Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Reactivity of Electrophilic Chlorine Atoms Due to σ-holes. A Mechanistic Assessment of the Chemical Reduction of the Trichloromethyl Group by Sulfur Nucleophiles

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Electronic Supplementary Information

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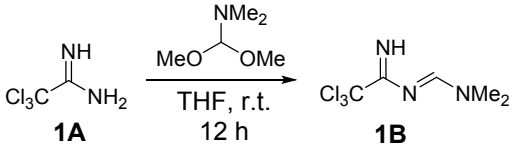
S1 Experimental Procedures and NMR data

In order to follow the chemical reduction of trichloromethyl group pyrimidine **1** was chosen as model substrate. We chose this compound for several reasons:

1. It is easily synthesized, a white solid with high molecular weight (313.5 g mol^{-1}) and easy to handle.
2. This compound does not show peaks within the aromatic region, thus enabling us to observe when the thiophenol incorporates to the molecule.
3. Pyrimidinic CH hydrogen atom can easily be followed, it appears as a singlet at 9.40 ppm.
4. We found that this reaction is quite fast. Other trichloromethyl compounds such as trichloroacetophenone or trichloroacetonitrile reacted too fast. Only compound **1** reacts slow enough to observe the formation of dichloromethylpyrimidine **2**.
5. All the intermediate generated form **1** (**2**, **3** and **4**) are solids and easily isolable. Trichloroacetonitrile, which presented itself as the simplest substrate is a liquid not so easy to follow in TLC and to isolate as well as its corresponding dichloro intermediate.

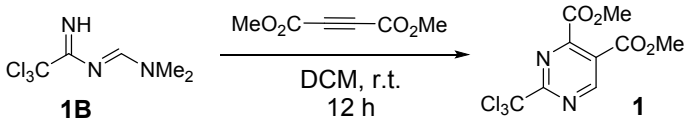
NMR spectra were acquired with a 300 MHz Bruker-Avace III apparatus, using chloroform-*d* as solvent.

Synthesis of trichloromethylpyrimidine 1 was carried out (gram-scale) accorded to the following procedure.



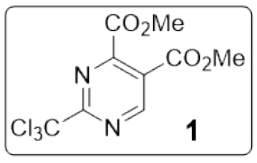
1A **1B**

Dimethyl 2-(trichloromethyl)pyrimidine-4,5-dicarboxylate (**1**).[1,2] In a 100 ml round-bottom flask, provided with nitrogen atmosphere and a magnetic stirrer, 3.14 g (19.4 mmol, 1.0 equiv.) of trichloroacetamidine **1A** were dissolved in 45 ml of anhydrous THF (dried with Na and freshly distillated from blue benzophenone). 3 ml of DMF dimethylacetal (22.6 mmol, 1.4 equiv.) were added in one portion at room temperature. After 12 h, the reaction was diluted with AcOEt and quenched with std. NaCl sln. The organic layer was separated and the aqueous phase extracted with AcOEt (3X30ml). The combined organic layers were dried over Na_2SO_4 and the solvent evaporated at reduced pressure to afford diazadiene **1B** as a yellowish oil, which was immediately used in the next reaction without further purification.



1B **1**

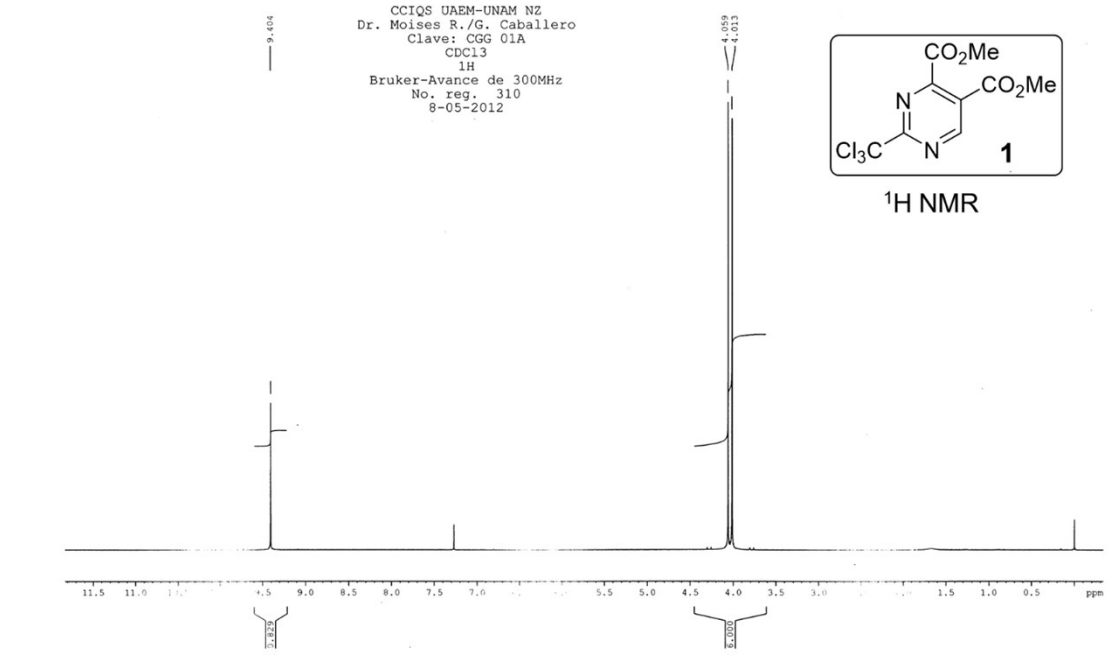
The crude diazadiene **1B** was dissolved in 30 ml of anhydrous DCM (freshly distillated from CaH_2) and 4.5 ml (36.61 mmol, 1.9 equiv.) of dimethyl acetylenedicarboxylate (DMAD) were dropwise added. After 12 h of stirring at room temperature, the reaction was diluted with DCM and quenched with std. NaCl sln. The organic layer was separated and the aqueous phase extracted with DCM (3X30ml). The combined organic layers were dried over Na_2SO_4 and the solvent evaporated at reduced pressure. Column chromatography (AcOEt:hexane 2:8) followed by recrystallization (DCM-hexane) yielded trichloromethylpyrimidine **1** as a white solid.

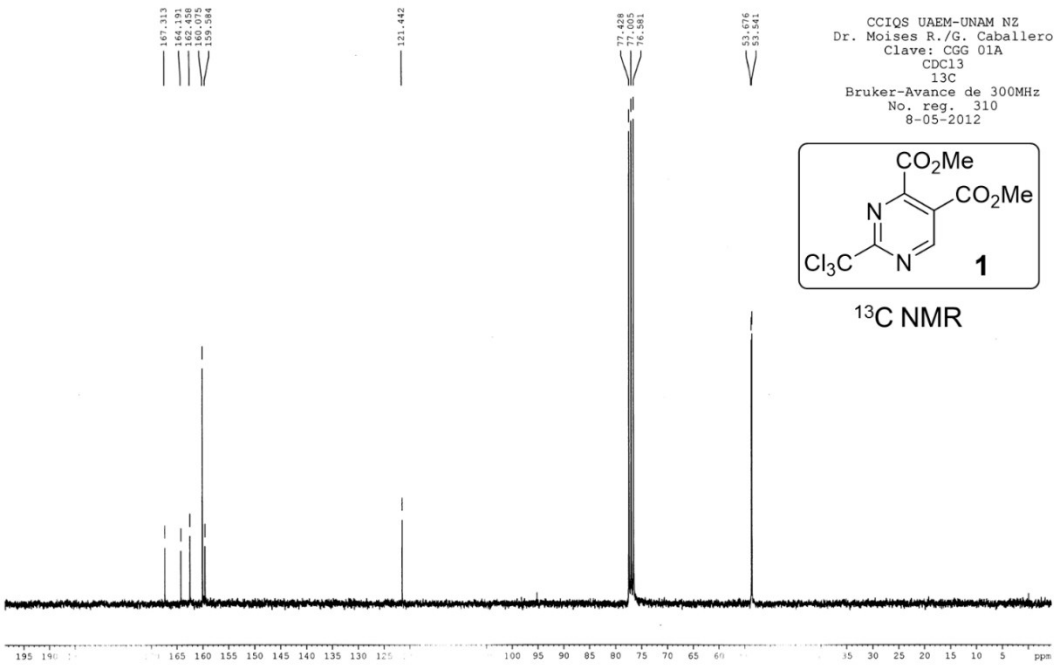


1

2.29 g, 37.54% yield, over two steps and recrystallization
R*f* = 0.37 (silica gel AcOEt:hexane 2:8)

melting point: 75-76 °C (determined with a MelTemp II apparatus, uncorrected)
^{1}H NMR (300 MHz, $CDCl_3$): δ ppm 9.40 (s, 1H), 4.04 (s, 3H), 4.01 (s, 3H)
^{13}C NMR (75 MHz, $CDCl_3$): δ ppm 167.3, 164.2, 162.5, 160.1, 159.6, 121.4, 95 (small peak, CCl_3), 53.7, 53.5



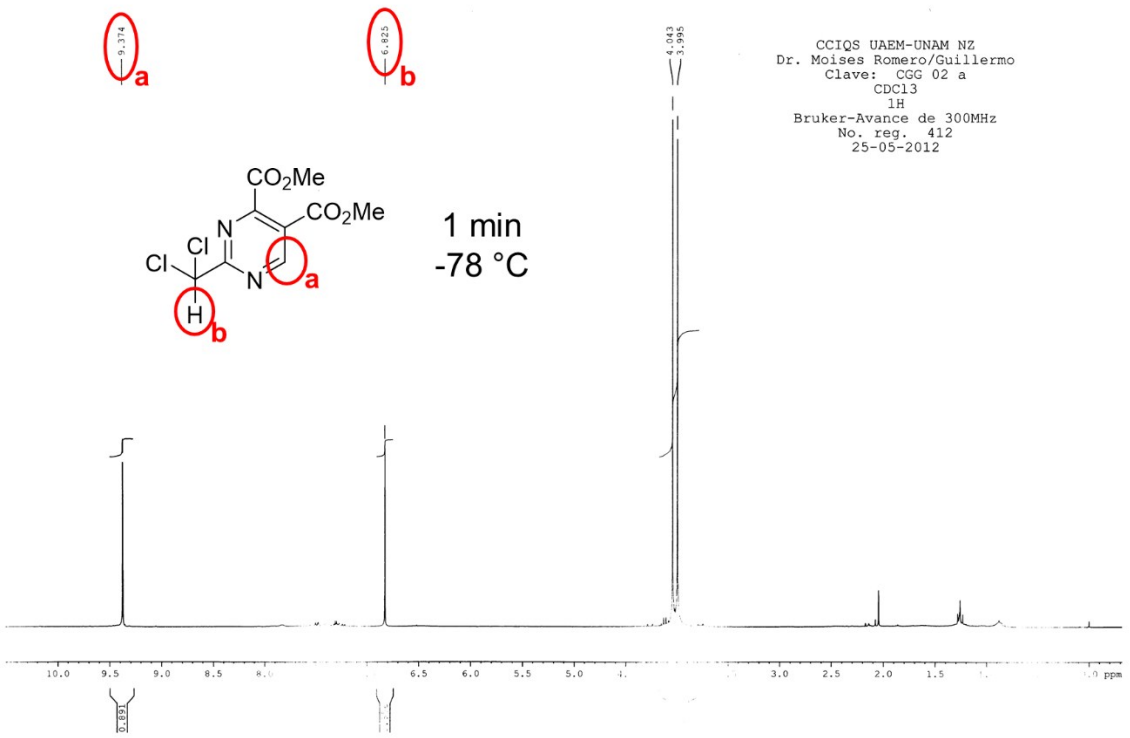


Reduction of trichloromethylpyrimidine (1)

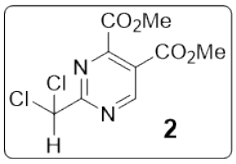
General Procedure to follow the reaction at -78 °C

In a 25 ml round-bottom flask, provided with a magnetic stirrer and under nitrogen atmosphere, 70 mg of NaH (60% suspension in mineral oil, 1.75 mmol, 3.5 equiv.) were suspended in 5 ml of anhydrous THF (dried with Na and freshly distillated from blue benzophenone). Then, the temperature was lowered to -78 °C (dry ice - acetone). 0.4 ml of thiophenol (4 mmol, 8 equiv.) were dropwise added to form sodium thiophenolate, the mixture was stirred at the aforementioned temperature for 5 minutes. 157 mg (0.5 mmol, 1 equiv.) of trichloromethyl pyrimidine **1** were added in one portion. Immediately after the addition the time started to count. Once the time (1, 5, 10, 30 or 90 minutes) was reached, NH_4Cl std. sln. was immediately added to quench the reaction. AcOEt was added to dilute the reaction, the organic layer was separated and the aqueous phase extracted with AcOEt (4X5ml), the combined organic layers were dried over Na_2SO_4 and the solvent evaporated at reduced pressure. Diphenyldisulfide (R*f* = 0.97, AcOEt:hexane 2:8) was removed through flash column chromatography (silica gel, AcOEt:hexane 2:8) and the remaining product(s) were collected. Details for each reaction time are provided as follows as well as their NMR spectra.

Time = 1 minute: Only one spot, apart from that corresponding to diphenyldisulfide, was observed in TLC (R*f* = 0.27 AcOEt:hexane 2:8). ^{1}H NMR spectrum indicates that after 1 minute only dichloromethyl pyrimidine **2** is isolated.



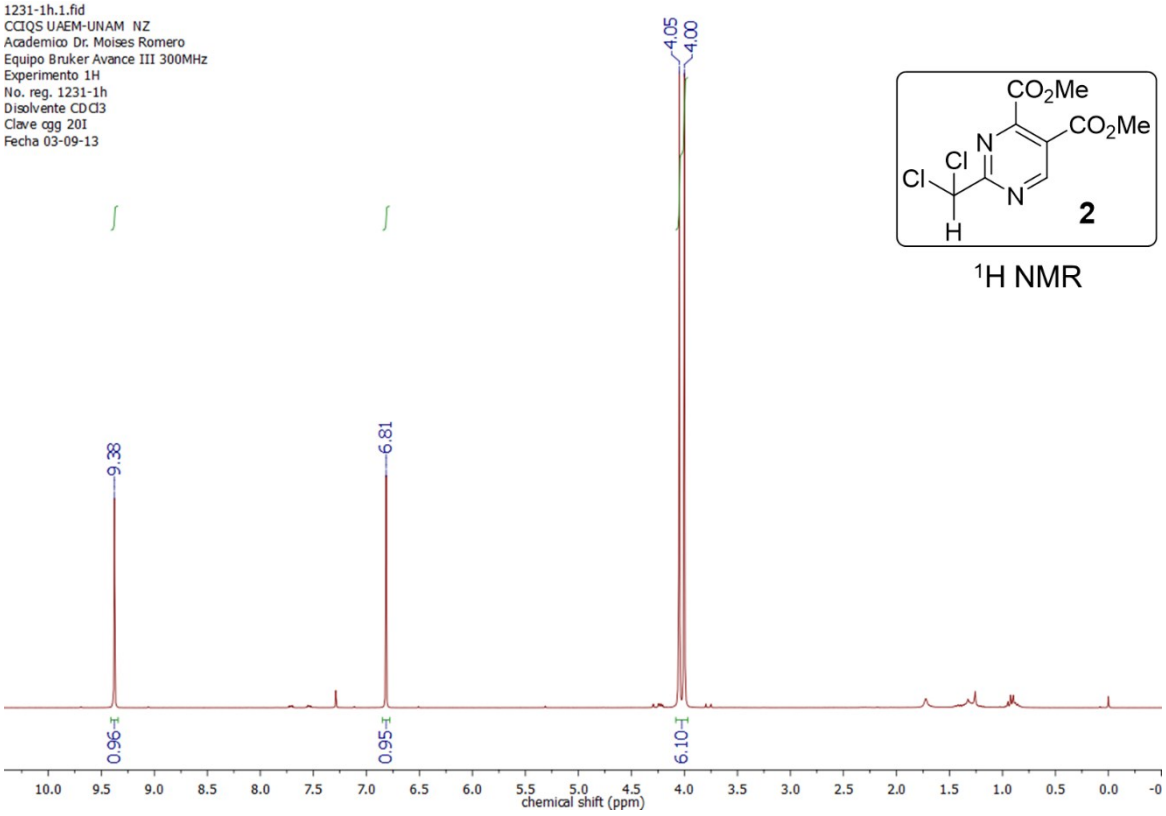
^{1}H NMR spectrum for the reaction at 1 minute shows that only compound **2** is isolated. Peak at 9.37 ppm corresponds to the CH pyrimidinic hydrogen atom and at 6.83 ppm corresponds to the hydrogen atom present in the dichloromethyl group. Otherwise, if starting material **1** remained unreacted, the peak at 9.40 ppm would still appear, which is not observed. This spectrum is clear for a single compound, indicating that dichloromethyl pyrimidine **2** is the first intermediate to yield sulfide **4**. NMR characterization for compound **2** is here presented.



R*f* = 0.27 (silica gel AcOEt:hexane 2:8)

^{1}H NMR (300 MHz, $CDCl_3$): δ ppm 9.38 (s, 1H), 6.81 (s, 1H), 4.05 (s, 3H), 4.00 (s, 3H)

^{13}C NMR (75 MHz, $CDCl_3$): δ ppm 167.5, 164.3, 162.6, 160.4, 159.4, 121.5, 69.7, 53.6, 53.4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Academico Dr. Moises Romero
Equipo Bruker Avance III 300MHz
Experimento 1H
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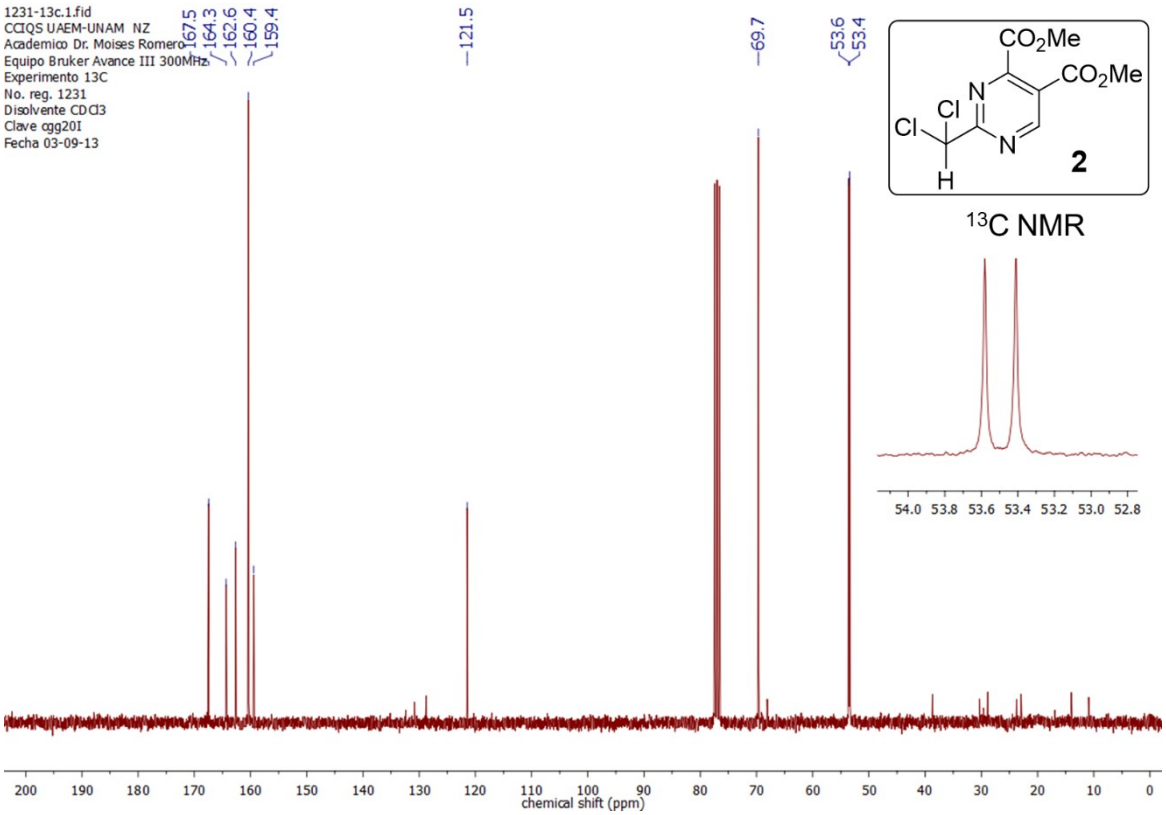
Disolvente CDCl3
Clave cgg 20I
Fecha 03-09-13
4.05
4.00
9.38
6.81
0.96
0.95
6.10
chemical shift (ppm)
CO2Me
CO2Me
N
Cl
Cl
N
H
2
1H NMR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Academico Dr. Moises Romero
Equipo Bruker Avance III 300MHz
Experimento 13C
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Clave cgg20I
Fecha 03-09-13
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160.4
159.4
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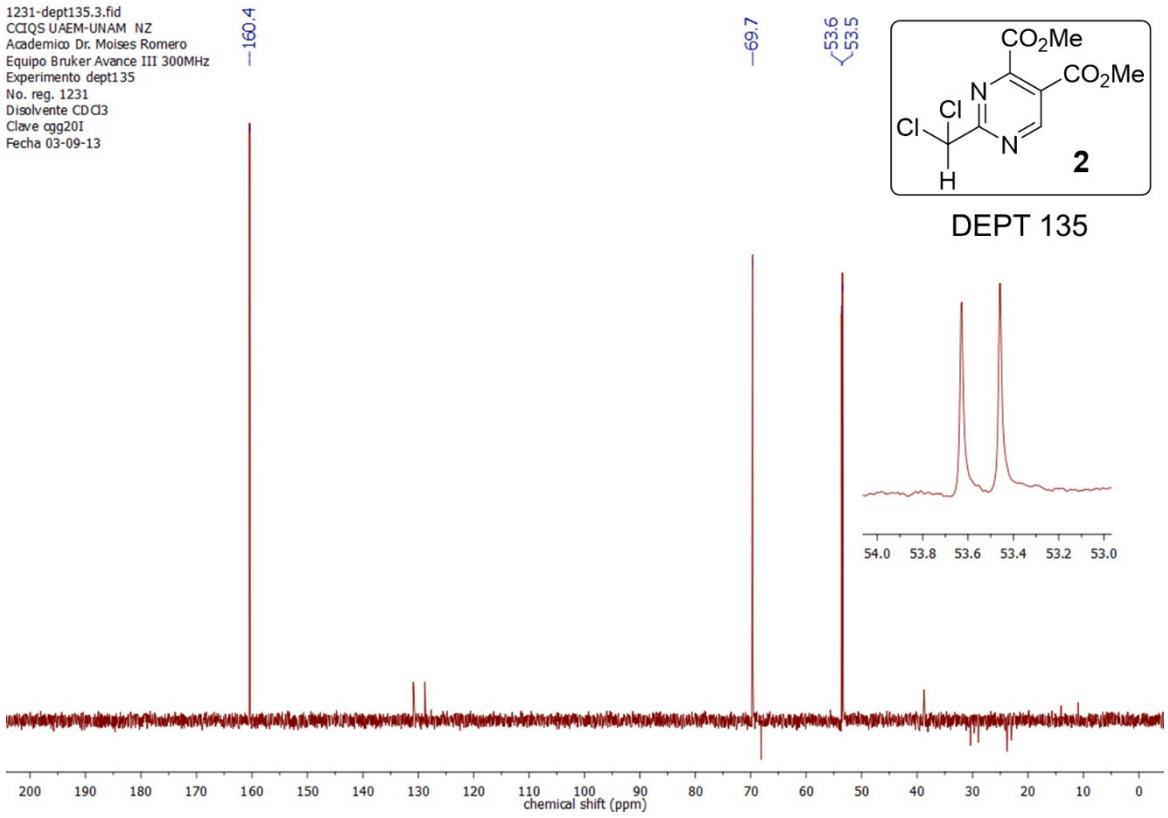
Cl
Cl
N
H
2
13C NMR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Equipo Bruker Avance III 300MHz
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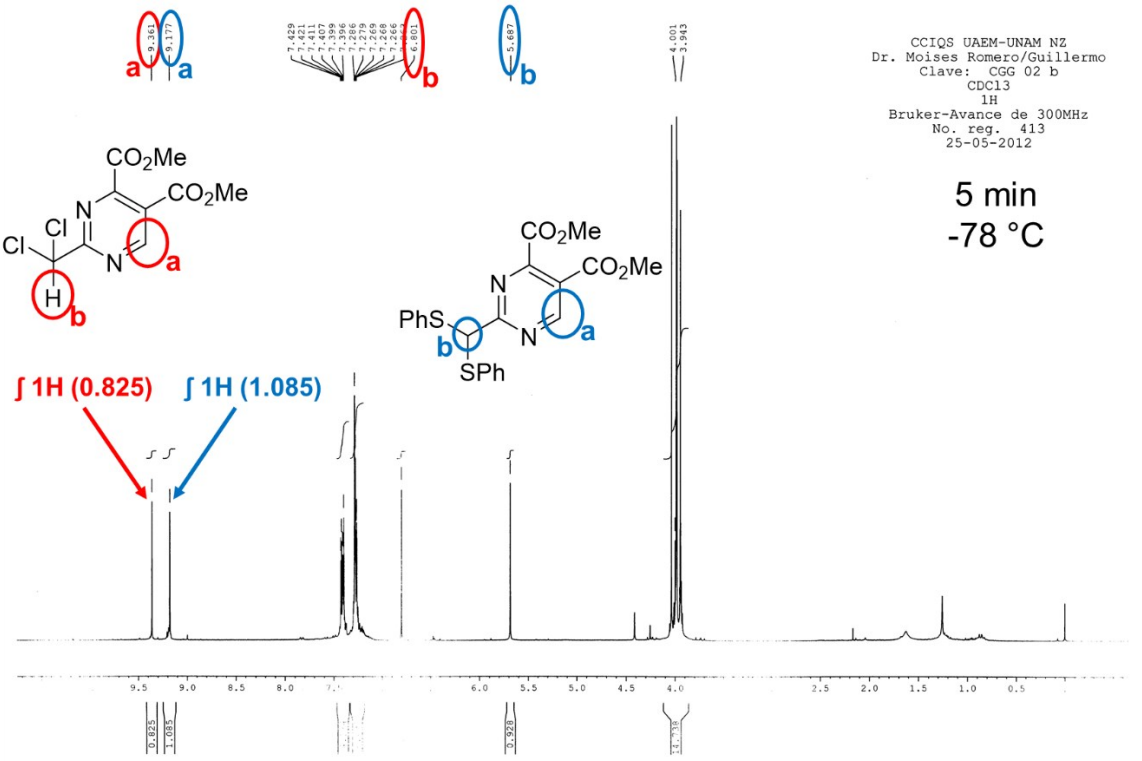
Fecha 03-09-13
160.4
69.7
53.6
53.5
CO2Me
CO2Me
N
Cl
Cl
N
H
2
DEPT 135
54.0 53.8 53.6 53.4 53.2 53.0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
chemical shift (ppm)

Time = 5 minutes: Two spots were observed in TLC, one at R*f* = 0.27 and the other at R*f* = 0.2 (AcOEt:hexane 2:8). ^{1}H NMR spectrum indicates that compounds **2** and **3** are obtained.

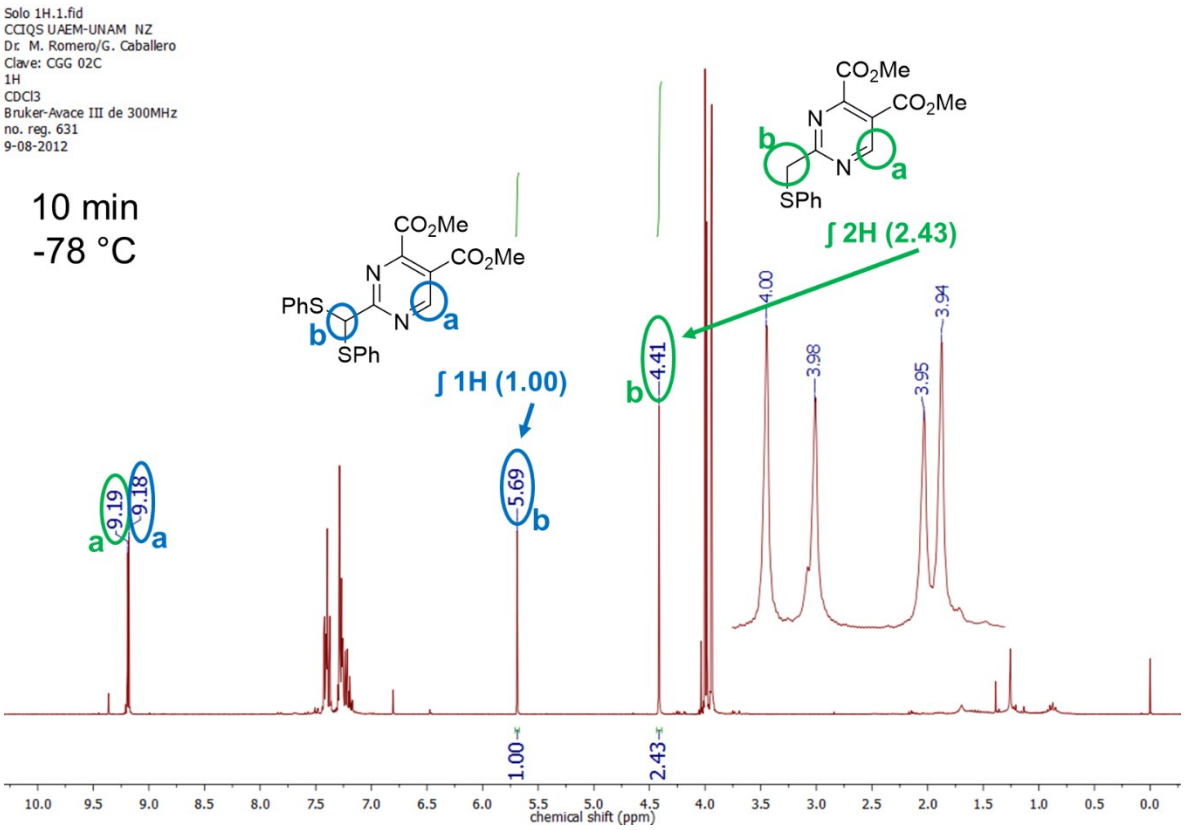


Integrals corresponding to the CH pyrimidinic hydrogen atoms in compounds **2** and **3** were taken in order to estimate the percentage of each compound. The sum of the two integrals **0.825** + **1.085** = **1.91** was taken as the 100%, thus:

(**0.825**/**1.91**)*100% = **43.2%** for dichloromethyl pyrimidine **2**

(**1.085**/**1.91**)*100% = **56.8%** for thioacetal **3**.

Time = 10 minutes: Two spots were observed in TLC, one at R*f* = 0.2 and the other at R*f* = 0.17 (AcOEt:hexane 2:8). ^{1}H NMR spectrum indicates that compounds **3** and **4** are obtained.



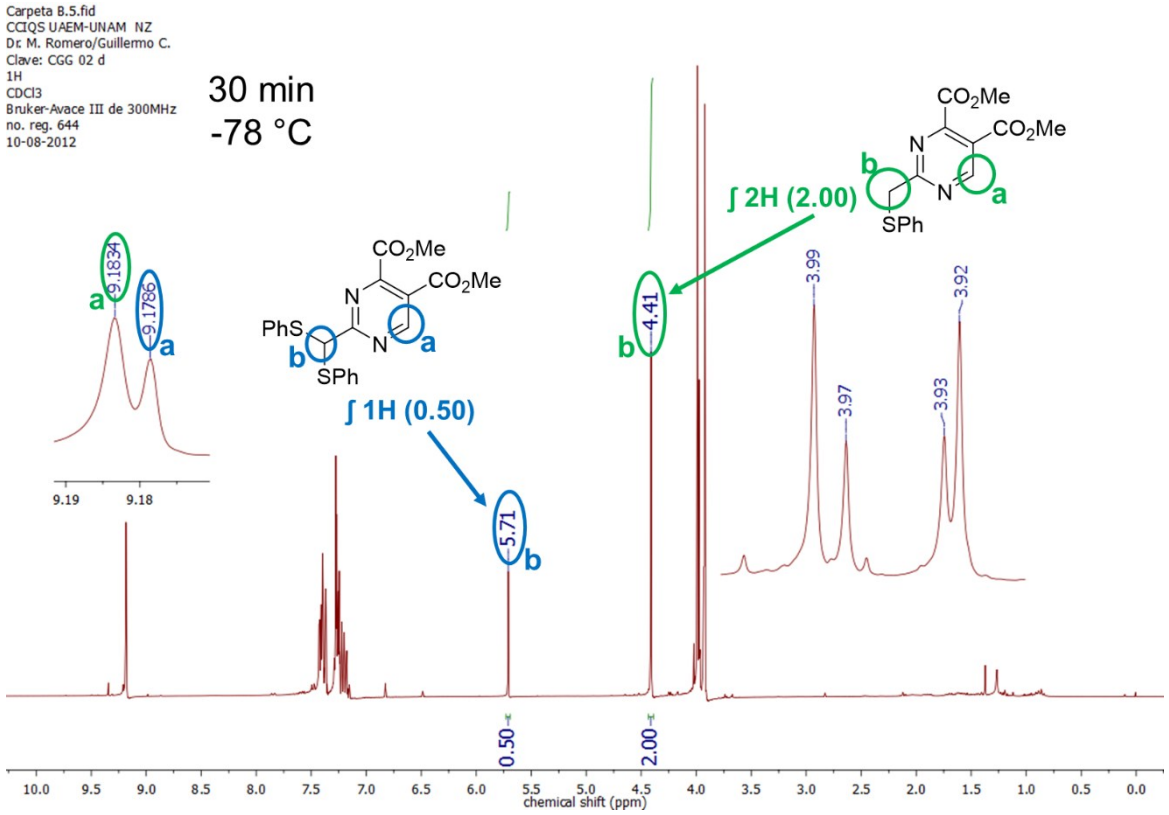
As peaks corresponding to pyrimidinic CH hydrogen atoms for thioacetal **3** and sulfide **4** are very close to each other, these singlets could not be integrated separately. To round this issue, peak at 5.69 ppm (hydrogen atom alpha to sulfur atoms) was considered for thioacetal **3** and that at 4.41 ppm (hydrogen atoms alpha to sulfur atom) for sulfide **4**. As peak b for compound **4** (labeled in green) corresponds to two hydrogen atoms, was divided by two in order to normalize the integral and compare it with that of thioacetal **3** (2.43/2 = **1.215**). The procedure to estimate the percentage of **3** and **4** was similar to that used previously.

The sum of the two integrals **1.00** + **1.215** = **2.215** was taken as the 100%, thus:

(**1.00**/**2.215**)*100% = **45.1%** for thioacetal **3**

(**1.215**/**2.215**)*100% = **54.9%** for sulfide **4**

Time = 30 minutes: Two spots were observed in TLC, one at R*f* = 0.2 and the other at R*f* = 0.17 (AcOEt:hexane 2:8). ^{1}H NMR spectrum indicates that compounds **3** and **4** are obtained, whereas compound **4** is obtained in a higher quantity respect to **3**, inferred both from the intensity of the spot in TLC and the integrals in ^{1}H NMR spectrum.



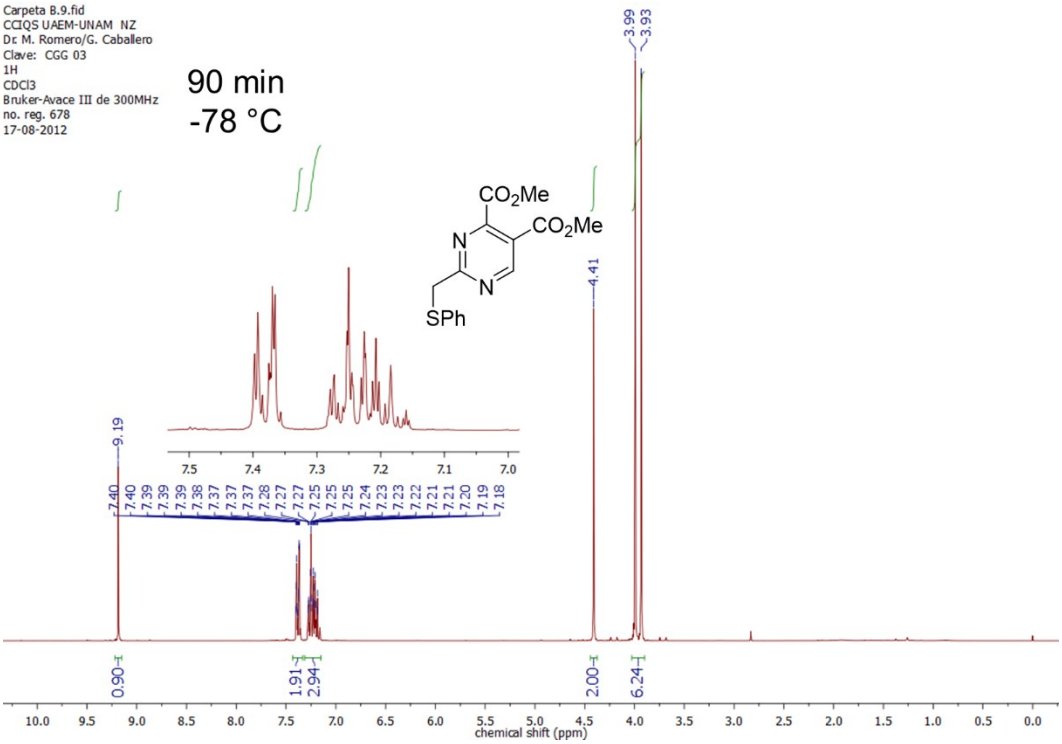
The procedure to estimate the percentage of **3** and **4** was exactly the same used for the reaction after 10 minutes. The integral for the peak at 4.41 ppm of sulfide **4** was divided by two in order to normalize it and compare it with that for **3** (2.00/2 = **1.00**).

The sum of the two integrals **0.50** + **1.00** = **1.50** was taken as the 100%, thus:

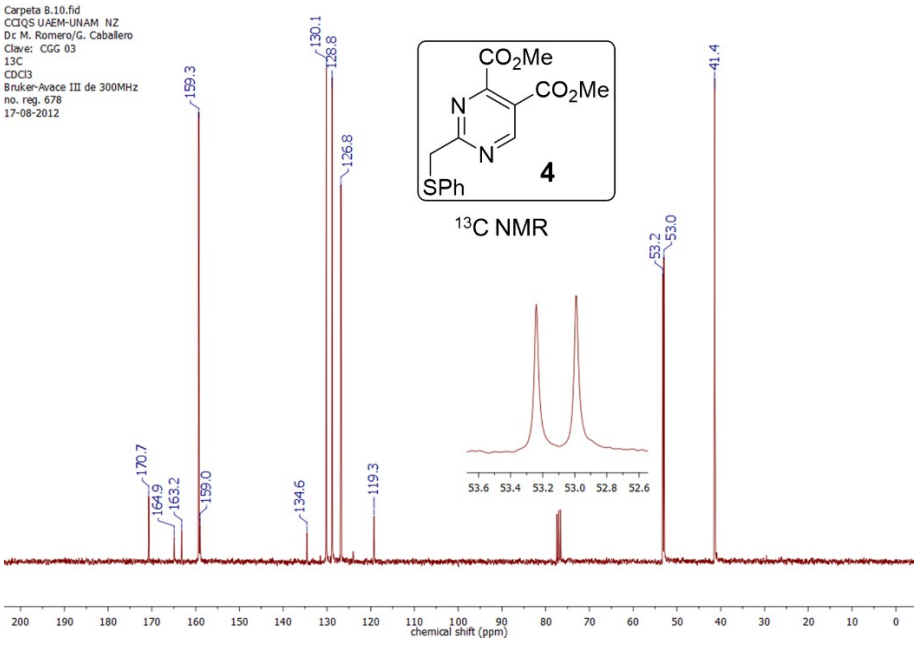
(**0.50**/**1.50**)*100% = **33.3%** for thioacetal **3**

(**1.00**/**1.50**)*100% = **66.7%** for sulfide **4**

Time = 90 minute: Only one spot was observed in TLC (R*f* = 0.17 AcOEt:hexane 2:8). ^{1}H NMR spectrum indicates that after 90 minutes only sulfide **4** is isolated.



^{1}H NMR spectrum for the reaction after 90 minutes shows that only compound **4** was isolated. Peak at 9.19 ppm corresponds to the CH pyrimidinic hydrogen atom and at 4.41 ppm corresponds to the hydrogen atoms alpha to the sulfur atom. Otherwise, if thioacetal intermediate **3** remained unreacted, the peak at 5.71 ppm would still appear, which is not observed. This spectrum is clear for a single compound, indicating that longer reaction time (>90 minutes) would only afford sulfide **4**. ^{13}C NMR spectrum of compound **4** is also provided.



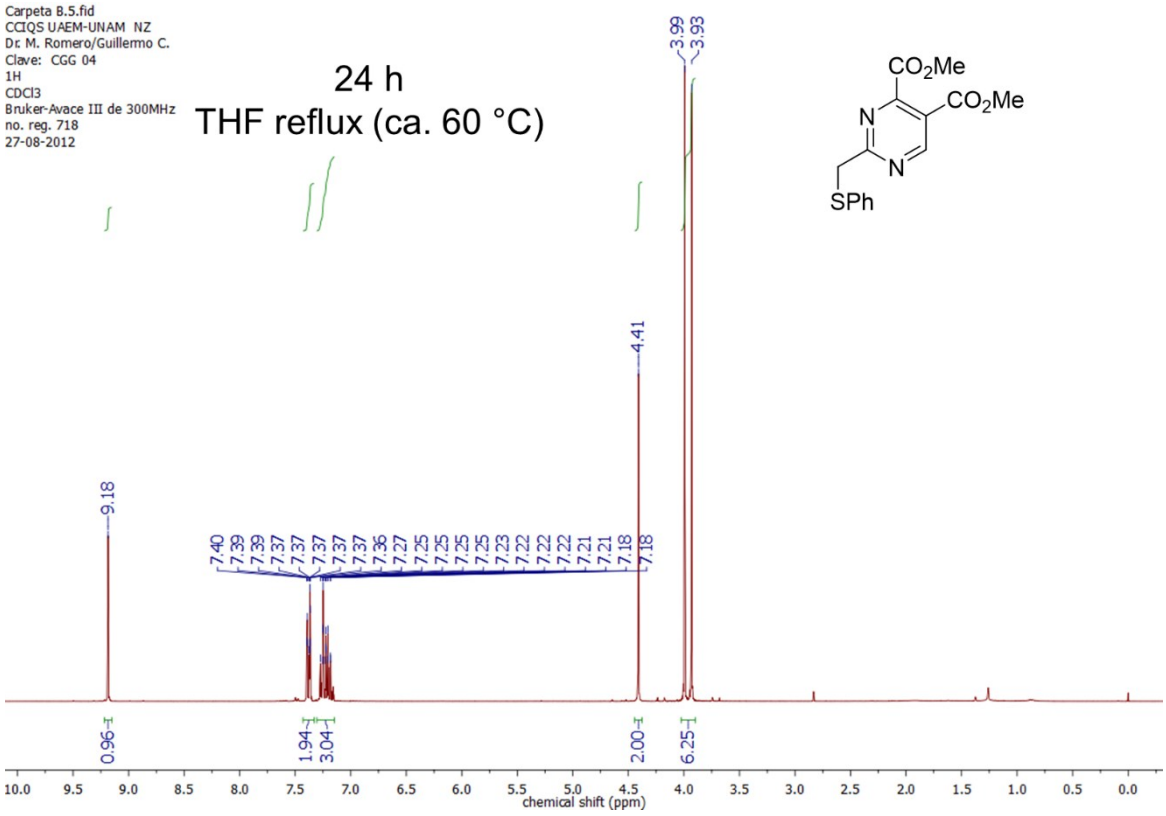
General Procedure for the reaction at THF reflux temperature

In a 25 ml round-bottom flask, provided with a magnetic stirrer and nitrogen atmosphere, 84 mg of NaH (60% suspension in mineral oil, 2.1 mmol, 4.2 equiv.) were suspended in 10 ml of anhydrous THF (dried with Na and freshly distillated from blue benzophenone). After that, 0.4 ml of thiophenol (4 mmol, 8 equiv.) were dropwise added at room temperature and the mixture was stirred for 5 minutes. 157 mg (0.5 mmol, 1 equiv.) of trichloromethyl pyrimidine **1** were added in one portion. Immediately after the addition the time started to count. The reaction then was left under vigorous THF reflux. Once the time (24 or 168 hours) was reached, NH_4Cl std. sln. was immediately added to quench the reaction. AcOEt was added to dilute the reaction, the organic layer was separated and the aqueous phase extracted with AcOEt (4X5ml), the combined organic layers were dried over Na_2SO_4 and the solvent evaporated at reduced pressure. Diphenyldisulfide (R*f* = 0.97, AcOEt:hexane 2:8) was removed through flash column chromatography (silica gel AcOEt:hexane 2:8) and the remaining product(s) were collected. Details for the two reactions are provided as follows as well as their NMR spectra.

Time = 24 h

THF reflux temperature

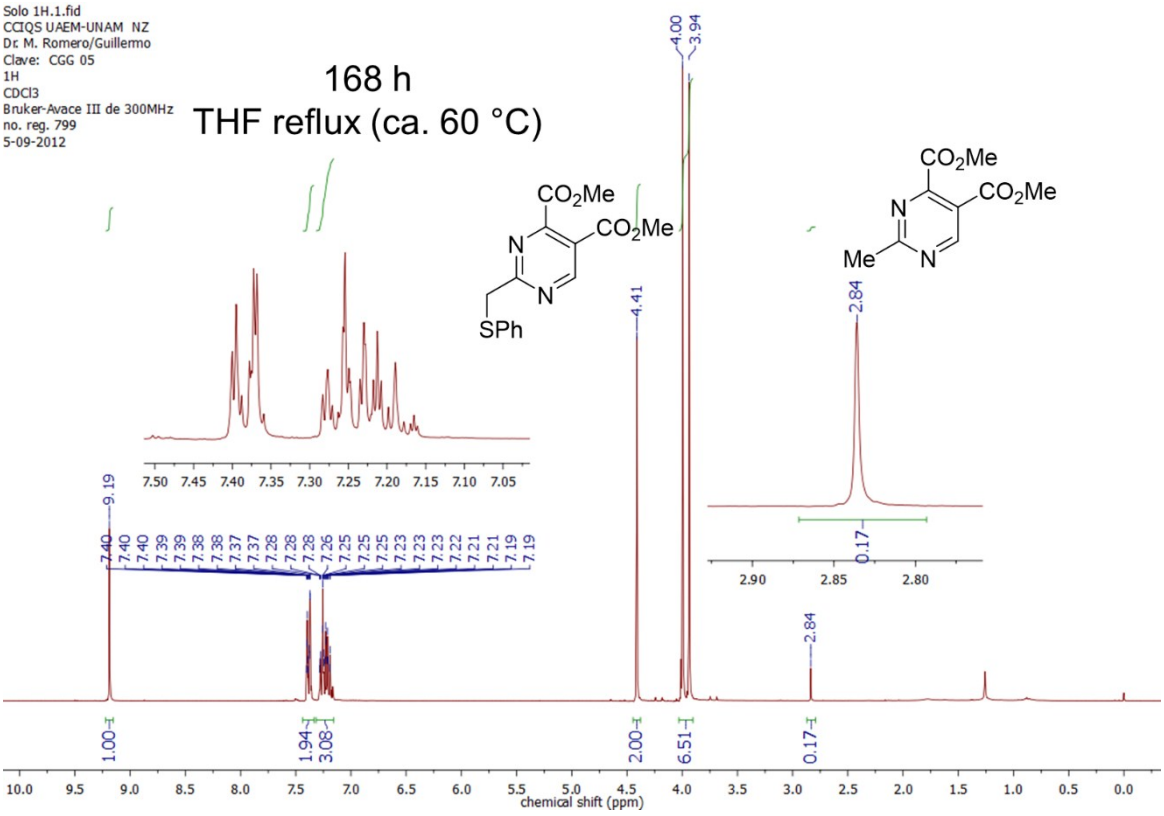
After all diphenyldisulfide was removed through flash column chromatography, the remaining product were collected, concentrated and sent to NMR. According to the ^{1}H NMR spectrum, only sulfide **4** was isolated.



Time = 168 h (7 days)

THF reflux temperature

After all diphenyldisulfide was removed through flash column chromatography, the remaining product were collected, concentrated and sent to NMR. According to the ^{1}H NMR spectrum, apparently only sulfide **4** was isolated, but a small peak at 2.84 ppm is observed.



The peak at 2.84 ppm presumably corresponds to the methyl group in methyl pyrimidine **5**, indicating that the total reduction of trichloromethyl group to a methyl group is possible although difficult with this reaction conditions.

In order to estimate the percentage of sulfide **4** and pyrimidine **5** a similar procedure to that previously described was used. The integral corresponding to the methylene group in sulfide **4** was divided by two so as to normalize it (2.00/2 = 1.00); the integral for the methyl group in compound **5** was also normalized dividing it by three (0.17/3 = 0.057).

The sum of the two normalized integrals (1.00 + 0.057 = 1.057) was taken as the 100%, thus:

(1/1.057)*100% = **94.6%** for sulfide **4**.

(0.057/1.057)*100% = **5.4%** for methyl pyrimidine **5**.

S2 Full Gaussian and Image Processing software References

Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Image processing software

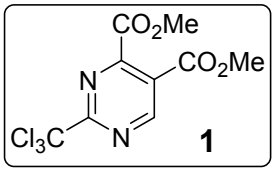
Electrostatic potential mapped onto the electronic density surface.

GaussView, **Version 5**, Roy Dennington, Todd Keith, and John Millam, *Semichem Inc*., Shawnee Mission, KS, 2009.

Transition state structures.

CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

S3 Cartesian coordinates of optimized structures at the BMK/6-31G(*d*,*p*). Absolut energies and Zero-point vibrational energies (ZPVE) are given in Ha



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Negative eigenvalues=0

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C	1.04947400	0.56372900	-0.39905400
C	2.17182200	1.88591700	-2.33292400
O	2.66465500	1.76775000	-3.42623200
O	2.34019200	2.92959100	-1.53125400
C	3.25947400	3.91975300	-1.99199100
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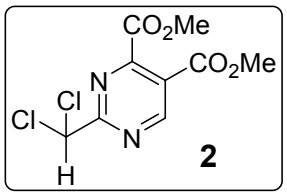

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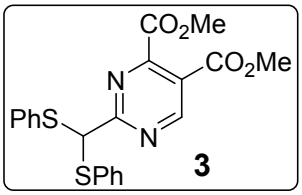
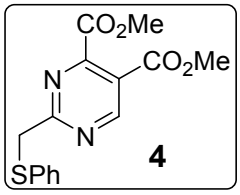
O	1.18151000	1.46231400	1.77558700
C	2.08307000	1.82408800	2.82095200
H	-0.02247600	0.64742400	-3.70653000
H	3.92065900	3.60177200	-2.14381500
H	2.59609900	4.48673800	-2.94824600
H	2.98200800	4.82959500	-1.22417600
H	1.45746100	2.05828200	3.68379000
H	2.67872400	2.69369800	2.52439900
H	2.75675800	0.99036000	3.04442900
H	-1.98358800	-1.69835900	0.70401400



E= -2016.89841661
ZPVE= 0.357430
Negative eigenvalues=0

N	0.09504200	-0.04999000	0.08365200
C	-0.90307100	-0.33591300	-0.75727000
N	-1.03001900	0.12901400	-2.00242100
C	-0.09841400	0.97874800	-2.42141200
C	0.97587900	1.38165200	-1.61460500
C	1.03622900	0.79119800	-0.34202700
C	1.92796600	2.40109100	-2.17257000
O	2.18171300	2.48433300	-3.34828800
O	2.38299000	3.23275200	-1.24119900

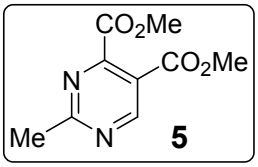
C	3.31573400	4.21208900	-1.69386200
C	-1.95949400	-1.29953700	-0.25243900
C	2.24421900	0.96230700	0.56567200
O	3.37521400	0.92250300	0.15523300
O	1.89627600	1.10831000	1.83504200
C	2.97953900	1.21175800	2.75713100
H	-0.19063400	1.37289400	-3.43282200
H	4.20655400	3.72371800	-2.10180200
H	2.86255200	4.83781300	-2.46959000
H	3.57102200	4.80763700	-0.81561700
H	2.52183500	1.33311600	3.74043400
H	3.60684900	2.07497500	2.51125200
H	3.59405300	0.30599500	2.72347200
H	-1.97097000	-1.28929000	0.84047200
S	-3.61712700	-0.76487500	-0.88875200
C	-4.66191000	-1.67070100	0.27711300
C	-5.09079300	-2.97187400	-0.02967100
C	-5.07878400	-1.05474900	1.46835200
C	-5.92734700	-3.65531400	0.86053100
H	-4.76314900	-3.43559100	-0.95662800
C	-5.91574300	-1.74319700	2.35322100
H	-4.75051900	-0.04175500	1.69065000
C	-6.33934600	-3.04306500	2.05011800
H	-6.25913100	-4.66376500	0.62249500
H	-6.23877500	-1.26395500	3.27500800
H	-6.99239300	-3.57603400	2.73808800
S	-1.52791800	-3.04182100	-0.76954500
C	-0.99434300	-3.78576500	0.78910500
C	-1.40314900	-5.10516900	1.04372500
C	-0.16206300	-3.11832300	1.70323900
C	-0.97588600	-5.75592200	2.20566700
H	-2.05951700	-5.61087600	0.33915400
C	0.23515800	-3.77101600	2.87623200
H	0.17252800	-2.10310700	1.49854000
C	-0.16208200	-5.08909400	3.12891700
H	-1.29461900	-6.77878600	2.39558400
H	0.87164900	-3.24803000	3.58729000
H	0.15945600	-5.59255200	4.03792800



4

E= -1387.94422905
ZPVE= 0.274618
Negative eigenvalues=0

N	-0.68992900	0.02944400	0.00760900
C	-1.43037500	-0.50672900	-0.97180400
N	-1.30974600	-0.23787300	-2.27267600
C	-0.39013500	0.66245900	-2.61640800
C	0.42422800	1.30721600	-1.67836600
C	0.23550900	0.91930700	-0.33957100
C	1.38352100	2.34725900	-2.17957300
O	1.83831600	2.33690500	-3.29660200
O	1.61232100	3.30231600	-1.28334600
C	2.53454400	4.31390800	-1.68314000
C	-2.47221600	-1.50950000	-0.52278900
C	1.16323700	1.37444700	0.77673300
O	2.36196300	1.30143700	0.69522800
O	0.49145900	1.79694000	1.83644300
C	1.28893600	2.16647200	2.95955100
H	-0.28383900	0.89799400	-3.67468800
H	3.51252500	3.87057700	-1.89627100
H	2.17036600	4.82568600	-2.57990800
H	2.60026100	5.00588000	-0.84176900
H	0.58629600	2.49299900	3.72816700
H	1.97437200	2.97671600	2.68979600
H	1.87320500	1.30832200	3.30786400
H	-1.96666400	-2.35804600	-0.04534900
H	-3.11498500	-1.03985500	0.23126100
S	-3.50357500	-2.11608700	-1.93441100
C	-4.59202500	-3.19915500	-0.97058900
C	-5.78431900	-2.69682800	-0.42467900
C	-4.26310800	-4.55325600	-0.79814300
C	-6.63405900	-3.54150600	0.29872800
H	-6.04085900	-1.65039100	-0.57531200
C	-5.11605000	-5.39480600	-0.07457600
H	-3.34518500	-4.93908100	-1.23629400
C	-6.30041400	-4.88985700	0.47533500
H	-7.55708300	-3.14777300	0.71940100
H	-4.85700000	-6.44353700	0.05575400
H	-6.96354700	-5.54584200	1.03541900

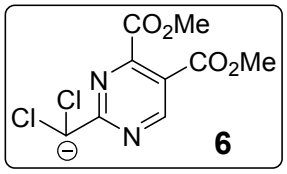


5

E= -758.994915581
ZPVE= 0.192137
Negative eigenvalues=0

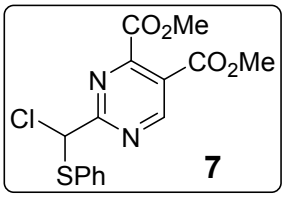
N	-0.30435200	0.36948400	0.04954500
C	-1.07966500	-0.21291400	-0.87552600
N	-0.99673100	-0.00013300	-2.19664000
C	-0.08926200	0.88124500	-2.60701000
C	0.75585300	1.56976000	-1.72601700
C	0.61037000	1.24207900	-0.36815100
C	1.69625400	2.58534200	-2.30382000
O	2.10893500	2.53093100	-3.43625200
O	1.96293500	3.57418400	-1.45511400
C	2.87481200	4.56267300	-1.92804900
C	-2.10266600	-1.21050800	-0.39073900
C	1.57208900	1.74559700	0.69733500

O	2.76782500	1.65781300	0.58875100
O	0.93313400	2.22851100	1.75218000
C	1.76415900	2.64607800	2.83277700
H	-0.01490500	1.07068800	-3.67753800
H	3.84423900	4.10611700	-2.15243800
H	2.48428500	5.03649800	-2.83453900
H	2.96994000	5.29056100	-1.12039900
H	1.08617700	3.02260200	3.60077800
H	2.45264300	3.43118300	2.50305300
H	2.34667800	1.79973200	3.21173200
H	-1.64015000	-2.20509500	-0.32795500
H	-2.93684600	-1.26586800	-1.09510600
H	-2.45217600	-0.93677100	0.60868900



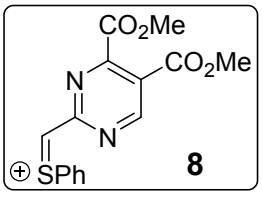
E= -1677.33656337
ZPVE= 0.160441
Negative eigenvalues=0

N	0.15687500	0.85374100	0.00013200
C	-0.68740300	0.25469200	-0.93315300
N	-0.74960000	0.65371700	-2.26906300
C	0.02748500	1.63822400	-2.62094600
C	0.92537800	2.32904700	-1.75229300
C	0.90988200	1.83483700	-0.41402100
C	1.73402800	3.40758300	-2.28514000
O	1.72753200	3.81143600	-3.43705100
O	2.55690400	3.97504900	-1.35714100
C	3.38212500	5.01039400	-1.84285500
C	-1.49595700	-0.77442000	-0.51384200
Cl	-2.60635200	-1.61376800	-1.59011600
Cl	-1.51339100	-1.36635600	1.14290800
C	1.79610200	2.40971200	0.68092500
O	2.85218400	1.95427500	1.03757000
O	1.21986400	3.47202900	1.25943500
C	1.97380400	4.06520500	2.30027600
H	-0.01429300	1.95756900	-3.66489900
H	4.01321100	4.65835000	-2.66780200
H	2.78443000	5.85422300	-2.21003900
H	4.00380900	5.32571900	-0.99977200
H	1.38527600	4.91539900	2.65527000
H	2.94761900	4.40183500	1.92541000
H	2.14404600	3.35074300	3.11424100



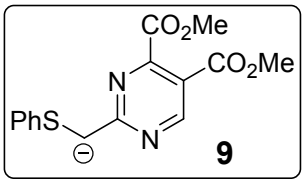
E= -1847.39976656
ZPVE= 0.265852
Negative eigenvalues=0

N	-0.49668300	-0.83364100	0.00959400
C	-1.38028300	-1.25610600	-0.89474300
N	-1.40359600	-0.93373200	-2.18939800
C	-0.46675900	-0.08843600	-2.60465400
C	0.50503500	0.44495500	-1.74363700
C	0.45178800	0.00419800	-0.41234600
C	1.47916800	1.43621500	-2.31635300
O	1.84051000	1.40629300	-3.46611300
O	1.82419500	2.37243700	-1.43954800
C	2.77004100	3.33340200	-1.90542900
C	-2.45371300	-2.19789700	-0.38440600
Cl	-2.05274500	-3.89878100	-0.91914900
C	1.54416700	0.33605400	0.59265300
O	2.71521600	0.26647100	0.32263900
O	1.04723700	0.65448900	1.77684000
C	2.01093900	0.90624300	2.79803500
H	-0.46959200	0.19503300	-3.65644900
H	3.70507700	2.83683700	-2.18373900
H	2.37273400	3.86478400	-2.77629100
H	2.93089200	4.01982900	-1.07242000
H	1.43729300	1.15736800	3.69180200
H	2.66367200	1.73644900	2.50857200
H	2.62349200	0.01469300	2.96802500
H	-2.42647200	-2.22216100	0.70546000
S	-4.10255900	-1.62293200	-0.95262600
C	-5.13634800	-2.48777100	0.25557300
C	-5.57473400	-3.79442700	-0.01071200
C	-5.52711500	-1.83681300	1.43638700
C	-6.39323800	-4.45183600	0.91468100
H	-5.27040100	-4.28391900	-0.93244800
C	-6.34937000	-2.49927900	2.35457600
H	-5.19009300	-0.82023300	1.62610600
C	-6.78053600	-3.80595700	2.09494200
H	-6.72983300	-5.46606000	0.71104300
H	-6.65355900	-1.99465300	3.26910100
H	-7.42046000	-4.31875500	2.80994700



E= -1847.34778449
ZPVE= 0.264480
Negative eigenvalues=0

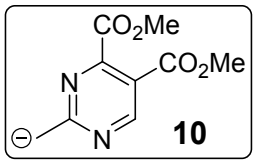
N	-0.44520600	-0.36847600	0.01564800
C	-1.58696100	-0.33987200	-0.69396700
N	-1.83140100	0.45129700	-1.75706200
C	-0.85091600	1.25484600	-2.13579000
C	0.39187500	1.30427100	-1.47742100
C	0.52897500	0.45016100	-0.36835100
C	1.43571000	2.22587500	-2.02168100
O	1.21798000	3.03346300	-2.89229000
O	2.63028800	2.03851300	-1.46222700
C	3.68109700	2.86308200	-1.96178400
C	-2.64226300	-1.23478100	-0.24680100
Cl	-4.09698800	-2.82104900	-2.87585100
C	1.78292600	0.35888900	0.49164900
O	2.54804200	-0.56509100	0.45705600
O	1.86272700	1.39659700	1.31702200
C	2.98178200	1.38656100	2.20090700
H	-1.02417800	1.89766300	-2.99794700
H	3.78792600	2.72599900	-3.04249900
H	3.46680500	3.91721900	-1.75665200
H	4.58472700	2.54230200	-1.44094300
H	2.89491100	2.29297300	2.80284800
H	3.91558700	1.38795100	1.62910700
H	2.95662100	0.49517500	2.83633800
H	-2.40932600	-1.96839100	0.51900800
S	-4.07455300	-1.30287900	-1.07421400
C	-5.06450700	-2.34149000	0.03366300
C	-6.18296300	-1.74277500	0.62179300
C	-4.71914000	-3.67414000	0.28279300
C	-6.96568400	-2.49969200	1.50256900
H	-6.43747100	-0.70860900	0.40063600
C	-5.50780900	-4.41385600	1.16827300
H	-3.87298900	-4.12300300	-0.23153300
C	-6.62633800	-3.82856600	1.77742900
H	-7.83834000	-2.04832400	1.96851500
H	-5.25453100	-5.45161200	1.37190600
H	-7.23846900	-4.41346500	2.46018600



9

E= -1387.38472076
ZPVE= 0.260979
Negative eigenvalues=0

N	-0.21189400	-0.09341300	0.03010400
C	-1.27776300	-0.52092400	-0.76513100
N	-1.22249300	-0.49288900	-2.15345400
C	-0.12828300	-0.03903500	-2.70029000
C	1.01252600	0.42540800	-1.98360500
C	0.85951900	0.35164000	-0.56872800
C	2.17529300	0.88739000	-2.72205600
O	2.27617000	0.95237700	-3.93552100
O	3.21142200	1.25815700	-1.91883200
C	4.37080400	1.68900800	-2.59780500
C	-2.39685800	-0.98146700	-0.09503900
C	1.94657500	0.79300800	0.39927600
O	2.71287300	0.06245300	0.97317000
O	1.90729000	2.11824300	0.59557700
C	2.88517200	2.61832300	1.48846300
H	-0.08481100	-0.01955200	-3.79191500
H	4.74846600	0.90732000	-3.26781600
H	4.16686300	2.58290800	-3.20038600
H	5.11089800	1.91385300	-1.82439600
H	2.73281300	3.70006300	1.53111500
H	3.89275400	2.38678600	1.12329700
H	2.76757400	2.17549600	2.48450900
H	-2.37827800	-0.98744600	0.98970100
S	-3.91397600	-1.43805000	-0.88339600
C	-3.80701400	-3.21701600	-1.17087400
C	-4.96079800	-3.88000000	-1.63106500
C	-2.63153300	-3.95654000	-0.96579400
C	-4.93678100	-5.25527000	-1.87981100
H	-5.87578600	-3.31064800	-1.79156900
C	-2.61599400	-5.33339600	-1.21343700
H	-1.74307700	-3.43605300	-0.61477800
C	-3.76396700	-5.99354800	-1.67075000
H	-5.83866800	-5.75246200	-2.23552400
H	-1.69556500	-5.89310800	-1.05122600
H	-3.74530000	-7.06471500	-1.86307800

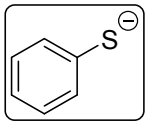


10

E= -758.410926607
ZPVE= 0.178597
Negative eigenvalues=0

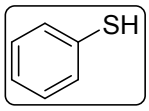
N	-0.11102800	0.05568100	0.08764800
C	-0.99894100	-0.50376100	-0.85284500
N	-1.11699600	0.01747400	-2.15762200
C	-0.35353500	1.02090200	-2.46972100
C	0.59488000	1.64632500	-1.59546000
C	0.62161000	1.06208400	-0.28750400
C	1.40361600	2.73107800	-2.09206200
O	1.35203100	3.23063700	-3.20821100
O	2.31152200	3.19895400	-1.17637100
C	3.13532100	4.24321600	-1.63689800
C	-1.76168100	-1.56823500	-0.48529500
C	1.52107200	1.59447200	0.81707700

O	2.54798700	1.09257700	1.19897800
O	0.99212100	2.69122800	1.38481800
C	1.78293700	3.27295900	2.40155500
H	-0.43952700	1.42271700	-3.48333700
H	3.70795700	3.93804200	-2.52176500
H	2.54488000	5.12789200	-1.90869900
H	3.81556300	4.48258700	-0.81327000
H	1.23237700	4.15040500	2.75243800
H	2.76125200	3.56946100	2.00384000
H	1.94493000	2.56820000	3.22606800
H	-2.45080700	-2.00950700	-1.19754800
H	-1.67783300	-1.97601800	0.51639400



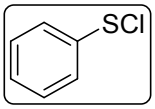
Thiophenolate
E= -629.592378432
ZPVE= 0.089852
Negative eigenvalues=0

C	2.04431900	-1.07964300	0.00000400
C	3.44813700	-1.05518300	0.00046100
C	4.14678800	0.15418700	-0.00004700
C	3.48589400	1.41724000	-0.00104300
C	2.06173900	1.35822200	-0.00148200
C	1.36376800	0.14847200	-0.00097500
H	1.49951300	-2.02278500	0.00039600
H	4.00571900	-1.99380500	0.00122000
H	5.23568100	0.15412100	0.00031700
H	1.51736200	2.30128800	-0.00224100
H	0.27212500	0.16229300	-0.00135100
S	4.36479200	2.93918600	-0.00169500



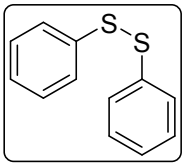
Thiophenol
E= -630.144570258
ZPVE= 0.099495
Negative eigenvalues=0

C	0.07386100	-0.64266100	0.00204700
C	1.46350600	-0.67484900	-0.14544200
C	2.17911100	0.52409700	-0.29317000
C	1.49576300	1.74960800	-0.29195700
C	0.10452000	1.76996700	-0.14323000
C	-0.61234400	0.57772700	0.00409800
H	-0.47232200	-1.57671100	0.11600200
H	1.99144800	-1.62638900	-0.14578700
H	2.04295200	2.68315400	-0.40622500
H	-0.41657300	2.72520000	-0.14332200
H	-1.69336200	0.59900800	0.11933600
S	3.96907700	0.40924500	-0.47958900
H	4.20220700	1.73523200	-0.57326500



Phenylsulfenyl chloride
E= -1089.59716803
ZPVE= 0.093018
Negative eigenvalues=0

C	0.09545900	-0.88487400	0.00323400
C	1.49347700	-0.88976200	0.01158600
C	2.19005100	0.33047500	0.01376700
C	1.49377500	1.55088100	0.00979600
C	0.09575800	1.54632100	0.00142900
C	-0.60089700	0.33080500	-0.00214600
H	-0.44900300	-1.82649300	0.00180600
H	2.04940900	-1.82420400	0.01532700
H	2.04993600	2.48519200	0.01218300
H	-0.44847300	2.48807100	-0.00139200
H	-1.68891000	0.33093500	-0.00787400
S	3.98485400	0.33029600	0.09996000
Cl	4.51425400	0.32922800	-1.91714300

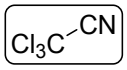


Diphenyldisulfide
E= -1259.11080203
ZPVE= 0.185049
Negative eigenvalues=0

C	-2.01597400	-1.71225800	0.31404600
C	-1.08318800	-0.66918100	0.36140200
C	-1.43987400	0.60437000	-0.11010300
C	-2.72582000	0.83396100	-0.62559000
C	-3.65084300	-0.21338900	-0.67186800
C	-3.29705300	-1.48545000	-0.20207200
H	-1.74142300	-2.69891300	0.68129700
H	-0.08586800	-0.83150500	0.76292100
H	-2.98933600	1.82588200	-0.98507700
H	-4.64770300	-0.03637300	-1.07005900
H	-4.02076600	-2.29716700	-0.23606000
S	-0.24637400	1.95787500	-0.00047000
S	0.66262300	1.95446400	-1.90994300

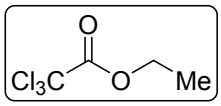
C	1.85647700	0.60167500	-1.79529100
C	1.50060500	-0.67336900	-2.26334900
C	3.14191500	0.83319400	-1.27939800
C	2.43370000	-1.71599900	-2.21216100
H	0.50367100	-0.83720400	-2.66521000
C	4.06722700	-0.21371800	-1.22923300
H	3.40481700	1.82625700	-0.92262200
C	3.71425400	-1.48726800	-1.69560800
H	2.15977700	-2.70381500	-2.57675100
H	5.06368900	-0.03520900	-0.83071200
H	4.43819400	-2.29865100	-1.65862300

Compounds in Chart 1



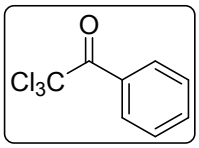
Trichloroacetonitrile
E= -1510.99855327
ZPVE= 0.018059
Negative eigenvalues=0

C	-0.32237700	-0.99920400	-0.01668700
Cl	-2.11966100	-0.99088200	-0.03088300
Cl	0.28493800	-2.69084800	-0.03137700
Cl	0.28497900	-0.14050100	1.44077700
C	0.16739100	-0.30655700	-1.21645600
N	0.55326000	0.23811400	-2.15934500



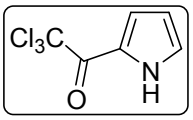
Ethyl trichloroacetate
E= -1685.87947066
ZPVE= 0.091727
Negative eigenvalues=0

C	-0.28221800	-0.15522200	0.00020000
O	0.89435600	-0.37322100	0.00141900
O	-0.86367900	1.02553000	-0.00101700
C	-1.36608600	-1.28899000	-0.00004400
Cl	-2.38676300	-1.11576500	1.47220600
Cl	-2.38522900	-1.11689100	-1.47347100
Cl	-0.57234500	-2.88641800	0.00096600
C	0.01922700	2.16323600	-0.00081200
H	0.65929200	2.10288400	0.88729200
H	0.66101400	2.10186600	-0.88760300
C	-0.85215600	3.41254100	-0.00237600
H	-1.49064300	3.43915200	0.88720800
H	-0.21330100	4.30317500	-0.00227500
H	-1.48892000	3.43811800	-0.89322500



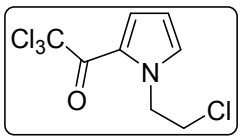
Trichloroacetophenone
E= -1762.99847511
ZPVE= 0.111181
Negative eigenvalues=0

C	0.18283700	-0.46201700	-0.07245700
C	1.57406500	-0.50578000	-0.21515200
C	2.33753700	0.65540000	-0.06735700
C	1.70659600	1.87864400	0.22747500
C	0.30442000	1.91415400	0.36857100
C	-0.45163300	0.75210200	0.21967000
H	-0.40468300	-1.37036200	-0.18887000
H	2.07116000	-1.44575600	-0.44273900
H	3.41265500	0.59218900	-0.18635200
H	-0.17095100	2.86424400	0.59504600
H	-1.53264200	0.79290700	0.33104900
C	2.39903500	3.20215900	0.41436900
C	3.97877100	3.30993400	0.30125400
O	1.79275700	4.21041000	0.65405100
Cl	4.50264700	4.99562400	0.57636100
Cl	4.49724700	2.80576600	-1.35199400
Cl	4.74361700	2.25521000	1.54942200



2-trichloromethylpyrrole
E= -1740.96338796
ZPVE= 0.094250
Negative eigenvalues=0

C	0.36810700	-1.18170000	0.00015300
C	1.76248200	-1.23680300	0.00074200
C	2.23165600	0.09654600	0.00048500
C	1.10660100	0.92781500	-0.00025300
N	-0.00252900	0.11608700	-0.00043300
H	-0.94133700	0.49152300	-0.00093900
H	-0.36665500	-1.97645800	0.00011700
H	2.36124800	-2.13791300	0.00128900
H	3.26128100	0.42821000	0.00079600
C	0.85955700	2.36713400	-0.00082000
O	-0.25732600	2.82847300	-0.00139200
C	2.10034900	3.34192300	-0.00066200
Cl	1.54715500	5.03869700	-0.00148800
Cl	3.09434300	3.03868200	-1.47436000
Cl	3.09312200	3.03972800	1.47407500



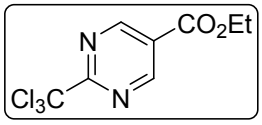
***N*-(2'-chloroethyl)-2-trichloroacetylpyrrole**

E= -2278.98163134

ZPVE= 0.142719

Negative eigenvalues=0

C	0.78522000	-1.03498500	-0.56638100
C	2.09370000	-0.65096700	-0.84773900
C	2.18603300	0.71887200	-0.54830600
C	0.92877800	1.13910800	-0.09160100
N	0.08420700	0.03255700	-0.11341700
H	0.32702000	-2.00889200	-0.66627000
H	2.87622800	-1.29623100	-1.22364300
H	3.06026800	1.34649300	-0.64747600
C	0.44496700	2.44584400	0.34850300
O	-0.68779000	2.66903200	0.70365000
C	1.47702700	3.65492900	0.36099100
Cl	0.66485200	5.13395800	0.94826300
Cl	2.08838600	3.95352200	-1.31014100
Cl	2.85476600	3.27348100	1.46176900
C	-1.32733100	0.02313300	0.28791100
H	-1.41080100	0.39050800	1.31455900
H	-1.88870600	0.71528800	-0.34691800
C	-1.93976300	-1.37829400	0.19072000
H	-1.94893200	-1.75874600	-0.83400600
H	-1.44466100	-2.09371900	0.85270000
Cl	-3.66647000	-1.28619600	0.72184200



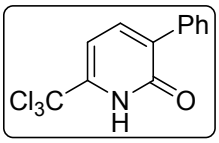
Ethyl 2-trichloromethylpyrimidin-5-carboxylate

E= -1948.86820332

ZPVE= 0.149445

Negative eigenvalues=0

C	-2.24029300	-1.22327300	0.00612500
N	-0.91207500	-1.23021700	-0.09632700
C	-0.30965400	-0.04545500	-0.07011700
C	-1.03715900	1.14749500	0.05858400
C	-2.42560700	1.02283000	0.15804700
N	-3.03076100	-0.16693400	0.13190900
H	0.77546100	-0.03592900	-0.15289800
H	-3.05196200	1.90777700	0.26053300
C	-2.89681600	-2.62461300	-0.02907200
Cl	-4.67807700	-2.54693100	0.10928300
Cl	-2.46269800	-3.42359400	-1.58597800
Cl	-2.24354600	-3.59896000	1.34058500
C	-0.41529800	2.51172700	0.09319700
O	-1.05537800	3.52854400	0.20253600
O	0.90972400	2.45942600	-0.01043400
C	1.59620900	3.72081300	0.01216200
H	1.35381600	4.23340000	0.95071500
H	1.22023400	4.33754900	-0.81285400
C	3.08723200	3.43312800	-0.11773300
H	3.64573100	4.37609800	-0.10499800
H	3.43565500	2.81071400	0.71389500
H	3.30120600	2.91432300	-1.05873700



3-phenyl-6-trichloromethyl-pyrimidin-2-one

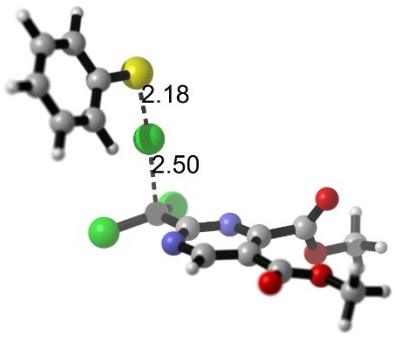
E= -1971.87692251

ZPVE= 0.175558

Negative eigenvalues=0

C	0.48250700	-0.74613700	0.07755100
C	1.79318400	1.74344200	-0.21381200
C	0.43827600	1.68401500	-0.35638100
C	-0.20111400	0.41214800	-0.20054700
H	-0.13821700	2.57326600	-0.57449600
H	-1.28437800	0.37385500	-0.29288900
N	2.48650900	0.60278400	0.07494200
H	3.49482900	0.63095700	0.18810300
C	1.95136600	-0.67570700	0.25813500
O	2.69974500	-1.59554600	0.53631400
C	2.63801300	3.00071700	-0.34128300
Cl	1.65588600	4.45131500	-0.72189100
Cl	3.52655400	3.29683000	1.21135700
Cl	3.86773200	2.77622800	-1.65421200
C	-0.21209200	-2.05518500	0.19279200
C	0.22485900	-3.04832800	1.09249800
C	-1.35498000	-2.31151200	-0.59234300
C	-0.48198400	-4.24787400	1.21600600
H	1.11806300	-2.87607400	1.68250100
C	-2.05499500	-3.51331100	-0.46844300
H	-1.67955000	-1.57533500	-1.32492500
C	-1.62283700	-4.48577300	0.44130700
H	-0.13528700	-5.00095900	1.92051600
H	-2.92951600	-3.69414900	-1.08981700
H	-2.16469500	-5.42425000	0.53735800

Transition state structures



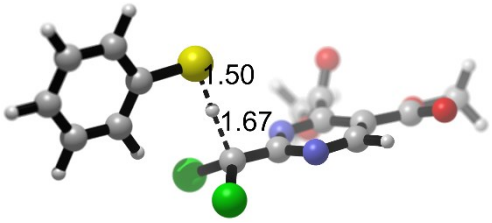
TS 1-6

E= -2766.93492764

ZPVE= 0.253882

Negative eigenvalues=-228.31

N	-1.45477800	0.25010100	0.11928000
C	-1.07947000	-0.36612200	-1.04217000
N	0.22456300	-0.52455100	-1.43205800
C	1.14343500	-0.01312200	-0.64682000
C	0.86941000	0.67601300	0.55956600
C	-0.50693100	0.74126900	0.88666300
C	1.98765800	1.27589800	1.29974700
O	3.16383300	1.09299300	1.05704100
O	1.58598300	2.10301800	2.28709100
C	2.62590500	2.67503500	3.05754600
C	-2.09453800	-0.96437100	-1.84282900
Cl	-2.00909700	-3.26118800	-0.86719200
Cl	-1.72831500	-1.30441000	-3.54440200
Cl	-3.77601300	-0.45924700	-1.59820200
C	-1.02795000	1.30422400	2.20066000
O	-0.89862500	0.76882300	3.27098200
O	-1.71155200	2.43456000	2.01059300
C	-2.33100100	2.96554300	3.17114100
H	2.18386300	-0.12076200	-0.95734100
H	3.23684500	1.89511000	3.52629000
H	3.27845800	3.29505400	2.43155900
H	2.13633300	3.28459400	3.82113700
H	-2.84360300	3.87510300	2.84895100
H	-1.58346100	3.19522700	3.93902500
H	-3.04783300	2.24781400	3.58568100
C	1.58012300	-7.24657700	-2.41973500
C	1.50640200	-5.85176500	-2.32575900
C	0.44310800	-5.22982900	-1.66182800
C	-0.57563700	-6.01182900	-1.09059000
C	-0.51086300	-7.41515700	-1.19739800
C	0.56522400	-8.02468800	-1.84876400
H	2.41291400	-7.72062100	-2.93540400
H	2.28486600	-5.23322700	-2.76907200
H	0.39587100	-4.14609800	-1.59719200
H	-1.30803500	-8.02229200	-0.77205600
H	0.60167200	-9.11077400	-1.91996400
S	-1.95803900	-5.32708900	-0.16930100



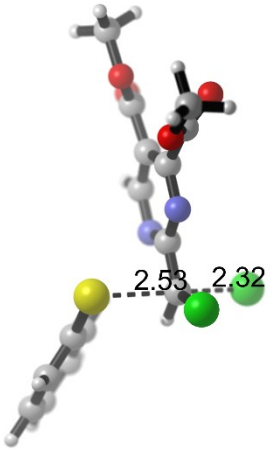
TS 6-2

E= -2307.48992368

ZPVE= 0.259529

Negative eigenvalues=-309.61

N	-0.04115500	-0.06616900	0.17025700
C	-0.83607800	-0.63766700	-0.78061100
N	-0.66808900	-0.44555900	-2.12305100
C	0.28240400	0.38440800	-2.49102400
C	1.12954300	1.07169200	-1.59129300
C	0.90917000	0.75185900	-0.23119700
C	2.08866600	2.05055300	-2.12993000
O	2.37720800	2.16807300	-3.30310900
O	2.60478400	2.85853500	-1.18342900
C	3.56699500	3.79064000	-1.64095600
C	-1.80795300	-1.60269300	-0.35078200
Cl	-3.15879100	-1.93296800	-1.47662600
Cl	-2.38607100	-1.45966000	1.33799000
C	1.81822200	1.22671600	0.89230900
O	2.97338000	0.90740200	1.01031500
O	1.16048400	1.98503800	1.76956700
C	1.90634500	2.36811800	2.91417000
H	0.40915500	0.55766400	-3.56070600
H	4.41416700	3.27631500	-2.10884000
H	3.12705800	4.47369800	-2.37693700
H	3.89793600	4.34148900	-0.75711400
H	1.23365000	2.97975400	3.51996500
H	2.79441400	2.94120300	2.62413100
H	2.22903200	1.48352000	3.47464700
C	-2.14251800	-7.84689000	0.37793300
C	-1.18454100	-6.88509300	0.04575600
C	-1.49607600	-5.50989500	0.08383600
C	-2.79810500	-5.12832200	0.46418900
C	-3.75212600	-6.09793300	0.79066500
C	-3.43619900	-7.46167200	0.75240800
H	-1.87588700	-8.90260100	0.34046900
H	-0.18267400	-7.19175300	-0.24934800
H	-3.05980000	-4.07413800	0.50450400
H	-4.75251900	-5.77808400	1.07913700
H	-4.18357000	-8.21024500	1.00871500
S	-0.21417600	-4.33667900	-0.33994300
H	-0.98769300	-3.05380300	-0.33526300



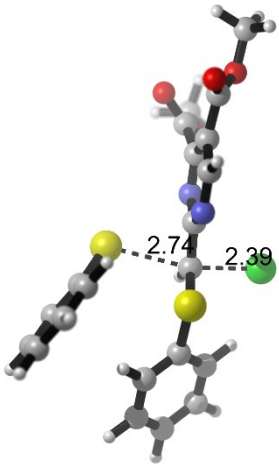
TS 2-7

E= -2307.48788530

ZPVE= 0.263769

Negative eigenvalues=-477.56

N	1.76288000	-0.18182000	0.56321800
C	0.49409900	-0.60005800	0.53859300
N	-0.51463300	-0.00857400	-0.13035700
C	-0.22685100	1.11795600	-0.74881000
C	1.06055300	1.69466200	-0.74352900
C	2.04302100	0.94855800	-0.07318800
C	1.23964800	3.01714700	-1.40057000
O	0.51117700	3.45046100	-2.26399300
O	2.26019800	3.71631500	-0.88941600
C	2.50294500	4.97423000	-1.49842600
C	0.15011300	-1.85470400	1.25699400
Cl	1.37901000	-2.72993200	2.14981200
C	3.52192800	1.29426600	-0.14390800
O	4.11116900	1.50559400	-1.17393500
O	4.09040000	1.27953800	1.05640700
C	5.49510800	1.48371000	1.06682200
H	-1.03210700	1.62479100	-1.28002600
H	2.72393400	4.84922900	-2.56419500
H	1.62874300	5.62673900	-1.39492100
H	3.36360700	5.39887100	-0.97682000
H	5.79520100	1.43981700	2.11590900
H	5.74698200	2.45769700	0.63188400
H	5.99900400	0.70066900	0.48934800
H	-0.87174000	-2.18358900	1.35709500
Cl	0.22031300	-3.08908300	-0.70311700
S	-0.49833500	-0.32310200	3.16551200
C	-2.23339000	-0.73046100	3.22747800
C	-2.82995800	-1.08571200	4.45967000
C	-3.05597700	-0.71366800	2.07728800
C	-4.19051500	-1.39262500	4.54173000
H	-2.20460100	-1.11708000	5.34951800
C	-4.41342600	-1.04434800	2.16339400
H	-2.61711100	-0.44028200	1.11922200
C	-4.99398900	-1.37886800	3.39283700
H	-4.62341900	-1.65676100	5.50633000
H	-5.02178300	-1.03211700	1.25967000
H	-6.05166400	-1.62875500	3.45544300



TS 7-3

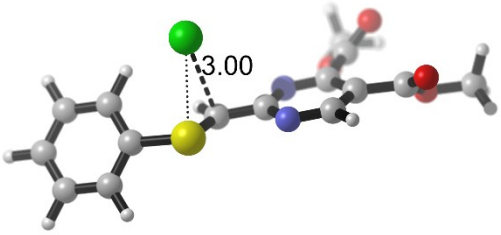
E= -2476.99629407

ZPVE= 0.355627

Negative eigenvalues=-342.45

N	-0.50536500	-0.22419700	-0.06499200
C	-1.45050400	-1.06799200	-0.51458400
N	-1.30208100	-1.94719500	-1.51529800
C	-0.12995200	-1.94822700	-2.13314000
C	0.92121600	-1.09018500	-1.78016200
C	0.66476500	-0.24914700	-0.67300300
C	2.15207600	-1.11290700	-2.61824800
O	2.52506100	-2.07566400	-3.24901000
O	2.76732300	0.07397000	-2.66670000
C	3.96920700	0.10693300	-3.41899000
C	-2.78792800	-0.98328400	0.11626600
C	1.76589100	0.56704300	-0.01588100
O	2.87395300	0.14018000	0.19461900
O	1.34819900	1.77583500	0.33865900
C	2.28927500	2.55749800	1.05786300
H	0.00454200	-2.64426800	-2.96077300
H	4.69852300	-0.59991200	-3.00819200
H	3.77613200	-0.15519800	-4.46535900
H	4.34329900	1.13031600	-3.34178900
H	1.78950600	3.50507300	1.26968200
H	3.19301100	2.72096100	0.45945000
H	2.57147700	2.05411300	1.98928200
H	-2.92801100	-0.37485000	0.99609000
Cl	-3.34051000	0.94108400	-1.18701900
S	-1.47850900	-2.32627000	2.11935300
C	-2.49919400	-3.73299800	2.44418800
C	-2.65624000	-4.76905400	1.49087600
C	-3.19612100	-3.87017000	3.67070500
C	-3.46394000	-5.88195800	1.75284000
H	-2.13150900	-4.68056900	0.54249300
C	-3.99034500	-4.98788500	3.93550700
H	-3.09854900	-3.07780600	4.40976200
C	-4.13633700	-6.00285000	2.97655700
H	-3.56431600	-6.66075800	0.99735800
H	-4.50625500	-5.06585100	4.89228200
H	-4.75862900	-6.87224300	3.18207600
S	-3.98983000	-2.17398100	-0.33686900

C	-5.31854400	-1.76028100	0.81939400
C	-5.83465500	-2.78896100	1.62133400
C	-5.87125800	-0.46986000	0.86543000
C	-6.91527300	-2.52306200	2.47079300
H	-5.37907600	-3.77667800	1.59790400
C	-6.93875000	-0.21486200	1.73357200
H	-5.45656600	0.31183400	0.23031500
C	-7.46675300	-1.23826200	2.53152000
H	-7.30797500	-3.32033500	3.09879900
H	-7.36280900	0.78674300	1.77825200
H	-8.30056900	-1.03323600	3.20094500



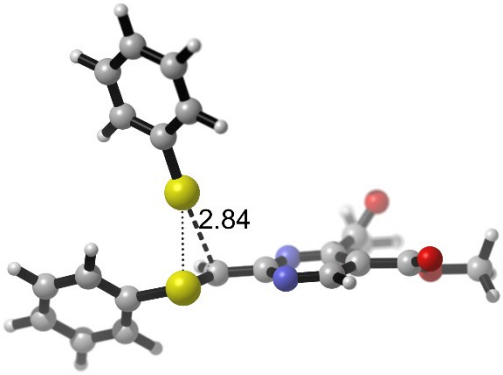
TS 7-8

E= -1847.32776691

ZPVE= 0.263711

Negative eigenvalues=-265.18

N	-1.04444800	0.60586600	-0.01922300
C	-2.19105600	0.64508100	-0.71004900
N	-2.42051000	1.33392400	-1.83755600
C	-1.40565600	2.04270300	-2.30897200
C	-0.15431400	2.08800300	-1.66805200
C	-0.02468900	1.30833500	-0.50394800
C	0.89714600	2.98316100	-2.26422100
O	0.96776000	3.20266800	-3.44708900
O	1.66196300	3.55051500	-1.33960200
C	2.70311500	4.39270000	-1.83359000
C	-3.28812500	-0.14844300	-0.16319400
Cl	-3.11959400	-2.41617500	-2.11892600
C	1.31630600	1.10686800	0.18710400
O	2.33352700	0.90949600	-0.42416900
O	1.20178900	1.12936600	1.50458400
C	2.40290600	0.86114900	2.22744700
H	-1.56270200	2.60995500	-3.22534400
H	3.38715300	3.81426100	-2.46259500
H	2.27947200	5.21281700	-2.42221600
H	3.21952200	4.77439500	-0.95129100
H	2.13426000	0.92611800	3.28310200
H	3.17110800	1.59939100	1.97483100
H	2.77531000	-0.13889100	1.98241600
H	-3.10802700	-0.71002900	0.75054900
S	-4.73298900	-0.25700500	-0.94722700
C	-5.70222300	-1.31256000	0.15456900
C	-6.95832900	-0.83122100	0.54996500
C	-5.23155600	-2.57348000	0.54369900
C	-7.74987700	-1.62546200	1.38570800
H	-7.30684000	0.14561700	0.22122500
C	-6.03719700	-3.34962900	1.38385500
H	-4.28520900	-2.93856300	0.14619500
C	-7.28723300	-2.87895600	1.80541200
H	-8.72346200	-1.26329300	1.70729400
H	-5.69061300	-4.33297800	1.69297800
H	-7.90752100	-3.49436500	2.45329400



TS 8-3

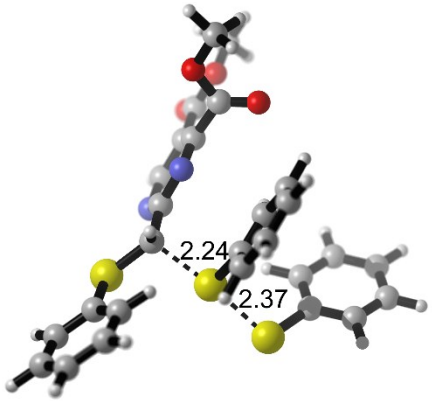
E= -2016.81941955

ZPVE= 0.354905

Negative eigenvalues=-55.13

N	-0.46283000	-0.24894600	-0.00117100
C	-1.66538500	-0.08230900	-0.58677100
N	-1.96751000	0.85616000	-1.50739800
C	-0.99163100	1.67800400	-1.85550400
C	0.30238300	1.60470700	-1.30733000
C	0.50973100	0.57574800	-0.36743900
C	1.29767800	2.63538600	-1.73737700
O	1.19751900	3.26003300	-2.76594600
O	2.26083200	2.82674400	-0.83868700
C	3.26002900	3.77648800	-1.20013500
C	-2.71003200	-0.99517600	-0.17656100
C	1.88237600	0.23761700	0.19623300
O	2.82925900	-0.01837500	-0.49984100
O	1.87356700	0.20268500	1.52115700
C	3.09856400	-0.20141000	2.12872600
H	-1.21352100	2.44665000	-2.59506400
H	3.76030500	3.46703800	-2.12342700
H	2.80922300	4.76277600	-1.35203000
H	3.96605400	3.79746500	-0.36813800
H	2.92203500	-0.16761500	3.20532100
H	3.90761800	0.48018300	1.84600600
H	3.36209200	-1.21569800	1.81100000
H	-2.49043700	-1.75227200	0.56947400
S	-4.25759400	-0.88121700	-0.83392800
C	-5.19950000	-1.97927900	0.25525000
C	-5.21607900	-1.74929800	1.63885000
C	-5.97000000	-2.99856500	-0.31886800
C	-6.00420400	-2.56634500	2.45655200
H	-4.62583100	-0.94230700	2.06650400

C	-6.76446300	-3.79794700	0.50935600
H	-5.91756900	-3.17635900	-1.38994100
C	-6.78040700	-3.58615200	1.89351300
H	-6.01533200	-2.39849100	3.53113100
H	-7.36054200	-4.59534000	0.07145800
H	-7.39512900	-4.21610300	2.53254400
S	-3.01124300	-2.75743000	-2.38873200
C	-2.94672100	-3.98556600	-3.66355000
C	-2.57238200	-3.63797700	-4.98354800
C	-3.27243200	-5.33521100	-3.38816500
C	-2.52556700	-4.60564000	-5.98853500
H	-2.32102000	-2.60168600	-5.19794300
C	-3.22196600	-6.30046600	-4.39508200
H	-3.55703200	-5.60629200	-2.37378500
C	-2.84985700	-5.93869000	-5.69801600
H	-2.23520800	-4.32422800	-6.99891600
H	-3.47116500	-7.33532200	-4.16809200
H	-2.81186100	-6.69194200	-6.48247100



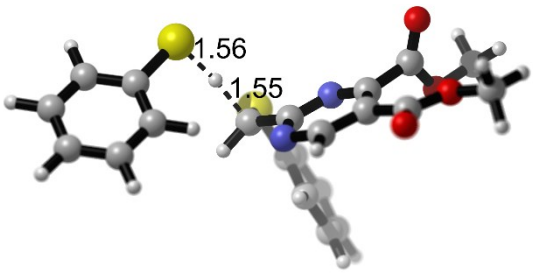
TS 3-9

E= -2646.48970364

ZPVE= 0.447215

Negative eigenvalues=-137.37

N	-0.21048300	0.24641200	-0.26078500
C	-0.94182800	0.84402400	-1.24520400
N	-0.38911800	1.56044700	-2.26719000
C	0.92357600	1.64165000	-2.30407600
C	1.77668800	1.02443500	-1.36144100
C	1.10212100	0.31964700	-0.33713900
C	3.23356100	1.18422200	-1.50683100
O	3.78094900	1.79704400	-2.39924300
O	3.92847600	0.57093200	-0.52847000
C	5.33824600	0.66173700	-0.63763200
C	-2.36126800	0.63162400	-1.22888800
C	1.80214900	-0.47480400	0.75389500
O	2.07251400	-1.64481900	0.66863600
O	2.00623800	0.26334300	1.84529200
C	2.57373100	-0.43208800	2.94594100
H	1.37110300	2.22117500	-3.11255500
H	5.68032500	0.23870400	-1.58872900
H	5.66472300	1.70685700	-0.58554000
H	5.74361800	0.09117900	0.20118100
H	2.67839300	0.30486400	3.74565400
H	3.54997300	-0.84943600	2.67527700
H	1.91788700	-1.25116600	3.26109700
H	-2.75162000	0.38201000	-0.24338900
S	-2.69423000	-1.18179200	-2.49644800
C	-2.35633800	-2.27621700	-1.08762600
C	-3.41612600	-2.76628400	-0.30469300
C	-1.03990500	-2.63459000	-0.76339300
C	-3.15850900	-3.58637400	0.79767600
H	-4.43821800	-2.52201500	-0.58650200
C	-0.78255200	-3.44937900	0.34648700
H	-0.21788800	-2.27341900	-1.37369200
C	-1.83891900	-3.92473700	1.12986800
H	-3.98718600	-3.96325100	1.39536000
H	0.24880900	-3.69117700	0.59409100
H	-1.63896400	-4.55846200	1.99248100
C	0.71599600	-5.17886400	-4.80355200
C	0.70079500	-3.78908300	-4.62662900
C	-0.49279100	-3.11830700	-4.34115800
C	-1.70476100	-3.82808500	-4.21323900
C	-1.67638700	-5.22882700	-4.37965300
C	-0.48271400	-5.89274000	-4.68029500
H	1.64671800	-5.69668700	-5.02823400
H	1.62443800	-3.21865500	-4.71630900
H	-0.49953400	-2.03858900	-4.21070500
H	-2.60278800	-5.78851200	-4.26732100
H	-0.48859700	-6.97496200	-4.80703600
S	-3.26653300	-3.01410500	-3.88509200
S	-3.29183400	1.93659300	-2.08914300
C	-4.97946600	1.64179700	-1.56742800
C	-5.41962200	0.53721900	-0.81739500
C	-5.92118400	2.61928900	-1.95262500
C	-6.76890700	0.42600800	-0.45761900
H	-4.72229400	-0.24344100	-0.53300400
C	-7.26403900	2.49544500	-1.59487100
H	-5.58878900	3.47911100	-2.53237800
C	-7.69902100	1.39725500	-0.83956100
H	-7.09033400	-0.43782200	0.12208800
H	-7.97265200	3.26215400	-1.90438700
H	-8.74554800	1.30078900	-0.55797500



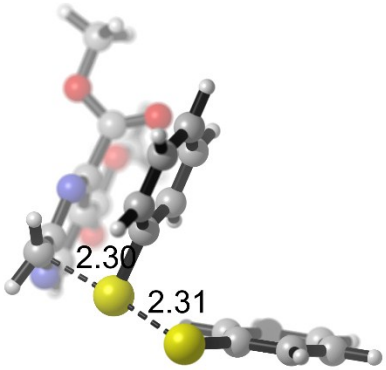
TS 9-4

E= -2017.53993221

ZPVE= 0.359989

Negative eigenvalues=-678.66

N	-0.49994000	-0.31770200	-0.03210500
C	-0.93070800	-1.41991900	-0.71297100
N	-0.69979800	-1.60747300	-2.05511500
C	-0.05021700	-0.66122500	-2.69472700
C	0.41484800	0.52828000	-2.08766600
C	0.15061300	0.61113800	-0.70074700
C	1.07178700	1.54170100	-2.92683000
O	1.35325900	1.40037200	-4.09944200
O	1.32555800	2.68926800	-2.26630400
C	1.99177300	3.68691800	-3.01794200
C	-1.59240600	-2.48745500	-0.03266200
C	0.64227400	1.75072100	0.18024700
O	1.75880200	1.84202500	0.61971600
O	-0.34574000	2.60021900	0.46526600
C	-0.00768300	3.63508800	1.37536400
H	0.12827300	-0.80448700	-3.76149300
H	2.95227300	3.31458600	-3.39183200
H	1.38398600	3.99811400	-3.87566600
H	2.14826200	4.52556400	-2.33527000
H	-0.91338400	4.23317100	1.50032900
H	0.80903000	4.24819700	0.97769500
H	0.30808900	3.21236400	2.33571200
C	-0.51330200	-7.96130500	-1.76010000
C	-0.07700100	-7.12910500	-0.72457600
C	-0.06708100	-5.72701000	-0.87661800
C	-0.51529800	-5.18224600	-2.09943400
C	-0.96697700	-6.02190300	-3.12412000
C	-0.96638500	-7.41376700	-2.96733200
H	-0.50809400	-9.04167200	-1.61837800
H	0.25668700	-7.55633500	0.21898400
H	-0.50501800	-4.10256200	-2.24572300
H	-1.31354700	-5.57947700	-4.05737600
H	-1.31305700	-8.06077300	-3.77127000
S	0.53463000	-4.69491200	0.45736500
H	-0.46942900	-3.52101600	0.22979600
H	-2.17685500	-3.14523400	-0.67669600
S	-2.22950900	-2.28732000	1.62997100
C	-3.67550500	-1.22561300	1.48123500
C	-4.12914200	-0.68494200	0.26732100
C	-4.38772200	-0.93869400	2.66292200
C	-5.27112100	0.12421300	0.23994300
H	-3.58488900	-0.90004500	-0.64846500
C	-5.52606500	-0.13019400	2.62746000
H	-4.04149500	-1.35376700	3.60852400
C	-5.97750000	0.40787700	1.41432300
H	-5.60695800	0.53643700	-0.71054200
H	-6.06277500	0.08021100	3.55166100
H	-6.86402500	1.03838100	1.38663300



TS 4-10

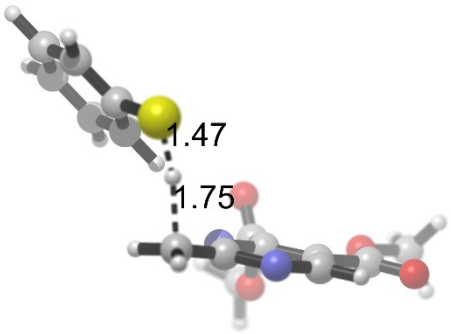
E= -2017.53012484

ZPVE= 0.364735

Negative eigenvalues=-183.65

N	-0.92698600	-0.42950300	-0.01453400
C	-1.67797900	0.18078700	-0.99189100
N	-1.11348600	0.87582800	-2.03966200
C	0.19563100	0.91894500	-2.09782800
C	1.05911300	0.29123500	-1.16290000
C	0.38185100	-0.38760800	-0.12065900
C	2.50888300	0.41746000	-1.33412700
O	3.06250500	1.00100900	-2.24528000
O	3.21253500	-0.19044400	-0.35161100
C	4.61905100	-0.12962400	-0.49012700
C	-3.08186500	0.01893600	-0.96294300
C	1.08608600	-1.19699600	0.95636800
O	1.34644400	-2.36948700	0.86445600
O	1.31127900	-0.47019100	2.05376700
C	1.88854100	-1.18163100	3.13712200
H	0.64623100	1.47664300	-2.92099800
H	4.93685400	-0.58048600	-1.43725300
H	4.96883500	0.90939500	-0.46924700
H	5.03131300	-0.68843300	0.35380000
H	2.01369100	-0.45442600	3.94318800
H	2.85636800	-1.60634100	2.84760300
H	1.23065100	-1.99819400	3.45537900
H	-3.51517900	-0.29845500	-0.01855800
H	-3.65228500	0.72432100	-1.56085400
S	-3.56862400	-1.78783300	-2.30595100
C	-3.17557800	-2.89058300	-0.91840900
C	-4.19917300	-3.35204600	-0.07394300
C	-1.85062800	-3.27559800	-0.67192400
C	-3.89694100	-4.18717700	1.00504600
H	-5.22623100	-3.05818600	-0.27887400
C	-1.54814000	-4.10296300	0.41738700

H	-1.05628400	-2.91968800	-1.32103100
C	-2.56878400	-4.56197200	1.25540100
H	-4.69703700	-4.54299100	1.65277300
H	-0.50947100	-4.36226800	0.60999000
H	-2.33382700	-5.20556800	2.10178900
C	-0.49560400	-5.59668300	-5.30896600
C	-0.41997500	-4.27472500	-4.85250600
C	-1.55109100	-3.62663900	-4.34505200
C	-2.78879200	-4.29613300	-4.27450600
C	-2.85479300	-5.63062700	-4.72676600
C	-1.72307500	-6.26863100	-5.24402400
H	0.38725000	-6.09610200	-5.70381700
H	0.52659800	-3.73742700	-4.89313700
H	-1.48753200	-2.59799400	-3.99734400
H	-3.80293400	-6.16133800	-4.66433900
H	-1.80001200	-7.29953000	-5.58838800
S	-4.28683100	-3.51426900	-3.66746000



TS 10-5

E= -1388.57519480

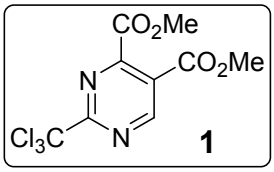
ZPVE= 0.278356

Negative eigenvalues=-123.88

N	-0.48141100	-0.64658400	-0.11060300
C	-0.78629900	-1.33076000	-1.28352700
N	-0.53876000	-0.78848700	-2.54074900
C	-0.01023800	0.40415000	-2.58636500
C	0.32504300	1.19077200	-1.44624300
C	0.03903100	0.55025100	-0.20978700
C	0.93138200	2.49983000	-1.64329000
O	1.12801200	3.04026100	-2.71766400
O	1.29789600	3.10443700	-0.48183800
C	1.91890600	4.36361200	-0.63091600
C	-1.31115200	-2.61127300	-1.18859100
C	0.28541900	1.21037000	1.13801600
O	1.18730200	0.95169800	1.89173200
O	-0.68703800	2.08711900	1.42479800
C	-0.54250500	2.75228600	2.66649800
H	0.18807000	0.82931800	-3.57287600
H	2.82065700	4.28558100	-1.24975000
H	1.24140300	5.08396400	-1.10583300
H	2.17972700	4.69532000	0.37799600
H	-1.39309800	3.43428300	2.74644800
H	0.40103000	3.30988100	2.69513500
H	-0.54682600	2.03554600	3.49600500
H	-1.69757000	-3.07387500	-2.09240500
H	-1.68375200	-2.95025500	-0.22564600
C	0.91338700	-3.49327300	2.97601500
C	0.83282500	-3.48877700	1.57874900
C	1.17041200	-4.64835700	0.85215300
C	1.58994300	-5.79502200	1.55410300
C	1.67887400	-5.78387600	2.94974200
C	1.33794800	-4.63285600	3.67094500
H	0.65203400	-2.58639400	3.51852400
H	0.51193000	-2.58484000	1.06162600
H	1.84118000	-6.69532600	0.99631300
H	2.00907400	-6.68049300	3.47327800
H	1.40421200	-4.62371200	4.75748600
S	1.11479800	-4.70069300	-0.94152500
H	0.09620900	-3.65162500	-1.10770700

S4 List of maximum surface electrostatic potentials calculated at the MP2/cc-pVQZ

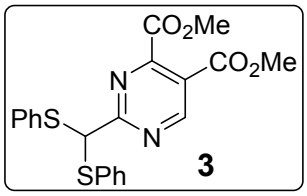
Herein, the list of surface maxima for the compounds that such values were calculated is presented. Maxima were located using the visualizer provided within MultiWFN program.



1

Number of surface maxima: 17

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	0.01539404	0.418893	9.659914	-4.980241	-2.922649	-0.539621
	2	-0.00573080	-0.155943	-3.596137	-4.813626	0.656839	-0.060433
	3	0.01658407	0.451275	10.406668	-3.491891	1.586314	3.176436
	4	0.01708663	0.464951	10.722029	-3.129697	2.266767	-2.890215
	5	0.02450502	0.666815	15.377144	-0.157854	-0.784199	1.747324
	6	0.02745928	0.747205	17.230975	0.008034	-0.708700	-1.655010
	7	0.03270661	0.889992	20.523723	0.616481	-4.396316	-0.243141
	8	0.01069387	0.290995	6.710507	1.888451	-1.148549	1.949634
	9	0.03623747	0.986072	22.739373	1.991348	5.329683	-1.748996
	10	0.03701179	1.007142	23.225268	2.124119	-2.263205	-1.546319
	11	0.02934326	0.798471	18.413188	2.201988	4.829064	1.812215
	12	0.03379101	0.919500	21.204195	3.354423	5.088380	-0.056973
	13	0.03403690	0.926191	21.358493	4.733957	3.167861	-0.809350
	14	0.03165118	0.861273	19.861435	5.554032	-2.955877	-1.916068
*	15	0.04001581	1.088886	25.110321	6.126769	0.646801	-1.895965
	16	0.02879707	0.783608	18.070447	6.346034	-0.954588	1.269089
	17	0.03456065	0.940443	21.687155	6.705084	-1.313095	-0.773191

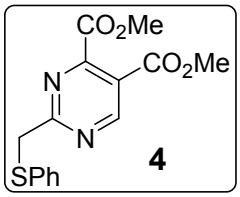


3

Number of surface maxima: 29

#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
1	0.03019809	0.821732	18.949601	-8.544472	-1.090303	0.699398
2	0.02462535	0.670090	15.452656	-8.230965	0.253588	-0.918611
3	0.02734295	0.744039	17.157972	-7.620410	-3.188647	0.625076
4	0.03626149	0.986725	22.754448	-7.578534	-0.129500	2.623829
5	0.03176970	0.864497	19.935804	-5.759694	2.642816	3.008032
6	0.02869651	0.780872	18.007350	-4.213538	-2.755347	0.344207
7	0.03278558	0.892141	20.573277	-4.173809	4.371532	3.068175
8	0.00153444	0.041754	0.962874	-4.000385	0.102210	-1.968732

	9	0.01139102	0.309966	7.147981	-3.377033	-0.453426	1.858992
	10	0.02458864	0.669091	15.429616	-3.055868	-4.021200	-2.070079
	11	0.02919933	0.794554	18.322870	-3.073618	4.995709	1.172351
*	12	0.03662495	0.996616	22.982524	-2.522321	3.587842	4.402028
	13	0.01913147	0.520594	12.005191	-2.086767	2.434791	-0.074125
	14	0.01606297	0.437096	10.079677	-1.866026	-1.801628	1.023647
	15	0.01027425	0.279576	6.447192	-1.805439	0.022834	-1.865673
	16	0.02778295	0.756013	17.434080	0.363680	4.935428	1.731555
	17	-0.01683571	-0.458123	-10.564579	0.974619	-1.754617	-2.581154
	18	0.01803700	0.490812	11.318396	1.379033	0.174853	1.891921
	19	-0.02310171	-0.628629	-14.496553	1.699587	3.600173	-2.155621
	20	0.02249241	0.612050	14.114213	1.947541	-2.116592	3.797002
	21	-0.00288231	-0.078432	-1.808681	2.727849	-4.201954	0.378761
	22	0.02618667	0.712576	16.432399	3.674923	6.430191	0.461660
	23	0.01553459	0.422718	9.748108	4.719379	-1.946703	-2.599262
	24	-0.02028688	-0.552034	-12.730219	4.878132	-3.443006	1.194299
	25	0.02228242	0.606335	13.982442	4.951347	1.222998	-3.088633
	26	0.02752282	0.748934	17.270846	5.097238	-1.366953	4.871026
	27	0.02592880	0.705559	16.270584	5.828608	4.467453	-1.991196
	28	0.02647352	0.720381	16.612399	7.509631	-1.163868	-1.286456
	29	0.02728283	0.742404	17.120252	8.042363	-0.852850	2.441823

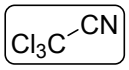


4

Number of surface maxima: 26

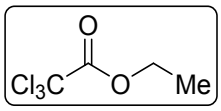
#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
1	0.02705268	0.736141	16.974477	-8.842310	2.188424	0.035457
2	0.02647279	0.720361	16.610618	-7.334155	0.859613	3.269153
3	0.02689456	0.731838	16.875263	-7.067736	1.671649	-3.251110
4	-0.01963967	-0.534422	-12.323104	-6.361707	-1.257230	-0.243696
5	-0.00536545	-0.146001	-3.366606	-4.439909	-2.577998	-0.305778
6	0.02043685	0.556115	12.823305	-4.333991	-0.797309	3.360087
7	0.02138419	0.581894	13.417727	-4.063419	0.017973	-3.497262
8	0.02129895	0.579574	13.364242	-2.163568	1.048453	2.278115
9	0.02169674	0.590398	13.613837	-2.002119	1.433519	-1.900511
10	0.01465955	0.398907	9.198280	-0.732762	-0.142271	1.977442
11	0.01565176	0.425906	9.820853	-0.577803	0.092100	-1.758885
12	0.01452807	0.395329	9.115785	0.906600	-0.716272	1.777063
13	0.01707815	0.464720	10.715855	0.987975	-0.477101	-1.632669
14	0.00482530	0.131303	3.027681	1.461604	-2.694063	1.690709
15	0.02205915	0.600260	13.841236	1.573525	-4.257973	-0.408139
16	0.02613549	0.711183	16.398974	3.127038	5.157849	1.310825
17	0.02805053	0.763294	17.600584	3.328572	-1.645674	-1.815754
18	0.03425310	0.932074	21.492452	3.548008	5.019891	-2.251536
19	0.01466299	0.399000	9.200437	4.077710	-0.954391	1.690285
20	0.03052411	0.830603	19.152661	4.637104	5.046708	-0.301224

	21	0.01564752	0.425791	9.818195	5.118331	-1.030263	1.469041
	22	0.03152319	0.857790	19.779542	5.998084	2.949506	-0.500013
	23	0.02865207	0.779663	17.978030	6.641245	-2.299391	-2.253032
	24	0.02630588	0.715819	16.505888	7.258025	-1.351633	1.446311
*	25	0.03770816	1.026091	23.660364	7.200800	1.117741	-1.206766
	26	0.03157706	0.859256	19.813344	7.744529	-1.096886	-0.657098



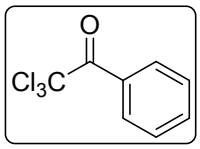
Number of surface maxima: 7

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	0.03037307	0.826493	19.059404	-1.009676	1.435548	1.263550
	2	0.03040917	0.827476	19.082061	-0.979791	-1.834118	0.583426
	3	0.03032829	0.825275	19.031306	-0.943202	0.351457	-1.905791
*	4	0.03669079	0.998407	23.023837	1.212869	-2.621861	-2.317600
	5	0.03666839	0.997798	23.009783	1.148459	-0.738626	3.442349
	6	0.03667574	0.997998	23.014391	1.195345	3.333227	-1.083482
	7	0.02057041	0.559749	12.908141	2.134013	0.033069	0.008253



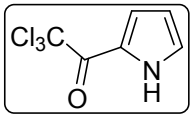
Number of surface maxima: 16

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	0.03295283	0.896692	20.678229	-5.948026	0.682606	-0.021312
*	2	0.03308798	0.900370	20.763041	-4.325338	1.645144	0.002784
	3	0.02677976	0.728714	16.804568	-3.755334	-1.778068	2.083487
	4	0.02678559	0.728873	16.808224	-3.706480	-1.737356	-2.104693
	5	0.03115651	0.847812	19.551023	-3.423623	1.649692	-2.040773
	6	0.03115988	0.847903	19.553136	-3.427927	1.720134	2.008452
	7	0.02589648	0.704679	16.250298	-1.385088	0.920736	-1.707921
	8	0.02589363	0.704601	16.248510	-1.327337	0.913255	1.710493
	9	0.02590011	0.704778	16.252575	-1.072620	0.838957	-1.757208
	10	0.02588697	0.704420	16.244335	-1.142583	0.844291	1.743767
	11	0.02588191	0.704283	16.241157	-0.948027	0.802160	1.784225
	12	-0.01094726	-0.297890	-6.869517	-0.338878	-2.247814	0.006794
	13	0.02194116	0.597049	13.768297	0.897772	-2.213131	-3.056727
	14	0.02194618	0.597186	13.771447	0.899928	-2.208520	3.059881
	15	-0.00031089	-0.008460	-0.195087	2.696729	-1.301809	0.014784
	16	0.01803977	0.490887	11.320135	3.833473	2.185601	-0.015815



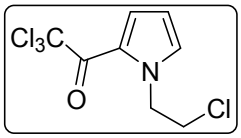
Number of surface maxima: 13

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
*	1	0.03597918	0.979043	22.577293	-6.273752	-1.033430	0.050919
	2	0.03469424	0.944078	21.770982	-5.368472	2.639277	0.002064
	3	0.03575998	0.973079	22.439748	-3.560497	-3.683986	0.025796
	4	-0.00732351	-0.199283	-4.595576	-2.513517	0.002953	-1.762684
	5	-0.00731255	-0.198985	-4.588701	-2.492844	0.017317	1.759240
	6	0.02348382	0.639027	14.736329	-2.498532	3.651307	-0.000362
	7	0.02849716	0.775447	17.882255	-0.681758	-3.086781	-0.004769
	8	0.01686010	0.458787	10.579883	0.026012	0.956018	1.888772
	9	0.01676927	0.456315	10.522887	0.113548	0.960750	-1.910497
	10	0.02319362	0.631131	14.554230	1.242881	-2.216701	3.047841
	11	0.02331027	0.634305	14.627430	1.280952	-2.231244	-3.037221
	12	-0.00019441	-0.005290	-0.121997	3.081486	-1.502312	0.010594
	13	0.01648689	0.448631	10.345690	4.616629	1.826119	-0.018000



Number of surface maxima: 10

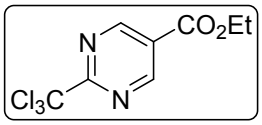
	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	0.04692022	1.276764	29.442904	-5.616463	1.751768	0.007074
	2	0.03419941	0.930613	21.460472	-4.959212	-2.697547	0.012696
*	3	0.07624184	2.074646	47.842516	-2.753532	3.276968	0.014742
	4	0.02756558	0.750098	17.297678	-0.919276	-3.195990	0.000799
	5	0.01279826	0.348258	8.031035	-0.127832	0.948790	-1.911288
	6	0.01278969	0.348025	8.025661	-0.143454	1.006497	1.898822
	7	0.02060532	0.560699	12.930046	1.063102	-2.243798	3.026082
	8	0.02062434	0.561217	12.941982	1.116120	-2.198405	-3.060287
	9	-0.00259633	-0.070650	-1.629223	2.899192	-1.431917	0.004311
	10	0.01547520	0.421102	9.710845	4.299830	1.965846	-0.011624



Number of surface maxima: 10

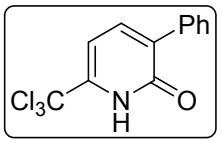
	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	-0.00340241	-0.092584	-2.135045	-4.409332	-0.294293	0.082282
	2	0.01490988	0.405718	9.356098	-3.588016	-3.859268	0.019515
	3	0.02083467	0.566940	13.073966	-3.451027	1.377405	-3.033753
	4	0.02080393	0.566104	13.054675	-3.365053	1.365510	3.082236
	5	0.02741635	0.746037	17.204031	-2.409673	3.282955	0.013840

	6	0.01473325	0.400912	9.245262	-0.500734	-0.466292	-1.927819
	7	0.01558554	0.424104	9.780080	-0.401870	-0.510277	1.867243
	8	0.03680261	1.001450	23.094004	0.874229	5.380744	0.036074
*	9	0.05522085	1.502636	34.651637	4.274664	2.577085	-0.056742
	10	0.01028412	0.279845	6.453390	6.011715	-2.983460	0.017040



Number of surface maxima: 16

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	-0.00888365	-0.241736	-5.574578	-4.753726	-0.688993	0.001552
	2	0.01360826	0.370300	8.539321	-4.611024	2.999304	0.013722
	3	0.01503358	0.409085	9.433722	-3.460185	-2.115437	-3.054074
	4	0.01501761	0.408650	9.423701	-3.436641	-2.062856	3.093225
	5	0.02274126	0.618821	14.270370	0.129897	0.324432	-1.705751
	6	0.02272173	0.618290	14.258111	0.129897	0.324431	1.706436
	7	0.02919524	0.794443	18.320306	1.040282	3.914366	0.020062
*	8	0.03789479	1.031170	23.779361	2.193688	-2.843775	0.014687
	9	0.03524794	0.959145	22.118435	2.844186	0.476448	-1.803415
	10	0.03524274	0.959004	22.115172	2.817310	0.538402	1.808826
	11	0.03118564	0.848604	19.569299	5.137127	-2.709490	-2.061683
	12	0.03118094	0.848477	19.566351	5.136878	-2.710550	2.063129
	13	0.03263700	0.888098	20.480047	6.118958	0.579124	-2.062239
	14	0.03262926	0.887887	20.475190	6.101723	0.561325	2.072128
	15	0.03407905	0.927338	21.384942	7.000707	0.270224	-0.015936
	16	0.03481158	0.947271	21.844617	8.203813	-1.207897	-0.012658



Number of surface maxima: 17

	#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
	1	0.00748154	0.203583	4.694739	-5.050321	-0.164335	0.065082
	2	0.03166601	0.861676	19.870735	-4.496622	3.360430	-0.731177
	3	0.02629499	0.715523	16.500370	-3.956776	-2.400105	-2.569724
	4	0.02626986	0.714839	16.484598	-3.878168	-1.129528	3.364842
	5	0.01287655	0.350389	8.080165	-2.205908	0.859033	-2.018355
	6	0.01293178	0.351892	8.114821	-2.213403	1.613941	1.491368
*	7	0.06245841	1.699580	39.193275	-1.752899	-2.821688	0.599719
	8	0.04099851	1.115626	25.726973	-1.304869	3.584009	-0.795954
	9	0.00753428	0.205018	4.727836	-1.063932	0.400959	1.914978
	10	0.01037400	0.282291	6.509787	0.024950	-0.486467	-1.688364
	11	0.00939911	0.255763	5.898038	-0.027524	0.321682	1.680935
	12	0.01016515	0.276608	6.378730	0.331104	-0.887846	-1.707218
	13	0.03821347	1.039841	23.979337	1.657598	3.525743	-0.671330
	14	0.00789095	0.214724	4.951652	3.428272	-2.964797	-1.530756

15	0.02749101	0.748068	17.250884	6.168308	3.353234	1.186532
16	0.02239318	0.609349	14.051942	6.498667	-2.787231	-1.207436
17	0.02585725	0.703612	16.225682	8.234230	0.331005	0.002108

S5 References

1 A. Guzman, M. Romero, F. X. Talamás and J. M. Muchowski, *Tetrahedron Lett.*, 1992, **33**, 3449–3452.

2 A. Guzma, F. X. Talama and R. Villena, *J. Org. Chem.*, 1996, **61**, 2470–2483.