103.089 | -1127.200421 | 18.6 |
| **IN2b** | -1127.322843 | 13.4 | 0.105254 | 119.456 | -1127.217589 | 2.9 |
| **TS4b** | -1127.301022 | 27.1 | 0.103937 | 99.648 | -1127.197085 | 21.7 |
| $RSO_2^+$ | -666.920533 | | 0.107177 | 86.171 | -666.813356 | |
| $R^+$ | -118.313614 | | 0.090792 | 66.576 | -118.222822 | |

[a] Structures fully optimized, unless otherwise indicated. [b] Relative to **2b**. [c] From **Table S1** [d] In **IN1b**, the distance C---H and the rotation of the methyl are frozen (see figure S4b). [e] In **TS2b** (in dichloromethane and acetonitrile), the rotation of the two methyl are frozen.

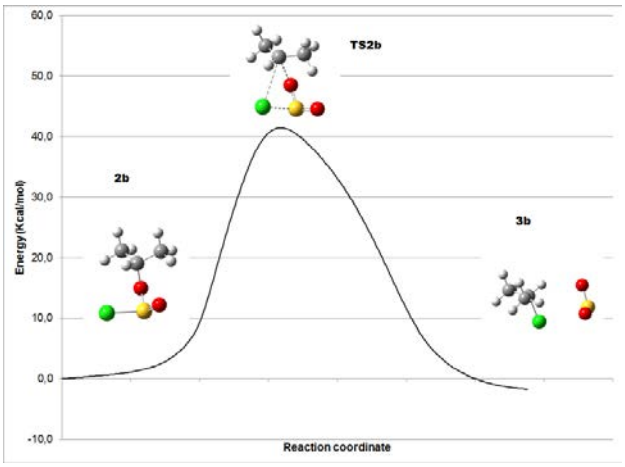



**Figure S1b-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS2b** in **gas-phase**

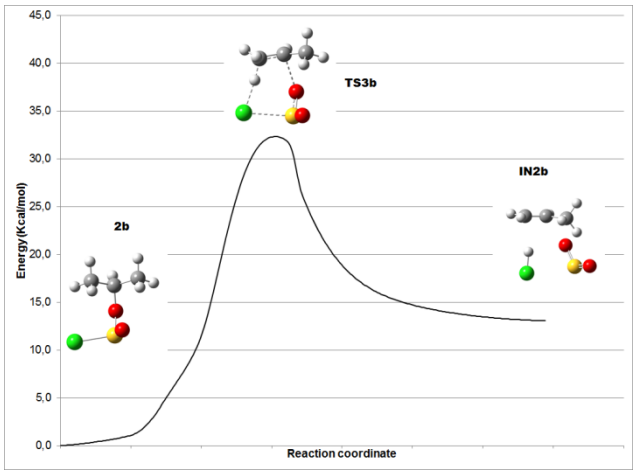



**Figure S2b-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3b** in **gas-phase**

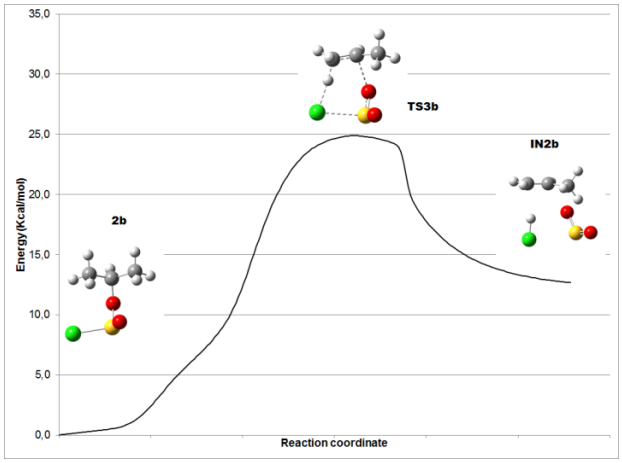



**Figure S2b-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3b** in **DCM**

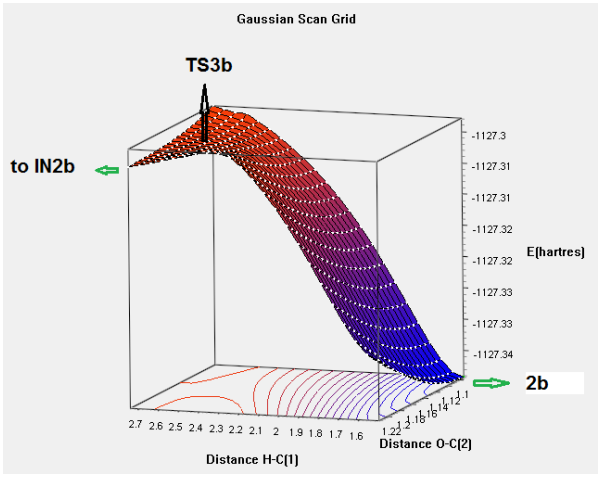



**Figure S2b-3'**. Energy profile (Scan Grid, Δ*E*) corresponding to the transition state **TS3b** in **acetonitrile**

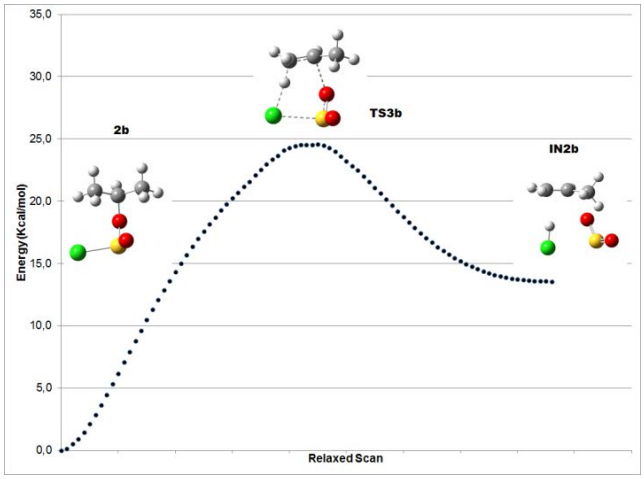



**Figure S2b-3**. Energy profile (Relaxed Scan, Δ*E*) corresponding to the transition state **TS3b** in **acetonitrile**

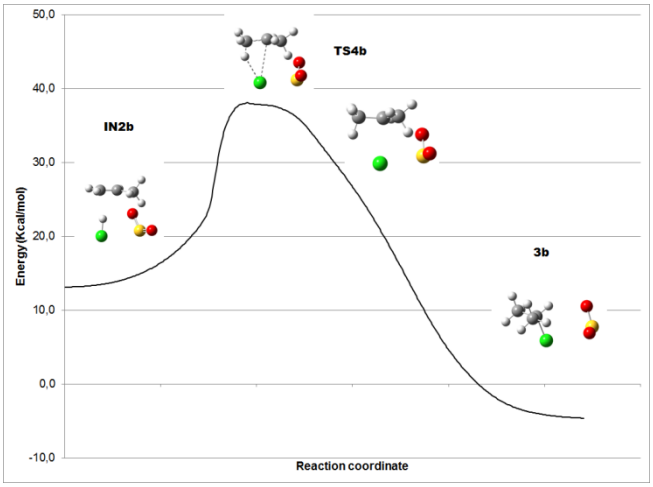



**Figure S3b-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS4b** in **gas-phase**

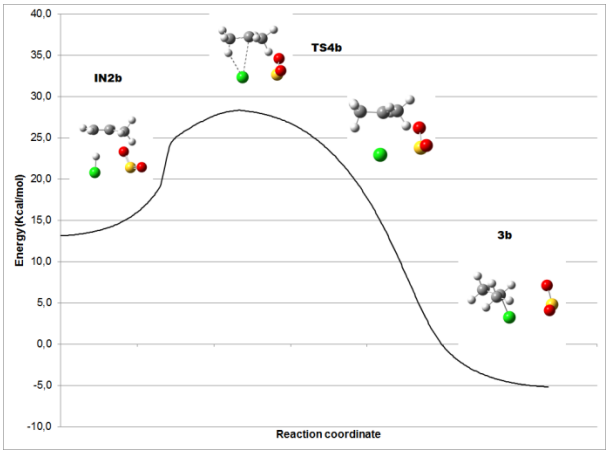



**Figure S3b-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS4b** in **DCM**

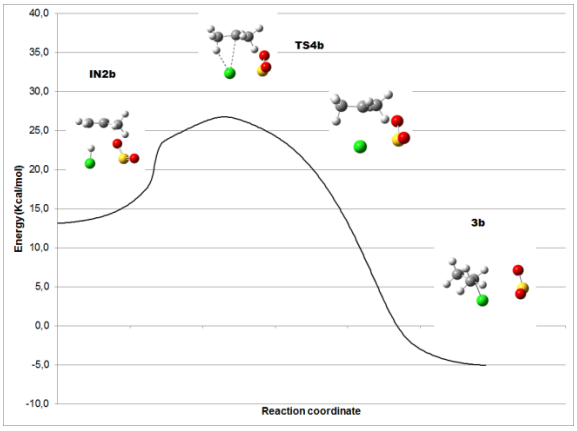
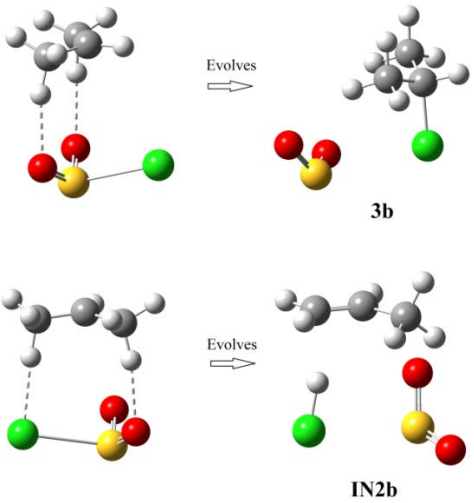



**Figure S3b-3**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS4b** in **acetonitrile**



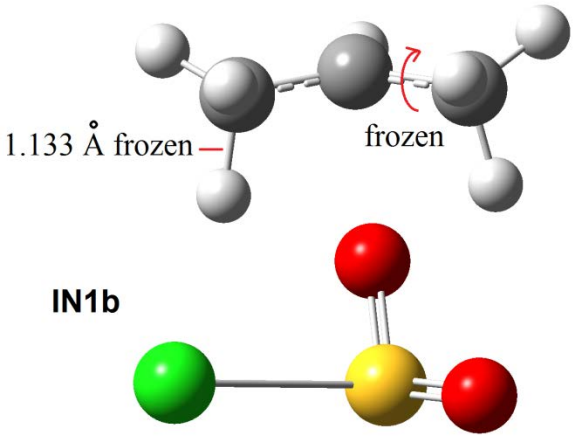
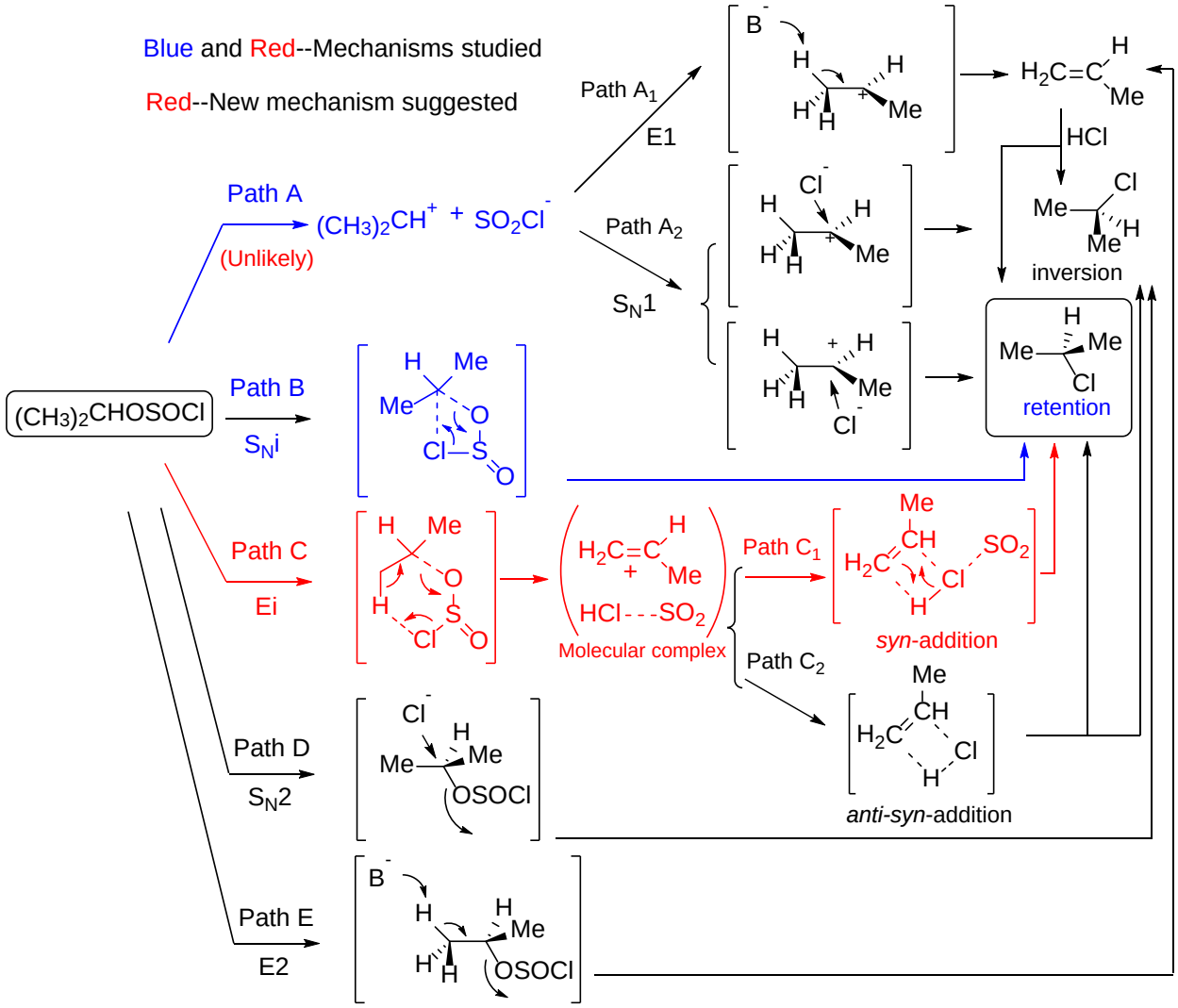




**Figure S4b**. Attempts to obtain the ion pair **IN1b**, in **acetonitrile**, starting from different initial geometries (above), and **IN1b** with the distance C-H and the rotation of the methyl frozen (down).

**Scheme S1b.** Global mechanistic pathways for the conversion of secondary alkanenesulfonyl chlorides into chloroalkanes or alkenes.




The routes paths D and E (Scheme **S1b**) correspond to the classical mechanisms $S_N2$ and E2, typical of secondary substrates with good leaving groups, which lead to a chloroalkane or an olefin, respectively. The olefin can suffer a non-selective addition by HCl to give the chloroalkane. These mechanisms can compete, depending on the reaction conditions and used solvent, with the routes path A-C herein studied.

According to our results, to obtain the chloroalkane with retention of configuration, it is preferred the mechanism suggested by us (path C and path $C_1$) over the suggested by the literature (path B). However, this mechanism can lead to chloroalkanes with inversion of configuration through the path $C_2$. The calculations give a very high energy for the ions $(CH_3)_2CH^+$ and $SO_2Cl^-$ in solvents such as $CH_3CN$ and DCM (path A), which makes this mechanism very unlikely. These ions could suffer either an E1 elimination reaction to give the corresponding olefin (path $A_1$) or a $S_N1$ substitution (path $A_2$) to give the chloroalkanes with inversion and retention of configuration.

**Table S5**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of all species involved in the decomposition of *t*-butyl chlorosulfite **2c** in gas phase, dichloromethane and acetonitrile.

| | Gas phase[a] | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2c** | -1166.658478 | 0.0 | 0.138448 | 99.565 | -1166.520030 | 0.0 |
| **3c** | -1166.664485 | -3.8 | 0.138076 | 112.914 | -1166.526409 | -8.0 |
| **TS3c** | -1166.615927 | 26.7 | 0.133338 | 105.198 | -1166.482589 | 21.8 |
| **IN2c** | -1166.640313 | 11.4 | 0.133985 | 122.390 | -1166.506327 | 1.8 |
| **TS4c** | -1166.614312 | 27.7 | 0.133638 | 105.878 | -1166.480674 | 22.8 |
| **$RSO_2^+$** | -706.169335 | | 0.130577 | 100.216 | -706.038758 | |
| **$R^+$** | -157.567718 | | 0.118537 | 73.639 | -157.449181 | |
| **$RSO_2^+$+$Cl^-$** [c] | -1166.421568 | 148.7 | | | | |
| **$R^+$+$SO_2Cl^-$** [c] | -1166.450887 | 130.3 | | | | |
| | Dichloromethane (DCM)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2c** | -1166.664152 | 0.0 | 0.138119 | 100.737 | -1166.526033 | 0.0 |
| **IN1c** | -1166.637496 | 16.7 | 0.134377 | 112.875 | -1166.503119 | 10.8 |
| **3c** | -1166.669956 | -3.6 | 0.137835 | 114.118 | -1166.532121 | -7.8 |
| **TS1c** | -1166.635555 | 17.9 | 0.133737 | 111.363 | -1166.501818 | 12.0 |
| **IN2c** | -1166.645627 | 11.6 | 0.133500 | 128.315 | -1166.512127 | 0.5 |
| **TS6c** | -1166.634352 | 18.7 | 0.134052 | 110.709 | -1166.500300 | 13.2 |
| **TS5c** | -1166.636382 | 17.4 | 0.130206 | 107.931 | -1166.506176 | 10.3 |
| **$RSO_2^+$** | -706.242105 | | 0.131625 | 108.913 | -706.110480 | |
| **$R^+$** | -157.645196 | | 0.119561 | 76.051 | -157.525635 | |
| | Acetonitrile ($CH_3CN$)[a] | | | | | |
| species | *E* | Δ*E* [b] | Thermal correction to *H* | *S* | *H* | Δ*G* [b] |
| **2c** | -1166.665122 | 0.0 | 0.138062 | 100.820 | -1166.527060 | 0.0 |
| **IN1c** | -1166.640680 | 15.3 | 0.134466 | 114.557 | -1166.506214 | 9.0 |
| **3c** | -1166.670852 | -3.6 | 0.137788 | 114.457 | -1166.533064 | -7.8 |
| **TS1c** | -1166.639300 | 16.2 | 0.132809 | 107.220 | -1166.506491 | 11.0 |
| **IN2c** | -1166.646497 | 11.7 | 0.133457 | 127.334 | -1166.513040 | 0.9 |
| **TS6c** | -1166.638035 | 17.0 | 0.134062 | 111.684 | -1166.503973 | 11.2 |
| **TS5c** | -1166.638450 | 16.7 | 0.130524 | 115.927 | -1166.507926 | 7.5 |
| **$RSO_2^+$** | -706.249326 | | 0.131529 | 110.651 | -706.117797 | |
| **$R^+$** | -157.652731 | | 0.118812 | 73.964 | -157.533919 | |

[a] Structures fully optimized. [b] Relative to **2c**. [c] From **Table S1**.

**Table S6**. B3LYP/6-31G** total energies (*E* and *H*, au), thermal correction to *H* (au, 298.15 K), *S* (Cal/Mol-Kelvin, 298.15 K) and relative energies (Δ*E* and Δ*G*, kcal/mol) of the species involved in the decomposition of isopropyl chlorosulfite **2b** and *t*-butyl chlorosulfite **2c** in acetonitrile. All species surrounded by four molecules of acetonitrile.

| | Acetonitrile ($CH_3CN$) | | | | | |
|---|---|---|---|---|---|---|
| species | *E* | $\Delta E$ [a] | Thermal correction to *H* | *S* | *H* | $\Delta G$ [a] |
| **2b-s** [b] | -1658.417201 | 0.0 | 0.306098 | 231.904 | -1658.111103 | 0.0 |
| **IN1b-contact-s** [b] | -1658.376035 | 25.8 | 0.295180 | 200.959 | -1658.080855 | 28.2 |
| **IN1b-shared-s** [c] | -1658.378836 | 24.1 | 0.303757 | 233.796 | -1658.075079 | 22.0 |
| **TS3b-s** [b] | -1658.382065 | 22.0 | 0.299618 | 233.704 | -1658.082447 | 17.4 |
| **IN2b-s** [b] | -1658.395329 | 13.7 | 0.298085 | 244.256 | -1658.097244 | 5.0 |
| **TS4b-s** [b] | -1658.375671 | 26.1 | 0.301679 | 246.340 | -1658.073992 | 19.0 |
| **2c-s** [b] | -1697.737706 | 0.0 | 0.335888 | 246.468 | -1697.401818 | 0.0 |
| **IN1c-contact-s** [c] | -1697.718090 | 12.3 | 0.332373 | 265.113 | -1697.385717 | 4.5 |
| **IN1c-shared-s** [c] | -1697.716519 | 13.3 | 0.333623 | 239.080 | -1697.382896 | 14.1 |
| **TS1c-s** [b] | -1697.713743 | 15.0 | 0.329606 | 256.728 | -1697.384137 | 8.1 |
| **IN2c-s** [b] | -1697.720042 | 11.1 | 0.328390 | 260.991 | -1697.391652 | 2.0 |
| **TS6c-s** [b] | -1697.713943 | 14.9 | 0.329823 | 253.649 | -1697.384120 | 9.0 |
| **TS5c-s** [b] | -1697.713285 | 15.3 | 0.326354 | 257.077 | -1697.386931 | 6.2 |

[a] Relative to **2b-s** or **2c-s**. [b] Keeping the core frozen. Acetonitrile molecules aligned with the nearest proton. [c] Structures fully optimized.

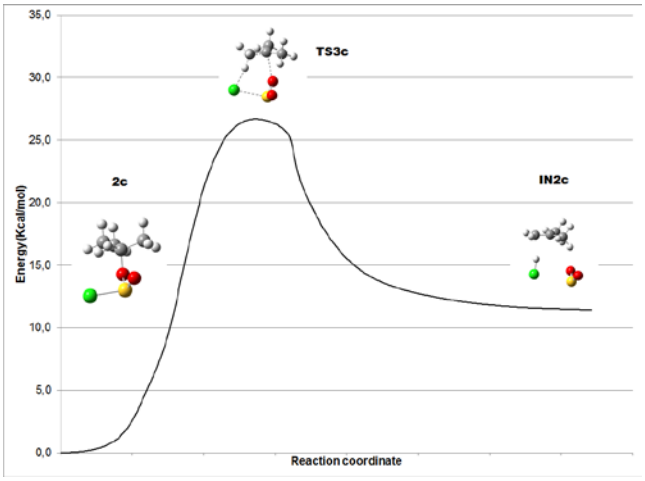



**Figure S1c-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS3c** in **gas-phase**

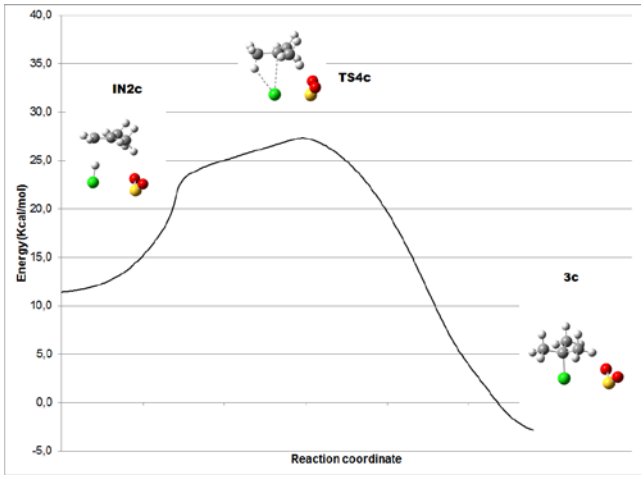



**Figure S2c-1**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS4c** in **gas-phase**

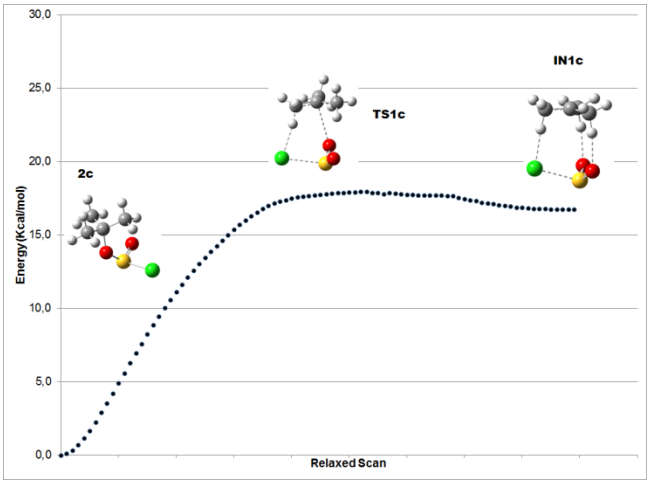



**Figure S1c-2**. Energy profile (Relaxed Scan, Δ*E*) corresponding to the transition state **TS1c** in **DCM**

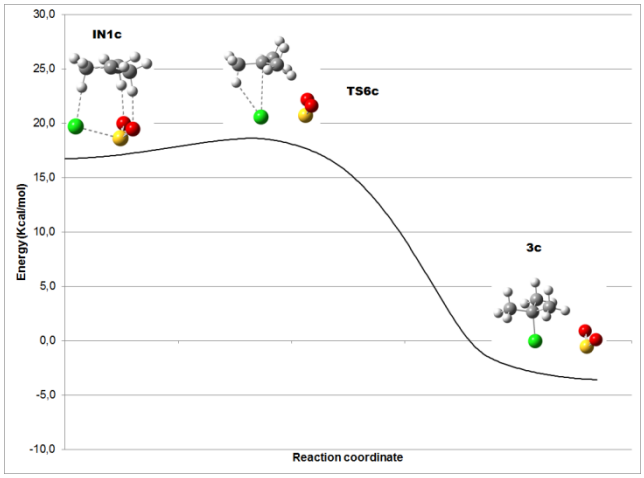



**Figure S2c-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS6c** in **DCM**

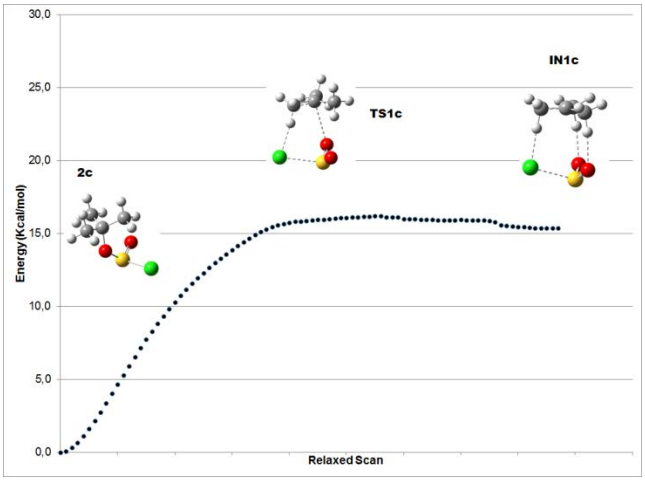



**Figure S1c-3**. Energy profile (Relaxed Scan, Δ*E*) corresponding to the transition state **TS1c** in **acetonitrile**

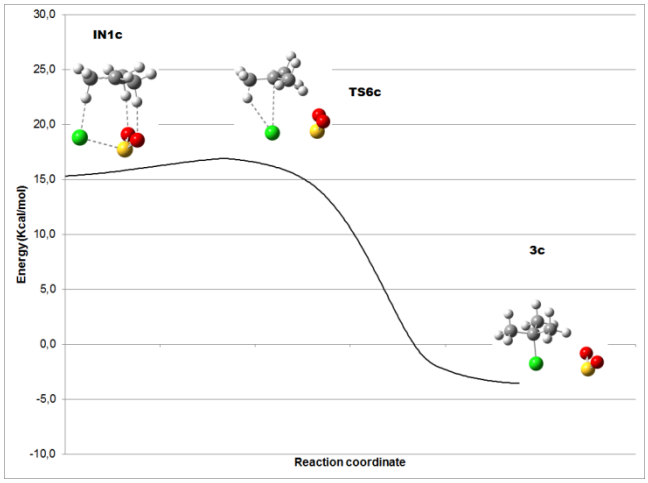



**Figure S2c-3**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS6c** in **acetonitrile**

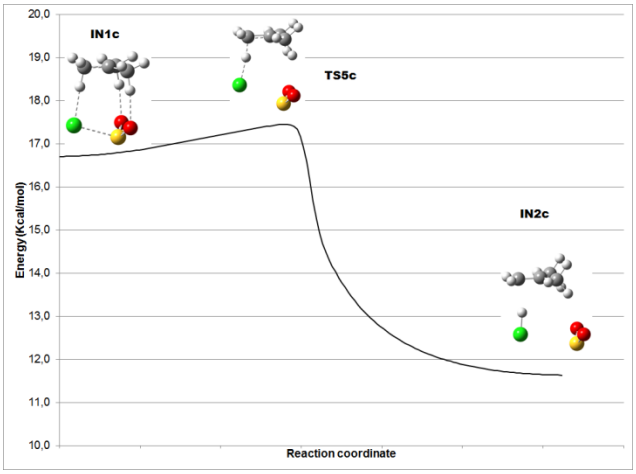



**Figure S3c-2**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS5c** in **DCM**

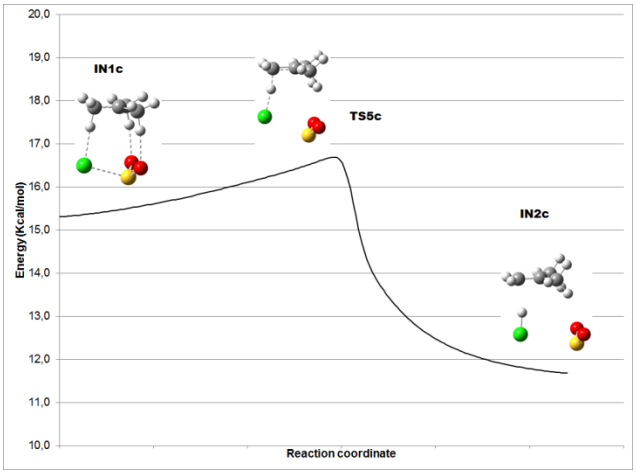
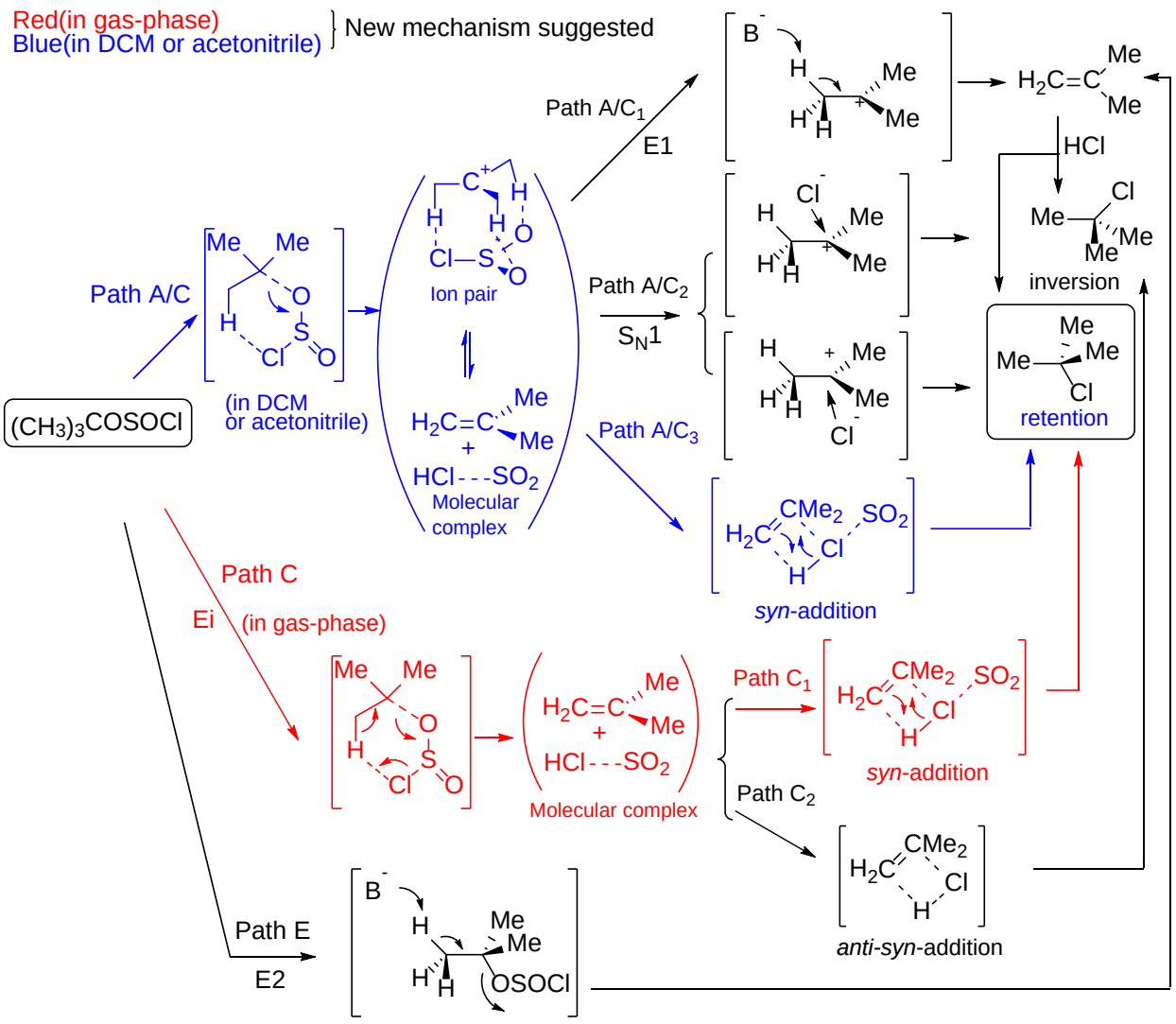



**Figure S3c-3**. Energy profile (IRC, Δ*E*) corresponding to the transition state **TS5c** in **acetonitrile**

**Scheme S1c.** Global mechanistic pathways for the conversion of tertiary alkanenesulfonyl chlorides into chloroalkanes or alkenes.




The route path E (Scheme **S1c**) corresponds to the classical mechanisms E2, typical of tertiary substrates with good leaving groups, which leads to an olefin. The olefin can suffer a non-selective addition by HCl to give the chloroalkane. This mechanism can compete, depending on the reaction conditions and used solvent, with the routes path C, A/C herein studied.

According to our results, to obtain the chloroalkane with retention of configuration in gas-phase, the most likely mechanism is the one suggested by us (path C and path $C_1$). However, this mechanism can lead to chloroalkanes with inversion of configuration through the path $C_2$. However in solvent, the mechanism changes to that represented by the path A/C (and path $A/C_3$) through the ion pair in equilibrium with a molecular complex. These ions could suffer either an E1 elimination reaction to give the corresponding olefin (path $A/C_1$) or a $S_N1$ substitution (path $A/C_2$) to give the chloroalkanes with inversion and retention of configuration.

**Table S7**. MPWB1K/6-31++G** total energies (*E*, au) [a] (in dichloromethane and acetonitrile), B3LYP-D3/def2TZVP//MPWB1K/6-31++G** (*E*, au) [b] (in acetonitrile), M062X/cc-pVTZ//MPWB1K/6-31++G** (*E*, au) [b] (in acetonitrile), and relative energies ($\Delta E$ and $\Delta G$, kcal/mol) of species involved in the decomposition of ethyl chlorosulfite **2a**, isopropyl chlorosulfite **2b** and *t*-butyl chlorosulfite **2c** in dichloromethane and acetonitrile.

| | Dichloromethane (DCM) | | |
|---|---|---|---|
| | MPWB1K/6-31++G** | | |
| species | *E* | $\Delta E$ [c] | $\Delta G$ [c, d] |
| **2a** | -1088.001923 | 0.0 | 0.0 |
| **TS3a** | -1087.932723 | 43.4 | 38.8 |
| **IN2a** | -1087.967960 | 21.3 | 10.3 |
| **TS4a** | -1087.928728 | 45.9 | 39.7 |
| **3a** | -1088.004910 | -1.9 | -5.6 |
| | | | |
| **2b** | -1127.295206 | 0.0 | 0.0 |
| **TS3b** | -1127.246317 | 30.7 | 24.5 |
| **IN2b** | -1127.26755 | 17.4 | 6.7 |
| **TS4b** | -1127.244189 | 32.0 | 26.6 |
| **3b** | -1127.302327 | -4.5 | -9.5 |
| | | | |
| **2c** | -1166.593451 | 0.0 | 0.0 |
| **TS1c** | -1166.558743 | 21.8 | 15.9 |
| **IN1c** | -1166.559668 | 21.2 | 15.2 |
| **TS6c** | -1166.558880 | 21.7 | 15.8 |
| **3c** | -1166.598393 | -3.1 | -7.3 |
| **TS5c** | -1166.554355 | 24.5 | 17.4 |
| **IN2c** | -1166.566633 | 16.8 | 5.7 |

| | Acetonitrile ($CH_3CN$) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | MPWB1K/6-31++G** | | | B3LYP-D3/def2TZVP | | | M062X/cc-pVTZ | | |
| species | *E* | $\Delta E$ [c] | $\Delta G$ [c, d] | *E* | $\Delta E$ [c] | $\Delta G$ [c, d] | *E* | $\Delta E$ [c] | $\Delta G$ [c, d] |
| **2a** | -1088.002763 | 0.0 | 0.0 | -1088.221586 | 0.0 | 0.0 | -1088.044261 | 0.0 | 0.0 |
| **TS3a** | -1087.935470 | 42.2 | 37.5 | -1088.168286 | 33.4 | 28.7 | -1087.974352 | 43.9 | 39.1 |
| **IN2a** | -1087.969088 | 21.1 | 8.7 | -1088.201201 | 12.8 | 0.4 | -1088.010379 | 21.3 | 8.8 |
| **TS4a** | -1087.932133 | 44.3 | 38.1 | -1088.159706 | 38.8 | 32.6 | -1087.970736 | 46.1 | 39.9 |
| **3a** | -1088.005831 | -1.9 | -5.8 | -1088.228501 | -4.3 | -8.3 | -1088.044445 | -0.1 | -4.0 |
| | | | | | | | | | |
| **2b** | -1127.296096 | 0.0 | 0.0 | -1127.554185 | 0.0 | 0.0 | -1127.352654 | 0.0 | 0.0 |
| **TS3b** | -1127.249597 | 29.2 | 23.2 | -1127.519226 | 21.9 | 16.0 | -1127.301440 | 32.1 | 26.2 |
| **IN2b** | -1127.268466 | 17.3 | 6.9 | -1127.539460 | 9.2 | -1.2 | -1127.324184 | 17.9 | 7.4 |
| **TS4b** | -1127.247841 | 30.3 | 24.9 | -1127.515856 | 24.1 | 18.7 | -1127.300360 | 32.8 | 27.4 |
| **3b** | -1127.303305 | -4.5 | -8.1 | -1127.564765 | -6.6 | -10.2 | -1127.356735 | -2.6 | -6.1 |
| | | | | | | | | | |
| **2c** | -1166.594326 | 0.0 | 0.0 | -1166.890460 | 0.0 | 0.0 | -1166.665758 | 0.0 | 0.0 |
| **TS1c** | -1166.561784 | 20.4 | 15.2 | -1166.867281 | 14.5 | 9.3 | -1166.626777 | 24.5 | 19.3 |
| **IN1c** | -1166.563512 | 19.3 | 13.0 | -1166.868852 | 13.6 | 7.2 | -1166.630591 | 22.1 | 15.7 |
| **TS6c** | -1166.562720 | 19.8 | 14.0 | -1166.867920 | 14.1 | 9.0 | -1166.628458 | 23.4 | 18.2 |
| **3c** | -1166.599421 | -3.2 | -7.4 | -1166.898896 | -5.3 | -9.5 | -1166.667622 | -1.2 | -5.4 |
| **TS5c** | -1166.556621 | 23.7 | 14.4 | -1166.866538 | 15.0 | 5.8 | -1166.626056 | 24.9 | 15.7 |
| **IN2c** | -1166.567674 | 16.7 | 5.9 | -1166.877527 | 8.1 | -2.7 | -1166.638064 | 17.4 | 6.6 |

[a] Structures fully optimized. [b] Single point. [c] Relative to **2a**, **2b** and **2c**. [d] Thermal correction to *H* and *S* from **Table S1**, **S4** and **S6**.

**Table S8**. Natural charges corresponding to the hydrocarbon fragment of the species involved in the decomposition of ethyl chlorosulfite **2a** in gas-phase, dichloromethane (DCM) and acetonitrile ($CH_3CN$).

| specie | fragment | Gas-phase | DCM | $CH_3CN$ |
|---|---|---|---|---|
| **2a** | $CH_3CH_2$ | 0.372 | 0.393 | 0.397 |
| **TS2a** | $CH_3CH_2$ | 0.619 | 0.768 | 0.795 |
| **3a** | $CH_3CH_2$ | 0.122 | 0.144 | 0.149 |
| **TS3a** | $CH_3CH_2$ | 0.503 | 0.616 | 0.637 |
| **IN2a** | $CH_2$=$CH_2$ | 0.033 | 0.039 | 0.040 |
| **TS4a** | $CH_3CH_2$ | 0.650 | 0.828 | 0.850 |

**Table S9.** Natural charges corresponding to the hydrocarbon fragment of the species involved in the decomposition of isopropyl chlorosulfite **2b** in gas-phase, dichloromethane (DCM) and acetonitrile ($CH_3CN$).

| specie | fragment | Gas-phase | DCM | $CH_3CN$ |
|---|---|---|---|---|
| **2b** | $(CH_3)_2CH$ | 0.396 | 0.420 | 0.422 |
| **3b** | $(CH_3)_2CH$ | 0.139 | 0.161 | 0.163 |
| **TS3b** | $(CH_3)_2CH$ | 0.594 | 0.754 | 0.781 |
| **IN2b** | $CH_3CH$=$CH_2$ | 0.040 | 0.048 | 0.047 |
| **TS4b** | $(CH_3)_2CH$ | 0.758 | 0.875 | 0.909 |

**Table S10**. Natural charges corresponding to the hydrocarbon fragment of the species involved in the decomposition of *tert*-butyl chlorosulfite **2c** in gas-phase, dichloromethane (DCM) and acetonitrile ($CH_3CN$).

| specie | fragment | Gas-phase | DCM | $CH_3CN$ |
|---|---|---|---|---|
| **2c** | $(CH_3)_3C$ | 0.406 | 0.433 | 0.434 |
| **IN1c** | $(CH_3)_3C$ | | 0.836 | 0.860 |
| **3c** | $(CH_3)_3C$ | 0.145 | 0.172 | 0.176 |
| **TS3c/TS1c** | $(CH_3)_3C$ | 0.675 | 0.858 | 0.885 |
| **IN2c** | $(CH_3)_2C$=$CH_2$ | 0.045 | 0.055 | 0.055 |
| **TS4c/TS6c** | $(CH_3)_3C$ | 0.773 | 0.902 | 0.917 |
| **TS5c** | $(CH_3)_3C$ | | 0.654 | 0.626 |

**2.3.1-extended. Conversion of ethyl chlorosulfite (2a) into chloroethane (3a) in gas-phase.**

When we calculated the relative electronic energies ($\Delta E$) of ions $CH_3CH_2OSO^+ + Cl^-$ and $CH_3CH_2^+ + SO_2Cl^-$ in gas-phase ( Table S1), these were 162.9, and 168.6 kcal $mol^{-1}$, respectively, above the energy value of ethyl chlorosulfite **2a**. These values indicate a higher stability of ions $CH_3CH_2OSO^+ + Cl^-$ and therefore, the preference of an ionization process through path A' in Scheme 2 (see manuscript). These high values of $\Delta E$ are similar to the ones calculated by Schreiner, Schleyer and Hill[17] and are so high to be taken into account and no attempt was made to obtain the corresponding **TS1a** and **TS1'a**.

It should be noted that in the carbocation $CH_3CH_2^+$ the positive charge is delocalized between the two carbon atoms and a proton adopting a triangular arrangement (see Fig. S4a).

It was possible to locate the transition structure **TS2a** corresponding to the path B (Scheme 2), and the transition structures **TS3a** and **TS4a**, and intermediate **IN2a** corresponding to the path C suggested by us. The transition structure **TS2a** corresponding to the path B is a 4-center *syn*-rearrangement. Its geometry and relative energy to **2a** ($\Delta G$ = 46.6 kcal $mol^{-1}$, Table S1 ) are similar to the found by Schreiner et al.[1] With regard to the transition structures **TS3a** and **TS4a** corresponding to the path C, the free energy barrier ($\Delta G$ = 36.8 kcal $mol^{-1}$, Table S1) of **TS3a** is 9.8 kcal $mol^{-1}$ lower to the one obtained for **TS2a**. The **TS3a** is a 6-center *syn*-rearrangement, similar to the Ei pyrolitic eliminations of esters,[2] and leads to the corresponding olefin by simultaneous expulsion of HCl and $SO_2$. The olefin, HCl and $SO_2$ form a molecular complex **IN2a** quite stable with a free Gibbs energy ($\Delta G$, Table S1) of 7.8 kcal mol-1 higher than **2a**. The regio- and stereoselective addition of HCl to the olefin through the transition structure **TS4a** finally leads to chloroethane **3a**. It should be noted that a carbocation is never formed, as it is postulated in the normal mechanism of HCl addition to olefins.

The energy profile (IRC, $\Delta E$**,** Fig. S3a-1) corresponding to the transition structure **TS4a** in gas-phase shows that initially the approach of the HCl molecule to the double bond occurs until the distances C(2)-HCl and C(1)-ClH are 1.790 and 2.747 Å, respectively. Subsequently, the H atom of HCl approximates to the C(2) passing through 1.248 Å (**TS4a**) and reaching up to 1.093 Å, keeping the distance C(1)-Cl almost intact. Finally the chlorine atom binds to the carbon C(1). During the process the appearing negative charge on the Cl atom is stabilized by the $SO_2$ molecule. The distance Cl-$SO_2$ goes from 3.538 Å in **IN2a** to 3.422 Å in **3a** through a minimum of 3.007 Å. The Gibbs free energy of the transition structure **TS4a** is 45.2 kcal $mol^{-1}$ higher than that of **2a** (but 1.4 kcal $mol^{-1}$ lower to $\Delta G$ of **TS2a**), being in this case the rate limiting step for the conversion of **2a** into **3a**. Therefore, in terms of energy in gas-phase, the path C (Scheme 2) is more favorable than the path B (Scheme 2).

**2.4.1-extended. Conversion of isopropyl chlorosulfite (2b) into 2-chloropropane (3b) in gas-phase.**

In this case, again, the relative energies of species $(CH_3)_2CHOSO^+ + Cl^-$, $(CH_3)_2CH^+ + SO_2Cl^-$ (more favorable) are so high to be taken into account (see Table S4) and no attempt was made to obtain the corresponding **TS1b** and **TS1'b**. It was possible to locate **TS2b** corresponding to the path B (Scheme 2), and **TS3b**, **TS4b**, **IN2b** corresponding to the path C suggested by us. The transition structure **TS2b** has a free energy barrier of 34.4 kcal $mol^{-1}$, appreciably lower than that found for the transition structure **TS2a**.With regard to the transition structure **TS3b**, the free energy barrier ($\Delta G$ = 27.5 kcal $mol^{-1}$, Table 3) is 6.9 kcal $mol^{-1}$ lower to the one obtained for **TS2b**.

The Gibbs free energy of the transition structure **TS4b** is 33.4 kcal $mol^{-1}$ higher than that of **2b (**but 1.0 kcal $mol^{-1}$ lower to $\Delta G$ of **TS2b**), being in this case the rate limiting step for the conversion of **2b** into **3b**. Therefore, in terms of energy in gas-phase, the path C (Scheme 2) is more favorable than the path B (Scheme 2) .

The energy profile (IRC, $\Delta E$**,** Fig. S3b-1) corresponding to the transition structure **TS4b** in gas-phase shows the initial transference of the H atom of HCl to the olefinic C(2) before the formation of the bond C(1)-Cl.

**2.5.1-extended. Conversion of *tert*-butyl chlorosulfite (2c) into 2-chloro-2-methylpropane (3c) in gas-phase.**

In this case, again, the relative energies of species *t*-$BuOSO^+ + Cl^-$ and *t*-$Bu^+ + SO_2Cl^-$ (more favorable) are so high to be taken into account (see Table S6) and no attempt was made to obtain the corresponding **TS1c** and **TS1'c**. Also, all attempts to locate **TS2c** corresponding to the path B (Scheme 2) were unsuccessful. It was only possible to locate **TS3c**, **TS4c** and intermediate **IN2c** corresponding to the path C suggested by us. **TS3c** and **TS4c** have free energy barriers of 21.8 and 22.8 kcal $mol^{-1}$, respectively, appreciably lower than that found for **TS3a**/**TS4a** and **TS3b**/**TS4b**. Therefore, in terms of energy in gas-phase, the path C (Scheme 2) is the only possible one.

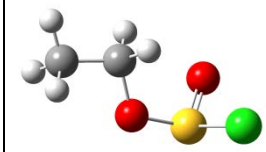
1 P. R. Schreiner, P. von R. Schleyer and R. K. Hill, *J. Org. Chem.*, 1994, **59**,1849–1854.

2 D. Y. Curtin, and D. B. Kellom, *J. Am. Chem. Soc.*, 1953, **75**, 6011-6018.

**Z-matrices**

**2a** in DCM

0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
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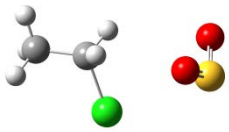
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.513057 |
| 3 | 1 | 0 | 1.019162 | 0.000000 | -0.394061 |
| 4 | 8 | 0 | 0.686894 | 1.232716 | 1.941676 |
| 5 | 16 | 0 | 0.730435 | 1.627378 | 3.507188 |
| 6 | 8 | 0 | -0.464973 | 1.120746 | 4.191513 |
| 7 | 17 | 0 | 2.397058 | 0.245066 | 4.149977 |
| 8 | 1 | 0 | -0.534504 | 0.868859 | -0.392161 |
| 9 | 1 | 0 | -0.506436 | -0.903880 | -0.351550 |
| 10 | 1 | 0 | -1.008374 | 0.009255 | 1.930395 |
| 11 | 1 | 0 | 0.558656 | -0.842537 | 1.929940 |

**3a** in DCM

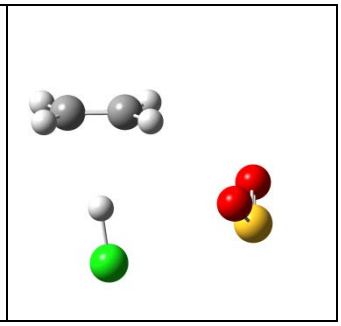
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.515004 |
| 3 | 1 | 0 | 1.017382 | 0.000000 | 1.913766 |
| 4 | 17 | 0 | 0.840001 | 1.492593 | -0.670107 |
| 5 | 16 | 0 | -0.200547 | 0.380232 | -3.761969 |
| 6 | 8 | 0 | 0.565134 | -0.860850 | -3.609744 |
| 7 | 8 | 0 | -1.580808 | 0.392231 | -3.266426 |
| 8 | 1 | 0 | -0.505736 | -0.907383 | 1.863432 |
| 9 | 1 | 0 | -0.535339 | 0.865161 | 1.913732 |
| 10 | 1 | 0 | -1.005800 | 0.026610 | -0.419362 |
| 11 | 1 | 0 | 0.544254 | -0.845841 | -0.419761 |

**IN2a** in DCM

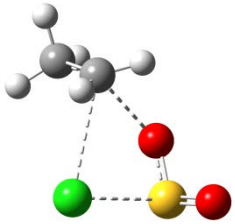
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.336176 |
| 3 | 1 | 0 | 2.240065 | 0.000000 | 0.768566 |
| 4 | 8 | 0 | 1.869738 | 0.577300 | 4.412856 |
| 5 | 16 | 0 | 2.564240 | -0.713125 | 4.382739 |
| 6 | 8 | 0 | 1.805134 | -1.885208 | 3.935300 |
| 7 | 17 | 0 | 3.540462 | -0.029914 | 0.922853 |
| 8 | 1 | 0 | -0.029304 | 0.923810 | -0.571457 |
| 9 | 1 | 0 | 0.016583 | -0.924448 | -0.571003 |
| 10 | 1 | 0 | -0.026840 | 0.923013 | 1.908779 |
| 11 | 1 | 0 | 0.021321 | -0.922930 | 1.909171 |

**TS2a** in DCM

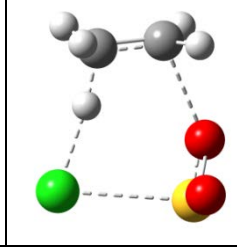
1 imaginary frequencies= -383.2121



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 17 | 0 | 0.000000 | 0.000000 | 2.968372 |
| 3 | 8 | 0 | 2.269740 | 0.000000 | 0.908768 |
| 4 | 16 | 0 | 2.463655 | 0.561018 | 2.280095 |
| 5 | 6 | 0 | 0.000114 | -1.395326 | -0.363230 |
| 6 | 1 | 0 | 0.959620 | -1.761600 | -0.725137 |
| 7 | 8 | 0 | 2.502146 | 2.032144 | 2.342826 |
| 8 | 1 | 0 | -0.461157 | -2.043946 | 0.381181 |
| 9 | 1 | 0 | -0.693201 | -1.378688 | -1.237953 |
| 10 | 1 | 0 | -0.795680 | 0.408783 | 0.611335 |
| 11 | 1 | 0 | 0.663340 | 0.700359 | -0.492477 |

**TS3a** in DCM

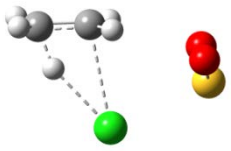
1 imaginary frequencies= -233.2404



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.398324 |
| 3 | 1 | 0 | 1.175995 | 0.000000 | -0.310537 |
| 4 | 8 | 0 | 2.209029 | 0.187628 | 2.146856 |
| 5 | 16 | 0 | 3.247584 | -0.748970 | 1.637907 |
| 6 | 8 | 0 | 2.856025 | -2.164375 | 1.615249 |
| 7 | 17 | 0 | 2.881401 | -0.050933 | -1.053509 |
| 8 | 1 | 0 | -0.338396 | 0.919121 | -0.479066 |
| 9 | 1 | 0 | -0.324249 | -0.926082 | -0.476307 |
| 10 | 1 | 0 | -0.062241 | 0.919050 | 1.969432 |
| 11 | 1 | 0 | -0.014168 | -0.923626 | 1.966174 |

**TS4a** in DCM

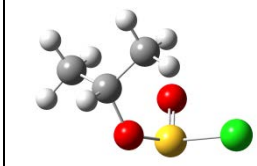
1 imaginary frequencies= -711.2527



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.391374 |
| 3 | 1 | 0 | 1.168916 | 0.000000 | 1.080978 |
| 4 | 17 | 0 | 2.847228 | 0.012535 | -0.275372 |
| 5 | 16 | 0 | 2.507097 | 2.701435 | -1.303675 |
| 6 | 8 | 0 | 2.816524 | 2.500608 | -2.726601 |
| 7 | 8 | 0 | 1.075062 | 2.826227 | -0.962121 |
| 8 | 1 | 0 | -0.170005 | -0.928905 | 1.927965 |
| 9 | 1 | 0 | -0.163980 | 0.934285 | 1.920887 |
| 10 | 1 | 0 | 0.047832 | 0.933879 | -0.557140 |
| 11 | 1 | 0 | 0.031736 | -0.929026 | -0.560866 |

**2b** in DCM

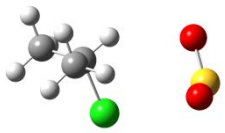
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.520340 |
| 3 | 6 | 0 | 1.378002 | 0.000000 | 2.164706 |
| 4 | 1 | 0 | -1.016885 | 0.004502 | -0.396674 |
| 5 | 1 | 0 | 1.885436 | -0.934009 | 1.904547 |
| 6 | 1 | 0 | 1.295311 | 0.049910 | 3.253365 |
| 7 | 8 | 0 | -0.820202 | 1.128113 | 2.080815 |
| 8 | 16 | 0 | -0.654060 | 2.687142 | 1.738340 |
| 9 | 8 | 0 | 0.663409 | 2.977862 | 1.158839 |
| 10 | 17 | 0 | -2.116305 | 2.871807 | -0.002307 |
| 11 | 1 | 0 | 0.495063 | -0.915410 | -0.338461 |
| 12 | 1 | 0 | 0.547325 | 0.853149 | -0.405901 |
| 13 | 1 | 0 | 1.986161 | 0.835010 | 1.812019 |
| 14 | 1 | 0 | -0.581801 | -0.847558 | 1.889738 |

**3b** in DCM

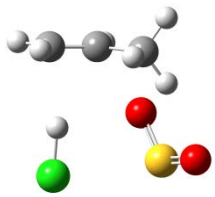
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | 1.093652 |
| 3 | 6 | 0 | 1.417801 | 0.000000 | -0.546365 |
| 4 | 6 | 0 | 2.266202 | 1.171157 | -0.077748 |
| 5 | 1 | 0 | 1.803076 | 2.101343 | -0.425553 |
| 6 | 1 | 0 | 3.278871 | 1.121736 | -0.483992 |
| 7 | 1 | 0 | 2.324138 | 1.203557 | 1.013888 |
| 8 | 16 | 0 | 4.320156 | -1.364729 | -2.777867 |
| 9 | 8 | 0 | 3.181772 | -0.787968 | -3.501924 |
| 10 | 8 | 0 | 5.285662 | -0.436470 | -2.180494 |
| 11 | 1 | 0 | -0.566632 | -0.864445 | -0.353177 |
| 12 | 1 | 0 | -0.508533 | 0.907546 | -0.344095 |
| 13 | 17 | 0 | 2.256968 | -1.586495 | -0.040345 |
| 14 | 1 | 0 | 1.417829 | -0.064935 | -1.636020 |

**IN2b** in DCM

0 imaginary frequencies



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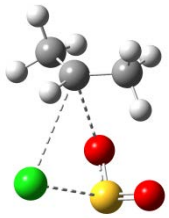
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.340564 |
| 3 | 6 | 0 | 1.222450 | 0.000000 | 2.208519 |
| 4 | 1 | 0 | -0.170303 | 2.133660 | 0.348928 |
| 5 | 1 | 0 | 1.246102 | -0.901906 | 2.832649 |
| 6 | 1 | 0 | 1.210458 | 0.853223 | 2.896565 |
| 7 | 8 | 0 | -2.066709 | 2.069929 | 3.418386 |
| 8 | 16 | 0 | -1.261408 | 3.246854 | 3.758726 |
| 9 | 8 | 0 | 0.112484 | 3.021898 | 4.219395 |
| 10 | 17 | 0 | -0.294763 | 3.444730 | 0.306799 |
| 11 | 1 | 0 | -0.925209 | -0.027195 | -0.568578 |
| 12 | 1 | 0 | 0.926935 | -0.015421 | -0.568964 |
| 13 | 1 | 0 | 2.141834 | 0.034793 | 1.617549 |
| 14 | 1 | 0 | -0.955324 | 0.006438 | 1.865064 |

**TS2b** in DCM

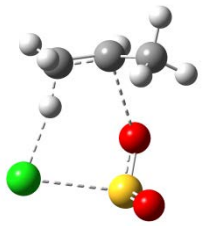
1 imaginary frequencies= -166.8450



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 17 | 0 | 0.000000 | 0.000000 | 3.188281 |
| 3 | 8 | 0 | 2.528093 | 0.000000 | 1.214510 |
| 4 | 16 | 0 | 2.420046 | 0.841816 | 2.432265 |
| 5 | 6 | 0 | 0.445098 | -1.262958 | -0.550659 |
| 6 | 1 | 0 | 1.353055 | -1.197702 | -1.148423 |
| 7 | 8 | 0 | 2.136834 | 2.268542 | 2.159546 |
| 8 | 1 | 0 | 0.477851 | -2.055499 | 0.199674 |
| 9 | 6 | 0 | 0.338432 | 1.308196 | -0.523464 |
| 10 | 1 | 0 | -0.397057 | -1.533944 | -1.224614 |
| 11 | 1 | 0 | 0.631154 | 1.962964 | 0.312278 |
| 12 | 1 | 0 | 1.099439 | 1.300530 | -1.301548 |
| 13 | 1 | 0 | -0.604602 | 1.751506 | -0.890177 |
| 14 | 1 | 0 | -0.731502 | -0.034725 | 0.807026 |

**TS3b** in DCM

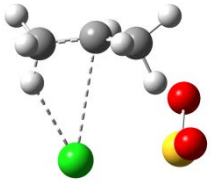
1 imaginary frequencies= -93.8156



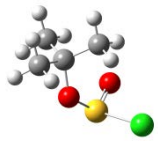
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.414647 |
| 3 | 6 | 0 | 1.207677 | 0.000000 | 2.243518 |
| 4 | 1 | 0 | -0.108622 | 1.134130 | -0.284694 |
| 5 | 1 | 0 | 1.340137 | -1.051383 | 2.557735 |
| 6 | 1 | 0 | 1.071889 | 0.580573 | 3.157543 |
| 7 | 8 | 0 | -0.763861 | 2.359706 | 2.051426 |
| 8 | 16 | 0 | -0.220959 | 3.640192 | 1.532700 |
| 9 | 8 | 0 | 1.212129 | 3.862836 | 1.779868 |
| 10 | 17 | 0 | -0.215197 | 2.940812 | -1.162227 |
| 11 | 1 | 0 | -0.884541 | -0.442568 | -0.460505 |
| 12 | 1 | 0 | 0.946946 | -0.278734 | -0.465588 |
| 13 | 1 | 0 | 2.103352 | 0.301728 | 1.698054 |
| 14 | 1 | 0 | -0.954502 | -0.055013 | 1.931550 |

**TS4b** in DCM

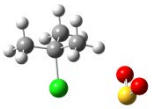
1 imaginary frequencies= -154.6220



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | 1.119173 |
| 3 | 6 | 0 | 1.412310 | 0.000000 | -0.285679 |
| 4 | 6 | 0 | 2.180723 | 1.106282 | -0.763471 |
| 5 | 1 | 0 | 2.994749 | 0.784711 | -1.424510 |
| 6 | 1 | 0 | 2.770045 | 1.421799 | 0.153608 |
| 7 | 1 | 0 | 1.607359 | 1.948919 | -1.145873 |
| 8 | 16 | 0 | 3.971939 | 0.433527 | 2.489637 |
| 9 | 8 | 0 | 4.160694 | -0.797648 | 1.683040 |
| 10 | 8 | 0 | 3.890654 | 1.676432 | 1.683039 |
| 11 | 1 | 0 | -0.461285 | -0.962017 | -0.253331 |
| 12 | 1 | 0 | -0.550500 | 0.857574 | -0.382105 |
| 13 | 17 | 0 | 1.431894 | 0.163890 | 3.133914 |
| 14 | 1 | 0 | 1.969785 | -0.900002 | -0.021179 |

| **2c** in DCM<br><br>0 imaginary frequencies |  |
|---|---|

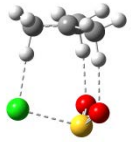
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.525299 |
| 3 | 6 | 0 | 1.404877 | 0.000000 | 2.123143 |
| 4 | 1 | 0 | -1.017109 | 0.038213 | -0.394960 |
| 5 | 1 | 0 | 1.895705 | -0.945293 | 1.872683 |
| 6 | 1 | 0 | 1.359490 | 0.083318 | 3.212208 |
| 7 | 6 | 0 | -0.862903 | -1.120531 | 2.096685 |
| 8 | 1 | 0 | -0.899239 | -1.066950 | 3.187715 |
| 9 | 1 | 0 | -1.881470 | -1.066903 | 1.704714 |
| 10 | 1 | 0 | -0.431282 | -2.084569 | 1.812285 |
| 11 | 8 | 0 | -0.720701 | 1.238972 | 2.047273 |
| 12 | 16 | 0 | -0.484677 | 2.765820 | 1.631422 |
| 13 | 8 | 0 | 0.830383 | 2.973278 | 1.010698 |
| 14 | 17 | 0 | -1.980739 | 2.955761 | -0.088724 |
| 15 | 1 | 0 | 0.467012 | -0.928407 | -0.342116 |
| 16 | 1 | 0 | 0.572064 | 0.836168 | -0.405361 |
| 17 | 1 | 0 | 2.008573 | 0.817816 | 1.726709 |

| **3c** in DCM<br><br>0 imaginary frequencies |  |
|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | 1.092723 |
| 3 | 6 | 0 | 1.420436 | 0.000000 | -0.556224 |
| 4 | 6 | 0 | 2.249748 | -1.164645 | -0.023253 |
| 5 | 6 | 0 | 1.443529 | 0.080042 | -2.079911 |
| 6 | 1 | 0 | 0.988595 | -0.830475 | -2.486662 |
| 7 | 1 | 0 | 1.804586 | -2.102515 | -0.374462 |
| 8 | 1 | 0 | 2.464116 | 0.152489 | -2.462625 |
| 9 | 1 | 0 | 3.280852 | -1.119659 | -0.381464 |
| 10 | 1 | 0 | 2.257444 | -1.178081 | 1.069384 |
| 11 | 1 | 0 | 0.870836 | 0.938141 | -2.440198 |
| 12 | 16 | 0 | 5.434639 | 1.515962 | -1.253606 |
| 13 | 8 | 0 | 5.816440 | 0.220607 | -0.681561 |
| 14 | 8 | 0 | 4.944550 | 1.529908 | -2.635710 |
| 15 | 1 | 0 | -0.511162 | -0.907163 | -0.342147 |
| 16 | 1 | 0 | -0.565527 | 0.865202 | -0.354448 |
| 17 | 17 | 0 | 2.240142 | 1.584152 | 0.079410 |

**IN1c** in DCM

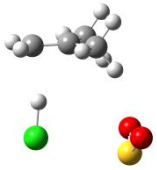
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.444901 |
| 3 | 6 | 0 | 1.268186 | 0.000000 | 2.182559 |
| 4 | 1 | 0 | -0.936055 | -0.335848 | -0.447956 |
| 5 | 1 | 0 | 2.089725 | -0.456310 | 1.630032 |
| 6 | 1 | 0 | 1.171726 | -0.414120 | 3.188311 |
| 7 | 6 | 0 | -1.247808 | 0.231410 | 2.181208 |
| 8 | 1 | 0 | -1.243880 | 1.320917 | 2.410178 |
| 9 | 1 | 0 | -2.143695 | 0.013061 | 1.600679 |
| 10 | 1 | 0 | -1.256721 | -0.274824 | 3.149436 |
| 11 | 8 | 0 | -0.882431 | 3.439475 | 2.521442 |
| 12 | 16 | 0 | 0.392179 | 4.002380 | 2.017540 |
| 13 | 8 | 0 | 1.597737 | 3.227379 | 2.393651 |
| 14 | 17 | 0 | 0.204265 | 3.310534 | -0.550772 |
| 15 | 1 | 0 | 0.882111 | -0.453757 | -0.452168 |
| 16 | 1 | 0 | 0.064617 | 1.112211 | -0.237428 |
| 17 | 1 | 0 | 1.513030 | 1.078254 | 2.317722 |

**IN2c** in DCM

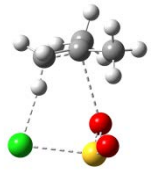
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.346193 |
| 3 | 6 | 0 | 1.278359 | 0.000000 | 2.143364 |
| 4 | 1 | 0 | 0.010351 | 2.069793 | 0.145576 |
| 5 | 1 | 0 | 1.316964 | -0.878134 | 2.799644 |
| 6 | 1 | 0 | 1.330913 | 0.880413 | 2.795068 |
| 7 | 6 | 0 | -1.277962 | 0.001671 | 2.143945 |
| 8 | 1 | 0 | -1.326970 | 0.879176 | 2.799744 |
| 9 | 1 | 0 | -2.161702 | -0.002807 | 1.501316 |
| 10 | 1 | 0 | -1.319336 | -0.879375 | 2.796215 |
| 11 | 8 | 0 | -1.255368 | 3.449300 | 3.649565 |
| 12 | 16 | 0 | 0.002009 | 4.165440 | 3.411300 |
| 13 | 8 | 0 | 1.253439 | 3.445830 | 3.669601 |
| 14 | 17 | 0 | 0.019815 | 3.385244 | -0.011578 |
| 15 | 1 | 0 | -0.926286 | -0.034054 | -0.567424 |
| 16 | 1 | 0 | 0.926307 | -0.036350 | -0.567270 |
| 17 | 1 | 0 | 2.161750 | -0.010408 | 1.500325 |

**TS1c** in DCM

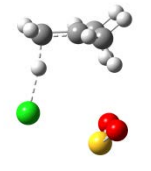
1 imaginary frequencies= -61.7570



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.439659 |
| 3 | 6 | 0 | 1.279048 | 0.000000 | 2.172960 |
| 4 | 1 | 0 | -0.108843 | 1.099665 | -0.283687 |
| 5 | 1 | 0 | 1.770071 | -0.964708 | 1.975438 |
| 6 | 1 | 0 | 1.161945 | 0.141090 | 3.246414 |
| 7 | 6 | 0 | -1.265462 | -0.026953 | 2.188067 |
| 8 | 1 | 0 | -1.241699 | 0.709302 | 2.996512 |
| 9 | 1 | 0 | -2.145858 | 0.099442 | 1.558812 |
| 10 | 1 | 0 | -1.313837 | -1.013896 | 2.678020 |
| 11 | 8 | 0 | -0.106355 | 2.848918 | 2.033004 |
| 12 | 16 | 0 | 0.793116 | 3.719083 | 1.239313 |
| 13 | 8 | 0 | 2.183960 | 3.231197 | 1.133576 |
| 14 | 17 | 0 | -0.169776 | 3.085824 | -1.226953 |
| 15 | 1 | 0 | -0.883424 | -0.470611 | -0.437212 |
| 16 | 1 | 0 | 0.936670 | -0.325433 | -0.453864 |
| 17 | 1 | 0 | 1.942537 | 0.766888 | 1.755318 |

**TS5c** in DCM

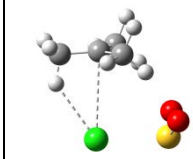
1 imaginary frequencies= -213.2930



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.393996 |
| 3 | 6 | 0 | 1.276972 | 0.000000 | 2.157444 |
| 4 | 1 | 0 | -0.940360 | -0.194090 | -0.512984 |
| 5 | 1 | 0 | 2.137391 | -0.254146 | 1.537876 |
| 6 | 1 | 0 | 1.211888 | -0.689304 | 3.005955 |
| 7 | 6 | 0 | -1.260278 | 0.205803 | 2.157444 |
| 8 | 1 | 0 | -1.250093 | 1.219875 | 2.585217 |
| 9 | 1 | 0 | -2.150409 | 0.093649 | 1.537876 |
| 10 | 1 | 0 | -1.307138 | -0.484979 | 3.005955 |
| 11 | 16 | 0 | 0.341241 | 4.195854 | 2.121354 |
| 12 | 8 | 0 | -0.952142 | 3.705114 | 2.624011 |
| 13 | 8 | 0 | 1.538328 | 3.502569 | 2.624011 |
| 14 | 1 | 0 | 0.102816 | 1.268849 | -0.142988 |
| 15 | 17 | 0 | 0.238833 | 2.951262 | -0.586354 |
| 16 | 1 | 0 | 0.896786 | -0.343106 | -0.512984 |
| 17 | 1 | 0 | 1.430353 | 1.002456 | 2.585217 |

**TS6c** in DCM

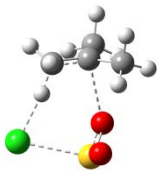
1 imaginary frequencies= -103.2469



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.460792 |
| 3 | 6 | 0 | 1.260271 | 0.000000 | 2.207877 |
| 4 | 1 | 0 | -0.919753 | -0.394892 | -0.434710 |
| 5 | 1 | 0 | 2.143993 | 0.013812 | 1.572127 |
| 6 | 1 | 0 | 1.268924 | -0.899950 | 2.842962 |
| 7 | 6 | 0 | -1.274612 | -0.060878 | 2.187605 |
| 8 | 1 | 0 | -1.232971 | 0.419344 | 3.167619 |
| 9 | 1 | 0 | -2.108349 | 0.311385 | 1.590932 |
| 10 | 1 | 0 | -1.451242 | -1.140348 | 2.348136 |
| 11 | 8 | 0 | -1.261535 | 2.496586 | 4.336977 |
| 12 | 16 | 0 | -0.076711 | 3.301961 | 3.969044 |
| 13 | 8 | 0 | 1.221355 | 2.608129 | 4.142354 |
| 14 | 17 | 0 | -0.235190 | 3.206102 | 1.278840 |
| 15 | 1 | 0 | 0.900395 | -0.439208 | -0.432733 |
| 16 | 1 | 0 | 0.024874 | 1.087143 | -0.224383 |
| 17 | 1 | 0 | 1.273680 | 0.839596 | 2.922099 |

**TS3c** in gas-phase

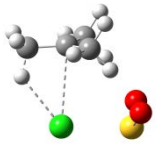
1 imaginary frequencies= -143.2387



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.425462 |
| 3 | 6 | 0 | 1.283651 | 0.000000 | 2.174290 |
| 4 | 1 | 0 | -0.229608 | 1.105071 | -0.339855 |
| 5 | 1 | 0 | 1.639515 | -1.042962 | 2.192111 |
| 6 | 1 | 0 | 1.166101 | 0.343564 | 3.201899 |
| 7 | 6 | 0 | -1.272329 | -0.201265 | 2.164744 |
| 8 | 1 | 0 | -1.271193 | 0.323081 | 3.120438 |
| 9 | 1 | 0 | -2.139154 | 0.095490 | 1.571578 |
| 10 | 1 | 0 | -1.356759 | -1.280745 | 2.369566 |
| 11 | 8 | 0 | -0.268399 | 2.437217 | 1.979410 |
| 12 | 16 | 0 | 0.498972 | 3.422519 | 1.161324 |
| 13 | 8 | 0 | 1.905836 | 3.044245 | 0.930583 |
| 14 | 17 | 0 | -0.617838 | 2.815062 | -1.164467 |
| 15 | 1 | 0 | -0.846421 | -0.523529 | -0.451080 |
| 16 | 1 | 0 | 0.958964 | -0.226319 | -0.467390 |
| 17 | 1 | 0 | 2.037379 | 0.602055 | 1.663102 |

**TS4c** in gas-phase

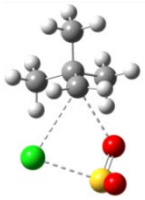
1 imaginary frequencies= -205.4841



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | 1.111812 |
| 3 | 6 | 0 | 1.428264 | 0.000000 | -0.336817 |
| 4 | 6 | 0 | 2.141803 | -1.266135 | -0.554803 |
| 5 | 6 | 0 | 2.141803 | 1.266135 | -0.554803 |
| 6 | 1 | 0 | 2.538932 | 1.273715 | -1.580590 |
| 7 | 1 | 0 | 2.538932 | -1.273715 | -1.580590 |
| 8 | 1 | 0 | 3.039365 | 1.312628 | 0.094070 |
| 9 | 1 | 0 | 3.039365 | -1.312628 | 0.094070 |
| 10 | 1 | 0 | 1.518238 | -2.144186 | -0.390168 |
| 11 | 1 | 0 | 1.518238 | 2.144186 | -0.390168 |
| 12 | 16 | 0 | 4.351408 | 0.000833 | 2.295763 |
| 13 | 8 | 0 | 4.453794 | -1.246758 | 1.498739 |
| 14 | 8 | 0 | 4.453316 | 1.248462 | 1.498739 |
| 15 | 1 | 0 | -0.513914 | -0.907083 | -0.324934 |
| 16 | 1 | 0 | -0.513895 | 0.907122 | -0.324854 |
| 17 | 17 | 0 | 1.780140 | 0.000000 | 2.708247 |

**TS2a1** in acetonitrile

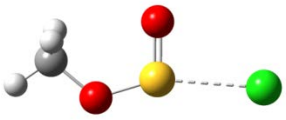
1 imaginary frequencies= -271.2286



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.442907 |
| 3 | 8 | 0 | 2.596339 | 0.000000 | 1.756637 |
| 4 | 16 | 0 | 3.145243 | -0.778910 | 2.900230 |
| 5 | 8 | 0 | 3.086848 | -0.090269 | 4.202211 |
| 6 | 17 | 0 | 1.063403 | -2.432827 | 3.004928 |
| 7 | 1 | 0 | 0.406623 | 0.822338 | 2.023601 |
| 8 | 1 | 0 | -0.536036 | -0.770801 | 1.987744 |
| 9 | 6 | 0 | 0.888660 | 1.091299 | -0.619899 |
| 10 | 1 | 0 | 1.934852 | 0.923896 | -0.360763 |
| 11 | 1 | 0 | 0.790129 | 1.076062 | -1.708291 |
| 12 | 1 | 0 | 0.596391 | 2.084690 | -0.266930 |
| 13 | 6 | 0 | -1.504490 | 0.244111 | -0.444334 |
| 14 | 1 | 0 | -1.479946 | 0.206232 | -1.535662 |
| 15 | 1 | 0 | -2.173532 | -0.531620 | -0.068233 |
| 16 | 1 | 0 | -1.863569 | 1.224307 | -0.126343 |
| 17 | 6 | 0 | 0.388335 | -1.419772 | -0.525314 |
| 18 | 1 | 0 | -0.263009 | -2.191616 | -0.111261 |
| 19 | 1 | 0 | 0.289693 | -1.412713 | -1.613861 |
| 20 | 1 | 0 | 1.420944 | -1.644606 | -0.256149 |

**TS-I** in acetonitrile

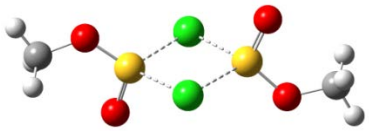
1 imaginary frequencies= -156.7914



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 16 | 0 | 0.000000 | 0.000000 | 1.605453 |
| 3 | 8 | 0 | 1.390460 | 0.000000 | 2.038835 |
| 4 | 17 | 0 | -0.973035 | 0.000229 | 4.101135 |
| 5 | 6 | 0 | 1.227100 | 0.002883 | -0.800577 |
| 6 | 1 | 0 | 1.762493 | 0.935386 | -0.617769 |
| 7 | 1 | 0 | 0.888600 | -0.067854 | -1.830858 |
| 8 | 1 | 0 | 1.840310 | -0.853189 | -0.517749 |

**TS-II** in acetonitrile

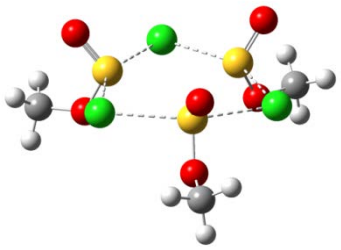
1 imaginary frequencies= -128.1160



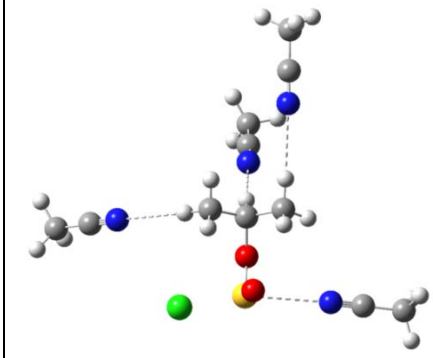
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 17 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 17 | 0 | 0.000000 | 0.000000 | 4.566919 |
| 3 | 16 | 0 | 1.700084 | 0.000000 | 2.283182 |
| 4 | 16 | 0 | -1.700421 | 0.082673 | 2.283842 |
| 5 | 8 | 0 | 2.345400 | -1.306486 | 2.283209 |
| 6 | 8 | 0 | -2.164951 | 1.463405 | 2.283770 |
| 7 | 8 | 0 | 2.809034 | 1.148296 | 2.283120 |
| 8 | 8 | 0 | -2.956465 | -0.902692 | 2.283953 |
| 9 | 6 | 0 | 4.245955 | 0.838983 | 2.283098 |
| 10 | 6 | 0 | -4.336226 | -0.395996 | 2.283972 |
| 11 | 1 | 0 | 4.728383 | 1.812986 | 2.283056 |
| 12 | 1 | 0 | -4.950225 | -1.292830 | 2.284053 |
| 13 | 1 | 0 | 4.492500 | 0.273547 | 1.384877 |
| 14 | 1 | 0 | 4.492535 | 0.273585 | 3.181337 |
| 15 | 1 | 0 | -4.500678 | 0.198690 | 1.385805 |
| 16 | 1 | 0 | -4.500615 | 0.198817 | 3.182063 |

**TS-III** in acetonitrile

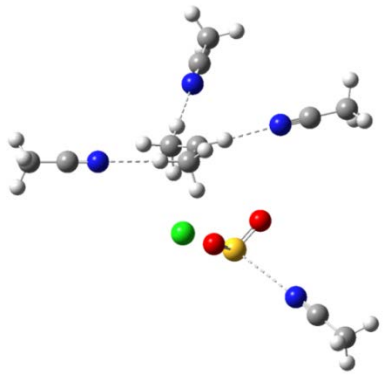
1 imaginary frequencies= -163.3732



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 17 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 17 | 0 | 0.000000 | 0.000000 | 5.266174 |
| 3 | 17 | 0 | 4.562447 | 0.000000 | 2.634566 |
| 4 | 16 | 0 | 2.644230 | -0.046439 | 0.690365 |
| 5 | 16 | 0 | -0.729034 | -0.016716 | 2.628594 |
| 6 | 16 | 0 | 2.629918 | -0.124214 | 4.565330 |
| 7 | 8 | 0 | 2.981226 | 1.393266 | 0.089923 |
| 8 | 8 | 0 | 3.149818 | -1.096117 | -0.185854 |
| 9 | 8 | 0 | 3.034643 | 1.254907 | 5.259302 |
| 10 | 8 | 0 | 3.088111 | -1.252681 | 5.367134 |
| 11 | 8 | 0 | -1.370527 | 1.444775 | 2.638273 |
| 12 | 8 | 0 | -1.774622 | -1.032481 | 2.627967 |
| 13 | 6 | 0 | 3.759858 | 1.261810 | 6.532116 |
| 14 | 1 | 0 | 4.737371 | 0.798788 | 6.396093 |
| 15 | 1 | 0 | 3.856264 | 2.316571 | 6.777568 |
| 16 | 1 | 0 | 3.179826 | 0.733250 | 7.288595 |
| 17 | 6 | 0 | 3.677299 | 1.524329 | -1.192680 |
| 18 | 1 | 0 | 3.896717 | 2.586476 | -1.269873 |
| 19 | 1 | 0 | 4.592421 | 0.932820 | -1.181739 |
| 20 | 1 | 0 | 3.012956 | 1.200655 | -1.994423 |
| 21 | 6 | 0 | -2.824667 | 1.621209 | 2.675559 |
| 22 | 1 | 0 | -2.968514 | 2.690320 | 2.538830 |
| 23 | 1 | 0 | -3.287080 | 1.054935 | 1.867620 |
| 24 | 1 | 0 | -3.200095 | 1.294612 | 3.645588 |

| **2b-s** in acetonitrile<br><br>0 imaginary frequencies |  |
|---|---|

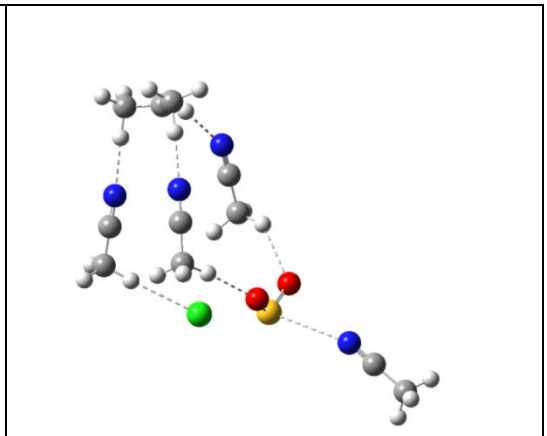
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.519717 |
| 3 | 6 | 0 | 1.376571 | 0.000000 | 2.165551 |
| 4 | 1 | 0 | -1.013321 | -0.076710 | -0.400050 |
| 5 | 1 | 0 | 1.856059 | -0.958985 | 1.945725 |
| 6 | 1 | 0 | 1.292649 | 0.105111 | 3.250068 |
| 7 | 8 | 0 | -0.832650 | 1.135894 | 2.061657 |
| 8 | 16 | 0 | -0.590487 | 2.697137 | 1.835608 |
| 9 | 8 | 0 | 0.745627 | 2.977014 | 1.300454 |
| 10 | 17 | 0 | -1.997107 | 3.062889 | 0.010009 |
| 11 | 1 | 0 | 0.563632 | -0.877288 | -0.333834 |
| 12 | 1 | 0 | 0.487112 | 0.889214 | -0.406335 |
| 13 | 1 | 0 | 2.006664 | 0.803401 | 1.779485 |
| 14 | 1 | 0 | -0.585413 | -0.842384 | 1.894224 |
| 15 | 7 | 0 | 0.574676 | 2.758271 | 4.662788 |
| 16 | 7 | 0 | 2.986246 | -3.322352 | 1.325096 |
| 17 | 7 | 0 | -3.695239 | -0.379546 | -1.483212 |
| 18 | 7 | 0 | -1.889045 | -2.780469 | 2.832389 |
| 19 | 6 | 0 | 1.003793 | 2.819656 | 5.739230 |
| 20 | 6 | 0 | -4.770870 | -0.460367 | -1.912258 |
| 21 | 6 | 0 | 3.438799 | -4.359833 | 1.067153 |
| 22 | 6 | 0 | -2.523798 | -3.658495 | 3.248700 |
| 23 | 6 | 0 | 1.543892 | 2.898670 | 7.091289 |
| 24 | 1 | 0 | 1.019214 | 2.197304 | 7.744654 |
| 25 | 1 | 0 | 2.607722 | 2.648898 | 7.083168 |
| 26 | 1 | 0 | 1.419634 | 3.910858 | 7.483990 |
| 27 | 6 | 0 | -6.122419 | -0.560449 | -2.451680 |
| 28 | 1 | 0 | -6.235466 | -1.494583 | -3.007467 |
| 29 | 1 | 0 | -6.852270 | -0.541184 | -1.638581 |
| 30 | 1 | 0 | -6.319530 | 0.277775 | -3.124534 |
| 31 | 6 | 0 | 4.008252 | -5.663129 | 0.743057 |
| 32 | 1 | 0 | 3.385103 | -6.169511 | 0.001768 |
| 33 | 1 | 0 | 5.014674 | -5.540583 | 0.335094 |
| 34 | 1 | 0 | 4.062757 | -6.281782 | 1.642289 |
| 35 | 6 | 0 | -3.322692 | -4.761459 | 3.770712 |
| 36 | 1 | 0 | -3.254654 | -5.622144 | 3.100676 |
| 37 | 1 | 0 | -2.959175 | -5.051678 | 4.759524 |
| 38 | 1 | 0 | -4.369338 | -4.458070 | 3.852768 |

| **IN1b-contact-s** in acetonitrile<br><br>0 imaginary frequencies |  |
|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.457851 |
| 3 | 6 | 0 | 1.263792 | 0.000000 | 2.196417 |
| 4 | 1 | 0 | -0.946964 | -0.342901 | -0.421007 |
| 5 | 1 | 0 | 2.094378 | -0.426050 | 1.632680 |
| 6 | 1 | 0 | 1.156945 | -0.444433 | 3.188906 |
| 7 | 8 | 0 | -0.928709 | 3.528794 | 2.388961 |
| 8 | 16 | 0 | 0.373367 | 4.095625 | 1.971549 |
| 9 | 8 | 0 | 1.552438 | 3.284564 | 2.354174 |
| 10 | 17 | 0 | 0.278538 | 3.511010 | -0.671906 |
| 11 | 1 | 0 | 0.872611 | -0.492896 | -0.429698 |
| 12 | 1 | 0 | 0.084286 | 1.086019 | -0.259940 |
| 13 | 1 | 0 | 1.477711 | 1.078171 | 2.362408 |
| 14 | 1 | 0 | -0.914178 | 0.168523 | 1.987737 |
| 15 | 7 | 0 | -3.061314 | -1.070414 | -1.273826 |
| 16 | 6 | 0 | -4.078371 | -1.403945 | -1.722047 |
| 17 | 6 | 0 | -5.354171 | -1.828969 | -2.286139 |
| 18 | 1 | 0 | -5.614661 | -1.196992 | -3.138841 |
| 19 | 1 | 0 | -5.286886 | -2.867019 | -2.621181 |
| 20 | 1 | 0 | -6.141526 | -1.749480 | -1.532415 |
| 21 | 7 | 0 | 3.951575 | -1.285041 | 0.400383 |
| 22 | 6 | 0 | 4.830653 | -1.702965 | -0.231500 |
| 23 | 6 | 0 | 5.938961 | -2.226467 | -1.021230 |
| 24 | 1 | 0 | 5.567568 | -2.943865 | -1.757292 |
| 25 | 1 | 0 | 6.442844 | -1.409950 | -1.544361 |
| 26 | 1 | 0 | 6.658228 | -2.727971 | -0.368969 |
| 27 | 7 | 0 | 0.508034 | 5.965739 | 4.611575 |
| 28 | 6 | 0 | 0.560813 | 6.668404 | 5.533887 |
| 29 | 6 | 0 | 0.632186 | 7.551266 | 6.692629 |
| 30 | 1 | 0 | -0.243699 | 7.404528 | 7.329517 |
| 31 | 1 | 0 | 1.532740 | 7.334413 | 7.272528 |
| 32 | 1 | 0 | 0.662823 | 8.593886 | 6.366565 |
| 33 | 7 | 0 | -2.806705 | 0.439526 | 3.085069 |
| 34 | 6 | 0 | -3.798119 | 0.622177 | 3.658558 |
| 35 | 6 | 0 | -5.042032 | 0.853496 | 4.382647 |
| 36 | 1 | 0 | -5.648035 | 1.594486 | 3.855427 |
| 37 | 1 | 0 | -5.607621 | -0.078341 | 4.460153 |
| 38 | 1 | 0 | -4.824679 | 1.222349 | 5.388121 |

**IN1b-shared-s** in acetonitrile

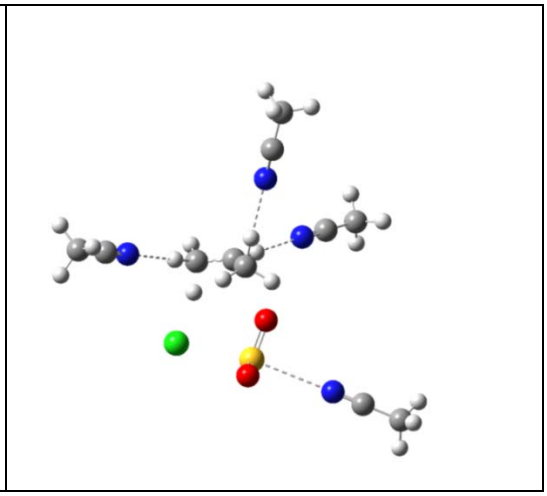
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.437369 |
| 3 | 6 | 0 | 1.164112 | 0.000000 | 2.272973 |
| 4 | 1 | 0 | -0.866880 | -0.539013 | -0.400653 |
| 5 | 1 | 0 | 2.079357 | -0.359124 | 1.802915 |
| 6 | 1 | 0 | 0.979728 | -0.408785 | 3.270068 |
| 7 | 8 | 0 | -3.823914 | 6.066859 | 4.730057 |
| 8 | 16 | 0 | -2.892156 | 7.153820 | 4.363710 |
| 9 | 8 | 0 | -1.458389 | 6.824610 | 4.507581 |
| 10 | 17 | 0 | -3.116966 | 7.122427 | 1.604554 |
| 11 | 1 | 0 | 0.941744 | -0.280652 | -0.469564 |
| 12 | 1 | 0 | -0.245093 | 1.067613 | -0.247891 |
| 13 | 1 | 0 | 1.283184 | 1.108296 | 2.459174 |
| 14 | 7 | 0 | -0.801871 | 3.063744 | -0.689886 |
| 15 | 6 | 0 | -1.163120 | 4.114726 | -1.023264 |
| 16 | 6 | 0 | -1.621384 | 5.435516 | -1.433281 |
| 17 | 1 | 0 | -2.375257 | 5.337828 | -2.218866 |
| 18 | 1 | 0 | -2.059110 | 5.960260 | -0.575531 |
| 19 | 1 | 0 | -0.779960 | 6.016192 | -1.820224 |
| 20 | 7 | 0 | 1.469593 | 3.153863 | 2.719911 |
| 21 | 6 | 0 | 1.352388 | 4.307715 | 2.732629 |
| 22 | 6 | 0 | 1.205343 | 5.756588 | 2.753210 |
| 23 | 1 | 0 | 1.054071 | 6.126641 | 1.735778 |
| 24 | 1 | 0 | 0.343694 | 6.037759 | 3.366604 |
| 25 | 1 | 0 | 2.108041 | 6.213880 | 3.166881 |
| 26 | 7 | 0 | -3.046887 | 8.316315 | 7.375246 |
| 27 | 6 | 0 | -3.403070 | 9.071364 | 8.181792 |
| 28 | 6 | 0 | -3.848547 | 10.020582 | 9.195527 |
| 29 | 1 | 0 | -4.341983 | 10.871344 | 8.718998 |
| 30 | 1 | 0 | -4.553658 | 9.537389 | 9.876396 |
| 31 | 1 | 0 | -2.992551 | 10.383293 | 9.769997 |
| 32 | 7 | 0 | -2.796522 | 1.185585 | 2.553635 |
| 33 | 6 | 0 | -3.364875 | 2.196949 | 2.596665 |
| 34 | 6 | 0 | -4.077191 | 3.466273 | 2.651480 |
| 35 | 1 | 0 | -3.659250 | 4.166247 | 1.922073 |
| 36 | 1 | 0 | -5.135981 | 3.307852 | 2.430576 |
| 37 | 1 | 0 | -3.979168 | 3.920539 | 3.641336 |
| 38 | 1 | 0 | -0.970468 | 0.139585 | 1.925282 |

**TS3b-s** in acetonitrile

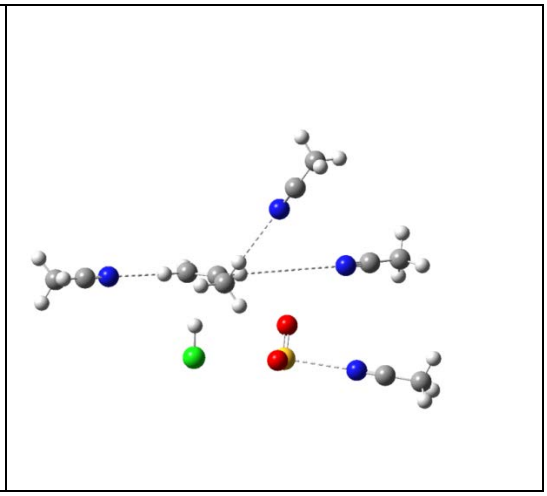
1 imaginary frequencies= -57.1037



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.414736 |
| 3 | 6 | 0 | 1.202157 | 0.000000 | 2.246544 |
| 4 | 1 | 0 | -0.072479 | 1.137819 | -0.268029 |
| 5 | 1 | 0 | 1.288375 | -1.035243 | 2.624928 |
| 6 | 1 | 0 | 1.077234 | 0.631723 | 3.128833 |
| 7 | 8 | 0 | -0.781176 | 2.430722 | 2.063296 |
| 8 | 16 | 0 | -0.253983 | 3.715078 | 1.545876 |
| 9 | 8 | 0 | 1.162103 | 3.984809 | 1.840596 |
| 10 | 17 | 0 | -0.113166 | 2.967224 | -1.163838 |
| 11 | 1 | 0 | -0.896222 | -0.416179 | -0.461892 |
| 12 | 1 | 0 | 0.939518 | -0.303369 | -0.465187 |
| 13 | 1 | 0 | 2.112255 | 0.237618 | 1.694256 |
| 14 | 1 | 0 | -0.956441 | -0.025279 | 1.931320 |
| 15 | 7 | 0 | -1.206868 | 5.228190 | 4.096157 |
| 16 | 7 | 0 | 1.408310 | -3.194619 | 3.470707 |
| 17 | 7 | 0 | -3.031648 | -0.049987 | 2.966361 |
| 18 | 7 | 0 | 3.054551 | -1.039586 | -1.444294 |
| 19 | 6 | 0 | -1.523224 | 5.800401 | 5.054937 |
| 20 | 6 | 0 | 1.508517 | -4.269801 | 3.895200 |
| 21 | 6 | 0 | -4.055361 | -0.036898 | 3.512150 |
| 22 | 6 | 0 | 4.078484 | -1.366831 | -1.881706 |
| 23 | 6 | 0 | -1.923323 | 6.520522 | 6.258497 |
| 24 | 1 | 0 | -1.129045 | 6.467049 | 7.007169 |
| 25 | 1 | 0 | -2.115573 | 7.569367 | 6.019047 |
| 26 | 1 | 0 | -2.832668 | 6.078268 | 6.672943 |
| 27 | 6 | 0 | 1.611721 | -5.618485 | 4.440384 |
| 28 | 1 | 0 | 1.126362 | -6.330870 | 3.768692 |
| 29 | 1 | 0 | 2.662156 | -5.897337 | 4.554495 |
| 30 | 1 | 0 | 1.124233 | -5.661959 | 5.417526 |
| 31 | 6 | 0 | -5.341399 | -0.015424 | 4.199560 |
| 32 | 1 | 0 | -5.896870 | 0.884234 | 3.923219 |
| 33 | 1 | 0 | -5.928219 | -0.894534 | 3.922037 |
| 34 | 1 | 0 | -5.186234 | -0.018845 | 5.281304 |
| 35 | 6 | 0 | 5.365511 | -1.778912 | -2.430481 |
| 36 | 1 | 0 | 5.239757 | -2.671672 | -3.048078 |
| 37 | 1 | 0 | 5.783208 | -0.977750 | -3.045230 |
| 38 | 1 | 0 | 6.062204 | -2.003781 | -1.619077 |

**IN2b-s** in acetonitrile

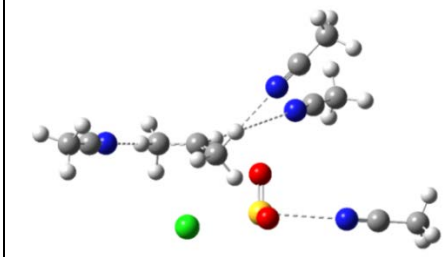
0 imaginary frequencies



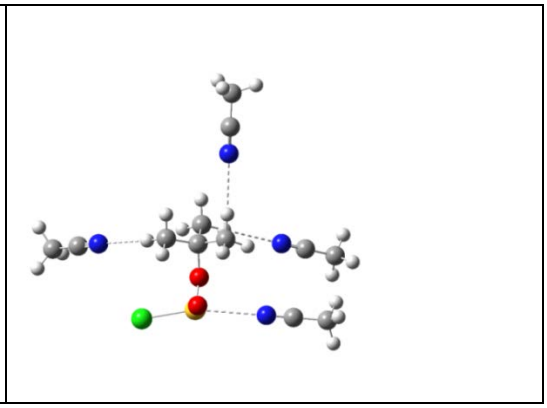
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.340411 |
| 3 | 6 | 0 | 1.222410 | 0.000000 | 2.208461 |
| 4 | 1 | 0 | -0.171706 | 2.142901 | 0.344019 |
| 5 | 1 | 0 | 1.248469 | -0.904027 | 2.829417 |
| 6 | 1 | 0 | 1.208049 | 0.851481 | 2.898607 |
| 7 | 8 | 0 | -2.086888 | 2.063019 | 3.484220 |
| 8 | 16 | 0 | -1.297827 | 3.264970 | 3.771331 |
| 9 | 8 | 0 | 0.109489 | 3.083145 | 4.141909 |
| 10 | 17 | 0 | -0.294042 | 3.453137 | 0.289547 |
| 11 | 1 | 0 | -0.925045 | -0.029477 | -0.568711 |
| 12 | 1 | 0 | 0.927063 | -0.012246 | -0.568841 |
| 13 | 1 | 0 | 2.141544 | 0.039321 | 1.617396 |
| 14 | 1 | 0 | -0.955505 | 0.002438 | 1.864716 |
| 15 | 7 | 0 | -2.194520 | 3.566444 | 6.547996 |
| 16 | 7 | 0 | 1.237094 | -3.241246 | 4.508926 |
| 17 | 7 | 0 | -5.313686 | 0.032978 | 4.456798 |
| 18 | 7 | 0 | 3.258264 | -0.110356 | -1.922579 |
| 19 | 6 | 0 | -2.512036 | 3.698563 | 7.655936 |
| 20 | 6 | 0 | 1.272948 | -4.182109 | 5.188052 |
| 21 | 6 | 0 | -6.322477 | 0.006008 | 5.031065 |
| 22 | 6 | 0 | 4.281202 | -0.148397 | -2.470003 |
| 23 | 6 | 0 | -2.908550 | 3.856506 | 9.049826 |
| 24 | 1 | 0 | -2.967071 | 2.877931 | 9.532874 |
| 25 | 1 | 0 | -2.175551 | 4.470976 | 9.578466 |
| 26 | 1 | 0 | -3.886498 | 4.340743 | 9.107186 |
| 27 | 6 | 0 | 1.316059 | -5.363723 | 6.042442 |
| 28 | 1 | 0 | 2.200678 | -5.329936 | 6.683312 |
| 29 | 1 | 0 | 0.423760 | -5.403392 | 6.672204 |
| 30 | 1 | 0 | 1.357154 | -6.267318 | 5.428978 |
| 31 | 6 | 0 | -7.589878 | -0.029233 | 5.752677 |
| 32 | 1 | 0 | -8.238989 | 0.780443 | 5.409789 |
| 33 | 1 | 0 | -8.093464 | -0.983724 | 5.579886 |
| 34 | 1 | 0 | -7.412941 | 0.088725 | 6.824712 |
| 35 | 6 | 0 | 5.566056 | -0.197087 | -3.158870 |
| 36 | 1 | 0 | 5.776321 | 0.767714 | -3.627244 |
| 37 | 1 | 0 | 6.363309 | -0.427150 | -2.447606 |
| 38 | 1 | 0 | 5.546856 | -0.969600 | -3.931739 |

**TS4b-s** in acetonitrile

1 imaginary frequencies= -138.7113



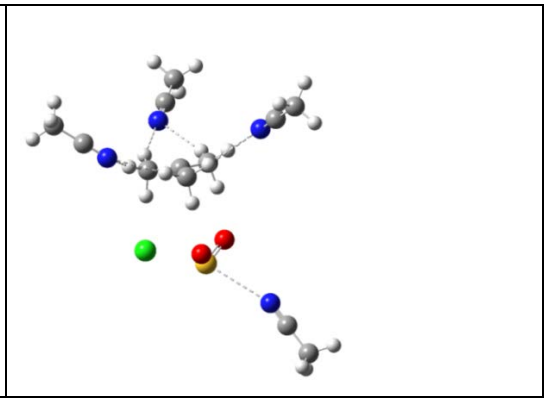
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | 1.130338 |
| 3 | 6 | 0 | 1.420535 | 0.000000 | -0.173258 |
| 4 | 6 | 0 | 2.243459 | 1.154916 | -0.436656 |
| 5 | 1 | 0 | 2.875451 | 0.913583 | -1.309065 |
| 6 | 1 | 0 | 2.994902 | 1.220842 | 0.377534 |
| 7 | 1 | 0 | 1.699878 | 2.086361 | -0.582204 |
| 8 | 16 | 0 | 3.838003 | -0.638794 | 2.585563 |
| 9 | 8 | 0 | 3.606820 | -1.640325 | 1.520778 |
| 10 | 8 | 0 | 4.248556 | 0.697362 | 2.093938 |
| 11 | 1 | 0 | -0.479814 | -0.945524 | -0.264449 |
| 12 | 1 | 0 | -0.519450 | 0.890507 | -0.350251 |
| 13 | 17 | 0 | 1.268917 | -0.103860 | 3.232556 |
| 14 | 1 | 0 | 1.952427 | -0.939487 | -0.008076 |
| 15 | 7 | 0 | 6.872339 | -1.578454 | 2.864312 |
| 16 | 7 | 0 | 4.183469 | 0.365153 | -3.034184 |
| 17 | 7 | 0 | 4.312214 | -5.366827 | 0.635999 |
| 18 | 7 | 0 | -1.596827 | 2.867357 | -1.169782 |
| 19 | 6 | 0 | 7.985369 | -1.900398 | 2.931648 |
| 20 | 6 | 0 | 4.891662 | 0.069252 | -3.903991 |
| 21 | 6 | 0 | 4.839418 | -6.384515 | 0.821671 |
| 22 | 6 | 0 | -2.084139 | 3.845240 | -1.560941 |
| 23 | 6 | 0 | 9.385470 | -2.298207 | 3.024089 |
| 24 | 1 | 0 | 9.645285 | -2.951209 | 2.187167 |
| 25 | 1 | 0 | 10.027199 | -1.414029 | 2.996655 |
| 26 | 1 | 0 | 9.560172 | -2.834638 | 3.960115 |
| 27 | 6 | 0 | 5.775377 | -0.309411 | -5.000021 |
| 28 | 1 | 0 | 6.806212 | -0.037342 | -4.760078 |
| 29 | 1 | 0 | 5.721907 | -1.388338 | -5.165363 |
| 30 | 1 | 0 | 5.475607 | 0.206141 | -5.915830 |
| 31 | 6 | 0 | 5.503907 | -7.662117 | 1.054790 |
| 32 | 1 | 0 | 5.174744 | -8.396126 | 0.314996 |
| 33 | 1 | 0 | 6.587109 | -7.540564 | 0.975139 |
| 34 | 1 | 0 | 5.261910 | -8.033489 | 2.053758 |
| 35 | 6 | 0 | -2.697657 | 5.073534 | -2.052242 |
| 36 | 1 | 0 | -2.573401 | 5.872860 | -1.317455 |
| 37 | 1 | 0 | -2.226341 | 5.377119 | -2.990319 |
| 38 | 1 | 0 | -3.764711 | 4.914155 | -2.226360 |

| **2c-s** in acetonitrile<br><br>0 imaginary frequencies |  |
|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.524863 |
| 3 | 6 | 0 | 1.400735 | 0.000000 | 2.129629 |
| 4 | 1 | 0 | -1.016663 | -0.061293 | -0.394496 |
| 5 | 1 | 0 | 1.864655 | -0.967092 | 1.913398 |
| 6 | 1 | 0 | 1.349547 | 0.127756 | 3.213826 |
| 7 | 6 | 0 | -0.859921 | -1.122110 | 2.097135 |
| 8 | 1 | 0 | -0.887189 | -1.075135 | 3.188753 |
| 9 | 1 | 0 | -1.879659 | -1.066966 | 1.707535 |
| 10 | 1 | 0 | -0.428211 | -2.082857 | 1.801085 |
| 11 | 8 | 0 | -0.745291 | 1.238580 | 2.027912 |
| 12 | 16 | 0 | -0.425093 | 2.772692 | 1.746475 |
| 13 | 8 | 0 | 0.910640 | 2.971572 | 1.174451 |
| 14 | 17 | 0 | -1.853802 | 3.163784 | -0.066223 |
| 15 | 1 | 0 | 0.550135 | -0.884260 | -0.337188 |
| 16 | 1 | 0 | 0.500462 | 0.881230 | -0.405238 |
| 17 | 1 | 0 | 2.022995 | 0.789754 | 1.706668 |
| 18 | 7 | 0 | 0.780573 | 2.839273 | 4.543192 |
| 19 | 7 | 0 | -0.878385 | -0.898647 | 5.956422 |
| 20 | 7 | 0 | -3.632188 | -0.314317 | -1.386421 |
| 21 | 7 | 0 | 2.913654 | -3.334918 | 1.341223 |
| 22 | 6 | 0 | 3.354460 | -4.386986 | 1.123351 |
| 23 | 6 | 0 | -0.905986 | -0.850499 | 7.116025 |
| 24 | 6 | 0 | -4.715616 | -0.378496 | -1.798453 |
| 25 | 6 | 0 | 1.203182 | 2.856558 | 5.623738 |
| 26 | 6 | 0 | 3.908168 | -5.708736 | 0.849526 |
| 27 | 1 | 0 | 4.404847 | -6.098527 | 1.741755 |
| 28 | 1 | 0 | 3.109089 | -6.395810 | 0.559559 |
| 29 | 1 | 0 | 4.635440 | -5.648548 | 0.036083 |
| 30 | 6 | 0 | -0.945995 | -0.793572 | 8.573213 |
| 31 | 1 | 0 | -0.015523 | -0.368743 | 8.957811 |
| 32 | 1 | 0 | -1.782480 | -0.171125 | 8.900725 |
| 33 | 1 | 0 | -1.070859 | -1.799067 | 8.982815 |
| 34 | 6 | 0 | 1.733283 | 2.877544 | 6.981770 |
| 35 | 1 | 0 | 2.821729 | 2.971428 | 6.956636 |
| 36 | 1 | 0 | 1.316078 | 3.724400 | 7.532262 |
| 37 | 1 | 0 | 1.468082 | 1.952189 | 7.498979 |
| 38 | 6 | 0 | -6.076824 | -0.454981 | -2.317252 |
| 39 | 1 | 0 | -6.309730 | 0.446724 | -2.888932 |
| 40 | 1 | 0 | -6.180318 | -1.324897 | -2.970611 |
| 41 | 1 | 0 | -6.787570 | -0.544729 | -1.491826 |

**IN1c-contact-s** in acetonitrile

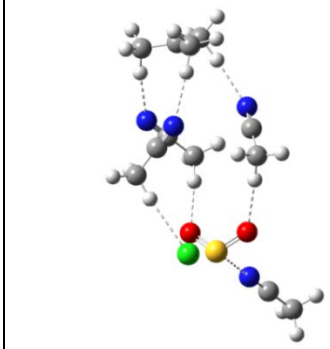
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.450936 |
| 3 | 6 | 0 | 1.265884 | 0.000000 | 2.189570 |
| 4 | 1 | 0 | -0.935294 | -0.366802 | -0.428479 |
| 5 | 1 | 0 | 2.088753 | -0.437012 | 1.621466 |
| 6 | 1 | 0 | 1.158444 | -0.429427 | 3.188736 |
| 7 | 6 | 0 | -1.253533 | 0.186088 | 2.187225 |
| 8 | 1 | 0 | -1.287094 | 1.276652 | 2.400222 |
| 9 | 1 | 0 | -2.139744 | -0.070794 | 1.603718 |
| 10 | 1 | 0 | -1.224057 | -0.307096 | 3.161545 |
| 11 | 8 | 0 | -0.967803 | 3.451206 | 2.477487 |
| 12 | 16 | 0 | 0.305238 | 4.052229 | 2.023195 |
| 13 | 8 | 0 | 1.515754 | 3.281890 | 2.385689 |
| 14 | 17 | 0 | 0.161262 | 3.413468 | -0.622393 |
| 15 | 1 | 0 | 0.894863 | -0.447668 | -0.435342 |
| 16 | 1 | 0 | 0.042268 | 1.099479 | -0.250130 |
| 17 | 1 | 0 | 1.494482 | 1.077920 | 2.341501 |
| 18 | 7 | 0 | -0.255020 | -1.443125 | 5.152816 |
| 19 | 6 | 0 | 0.194584 | -1.973915 | 6.081950 |
| 20 | 6 | 0 | 0.764612 | -2.638463 | 7.248022 |
| 21 | 1 | 0 | 1.736241 | -3.069526 | 6.994058 |
| 22 | 1 | 0 | 0.895480 | -1.919820 | 8.061051 |
| 23 | 1 | 0 | 0.099108 | -3.437478 | 7.584473 |
| 24 | 7 | 0 | -3.328726 | -1.117124 | -0.570502 |
| 25 | 6 | 0 | -4.394486 | -1.577066 | -0.573519 |
| 26 | 6 | 0 | -5.732994 | -2.155538 | -0.575660 |
| 27 | 1 | 0 | -5.939583 | -2.619635 | 0.392075 |
| 28 | 1 | 0 | -6.476487 | -1.376645 | -0.762128 |
| 29 | 1 | 0 | -5.810859 | -2.915371 | -1.357444 |
| 30 | 7 | 0 | 3.263526 | -1.585311 | -0.353924 |
| 31 | 6 | 0 | 3.590971 | -2.353462 | -1.160394 |
| 32 | 6 | 0 | 4.011046 | -3.318572 | -2.169545 |
| 33 | 1 | 0 | 3.242164 | -4.084759 | -2.296738 |
| 34 | 1 | 0 | 4.171400 | -2.813788 | -3.125534 |
| 35 | 1 | 0 | 4.942824 | -3.799023 | -1.860598 |
| 36 | 7 | 0 | 0.492237 | 5.851483 | 4.651808 |
| 37 | 6 | 0 | 0.621378 | 6.811141 | 5.291768 |
| 38 | 6 | 0 | 0.783101 | 8.014483 | 6.099597 |
| 39 | 1 | 0 | 0.392371 | 7.844244 | 7.105869 |
| 40 | 1 | 0 | 1.841334 | 8.278087 | 6.169622 |
| 41 | 1 | 0 | 0.239877 | 8.846292 | 5.644200 |

**IN1c-shared-s** in acetonitrile

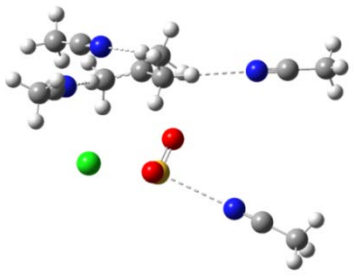
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.460411 |
| 3 | 6 | 0 | 1.267684 | 0.000000 | 2.187060 |
| 4 | 1 | 0 | -0.762550 | -0.685775 | -0.386540 |
| 5 | 1 | 0 | 1.922772 | -0.790365 | 1.800481 |
| 6 | 1 | 0 | 1.162382 | -0.057686 | 3.269204 |
| 7 | 6 | 0 | -1.259223 | 0.120910 | 2.189706 |
| 8 | 1 | 0 | -1.242744 | 1.140106 | 2.632302 |
| 9 | 1 | 0 | -2.147356 | 0.005964 | 1.570383 |
| 10 | 1 | 0 | -1.272441 | -0.549995 | 3.056069 |
| 11 | 8 | 0 | 0.133423 | 7.726192 | 2.241230 |
| 12 | 16 | 0 | 0.763922 | 8.469319 | 1.128332 |
| 13 | 8 | 0 | 1.899457 | 7.776270 | 0.481827 |
| 14 | 17 | 0 | -1.146072 | 8.194355 | -0.805301 |
| 15 | 1 | 0 | 0.976348 | -0.183142 | -0.445981 |
| 16 | 1 | 0 | -0.362295 | 1.007659 | -0.295970 |
| 17 | 1 | 0 | 1.782522 | 0.941667 | 1.904715 |
| 18 | 7 | 0 | -0.838954 | 3.180821 | 3.468110 |
| 19 | 6 | 0 | 0.039310 | 3.926871 | 3.613784 |
| 20 | 6 | 0 | 1.136118 | 4.869807 | 3.787625 |
| 21 | 1 | 0 | 2.039810 | 4.460022 | 3.329009 |
| 22 | 1 | 0 | 0.885321 | 5.819068 | 3.302314 |
| 23 | 1 | 0 | 1.316248 | 5.041034 | 4.852008 |
| 24 | 7 | 0 | -1.209040 | 3.055753 | -0.584302 |
| 25 | 6 | 0 | -1.797092 | 3.897508 | -0.041577 |
| 26 | 6 | 0 | -2.524455 | 4.961233 | 0.637337 |
| 27 | 1 | 0 | -2.371734 | 4.870421 | 1.715929 |
| 28 | 1 | 0 | -2.157238 | 5.936449 | 0.296099 |
| 29 | 1 | 0 | -3.592265 | 4.880671 | 0.417843 |
| 30 | 7 | 0 | 2.578624 | 2.866636 | 1.074178 |
| 31 | 6 | 0 | 2.379438 | 3.647797 | 0.237951 |
| 32 | 6 | 0 | 2.125529 | 4.635476 | -0.802335 |
| 33 | 1 | 0 | 1.158358 | 4.427819 | -1.267532 |
| 34 | 1 | 0 | 2.104926 | 5.639475 | -0.365560 |
| 35 | 1 | 0 | 2.909361 | 4.586561 | -1.562574 |
| 36 | 7 | 0 | 2.826102 | 9.899617 | 3.199531 |
| 37 | 6 | 0 | 3.694078 | 10.605375 | 3.509398 |
| 38 | 6 | 0 | 4.784841 | 11.491761 | 3.899074 |
| 39 | 1 | 0 | 4.686665 | 12.452253 | 3.387047 |
| 40 | 1 | 0 | 4.761925 | 11.661333 | 4.978440 |
| 41 | 1 | 0 | 5.744718 | 11.043432 | 3.630735 |

**TS1c-s** in acetonitrile

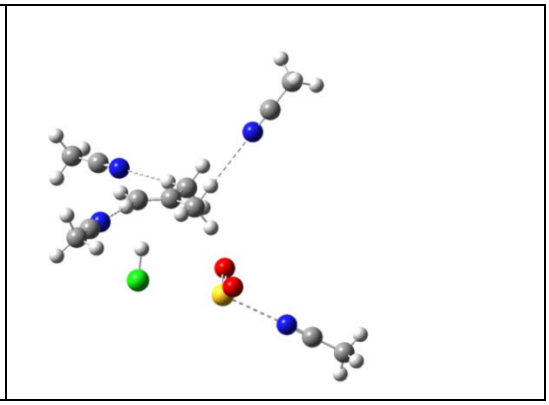
1 imaginary frequencies= -115.2180



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.444226 |
| 3 | 6 | 0 | 1.276748 | 0.000000 | 2.176491 |
| 4 | 1 | 0 | -0.128593 | 1.089469 | -0.283211 |
| 5 | 1 | 0 | 1.706805 | -1.006405 | 2.045895 |
| 6 | 1 | 0 | 1.166376 | 0.207667 | 3.239871 |
| 7 | 6 | 0 | -1.262246 | -0.016276 | 2.195568 |
| 8 | 1 | 0 | -1.264901 | 0.828625 | 2.894182 |
| 9 | 1 | 0 | -2.150004 | -0.006923 | 1.565029 |
| 10 | 1 | 0 | -1.260042 | -0.917742 | 2.827485 |
| 11 | 8 | 0 | -0.034490 | 2.885867 | 2.001161 |
| 12 | 16 | 0 | 0.856592 | 3.742583 | 1.184911 |
| 13 | 8 | 0 | 2.234225 | 3.232008 | 1.031229 |
| 14 | 17 | 0 | -0.188223 | 3.141972 | -1.266783 |
| 15 | 1 | 0 | -0.871558 | -0.497715 | -0.431121 |
| 16 | 1 | 0 | 0.943089 | -0.315189 | -0.448198 |
| 17 | 1 | 0 | 1.984396 | 0.693609 | 1.709975 |
| 18 | 7 | 0 | 3.066939 | -1.071010 | -1.383874 |
| 19 | 7 | 0 | 0.837458 | 0.714022 | 5.642544 |
| 20 | 7 | 0 | -4.113965 | 0.060451 | 0.081258 |
| 21 | 7 | 0 | 1.720771 | 5.516478 | 3.676491 |
| 22 | 6 | 0 | 2.075132 | 6.157113 | 4.577089 |
| 23 | 6 | 0 | 0.714243 | 0.977385 | 6.766097 |
| 24 | 6 | 0 | -5.014767 | 0.089446 | -0.649946 |
| 25 | 6 | 0 | 4.094669 | -1.397893 | -1.812482 |
| 26 | 6 | 0 | 2.522477 | 6.967767 | 5.704724 |
| 27 | 1 | 0 | 2.713831 | 6.329823 | 6.571102 |
| 28 | 1 | 0 | 3.442464 | 7.495755 | 5.442034 |
| 29 | 1 | 0 | 1.754048 | 7.699725 | 5.965706 |
| 30 | 6 | 0 | 0.565318 | 1.304987 | 8.179842 |
| 31 | 1 | 0 | 1.493215 | 1.083680 | 8.713367 |
| 32 | 1 | 0 | 0.334123 | 2.366854 | 8.294970 |
| 33 | 1 | 0 | -0.244744 | 0.715885 | 8.616393 |
| 34 | 6 | 0 | -6.149557 | 0.126460 | -1.566096 |
| 35 | 1 | 0 | -6.653289 | 1.093817 | -1.496754 |
| 36 | 1 | 0 | -5.805482 | -0.021433 | -2.592767 |
| 37 | 1 | 0 | -6.860240 | -0.663646 | -1.311805 |
| 38 | 6 | 0 | 5.386269 | -1.808286 | -2.352430 |
| 39 | 1 | 0 | 5.938743 | -0.933293 | -2.703528 |
| 40 | 1 | 0 | 5.971642 | -2.310904 | -1.578402 |
| 41 | 1 | 0 | 5.239431 | -2.495620 | -3.189274 |

**IN2c-s** in acetonitrile

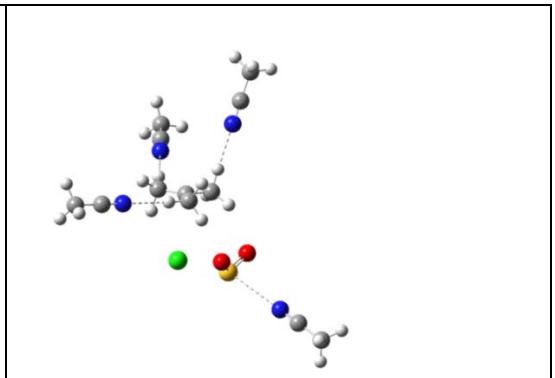
0 imaginary frequencies



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.346193 |
| 3 | 6 | 0 | 1.278359 | 0.000000 | 2.143364 |
| 4 | 1 | 0 | 0.010353 | 2.069793 | 0.145576 |
| 5 | 1 | 0 | 1.316963 | -0.878134 | 2.799644 |
| 6 | 1 | 0 | 1.330913 | 0.880413 | 2.795068 |
| 7 | 6 | 0 | -1.277962 | 0.001672 | 2.143944 |
| 8 | 1 | 0 | -1.326970 | 0.879178 | 2.799743 |
| 9 | 1 | 0 | -2.161702 | -0.002806 | 1.501316 |
| 10 | 1 | 0 | -1.319336 | -0.879373 | 2.796214 |
| 11 | 8 | 0 | -1.255367 | 3.449301 | 3.649563 |
| 12 | 16 | 0 | 0.002010 | 4.165441 | 3.411299 |
| 13 | 8 | 0 | 1.253440 | 3.445830 | 3.669601 |
| 14 | 17 | 0 | 0.019817 | 3.385243 | -0.011580 |
| 15 | 1 | 0 | -0.926286 | -0.034055 | -0.567424 |
| 16 | 1 | 0 | 0.926306 | -0.036351 | -0.567270 |
| 17 | 1 | 0 | 2.161751 | -0.010409 | 1.500325 |
| 18 | 7 | 0 | -0.014891 | 5.551181 | 5.990246 |
| 19 | 7 | 0 | 3.233865 | -0.190818 | -1.902375 |
| 20 | 7 | 0 | 1.335088 | -3.078923 | 4.513617 |
| 21 | 7 | 0 | -4.391087 | 0.057350 | -0.202395 |
| 22 | 6 | 0 | 0.017938 | 6.107785 | 7.007557 |
| 23 | 6 | 0 | 4.256702 | -0.251547 | -2.447947 |
| 24 | 6 | 0 | 1.382739 | -3.997539 | 5.221831 |
| 25 | 6 | 0 | -5.288182 | 0.080446 | -0.938905 |
| 26 | 6 | 0 | 0.057834 | 6.807307 | 8.285853 |
| 27 | 1 | 0 | 1.085781 | 6.852896 | 8.653898 |
| 28 | 1 | 0 | -0.322690 | 7.824673 | 8.165758 |
| 29 | 1 | 0 | -0.559393 | 6.280741 | 9.017972 |
| 30 | 6 | 0 | 5.542236 | -0.327864 | -3.132854 |
| 31 | 1 | 0 | 6.352232 | -0.108078 | -2.432882 |
| 32 | 1 | 0 | 5.689346 | -1.330685 | -3.541634 |
| 33 | 1 | 0 | 5.574097 | 0.396452 | -3.950582 |
| 34 | 6 | 0 | 1.439408 | -5.158273 | 6.103508 |
| 35 | 1 | 0 | 0.753787 | -5.931216 | 5.747362 |
| 36 | 1 | 0 | 2.453593 | -5.565061 | 6.121649 |
| 37 | 1 | 0 | 1.154246 | -4.872194 | 7.118990 |
| 38 | 6 | 0 | -6.417096 | 0.109890 | -1.862185 |
| 39 | 1 | 0 | -6.403114 | -0.778210 | -2.498941 |
| 40 | 1 | 0 | -7.356305 | 0.130737 | -1.303723 |
| 41 | 1 | 0 | -6.360716 | 0.999816 | -2.494028 |

**TS6c-s** in acetonitrile

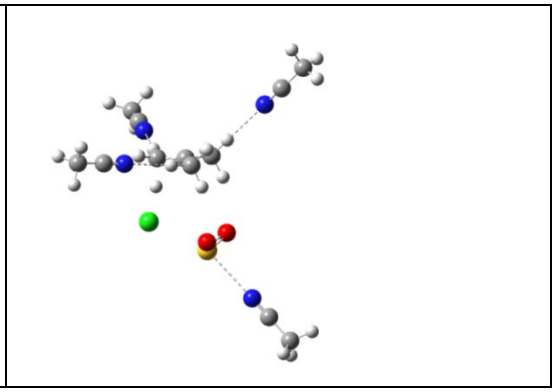
1 imaginary frequencies= -79.7621



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.459555 |
| 3 | 6 | 0 | 1.261289 | 0.000000 | 2.204596 |
| 4 | 1 | 0 | -0.923406 | -0.382404 | -0.437376 |
| 5 | 1 | 0 | 2.143067 | 0.047052 | 1.567761 |
| 6 | 1 | 0 | 1.282710 | -0.929670 | 2.796537 |
| 7 | 6 | 0 | -1.274532 | -0.050443 | 2.185340 |
| 8 | 1 | 0 | -1.227837 | 0.411736 | 3.173053 |
| 9 | 1 | 0 | -2.102586 | 0.339790 | 1.591634 |
| 10 | 1 | 0 | -1.468285 | -1.130107 | 2.325213 |
| 11 | 8 | 0 | -1.258459 | 2.556029 | 4.335515 |
| 12 | 16 | 0 | -0.057720 | 3.345532 | 3.987210 |
| 13 | 8 | 0 | 1.228492 | 2.635071 | 4.173339 |
| 14 | 17 | 0 | -0.192287 | 3.271447 | 1.279236 |
| 15 | 1 | 0 | 0.896891 | -0.446499 | -0.432676 |
| 16 | 1 | 0 | 0.039887 | 1.088091 | -0.219726 |
| 17 | 1 | 0 | 1.263356 | 0.806674 | 2.953168 |
| 18 | 7 | 0 | 0.188933 | 4.624272 | 6.950999 |
| 19 | 7 | 0 | 4.136436 | 0.070155 | 0.102609 |
| 20 | 7 | 0 | -1.917548 | -3.329672 | 2.670201 |
| 21 | 7 | 0 | -3.011079 | -1.155363 | -1.406243 |
| 22 | 6 | 0 | 0.317670 | 5.079950 | 8.010613 |
| 23 | 6 | 0 | 5.094498 | 0.072871 | -0.552332 |
| 24 | 6 | 0 | -2.115664 | -4.454793 | 2.871981 |
| 25 | 6 | 0 | -4.008010 | -1.493273 | -1.894728 |
| 26 | 6 | 0 | 0.475925 | 5.649599 | 9.344633 |
| 27 | 1 | 0 | -0.228582 | 5.180840 | 10.036313 |
| 28 | 1 | 0 | 1.493697 | 5.479579 | 9.704342 |
| 29 | 1 | 0 | 0.283972 | 6.725064 | 9.318125 |
| 30 | 6 | 0 | 6.298967 | 0.076966 | -1.374934 |
| 31 | 1 | 0 | 7.179095 | 0.234988 | -0.746609 |
| 32 | 1 | 0 | 6.400714 | -0.879329 | -1.894000 |
| 33 | 1 | 0 | 6.241183 | 0.878879 | -2.115170 |
| 34 | 6 | 0 | -2.373720 | -5.868030 | 3.122870 |
| 35 | 1 | 0 | -1.506917 | -6.326704 | 3.604688 |
| 36 | 1 | 0 | -3.243159 | -5.976701 | 3.776113 |
| 37 | 1 | 0 | -2.569969 | -6.383874 | 2.179723 |
| 38 | 6 | 0 | -5.264056 | -1.912604 | -2.506739 |
| 39 | 1 | 0 | -5.201191 | -2.960821 | -2.809550 |
| 40 | 1 | 0 | -6.083314 | -1.798259 | -1.792710 |
| 41 | 1 | 0 | -5.471737 | -1.300203 | -3.387681 |

**TS5c-s** in acetonitrile

1 imaginary frequencies= -414.9982



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | 1.387245 |
| 3 | 6 | 0 | 1.276915 | 0.000000 | 2.155268 |
| 4 | 1 | 0 | -0.938328 | -0.180078 | -0.521079 |
| 5 | 1 | 0 | 2.143644 | -0.207825 | 1.526974 |
| 6 | 1 | 0 | 1.225322 | -0.735703 | 2.965378 |
| 7 | 6 | 0 | -1.263703 | 0.183216 | 2.155266 |
| 8 | 1 | 0 | -1.253014 | 1.172141 | 2.635188 |
| 9 | 1 | 0 | -2.151282 | 0.101901 | 1.526972 |
| 10 | 1 | 0 | -1.318204 | -0.552276 | 2.965375 |
| 11 | 16 | 0 | 0.304307 | 4.217337 | 2.207908 |
| 12 | 8 | 0 | -0.985353 | 3.715406 | 2.705461 |
| 13 | 8 | 0 | 1.508548 | 3.535454 | 2.705462 |
| 14 | 1 | 0 | 0.094475 | 1.309889 | -0.127240 |
| 15 | 17 | 0 | 0.211855 | 2.937164 | -0.563446 |
| 16 | 1 | 0 | 0.902784 | -0.312849 | -0.521077 |
| 17 | 1 | 0 | 1.408231 | 0.980227 | 2.635189 |
| 18 | 7 | 0 | 0.463454 | 6.405954 | 4.271684 |
| 19 | 7 | 0 | 4.213223 | -0.782457 | 0.073550 |
| 20 | 7 | 0 | -1.507639 | -2.185407 | 4.850644 |
| 21 | 7 | 0 | -3.043570 | -0.516966 | -1.745832 |
| 22 | 6 | 0 | 0.564423 | 7.252640 | 5.059268 |
| 23 | 6 | 0 | 5.163469 | -1.027608 | -0.546586 |
| 24 | 6 | 0 | -1.555149 | -2.946331 | 5.725736 |
| 25 | 6 | 0 | -4.015947 | -0.681530 | -2.357927 |
| 26 | 6 | 0 | 0.688416 | 8.319876 | 6.044008 |
| 27 | 1 | 0 | 0.386099 | 7.956079 | 7.028644 |
| 28 | 1 | 0 | 1.724501 | 8.662173 | 6.094622 |
| 29 | 1 | 0 | 0.049606 | 9.160901 | 5.764511 |
| 30 | 6 | 0 | 6.358093 | -1.331138 | -1.326433 |
| 31 | 1 | 0 | 6.082287 | -1.560460 | -2.358742 |
| 32 | 1 | 0 | 7.034695 | -0.472848 | -1.322701 |
| 33 | 1 | 0 | 6.875963 | -2.192861 | -0.897996 |
| 34 | 6 | 0 | -1.616691 | -3.902411 | 6.825458 |
| 35 | 1 | 0 | -1.172818 | -4.853046 | 6.519580 |
| 36 | 1 | 0 | -1.067997 | -3.515993 | 7.688006 |
| 37 | 1 | 0 | -2.656765 | -4.073252 | 7.114261 |
| 38 | 6 | 0 | -5.235628 | -0.889168 | -3.130086 |
| 39 | 1 | 0 | -4.989854 | -1.298439 | -4.113168 |
| 40 | 1 | 0 | -5.893683 | -1.588919 | -2.608919 |
| 41 | 1 | 0 | -5.760616 | 0.060165 | -3.262289 |