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

Supporting Information

EXPERIMENTAL AND THEORETICAL STUDY OF THE PHOTOISOMERIZATION AND THERMAL REVERSION OF 5-ARYLMETHYLENE-2-THIOXOIMIDAZOLIDIN-4-ONE.

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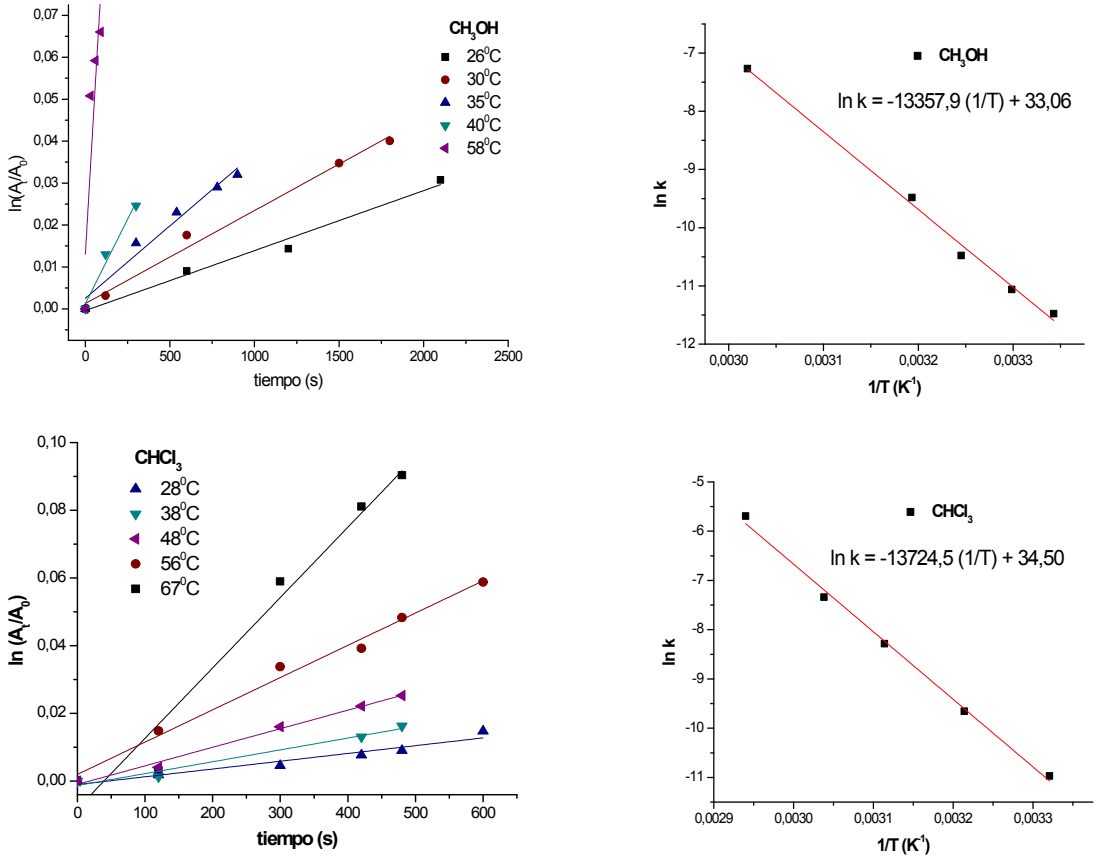


Figure S.0: Plot of thermal reversion progress in CH_3OH and $CHCl_3$ at different temperatures

Cartesian Coordinates and energy from B3LYP/6-31++G(d,p)

S_0: Z(min)

Energy (a.u.): -968.696089 (in vacuo)
Energy (a.u.): -968.710645 (in Acetonitrile)

C	-1.98465200	-0.95640400	0.48235800
C	-3.20204700	-1.63336800	0.42473200
C	-4.34752400	-0.98875800	-0.05225200
C	-4.27038500	0.34856100	-0.45373900
C	-3.05675200	1.02929900	-0.38931900
C	-1.88412000	0.38697600	0.06140300
H	-1.12546400	-1.46192400	0.91138500
H	-3.25905600	-2.66341800	0.76405100
H	-5.29344200	-1.51980000	-0.09795200
H	-5.15727600	0.86184200	-0.81322400
H	-3.00308200	2.06916500	-0.69984400
C	-0.64219000	1.15299800	0.08921500
H	-0.73355700	2.23668200	0.09461100
C	0.63819000	0.71922900	0.07200000

C	1.82226900	1.62792400	0.12537000
C	2.54788000	-0.56653700	-0.06687900
S	3.54781300	-1.87269300	-0.23307700
O	1.86418100	2.84038400	0.21732200
N	2.91451700	0.76186000	0.04993600
N	1.17532300	-0.56851800	-0.01807100
H	0.66065200	-1.41587700	-0.20386400
H	3.87986900	1.06042300	0.05510400

S_0: E(min)

Energy (a.u.): -968.692480 in vacuo)
Energy (a.u.): -968.709532 (in Acetonitrile)

C	2.33692200	0.87339500	-0.00007100
C	3.69694500	1.17722600	-0.00011200
C	4.65978300	0.16274000	-0.00007200
C	4.25255900	-1.17493200	0.00002400
C	2.89612000	-1.48636700	0.00012900
C	1.90859900	-0.47306300	0.00007600
H	1.60234000	1.66830200	-0.00023400
H	4.00673300	2.21821800	-0.00016700
H	5.71688300	0.41183300	-0.00012200
H	4.98983700	-1.97223200	-0.00002500
H	2.58724900	-2.52877500	0.00026500
C	0.52222700	-0.92039200	0.00019300
H	0.42999600	-2.00707200	0.00036500
C	-0.67745100	-0.27978400	-0.00015600
C	-1.08105400	1.16023300	0.00006900
C	-2.99458500	-0.15954400	-0.00000200
S	-4.59232300	-0.59430800	-0.00003800
O	-0.41184200	2.18088600	0.00003400
N	-2.47329000	1.12228200	0.00030900
N	-1.90141500	-0.97568600	-0.00032700
H	-2.00317700	-1.97998900	0.00005300
H	-3.05542100	1.94831000	-0.00013200

S_0 (max)

Energy (a.u.): -968.561227 (in vacuo)
Energy (a.u.): -968.601001(in Acetonitrile)

C	-1.73066300	-0.75795100	0.58987400
C	-2.83225000	-1.43983300	1.06838900
C	-4.08743400	-1.19723500	0.53721600
C	-4.23640500	-0.26483700	-0.47609300
C	-3.13742000	0.41841800	-0.95629200
C	-1.86775900	0.18062600	-0.43106900
H	-0.76247800	-0.95269900	1.00571500
H	-2.71159000	-2.15875200	1.85386800

H	-4.94045600	-1.72850900	0.90906600
H	-5.20596800	-0.07164800	-0.88969900
H	-3.25812100	1.14202800	-1.73897700
C	-0.72008700	0.90326000	-0.96623800
H	-0.86471600	1.59708400	-1.77177900
C	0.65140000	0.72658200	-0.42930600
C	1.33385500	1.48546900	0.65971000
C	2.76535300	-0.10905200	-0.19990900
S	4.15302000	-1.06613000	-0.44326700
O	0.93850000	2.39053000	1.34861500
N	2.60251300	0.88890600	0.70549500
N	1.59232400	-0.19773200	-0.87464700
H	1.44757800	-0.86592000	-1.60043600
H	3.32535200	1.16669900	1.33441100

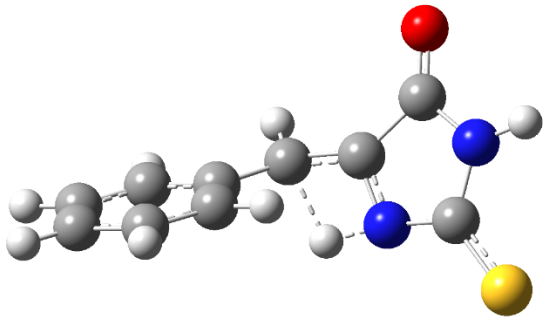
T_1 (min)

Energy (a.u.): -968.634707 (in vacuo)
Energy (a.u.): -968.651895(in Acetonitrile)

C	-1.86227200	-0.59772600	0.75175400
C	-3.03773000	-1.12461500	1.27029700
C	-4.26593700	-0.89365300	0.63020600
C	-4.30538100	-0.12157700	-0.54275900
C	-3.13848000	0.41202600	-1.07102000
C	-1.87804200	0.18826200	-0.43919200
H	-0.91916500	-0.78327300	1.25674900
H	-3.00446700	-1.71968500	2.17812100
H	-5.18097800	-1.30956700	1.04022000
H	-5.25358400	0.05975200	-1.04011000
H	-3.17281900	1.00914900	-1.97793700
C	-0.70121900	0.74117500	-1.00454200
H	-0.78929800	1.34900100	-1.90333600
C	0.63761300	0.57575800	-0.44800900
C	1.39440600	1.48157100	0.40037000
C	2.69073800	-0.36362900	-0.08262300
S	3.95027400	-1.45777600	-0.15010900
O	1.08090000	2.57538100	0.88158300
N	2.63035600	0.83328800	0.57524000
N	1.46208000	-0.48800800	-0.69654200
H	1.22446200	-1.29127000	-1.26625000
H	3.39503400	1.20473000	1.12384900

1,3-H-shift TS

Energy (a.u.): -968.583196 (in vacuo)
Energy (a.u.): -968.602754(in Acetonitrile)



C	-3.05675100	0.70780800	-0.83902400
C	-4.21974100	0.06184200	-0.42190800
C	-4.15893000	-0.95440000	0.53548100
C	-2.91774800	-1.31121900	1.07256400
C	-1.75183000	-0.66817300	0.65983900
C	-1.80139700	0.35826700	-0.30343100
H	-3.11640500	1.49746200	-1.58316100
H	-5.17538600	0.35546300	-0.84673200
H	-5.06357700	-1.45816700	0.86154500
H	-2.85493000	-2.09239300	1.82475200
H	-0.80294000	-0.96484900	1.09500300
C	0.71831400	0.89363700	-0.31664200
C	1.82278300	1.60486200	0.42062000
C	2.40639900	-0.58250300	-0.14428500
S	3.30511500	-1.94995700	-0.28168400
O	1.88112700	2.73391900	0.86321600
N	2.78303200	0.59703000	0.50858000
N	1.15923200	-0.30291500	-0.69899700
C	-0.60594200	1.10389900	-0.79519300
H	0.03507000	-0.15777300	-1.42858400
H	-0.83800900	2.10146400	-1.16474100
H	3.67853300	0.70383600	0.96792800

Table S.0. Energies and geometrical parameters of the main structures at SA-2-CAS(6/5)/6-31G level.

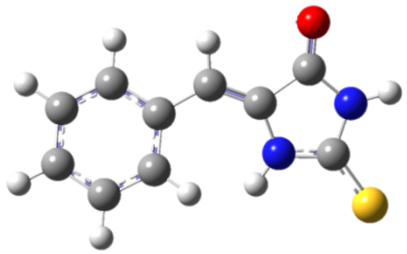
Structure	***State***	***Energy***	***ΔE (kcalmol^{-1})***	***dC-C***	***φ***
Z	S_0	-964,66055510	---	1.32356	1.355
TS	S_0	-964.52345910	77.7	1.48376	89.066
E	S_0	-964,64813980	7.8	1.32466	179.980
ZFC	S_1	-964,51246310	92.9	1.32356	1.355
Z(min)	S_1	-964.56236770	61.6	1.35197	2.256
CI	S_1	-964.54449379	72.8	1.46846	135.022
EFC	S_1	-964.54810490	70.6	1.36000	179.980
E(min)	S_1	-964,57992520	40.0	1.41270	171.661
ZFC	S_2	-964.49799044	102.0	1.32356	1.355

Z(min)	S_2	-964.51130170	93.6	1.45880	50.626
CI	S_2	-964.48658413	91.7	1.45559	117.121
EFC	S_2	-964.50474220	97.8	1.36000	179.980
E(min)	S_2	-964.49902285	85.2	1.41641	179.976
ZFC	T_1	-964,51781150	89.6	1.32356	1.355
TW(min)	T_1	-964.57167560 (in vacuo) -964.60151770 (acetonitrile)	55.8	1.45937	76.683
EFC	T_1	-964.54058300	75.3	1.36000	179.980
E(min)	T_1	-964.56387450	60.7	1.49873	179.858

Cartesian Coordinates and energy from CAS(6/5)/6-31G(d)

S_0: Z(min)

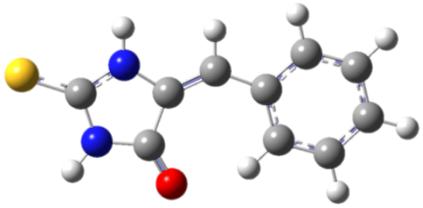
Energy (a.u.): -964.66055510



C	-1.99545400	-0.81071400	0.71270500
C	-3.17408900	-1.50766200	0.63295000
C	-4.26418000	-0.97711500	-0.06721700
C	-4.15795600	0.25441500	-0.66290800
C	-2.96039600	0.97416400	-0.57908100
C	-1.86490100	0.44555000	0.08887400
H	-1.18090200	-1.21008000	1.28961000
H	-3.26464300	-2.46184500	1.11996400
H	-5.18332700	-1.53135600	-0.12639500
H	-4.99251300	0.67456100	-1.19446200
H	-2.88480700	1.93880900	-1.04900800
C	-0.60883800	1.22037900	0.13955800
H	-0.68822600	2.29143700	0.19441700
C	0.62906400	0.75445100	0.09151200
C	1.85281300	1.60408600	0.15744200
C	2.46290600	-0.59086200	-0.09673300
S	3.41525900	-1.92310300	-0.30150100
O	1.94522800	2.78087700	0.27663800
N	2.88854200	0.69797700	0.04856600
N	1.11834400	-0.54988900	-0.04173700
H	0.57282100	-1.36107800	-0.22373800
H	3.85361000	0.94542700	0.05010100

S_0-E

Energy (a.u.): -964,64813980



C	2.33692200	0.87339500	-0.00007100
C	3.69694500	1.17722600	-0.00011200
C	4.65978300	0.16274000	-0.00007200
C	4.25255900	-1.17493200	0.00002400
C	2.89612000	-1.48636700	0.00012900
C	1.90859900	-0.47306300	0.00007600
H	1.60234000	1.66830200	-0.00023400
H	4.00673300	2.21821800	-0.00016700
H	5.71688300	0.41183300	-0.00012200
H	4.98983700	-1.97223200	-0.00002500
H	2.58724900	-2.52877500	0.00026500
C	0.52222700	-0.92039200	0.00019300
H	0.42999600	-2.00707200	0.00036500
C	-0.67745100	-0.27978400	-0.00015600
C	-1.08105400	1.16023300	0.00006900
C	-2.99458500	-0.15954400	-0.00000200
S	-4.59232300	-0.59430800	-0.00003800
O	-0.41184200	2.18088600	0.00003400
N	-2.47329000	1.12228200	0.00030900
N	-1.90141500	-0.97568600	-0.00032700
H	-2.00317700	-1.97998900	0.00005300
H	-3.05542100	1.94831000	-0.00013200

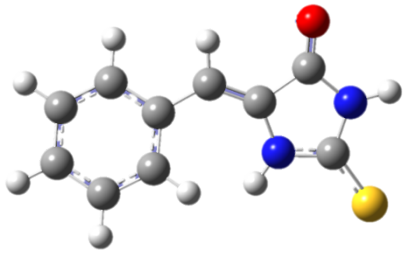
S_0-TS

Energy (a.u.): -964.52345910

C	-1.51398000	-0.61134600	0.58621000
C	-2.55721300	-1.30611900	1.14965700
C	-3.84449100	-1.13528300	0.64248000
C	-4.11294700	-0.27884800	-0.42917900
C	-3.07583200	0.41435900	-0.99791000
C	-1.75294600	0.26393100	-0.50411200
H	-0.51535000	-0.72228700	0.95904800
H	-2.38712100	-1.97074800	1.97519300
H	-4.65749600	-1.67866400	1.09025600
H	-5.11672800	-0.16839500	-0.79359400
H	-3.25450700	1.08241500	-1.82132600
C	-0.71496200	0.98272100	-1.09857900
H	-1.02215600	1.61201900	-1.92471100
C	0.70216100	0.97206100	-0.71532700
C	1.10028700	1.39786500	0.56307200
C	2.49270600	-0.29556000	-0.11828600
S	3.81498600	-1.32978800	-0.20274900
O	0.61827300	2.19071300	1.35149500
N	2.23716600	0.61582200	0.83763200
N	1.49264000	-0.19855000	-1.01163300
H	1.70579500	-0.48577700	-1.94186700
H	2.81626300	0.73876200	1.63887700

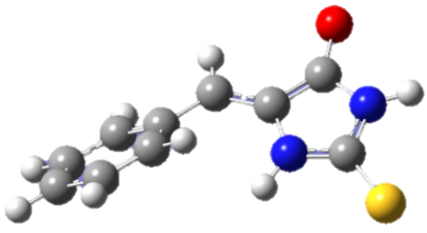
S_1-Z(FC)

Energy (a.u.): -964,51246310



S_1-Z(min)

Energy (a.u.): -964.56236770



C	-1.95755200	-0.71884200	0.75224900
C	-3.11752500	-1.46344600	0.72589300

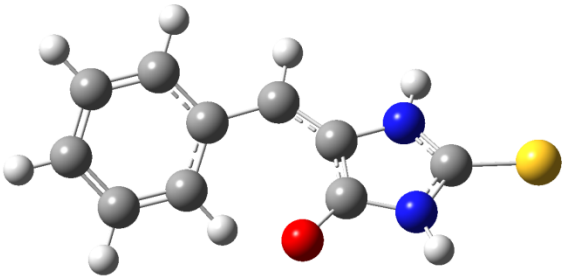
C	-4.23309600	-1.00873800	0.00295800
C	-4.16244800	0.18378100	-0.66521000
C	-2.98341400	0.94119100	-0.64069300
C	-1.87138200	0.50586800	0.04578400
H	-1.12750100	-1.05400500	1.34754400
H	-3.17224700	-2.38724500	1.27303800
H	-5.13595600	-1.59188200	-0.01475000
H	-5.01079800	0.54786000	-1.21650900
H	-2.94630800	1.87402200	-1.17554700
C	-0.65509800	1.33118300	0.05897400
H	-0.77496800	2.39732900	0.01690800
C	0.67248100	0.85317500	0.05257600
C	1.85722200	1.52964600	0.16404700
C	2.42218000	-0.61996700	-0.10953000
S	3.31775200	-2.02056100	-0.29988600
O	2.11596300	2.84842500	0.33522800
N	2.90556600	0.62886500	0.06791300
N	1.08853100	-0.48879300	-0.10291500
H	0.49040600	-1.25691200	-0.30409300
H	3.87874500	0.82880000	0.11248500

S_1-E(FC)

Energy (a.u.): -964.54810490

C	2.33692200	0.87339500	-0.00007100
C	3.69694500	1.17722600	-0.00011200
C	4.65978300	0.16274000	-0.00007200
C	4.25255900	-1.17493200	0.00002400
C	2.89612000	-1.48636700	0.00012900
C	1.90859900	-0.47306300	0.00007600
H	1.60234000	1.66830200	-0.00023400
H	4.00673300	2.21821800	-0.00016700
H	5.71688300	0.41183300	-0.00012200
H	4.98983700	-1.97223200	-0.00002500
H	2.58724900	-2.52877500	0.00026500
C	0.52222700	-0.92039200	0.00019300
H	0.42999600	-2.00707200	0.00036500
C	-0.67745100	-0.27978400	-0.00015600
C	-1.08105400	1.16023300	0.00006900
C	-2.99458500	-0.15954400	-0.00000200
S	-4.59232300	-0.59430800	-0.00003800
O	-0.41184200	2.18088600	0.00003400
N	-2.47329000	1.12228200	0.00030900
N	-1.90141500	-0.97568600	-0.00032700
H	-2.00317700	-1.97998900	0.00005300
H	-3.05542100	1.94831000	-0.00013200

S_1-E(min)

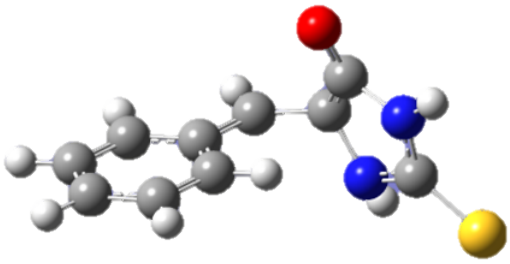


Energy (a.u.): -959.55754290

C	-2.22664200	0.70278200	0.51620100
C	-3.52961100	1.15704400	0.41781000
C	-4.52954200	0.31845300	-0.03867900
C	-4.22160300	-0.98499000	-0.39273000
C	-2.92225100	-1.44030000	-0.29816000
C	-1.90264900	-0.59982000	0.14716000
H	-1.47179400	1.35737700	0.90037000
H	-3.76196000	2.16259400	0.70647300
H	-5.53813500	0.67264500	-0.11231700
H	-4.99179000	-1.64286200	-0.74286700
H	-2.68851200	-2.44897600	-0.57828800
C	-0.53690800	-1.12772900	0.24320100
H	-0.41980600	-2.17815000	0.42148100
C	0.64297600	-0.37403500	0.05464900
C	0.90980200	0.89110500	-0.44633400
C	2.92076600	-0.02701500	0.03216400
S	4.62455500	-0.24842900	0.21483600
O	0.10487400	1.91580500	-0.90804700
N	2.29727200	1.07582600	-0.43996700
N	1.94188500	-0.89317700	0.32798700
H	2.12691600	-1.79192200	0.71639200
H	2.78643400	1.88987000	-0.74122800

S_1-CI1

Energy (a.u.): -964.51958580



C	-1.43987400	-0.57262500	0.57446900
C	-2.45969000	-1.26567600	1.16569000

C	-3.75548700	-1.10217100	0.67548000
C	-4.07090900	-0.25953800	-0.40844800
C	-3.06346900	0.42900500	-1.00298600
C	-1.71333700	0.29567500	-0.53285900
H	-0.43184800	-0.66050400	0.91864400
H	-2.27566300	-1.91902800	1.99548500
H	-4.55477000	-1.64521700	1.14713600
H	-5.08670700	-0.17158900	-0.74081500
H	-3.25730800	1.08615200	-1.83012300
C	-0.70760400	1.00391700	-1.13786400
H	-1.05375200	1.62265200	-1.95979700
C	0.71631200	1.02652000	-0.78457400
C	1.01518000	1.37336800	0.52258600
C	2.39795800	-0.35557300	-0.09661600
S	3.69012200	-1.45189100	-0.13187200
O	0.47704400	2.11537200	1.34617700
N	2.12381900	0.53862400	0.85307700
N	1.45907800	-0.20624800	-1.05132600
H	1.78062000	-0.42287100	-1.96982600
H	2.66483300	0.63094900	1.68300900

S_2-Z(FC)

Energy (a.u.): -964.49799044

C	-1.99545400	-0.81071400	0.71270500
C	-3.17408900	-1.50766200	0.63295000
C	-4.26418000	-0.97711500	-0.06721700
C	-4.15795600	0.25441500	-0.66290800
C	-2.96039600	0.97416400	-0.57908100
C	-1.86490100	0.44555000	0.08887400
H	-1.18090200	-1.21008000	1.28961000
H	-3.26464300	-2.46184500	1.11996400
H	-5.18332700	-1.53135600	-0.12639500
H	-4.99251300	0.67456100	-1.19446200
H	-2.88480700	1.93880900	-1.04900800
C	-0.60883800	1.22037900	0.13955800
H	-0.68822600	2.29143700	0.19441700
C	0.62906400	0.75445100	0.09151200
C	1.85281300	1.60408600	0.15744200
C	2.46290600	-0.59086200	-0.09673300
S	3.41525900	-1.92310300	-0.30150100
O	1.94522800	2.78087700	0.27663800
N	2.88854200	0.69797700	0.04856600
N	1.11834400	-0.54988900	-0.04173700
H	0.57282100	-1.36107800	-0.22373800
H	3.85361000	0.94542700	0.05010100

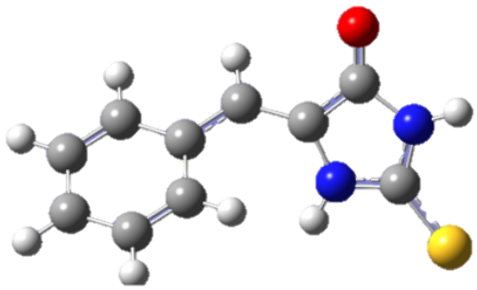
S_2-E(FC)

Energy (a.u.): -964.50474220

C	2.33692200	0.87339500	-0.00007100
C	3.69694500	1.17722600	-0.00011200
C	4.65978300	0.16274000	-0.00007200
C	4.25255900	-1.17493200	0.00002400
C	2.89612000	-1.48636700	0.00012900
C	1.90859900	-0.47306300	0.00007600
H	1.60234000	1.66830200	-0.00023400
H	4.00673300	2.21821800	-0.00016700
H	5.71688300	0.41183300	-0.00012200
H	4.98983700	-1.97223200	-0.00002500
H	2.58724900	-2.52877500	0.00026500
C	0.52222700	-0.92039200	0.00019300
H	0.42999600	-2.00707200	0.00036500
C	-0.67745100	-0.27978400	-0.00015600
C	-1.08105400	1.16023300	0.00006900
C	-2.99458500	-0.15954400	-0.00000200
S	-4.59232300	-0.59430800	-0.00003800
O	-0.41184200	2.18088600	0.00003400
N	-2.47329000	1.12228200	0.00030900
N	-1.90141500	-0.97568600	-0.00032700
H	-2.00317700	-1.97998900	0.00005300
H	-3.05542100	1.94831000	-0.00013200

S_2-Z(min)

Energy (a.u.): -964.51130170



C	-1.84656200	-0.77842100	0.66192800
C	-2.95451900	-1.48147300	0.89997700
C	-4.23178600	-1.09262600	0.32450600
C	-4.28461400	0.11999200	-0.48045000
C	-3.18317000	0.82938300	-0.72053000
C	-1.87452600	0.41406800	-0.19797000
H	-0.91698400	-1.06893400	1.11525300
H	-2.91806000	-2.34781100	1.53561900
H	-5.11174800	-1.68000700	0.49308400
H	-5.23221900	0.43541100	-0.87812300
H	-3.22710900	1.72392000	-1.31605400
C	-0.71238100	1.16186600	-0.53065200
H	-0.82881300	2.09394100	-1.05155200
C	0.65545900	0.77340200	-0.20477500
C	1.70668500	1.57567900	0.34446400
C	2.54032700	-0.49864300	-0.12546600
S	3.56282600	-1.79576900	-0.28786300
O	1.68545000	2.72956900	0.72206100
N	2.82389200	0.72449200	0.36292500
N	1.22664900	-0.45845700	-0.46341800
H	0.77424300	-1.23819100	-0.88499000
H	3.72860400	0.97582000	0.69334600

T_1-E(FC)

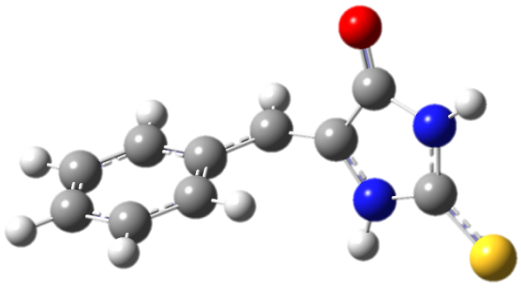
Energy (a.u.): -964.54058300

C	2.33692200	0.87339500	-0.00007100
C	3.69694500	1.17722600	-0.00011200
C	4.65978300	0.16274000	-0.00007200
C	4.25255900	-1.17493200	0.00002400
C	2.89612000	-1.48636700	0.00012900
C	1.90859900	-0.47306300	0.00007600
H	1.60234000	1.66830200	-0.00023400
H	4.00673300	2.21821800	-0.00016700

H	5.71688300	0.41183300	-0.00012200
H	4.98983700	-1.97223200	-0.00002500
H	2.58724900	-2.52877500	0.00026500
C	0.52222700	-0.92039200	0.00019300
H	0.42999600	-2.00707200	0.00036500
C	-0.67745100	-0.27978400	-0.00015600
C	-1.08105400	1.16023300	0.00006900
C	-2.99458500	-0.15954400	-0.00000200
S	-4.59232300	-0.59430800	-0.00003800
O	-0.41184200	2.18088600	0.00003400
N	-2.47329000	1.12228200	0.00030900
N	-1.90141500	-0.97568600	-0.00032700
H	-2.00317700	-1.97998900	0.00005300
H	-3.05542100	1.94831000	-0.00013200

T_1-TW

Energy (a.u.): -964.57167560



C	-1.83935400	-0.66716100	0.69789300
C	-3.00508800	-1.26040500	1.16208800
C	-4.24094000	-0.96678800	0.56620400
C	-4.29804200	-0.06171900	-0.50600500
C	-3.14117500	0.53822200	-0.97889100
C	-1.87143900	0.25211800	-0.39314900
H	-0.89071600	-0.89459200	1.17448800
H	-2.95844200	-1.95429600	1.99635900
H	-5.14877100	-1.43460700	0.93433100
H	-5.25321500	0.17176200	-0.96721800

H	-3.18952500	1.23977300	-1.80723300
C	-0.70419400	0.87307400	-0.90252200
H	-0.81324600	1.60144800	-1.70420900
C	0.64305000	0.65199700	-0.38695700
C	1.46817500	1.53461200	0.41186900
C	2.66495300	-0.39576000	-0.07499900
S	3.81664300	-1.58517600	-0.22324400
O	1.22552400	2.64822900	0.86511800
N	2.70341500	0.82043300	0.57374100
N	1.40121000	-0.45813700	-0.63879600
H	1.12261800	-1.25342400	-1.19801600
H	3.47276400	1.17570200	1.10466900

T_1-E(min)

Energy (a.u.): -964.56387450

C	2.33122400	0.81848800	0.00078600
C	3.67552600	1.14859900	0.00138400
C	4.64842600	0.16379900	0.00088800
C	4.27079300	-1.17287500	-0.00021000
C	2.93560200	-1.51135900	-0.00079400
C	1.93497800	-0.52407700	-0.00032100
H	1.59555500	1.59661700	0.00104000
H	3.96063600	2.18523700	0.00214200
H	5.68979000	0.43087300	0.00133100
H	5.01799800	-1.94596800	-0.00063500
H	2.65267200	-2.54954700	-0.00171200
C	0.56745700	-0.97418300	-0.00113900
H	0.40644100	-2.03550900	-0.00197900
C	-0.71302000	-0.19535100	-0.00084000
C	-1.10887300	1.19656200	-0.00232400
C	-2.98851200	-0.11873300	0.00118200
S	-4.55682900	-0.63207400	0.00387000
O	-0.47824500	2.21615600	-0.00361600
N	-2.50675200	1.13792200	-0.00132600
N	-1.87742800	-0.90895500	0.00119100
H	-1.95451500	-1.90168200	0.00291400
H	-3.08728800	1.94734100	-0.00177400

ISC- E

N	1.401109	-0.535364	0.589936
C	0.629317	0.617303	0.414975
C	1.531246	1.583154	-0.280922
N	2.723842	0.875151	-0.439702

C	2.659179	-0.415848	0.052075
C	-0.654053	0.890101	0.741116
C	-1.881690	0.217422	0.328366
C	-1.930041	-1.123172	-0.110328
C	-3.136781	-1.704903	-0.496359
C	-4.323238	-0.966214	-0.453824
C	-4.296776	0.356875	-0.001826
C	-3.093379	0.937508	0.392080
O	1.314526	2.726203	-0.636932
S	3.842137	-1.569751	0.000625
H	-1.034832	-1.736564	-0.097341
H	-3.152686	-2.741357	-0.820239
H	-5.260854	-1.421778	-0.757456
H	-5.214964	0.934609	0.047350
H	-3.078975	1.965001	0.745180
H	-0.763324	1.761537	1.382525
H	1.066877	-1.432136	0.908545
H	3.550992	1.245219	-0.886855

ISC-Z

N	-1.955647	-1.039222	0.166736
C	-0.691152	-0.566075	-0.196719
C	-0.915516	0.849198	-0.617768
N	-2.287088	1.039384	-0.440617
C	-2.930603	-0.077780	0.059923
C	0.522346	-1.161964	-0.183947
C	1.842716	-0.578599	0.031142
C	2.060556	0.629641	0.727336
C	3.348993	1.135669	0.893213
C	4.450300	0.450498	0.370895
C	4.254492	-0.758816	-0.303481
C	2.968695	-1.270344	-0.463260
O	-0.117308	1.670730	-1.027914
S	-4.530722	-0.223829	0.449563
H	1.230463	1.150903	1.193220
H	3.494634	2.061518	1.441832
H	5.452094	0.848760	0.499935
H	5.104609	-1.305028	-0.701246
H	2.822516	-2.211847	-0.985593
H	0.485101	-2.227721	-0.397304
H	-2.153605	-1.916227	0.624008
H	-2.771599	1.905368	-0.631384