APPENDIX

ORGANOCATALYTIC CS_2 INSERTION INTO EPOXIDES IN NEAT CONDITIONS: A STRAIGHTFORWARD APPROACH FOR THE EFFICIENT SYNTHESIS OF DI- AND TRI-THIOCARBONATES

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Contents

1. Computational details

All electronic structure calculations were conducted at the DFT level using Gaussian16, revision C.01. [1] The M06-2X Minnesota functional was employed in conjunction with the Karlsruhe (def2) basis sets as implemented in Gaussian16, chosen for its accurate description of common organic species involving non-covalent interactions and prominent charge separation. [2]

Geometry optimizations, frequency analyses, and wavefunction generation were performed at the M06-2X/def2-SVP level of theory. A single-point energy refinement was subsequently carried out at the M06-2X/def2-TZVP level to ensure a more accurate energy evaluation. The nature of the stationary points, unless otherwise stated, was determined as either local minima or first-order saddle points (for transition states) by examining the eigenvalues of the Hessian matrix. Likewise, the progress of chemical transformations was evaluated through Intrinsic Reaction Coordinate (IRC) calculations, using the Gaussian16 implementation. [1] The Local Quadratic Approximation (LQA) was employed to handle flat and fuzzy potential energy surfaces. Unless explicitly specified, all reactions were modeled under neat conditions (i.e., in the presence of CS_2). Solvent effects were implicitly included for both energy and gradient evaluations using the SMD solvation model as implemented in Gaussian16. [1]

Wavefunction analyses were conducted on selected compounds and stationary points to elucidate the electron redistribution taking place throughout various reaction steps. These single-determinant wave functions were generated at the M06-2X/def2-SVP level of theory in the gas phase with Gaussian16. [1] Quantum Theory of Atoms in Molecules (QTAIM) calculations were then performed with the AIMAll [3] and PROMOLDEN [4] suites, using default integration grids.

All energies presented in the reaction profiles are reported as Gibbs free energies (373.15 K), computed at the M06-2X/def2-TZVP level, with corrections for translational entropy contributions following the Morokuma scheme. Visualization and molecular representations were done using Jmol [5] with default rendering options.

To mimic the reaction conditions, calculations were performed in the presence of various ionic species, including lithium chloride, choline chloride, and tetrabutylammonium chloride. However, due to the high computational cost of simulating the latter, we opted to use tetramethylammonium chloride as an equivalent system instead.

[1] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[2] https://pubs.acs.org/doi/abs/10.1021/jp408166m

[3] AIMAll (Version 19.10.12), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2019 (aim.tkgristmill.com).

[4] PROMOLDEN: A QTAIM/IQA code. Available from the authors upon request by writing to ampendas@uniovi.es.

[5] Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/.

[6] Bader, R. Atoms in Molecules: A Quantum Theory. International Series of Monographs on Chemistry (Oxford University Press, Oxford, 1990).

2. General reaction mechanism

The current section comprises the general reaction profile and mechanism for the formation of trithiocarbonates (TTC) starting from the corresponding oxiranes. For the sake of computational efficiency, Li^+ was used a single-point charge counter cation of CS_2Cl^-.

Formation of the Thiirane from the Oxirane: **(*S*)/(*R*)-1a** to **4-S**/**R**

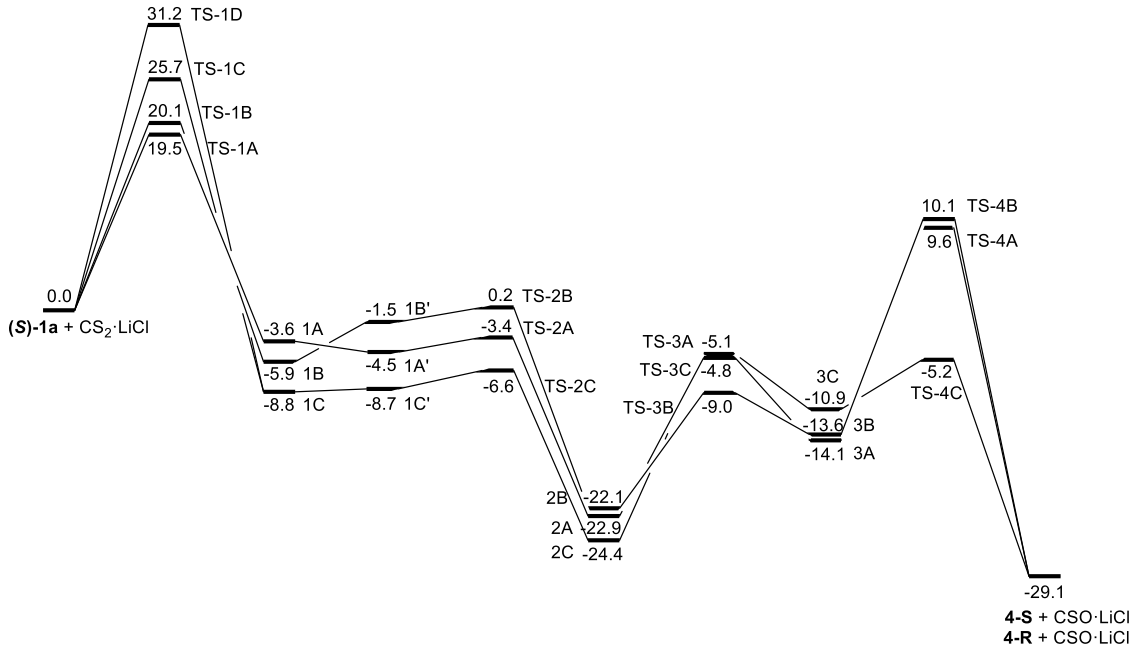


Figure S1. Reaction energy profile for the transformation of **(*S*)-1a** to **4-S**/**4-R**. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

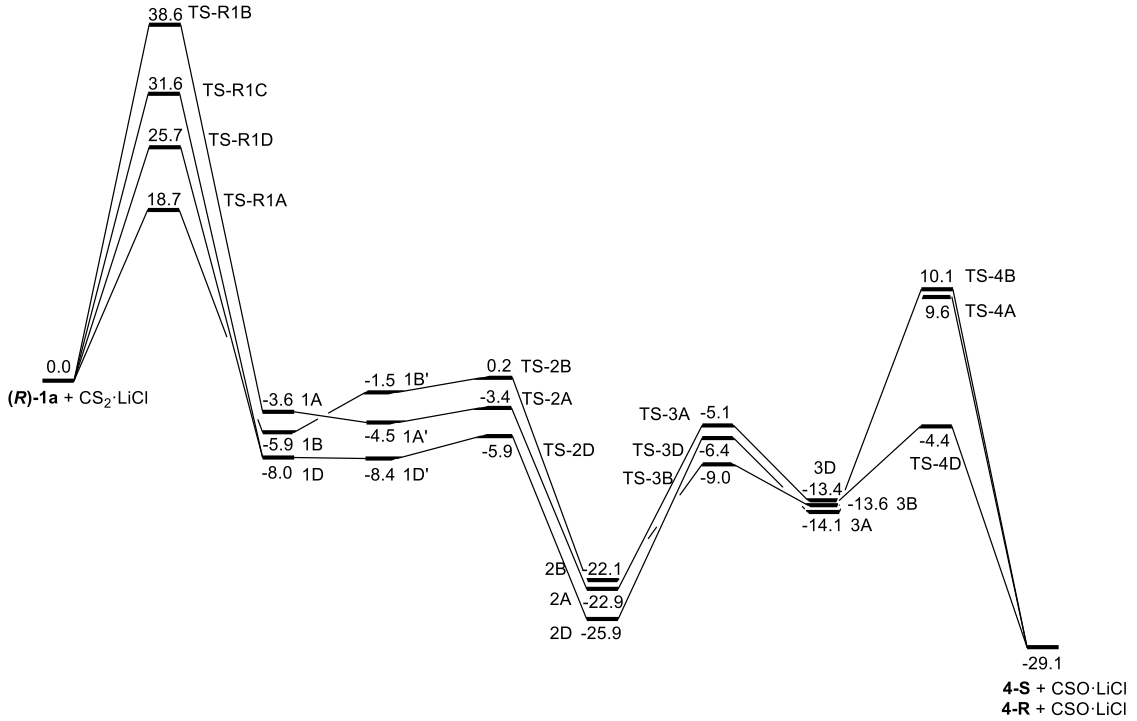
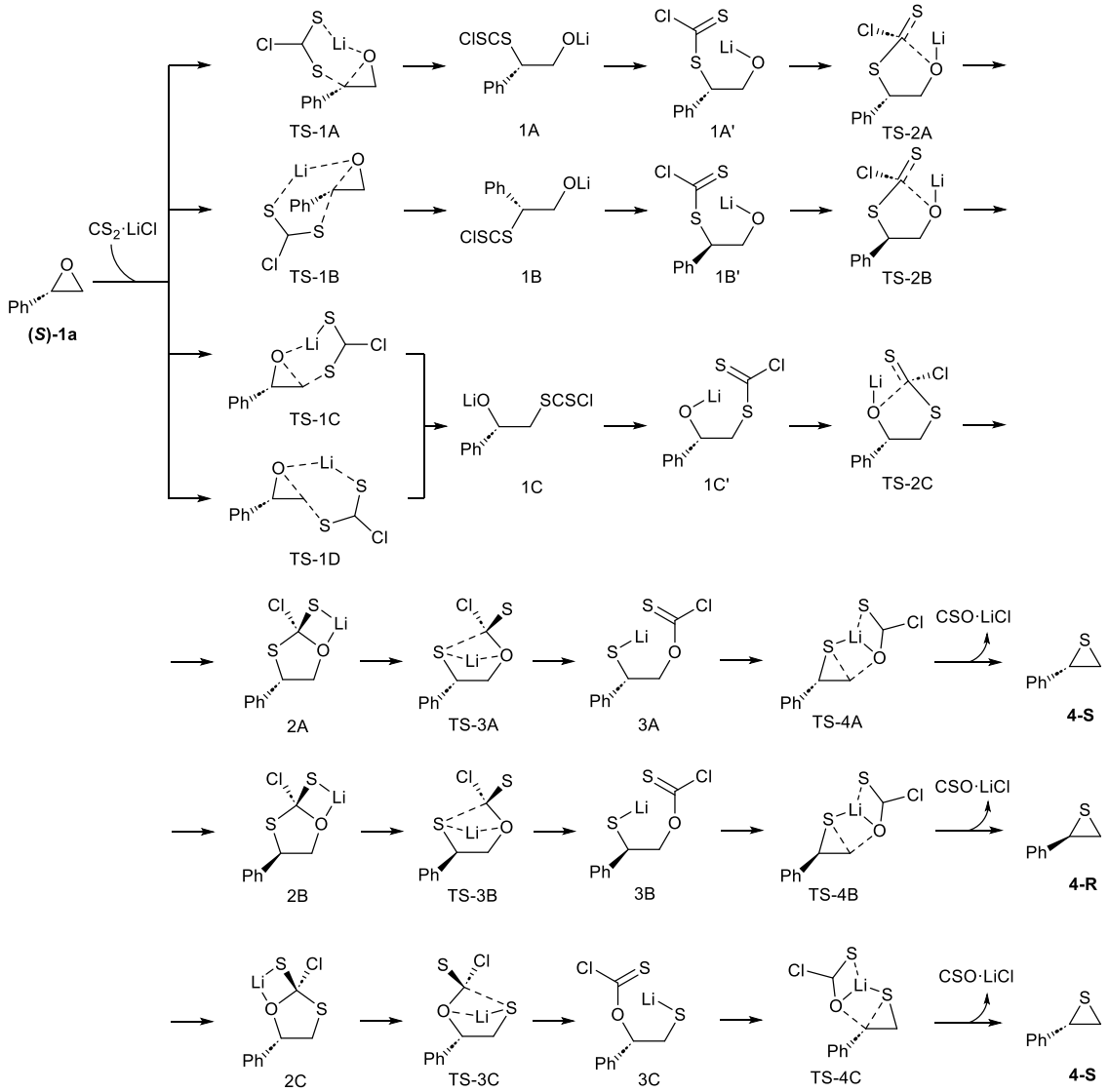
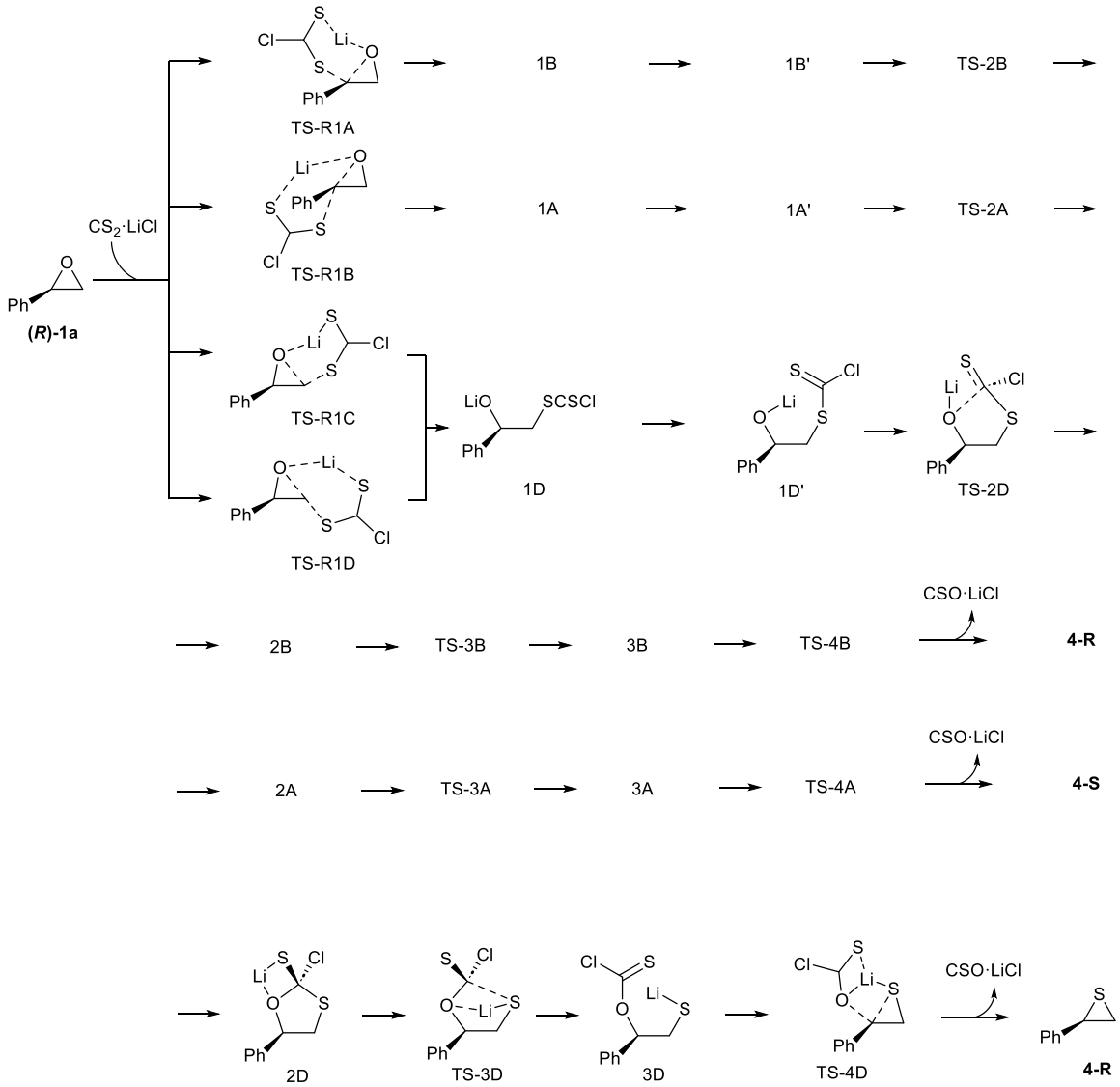


Figure S2. Reaction energy profile for the transformation of **(*R*)-1a** to **4-S**/**4-R**. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).



Scheme S1. Structures of the different stationary states involved in the transformation of **(*S*)-1a** to **4-S**/**4-R**.



Scheme S2. Structures of the different stationary states involved in the transformation of **(*R*)-1a** to **4-S**/**4-R**.

Formation of the trithiocarbonates (TTC) from the Thiirane: **4-S**/**R** to **(*S*)-2a**/**(*R*)-2a**

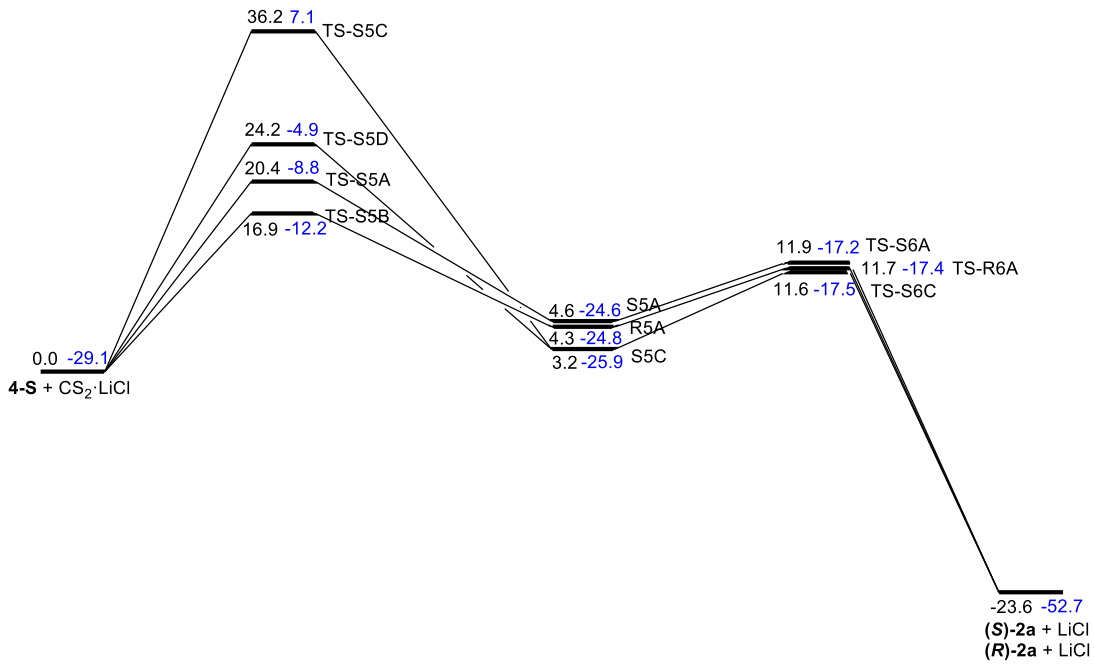


Figure S3. Reaction energy profile for the transformation of **4-S** to **(*S*)-2a**/**(*R*)-2a**. Energies are reported, relative to the reactant complex (black) and to **(*S*)-1a**/**(*R*)-1a** (blue), as the Morokuma-corrected Gibbs free energies (373.15 K).

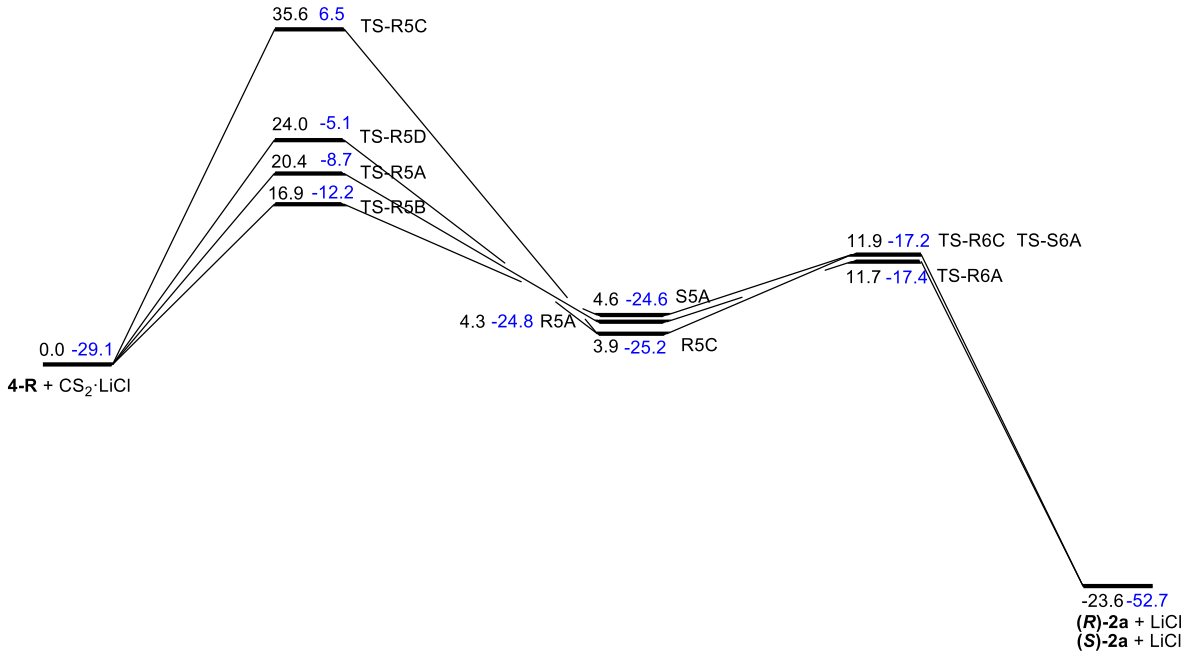
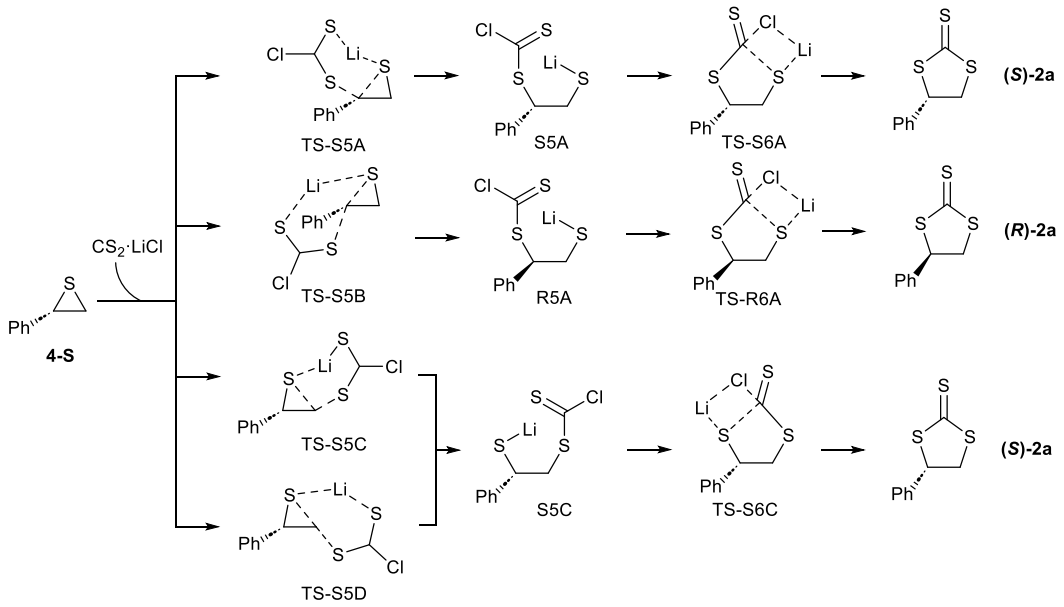
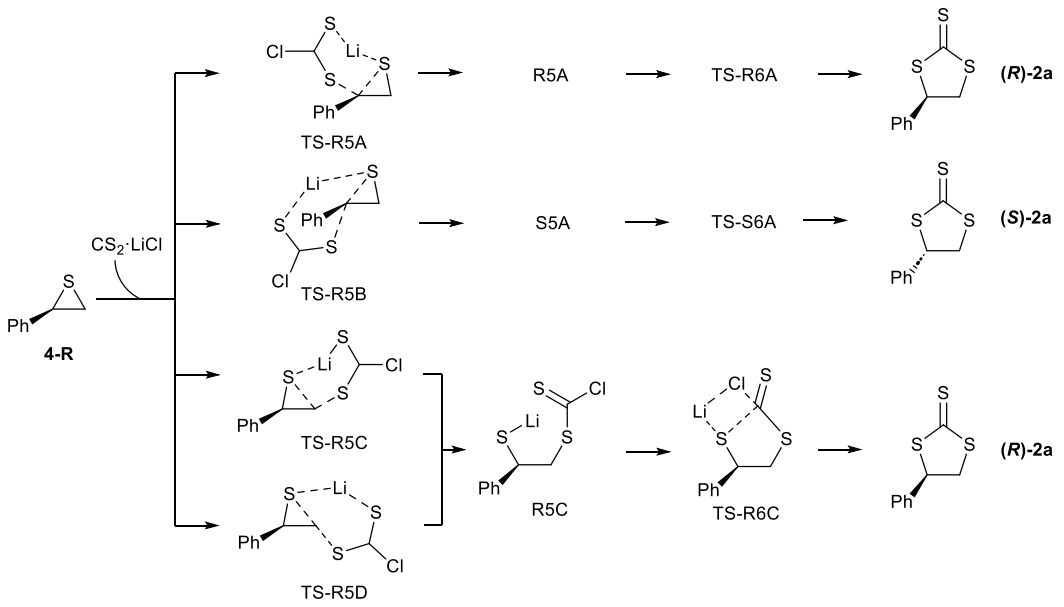


Figure S4. Reaction energy profile for the transformation of **4-R** to **(*S*)-2a**/**(*R*)-2a**. Energies are reported, relative to the reactant complex (black) and to **(*S*)-1a**/**(*R*)-1a** (blue), as the Morokuma-corrected Gibbs free energies (373.15 K).



Scheme S3. Structures of the different stationary states involved in the transformation of **4-S** to (***S***)-**2a**/(***R***)-**2a**.

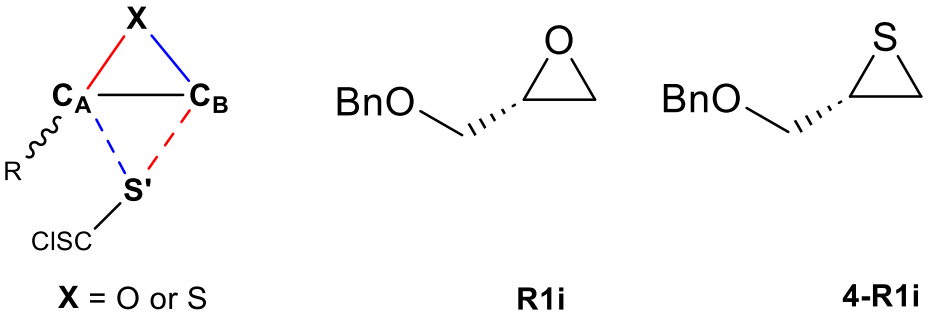


Scheme S4. Structures of the different stationary states involved in the transformation of **4-R** to (***S***)-**2a**/(***R***)-**2a**.

3. Wavefunction analysis

Trying to investigate the nucleophilic attack of the adduct on the starting oxiranes and thiiranes, wave function analyses were conducted. Specifically, we examined the electronic redistribution occurring at this reaction stage using the Quantum Theory of Atoms in Molecules (QTAIM) framework. **[6]** For such a purpose, we focused on two key aspects: electronic transfer, assessed through the atomic charge distribution (Q), and electronic sharing, evaluated via the delocalization index (DI).

Oxirane **R1i** and its corresponding thiirane **4-R1i** were used as prototypical models. The nucleophilic attack was modeled at both the more substituted (A) and less substituted (B) carbon atoms, considering upward (U) and downward (D) approaches, as illustrated in **Scheme S5**. Both gas-phase and solvated calculations were performed as indicated in the computational details.



Scheme S5. Schematic representation of the nomenclature employed to refer to the most relevant atoms involved in the nucleophilic attack to the oxirane (**X** = O) or thiirane (**X** = S). The structures of the target oxirane (**R1i**) and thiirane (**4-R1i**) used as prototypical models are also shown.

Nucleophilic attack to the oxirane

Gas-Phase studies

Anionic reaction (without counter cation):

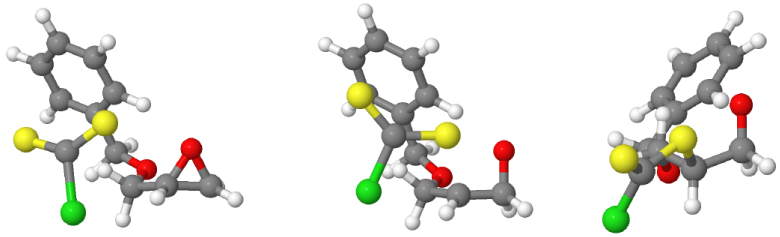


Figure S5. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (upward attack to C_A).

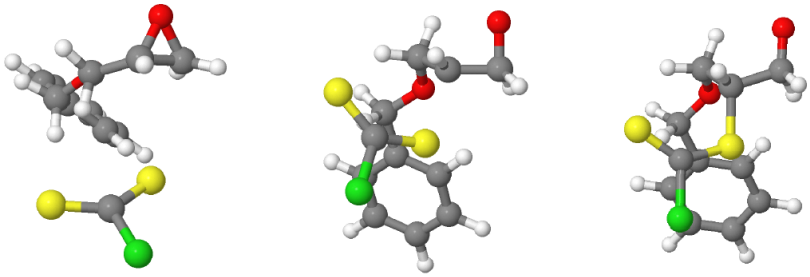


Figure S6. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (downward attack to C_A).

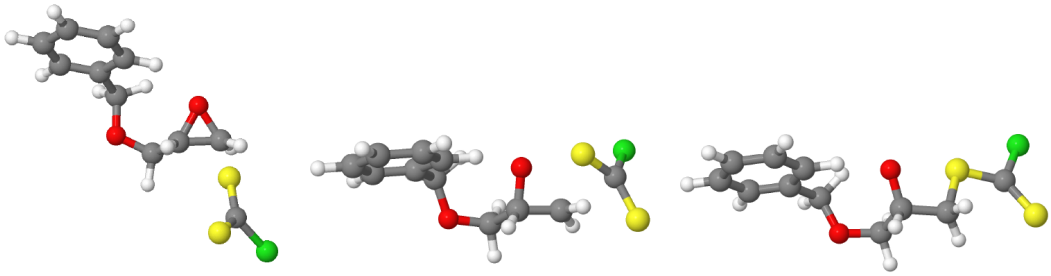


Figure S7. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (upward attack to C_B).

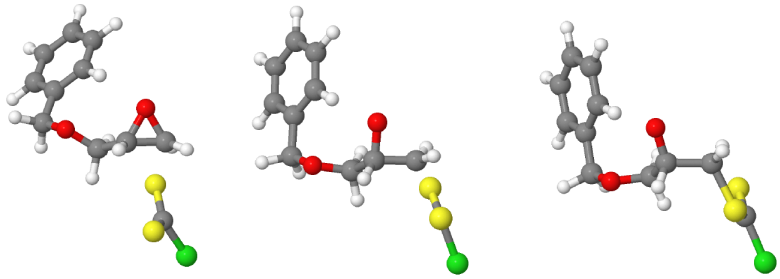


Figure S8. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	56.6	14.5
A	downward	0.0	32.4	22.0
B	upward	0.0	52.6	11.6
B	downward	0.0	26.5	15.8

Table S1. Energies of the reactants (R), transition state (TS) and products (P) involved in the gas-phase reaction between CS_2Cl^- and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

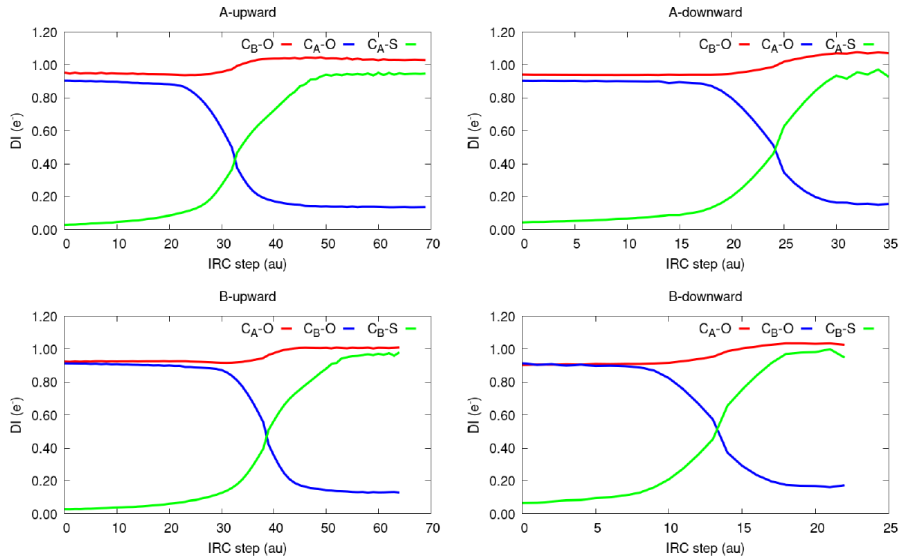


Figure S9. Evolution of the electron delocalization (DI) across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- to R1i. The results for different spatial approximations are shown. All values are reported in electron pairs.

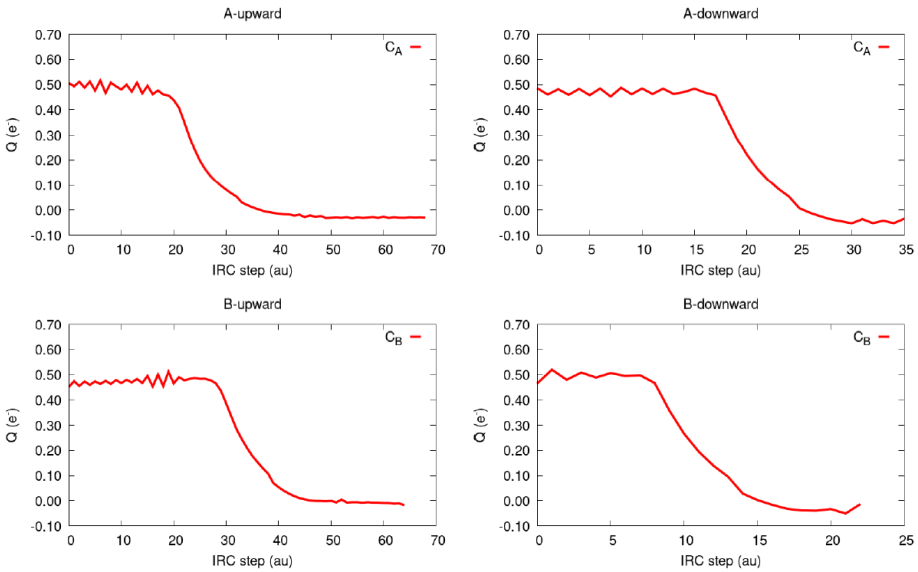


Figure S10. Evolution of the atomic charges (Q) of the electrophilic carbon across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- to R1i. The results for different spatial approximations are shown. All values are reported in electrons.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A, Orientation: Upward]

C	-2.530361	2.773350	-0.643218
C	-2.129996	1.452348	-0.139281
O	-1.714977	1.911101	-1.403644
H	-3.546063	2.924016	-1.027248
H	-2.832847	0.611942	-0.158022
S	0.520983	-2.319931	0.792305
C	-0.858726	-1.930579	-0.014546
S	-1.224304	-1.583389	-1.583155
Cl	-2.390630	-1.778078	1.155381
H	-2.023441	3.658501	-0.245423
C	-1.069617	1.330911	0.926707
H	-1.560209	1.299110	1.918497
H	-0.532110	0.377363	0.807476
O	-0.189999	2.430061	0.836393
C	1.105055	2.163592	1.287791
H	1.090147	1.776305	2.326470
H	1.625026	3.135421	1.312334
C	1.882425	1.192052	0.419053
C	1.434082	0.849814	-0.857665
C	3.056736	0.614320	0.911524
C	2.140257	-0.082244	-1.617909
H	0.501205	1.274331	-1.235868
C	3.778508	-0.289876	0.138063
H	3.396883	0.860826	1.921753
C	3.314978	-0.646438	-1.128617
H	1.733502	-0.396458	-2.579813
H	4.687615	-0.744173	0.537775
H	3.853909	-1.389515	-1.719213

[TS, Approximation: A, Orientation: Upward]

C	1.440027	-3.007989	-0.839122
C	1.452228	-1.912713	0.144443
O	0.691696	-2.286258	-1.713548
H	2.468763	-3.275308	-1.181877
H	2.368459	-1.500524	0.569089
S	1.177711	2.987854	-0.168852
C	1.684343	1.435307	-0.031653
S	1.689837	0.185270	-1.141267
Cl	2.314703	0.934608	1.653837
H	0.976944	-3.943192	-0.434407
C	0.285603	-1.729612	1.059915
H	0.646757	-2.068172	2.058009
H	0.053175	-0.657457	1.172392
O	-0.835967	-2.478715	0.683506
C	-2.067523	-1.905152	1.010881
H	-2.172848	-1.774960	2.108456
H	-2.827573	-2.639297	0.699303
C	-2.316223	-0.573096	0.330246
C	-1.615025	-0.254404	-0.836957
C	-3.201717	0.355488	0.884712
C	-1.772786	1.007316	-1.411485
H	-0.900648	-0.979674	-1.250392
C	-3.388747	1.598199	0.281607
H	-3.733040	0.112582	1.809999
C	-2.660489	1.931045	-0.861227
H	-1.156158	1.276556	-2.270921

H	-4.075167	2.322273	0.725885
H	-2.763358	2.922314	-1.306691

[P, Approximation: A, Orientation: Upward]

C	-0.104037	1.389204	1.521713
C	-0.951897	0.206408	0.948037
O	0.405167	2.105665	0.531590
H	-0.800159	1.932913	2.229380
H	-1.488511	-0.383240	1.705192
S	-4.863187	0.483836	-1.124879
C	-3.510611	0.031449	-0.332331
S	-2.161931	1.076463	-0.119931
Cl	-3.401828	-1.615188	0.328535
H	0.631894	0.868997	2.205615
C	-0.079430	-0.658943	0.054849
H	-0.672699	-1.430327	-0.473701
H	0.378888	0.025556	-0.679023
O	0.900366	-1.276342	0.860435
C	1.992295	-1.781908	0.161179
H	1.666115	-2.227261	-0.801736
H	2.405989	-2.608662	0.762559
C	3.110850	-0.787034	-0.109004
C	2.942117	0.596883	0.020384
C	4.355464	-1.296399	-0.502417
C	4.026133	1.438833	-0.250143
H	1.976383	1.081323	0.284192
C	5.427958	-0.449112	-0.768454
H	4.486541	-2.379564	-0.594171
C	5.263921	0.931206	-0.639834
H	3.876324	2.516166	-0.152031
H	6.391957	-0.865151	-1.070038
H	6.099398	1.604554	-0.844457

[R, Approximation: A, Orientation: Downward]

C	0.397618	2.879318	-1.266025
C	0.872780	2.845108	0.114048
O	0.027043	3.883191	-0.336754
H	1.082378	3.193843	-2.061060
H	1.907021	3.151109	0.318960
S	2.240101	-1.436807	1.584282
C	2.538270	-1.054042	-0.003264
S	1.566843	-0.422730	-1.193892
Cl	4.275971	-1.373720	-0.542734
H	-0.395462	2.180206	-1.543565
C	0.311337	1.869378	1.111478
H	1.037436	1.046098	1.240197
H	0.192793	2.378872	2.091270
O	-0.921428	1.380247	0.663008
C	-1.287747	0.169846	1.277424
H	-1.578750	0.341088	2.334028
H	-0.428340	-0.527126	1.268029
C	-2.442040	-0.428523	0.517523
C	-3.728074	-0.497490	1.054838
C	-2.217982	-0.912255	-0.777866
C	-4.780396	-1.045193	0.317951
H	-3.906618	-0.115030	2.062860
C	-3.266515	-1.454599	-1.515845
H	-1.200347	-0.865004	-1.177201
C	-4.551195	-1.522696	-0.970463
H	-5.781750	-1.094235	0.750787
H	-3.080567	-1.834109	-2.522524
H	-5.371673	-1.950488	-1.550368

[TS, Approximation: A, Orientation: Downward]

C	1.521936	2.747055	-1.226153
C	1.680556	1.729057	-0.154481
O	2.137065	3.655361	-0.450696
H	2.029680	2.439054	-2.175488
H	2.718302	1.443983	0.031565
S	2.735285	-1.185835	1.401031
C	2.001254	-1.368203	-0.057524
S	1.093060	-0.275064	-0.964957
Cl	2.160120	-2.976270	-0.869034
H	0.443318	2.921578	-1.478715
C	0.814222	1.863503	1.077376
H	1.162774	1.157164	1.846809
H	0.957462	2.893135	1.429594
O	-0.558980	1.667232	0.800569
C	-1.124765	0.535479	1.385566
H	-1.389929	0.722591	2.446849
H	-0.407557	-0.308395	1.375206
C	-2.364299	0.122172	0.631379
C	-3.336140	-0.675306	1.243346
C	-2.539697	0.501463	-0.702135
C	-4.460224	-1.097471	0.536022
H	-3.208565	-0.968059	2.289022
C	-3.666334	0.083176	-1.409131
H	-1.777947	1.130465	-1.163908
C	-4.629298	-0.717738	-0.795599
H	-5.209515	-1.721510	1.027379
H	-3.791496	0.385111	-2.450801
H	-5.510038	-1.044002	-1.352093

[P, Approximation: A, Orientation: Downward]

C	1.862801	2.529395	-1.120465
C	1.874854	1.291037	-0.110439
O	2.297086	3.599270	-0.533786
H	2.451352	2.129213	-2.013888
H	2.925380	1.051532	0.113576
S	2.545376	-1.661552	1.250284
C	1.700937	-1.529732	-0.134507
S	1.163704	-0.140663	-0.980313
Cl	1.180150	-2.994207	-1.008141
H	0.784369	2.538489	-1.523273
C	1.163771	1.665543	1.178493
H	1.457513	1.017859	2.021872
H	1.510022	2.698780	1.344660
O	-0.244022	1.684120	1.040129
C	-0.911973	0.563378	1.523235
H	-1.193743	0.696668	2.588874
H	-0.267599	-0.336524	1.483120
C	-2.160717	0.297952	0.714921
C	-3.150209	-0.562577	1.200995
C	-2.329425	0.889205	-0.539683
C	-4.287111	-0.839066	0.444450
H	-3.026040	-1.021147	2.186015
C	-3.469423	0.614862	-1.295359
H	-1.551660	1.563682	-0.902274
C	-4.450300	-0.248980	-0.809485
H	-5.050393	-1.514856	0.835750
H	-3.590026	1.081658	-2.274874
H	-5.340736	-0.461621	-1.404364

[R, Approximation: B, Orientation: Upward]

C	-0.293356	0.986012	0.306222
C	0.658213	1.722282	-0.524061
O	-0.629905	1.384876	-1.019099
H	1.495846	1.169078	-0.963616
S	3.235775	-0.870618	-1.273234
C	3.909982	-0.148927	0.063407
Cl	5.760703	-0.172751	0.070021
S	3.239554	0.594601	1.386240
H	-0.850730	1.526350	1.083424
C	-0.114780	-0.485692	0.551354
H	0.469756	-0.621307	1.471103
H	0.480188	-0.920122	-0.272461
O	-1.347828	-1.155170	0.732527
C	-2.134046	-1.279532	-0.430129
H	-2.276982	-2.353112	-0.649150
H	-1.630047	-0.815738	-1.292186
C	-3.487942	-0.633430	-0.231942
C	-4.553668	-1.371558	0.290968
C	-3.682475	0.723373	-0.519100
C	-5.792953	-0.775092	0.521975
H	-4.404212	-2.429489	0.520648
C	-4.920752	1.321692	-0.289271
H	-2.847736	1.303578	-0.921412
C	-5.979087	0.575709	0.231085
H	-6.615474	-1.365928	0.930073
H	-5.060888	2.379657	-0.519694
H	-6.947916	1.046660	0.408880
H	0.818029	2.786762	-0.324530

[TS, Approximation: B, Orientation: Upward]

C	-0.298311	0.567628	0.993024
C	1.078690	1.051804	0.975983
O	-0.300486	0.760993	-0.373549
H	1.912087	0.532390	1.463104
S	2.414301	0.351219	-0.938547
C	3.919493	0.131598	-0.237657
Cl	5.047355	-0.908480	-1.227285
S	4.495279	0.677711	1.208350
H	-1.035180	1.183455	1.565616
C	-0.451618	-0.882946	1.435792
H	-0.197621	-0.980058	2.504180
H	0.263981	-1.490306	0.846762
O	-1.765132	-1.371916	1.305649
C	-2.241947	-1.489763	-0.020987
H	-2.523750	-2.544419	-0.195164
H	-1.456956	-1.195644	-0.733151
C	-3.458974	-0.615081	-0.230703
C	-4.746918	-1.140731	-0.099707
C	-3.304681	0.748383	-0.519563
C	-5.871301	-0.328308	-0.253923
H	-4.867941	-2.203321	0.127385
C	-4.428262	1.559090	-0.671751
H	-2.282567	1.138152	-0.629146
C	-5.712675	1.026412	-0.540015
H	-6.871745	-0.753841	-0.150020
H	-4.300660	2.619235	-0.900957
H	-6.588818	1.666760	-0.663212
H	1.214828	2.127757	0.871847

[P, Approximation: B, Orientation: Upward]

C	0.000178	0.741426	0.687182
C	-1.530640	0.857945	0.930871

O	0.350288	-0.546501	0.627085
H	-2.023705	1.785452	0.600690
S	-2.209101	-0.547261	-0.011717
C	-3.890828	-0.198622	0.030778
Cl	-4.755190	-1.447583	-0.909638
S	-4.735382	0.980265	0.773037
H	0.475756	1.332919	1.526013
C	0.352563	1.542328	-0.585079
H	0.052688	2.600392	-0.482784
H	-0.201520	1.107643	-1.444550
O	1.737099	1.555121	-0.842992
C	2.266031	0.353044	-1.360621
H	2.543559	0.505698	-2.423706
H	1.516773	-0.446155	-1.272751
C	3.495489	-0.054106	-0.581606
C	4.779700	0.115963	-1.101770
C	3.339291	-0.591627	0.705869
C	5.906314	-0.245253	-0.358320
H	4.898860	0.539210	-2.103123
C	4.464806	-0.948634	1.444955
H	2.303914	-0.722474	1.061731
C	5.749446	-0.777237	0.919372
H	6.905839	-0.107156	-0.777116
H	4.341550	-1.372076	2.444607
H	6.626473	-1.060838	1.506012
H	-1.783427	0.677883	1.985153

[R, Approximation: B, Orientation: Downward]

C	0.156793	2.299509	-0.208077
C	0.896583	1.988135	-1.425771
O	-0.480486	2.337042	-1.473547
H	1.141999	0.938433	-1.623379
H	1.585024	2.736764	-1.830396
S	3.373850	0.878210	0.657114
C	3.215111	-0.651933	0.034391
Cl	4.804160	-1.602456	-0.038783
S	1.903481	-1.495005	-0.538537
H	0.288984	3.282563	0.261414
C	-0.270098	1.202412	0.714313
H	0.517680	1.023988	1.467827
H	-0.383202	0.269544	0.136035
O	-1.489805	1.593892	1.327889
C	-2.234854	0.531785	1.826918
H	-2.919215	0.943950	2.587438
H	-1.588228	-0.206350	2.341189
C	-3.063222	-0.182490	0.772875
C	-3.824060	-1.301345	1.128400
C	-3.100681	0.276292	-0.545942
C	-4.618717	-1.950212	0.186944
H	-3.789409	-1.669156	2.157943
C	-3.891183	-0.380605	-1.490640
H	-2.487147	1.132546	-0.834981
C	-4.654783	-1.489025	-1.129988
H	-5.206234	-2.823123	0.478505
H	-3.901565	-0.021608	-2.521399
H	-5.269694	-1.999699	-1.873399

[TS, Approximation: B, Orientation: Downward]

C	-0.251933	1.880556	-0.328225
C	-1.294579	1.822411	0.715731
O	0.563556	2.402641	0.618637
H	-1.166378	1.047716	1.472439

H	-1.677146	2.787982	1.041137
S	-3.301547	1.103890	-0.017850
C	-3.282044	-0.553170	0.311835
Cl	-4.784406	-1.371558	-0.288040
S	-2.163911	-1.491078	1.054953
H	-0.512368	2.544715	-1.188293
C	0.160257	0.529841	-0.889552
H	-0.677540	0.043584	-1.427513
H	0.450941	-0.118454	-0.043687
O	1.251023	0.735864	-1.770735
C	2.134137	-0.330219	-1.861773
H	2.699477	-0.203095	-2.800832
H	1.595217	-1.296576	-1.943487
C	3.128381	-0.412493	-0.715209
C	4.067968	-1.449451	-0.694428
C	3.136175	0.545222	0.303570
C	5.015286	-1.532781	0.322965
H	4.056083	-2.201452	-1.489462
C	4.083799	0.451165	1.326055
H	2.379054	1.341521	0.318946
C	5.025483	-0.576488	1.339972
H	5.743974	-2.346353	0.326046
H	4.074621	1.195229	2.125077
H	5.762069	-0.638911	2.143797

[P, Approximation: B, Orientation: Downward]

C	0.267417	1.724105	0.371730
C	1.517697	1.699241	-0.589386
O	-0.684521	2.400934	-0.222861
H	1.302027	1.109207	-1.491426
H	1.692462	2.745076	-0.873833
S	3.109318	1.141668	0.105897
C	3.279355	-0.496316	-0.380638
Cl	4.772188	-1.155151	0.339885
S	2.334455	-1.424461	-1.315127
H	0.664160	2.148307	1.352510
C	-0.100318	0.265147	0.717959
H	0.769926	-0.327982	1.068965
H	-0.493948	-0.203870	-0.203733
O	-1.087009	0.281711	1.733759
C	-2.010846	-0.748822	1.673666
H	-2.484514	-0.817157	2.668586
H	-1.518535	-1.727624	1.490493
C	-3.106828	-0.545689	0.639853
C	-4.091026	-1.528018	0.480435
C	-3.157129	0.620896	-0.131532
C	-5.129044	-1.355702	-0.432488
H	-4.043124	-2.440655	1.083345
C	-4.197560	0.780147	-1.051550
H	-2.357498	1.381966	-0.044275
C	-5.184301	-0.193322	-1.203894
H	-5.892737	-2.128700	-0.545602
H	-4.225746	1.685551	-1.661872
H	-5.992307	-0.053002	-1.925625

Neutral reaction (using $N(CH_3)_4^+$ as a counter cation):

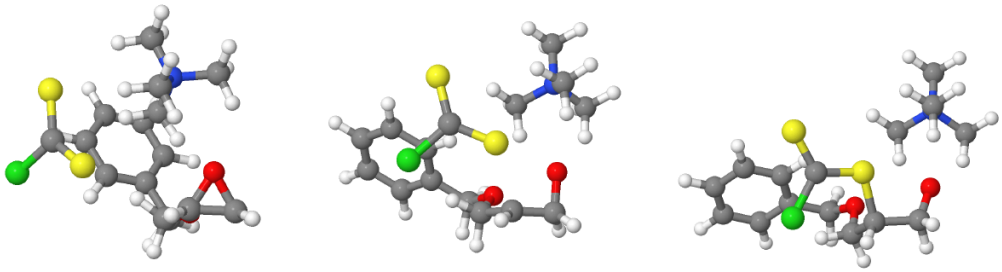


Figure S11. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_A).

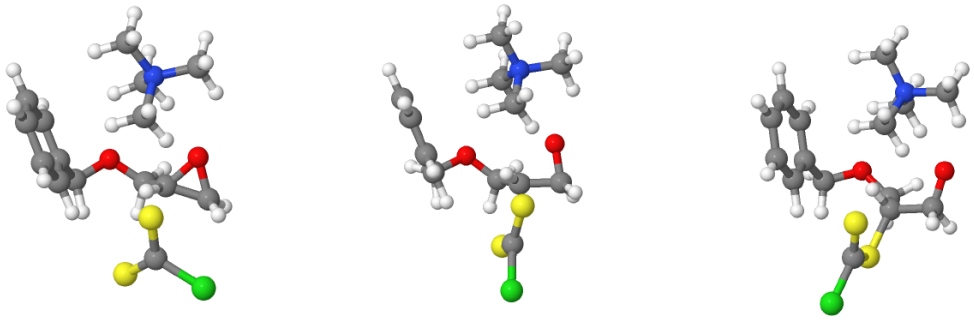


Figure S12. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_A).

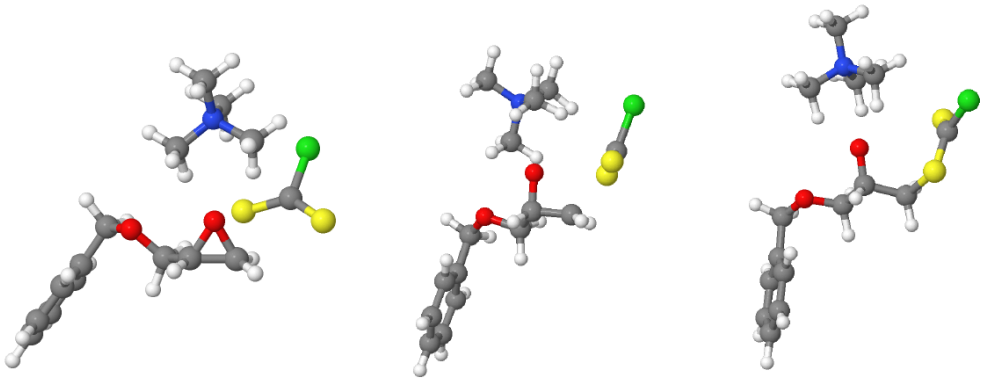


Figure S13. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_B).

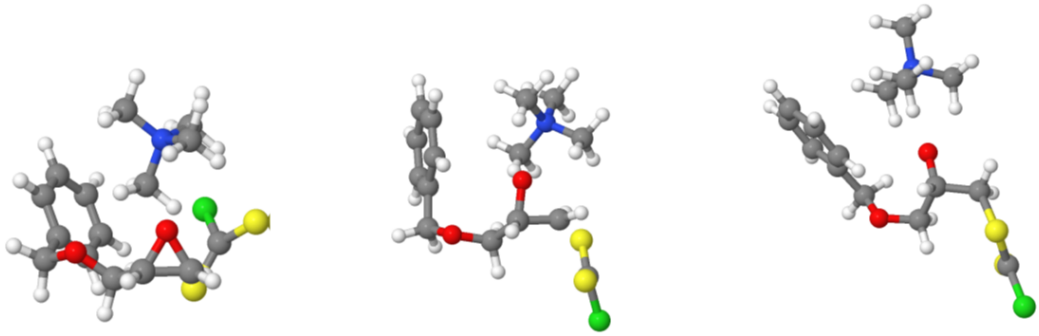


Figure S14. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	57.0	13.3
A	downward	0.0	23.6	3.8
B	upward	0.0	53.9	4.0
B	downward	0.0	32.9	6.5

Table S2. Energies of the reactants (R), transition state (TS) and products (P) involved in the gas-phase reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

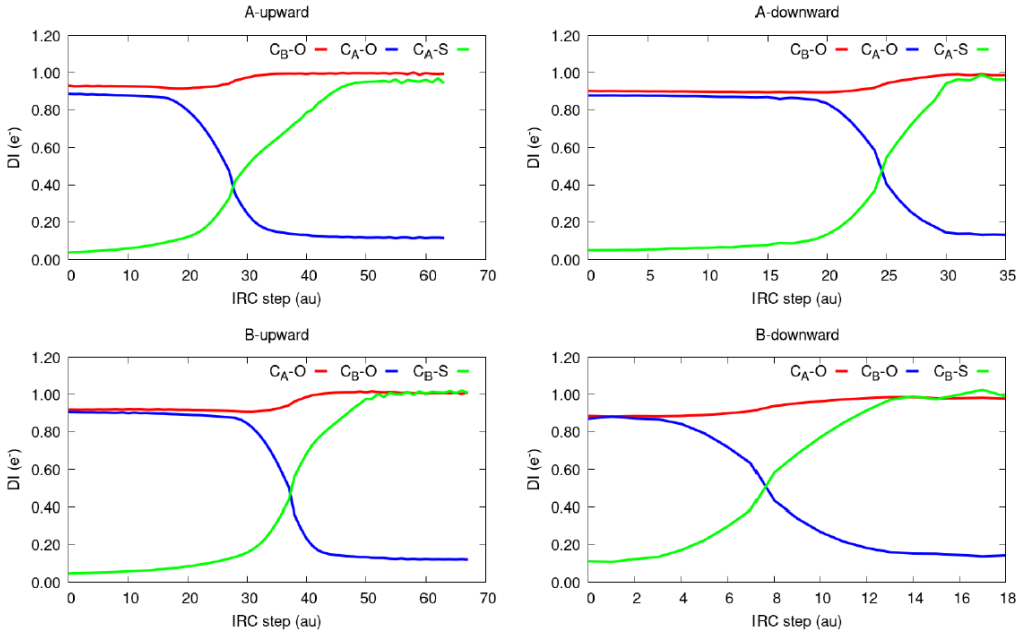


Figure S15. Evolution of the electron delocalization (DI) across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- + $N(CH_3)_4^+$ to R1i. The results for different spatial approximations are shown. All values are reported in electron pairs.

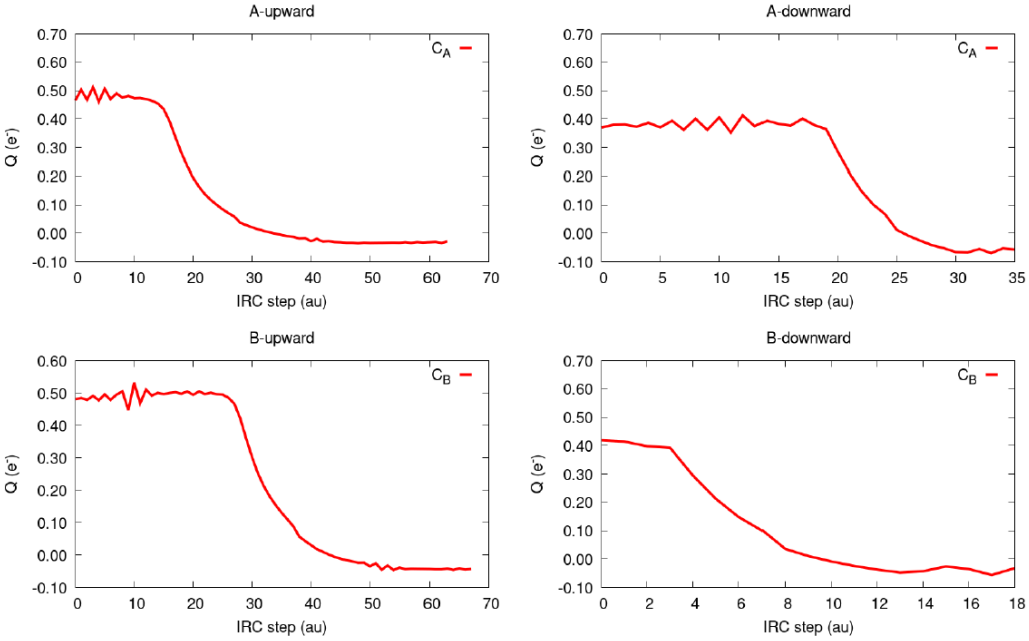


Figure S16. Evolution of the atomic charges (Q) of the electrophilic carbon across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- + $N(CH_3)_4^+$ to R1i. The results for different spatial approximations are shown. All values are reported in electrons.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A, Orientation: Upward]

C	-3.942144	0.673425	-1.656523
C	-2.511234	0.687494	-1.977280
O	-2.987114	1.164414	-0.729488
H	-4.602844	1.430508	-2.088931
H	-2.120487	1.469483	-2.638725
S	2.816554	1.422940	0.593854
C	2.298341	1.097788	-0.957553
S	1.012978	1.697642	-1.824086
Cl	3.314659	-0.121358	-1.847162
H	-4.395719	-0.280985	-1.377328
C	-1.686582	-0.571383	-1.970238
H	-1.603807	-0.935123	-3.013618
H	-0.666515	-0.319782	-1.633387
O	-2.291564	-1.533519	-1.149855
C	-1.550256	-2.733509	-1.042946
H	-1.128018	-2.999571	-2.028672
H	-2.271596	-3.513055	-0.761460
C	-0.449518	-2.666827	-0.007352
C	0.814446	-2.143361	-0.311149
C	-0.700583	-3.110989	1.296727
C	1.799002	-2.043377	0.673912
H	1.051792	-1.802929	-1.323483
C	0.284282	-3.026413	2.280487
H	-1.678690	-3.534746	1.538070
C	1.532794	-2.483254	1.970746
H	2.765779	-1.605975	0.418630
H	0.079284	-3.390549	3.289110
H	2.305867	-2.410623	2.737586
C	-0.610835	0.364410	1.231192
H	0.349635	0.473930	0.714074
H	-0.548853	-0.436598	1.978463
N	-0.899335	1.652608	1.942659
C	-0.761973	2.793243	0.984504
H	-0.993095	3.719571	1.525771
H	0.265452	2.793214	0.596079
H	-1.468734	2.629887	0.163266
C	-2.285347	1.611275	2.473995
H	-2.965993	1.501149	1.621274
H	-2.377305	0.751655	3.148718
H	-2.487348	2.542446	3.017349
C	0.083313	1.828899	3.046395
H	1.085144	1.834410	2.596736
H	-0.121675	2.780100	3.552525
H	-0.020881	0.992236	3.747285
H	-1.430584	0.165172	0.532767

[TS, Approximation: A, Orientation: Upward]

C	1.890322	-1.501793	2.673906
C	0.718239	-0.611183	2.650835
O	2.347416	-1.052642	1.458828
H	2.565546	-1.306143	3.531950
H	0.585956	0.179977	3.389111
S	0.018600	2.883395	-1.031726
C	-0.014214	2.259265	0.501896
S	1.253346	1.515276	1.308223
Cl	-1.568059	2.350632	1.401061
H	1.596724	-2.574745	2.707366
C	-0.553108	-1.065431	2.029080

H	-1.073232	-1.601449	2.860473
H	-1.193380	-0.212051	1.754179
O	-0.337138	-1.939548	0.961196
C	-1.499966	-2.543929	0.462549
H	-2.062708	-3.036202	1.279658
H	-1.154706	-3.340685	-0.214713
C	-2.421815	-1.602580	-0.287528
C	-1.975736	-0.354970	-0.725820
C	-3.736851	-1.989575	-0.565973
C	-2.828919	0.504171	-1.418551
H	-0.959002	-0.034113	-0.490972
C	-4.584983	-1.144766	-1.277917
H	-4.101469	-2.959973	-0.218267
C	-4.133744	0.106831	-1.702036
H	-2.459927	1.490916	-1.707941
H	-5.608750	-1.457645	-1.490217
H	-4.805315	0.776022	-2.241941
C	1.409617	-0.583377	-1.382109
H	1.014480	0.423194	-1.582784
H	0.945994	-1.324853	-2.046519
N	2.883272	-0.574145	-1.659511
C	3.539710	0.492524	-0.838489
H	4.598020	0.533462	-1.127251
H	3.028611	1.442651	-1.037402
H	3.406402	0.214859	0.216094
C	3.445449	-1.895379	-1.258486
H	3.222708	-2.013384	-0.185356
H	2.958957	-2.676590	-1.855256
H	4.525972	-1.889680	-1.448986
C	3.116161	-0.308563	-3.098567
H	2.683692	0.668945	-3.343797
H	4.195296	-0.304349	-3.294487
H	2.628282	-1.091993	-3.690559
H	1.281622	-0.856593	-0.324720

[P, Approximation: A, Orientation: Upward]

C	1.777844	0.954435	2.442646
C	0.312942	1.033144	1.920444
O	2.611527	0.384168	1.554455
H	2.051543	2.006696	2.713329
H	-0.247688	1.822633	2.442175
S	-1.178601	2.544120	-1.979587
C	-0.980486	2.149296	-0.414608
S	0.534895	1.555458	0.171278
Cl	-2.300056	2.332121	0.730731
H	1.692905	0.420632	3.426009
C	-0.492224	-0.253368	2.023027
H	-0.456441	-0.587275	3.079351
H	-1.548430	-0.053278	1.771688
O	0.017367	-1.262135	1.185047
C	-0.852510	-2.349121	1.032217
H	-1.159096	-2.754894	2.015578
H	-0.270769	-3.135861	0.525414
C	-2.086062	-2.015980	0.214532
C	-2.013475	-1.046872	-0.791069
C	-3.302180	-2.660878	0.449911
C	-3.142051	-0.716727	-1.538611
H	-1.066006	-0.531378	-0.963504
C	-4.427773	-2.349062	-0.312739
H	-3.373110	-3.407833	1.244815
C	-4.351384	-1.371911	-1.304436
H	-3.073754	0.067616	-2.295079

H	-5.373057	-2.858761	-0.118815
H	-5.236519	-1.113445	-1.887611
C	2.438586	-1.397989	-0.716532
H	1.809156	-1.106190	-1.566815
H	2.514594	-2.491200	-0.653170
N	3.816947	-0.852377	-0.940921
C	3.731421	0.638821	-1.061779
H	4.739232	1.021189	-1.267591
H	3.051116	0.879784	-1.888018
H	3.330872	0.987641	-0.088088
C	4.646928	-1.176603	0.261902
H	4.133761	-0.705566	1.122403
H	4.696662	-2.268378	0.358245
H	5.652059	-0.765189	0.105242
C	4.413223	-1.436405	-2.162570
H	3.784017	-1.178310	-3.022860
H	5.421552	-1.027766	-2.301743
H	4.463273	-2.526380	-2.051517
H	2.077814	-0.948097	0.227508

[R, Approximation: A, Orientation: Downward]

C	1.823493	-1.995519	1.297278
C	0.846198	-0.912918	1.383750
O	0.440698	-2.252663	1.075081
H	2.464346	-2.049194	0.411518
H	0.793740	-0.223740	0.531230
S	1.745037	0.047641	-1.883727
C	2.943801	0.415436	-0.779907
S	2.981122	1.504436	0.471932
Cl	4.451028	-0.593072	-0.952392
H	2.224517	-2.428457	2.219923
C	0.391567	-0.343097	2.699011
H	0.187049	-1.164756	3.403090
H	1.205991	0.277667	3.112191
O	-0.791548	0.414011	2.570667
C	-0.600983	1.744941	2.108886
H	0.470968	1.956836	1.966911
H	-0.993250	2.427388	2.881762
C	-1.319426	1.994956	0.802823
C	-2.719976	1.943699	0.745150
C	-0.598635	2.262196	-0.364746
C	-3.388245	2.148909	-0.461261
H	-3.286306	1.754717	1.661674
C	-1.267867	2.467710	-1.574818
H	0.495530	2.276193	-0.335171
C	-2.659086	2.410683	-1.627338
H	-4.480176	2.127959	-0.491531
H	-0.683125	2.650958	-2.477513
H	-3.180651	2.580090	-2.571284
C	-1.341696	-1.102548	-1.209243
H	-1.348865	-1.251859	-2.295797
H	-0.385736	-1.432005	-0.792233
N	-2.436996	-1.935157	-0.608479
C	-2.116400	-3.372315	-0.824557
H	-1.152967	-3.570003	-0.338435
H	-2.909721	-3.985498	-0.380187
H	-2.047275	-3.561021	-1.902272
C	-3.727441	-1.577517	-1.251083
H	-3.652755	-1.769017	-2.327896
H	-4.528744	-2.184131	-0.812367
H	-3.909809	-0.510277	-1.072821
C	-2.525303	-1.673026	0.862494

H	-1.612927	-2.053457	1.331886
H	-2.589967	-0.592344	1.028965
H	-3.411808	-2.190572	1.249113
H	-1.528300	-0.050704	-0.966651

[TS, Approximation: A, Orientation: Downward]

C	-0.811432	-2.735272	-0.425740
C	-0.661043	-1.378400	-0.962183
O	0.563754	-2.675186	-0.330554
H	-1.371229	-2.786531	0.524848
H	-0.412421	-0.610362	-0.231955
S	-1.912000	-0.124277	1.849494
C	-3.020652	-0.090824	0.626651
S	-2.831505	-0.417901	-1.024747
Cl	-4.686839	0.371051	1.053997
H	-1.213821	-3.476360	-1.143566
C	-0.203546	-1.195988	-2.392102
H	0.278413	-2.131848	-2.704478
H	-1.067619	-1.014909	-3.055577
O	0.754717	-0.176668	-2.551226
C	0.259928	1.148712	-2.531107
H	-0.840553	1.155130	-2.597700
H	0.661623	1.663868	-3.419078
C	0.692589	1.896294	-1.287918
C	2.012269	2.352864	-1.165624
C	-0.197431	2.118766	-0.234279
C	2.435105	3.008743	-0.009792
H	2.708300	2.201651	-1.995600
C	0.220475	2.775852	0.925546
H	-1.226874	1.763285	-0.320984
C	1.536647	3.220113	1.041203
H	3.460958	3.376269	0.065161
H	-0.491156	2.924268	1.739246
H	1.862193	3.741420	1.943121
C	1.732145	-0.534647	1.482079
H	1.781231	-0.495606	2.577251
H	0.926501	-1.194920	1.140364
N	3.014590	-1.121340	0.973453
C	3.080908	-2.550791	1.396965
H	2.212551	-3.053973	0.944247
H	4.025011	-2.978029	1.037398
H	3.038978	-2.591820	2.492204
C	4.160352	-0.351361	1.513082
H	4.152289	-0.416328	2.607666
H	5.093529	-0.770189	1.117552
H	4.049536	0.694219	1.198961
C	3.029713	-1.065621	-0.523352
H	2.179229	-1.659653	-0.882150
H	2.910112	-0.021964	-0.831560
H	3.989573	-1.471659	-0.866216
H	1.619939	0.474570	1.066448

[P, Approximation: A, Orientation: Downward]

C	0.599033	-2.643240	0.407913
C	0.821268	-1.194339	0.951404
O	-0.710255	-2.848615	0.215451
H	1.241644	-2.732394	-0.504057
H	0.307175	-0.494408	0.278688
S	1.813745	-0.194765	-1.960336
C	2.853223	-0.257519	-0.718183
S	2.580226	-0.693838	0.934531
Cl	4.540557	0.202715	-0.913157

H	1.085540	-3.320364	1.164047
C	0.248467	-1.053134	2.367290
H	-0.400313	-1.925581	2.526225
H	1.053182	-1.082788	3.128285
O	-0.578015	0.070020	2.580295
C	0.025471	1.337885	2.455513
H	1.125681	1.260909	2.453233
H	-0.267623	1.932195	3.336678
C	-0.443161	2.045616	1.201365
C	-1.781839	2.446468	1.091999
C	0.415482	2.269927	0.124164
C	-2.250640	3.051309	-0.072822
H	-2.455513	2.286206	1.938059
C	-0.050489	2.868461	-1.048909
H	1.461257	1.962979	0.201699
C	-1.384299	3.258394	-1.150788
H	-3.291132	3.377148	-0.137923
H	0.635245	3.020868	-1.883986
H	-1.748341	3.733377	-2.063279
C	-1.778986	-0.608049	-1.433616
H	-1.915958	-0.585778	-2.522319
H	-1.010420	-1.334189	-1.124345
N	-3.048129	-1.100208	-0.809009
C	-3.243507	-2.523327	-1.224969
H	-2.348780	-3.069815	-0.874414
H	-4.161070	-2.896885	-0.753649
H	-3.340135	-2.553210	-2.317597
C	-4.185131	-0.253310	-1.230788
H	-4.281550	-0.296383	-2.322672
H	-5.103174	-0.622916	-0.757883
H	-3.983877	0.777518	-0.912819
C	-2.899013	-1.067771	0.683232
H	-2.066999	-1.768464	0.904939
H	-2.640896	-0.047319	0.987563
H	-3.853342	-1.383405	1.123960
H	-1.565811	0.400181	-1.051638

[R, Approximation: B, Orientation: Upward]

C	0.807469	-0.244124	-2.328712
C	-0.411536	-1.020010	-2.598686
O	-0.467920	0.364441	-2.298152
H	-0.820882	-1.678819	-1.822553
S	-3.421834	-2.307464	-0.986115
C	-2.953414	-1.678062	0.456005
Cl	-4.335787	-0.985568	1.479848
S	-1.440984	-1.482512	1.151790
H	1.433256	0.075251	-3.171026
C	1.500681	-0.375931	-1.007845
H	2.368211	-1.053199	-1.111277
H	0.800388	-0.819547	-0.275857
O	1.917817	0.905029	-0.577879
C	2.565924	0.877016	0.667311
H	1.950080	0.340234	1.415332
H	2.647643	1.926680	0.992267
C	3.947832	0.259952	0.609399
C	4.439207	-0.507643	1.666816
C	4.758279	0.478717	-0.509528
C	5.728867	-1.037433	1.617047
H	3.804612	-0.699287	2.535489
C	6.042812	-0.056707	-0.564645
H	4.361824	1.065619	-1.340783
C	6.532942	-0.813008	0.501215

H	6.101868	-1.636984	2.448811
H	6.666587	0.116201	-1.443202
H	7.539020	-1.232757	0.458078
H	-0.658087	-1.278476	-3.632898
C	-0.706683	2.107370	0.117340
H	-0.238518	2.814447	0.813417
H	-0.388504	2.286810	-0.913684
N	-2.190986	2.260365	0.212542
C	-2.582245	3.656540	-0.099140
H	-3.675778	3.730586	-0.069799
H	-2.139951	4.328309	0.646106
H	-2.215100	3.911270	-1.099925
C	-2.622884	1.914237	1.600608
H	-2.132569	2.610593	2.292043
H	-3.713107	2.003298	1.663798
H	-2.327121	0.875315	1.807531
C	-2.835384	1.328827	-0.771288
H	-2.643311	1.710220	-1.779854
H	-2.365057	0.347343	-0.670427
H	-3.906886	1.263676	-0.548448
H	-0.468609	1.070718	0.383714

[TS, Approximation: B, Orientation: Upward]

C	-0.498350	-1.062377	1.227663
C	0.307838	-2.258229	0.941347
O	0.628289	-0.311393	1.438922
H	0.410093	-2.592369	-0.094421
S	2.706562	-2.222574	0.932774
C	3.028006	-1.502209	-0.537634
Cl	4.731466	-0.858365	-0.626542
S	2.074303	-1.229313	-1.855974
H	-1.159769	-1.168110	2.119951
C	-1.366247	-0.628221	0.053851
H	-2.212992	-1.330669	-0.072928
H	-0.760347	-0.646534	-0.874466
O	-1.844109	0.680287	0.290025
C	-2.810987	1.097307	-0.629908
H	-2.482837	0.897356	-1.668687
H	-2.897448	2.190763	-0.518349
C	-4.171347	0.468166	-0.400055
C	-5.077565	0.316045	-1.451965
C	-4.545092	0.064144	0.884942
C	-6.345002	-0.218619	-1.223676
H	-4.787126	0.614849	-2.462479
C	-5.808365	-0.478282	1.113107
H	-3.825238	0.172001	1.698696
C	-6.713317	-0.617475	0.060569
H	-7.044082	-0.333267	-2.053686
H	-6.088832	-0.795077	2.119086
H	-7.702077	-1.042460	0.239756
H	0.400931	-3.031892	1.704854
C	0.872752	1.940135	-0.240978
H	0.575806	2.620353	-1.050166
H	0.154482	1.930091	0.583792
N	2.208791	2.394984	0.261348
C	2.091894	3.784367	0.767979
H	3.079058	4.131192	1.095978
H	1.713450	4.428287	-0.034653
H	1.392532	3.786755	1.611629
C	3.189655	2.340471	-0.859374
H	2.883749	3.061869	-1.626846
H	4.184858	2.590179	-0.472378

H	3.192211	1.322597	-1.271269
C	2.678686	1.509043	1.376176
H	1.870288	1.400246	2.106316
H	2.876527	0.510306	0.979693
H	3.587798	1.958646	1.794385
H	0.979886	0.905646	-0.584659

[P, Approximation: B, Orientation: Upward]

C	0.303534	-0.571351	-0.319227
C	-0.190317	-1.939712	0.233955
O	-0.654669	0.361072	-0.273018
H	-0.444716	-1.864749	1.301459
S	-1.693984	-2.432681	-0.643816
C	-2.975398	-1.800968	0.319336
Cl	-4.483969	-1.958337	-0.601798
S	-2.983461	-1.177919	1.812861
H	0.679969	-0.781517	-1.358185
C	1.548929	-0.188943	0.487313
H	2.300690	-1.004014	0.487317
H	1.245243	0.004107	1.536546
O	2.098973	0.982151	-0.069883
C	3.266140	1.411018	0.559286
H	3.141134	1.438309	1.659960
H	3.438660	2.447855	0.226712
C	4.486174	0.576974	0.214550
C	5.577550	0.507767	1.083638
C	4.544255	-0.104537	-1.004612
C	6.716056	-0.219204	0.737460
H	5.534524	1.026272	2.045070
C	5.677850	-0.838571	-1.348867
H	3.680479	-0.056388	-1.670888
C	6.768707	-0.895148	-0.480891
H	7.561939	-0.265235	1.425525
H	5.710894	-1.370634	-2.301292
H	7.655970	-1.469894	-0.751029
H	0.522156	-2.764232	0.079185
C	-1.463049	3.001075	-0.973433
H	-1.096417	3.909266	-0.478755
H	-1.725085	3.217827	-2.016616
N	-2.706831	2.557344	-0.264189
C	-3.722659	3.633297	-0.268413
H	-4.623773	3.273688	0.242862
H	-3.320020	4.509213	0.254651
H	-3.962170	3.895521	-1.306068
C	-2.339178	2.192142	1.141179
H	-1.930127	3.086759	1.627744
H	-3.246458	1.852420	1.655939
H	-1.589032	1.381897	1.049728
C	-3.242567	1.335988	-0.950109
H	-3.546503	1.621360	-1.965124
H	-2.409265	0.605186	-0.946831
H	-4.104821	0.967370	-0.379417
H	-0.749430	2.154772	-0.887125

[R, Approximation: B, Orientation: Downward]

C	-0.280438	-3.375569	-0.309461
C	1.180250	-3.257612	-0.425393
O	0.503260	-2.914502	0.771881
H	1.613641	-2.415500	-0.981613
H	1.789253	-4.164739	-0.366577
S	1.307010	0.013622	-2.550247
C	2.186857	0.618038	-1.292000

Cl	1.815096	2.387328	-0.874556
S	3.328334	-0.094116	-0.307011
H	-0.726951	-4.363987	-0.147283
C	-1.171298	-2.362172	-0.962818
H	-1.496120	-2.743162	-1.951032
H	-0.593087	-1.438128	-1.141504
O	-2.291339	-2.135159	-0.138263
C	-3.260037	-1.275936	-0.702358
H	-4.186977	-1.447509	-0.137821
H	-3.442037	-1.558925	-1.755578
C	-2.869621	0.183372	-0.620207
C	-2.029393	0.754768	-1.582004
C	-3.278968	0.964982	0.466745
C	-1.572567	2.065706	-1.447216
H	-1.696910	0.167268	-2.440347
C	-2.847999	2.286038	0.593600
H	-3.944832	0.531594	1.217843
C	-1.984170	2.834559	-0.358512
H	-0.866022	2.463084	-2.176860
H	-3.190264	2.892533	1.435105
H	-1.629569	3.861327	-0.252956
N	0.539807	0.296872	2.428795
C	1.432506	1.492486	2.369772
H	0.842154	2.350185	2.027303
H	2.235141	1.288876	1.646058
H	1.837720	1.668999	3.374032
C	1.336092	-0.886843	2.865768
H	1.701575	-0.704245	3.883840
H	2.169177	-1.001401	2.160075
H	0.702344	-1.778135	2.811678
C	-0.033940	0.028642	1.069989
H	-0.423203	0.971178	0.668514
H	-0.825700	-0.723567	1.166783
H	0.770632	-0.358382	0.438287
C	-0.574841	0.547382	3.375634
H	-0.162740	0.809290	4.357707
H	-1.184119	-0.361074	3.447298
H	-1.183864	1.369897	2.980869

[TS, Approximation: B, Orientation: Downward]

C	-0.542054	0.982457	1.892044
C	-1.456651	-0.153447	1.756277
O	0.376556	-0.043098	2.030570
H	-1.419842	-0.707594	0.821058
H	-1.777660	-0.658128	2.665993
S	-3.625256	0.467132	1.110135
C	-3.625238	-0.077912	-0.486183
Cl	-5.065200	0.447736	-1.392917
S	-2.536243	-1.005119	-1.330144
H	-0.680724	1.607321	2.794291
C	-0.422719	1.864196	0.668095
H	-1.375461	2.401011	0.509255
H	-0.252941	1.223518	-0.217009
O	0.630542	2.789450	0.838614
C	1.390171	3.025459	-0.305803
H	1.867594	4.010281	-0.174705
H	0.759045	3.092881	-1.211489
C	2.482095	1.991866	-0.508054
C	2.991006	1.712697	-1.779832
C	3.043835	1.359807	0.606853
C	4.066767	0.837396	-1.939251
H	2.546186	2.192264	-2.655471

C	4.131865	0.502730	0.449773
H	2.602460	1.540922	1.588337
C	4.648810	0.238092	-0.821060
H	4.459187	0.633995	-2.937193
H	4.585850	0.042103	1.330116
H	5.508856	-0.424126	-0.939702
N	1.388335	-2.561776	0.117587
C	1.859149	-3.623242	-0.804354
H	2.779684	-3.282566	-1.293007
H	1.081790	-3.804795	-1.555895
H	2.050681	-4.539044	-0.232077
C	0.104446	-2.973367	0.762671
H	0.234186	-3.979218	1.180675
H	-0.697161	-2.952742	0.012324
H	-0.104601	-2.238001	1.547810
C	1.181394	-1.283764	-0.639584
H	2.135412	-0.996038	-1.101381
H	0.870969	-0.540816	0.109615
H	0.398147	-1.443701	-1.390447
C	2.394255	-2.313675	1.192534
H	2.483911	-3.222722	1.800343
H	2.027980	-1.463786	1.788933
H	3.350909	-2.068884	0.718026

[P, Approximation: B, Orientation: Downward]

C	0.751043	0.140439	0.364432
C	1.911285	1.162022	0.255361
O	-0.381981	0.699417	-0.117020
H	2.163539	1.361580	-0.796416
H	1.572321	2.097094	0.723278
S	3.437707	0.735804	1.144768
C	4.490152	0.092410	-0.072936
Cl	6.002987	-0.375446	0.697826
S	4.255457	-0.096486	-1.661526
H	0.685170	-0.134359	1.454086
C	1.124232	-1.162230	-0.349905
H	2.066812	-1.578474	0.039958
H	1.261237	-0.951271	-1.427361
O	0.140301	-2.157542	-0.159034
C	-0.957051	-2.119002	-1.018453
H	-0.971380	-3.031537	-1.645204
H	-0.888140	-1.248666	-1.694115
C	-2.271419	-2.028230	-0.276336
C	-3.469972	-2.335295	-0.929193
C	-2.313911	-1.591516	1.049662
C	-4.695571	-2.188685	-0.279194
H	-3.442241	-2.697201	-1.960772
C	-3.537901	-1.452824	1.704542
H	-1.369678	-1.366503	1.546190
C	-4.733784	-1.742181	1.043050
H	-5.622003	-2.437330	-0.800335
H	-3.559452	-1.124635	2.746335
H	-5.688983	-1.642704	1.561894
N	-2.975279	2.338552	-0.234538
C	-4.229721	3.122692	-0.271785
H	-5.033424	2.525686	0.175683
H	-4.475237	3.356996	-1.314772
H	-4.090334	4.049959	0.297111
C	-1.848771	3.106031	-0.850677
H	-1.715744	4.036818	-0.285071
H	-2.115037	3.330843	-1.890936
H	-0.963013	2.445783	-0.778810

C	-3.138001	1.055259	-0.990862
H	-3.920682	0.458958	-0.503469
H	-2.161074	0.546710	-0.929590
H	-3.422040	1.300181	-2.022150
C	-2.604034	2.003882	1.177629
H	-2.472963	2.944415	1.727772
H	-1.661460	1.421373	1.089154
H	-3.416648	1.408256	1.610814

Neutral reaction (using Choline as a counter cation):

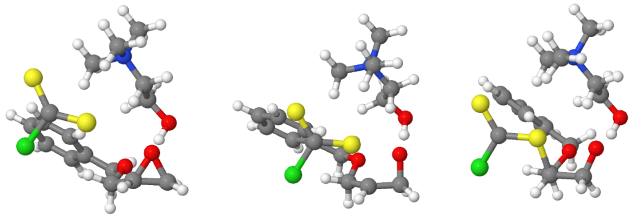


Figure S17. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_A).

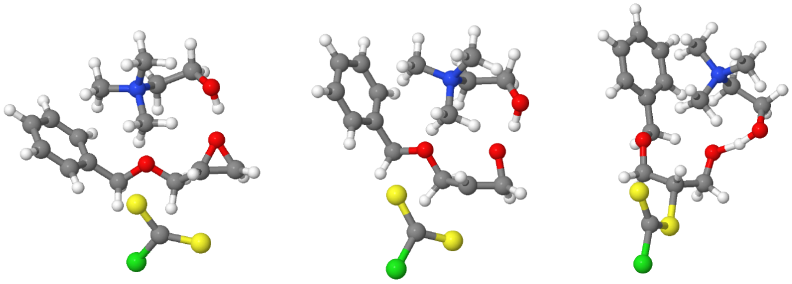


Figure S18. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_A).

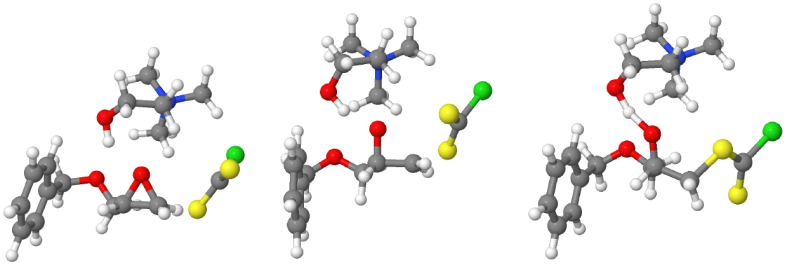


Figure S19. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_B).

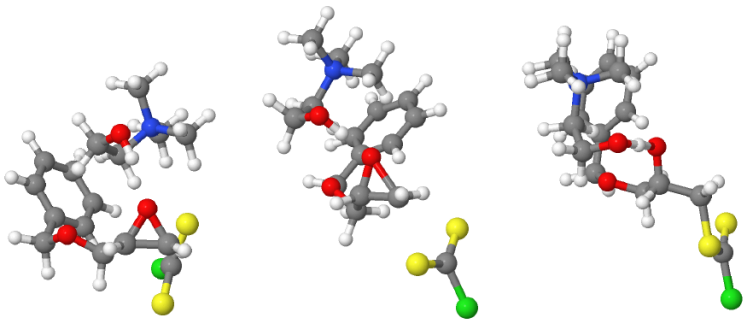


Figure S20. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	49.4	9.4
A	downward	0.0	22.6	-4.9
B	upward	0.0	47.0	-1.9
B	downward	0.0	29.5	-2.9

Table S3. Energies of the reactants (R), transition state (TS) and products (P) involved in the gas-phase reaction between CS_2Cl^- + Choline and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

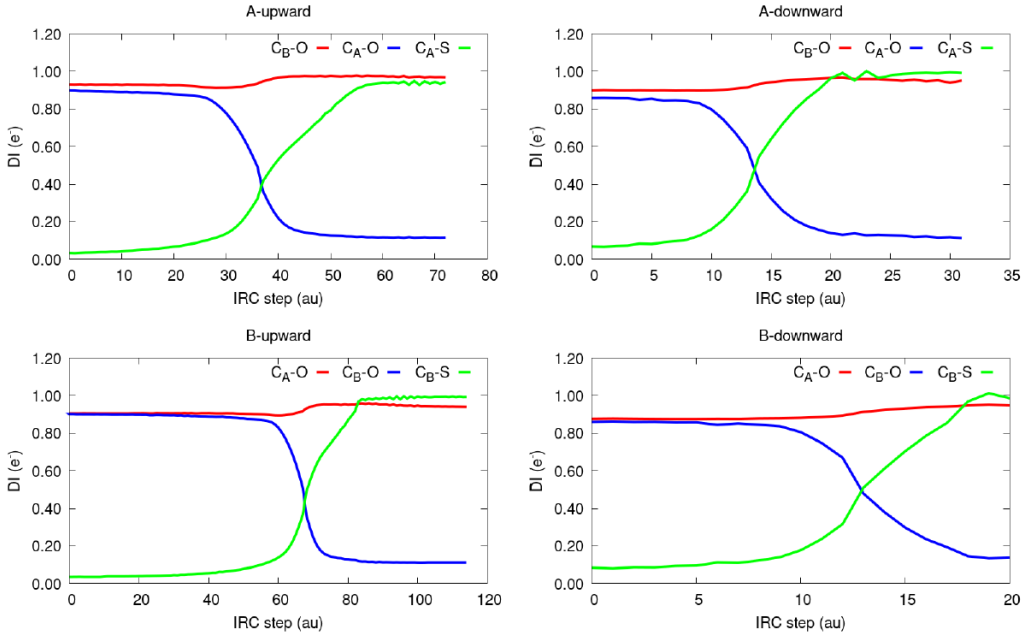


Figure S21. Evolution of the electron delocalization (DI) across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- + Choline to R1i. The results for different spatial approximations are shown. All values are reported in electron pairs.

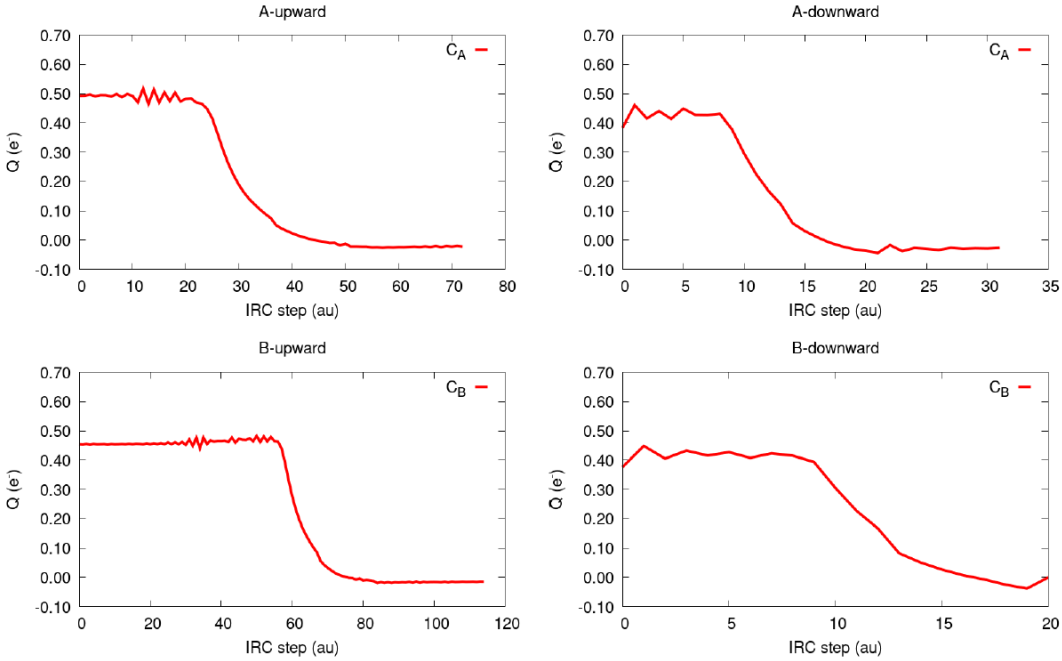


Figure S22. Evolution of the atomic charges (Q) of the electrophilic carbon across the gas-phase reaction coordinate attributed to the nucleophilic attack of CS_2Cl^- + Choline to R1i. The results for different spatial approximations are shown. All values are reported in electrons.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A, Orientation: Upward]

C	-1.249424	3.430123	2.246682
C	-0.429916	2.238005	2.498818
O	-1.604370	2.163017	1.725780
H	-1.906909	3.815632	3.031718
H	-0.490923	1.741054	3.472605
S	-0.294360	-3.564185	0.608898
C	-0.000512	-2.226007	1.541845
S	-1.005424	-0.945583	1.945126
Cl	1.669868	-2.089909	2.224880
H	-0.909526	4.160218	1.503230
C	0.870041	2.012492	1.759609
H	1.662558	2.646628	2.199466
H	1.168010	0.955678	1.859737
O	0.649796	2.369894	0.414653
C	1.774448	2.523754	-0.408914
H	2.551555	3.114346	0.112138
H	1.430319	3.122603	-1.267793
C	2.370485	1.222796	-0.908199
C	1.807224	-0.013195	-0.589010
C	3.505166	1.262315	-1.727562
C	2.370985	-1.198312	-1.071619
H	0.931135	-0.055939	0.062943
C	4.060519	0.085461	-2.221021
H	3.957118	2.225278	-1.980677
C	3.494429	-1.149152	-1.892869
H	1.931248	-2.155326	-0.776943
H	4.944730	0.129122	-2.859208
H	3.939291	-2.072173	-2.267485
C	-2.380761	0.649271	-1.061777
N	-2.525729	-0.733925	-1.649119
C	-3.316117	-1.573145	-0.693491
H	-3.460574	-2.562941	-1.141848
H	-2.743542	-1.658570	0.243396
H	-4.279293	-1.077623	-0.522269
C	-3.232032	-0.681905	-2.954068
H	-4.227793	-0.249607	-2.801318
H	-2.660112	-0.068002	-3.657291
H	-3.321733	-1.703081	-3.342690
C	-1.179994	-1.359590	-1.826815
H	-0.652558	-1.296841	-0.868784
H	-1.316850	-2.415488	-2.084752
H	-0.633771	-0.830561	-2.615530
C	-1.419281	1.579273	-1.804255
H	-2.035224	0.519015	-0.025129
H	-3.383260	1.099372	-1.045081
O	-1.490535	2.842529	-1.226884
H	-1.699324	1.680230	-2.865945
H	-0.393794	1.170055	-1.762661
H	-1.022571	2.772508	-0.375874

[TS, Approximation: A, Orientation: Upward]

C	0.959071	-2.240911	2.913317
C	-0.079760	-1.219158	2.740976
O	1.650741	-1.761412	1.820263
H	1.503346	-2.166105	3.874407
H	-0.282620	-0.466322	3.504754
S	0.170424	3.401751	0.287305
C	-0.095569	2.153974	1.329550

S	0.935282	0.863662	1.683391
Cl	-1.677782	2.088503	2.174347
H	0.569804	-3.276521	2.809863
C	-1.224890	-1.470003	1.821434
H	-1.922507	-2.110602	2.412742
H	-1.757585	-0.531273	1.601508
O	-0.809268	-2.136328	0.670824
C	-1.818742	-2.467585	-0.238549
H	-2.634131	-3.026198	0.261404
H	-1.344736	-3.155156	-0.956523
C	-2.405771	-1.277132	-0.975623
C	-1.812064	-0.014304	-0.903134
C	-3.556741	-1.437500	-1.753904
C	-2.364114	1.075223	-1.579166
H	-0.924253	0.118723	-0.281345
C	-4.097769	-0.358121	-2.449146
H	-4.036848	-2.417942	-1.813307
C	-3.505823	0.903129	-2.359713
H	-1.903979	2.060020	-1.465826
H	-4.995485	-0.498349	-3.053657
H	-3.943403	1.752083	-2.887028
C	2.722475	-0.840626	-0.831151
N	2.780041	0.427512	-1.663308
C	3.516127	1.470536	-0.889326
H	3.675966	2.341030	-1.537361
H	2.899380	1.749079	-0.024260
H	4.474705	1.048582	-0.565136
C	3.488651	0.155110	-2.939348
H	4.527255	-0.115169	-2.717108
H	2.989769	-0.674884	-3.451633
H	3.458001	1.055732	-3.564254
C	1.410036	0.947187	-1.959011
H	0.880254	1.069644	-1.008137
H	1.512311	1.924354	-2.445819
H	0.885979	0.241598	-2.612321
C	1.626381	-1.837949	-1.219120
H	2.560665	-0.546680	0.214135
H	3.707453	-1.319781	-0.921378
O	1.772853	-2.968281	-0.443621
H	1.710277	-2.118863	-2.286552
H	0.641330	-1.358551	-1.071144
H	1.636153	-2.645224	0.503865

[P, Approximation: A, Orientation: Upward]

C	1.134942	1.591821	2.827830
C	-0.024312	1.945288	1.840291
O	1.923057	0.612193	2.335620
H	1.687032	2.544756	3.008673
H	-0.339082	2.996535	1.896883
S	0.169988	2.112904	-2.594626
C	-0.182474	2.352988	-1.016561
S	0.814132	1.679199	0.222245
Cl	-1.569957	3.314213	-0.551439
H	0.630276	1.350478	3.795152
C	-1.229891	1.033523	1.988907
H	-1.695348	1.244980	2.972825
H	-1.991159	1.233417	1.211576
O	-0.773266	-0.285693	1.937432
C	-1.739869	-1.288212	1.961421
H	-2.503236	-1.092249	2.739351
H	-1.200760	-2.203980	2.254490
C	-2.423294	-1.497327	0.621645

C	-1.930793	-0.888839	-0.536440
C	-3.545036	-2.326179	0.520197
C	-2.546566	-1.098452	-1.770872
H	-1.062791	-0.232435	-0.454871
C	-4.154525	-2.548757	-0.713033
H	-3.946044	-2.802652	1.418597
C	-3.658259	-1.934029	-1.863844
H	-2.158188	-0.591944	-2.657139
H	-5.028352	-3.199513	-0.775960
H	-4.144161	-2.098990	-2.826643
C	2.721106	-1.277876	0.344704
N	2.810562	-1.367718	-1.173421
C	3.597364	-0.202364	-1.665093
H	3.790089	-0.327314	-2.738188
H	3.007055	0.705800	-1.490749
H	4.538997	-0.156732	-1.106069
C	3.489186	-2.633410	-1.552289
H	4.519694	-2.606509	-1.180745
H	2.950851	-3.468634	-1.090525
H	3.482357	-2.735438	-2.644453
C	1.462134	-1.326951	-1.814818
H	0.942819	-0.422420	-1.479630
H	1.603056	-1.290121	-2.902260
H	0.895610	-2.219378	-1.529849
C	1.533039	-2.001101	0.991728
H	2.655756	-0.218580	0.635357
H	3.663672	-1.686730	0.734934
O	1.619238	-1.840846	2.348850
H	1.549474	-3.080836	0.731844
H	0.599898	-1.575595	0.571183
H	1.653155	-0.793138	2.494863

[R, Approximation: A, Orientation: Downward]

C	-2.158167	2.839766	1.519041
C	-1.533794	1.658968	0.927985
O	-0.745799	2.781066	1.350214
H	-2.685176	3.535393	0.861222
H	-1.609663	1.520519	-0.157538
S	-1.662183	-0.767311	-1.777191
C	-3.098309	-0.705230	-0.925069
S	-4.173534	0.522644	-0.697523
Cl	-3.515222	-2.277185	-0.057083
H	-2.492047	2.812600	2.560357
C	-1.355328	0.403034	1.722137
H	-1.341451	0.640033	2.802821
H	-2.217668	-0.254068	1.515119
O	-0.148508	-0.223275	1.343807
C	-0.191077	-1.629362	1.515947
H	-1.064483	-2.036257	0.980249
H	-0.293589	-1.868268	2.591250
C	1.074710	-2.233142	0.972285
C	1.099807	-2.747757	-0.329710
C	2.242922	-2.259141	1.743222
C	2.280171	-3.283152	-0.847860
H	0.184024	-2.707620	-0.927641
C	3.423768	-2.789971	1.223700
H	2.219341	-1.866912	2.763011
C	3.442917	-3.302722	-0.075291
H	2.289372	-3.694471	-1.858887
H	4.326998	-2.816595	1.835837
H	4.361844	-3.731657	-0.479038
H	0.224466	3.639910	0.192819

O	1.051164	3.876206	-0.276571
C	2.098484	3.420149	0.519980
H	3.013693	3.944518	0.203797
H	1.949414	3.658857	1.587612
C	2.319269	1.911551	0.456201
H	3.265801	1.665296	0.959282
H	1.507083	1.351174	0.944958
N	2.407712	1.351875	-0.950557
C	3.171289	0.073863	-0.892805
H	2.701746	-0.576104	-0.146389
H	3.131196	-0.407194	-1.876811
H	4.209385	0.291041	-0.613362
C	3.080135	2.291913	-1.886609
H	4.073399	2.541803	-1.493335
H	3.179316	1.790585	-2.856422
H	2.460589	3.189889	-1.981936
C	1.022491	1.043581	-1.449720
H	0.555615	0.331883	-0.757682
H	0.455825	1.978127	-1.477899
H	1.100650	0.605140	-2.451872

[TS, Approximation: A, Orientation: Downward]

C	-1.659311	-2.790553	-1.321450
C	-1.596769	-1.402455	-0.860835
O	-0.284110	-2.673931	-1.202526
H	-2.155784	-3.489639	-0.627386
H	-1.419738	-1.240147	0.199055
S	-2.032774	1.268516	1.028281
C	-3.492221	0.649571	0.545913
S	-3.831336	-0.671576	-0.444977
Cl	-4.954478	1.474248	1.141436
H	-2.034773	-2.942973	-2.349116
C	-1.131896	-0.326820	-1.810703
H	-1.001254	-0.770198	-2.813378
H	-1.897449	0.460486	-1.867595
O	0.082738	0.248899	-1.369968
C	0.208303	1.589899	-1.782243
H	-0.695646	2.150506	-1.485260
H	0.304797	1.645102	-2.883218
C	1.415098	2.203767	-1.127130
C	1.275413	2.918137	0.068188
C	2.691293	2.035132	-1.676431
C	2.394760	3.461041	0.700491
H	0.278009	3.046433	0.497459
C	3.811815	2.574102	-1.044668
H	2.800607	1.481562	-2.612136
C	3.664155	3.288336	0.146253
H	2.274425	4.026755	1.625869
H	4.801588	2.446838	-1.486508
H	4.538276	3.721477	0.635469
H	0.517571	-3.494004	-0.211449
O	1.296182	-3.827831	0.353339
C	2.412819	-3.290332	-0.265844
H	3.317192	-3.746698	0.171137
H	2.442927	-3.506332	-1.350292
C	2.496877	-1.768062	-0.157583
H	3.479915	-1.418989	-0.506515
H	1.703937	-1.285250	-0.749721
N	2.325801	-1.243890	1.261930
C	3.004283	0.075782	1.360830
H	2.618816	0.720260	0.564716
H	2.781722	0.517420	2.339684

H	4.085126	-0.067349	1.243263
C	2.900210	-2.174336	2.271847
H	3.956969	-2.347833	2.034971
H	2.812172	-1.702183	3.257557
H	2.333610	-3.110991	2.234072
C	0.866222	-1.041159	1.541151
H	0.477825	-0.297269	0.832349
H	0.368275	-2.002640	1.387999
H	0.757360	-0.689767	2.574705

[P, Approximation: A, Orientation: Downward]

C	-1.197212	0.887091	1.839845
C	-1.860426	0.019564	0.741909
O	0.107076	1.146494	1.551994
H	-1.815059	1.809196	1.932866
H	-1.723263	0.508414	-0.234175
S	-3.614640	-0.468337	-1.944529
C	-4.345907	-0.279447	-0.513060
S	-3.661221	0.000986	1.055765
Cl	-6.096455	-0.322766	-0.359550
H	-1.333319	0.342380	2.807492
C	-1.384841	-1.434544	0.660078
H	-1.531892	-1.915600	1.645371
H	-2.005374	-1.968006	-0.075411
O	-0.050712	-1.578060	0.237948
C	0.901458	-1.694493	1.267334
H	0.644654	-2.557615	1.914399
H	0.917443	-0.777181	1.880188
C	2.256429	-1.935186	0.651157
C	2.375708	-2.585822	-0.582650
C	3.419123	-1.533883	1.319189
C	3.633460	-2.836056	-1.131986
H	1.465507	-2.883575	-1.104539
C	4.677391	-1.783502	0.771090
H	3.332675	-1.016384	2.278022
C	4.788431	-2.436335	-0.457624
H	3.712945	-3.349269	-2.092063
H	5.575007	-1.467727	1.305693
H	5.771959	-2.635592	-0.886128
H	0.360446	2.375550	1.171257
O	0.814572	3.311293	0.778637
C	2.146008	3.130317	1.048411
H	2.737453	4.003958	0.710630
H	2.372111	3.016346	2.130650
C	2.717044	1.860053	0.409196
H	3.811205	1.818371	0.518260
H	2.257332	0.975749	0.868398
N	2.427950	1.736586	-1.080174
C	3.412958	0.789008	-1.664894
H	3.362326	-0.154113	-1.108505
H	3.158613	0.617240	-2.717993
H	4.417298	1.221454	-1.582979
C	2.533354	3.060423	-1.750998
H	3.525134	3.483963	-1.550718
H	2.398775	2.911680	-2.829185
H	1.744502	3.701761	-1.340393
C	1.048505	1.190523	-1.311394
H	0.956213	0.214608	-0.818461
H	0.341374	1.885870	-0.854636
H	0.907402	1.102994	-2.396499

[R, Approximation: B, Orientation: Upward]

C	-1.451224	-1.330704	0.724046
C	-0.375202	-1.681532	1.659871
O	-0.613272	-0.330790	1.285157
H	0.555059	-2.116003	1.277268
S	3.094220	-1.062622	1.746852
C	3.297492	-1.583343	0.175991
Cl	4.744529	-0.823345	-0.694852
S	2.414829	-2.617608	-0.760634
H	-2.485386	-1.300396	1.086571
C	-1.239664	-1.483108	-0.760960
H	-1.873367	-2.286336	-1.174061
H	-0.185119	-1.738829	-0.945960
O	-1.489734	-0.254181	-1.424535
C	-2.779741	-0.097428	-1.983251
H	-2.954805	-0.884283	-2.738292
H	-2.756445	0.873809	-2.496951
C	-3.882166	-0.121196	-0.950119
C	-4.754334	-1.207304	-0.855400
C	-3.988393	0.924311	-0.023584
C	-5.715425	-1.260049	0.155749
H	-4.677466	-2.024921	-1.576680
C	-4.945689	0.872865	0.985910
H	-3.299136	1.769560	-0.093893
C	-5.808781	-0.221618	1.079862
H	-6.389887	-2.115011	0.222252
H	-5.022045	1.689780	1.705262
H	-6.557061	-0.261334	1.872893
H	-0.635236	-1.916064	2.696141
C	1.661141	0.957875	-1.035708
H	0.732019	1.129542	-1.586026
H	1.540200	0.105882	-0.357563
N	1.974878	2.176723	-0.203809
C	1.738638	3.404825	-1.008811
H	1.959819	4.283092	-0.389288
H	2.415737	3.379058	-1.870881
H	0.695386	3.410946	-1.340096
C	3.414412	2.131636	0.203289
H	4.031554	2.052221	-0.697947
H	3.642013	3.052742	0.753348
H	3.574499	1.243516	0.832463
C	1.144394	2.163438	1.059547
H	2.506933	0.764778	-1.706840
C	-0.300843	2.626068	0.880086
H	1.646777	2.827214	1.777881
H	1.202497	1.133287	1.435359
O	-0.921271	2.180154	-0.286655
H	-0.836138	2.306187	1.790531
H	-0.334223	3.726380	0.848154
H	-1.015583	1.208783	-0.294843

[TS, Approximation: B, Orientation: Upward]

C	-1.124655	-1.204930	0.367648
C	-0.080030	-2.040136	0.962117
O	-0.494426	-0.082451	0.882618
H	0.575361	-2.657881	0.342036
S	2.239153	-1.198057	1.549079
C	3.146101	-1.650198	0.199300
Cl	4.881052	-1.156847	0.330494
S	2.689570	-2.400163	-1.188264
H	-2.138348	-1.386260	0.780652
C	-1.146708	-1.215066	-1.162987
H	-1.754714	-2.055651	-1.548604

H	-0.114462	-1.351747	-1.526554
O	-1.603559	0.015595	-1.678181
C	-2.971247	0.078209	-2.002518
H	-3.210155	-0.662374	-2.789364
H	-3.125615	1.082348	-2.422697
C	-3.890483	-0.135064	-0.820272
C	-4.734749	-1.245308	-0.759888
C	-3.858106	0.759747	0.257173
C	-5.535511	-1.470177	0.361311
H	-4.760044	-1.947800	-1.596975
C	-4.653756	0.534297	1.377102
H	-3.186332	1.620496	0.217203
C	-5.492076	-0.581791	1.433375
H	-6.189258	-2.343077	0.398354
H	-4.619167	1.231740	2.215689
H	-6.112468	-0.756523	2.313940
H	-0.187645	-2.313110	2.011697
C	1.403904	1.140363	-1.173506
H	0.366801	1.337365	-1.461378
H	1.437383	0.226708	-0.572688
N	1.909025	2.272984	-0.319323
C	1.703848	3.549835	-1.048208
H	2.036961	4.383299	-0.416888
H	2.294238	3.519010	-1.971813
H	0.636883	3.639416	-1.281201
C	3.362350	2.050750	-0.069252
H	3.872929	1.905382	-1.028350
H	3.769532	2.924516	0.453484
H	3.472906	1.150466	0.547706
C	1.224966	2.301270	1.036028
H	2.065769	1.065559	-2.045238
C	-0.181945	2.885373	1.025163
H	1.875841	2.891980	1.697097
H	1.197679	1.256875	1.373094
O	-0.996531	2.315160	0.059612
H	-0.563828	2.740125	2.054075
H	-0.146945	3.974749	0.854902
H	-0.969207	1.321949	0.237710

[P, Approximation: B, Orientation: Upward]

C	0.756104	-0.882649	-0.611206
C	-0.182890	-1.850456	-1.363057
O	0.479942	0.389674	-0.992248
H	-0.207259	-2.882598	-0.985384
S	-1.883128	-1.195378	-1.359381
C	-2.733092	-2.146146	-0.193666
Cl	-4.367543	-1.464680	-0.040118
S	-2.267733	-3.414710	0.690581
H	1.781693	-1.217964	-0.896754
C	0.605803	-1.092887	0.908862
H	1.015325	-2.074519	1.218917
H	-0.466074	-1.094474	1.169227
O	1.189947	-0.049335	1.655963
C	2.516235	-0.256447	2.070107
H	2.581167	-1.166134	2.698018
H	2.762190	0.607580	2.704979
C	3.517885	-0.361739	0.940819
C	4.304703	-1.505131	0.790826
C	3.640286	0.682732	0.015345
C	5.206232	-1.615072	-0.269229
H	4.204524	-2.324480	1.507552

C	4.535639	0.569912	-1.044688
H	3.009879	1.570270	0.112398
C	5.319338	-0.577128	-1.191270
H	5.813947	-2.515029	-0.377776
H	4.618685	1.382632	-1.768271
H	6.017666	-0.660563	-2.025891
H	0.086207	-1.849299	-2.427333
C	-1.455738	1.548617	1.154650
H	-0.366418	1.538207	1.262376
H	-1.781169	0.650419	0.620844
N	-1.861018	2.735022	0.328443
C	-1.492947	3.972792	1.065278
H	-1.737269	4.845071	0.446471
H	-2.062517	4.002083	2.002035
H	-0.416040	3.924720	1.265442
C	-3.331714	2.668330	0.129029
H	-3.822602	2.620646	1.108741
H	-3.664726	3.557159	-0.419642
H	-3.558827	1.758983	-0.441434
C	-1.198278	2.709331	-1.042802
H	-1.967076	1.634440	2.122513
C	0.256993	3.189604	-1.032066
H	-1.818697	3.342702	-1.694308
H	-1.219817	1.659688	-1.366648
O	1.016427	2.547250	-0.086221
H	0.607260	3.020342	-2.072052
H	0.281940	4.285992	-0.876594
H	0.919247	1.477250	-0.385270

[R, Approximation: B, Orientation: Downward]

C	-0.164521	-2.748790	1.579813
C	-0.533860	-3.423004	0.330492
O	0.738937	-2.805626	0.483210
H	-1.212078	-2.908195	-0.360062
H	-0.510378	-4.515895	0.296313
S	-3.601656	-1.139776	0.062441
C	-2.778557	-0.242935	-1.045584
Cl	-3.467882	1.406328	-1.395374
S	-1.385523	-0.597476	-1.912144
H	0.144586	-3.351294	2.441825
C	-0.731128	-1.401696	1.900510
H	-1.714761	-1.521794	2.390774
H	-0.905883	-0.862301	0.951998
O	0.161420	-0.720115	2.753044
C	-0.292139	0.559494	3.140788
H	0.227267	0.802721	4.078263
H	-1.377092	0.525003	3.345988
C	0.003325	1.619992	2.103248
C	1.173093	2.384856	2.198747
C	-0.854268	1.824875	1.015109
C	1.482808	3.337565	1.228093
H	1.840597	2.237711	3.051706
C	-0.536863	2.759737	0.028387
H	-1.790021	1.262921	0.936629
C	0.628214	3.521189	0.137700
H	2.385086	3.944038	1.327338
H	-1.219429	2.881565	-0.814764
H	0.862473	4.272620	-0.619525
N	2.375433	0.027826	-1.736567
C	2.096517	-1.296126	-2.377552
H	2.652113	-2.058168	-1.826088
H	2.420924	-1.245827	-3.424245

H	1.018756	-1.489878	-2.312904
C	1.652188	1.094664	-2.492351
H	0.570168	0.915317	-2.400924
H	1.964962	1.048233	-3.542849
H	1.912487	2.064855	-2.053492
C	3.837068	0.296901	-1.779442
H	4.358642	-0.533783	-1.291737
H	4.035782	1.240433	-1.256477
H	4.142142	0.380506	-2.829484
C	1.857935	0.029167	-0.307434
C	2.795177	-0.607883	0.709375
H	0.885563	-0.481001	-0.347722
H	1.688491	1.079393	-0.037487
O	3.286728	-1.868035	0.337638
H	2.218938	-0.639601	1.649876
H	3.666118	0.043361	0.882185
H	2.548757	-2.495080	0.426907

[TS, Approximation: B, Orientation: Downward]

C	-0.816975	-1.692728	0.570174
C	-1.613969	-1.784547	-0.643282
O	0.149120	-1.628768	-0.442871
H	-1.806431	-0.871216	-1.204085
H	-1.751505	-2.758206	-1.109456
S	-3.961290	-1.599144	0.024421
C	-4.245640	0.014245	-0.384832
Cl	-5.934422	0.518086	-0.072917
S	-3.244087	1.171574	-1.016486
H	-0.753970	-2.611230	1.180541
C	-0.970101	-0.450457	1.422250
H	-1.681900	-0.648013	2.242727
H	-1.388515	0.365111	0.811659
O	0.304829	-0.108216	1.940508
C	0.501229	1.253061	2.204344
H	1.182918	1.332805	3.065667
H	-0.449533	1.730477	2.505498
C	1.093991	2.022946	1.035489
C	1.989704	3.069408	1.280663
C	0.742011	1.736200	-0.291603
C	2.511922	3.829624	0.232925
H	2.279059	3.297263	2.309854
C	1.256743	2.502306	-1.338516
H	0.073325	0.902956	-0.517589
C	2.140875	3.551581	-1.082470
H	3.204955	4.645078	0.446650
H	0.953210	2.278403	-2.363021
H	2.534146	4.153169	-1.903423
N	3.686699	-0.862085	-0.597426
C	2.769377	-0.944962	-1.782403
H	2.427486	-1.977288	-1.878019
H	3.333674	-0.620552	-2.665521
H	1.905435	-0.299073	-1.595394
C	4.241386	0.519439	-0.527255
H	3.417394	1.217088	-0.331738
H	4.720447	0.759262	-1.484091
H	4.975282	0.564789	0.285768
C	4.786763	-1.847559	-0.767742
H	4.336605	-2.840154	-0.883095
H	5.433946	-1.815508	0.117390
H	5.360551	-1.578228	-1.662739
C	2.922944	-1.112655	0.690070
C	2.629386	-2.579808	0.986579

H	1.981165	-0.557704	0.602943
H	3.525909	-0.678076	1.501250
O	2.067151	-3.265243	-0.080994
H	1.975025	-2.551350	1.879577
H	3.552153	-3.102339	1.289510
H	1.216805	-2.767939	-0.305730

[P, Approximation: B, Orientation: Downward]

C	-0.982609	-1.056006	-0.088419
C	-2.212915	-1.261653	-0.995027
O	0.149994	-1.203008	-0.838127
H	-2.289767	-0.466067	-1.749746
H	-2.084851	-2.224100	-1.508047
S	-3.808780	-1.404989	-0.139005
C	-4.502122	0.180675	-0.242241
Cl	-6.067771	0.151217	0.561044
S	-3.929267	1.527591	-0.930496
H	-1.050405	-1.821399	0.724155
C	-1.031091	0.306768	0.602398
H	-1.952792	0.428623	1.202603
H	-1.020807	1.100483	-0.165319
O	0.103622	0.403592	1.443603
C	0.535435	1.698862	1.728655
H	1.013138	1.681335	2.721515
H	-0.323917	2.392871	1.804441
C	1.529361	2.245683	0.716680
C	2.373938	3.300919	1.079108
C	1.612569	1.724768	-0.580809
C	3.281718	3.836523	0.166921
H	2.322108	3.707311	2.092831
C	2.515543	2.271330	-1.496616
H	0.986423	0.869755	-0.862761
C	3.352528	3.324703	-1.129488
H	3.934658	4.657461	0.468153
H	2.562395	1.866562	-2.510248
H	4.054429	3.748676	-1.849417
N	3.660926	-1.550983	-0.119219
C	3.056287	-1.465812	-1.490740
H	2.418324	-2.340677	-1.632522
H	3.880877	-1.426401	-2.214176
H	2.431248	-0.569818	-1.537307
C	4.613432	-0.420709	0.046761
H	4.047114	0.518941	0.003033
H	5.352040	-0.453688	-0.763644
H	5.113700	-0.516139	1.017502
C	4.370894	-2.850680	0.003742
H	3.639397	-3.643549	-0.192411
H	4.778926	-2.940249	1.018057
H	5.182119	-2.877321	-0.734223
C	2.595369	-1.418743	0.959263
C	1.758748	-2.682303	1.163334
H	1.937680	-0.601049	0.642231
H	3.125707	-1.141938	1.882988
O	1.249745	-3.186385	-0.007962
H	0.983576	-2.364752	1.894183
H	2.368594	-3.447811	1.683596
H	0.695057	-2.332032	-0.467924

Solvated studies

Anionic reaction (without counter cation):

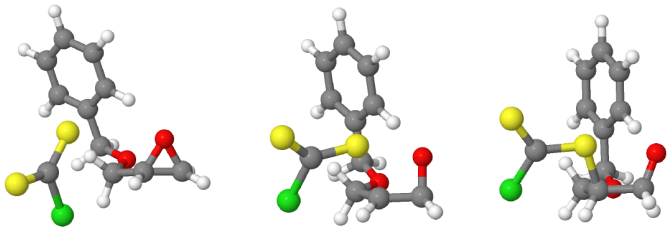


Figure S23. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (upward attack to C_A).

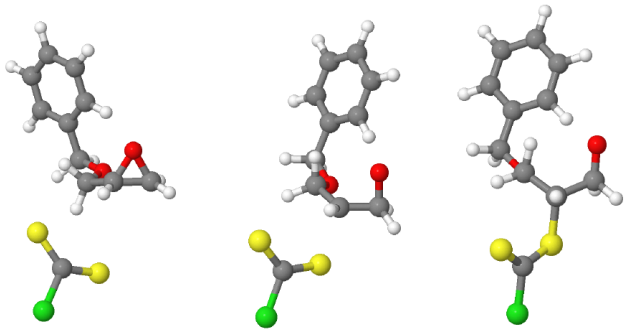


Figure S24. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (downward attack to C_A).

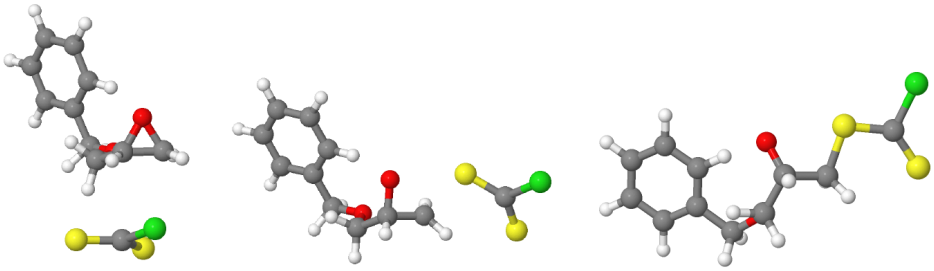


Figure S25. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (upward attack to C_B).

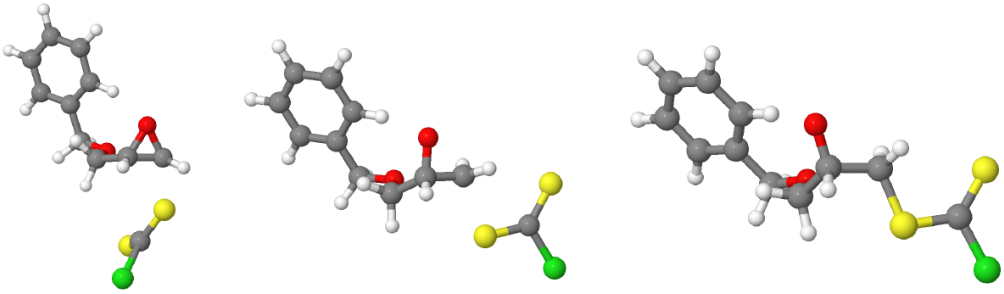


Figure S26. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	58.5	25.5
A	downward	0.0	32.2	18.0
B	upward	0.0	55.3	14.1
B	downward	0.0	26.0	13.2

Table S4. Energies of the reactants (R), transition state (TS) and products (P) involved in the solvated reaction between CS_2Cl^- and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A, Orientation: Upward]

C	0.279827	3.485469	-1.061148
C	-0.325798	2.271120	-0.504328
O	0.427083	2.230916	-1.696097
H	-0.348336	4.210117	-1.591027
H	-1.398504	2.087309	-0.625609
S	-4.438149	-1.728833	0.038303
C	-3.021696	-0.890599	-0.062991
S	-1.698357	-1.020382	-1.044854
Cl	-2.893813	0.513375	1.209901
H	1.188637	3.879499	-0.596415
C	0.270033	1.577517	0.690766
H	-0.293606	1.867746	1.596590
H	0.132916	0.489934	0.556462
O	1.628766	1.930732	0.814212
C	2.401468	0.995091	1.504214
H	1.900477	0.674882	2.438156
H	3.328898	1.511354	1.801318
C	2.760455	-0.226632	0.679834
C	2.524115	-0.255942	-0.697002
C	3.361954	-1.329617	1.295428
C	2.886719	-1.377711	-1.444330
H	2.036943	0.599097	-1.172159
C	3.733129	-2.443750	0.546138
H	3.537426	-1.315551	2.374774
C	3.494853	-2.470578	-0.829103
H	2.683286	-1.397187	-2.516574
H	4.199891	-3.299472	1.037876
H	3.773733	-3.347071	-1.416693

[TS, Approximation: A, Orientation: Upward]

C	0.342505	-2.884105	-1.243935
C	0.756941	-2.036128	-0.115471
O	-0.183467	-1.836922	-1.932708
H	1.216391	-3.387079	-1.721693
H	1.784288	-2.003717	0.246439
S	3.715868	2.063307	-0.151531
C	2.693834	0.789884	0.000625
S	1.635890	0.089548	-1.093492
Cl	2.682935	-0.023215	1.671813
H	-0.366560	-3.691117	-0.934852
C	-0.234735	-1.617234	0.918137
H	0.125577	-2.055303	1.875486
H	-0.199082	-0.522777	1.053773
O	-1.529111	-2.073593	0.643376
C	-2.543963	-1.293372	1.202940
H	-2.372561	-1.128588	2.285603

H	-3.468915	-1.885415	1.114327
C	-2.732886	0.041448	0.509116
C	-2.154056	0.268785	-0.743954
C	-3.501448	1.042965	1.112254
C	-2.350111	1.498288	-1.377578
H	-1.535294	-0.515354	-1.205423
C	-3.704426	2.261613	0.467637
H	-3.942284	0.867837	2.097997
C	-3.125209	2.492568	-0.781800
H	-1.880158	1.677806	-2.346731
H	-4.305799	3.037714	0.945511
H	-3.271665	3.450824	-1.284070

[P, Approximation: A, Orientation: Upward]

C	0.549197	2.442832	1.376824
C	1.081339	1.619878	0.155001
O	-0.188349	1.692557	2.178981
H	1.495333	2.864816	1.843282
H	2.010729	2.038069	-0.255726
S	3.340114	-2.168061	0.339060
C	2.574629	-0.785579	-0.066444
S	1.527047	0.053961	1.014494
Cl	2.791059	-0.124006	-1.705044
H	0.057182	3.346104	0.913884
C	0.062760	1.387070	-0.978363
H	0.485964	1.760734	-1.930515
H	-0.114964	0.306307	-1.116250
O	-1.152699	2.050848	-0.727962
C	-2.269257	1.427500	-1.284072
H	-2.125257	1.226514	-2.365435
H	-3.096074	2.151929	-1.203312
C	-2.658746	0.143901	-0.575373
C	-2.198936	-0.101772	0.724257
C	-3.492321	-0.784170	-1.208533
C	-2.584894	-1.279267	1.369925
H	-1.526260	0.620810	1.228715
C	-3.883015	-1.949427	-0.550088
H	-3.837811	-0.593577	-2.229000
C	-3.426147	-2.200218	0.744786
H	-2.214634	-1.475978	2.378529
H	-4.535391	-2.667278	-1.051757
H	-3.720661	-3.116471	1.260805

[R, Approximation: A, Orientation: Downward]

C	0.131523	2.906402	0.150313
C	0.275536	1.512337	0.565698
O	-0.687802	2.359281	1.170061
H	0.871869	3.641775	0.483237
S	3.358004	0.758056	-0.946753
C	3.592631	-0.511220	0.094232
Cl	5.315537	-1.199699	0.068345
S	2.578754	-1.285813	1.156673
H	-0.381948	3.124231	-0.790293
H	1.122903	1.224870	1.197480
C	-0.256014	0.381754	-0.268619
H	0.595056	-0.098314	-0.782022
H	-0.714515	-0.368380	0.402499
O	-1.200670	0.875675	-1.192900
C	-2.076736	-0.090626	-1.685045
H	-2.501389	0.311441	-2.619472
H	-1.539460	-1.020406	-1.952911
C	-3.212212	-0.414213	-0.732044

C	-4.045113	-1.511532	-0.976287
C	-3.460450	0.398885	0.377480
C	-5.117921	-1.788702	-0.131416
H	-3.848156	-2.156410	-1.837150
C	-4.530931	0.115311	1.227386
H	-2.791514	1.240240	0.576260
C	-5.364433	-0.973508	0.974817
H	-5.760453	-2.648227	-0.332156
H	-4.711615	0.751440	2.096058
H	-6.200537	-1.192230	1.641508

[TS, Approximation: A, Orientation: Downward]

C	0.181905	2.318240	-0.546582
C	0.706867	1.136132	0.161934
O	-0.723664	2.459438	0.451811
H	0.945525	3.125053	-0.653671
S	2.547581	0.411785	-0.993685
C	3.485892	-0.298064	0.211685
Cl	5.152257	-0.707819	-0.365580
S	3.127447	-0.661177	1.774548
H	-0.209566	2.080850	-1.561303
H	1.276470	1.341944	1.069784
C	-0.118427	-0.120857	0.209596
H	0.535321	-0.982473	0.434570
H	-0.843368	-0.023504	1.034744
O	-0.775700	-0.296905	-1.019844
C	-1.784995	-1.256090	-0.996660
H	-1.968356	-1.547406	-2.043739
H	-1.451924	-2.171294	-0.467640
C	-3.092245	-0.773946	-0.392909
C	-4.159093	-1.673112	-0.274292
C	-3.262781	0.553099	0.015267
C	-5.386378	-1.258187	0.237121
H	-4.024690	-2.711871	-0.590215
C	-4.494245	0.960913	0.536019
H	-2.424649	1.262766	-0.028273
C	-5.557590	0.066342	0.644774
H	-6.210478	-1.969543	0.321526
H	-4.615628	1.995694	0.863180
H	-6.516024	0.395913	1.050641

[P, Approximation: A, Orientation: Downward]

C	0.172438	2.231697	-0.419243
C	0.927250	1.019301	0.250842
O	-0.901624	2.551431	0.266675
H	0.974571	3.032072	-0.511857
S	2.271753	0.481117	-0.858231
C	3.437252	-0.243028	0.175913
Cl	4.828789	-0.766287	-0.798460
S	3.425970	-0.480955	1.782894
H	0.010358	1.902313	-1.495602
H	1.391641	1.350366	1.190434
C	-0.041846	-0.102177	0.545640
H	0.447137	-0.942900	1.075441
H	-0.812233	0.346981	1.196167
O	-0.597764	-0.550563	-0.667718
C	-1.634809	-1.467959	-0.529652
H	-1.705645	-2.012600	-1.485895
H	-1.391540	-2.223622	0.245065
C	-2.990989	-0.857635	-0.222700
C	-4.092472	-1.713018	-0.089579
C	-3.170276	0.525110	-0.103035

C	-5.365681	-1.204595	0.154936
H	-3.948427	-2.793837	-0.183962
C	-4.452146	1.025360	0.150159
H	-2.318377	1.231052	-0.152237
C	-5.549066	0.174580	0.275620
H	-6.215360	-1.883597	0.253274
H	-4.583983	2.104803	0.252748
H	-6.543947	0.580487	0.470593

[R, Approximation: B Orientation: Upward]

C	0.627320	1.055858	0.227102
C	0.951136	1.833724	-0.963724
O	-0.067968	2.254915	-0.066287
H	0.596476	1.472984	-1.932696
H	1.864396	2.437089	-0.965035
S	3.062950	-1.046399	-1.363307
C	3.384765	-0.600886	0.196679
S	3.061559	-1.331080	1.651574
Cl	4.264163	1.037657	0.358130
H	1.310246	1.107148	1.082798
C	-0.155630	-0.224414	0.140085
H	0.549176	-1.073245	0.205844
H	-0.845156	-0.280445	1.004346
O	-0.873166	-0.257051	-1.070921
C	-1.953655	-1.137228	-1.071649
H	-2.201153	-1.335812	-2.127157
H	-1.680100	-2.110167	-0.620405
C	-3.180805	-0.576976	-0.376628
C	-4.268872	-1.407510	-0.087704
C	-3.250933	0.780571	-0.049969
C	-5.416075	-0.890089	0.510582
H	-4.214192	-2.471622	-0.333537
C	-4.397911	1.295843	0.556183
H	-2.388142	1.418883	-0.258736
C	-5.483750	0.466314	0.833978
H	-6.258876	-1.548274	0.730665
H	-4.440701	2.355792	0.814286
H	-6.379359	0.873006	1.307189

[TS, Approximation: B Orientation: Upward]

C	-0.007202	-0.715542	-1.319779
C	-1.040214	-0.917559	-0.305053
O	0.079322	0.588415	-0.920549
H	-0.669780	-1.003997	0.716660
H	-2.006073	-1.395499	-0.497153
S	-2.529660	0.961750	-0.002385
C	-3.996922	0.210688	0.289969
S	-4.307574	-1.332410	0.784346
Cl	-5.448050	1.267225	-0.046198
H	-0.379299	-0.869773	-2.360877
C	1.276712	-1.527229	-1.181950
H	1.157895	-2.543077	-1.610380
H	2.053803	-0.996237	-1.764545
O	1.642367	-1.620384	0.174894
C	3.007336	-1.761437	0.412731
H	3.111462	-2.161860	1.434632
H	3.459172	-2.510617	-0.267933
C	3.780544	-0.458778	0.320774
C	5.176406	-0.471275	0.423105
C	3.110513	0.759341	0.170031
C	5.900479	0.718374	0.385340
H	5.700740	-1.424643	0.537150

C	3.842429	1.948526	0.124571
H	2.019741	0.765266	0.050931
C	5.232044	1.935270	0.235857
H	6.988987	0.696963	0.468913
H	3.313674	2.895270	-0.003021
H	5.796005	2.869415	0.201293

[P, Approximation: B Orientation: Upward]

C	-0.122139	0.148356	1.348905
C	-1.335471	0.691201	0.537975
O	0.214402	-1.063776	0.938078
H	-1.010679	1.003916	-0.464754
H	-1.912394	1.499405	1.011778
S	-2.399952	-0.763313	0.341555
C	-3.852835	-0.069788	-0.257564
S	-4.223297	1.461290	-0.670142
Cl	-5.068072	-1.360143	-0.446606
H	-0.449507	0.220960	2.439221
C	1.000078	1.206493	1.257782
H	0.705375	2.163575	1.738338
H	1.869131	0.799831	1.805611
O	1.335271	1.445754	-0.094776
C	2.667737	1.761318	-0.331989
H	2.712980	2.237038	-1.326127
H	3.039446	2.514451	0.393163
C	3.595409	0.558967	-0.329526
C	4.969235	0.748199	-0.521478
C	3.088669	-0.735025	-0.165586
C	5.837454	-0.340726	-0.559324
H	5.361885	1.761952	-0.646829
C	3.968429	-1.821077	-0.196784
H	2.012053	-0.885160	0.029015
C	5.335666	-1.633840	-0.396526
H	6.906897	-0.181570	-0.713151
H	3.571356	-2.828991	-0.056884
H	6.011883	-2.490902	-0.421430

[R, Approximation: B Orientation: Downward]

C	0.275809	0.675603	-0.270476
C	0.476218	1.265796	-1.588537
O	-0.394753	1.868033	-0.638565
H	-0.021983	0.815211	-2.451485
H	1.415212	1.798009	-1.769769
S	3.109910	-1.225574	-0.662903
C	3.981711	-0.089030	0.172223
Cl	5.404168	-0.789650	1.144166
S	3.831545	1.558279	0.303667
H	1.084776	0.800251	0.458555
C	-0.586166	-0.537938	-0.064325
H	0.071316	-1.417465	0.061273
H	-1.165800	-0.412069	0.869628
O	-1.446138	-0.709418	-1.164428
C	-2.588967	-1.462296	-0.895427
H	-2.990123	-1.783170	-1.870443
H	-2.340403	-2.383798	-0.334372
C	-3.662351	-0.687580	-0.154047
C	-4.757210	-1.359287	0.400009
C	-3.588231	0.704407	-0.047953
C	-5.770855	-0.651879	1.043309
H	-4.814900	-2.448788	0.326371
C	-4.600443	1.410530	0.604349

H	-2.718492	1.222097	-0.461242
C	-5.694873	0.738080	1.146784
H	-6.620828	-1.187206	1.470914
H	-4.529327	2.496527	0.689989
H	-6.484300	1.293814	1.656027

[TS, Approximation: B Orientation: Downward]

C	-0.045282	-0.759873	-1.510824
C	1.061880	-0.978462	-0.563594
O	-0.613888	-1.865593	-0.976623
H	0.839706	-0.752120	0.478044
H	1.717305	-1.826319	-0.754735
S	2.703444	0.571953	-0.787589
C	3.859845	-0.014474	0.290576
Cl	5.357349	1.006900	0.315554
S	3.825429	-1.322485	1.278585
H	0.266240	-0.825949	-2.582848
C	-0.816849	0.545373	-1.347860
H	-0.278816	1.385832	-1.831892
H	-1.789508	0.424549	-1.861500
O	-1.003918	0.822650	0.019685
C	-2.141532	1.564204	0.323325
H	-1.982301	1.996029	1.325140
H	-2.264450	2.418430	-0.372366
C	-3.416048	0.740205	0.346599
C	-4.650699	1.374514	0.526223
C	-3.366921	-0.652291	0.225376
C	-5.826503	0.630512	0.596225
H	-4.689449	2.464077	0.615994
C	-4.550277	-1.392400	0.288417
H	-2.401585	-1.144265	0.048029
C	-5.778300	-0.759993	0.478124
H	-6.783711	1.135890	0.740085
H	-4.506116	-2.478701	0.186198
H	-6.697649	-1.346597	0.529483

[P, Approximation: B Orientation: Downward]

C	0.018697	1.075005	1.192713
C	1.283007	1.011839	0.269249
O	-0.759968	2.053640	0.789708
H	0.964728	0.749932	-0.748849
H	1.762439	1.999282	0.264814
S	2.513167	-0.213732	0.819045
C	3.815702	-0.026349	-0.285499
Cl	5.109944	-1.172505	0.129925
S	3.971083	0.985580	-1.542814
H	0.435143	1.165327	2.254634
C	-0.654310	-0.318695	1.204273
H	-0.036602	-1.089640	1.714971
H	-1.596289	-0.209768	1.771472
O	-0.914447	-0.734252	-0.121658
C	-2.034220	-1.541133	-0.280628
H	-1.927051	-2.054509	-1.251091
H	-2.072197	-2.336427	0.492270
C	-3.346015	-0.776008	-0.281670
C	-4.552123	-1.474814	-0.411152
C	-3.359455	0.619945	-0.184365
C	-5.766660	-0.793516	-0.453300
H	-4.537735	-2.566678	-0.483018
C	-4.583161	1.294970	-0.220893
H	-2.414086	1.170629	-0.035839
C	-5.783941	0.599754	-0.359909

H	-6.701149	-1.348961	-0.557919
H	-4.590916	2.383955	-0.136516
H	-6.733147	1.138779	-0.390654

Neutral reaction (using $N(CH_3)_4^+$ as a counter cation):

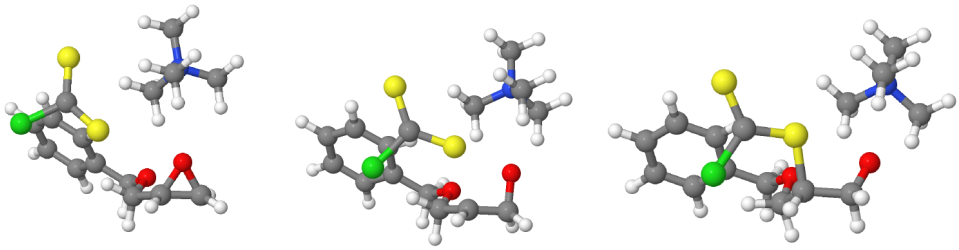


Figure S27. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_A).

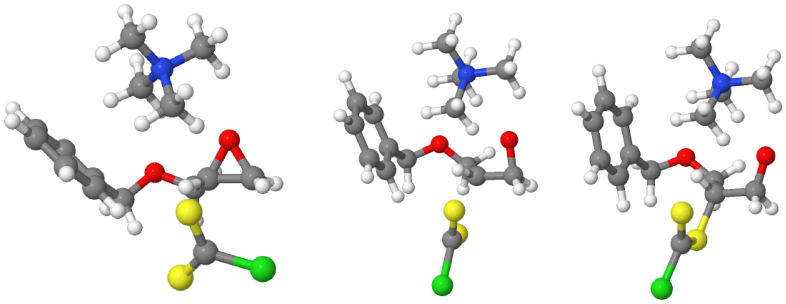


Figure S28. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_A).

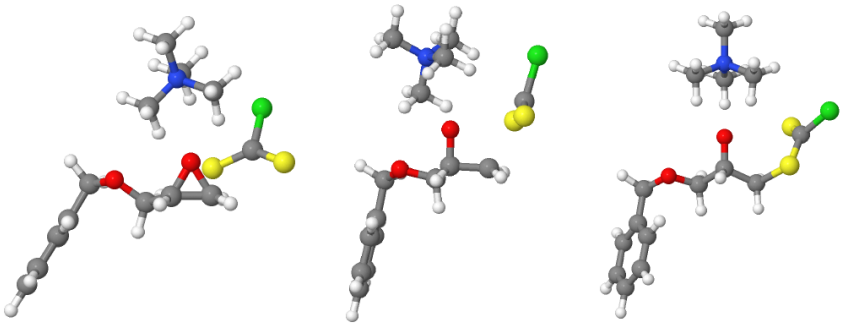


Figure S29. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_B).

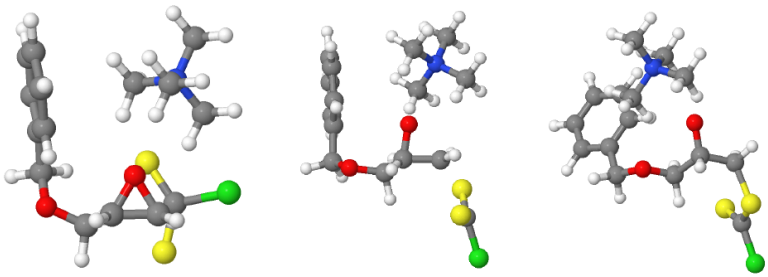


Figure S30. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	54.8	12.1
A	downward	0.0	28.0	11.2
B	upward	0.0	58.5	9.1
B	downward	0.0	26.2	4.6

Table S5. Energies of the reactants (R), transition state (TS) and products (P) involved in the solvated reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

Atom	R	TS	P
C_A	+0.49	+0.05	-0.02
C_B	+0.47	+0.79	+0.91
S'	+0.14	+0.29	+0.43
O	-1.02	-1.10	-1.32

Table S6. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.40	+0.03	-0.06
C_B	+0.47	+0.74	+0.92
S'	+0.17	+0.22	+0.35
O	-1.05	-1.12	-1.30

Table S7. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.47	+0.78	+0.90
C_B	+0.47	+0.07	-0.03
S'	+0.24	+0.40	+0.43
O	-1.03	-1.09	-1.32

Table S8. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.45	+0.71	+0.87
C_B	+0.44	+0.07	-0.02
S'	+0.23	+0.25	+0.35
O	-1.05	-1.11	-1.31

Table S9. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.90	0.39	0.12
O-C_B	0.93	0.95	0.98
C_A-S'	0.02	0.39	0.96

Table S10. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.89	0.46	0.13
O-C_B	0.91	0.94	1.00
C_A-S'	0.03	0.49	0.98

Table S11. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.91	0.96	0.97
O-C_B	0.92	0.41	0.12
C_B-S'	0.02	0.52	1.01

Table S12. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.89	0.92	0.96
O-C_B	0.92	0.50	0.13
C_B-S'	0.01	0.52	1.01

Table S13. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A Orientation: Upward]

C	-2.296475	-3.060882	-1.628479
C	-1.305132	-2.109745	-2.140400
O	-2.303048	-1.699922	-1.228375
H	-3.133953	-3.366868	-2.263364
H	-1.427271	-1.715441	-3.155702
S	-0.089962	3.184243	0.375716
C	0.191420	2.341017	-1.040424
S	-0.785109	1.308383	-1.897508
Cl	1.837574	2.614433	-1.764708
H	-1.988726	-3.766196	-0.850668
C	0.122478	-2.129825	-1.653732
H	0.685233	-2.856289	-2.271143
H	0.575616	-1.135180	-1.806107
O	0.135259	-2.512144	-0.302692
C	1.381019	-2.904373	0.205076
H	1.898809	-3.564839	-0.516467
H	1.171087	-3.513398	1.098709
C	2.301033	-1.766409	0.600185
C	1.911911	-0.428361	0.514766
C	3.570137	-2.073701	1.106990
C	2.771213	0.588942	0.940509
H	0.936584	-0.170226	0.096988
C	4.428004	-1.062430	1.529989
H	3.885148	-3.118825	1.174164
C	4.028065	0.273809	1.450911
H	2.444772	1.627882	0.857902
H	5.414011	-1.316271	1.923711
H	4.699644	1.067853	1.781347

C	-1.323816	-0.100584	1.419971
H	-0.757160	0.806313	1.170945
H	-0.936283	-0.556828	2.339923
N	-2.742992	0.305114	1.662336
C	-3.282176	0.971047	0.439101
H	-4.324059	1.253075	0.634798
H	-2.658004	1.847662	0.225757
H	-3.204972	0.264036	-0.394263
C	-3.550785	-0.903753	1.962442
H	-3.484534	-1.576376	1.098835
H	-3.141900	-1.391268	2.855315
H	-4.591225	-0.604579	2.136258
C	-2.790071	1.260947	2.799388
H	-2.170989	2.127637	2.536274
H	-3.829418	1.569586	2.962136
H	-2.394853	0.767284	3.694878
H	-1.302869	-0.819584	0.592913

[TS, Approximation: A Orientation: Upward]

C	1.899177	-0.721856	2.958826
C	0.672678	0.051388	2.709355
O	2.376658	-0.554183	1.684154
H	2.526804	-0.280630	3.761909
H	0.464439	0.982145	3.238281
S	-0.246373	2.736479	-1.591675
C	-0.176542	2.365696	0.019269
S	1.145422	1.801066	0.878012
Cl	-1.698045	2.569302	0.976844
H	1.670374	-1.771879	3.253899
C	-0.541642	-0.616129	2.179668
H	-1.047459	-0.989930	3.103634
H	-1.229571	0.111840	1.721954
O	-0.243981	-1.680168	1.327282
C	-1.357590	-2.446814	0.954185
H	-1.904919	-2.799663	1.849315
H	-0.952391	-3.340271	0.453535
C	-2.321282	-1.737955	0.023159
C	-1.943387	-0.585451	-0.670059
C	-3.609599	-2.250903	-0.163425
C	-2.841589	0.055604	-1.524057
H	-0.945566	-0.167239	-0.516326
C	-4.500591	-1.626043	-1.033452
H	-3.918302	-3.146776	0.381994
C	-4.119830	-0.466906	-1.712436
H	-2.531797	0.977530	-2.021011
H	-5.502503	-2.036702	-1.171390
H	-4.823969	0.033716	-2.379072
C	1.517696	-0.811051	-1.264917
H	1.143567	0.122490	-1.708727
H	1.057681	-1.681472	-1.750831
N	2.995936	-0.886498	-1.487205
C	3.646833	0.332559	-0.919651
H	4.721429	0.273845	-1.133611
H	3.201912	1.215554	-1.392652
H	3.444546	0.337147	0.160178
C	3.518218	-2.081433	-0.766246
H	3.276009	-1.937435	0.297518
H	3.025219	-2.974745	-1.168133
H	4.601524	-2.142169	-0.926813
C	3.284596	-0.984237	-2.938145
H	2.880965	-0.095204	-3.436807
H	4.369975	-1.038219	-3.084134

H	2.805170	-1.886708	-3.335619
H	1.353005	-0.822608	-0.178337

[P, Approximation: A Orientation: Upward]

C	1.738126	1.111344	2.392453
C	0.271936	1.143139	1.870731
O	2.589419	0.535095	1.533350
H	1.981177	2.182054	2.635459
H	-0.300708	1.938389	2.369718
S	-1.250382	2.576995	-2.045968
C	-1.035269	2.191004	-0.478173
S	0.484264	1.612143	0.104806
Cl	-2.350501	2.394513	0.672536
H	1.655826	0.614597	3.399155
C	-0.510074	-0.152634	2.012792
H	-0.475439	-0.448624	3.080527
H	-1.569981	0.020722	1.755426
O	0.020440	-1.177468	1.210355
C	-0.814312	-2.298578	1.117809
H	-1.108186	-2.660388	2.121548
H	-0.208991	-3.094051	0.653988
C	-2.057139	-2.054398	0.283278
C	-2.031820	-1.115907	-0.753810
C	-3.236505	-2.761976	0.529964
C	-3.169672	-0.882104	-1.524400
H	-1.113256	-0.553363	-0.936260
C	-4.370830	-2.542814	-0.252016
H	-3.270539	-3.486197	1.348031
C	-4.341338	-1.598944	-1.278410
H	-3.140544	-0.128673	-2.314038
H	-5.286407	-3.101157	-0.048527
H	-5.232960	-1.415336	-1.880170
C	2.501644	-1.430279	-0.675600
H	1.904496	-1.220819	-1.572062
H	2.570175	-2.513463	-0.512655
N	3.885518	-0.907961	-0.900139
C	3.808395	0.566950	-1.128958
H	4.824279	0.940032	-1.309451
H	3.176326	0.748638	-2.006842
H	3.365750	0.992023	-0.210396
C	4.682772	-1.149525	0.339663
H	4.156146	-0.622735	1.153728
H	4.725767	-2.231363	0.515935
H	5.693508	-0.752658	0.183981
C	4.513166	-1.578815	-2.061557
H	3.911055	-1.377528	-2.955664
H	5.527462	-1.184279	-2.196609
H	4.552638	-2.658076	-1.871848
H	2.106829	-0.904730	0.211228

[R, Approximation: A Orientation: Downward]

C	-1.891521	1.444177	1.782715
C	-0.939739	0.356830	1.565161
O	-0.490543	1.692525	1.793839
H	-2.435740	1.841661	0.920165
H	-0.800854	0.011025	0.532161
S	-1.889825	0.555672	-1.927621
C	-2.970794	-0.284824	-0.978736
S	-2.884157	-1.792060	-0.295083
Cl	-4.520544	0.628715	-0.614590
H	-2.384475	1.540688	2.756022
C	-0.613256	-0.644633	2.635842

H	-0.546313	-0.125691	3.604273
H	-1.425640	-1.390156	2.695371
O	0.626856	-1.268728	2.398158
C	0.578460	-2.378330	1.512129
H	-0.448055	-2.532306	1.142085
H	0.881605	-3.278599	2.072915
C	1.496831	-2.184196	0.330062
C	2.876130	-2.384266	0.465096
C	0.985070	-1.766800	-0.903900
C	3.733894	-2.170437	-0.613651
H	3.277457	-2.717667	1.425486
C	1.843071	-1.551300	-1.985217
H	-0.093569	-1.615894	-1.025843
C	3.217683	-1.751392	-1.842958
H	4.806271	-2.340083	-0.499846
H	1.424674	-1.236346	-2.943782
H	3.886242	-1.597058	-2.692340
C	1.012507	2.074703	-0.992745
H	0.865821	2.931707	-1.660828
H	0.162121	1.969487	-0.311629
N	2.238860	2.309285	-0.170570
C	2.001631	3.456141	0.749161
H	1.170947	3.187925	1.412058
H	2.917040	3.640149	1.323645
H	1.746045	4.338518	0.150582
C	3.391058	2.599850	-1.062949
H	3.183586	3.519801	-1.621297
H	4.292826	2.721812	-0.451530
H	3.515972	1.757824	-1.754001
C	2.531799	1.081868	0.627907
H	1.651566	0.815802	1.224543
H	2.771729	0.270647	-0.068249
H	3.387876	1.288911	1.281399
H	1.146342	1.152175	-1.569560

[TS, Approximation: A Orientation: Downward]

C	0.762329	-2.737139	0.455490
C	0.678598	-1.362954	0.968392
O	-0.606506	-2.665840	0.382487
H	1.310161	-2.826523	-0.501910
H	0.414214	-0.608439	0.227737
S	1.978792	-0.223088	-1.888644
C	3.057693	-0.157693	-0.647281
S	2.855167	-0.489649	0.999661
Cl	4.728985	0.356654	-1.042277
H	1.175458	-3.468462	1.181508
C	0.236449	-1.150276	2.400155
H	-0.249830	-2.077205	2.731799
H	1.107617	-0.971823	3.056196
O	-0.708283	-0.121413	2.556115
C	-0.200732	1.198967	2.507511
H	0.900461	1.195685	2.566896
H	-0.584204	1.731809	3.393084
C	-0.637296	1.937076	1.260846
C	-1.946598	2.425811	1.157074
C	0.238199	2.124743	0.187620
C	-2.371996	3.084753	0.003831
H	-2.633043	2.299028	1.998798
C	-0.182437	2.784425	-0.969357
H	1.261337	1.747566	0.260200
C	-1.487969	3.264459	-1.064217
H	-3.390443	3.474157	-0.057797

H	0.517206	2.916375	-1.796430
H	-1.815543	3.787840	-1.964318
C	-1.860817	-0.531899	-1.476278
H	-1.908084	-0.539423	-2.571944
H	-1.045717	-1.166344	-1.107610
N	-3.129802	-1.113330	-0.940604
C	-3.189589	-2.555598	-1.314609
H	-2.318949	-3.043823	-0.854117
H	-4.129408	-2.975135	-0.936067
H	-3.153480	-2.633185	-2.407859
C	-4.294154	-0.382852	-1.497181
H	-4.301368	-0.499879	-2.587105
H	-5.214028	-0.796587	-1.067604
H	-4.197813	0.677709	-1.233909
C	-3.124137	-1.002332	0.549714
H	-2.239604	-1.538045	0.916800
H	-3.062079	0.058434	0.815993
H	-4.053577	-1.444787	0.928964
H	-1.763691	0.496120	-1.103731

[P, Approximation: A Orientation: Downward]

C	0.457713	-2.695855	0.461948
C	0.730813	-1.238546	0.959625
O	-0.852082	-2.894246	0.305991
H	1.085526	-2.821814	-0.460335
H	0.232172	-0.536211	0.276904
S	1.741012	-0.335481	-1.990417
C	2.778072	-0.397064	-0.747488
S	2.508490	-0.810422	0.908739
Cl	4.475600	0.038851	-0.953499
H	0.961598	-3.358586	1.226215
C	0.190377	-1.043106	2.380512
H	-0.515664	-1.867413	2.554155
H	1.001807	-1.132173	3.130321
O	-0.548456	0.135401	2.600765
C	0.144325	1.358155	2.472657
H	1.236574	1.206984	2.496112
H	-0.121407	1.977306	3.345377
C	-0.253318	2.090192	1.208492
C	-1.573198	2.540670	1.063300
C	0.646668	2.298453	0.161675
C	-1.984238	3.176778	-0.106185
H	-2.279016	2.395189	1.885441
C	0.238034	2.930947	-1.015603
H	1.680752	1.960577	0.267325
C	-1.077827	3.367574	-1.153684
H	-3.010836	3.537599	-0.199407
H	0.954092	3.077167	-1.826196
H	-1.396220	3.867077	-2.070345
C	-1.855879	-0.599495	-1.457633
H	-1.996126	-0.619982	-2.545582
H	-1.123966	-1.349012	-1.124299
N	-3.144611	-0.985296	-0.807196
C	-3.437500	-2.403726	-1.168871
H	-2.581020	-2.998145	-0.810962
H	-4.370606	-2.702004	-0.675703
H	-3.548660	-2.468909	-2.258183
C	-4.232546	-0.085987	-1.253724
H	-4.338603	-0.164250	-2.342438
H	-5.166672	-0.382541	-0.761839
H	-3.969779	0.942192	-0.975451
C	-2.975757	-0.907050	0.677755

H	-2.184484	-1.639792	0.924266
H	-2.664901	0.109893	0.942823
H	-3.937889	-1.155068	1.143685
H	-1.581765	0.412079	-1.125882

[R, Approximation: B Orientation: Upward]

C	0.807626	-0.580792	-2.201085
C	-0.410864	-1.383869	-2.363605
O	-0.468487	0.026626	-2.251570
H	-0.814904	-1.933141	-1.504861
S	-3.590956	-2.347383	-0.807232
C	-3.101364	-1.609087	0.580759
Cl	-4.454626	-0.750991	1.512266
S	-1.598330	-1.461847	1.296007
H	1.435178	-0.381392	-3.078395
C	1.502651	-0.534503	-0.876132
H	2.342499	-1.253583	-0.876560
H	0.792178	-0.839606	-0.084999
O	1.966241	0.779217	-0.644677
C	2.651149	0.915943	0.572622
H	2.060993	0.487188	1.405296
H	2.740227	1.999052	0.754900
C	4.034218	0.297552	0.558130
C	4.590160	-0.242457	1.720463
C	4.784528	0.291562	-0.622475
C	5.882606	-0.767646	1.709197
H	4.004037	-0.256704	2.642750
C	6.072418	-0.240658	-0.637365
H	4.341623	0.701823	-1.532514
C	6.626468	-0.768176	0.529962
H	6.305803	-1.187582	2.623311
H	6.648147	-0.244014	-1.564671
H	7.634846	-1.185077	0.518483
H	-0.657557	-1.783752	-3.352311
C	-0.642385	2.094883	-0.059232
H	-0.138895	2.817561	0.594292
H	-0.298919	2.189091	-1.093486
N	-2.112139	2.352997	-0.003157
C	-2.400842	3.744295	-0.433967
H	-3.486030	3.899155	-0.419894
H	-1.912022	4.440291	0.257915
H	-2.012693	3.884996	-1.449225
C	-2.585742	2.152051	1.396150
H	-2.047707	2.852513	2.045858
H	-3.663895	2.344298	1.433010
H	-2.380691	1.113456	1.687928
C	-2.807154	1.392415	-0.913535
H	-2.547364	1.647331	-1.946097
H	-2.443884	0.384227	-0.693817
H	-3.887754	1.464722	-0.744840
H	-0.473929	1.066885	0.281747

[TS, Approximation: B Orientation: Upward]

C	0.420107	-1.102840	-1.387070
C	-0.371517	-2.291537	-1.038332
O	-0.703634	-0.342023	-1.567636
H	-0.416353	-2.614724	0.005129
S	-2.758272	-2.210246	-0.906694
C	-3.003628	-1.515753	0.590550
Cl	-4.689026	-0.843209	0.766630
S	-1.997738	-1.316842	1.883088
H	1.043996	-1.241110	-2.303408

C	1.346606	-0.654981	-0.265009
H	2.166237	-1.388744	-0.131847
H	0.772264	-0.611607	0.682274
O	1.865311	0.619815	-0.573949
C	2.752546	1.115080	0.386372
H	2.334107	1.006657	1.405936
H	2.855556	2.195402	0.190087
C	4.125100	0.472893	0.333077
C	4.939833	0.432302	1.467868
C	4.607300	-0.052896	-0.869585
C	6.221866	-0.112653	1.401054
H	4.565605	0.828557	2.415378
C	5.885310	-0.605844	-0.935860
H	3.962309	-0.030384	-1.750403
C	6.697845	-0.633911	0.198115
H	6.848394	-0.138272	2.294450
H	6.249850	-1.017437	-1.878835
H	7.698363	-1.066438	0.145895
H	-0.505779	-3.076472	-1.784803
C	-0.831216	1.926459	0.203375
H	-0.455866	2.585796	0.996613
H	-0.155139	1.881514	-0.655233
N	-2.158245	2.454406	-0.235831
C	-1.994032	3.843603	-0.733323
H	-2.974656	4.236288	-1.026491
H	-1.564669	4.458234	0.066527
H	-1.320671	3.825907	-1.597636
C	-3.093940	2.439150	0.921696
H	-2.708937	3.116185	1.693538
H	-4.082424	2.771433	0.582489
H	-3.151771	1.414221	1.309284
C	-2.712665	1.600914	-1.330275
H	-1.964603	1.515529	-2.123984
H	-2.883600	0.592942	-0.942593
H	-3.645996	2.061367	-1.676106
H	-0.979395	0.900022	0.556308

[P, Approximation: B Orientation: Upward]

C	0.331527	-0.493118	-0.374831
C	-0.121177	-1.882671	0.168370
O	-0.640289	0.419235	-0.317881
H	-0.350396	-1.832248	1.243028
S	-1.628807	-2.408032	-0.679483
C	-2.908889	-1.852720	0.329841
Cl	-4.436956	-2.083286	-0.544191
S	-2.903201	-1.259440	1.835980
H	0.712172	-0.694745	-1.417449
C	1.581508	-0.113552	0.429664
H	2.317585	-0.942973	0.449594
H	1.274510	0.098676	1.474267
O	2.160687	1.037717	-0.138412
C	3.317957	1.465034	0.510088
H	3.169816	1.508670	1.606893
H	3.506528	2.497238	0.170681
C	4.540687	0.620377	0.202785
C	5.619996	0.574525	1.089738
C	4.617823	-0.093461	-0.997124
C	6.763046	-0.162124	0.779930
H	5.563265	1.119834	2.035543
C	5.756274	-0.837153	-1.304986
H	3.766711	-0.063501	-1.680620
C	6.833875	-0.871120	-0.419200

H	7.598856	-0.189374	1.481536
H	5.803033	-1.394129	-2.242709
H	7.724805	-1.453357	-0.660527
H	0.608335	-2.686880	-0.013462
C	-2.450094	2.204860	1.142804
H	-2.063052	3.121922	1.604420
H	-1.666307	1.433605	1.035169
N	-2.894492	2.532817	-0.245812
C	-1.716335	3.050658	-1.006206
H	-2.031489	3.242744	-2.039349
H	-1.386344	3.983861	-0.533428
H	-0.944566	2.261104	-0.950900
C	-3.980284	3.539434	-0.217627
H	-3.616599	4.442755	0.286782
H	-4.273453	3.777200	-1.247149
H	-4.835295	3.123827	0.328932
C	-3.370444	1.274386	-0.898686
H	-2.500229	0.592671	-0.910685
H	-4.197122	0.868394	-0.302392
H	-3.717473	1.520152	-1.910100
H	-3.317483	1.834513	1.702870

[R, Approximation: B Orientation: Downward]

C	-0.353360	1.623001	2.042823
C	-1.321342	0.557015	2.320377
O	-0.070375	0.273597	1.706895
H	-2.201015	0.448632	1.676159
H	-1.428366	0.191126	3.346540
S	-3.844396	1.558394	-0.426857
C	-3.009129	0.202156	-0.851203
Cl	-3.689307	-1.372984	-0.104922
S	-1.671151	-0.027782	-1.810152
H	0.246270	2.005948	2.878300
C	-0.559265	2.580145	0.903805
H	-1.159702	3.428666	1.269822
H	-1.133595	2.081349	0.104842
O	0.660112	3.096273	0.418778
C	1.149478	2.557543	-0.777867
H	1.473807	3.396387	-1.417509
H	0.349102	2.027230	-1.325979
C	2.328099	1.625127	-0.591289
C	2.945445	1.066854	-1.718880
C	2.833822	1.323892	0.674079
C	4.052061	0.231738	-1.583397
H	2.557529	1.302276	-2.713757
C	3.935130	0.475368	0.813017
H	2.362940	1.772865	1.548868
C	4.551103	-0.069682	-0.313102
H	4.530311	-0.184518	-2.472201
H	4.324687	0.254708	1.809043
H	5.422951	-0.717583	-0.205116
N	0.737297	-2.733217	0.246346
C	1.096709	-4.058499	-0.318998
H	2.185856	-4.114651	-0.429024
H	0.612702	-4.165777	-1.296286
H	0.743913	-4.841909	0.362146
C	-0.747719	-2.621535	0.362126
H	-1.107735	-3.410109	1.033964
H	-1.190275	-2.715781	-0.634737
H	-0.987763	-1.626327	0.748517
C	1.233339	-1.645391	-0.649170
H	2.327845	-1.697204	-0.686650

H	0.900800	-0.687914	-0.230635
H	0.795781	-1.786552	-1.643821
C	1.357691	-2.571226	1.590395
H	0.972156	-3.355609	2.252520
H	1.091982	-1.576809	1.968397
H	2.445442	-2.662973	1.486336

[TS, Approximation: B Orientation: Downward]

C	0.689850	-0.401583	1.875449
C	1.542531	0.747360	1.552369
O	-0.297455	0.558749	1.887825
H	1.474347	1.143487	0.539860
H	1.799187	1.419989	2.369247
S	3.759535	0.146560	1.170973
C	3.802025	0.061009	-0.514540
Cl	5.383641	-0.526207	-1.127997
S	2.661762	0.425116	-1.648980
H	0.900781	-0.879739	2.852965
C	0.593138	-1.468823	0.806715
H	1.590148	-1.914279	0.626066
H	0.263440	-0.996015	-0.135580
O	-0.313615	-2.470529	1.217409
C	-1.045498	-3.039718	0.173813
H	-1.370067	-4.036069	0.516858
H	-0.420688	-3.199751	-0.724144
C	-2.278930	-2.233506	-0.183817
C	-2.808657	-2.250083	-1.477616
C	-2.944889	-1.516177	0.816468
C	-4.003814	-1.587843	-1.764515
H	-2.285135	-2.795269	-2.267126
C	-4.148991	-0.871888	0.535533
H	-2.498970	-1.469465	1.811380
C	-4.684456	-0.906434	-0.754431
H	-4.409182	-1.613282	-2.777774
H	-4.677224	-0.343599	1.332250
H	-5.631487	-0.408101	-0.971206
N	-1.921641	2.589324	-0.185611
C	-2.665759	3.452603	-1.135369
H	-3.553806	2.910692	-1.480911
H	-2.013750	3.685416	-1.985451
H	-2.961216	4.375552	-0.622295
C	-0.676397	3.274889	0.264028
H	-0.947278	4.251537	0.682771
H	-0.011472	3.399687	-0.599030
H	-0.212072	2.633541	1.022927
C	-1.558292	1.296614	-0.844098
H	-2.481637	0.791875	-1.156503
H	-1.025674	0.706738	-0.085133
H	-0.923597	1.515560	-1.711126
C	-2.758831	2.295268	1.013784
H	-2.952014	3.237108	1.541472
H	-2.193864	1.593635	1.644640
H	-3.699557	1.848313	0.674695

[P, Approximation: B Orientation: Downward]

C	-0.635443	1.234397	-0.138386
C	-1.833262	1.518519	0.804772
O	0.510834	1.465208	0.522934
H	-1.865796	0.797907	1.634665
H	-1.688286	2.524891	1.221141
S	-3.475280	1.586369	0.025703

C	-4.163267	0.022443	0.292552
Cl	-5.753960	-0.023165	-0.472447
S	-3.579569	-1.258455	1.090948
H	-0.787888	1.898817	-1.037599
C	-0.726187	-0.196335	-0.684810
H	-1.682339	-0.385525	-1.213408
H	-0.658592	-0.902674	0.162569
O	0.352294	-0.383138	-1.580215
C	0.700384	-1.713893	-1.804059
H	1.246736	-1.750518	-2.761048
H	-0.200943	-2.345118	-1.932173
C	1.579762	-2.311965	-0.719385
C	2.059951	-3.618735	-0.864538
C	1.930365	-1.577598	0.418623
C	2.883386	-4.186072	0.105458
H	1.785698	-4.197707	-1.750971
C	2.749843	-2.153165	1.393605
H	1.534994	-0.561741	0.541634
C	3.231805	-3.452508	1.241155
H	3.252329	-5.205493	-0.022296
H	3.003999	-1.580837	2.288939
H	3.870386	-3.897124	2.006535
N	3.487728	2.346872	-0.021156
C	4.891806	2.771141	-0.231992
H	5.539084	1.886672	-0.195942
H	5.174407	3.476033	0.558982
H	4.973851	3.254791	-1.212587
C	2.571308	3.525919	-0.056436
H	2.647119	3.992539	-1.045979
H	2.887897	4.232911	0.720096
H	1.561020	3.122483	0.139347
C	3.343965	1.678911	1.307898
H	3.966305	0.775444	1.306831
H	2.276591	1.438162	1.430854
H	3.692489	2.375677	2.080392
C	3.069393	1.390025	-1.090885
H	3.160687	1.898607	-2.058497
H	2.025935	1.107689	-0.874878
H	3.737238	0.520136	-1.056508

Neutral reaction (using Choline as a counter cation):

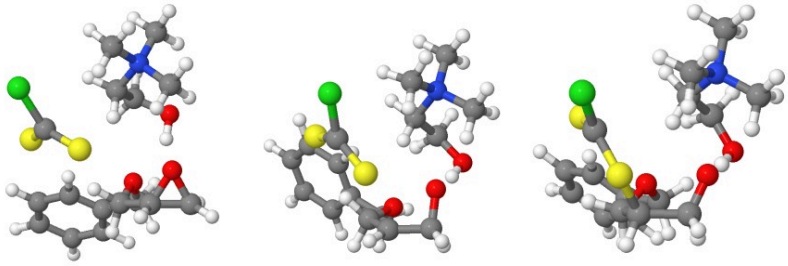


Figure S31. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_A).

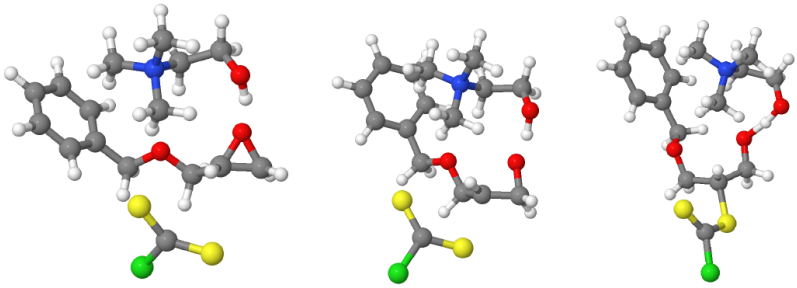


Figure S32. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_A).

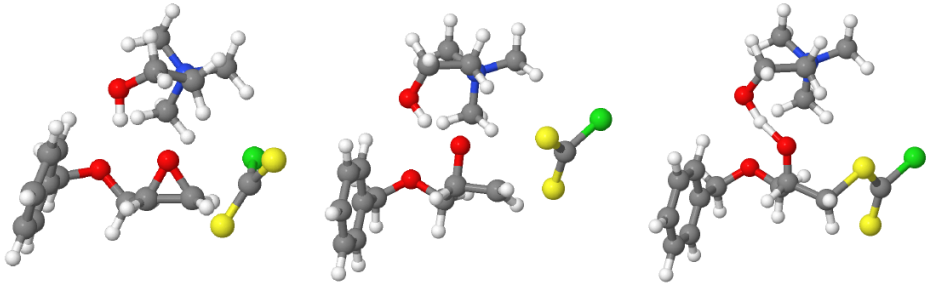


Figure S33. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_B).

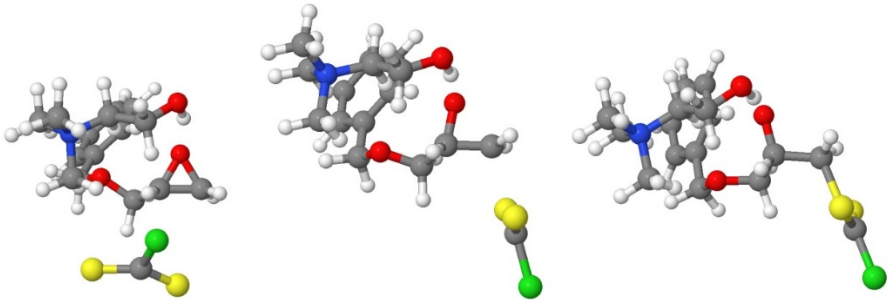


Figure S34. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	51.8	14.9
A	downward	0.0	26.1	1.0
B	upward	0.0	49.9	0.8
B	downward	0.0	25.8	5.2

Table S14. Energies of the reactants (R), transition state (TS) and products (P) involved in the solvated reaction between CS_2Cl^- + Choline and R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

Atom	R	TS	P
C_A	+0.48	+0.03	-0.03
C_B	+0.47	+0.80	+0.87
S'	+0.11	+0.25	+0.42
O	-1.02	-1.12	-1.28

Table S15. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.42	+0.08	-0.03
C_B	+0.48	+0.72	+0.83
S'	+0.20	+0.25	+0.35
O	-1.04	-1.08	-1.26

Table S16. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.43	+0.69	+0.82
C_B	+0.45	+0.07	-0.01
S'	+0.12	+0.27	+0.39
O	-1.03	-1.08	-1.28

Table S17. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.43	+0.64	+0.83
C_B	+0.48	+0.11	-0.02
S'	+0.15	+0.20	+0.34
O	-1.03	-1.06	-1.24

Table S18. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.89	0.34	0.11
O-C_B	0.93	0.95	0.96
C_A-S'	0.02	0.25	0.97

Table S19. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.88	0.47	0.11
O-C_B	0.91	0.93	0.96
C_A-S'	0.03	0.49	0.98

Table S20. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.91	0.93	0.94
O-C_B	0.91	0.42	0.11
C_B-S'	0.02	0.44	0.99

Table S21. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
O-C_A	0.88	0.92	0.96
O-C_B	0.90	0.52	0.12
C_B-S'	0.00	0.47	1.02

Table S22. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A Orientation: Upward]

C	0.474213	2.913126	2.364873
C	0.338885	1.455222	2.436362
O	-0.580460	2.235805	1.699968
H	0.170948	3.528417	3.217655
H	-0.069313	1.003743	3.347126
S	-0.370891	-2.554688	-0.100115
C	-1.773375	-2.200293	0.707617
S	-2.094893	-1.128704	1.943067
Cl	-3.243994	-3.128342	0.114123
H	1.230307	3.353133	1.704812
C	1.207338	0.539697	1.610474
H	2.119133	0.275886	2.172876
H	0.652527	-0.390521	1.402140
O	1.520943	1.172366	0.386217

C	2.869541	1.486344	0.157129
H	3.308840	1.989317	1.039255
H	2.874137	2.216621	-0.668329
C	3.713424	0.287199	-0.219529
C	3.127509	-0.952577	-0.482373
C	5.102442	0.424115	-0.324682
C	3.921581	-2.042043	-0.846414
H	2.045639	-1.071805	-0.388507
C	5.892735	-0.660772	-0.695559
H	5.567984	1.390791	-0.114202
C	5.302975	-1.899564	-0.957203
H	3.450476	-3.007503	-1.040369
H	6.974766	-0.542196	-0.776046
H	5.922279	-2.751734	-1.241959
C	-1.543664	0.516836	-1.273486
N	-2.898970	1.203001	-1.261937
C	-3.947478	0.158963	-1.068787
H	-4.922247	0.657357	-1.005282
H	-3.924199	-0.530664	-1.920407
H	-3.733908	-0.382271	-0.138556
C	-2.982299	2.164308	-0.121369
H	-2.823195	1.605580	0.808297
H	-2.192020	2.909439	-0.239876
H	-3.977901	2.623825	-0.137275
C	-3.150511	1.926623	-2.534682
H	-3.017843	1.231259	-3.372446
H	-4.180307	2.302317	-2.519490
H	-2.447350	2.763059	-2.610750
C	-0.418406	1.306899	-1.917292
H	-1.675775	-0.439668	-1.796948
H	-1.311526	0.294544	-0.221306
O	-0.187224	2.546968	-1.314971
H	-0.617047	1.480967	-2.985311
H	0.466294	0.648699	-1.860550
H	0.167002	2.350876	-0.428515

[TS, Approximation: A Orientation: Upward]

C	0.698696	-1.366361	3.009614
C	0.076520	-0.041926	2.839863
O	1.154114	-1.528171	1.729584
H	1.488938	-1.343267	3.786161
H	0.382416	0.840275	3.401815
S	0.363111	2.397322	-0.410255
C	1.836641	2.192402	0.317965
S	2.262829	1.472595	1.757242
Cl	3.262096	2.834521	-0.622316
H	-0.070605	-2.103297	3.339623
C	-1.101482	0.158010	1.995095
H	-1.875648	0.523463	2.711146
H	-0.916518	1.013558	1.307393
O	-1.504025	-0.999531	1.335238
C	-2.884105	-1.143751	1.128528
H	-3.431115	-1.066030	2.087444
H	-3.014890	-2.175923	0.766461
C	-3.471151	-0.168879	0.129761
C	-2.656261	0.486652	-0.796479
C	-4.850369	0.064168	0.106115
C	-3.209189	1.364033	-1.730134
H	-1.576422	0.329609	-0.766351
C	-5.405661	0.929678	-0.834166
H	-5.495297	-0.436185	0.833204
C	-4.585227	1.584144	-1.754762

H	-2.556639	1.882082	-2.435595
H	-6.483209	1.102902	-0.842621
H	-5.018629	2.270859	-2.483655
C	0.653710	-1.296540	-1.201085
N	2.083797	-1.620042	-1.586178
C	2.865323	-0.353722	-1.487925
H	3.865613	-0.519969	-1.905187
H	2.342357	0.434967	-2.041571
H	2.933608	-0.081615	-0.427839
C	2.700753	-2.620430	-0.661216
H	2.549169	-2.269175	0.368847
H	2.199337	-3.583083	-0.792346
H	3.765511	-2.690349	-0.915597
C	2.140927	-2.126930	-2.979977
H	1.752462	-1.353992	-3.653812
H	3.184741	-2.351961	-3.228801
H	1.538079	-3.037640	-3.059874
C	-0.264829	-2.492375	-0.986153
H	0.274846	-0.650818	-2.005833
H	0.714913	-0.721574	-0.264529
O	0.013271	-3.221835	0.155287
H	-0.245887	-3.164661	-1.864270
H	-1.282073	-2.050793	-0.974683
H	0.345049	-2.575361	0.860167

[P, Approximation: A Orientation: Upward]

C	0.803593	-0.084977	2.760993
C	0.299576	1.260306	2.157234
O	1.353247	-0.932696	1.870004
H	1.504917	0.197714	3.583961
H	0.146958	1.987499	2.970999
S	0.385281	1.833406	-1.426099
C	1.584468	2.142497	-0.385448
S	1.749234	2.033685	1.320610
Cl	3.142589	2.770823	-0.997812
H	-0.101153	-0.487154	3.286764
C	-1.041751	1.141998	1.439608
H	-1.799934	1.163477	2.243154
H	-1.236990	2.011950	0.791394
O	-1.154484	-0.060869	0.726151
C	-2.317564	-0.804085	0.974937
H	-2.567631	-0.784039	2.052245
H	-2.071596	-1.851065	0.740858
C	-3.511413	-0.337227	0.170030
C	-3.347072	0.532400	-0.910860
C	-4.795535	-0.798572	0.482406
C	-4.449009	0.935587	-1.667341
H	-2.342422	0.890316	-1.146246
C	-5.894663	-0.401398	-0.275534
H	-4.932984	-1.476350	1.329118
C	-5.724466	0.469304	-1.353939
H	-4.308327	1.619070	-2.506852
H	-6.890850	-0.768527	-0.021753
H	-6.585944	0.784636	-1.945011
C	1.145532	-1.550463	-0.941194
N	2.595105	-2.006686	-0.864526
C	3.426245	-0.778637	-0.721391
H	4.487061	-1.057709	-0.747106
H	3.192806	-0.097038	-1.548907
H	3.155256	-0.325644	0.242380
C	2.872988	-2.895236	0.308513
H	2.589800	-2.350557	1.218490

H	2.276729	-3.807533	0.212788
H	3.944272	-3.131580	0.288236
C	2.951601	-2.725478	-2.112923
H	2.850385	-2.038451	-2.961257
H	3.985567	-3.082864	-2.039551
H	2.270389	-3.575863	-2.235182
C	0.108221	-2.580552	-0.529813
H	0.997146	-1.213990	-1.976112
H	1.049845	-0.708922	-0.246655
O	0.057040	-2.792886	0.831790
H	0.269659	-3.537623	-1.069563
H	-0.844267	-2.173673	-0.935724
H	0.508374	-1.977902	1.326614

[R, Approximation: A Orientation: Downward]

C	-2.088330	-2.805650	-1.631485
C	-1.489181	-1.640310	-0.984055
O	-0.678681	-2.722097	-1.452508
H	-2.598495	-3.547959	-1.011612
H	-1.565567	-1.553258	0.106648
S	-1.749115	0.819237	1.752271
C	-3.186131	0.647020	0.930856
S	-4.214615	-0.636657	0.780883
Cl	-3.706908	2.164877	0.006030
H	-2.421193	-2.736526	-2.671606
C	-1.330991	-0.346458	-1.718151
H	-1.306959	-0.532224	-2.808673
H	-2.207074	0.287173	-1.494272
O	-0.141178	0.282216	-1.299766
C	-0.185160	1.687158	-1.466006
H	-1.048999	2.093387	-0.912692
H	-0.310979	1.931636	-2.537589
C	1.092611	2.286379	-0.946285
C	1.143037	2.824284	0.344511
C	2.254148	2.273381	-1.728013
C	2.337235	3.347819	0.842742
H	0.234443	2.817533	0.952740
C	3.449108	2.791794	-1.229773
H	2.214857	1.858953	-2.738556
C	3.491597	3.329984	0.058461
H	2.365277	3.774117	1.847240
H	4.347725	2.785485	-1.849454
H	4.423593	3.745280	0.446348
H	0.292499	-3.615866	-0.301805
O	1.090606	-3.889772	0.192496
C	2.184874	-3.408439	-0.524617
H	3.081342	-3.934215	-0.162516
H	2.109868	-3.629225	-1.604493
C	2.393314	-1.902597	-0.423412
H	3.350319	-1.644942	-0.898315
H	1.590396	-1.339824	-0.923926
N	2.443142	-1.364607	0.992210
C	3.186145	-0.073174	0.970582
H	2.712783	0.583722	0.232361
H	3.130866	0.380246	1.966820
H	4.229899	-0.268343	0.697855
C	3.119334	-2.305933	1.924282
H	4.118805	-2.538232	1.537154
H	3.202403	-1.815678	2.901247
H	2.513052	-3.214084	2.007640
C	1.048981	-1.093374	1.474401
H	0.581708	-0.371298	0.792814

H	0.497507	-2.037961	1.472305
H	1.107491	-0.683899	2.489888

[TS, Approximation: A Orientation: Downward]

C	1.701803	2.508891	-1.615945
C	1.658275	1.188539	-0.981154
O	0.331398	2.445544	-1.463882
H	2.227952	3.284261	-1.029883
H	1.495860	1.174318	0.094536
S	2.225424	-1.275171	1.177480
C	3.631585	-0.692749	0.541130
S	3.889214	0.523794	-0.599296
Cl	5.157096	-1.439641	1.115529
H	2.065323	2.523375	-2.660885
C	1.138042	0.006148	-1.760386
H	1.026171	0.294964	-2.821013
H	1.862796	-0.819933	-1.699920
O	-0.097670	-0.433533	-1.238937
C	-0.348818	-1.780684	-1.563789
H	0.436946	-2.425495	-1.129920
H	-0.325427	-1.914925	-2.662366
C	-1.698844	-2.177163	-1.032076
C	-1.816954	-3.059032	0.045399
C	-2.859349	-1.627965	-1.593341
C	-3.074627	-3.394453	0.552525
H	-0.914429	-3.484169	0.490866
C	-4.114807	-1.957650	-1.087433
H	-2.768909	-0.938097	-2.436147
C	-4.224311	-2.843101	-0.011626
H	-3.154751	-4.089572	1.390026
H	-5.013187	-1.530588	-1.537147
H	-5.207684	-3.108368	0.380533
H	-0.385002	3.349772	-0.475653
O	-1.084862	3.782207	0.123946
C	-2.285501	3.238709	-0.304874
H	-3.116233	3.782789	0.174732
H	-2.435200	3.348006	-1.396385
C	-2.421597	1.742937	-0.034924
H	-3.441493	1.413337	-0.279846
H	-1.695830	1.169395	-0.632165
N	-2.168388	1.345168	1.409692
C	-2.864389	0.056876	1.674171
H	-2.542669	-0.669527	0.920073
H	-2.587874	-0.292901	2.676254
H	-3.946984	0.217759	1.611307
C	-2.662622	2.375452	2.361494
H	-3.725417	2.561339	2.165240
H	-2.532641	1.989638	3.379433
H	-2.075330	3.288577	2.218661
C	-0.701456	1.136857	1.616420
H	-0.373386	0.326508	0.952501
H	-0.195854	2.070388	1.353810
H	-0.532380	0.875475	2.668006

[P, Approximation: A Orientation: Downward]

C	1.248312	1.146398	-1.796806
C	1.846246	0.133312	-0.791821
O	-0.096583	1.270433	-1.657192
H	1.795622	2.106443	-1.635727
H	1.643833	0.465569	0.237029
S	3.455984	-0.765578	1.879814
C	4.261777	-0.352935	0.536781

S	3.663543	0.179883	-0.998191
Cl	6.021293	-0.384467	0.477541
H	1.559088	0.804912	-2.817376
C	1.378738	-1.317444	-0.955491
H	1.451181	-1.601843	-2.021698
H	2.052870	-1.976473	-0.386352
O	0.082669	-1.544513	-0.462734
C	-0.938359	-1.592840	-1.430868
H	-0.714246	-2.390114	-2.168216
H	-0.998660	-0.628438	-1.962990
C	-2.246241	-1.912990	-0.753456
C	-2.278219	-2.626147	0.450478
C	-3.455714	-1.517423	-1.337705
C	-3.496114	-2.941210	1.054414
H	-1.334472	-2.922478	0.909898
C	-4.673598	-1.833523	-0.735921
H	-3.438574	-0.952454	-2.273301
C	-4.697459	-2.546723	0.463996
H	-3.506806	-3.500116	1.992133
H	-5.608170	-1.520357	-1.205050
H	-5.649539	-2.795215	0.936024
H	-0.422774	2.455945	-1.189483
O	-0.850033	3.368043	-0.730737
C	-2.202524	3.197544	-0.883433
H	-2.754978	4.053205	-0.449379
H	-2.527894	3.147895	-1.946298
C	-2.734932	1.899871	-0.272380
H	-3.833204	1.874672	-0.321127
H	-2.319591	1.032286	-0.801881
N	-2.363502	1.693725	1.185092
C	-3.307113	0.702881	1.767419
H	-3.285227	-0.201798	1.148939
H	-2.987781	0.466453	2.789428
H	-4.316153	1.131884	1.774115
C	-2.444816	2.970307	1.943436
H	-3.448595	3.395172	1.822379
H	-2.253995	2.753911	3.001241
H	-1.683211	3.649723	1.544948
C	-0.972016	1.151767	1.299659
H	-0.910345	0.200287	0.756673
H	-0.298518	1.875228	0.835464
H	-0.755991	1.009901	2.366289

[R, Approximation: B Orientation: Upward]

C	-1.486957	-1.344216	0.722873
C	-0.465983	-1.654198	1.730269
O	-0.838134	-0.312548	1.448820
H	0.540945	-1.946095	1.409266
S	3.211993	-1.121884	1.718508
C	3.270538	-1.711656	0.163661
Cl	4.602472	-0.955124	-0.885649
S	2.360154	-2.848861	-0.617235
H	-2.542250	-1.478556	0.985174
C	-1.128037	-1.338186	-0.740772
H	-1.618757	-2.170617	-1.273610
H	-0.039058	-1.463249	-0.842203
O	-1.452103	-0.096542	-1.343837
C	-2.726135	-0.007362	-1.954069
H	-2.826233	-0.794605	-2.721331
H	-2.735174	0.967010	-2.463527
C	-3.869750	-0.095118	-0.970689
C	-4.778904	-1.153753	-1.016558

C	-3.991326	0.868890	0.039171
C	-5.797122	-1.255527	-0.066055
H	-4.685522	-1.910487	-1.799611
C	-5.003251	0.766445	0.989615
H	-3.273363	1.692244	0.083295
C	-5.907614	-0.297699	0.939803
H	-6.501252	-2.088114	-0.109683
H	-5.089433	1.518942	1.775346
H	-6.699607	-0.377613	1.686351
H	-0.788589	-2.022652	2.709023
C	1.730898	1.259476	-1.263081
H	0.656182	1.278334	-1.468678
H	2.035384	0.277346	-0.882150
N	2.047735	2.290921	-0.224813
C	1.749548	3.645093	-0.766116
H	1.925546	4.387505	0.021474
H	2.425124	3.830243	-1.609364
H	0.706425	3.670034	-1.097298
C	3.502489	2.206540	0.103082
H	4.075313	2.280684	-0.828394
H	3.754950	3.035305	0.774768
H	3.697845	1.241786	0.590207
C	1.260709	2.003926	1.038239
H	2.303951	1.495525	-2.167725
C	-0.153743	2.566242	1.060935
H	1.828951	2.434321	1.874352
H	1.260213	0.911168	1.150578
O	-0.907824	2.291164	-0.081720
H	-0.618287	2.162699	1.976207
H	-0.122425	3.661110	1.167225
H	-1.049080	1.330346	-0.178290

[TS, Approximation: B Orientation: Upward]

C	1.098701	-1.208068	-0.367375
C	0.064051	-2.070502	-0.937623
O	0.472215	-0.101907	-0.917650
H	-0.583065	-2.682003	-0.302836
S	-2.244544	-1.227826	-1.533438
C	-3.173326	-1.673662	-0.203474
Cl	-4.909758	-1.177863	-0.363658
S	-2.750814	-2.440483	1.188899
H	2.113838	-1.406219	-0.771122
C	1.122052	-1.186559	1.160428
H	1.688089	-2.050132	1.559574
H	0.084323	-1.270924	1.525690
O	1.635732	0.027690	1.659068
C	3.000553	0.025769	1.996871
H	3.206750	-0.751379	2.756877
H	3.189501	1.005342	2.460642
C	3.928322	-0.169086	0.817648
C	4.814516	-1.247096	0.771138
C	3.874388	0.719731	-0.264517
C	5.640495	-1.441611	-0.338215
H	4.853967	-1.947546	1.609392
C	4.694734	0.524173	-1.372462
H	3.167074	1.552535	-0.237986
C	5.579007	-0.557250	-1.412942
H	6.327667	-2.289224	-0.363954
H	4.643540	1.217589	-2.213929
H	6.219090	-0.708871	-2.283910
H	0.177642	-2.373399	-1.978901
C	-1.388174	1.195478	1.187993

H	-0.334197	1.378449	1.417506
H	-1.471038	0.273600	0.603534
N	-1.916090	2.322770	0.348619
C	-1.696070	3.604428	1.065252
H	-2.038969	4.432874	0.433016
H	-2.269843	3.582023	1.999141
H	-0.626753	3.699026	1.283603
C	-3.375014	2.101626	0.140594
H	-3.859046	1.971042	1.115568
H	-3.795233	2.969199	-0.381596
H	-3.503326	1.196236	-0.464973
C	-1.267966	2.344271	-1.021285
H	-1.998613	1.146687	2.098228
C	0.142867	2.912887	-1.057132
H	-1.926960	2.943212	-1.665443
H	-1.262762	1.300035	-1.360073
O	1.004828	2.312553	-0.150964
H	0.472657	2.796185	-2.108185
H	0.125014	3.997321	-0.858589
H	0.947868	1.321690	-0.329818

[P, Approximation: B Orientation: Upward]

C	0.680377	-0.870447	-0.656455
C	-0.262197	-1.838058	-1.401467
O	0.421940	0.399966	-1.048330
H	-0.253867	-2.879388	-1.049440
S	-1.973830	-1.218589	-1.348309
C	-2.772431	-2.207037	-0.181187
Cl	-4.433040	-1.610304	-0.008760
S	-2.244136	-3.465911	0.688389
H	1.702579	-1.227833	-0.936330
C	0.530557	-1.072908	0.862525
H	0.879572	-2.078841	1.168449
H	-0.538097	-1.003445	1.129038
O	1.186844	-0.073083	1.611624
C	2.487324	-0.379687	2.038725
H	2.491792	-1.328117	2.609631
H	2.766603	0.425452	2.735975
C	3.515722	-0.462067	0.930728
C	4.334673	-1.585305	0.798436
C	3.645121	0.592347	0.016953
C	5.276920	-1.662653	-0.229463
H	4.228902	-2.414018	1.503479
C	4.581277	0.512080	-1.010937
H	2.988713	1.462757	0.097949
C	5.399417	-0.613586	-1.137949
H	5.909267	-2.547424	-0.323763
H	4.670173	1.333635	-1.724329
H	6.129700	-0.672228	-1.947191
H	-0.017026	-1.809763	-2.471726
C	-1.465309	1.665222	1.130093
H	-0.377250	1.580847	1.212349
H	-1.861298	0.805247	0.579360
N	-1.802221	2.899859	0.351482
C	-1.345665	4.089780	1.117224
H	-1.541817	4.993107	0.526875
H	-1.904871	4.128001	2.059660
H	-0.273499	3.974098	1.310429
C	-3.277231	2.950222	0.177855
H	-3.752772	2.900059	1.164597
H	-3.549343	3.884384	-0.326872
H	-3.584101	2.089127	-0.428242

C	-1.162946	2.860617	-1.026271
H	-1.946365	1.751891	2.112840
C	0.314539	3.255973	-1.040452
H	-1.750875	3.538781	-1.660810
H	-1.255122	1.821233	-1.369288
O	1.076081	2.541091	-0.146230
H	0.625019	3.112693	-2.097587
H	0.406737	4.341604	-0.846378
H	0.912119	1.495538	-0.448066

[R, Approximation: B Orientation: Downward]

C	-0.360881	-0.833026	1.068069
C	-0.492264	-1.431205	2.390670
O	0.224776	-0.210576	2.213185
H	0.126629	-2.293202	2.656563
H	-1.451630	-1.343074	2.908051
S	-2.428989	-1.485930	-2.100196
C	-2.859171	-1.956522	-0.573166
Cl	-3.855545	-0.629497	0.375482
S	-2.601460	-3.325399	0.298507
H	-1.233832	-0.306460	0.667401
C	0.600029	-1.351631	0.048292
H	0.079525	-2.062599	-0.618411
H	1.433585	-1.869923	0.553870
O	1.079036	-0.240050	-0.691120
C	2.195006	-0.532410	-1.491238
H	2.233515	0.236709	-2.279479
H	2.060689	-1.502840	-2.002453
C	3.501836	-0.524355	-0.722871
C	4.678091	-0.933213	-1.361530
C	3.562027	-0.090271	0.603854
C	5.897081	-0.899508	-0.689040
H	4.636324	-1.281955	-2.396788
C	4.783838	-0.063367	1.279547
H	2.644339	0.207820	1.115990
C	5.953230	-0.462973	0.636036
H	6.807467	-1.219952	-1.198640
H	4.818153	0.270368	2.318125
H	6.906777	-0.440855	1.166031
N	-0.909723	2.828574	-0.848434
C	-1.851165	3.977281	-0.922113
H	-2.789978	3.706045	-0.427709
H	-2.044751	4.198863	-1.977914
H	-1.394878	4.844944	-0.429818
C	0.293384	3.117076	-1.677604
H	0.760644	4.041590	-1.319633
H	-0.018337	3.225737	-2.722622
H	0.987244	2.274386	-1.572510
C	-1.565632	1.595197	-1.392246
H	-2.431746	1.322190	-0.778778
H	-0.826877	0.786952	-1.383793
H	-1.891722	1.800464	-2.418438
C	-0.441669	2.598825	0.562911
C	-1.528306	2.399747	1.620291
H	0.164292	3.471841	0.842626
H	0.214102	1.716233	0.519653
O	-0.901530	2.228672	2.853165
H	-2.192090	1.552875	1.364448
H	-2.159867	3.297943	1.694191
H	-0.448913	1.366370	2.821896

[TS, Approximation: B Orientation: Downward]

C	0.729454	-1.088297	0.337281
C	1.820753	-1.225108	1.292417
O	0.027226	-0.955950	1.529037
H	2.220450	-0.320127	1.748305
H	1.934657	-2.182945	1.795595
S	3.862257	-1.582916	0.086333
C	4.466621	-0.014552	-0.067968
Cl	6.002967	0.039517	-1.008645
S	3.893290	1.421141	0.494881
H	0.496219	-1.999878	-0.248858
C	0.714676	0.133339	-0.544702
H	1.484502	0.054536	-1.334087
H	0.937668	1.020921	0.069146
O	-0.578137	0.235580	-1.125796
C	-0.896231	1.521240	-1.588900
H	-1.614040	1.403367	-2.418505
H	-0.002334	2.010396	-2.017441
C	-1.509984	2.407963	-0.521347
C	-2.045454	3.647524	-0.891392
C	-1.569990	2.008588	0.817924
C	-2.635638	4.477101	0.058568
H	-1.997905	3.964863	-1.936766
C	-2.161906	2.844635	1.768631
H	-1.138517	1.051052	1.127214
C	-2.696787	4.075566	1.394634
H	-3.048705	5.441252	-0.243220
H	-2.195256	2.528701	2.812862
H	-3.155845	4.725454	2.141454
N	-3.603094	-1.702517	-0.729435
C	-4.780131	-2.609069	-0.657904
H	-4.436612	-3.647714	-0.621894
H	-5.396966	-2.453085	-1.550853
H	-5.353051	-2.368591	0.245062
C	-4.074873	-0.291498	-0.816409
H	-4.635306	-0.051380	0.094366
H	-4.713819	-0.184496	-1.700694
H	-3.196106	0.358620	-0.889231
C	-2.796105	-2.010439	-1.947043
H	-2.554451	-3.078170	-1.960691
H	-1.881502	-1.403199	-1.911038
H	-3.396793	-1.757653	-2.829232
C	-2.754901	-1.815028	0.511410
C	-2.059885	-3.156367	0.749171
H	-3.413233	-1.592513	1.362332
H	-1.995204	-1.024208	0.433784
O	-1.373490	-3.085313	1.948490
H	-1.396617	-3.394275	-0.106191
H	-2.800238	-3.971481	0.818247
H	-0.771047	-2.283345	1.893831

[P, Approximation: B Orientation: Downward]

C	0.833175	-0.771810	0.716747
C	2.225788	-0.857231	1.383330
O	-0.107924	-0.657770	1.681818
H	2.470712	0.074177	1.913484
H	2.185260	-1.676875	2.113954
S	3.612008	-1.293540	0.291991
C	4.340959	0.220925	-0.122039
Cl	5.696526	-0.092965	-1.206182
S	3.963064	1.724790	0.339794
H	0.729747	-1.704982	0.095281
C	0.769309	0.389186	-0.274732

H	1.603738	0.370277	-1.001358
H	0.821399	1.334318	0.293742
O	-0.460399	0.305976	-0.981183
C	-0.908435	1.521607	-1.511404
H	-1.528520	1.286999	-2.394201
H	-0.057770	2.123790	-1.882480
C	-1.731071	2.337999	-0.531253
C	-2.382757	3.492607	-0.981506
C	-1.865008	1.947762	0.806143
C	-3.163300	4.250627	-0.112186
H	-2.276987	3.799749	-2.025962
C	-2.648896	2.714111	1.673856
H	-1.339643	1.056332	1.174818
C	-3.299887	3.860350	1.221744
H	-3.666806	5.148708	-0.474902
H	-2.742992	2.409150	2.717934
H	-3.909364	4.453414	1.905921
N	-3.221041	-2.046791	-0.835578
C	-4.221369	-3.144427	-0.854024
H	-3.706012	-4.101885	-0.726140
H	-4.745463	-3.128902	-1.817152
H	-4.932117	-2.987826	-0.034142
C	-3.909858	-0.743208	-1.042689
H	-4.616309	-0.583965	-0.220016
H	-4.438741	-0.766000	-2.003044
H	-3.151250	0.048003	-1.031197
C	-2.235075	-2.242506	-1.938292
H	-1.825247	-3.255364	-1.878099
H	-1.439114	-1.494980	-1.818642
H	-2.756320	-2.111415	-2.894097
C	-2.516790	-1.974599	0.497962
C	-1.657382	-3.177208	0.901942
H	-3.297642	-1.815032	1.254410
H	-1.866289	-1.088571	0.464332
O	-1.051510	-2.888863	2.100642
H	-0.930425	-3.397504	0.089458
H	-2.290048	-4.080311	1.008187
H	-0.606360	-1.923207	2.003678

Nucleophilic attack to the Thiirane

Solvated studies

Neutral reaction (using $N(CH_3)_4^+$ as a counter cation):

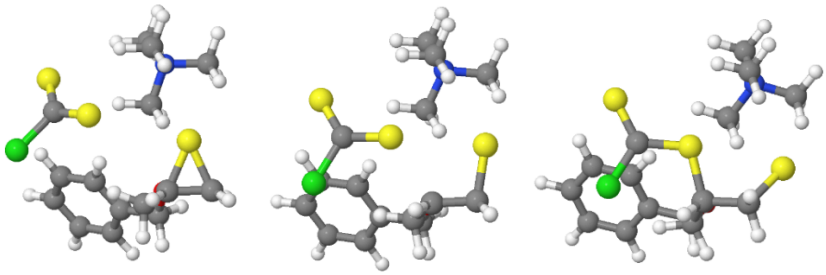


Figure S35. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_A).

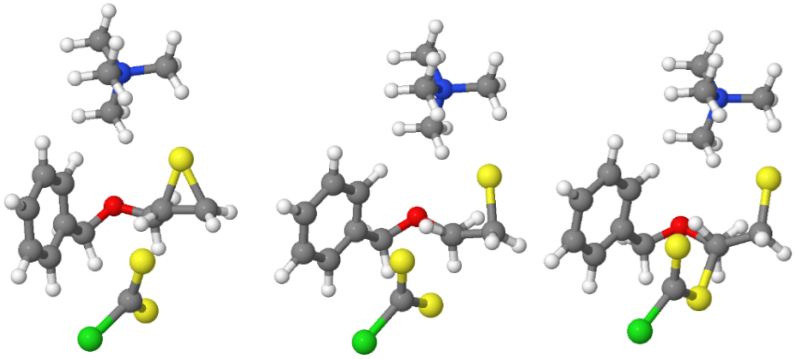


Figure S36. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_A).

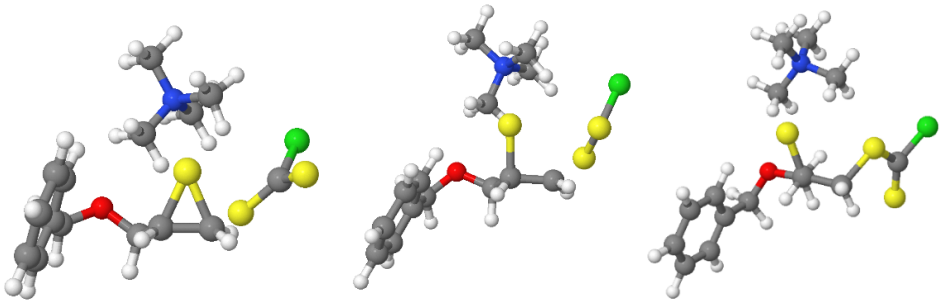


Figure S37. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_B).

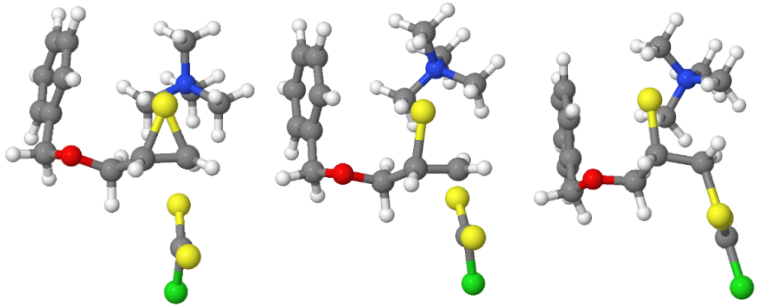


Figure S38. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	48.0	13.4
A	downward	0.0	19.5	2.7
B	upward	0.0	50.2	9.4
B	downward	0.0	23.4	11.6

Table S23. Energies of the reactants (R), transition state (TS) and products (P) involved in the solvated reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

Atom	R	TS	P
C_A	+0.01	+0.03	+0.01
C_B	-0.01	+0.07	+0.06
S'	+0.15	+0.30	+0.43
S	-0.10	-0.46	-0.62

Table S24. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	-0.04	-0.03	--
C_B	-0.01	+0.06	--
S'	+0.11	+0.19	--
S	-0.22	-0.52	--

Table S25. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	-0.04	+0.02	+0.03
C_B	-0.02	+0.03	+0.01
S'	+0.25	+0.41	+0.42
S	-0.13	-0.43	-0.61

Table S26. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	+0.00	+0.05	+0.05
C_B	-0.01	+0.01	+0.00
S'	+0.28	+0.28	+0.37
S	-0.14	-0.47	-0.61

Table S27. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.02	0.33	0.08
S-C_B	1.05	1.05	1.15
C_A-S'	0.02	0.42	0.95

Table S28. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.00	0.45	--
S-C_B	1.03	1.06	--
C_A-S'	0.04	0.45	--

Table S29. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.03	1.04	1.13
S-C_B	1.04	0.39	0.09
C_B-S'	0.03	0.48	0.99

Table S30. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.02	1.05	1.12
S-C_B	1.05	0.48	0.11
C_B-S'	0.01	0.50	0.98

Table S31. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + $N(CH_3)_4^+$ and 4-R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A Orientation: Upward]

C	2.427260	3.448845	-0.947274
C	1.465599	2.595405	-1.677745
S	2.875406	1.690228	-0.981742
H	3.080133	4.114635	-1.517258
H	1.489190	2.639672	-2.770747
S	-0.510328	-3.178684	-0.438851
C	-0.362608	-1.976760	-1.591528
S	0.926754	-1.018115	-2.003610
Cl	-1.877555	-1.669992	-2.555655
H	2.109879	3.817743	0.031444
C	0.075250	2.374139	-1.131320
H	-0.545122	3.238948	-1.437571
H	-0.355642	1.467628	-1.588843
O	0.119558	2.283046	0.270341
C	-1.030827	2.700827	0.951644
H	-1.387931	3.667811	0.548216

H	-0.719053	2.887821	1.992100
C	-2.170378	1.702661	0.957019
C	-2.027602	0.417747	0.430854
C	-3.387573	2.065166	1.547939
C	-3.079192	-0.500031	0.505783
H	-1.090680	0.132132	-0.053011
C	-4.436784	1.153479	1.622016
H	-3.510105	3.072110	1.956622
C	-4.282964	-0.134970	1.103493
H	-2.939374	-1.497931	0.085140
H	-5.380383	1.447851	2.085320
H	-5.105039	-0.850345	1.160747
C	1.005530	-0.499359	1.561926
H	0.329352	-1.155199	0.999359
H	0.511399	-0.122549	2.466613
N	2.180796	-1.324279	1.982327
C	2.873584	-1.848490	0.768934
H	3.730200	-2.451560	1.093363
H	2.153053	-2.444039	0.193993
H	3.197223	-0.996261	0.161532
C	3.117307	-0.483169	2.769668
H	3.428883	0.360808	2.142897
H	2.598489	-0.117277	3.663415
H	3.986495	-1.086833	3.056582
C	1.702210	-2.471238	2.799547
H	1.020262	-3.065200	2.178287
H	2.565636	-3.073699	3.106058
H	1.176311	-2.083326	3.679622
H	1.351025	0.332144	0.934745

[TS, Approximation: A Orientation: Upward]

C	-1.701189	-3.310870	0.074860
C	-0.656809	-2.667322	-0.718757
S	-2.999714	-1.998087	0.089222
H	-2.086274	-4.220343	-0.405015
H	-0.537672	-2.966147	-1.760681
S	0.233106	2.246319	-2.145093
C	0.186982	0.592615	-2.216436
S	-1.105173	-0.400584	-1.787917
Cl	1.666096	-0.247454	-2.798123
H	-1.358186	-3.521465	1.096412
C	0.607741	-2.278439	-0.031000
H	1.120969	-3.252125	0.153879
H	1.266763	-1.684185	-0.680801
O	0.340377	-1.644028	1.187606
C	1.449299	-1.528860	2.040623
H	1.927907	-2.515448	2.190049
H	1.046161	-1.216493	3.016878
C	2.485381	-0.526922	1.573765
C	2.158356	0.441866	0.623305
C	3.778915	-0.547078	2.106055
C	3.106787	1.371592	0.197544
H	1.154680	0.445338	0.194254
C	4.723509	0.392998	1.697982
H	4.049666	-1.307853	2.843037
C	4.391017	1.352547	0.739232
H	2.830263	2.095195	-0.572685
H	5.729831	0.368850	2.120082
H	5.137053	2.076941	0.408355
C	-1.267102	1.131034	1.251782
H	-0.674741	1.631220	0.473487
H	-0.810321	1.274221	2.239629

N	-2.621180	1.766439	1.270372
C	-3.236148	1.658499	-0.086188
H	-4.206748	2.168564	-0.064305
H	-2.556340	2.123428	-0.811587
H	-3.344397	0.594452	-0.328509
C	-3.475817	1.052900	2.258323
H	-3.513461	-0.006319	1.967881
H	-3.025059	1.160769	3.252172
H	-4.477767	1.498290	2.246422
C	-2.493008	3.199115	1.639057
H	-1.855328	3.692820	0.896117
H	-3.489965	3.655218	1.644655
H	-2.037710	3.271050	2.633634
H	-1.386705	0.063476	1.021026

[P, Approximation: A Orientation: Upward]

C	1.605087	-2.151656	-2.121115
C	0.273194	-1.914062	-1.396274
S	2.942448	-0.957764	-1.798369
H	1.941799	-3.165667	-1.848597
H	-0.305640	-2.849647	-1.395036
S	-0.721955	-1.435745	2.899075
C	-0.697552	-1.838730	1.318389
S	0.710722	-1.559924	0.357818
Cl	-2.094871	-2.598768	0.574508
H	1.358872	-2.190601	-3.196980
C	-0.636317	-0.839876	-1.981551
H	-0.697776	-1.017717	-3.073315
H	-1.654013	-0.967364	-1.571417
O	-0.177505	0.462073	-1.727601
C	-1.109340	1.452478	-2.063101
H	-1.505636	1.296217	-3.084091
H	-0.555414	2.404941	-2.080140
C	-2.260262	1.550554	-1.079637
C	-2.100814	1.099582	0.233981
C	-3.486140	2.101925	-1.463060
C	-3.150263	1.187123	1.147624
H	-1.145009	0.659095	0.525508
C	-4.531604	2.207927	-0.546123
H	-3.626024	2.445545	-2.491272
C	-4.368027	1.746456	0.760619
H	-3.014884	0.805145	2.161653
H	-5.484436	2.639723	-0.857609
H	-5.191640	1.815040	1.473162
C	1.719008	1.759075	0.325626
H	0.996491	1.513515	1.113897
H	1.535107	2.771275	-0.056456
N	3.089853	1.732760	0.922425
C	3.363533	0.368361	1.467866
H	4.357516	0.378296	1.931662
H	2.594488	0.134150	2.213838
H	3.320339	-0.342907	0.624469
C	4.077401	2.035836	-0.152369
H	3.914785	1.319153	-0.968482
H	3.905690	3.060100	-0.504094
H	5.088589	1.939244	0.259830
C	3.192181	2.737672	2.009077
H	2.468918	2.482852	2.792408
H	4.209809	2.719322	2.416789
H	2.967994	3.729676	1.599546
H	1.683994	1.012724	-0.484146

[R, Approximation: A Orientation: Downward]

C	0.033701	-2.569043	-0.951554
C	0.056947	-1.414934	-0.041565
S	-1.122837	-1.237869	-1.418881
H	0.895661	-2.676454	-1.615509
H	0.923827	-0.759947	-0.159400
S	3.098146	-0.784389	-1.757734
C	3.632433	-0.725359	-0.191859
S	3.222093	-1.600571	1.161315
Cl	4.921141	0.569599	0.116694
H	-0.438895	-3.494938	-0.610410
C	-0.487223	-1.574816	1.353960
H	-1.326982	-2.287968	1.342496
H	0.325530	-1.999678	1.972739
O	-0.972520	-0.392773	1.942892
C	0.020447	0.567536	2.247826
H	0.942592	0.067995	2.594078
H	-0.377966	1.159783	3.087023
C	0.348255	1.477528	1.084399
C	-0.680947	2.019391	0.305796
C	1.673078	1.762371	0.751142
C	-0.389413	2.827101	-0.790515
H	-1.717838	1.788495	0.562203
C	1.969111	2.559224	-0.355917
H	2.487245	1.318957	1.329420
C	0.939626	3.094333	-1.127199
H	-1.198013	3.243565	-1.395573
H	3.013523	2.725567	-0.624715
H	1.170705	3.708350	-1.999214
C	-4.181683	0.958971	-1.050006
H	-4.768901	0.950738	-1.975480
H	-3.154671	0.630039	-1.248749
N	-4.804984	0.011939	-0.080246
C	-4.802263	-1.363318	-0.658465
H	-3.760104	-1.659997	-0.835213
H	-5.281114	-2.041132	0.057299
H	-5.362928	-1.348323	-1.600353
C	-6.204883	0.432237	0.198656
H	-6.771646	0.414689	-0.739257
H	-6.644248	-0.266604	0.919394
H	-6.193655	1.446080	0.614987
C	-4.011901	0.015005	1.184398
H	-2.968443	-0.242154	0.960824
H	-4.059550	1.019483	1.621724
H	-4.447441	-0.715837	1.875460
H	-4.181188	1.962614	-0.608766

[TS, Approximation: A Orientation: Downward]

C	-0.113916	-2.783673	-0.484713
C	0.122137	-1.562916	0.279764
S	-1.717764	-2.068497	-0.998045
H	0.582860	-2.911468	-1.320787
H	0.384601	-0.678519	-0.299635
S	2.444349	-0.485187	-1.904785
C	3.098075	-0.785278	-0.432674
S	2.464443	-1.634289	0.885994
Cl	4.747632	-0.132849	-0.108568
H	-0.207249	-3.698048	0.115892
C	-0.437671	-1.415866	1.681820
H	-1.353155	-2.018770	1.752583
H	0.283430	-1.818301	2.416473
O	-0.787667	-0.100090	2.031851

C	0.288382	0.770947	2.295107
H	1.134884	0.219621	2.740901
H	-0.073321	1.486200	3.052886
C	0.773396	1.544330	1.085975
C	-0.085963	1.822093	0.019334
C	2.088219	2.015807	1.036267
C	0.356367	2.567497	-1.072781
H	-1.097490	1.412394	0.038725
C	2.532229	2.762311	-0.053737
H	2.782476	1.765751	1.842589
C	1.665690	3.045224	-1.109080
H	-0.318724	2.761897	-1.908768
H	3.568797	3.101013	-0.090936
H	2.018867	3.614911	-1.970106
C	-3.774460	0.874326	-1.394634
H	-4.455024	0.875244	-2.254417
H	-2.944972	0.171719	-1.555489
N	-4.538388	0.443938	-0.186133
C	-5.072631	-0.933704	-0.394544
H	-4.224317	-1.625870	-0.483013
H	-5.688138	-1.199326	0.472800
H	-5.679061	-0.940559	-1.307369
C	-5.662529	1.385037	0.056909
H	-6.342379	1.355133	-0.802818
H	-6.190568	1.077543	0.966698
H	-5.255757	2.395210	0.181178
C	-3.616177	0.433088	0.988511
H	-2.764855	-0.215805	0.748133
H	-3.274660	1.457688	1.176559
H	-4.160876	0.050923	1.859776
H	-3.388411	1.885245	-1.217856

[P, Approximation: A Orientation: Downward]

C	-0.518440	-2.601363	0.075228
C	0.092232	-1.287887	0.572538
S	-2.236956	-2.415991	-0.501748
H	0.120288	-2.969618	-0.743566
H	0.048064	-0.541954	-0.234297
S	2.061203	-0.739960	-1.960766
C	2.680161	-1.112862	-0.517619
S	1.881208	-1.513088	0.965547
Cl	4.425165	-1.172680	-0.246913
H	-0.451785	-3.349509	0.885638
C	-0.598682	-0.738223	1.822821
H	-1.642682	-1.077302	1.767429
H	-0.151977	-1.167549	2.741352
O	-0.642369	0.667121	1.917079
C	0.570618	1.319221	2.203255
H	1.228381	0.676524	2.815366
H	0.314277	2.196570	2.821141
C	1.321343	1.800205	0.977563
C	0.628997	2.204239	-0.166810
C	2.717152	1.889254	0.989184
C	1.316328	2.704123	-1.272919
H	-0.458030	2.111717	-0.186999
C	3.406868	2.383782	-0.116534
H	3.271466	1.544994	1.866337
C	2.706971	2.797896	-1.250174
H	0.763469	3.010571	-2.162915
H	4.497031	2.431950	-0.098403
H	3.246551	3.176984	-2.119510
C	-4.275212	0.244802	-1.755519

H	-5.227025	-0.070587	-2.199232
H	-3.539762	-0.574983	-1.757571
N	-4.521980	0.637354	-0.335933
C	-5.088314	-0.525369	0.409067
H	-4.336823	-1.330905	0.404248
H	-5.302638	-0.203325	1.434933
H	-6.012037	-0.841578	-0.089770
C	-5.469904	1.777555	-0.283736
H	-6.424717	1.465352	-0.722943
H	-5.614733	2.069191	0.763008
H	-5.049125	2.614557	-0.852947
C	-3.217343	1.019461	0.286848
H	-2.541212	0.161038	0.162908
H	-2.836666	1.907577	-0.230028
H	-3.380025	1.235655	1.349062
H	-3.879220	1.117351	-2.288512

[R, Approximation: B Orientation: Upward]

C	1.555047	-1.393331	0.242914
C	0.507829	-2.361972	-0.152646
S	0.644943	-0.933350	-1.259625
H	-0.424459	-2.387743	0.422666
S	-3.001781	-2.414759	-0.996754
C	-3.361513	-1.401543	0.246699
Cl	-4.938105	-0.438116	0.028591
S	-2.560654	-1.049641	1.670649
H	2.593947	-1.676408	0.049102
C	1.301173	-0.534888	1.461876
H	1.785716	-1.001966	2.340703
H	0.215651	-0.524297	1.644029
O	1.714498	0.808088	1.342209
C	3.057187	1.061380	1.673862
H	3.296864	0.638114	2.666633
H	3.143670	2.156168	1.754459
C	4.047334	0.546922	0.651207
C	5.158889	-0.205059	1.035747
C	3.838913	0.805680	-0.708744
C	6.053357	-0.689854	0.079000
H	5.322616	-0.422354	2.094190
C	4.723637	0.317386	-1.665655
H	2.958265	1.375658	-1.013108
C	5.834898	-0.432734	-1.272819
H	6.917193	-1.279038	0.391542
H	4.544803	0.515318	-2.723892
H	6.527347	-0.818875	-2.022633
H	0.820217	-3.313764	-0.589049
C	-0.708674	2.135558	0.343149
H	-0.498925	2.965152	1.028332
H	0.101077	2.014161	-0.383422
N	-1.981222	2.420776	-0.383720
C	-1.885244	3.725871	-1.085720
H	-2.809350	3.888604	-1.652767
H	-1.754317	4.520539	-0.342090
H	-1.025697	3.698240	-1.765246
C	-3.103869	2.463134	0.597807
H	-2.884493	3.243914	1.335848
H	-4.030532	2.692955	0.060116
H	-3.182903	1.480841	1.082703
C	-2.218386	1.332228	-1.379827
H	-1.489358	1.445133	-2.190675
H	-2.064809	0.365238	-0.888432
H	-3.242452	1.415221	-1.760820

H	-0.843326	1.198360	0.894729

[TS, Approximation: B Orientation: Upward]

C	1.108464	-1.291141	-0.089301
C	0.118144	-2.361832	-0.026177
S	0.378947	-0.499696	-1.582904
H	-0.428692	-2.513231	0.909117
S	-2.178079	-2.286170	-0.873965
C	-3.032109	-1.555052	0.353475
Cl	-4.658114	-0.938388	-0.196703
S	-2.630422	-1.257069	1.933491
H	2.104371	-1.679022	-0.353029
C	1.139561	-0.439883	1.175330
H	1.724620	-0.968376	1.951906
H	0.106116	-0.359299	1.550612
O	1.637759	0.867003	1.002495
C	2.933082	1.105348	1.478670
H	3.043352	0.744477	2.518737
H	3.046647	2.201341	1.508769
C	4.037811	0.520889	0.622680
C	5.281564	0.223350	1.188517
C	3.843983	0.315995	-0.747030
C	6.322033	-0.263586	0.398140
H	5.436374	0.371576	2.260599
C	4.881737	-0.182223	-1.535044
H	2.862659	0.519600	-1.187526
C	6.123697	-0.468534	-0.967481
H	7.287833	-0.493239	0.851958
H	4.713844	-0.350972	-2.600449
H	6.934099	-0.857592	-1.586393
H	0.307233	-3.258113	-0.619633
C	-1.007272	2.080984	0.428546
H	-0.823922	2.801391	1.234767
H	-0.169537	2.034475	-0.274488
N	-2.251437	2.485968	-0.294113
C	-2.128079	3.894288	-0.751956
H	-3.021517	4.158874	-1.329589
H	-2.038842	4.545602	0.125122
H	-1.232939	3.980415	-1.378443
C	-3.414120	2.357182	0.628123
H	-3.244192	3.009288	1.493004
H	-4.323327	2.659171	0.095080
H	-3.493515	1.311851	0.952926
C	-2.448633	1.598126	-1.477942
H	-1.632492	1.780532	-2.185252
H	-2.402167	0.551291	-1.157936
H	-3.421020	1.831385	-1.927863
H	-1.175365	1.076879	0.833529

[P, Approximation: B Orientation: Upward]

C	0.618974	-0.758946	-0.842600
C	-0.291671	-1.891550	-1.320083
S	0.348936	0.747178	-1.841572
H	-0.218763	-2.816892	-0.727858
S	-2.051273	-1.408326	-1.371919
C	-2.735681	-2.096479	0.052631
Cl	-4.445520	-1.618747	0.111755
S	-2.092036	-3.003359	1.232133
H	1.644404	-1.130166	-1.017645
C	0.449790	-0.559144	0.664222
H	0.594761	-1.521886	1.192026
H	-0.589808	-0.237454	0.858233

O	1.290171	0.417015	1.238381
C	2.484624	-0.032938	1.811620
H	2.332432	-1.005729	2.316302
H	2.742215	0.693638	2.600927
C	3.662604	-0.137967	0.862959
C	4.802995	-0.845120	1.261156
C	3.655189	0.503815	-0.378129
C	5.923652	-0.907969	0.435181
H	4.812149	-1.354440	2.228910
C	4.774855	0.429954	-1.208884
H	2.752293	1.025499	-0.711906
C	5.912095	-0.268725	-0.805665
H	6.806130	-1.464308	0.756854
H	4.749926	0.920828	-2.183783
H	6.785513	-0.322555	-1.458063
H	-0.063509	-2.113461	-2.370583
C	-0.652202	2.714454	1.080591
H	-0.158708	3.645069	1.386275
H	-0.019238	2.138799	0.388355
N	-1.915185	3.067006	0.363053
C	-1.560361	3.823893	-0.871106
H	-2.481788	4.061352	-1.415475
H	-1.039757	4.743844	-0.580377
H	-0.903996	3.180209	-1.471977
C	-2.792692	3.885925	1.234523
H	-2.262049	4.804927	1.510138
H	-3.710519	4.129587	0.686390
H	-3.034273	3.307470	2.133817
C	-2.611931	1.806524	-0.034457
H	-1.926021	1.255003	-0.698400
H	-2.835809	1.231259	0.872966
H	-3.541972	2.069510	-0.553408
H	-0.906301	2.111198	1.960020

[R, Approximation: B Orientation: Downward]

C	1.694369	-2.236776	1.477219
C	2.355300	-1.060055	2.072646
S	0.822905	-1.553228	2.922468
H	2.314718	-0.113231	1.521089
H	3.273930	-1.216020	2.643046
S	3.704424	-0.192689	-1.426641
C	2.530291	0.912286	-1.123727
Cl	0.926922	0.627711	-2.056481
S	2.515378	2.259890	-0.138948
H	2.146193	-3.216334	1.661272
C	1.045826	-2.078961	0.136067
H	1.824867	-2.104442	-0.649591
H	0.569371	-1.082801	0.079086
O	0.109941	-3.104528	-0.080146
C	-0.650576	-2.879543	-1.234640
H	-1.036417	-3.859015	-1.559776
H	-0.024306	-2.480329	-2.053214
C	-1.820726	-1.949495	-0.987370
C	-2.258457	-1.057169	-1.970446
C	-2.508351	-2.014169	0.230396
C	-3.390156	-0.267414	-1.756322
H	-1.709962	-0.983451	-2.912645
C	-3.638101	-1.226809	0.446981
H	-2.142847	-2.692121	1.003900
C	-4.088631	-0.359018	-0.550715
H	-3.731889	0.414400	-2.537843
H	-4.176052	-1.297449	1.394451

H	-4.986105	0.242112	-0.390485
N	-1.337137	2.552321	0.821530
C	-1.127214	3.023134	-0.578927
H	-1.690357	2.363895	-1.250936
H	-0.054659	2.960737	-0.804416
H	-1.490694	4.054912	-0.654043
C	-0.551245	3.407937	1.753375
H	-0.899114	4.443229	1.658303
H	0.506634	3.328687	1.476365
H	-0.706714	3.045805	2.776137
C	-0.866588	1.137304	0.940670
H	-1.414222	0.525270	0.213261
H	-1.053722	0.783490	1.961388
H	0.208261	1.126270	0.717954
C	-2.779847	2.630994	1.163586
H	-3.108036	3.674093	1.083880
H	-2.919123	2.265946	2.187892
H	-3.335654	1.998196	0.462736

[TS, Approximation: B Orientation: Downward]

C	0.861089	-1.162162	1.887062
C	1.688829	0.046148	1.903835
S	-0.434392	-0.153360	2.701393
H	1.506943	0.814483	1.152242
H	2.167356	0.339607	2.835974
S	3.744124	-0.467581	0.900555
C	3.575536	0.179695	-0.646188
Cl	4.981570	-0.178669	-1.695949
S	2.361204	1.070369	-1.324885
H	1.223712	-1.957411	2.552013
C	0.533660	-1.713093	0.520827
H	1.463389	-2.084574	0.045028
H	0.141679	-0.903758	-0.119531
O	-0.392673	-2.763387	0.643036
C	-1.096251	-3.025006	-0.535355
H	-1.470909	-4.058553	-0.457775
H	-0.432822	-2.990035	-1.419854
C	-2.278538	-2.095737	-0.735436
C	-2.747129	-1.785375	-2.015999
C	-2.953510	-1.586575	0.380071
C	-3.890279	-1.001464	-2.183485
H	-2.217372	-2.169227	-2.891729
C	-4.095170	-0.803227	0.213666
H	-2.554697	-1.793558	1.374852
C	-4.571656	-0.513198	-1.067244
H	-4.251547	-0.775856	-3.188638
H	-4.620838	-0.422984	1.092347
H	-5.474428	0.087518	-1.195945
N	-1.581261	2.675193	0.020154
C	-1.904877	3.674355	-1.029491
H	-2.809854	3.351419	-1.556992
H	-1.062347	3.732139	-1.728364
H	-2.069134	4.648900	-0.554737
C	-0.342901	3.083051	0.746207
H	-0.498565	4.082496	1.169258
H	0.492816	3.088073	0.035789
H	-0.160554	2.344686	1.539096
C	-1.364292	1.333568	-0.600876
H	-2.280406	1.036843	-1.127219
H	-1.146125	0.634479	0.218129
H	-0.516957	1.398645	-1.293599
C	-2.705286	2.569567	0.992197

H	-2.842137	3.541608	1.480562
H	-2.442629	1.797133	1.726725
H	-3.611377	2.281903	0.446383

[P, Approximation: B Orientation: Downward]

C	0.984373	-0.399071	1.883281
C	2.007268	0.675407	1.515280
S	-0.483563	0.471836	2.544254
H	1.642295	1.321429	0.705113
H	2.209806	1.296303	2.396861
S	3.664634	0.069201	1.002591
C	3.628461	0.127539	-0.723334
Cl	5.168637	-0.457972	-1.342539
S	2.461542	0.621943	-1.738260
H	1.417591	-1.034993	2.674988
C	0.689991	-1.313392	0.703360
H	1.633932	-1.681566	0.248508
H	0.155811	-0.747186	-0.080419
O	-0.066547	-2.421301	1.123407
C	-0.747720	-3.049786	0.080462
H	-0.991066	-4.067135	0.428156
H	-0.105935	-3.162345	-0.814926
C	-2.038208	-2.345080	-0.293906
C	-2.545795	-2.400323	-1.595481
C	-2.763949	-1.671523	0.696051
C	-3.776459	-1.816643	-1.903922
H	-1.976300	-2.912781	-2.375444
C	-3.995953	-1.094774	0.389102
H	-2.326002	-1.570770	1.691413
C	-4.509515	-1.168994	-0.908253
H	-4.165578	-1.874278	-2.922341
H	-4.560749	-0.584799	1.172820
H	-5.479985	-0.726490	-1.142962
N	-2.019408	2.591982	-0.386446
C	-2.550872	3.400448	-1.510961
H	-3.380914	2.856461	-1.976925
H	-1.748286	3.557544	-2.241038
H	-2.900282	4.364400	-1.122613
C	-0.864405	3.292524	0.249461
H	-1.201674	4.278689	0.590891
H	-0.070824	3.400515	-0.500344
H	-0.524907	2.669667	1.094352
C	-1.564460	1.255162	-0.874782
H	-2.419250	0.732263	-1.323633
H	-1.195919	0.712865	0.009647
H	-0.767808	1.405176	-1.613671
C	-3.079742	2.376161	0.640051
H	-3.367260	3.348118	1.058099
H	-2.657668	1.720343	1.414880
H	-3.937510	1.897017	0.153804

Neutral reaction (using Choline as a counter cation):

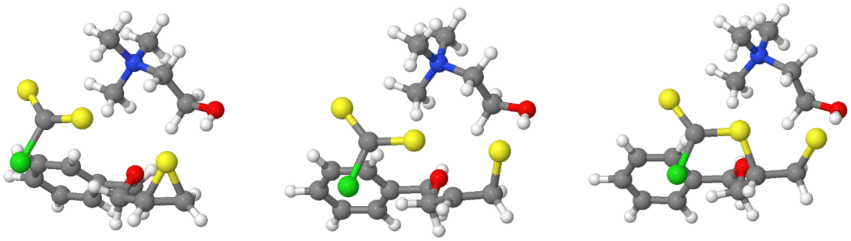


Figure S39. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_A).

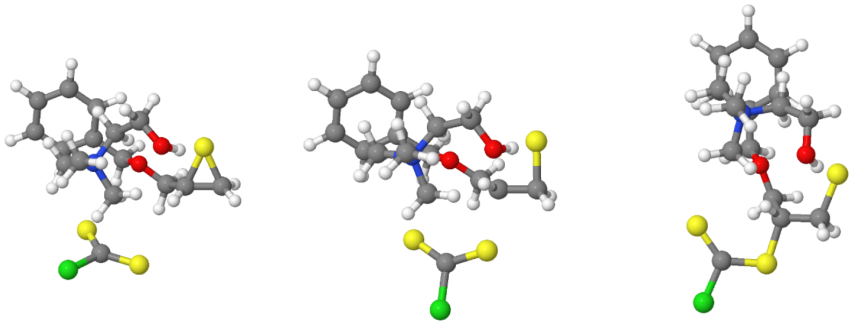


Figure S40. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_A).

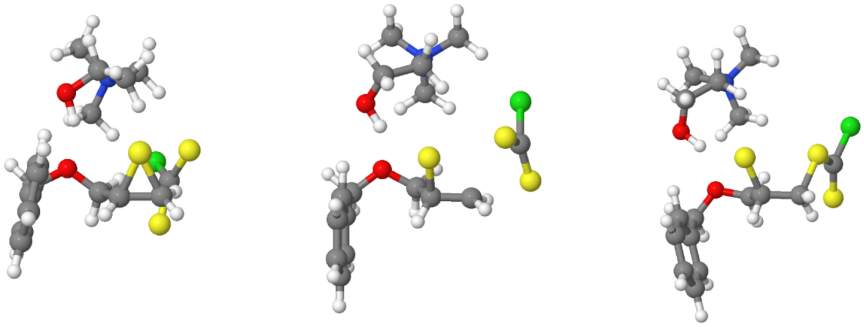


Figure S41. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_B).

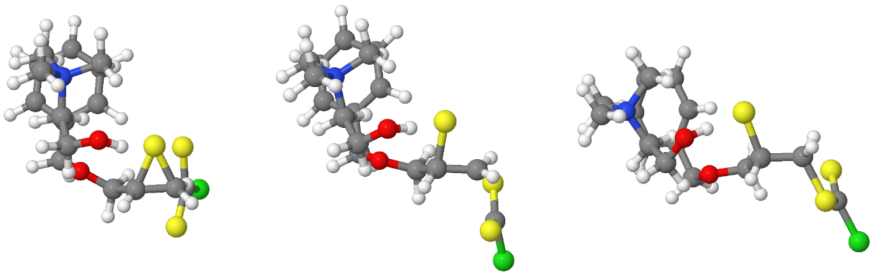


Figure S42. Reactant (left), transition state (center) and product (right) of the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_B).

Approximation	Orientation	R	TS	P
A	upward	0.0	44.8	10.9
A	downward	0.0	24.9	9.5
B	upward	0.0	47.9	9.8
B	downward	0.0	14.0	-2.8

Table S32. Energies of the reactants (R), transition state (TS) and products (P) involved in the solvated reaction between CS_2Cl^- + Choline and 4-R1i across various approximations and orientations. All energies are reported, relative to the reactant complex, as the Morokuma-corrected Gibbs free energies (373.15 K).

Atom	R	TS	P
C_A	-0.02	+0.05	+0.01
C_B	-0.02	+0.05	+0.03
S'	+0.11	+0.24	+0.43
S	-0.09	-0.41	-0.52

Table S33. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	-0.02	+0.01	+0.01
C_B	+0.01	+0.05	+0.05
S'	+0.16	+0.24	+0.38
S	-0.14	-0.43	-0.57

Table S34. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	-0.03	+0.01	+0.03
C_B	-0.03	+0.01	+0.01
S'	+0.08	+0.28	+0.41
S	-0.14	-0.43	-0.60

Table S35. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atom	R	TS	P
C_A	-0.01	+0.03	+0.05
C_B	-0.02	+0.01	+0.00
S'	+0.13	+0.21	+0.34
S	-0.20	-0.46	-0.60

Table S36. Atomic charges (in electrons) for the most relevant atoms involved in the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.01	0.36	0.09
S-C_B	1.05	1.07	1.16
C_A-S'	0.01	0.38	0.94

Table S37. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.00	0.42	0.09
S-C_B	1.04	1.08	1.15
C_A-S'	0.02	0.49	0.96

Table S38. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_A). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.02	1.04	1.12
S-C_B	1.04	0.42	0.09
C_B-S'	0.03	0.43	0.98

Table S39. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and 4-R1i (upward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

Atomic Pair	R	TS	P
S-C_A	1.00	1.04	1.12
S-C_B	1.01	0.51	0.10
C_B-S'	0.03	0.46	0.99

Table S40. Delocalization Index (DI, in electron pairs) for the most relevant atomic pairs involved in the reaction between CS_2Cl^- + Choline and 4-R1i (downward attack to C_B). The results for the reactants (R), transition state (TS) and product (P) are shown.

The upcoming section comprises the optimized geometries of the reactants (R), transition state (TS) and product (P) involved in the reaction across different approximations and orientations. All values are reported as XYZ Cartesian Coordinates in Angstroms.

[R, Approximation: A Orientation: Upward]

C	2.445016	-3.213720	0.977560
C	1.305162	-2.608048	1.693394
H	2.991567	-4.033252	1.450313
H	1.112624	-2.977212	2.705363
S	-1.656490	2.845067	1.030259
C	-0.990864	1.620837	1.928202
S	0.595810	1.164116	2.169100
Cl	-2.206135	0.566675	2.804879
H	2.381304	-3.253883	-0.113897
C	0.039379	-2.199048	0.981507
H	-0.626812	-3.081402	0.955853
H	-0.464276	-1.413843	1.568836
O	0.312478	-1.753296	-0.326204
C	-0.516022	-2.265448	-1.336169
H	-0.582906	-3.367368	-1.260354
H	-0.006084	-2.048416	-2.290309
C	-1.909389	-1.671285	-1.361198

C	-2.243098	-0.578398	-0.560262
C	-2.879318	-2.207482	-2.217403
C	-3.523977	-0.024321	-0.606734
H	-1.503630	-0.160295	0.122850
C	-4.155504	-1.652637	-2.271782
H	-2.631772	-3.068511	-2.844314
C	-4.481812	-0.558575	-1.465362
H	-3.749826	0.826062	0.040733
H	-4.903783	-2.079110	-2.942425
H	-5.484677	-0.130104	-1.504439
C	2.719822	1.266113	-1.127343
N	1.565380	2.095996	-1.616803
C	1.470981	3.309586	-0.749903
H	0.673128	3.952183	-1.137697
H	1.221437	2.986116	0.269561
H	2.436483	3.828498	-0.780243
C	1.769029	2.522600	-3.025952
H	2.694319	3.107268	-3.088661
H	1.831253	1.641832	-3.673427
H	0.912654	3.138269	-3.324658
C	0.294447	1.316098	-1.500947
H	0.264200	0.874015	-0.497207
H	-0.549988	1.998715	-1.643476
H	0.287287	0.531692	-2.266564
C	2.834145	-0.123757	-1.749792
H	2.577962	1.164035	-0.040489
H	3.635974	1.839808	-1.323500
O	4.029048	-0.709702	-1.319136
H	2.874960	-0.064157	-2.848527
H	1.963979	-0.732542	-1.456495
H	3.869658	-1.012843	-0.413392
S	2.780768	-1.550564	1.643583

[TS, Approximation: A Orientation: Upward]

C	1.773337	-3.095501	-0.705409
C	0.614243	-2.739620	0.101252
H	1.943948	-4.182352	-0.714764
H	0.397933	-3.355716	0.976378
S	-0.996677	1.453629	2.799647
C	-0.697304	-0.106871	2.367289
S	0.749701	-0.771790	1.782922
Cl	-2.051177	-1.280469	2.543168
H	1.713367	-2.701852	-1.728652
C	-0.572821	-2.133089	-0.570927
H	-0.961901	-2.966438	-1.202691
H	-1.362479	-1.867089	0.145091
O	-0.204413	-1.053753	-1.385595
C	-1.139045	-0.727128	-2.384129
H	-1.367919	-1.614387	-3.003560
H	-0.632292	-0.001771	-3.041082
C	-2.426291	-0.129870	-1.853983
C	-2.468694	0.469325	-0.593001
C	-3.586927	-0.149492	-2.634185
C	-3.648944	1.033481	-0.110347
H	-1.574140	0.473819	0.030848
C	-4.764117	0.429359	-2.162479
H	-3.570308	-0.625757	-3.617947
C	-4.799508	1.019440	-0.897594
H	-3.658242	1.469895	0.890853
H	-5.663516	0.408512	-2.780471
H	-5.726087	1.458241	-0.523987
C	3.006210	1.302894	-0.479677

N	2.061731	2.442171	-0.187633
C	2.164033	2.762168	1.266276
H	1.566803	3.658203	1.472160
H	1.767250	1.912014	1.834972
H	3.218513	2.939401	1.508152
C	2.430150	3.644425	-0.980026
H	3.428885	3.976013	-0.673142
H	2.428988	3.391522	-2.045697
H	1.693712	4.432392	-0.783397
C	0.654297	2.046619	-0.497377
H	0.475011	1.060337	-0.050531
H	-0.021518	2.797355	-0.071394
H	0.529731	2.000553	-1.585391
C	2.785557	0.579475	-1.808398
H	2.883169	0.572738	0.333471
H	4.023088	1.717331	-0.450437
O	3.860807	-0.274531	-2.032654
H	2.740907	1.295208	-2.646753
H	1.826797	0.032493	-1.766991
H	3.776205	-0.994358	-1.364510
S	3.082338	-2.258148	0.288763

[P, Approximation: A Orientation: Upward]

C	1.628353	-2.023124	-1.825849
C	0.373672	-2.095484	-0.937310
H	1.512297	-2.817561	-2.581993
H	0.095321	-3.141243	-0.747995
S	-0.724485	-0.541268	3.028886
C	-0.558958	-1.470746	1.691940
S	0.850778	-1.385840	0.699356
Cl	-1.741085	-2.725066	1.341882
H	1.605782	-1.067839	-2.374029
C	-0.796525	-1.350636	-1.560396
H	-0.925174	-1.740756	-2.589104
H	-1.737918	-1.534249	-1.017434
O	-0.507113	0.028607	-1.600698
C	-1.496264	0.799578	-2.230073
H	-1.751603	0.376347	-3.219187
H	-1.044908	1.788202	-2.413089
C	-2.755431	0.958665	-1.401933
C	-2.707966	0.830315	-0.010950
C	-3.976085	1.255750	-2.014709
C	-3.861255	0.987460	0.756426
H	-1.759644	0.585229	0.471558
C	-5.127761	1.430383	-1.248181
H	-4.026677	1.345478	-3.102870
C	-5.074332	1.292881	0.139382
H	-3.808382	0.860842	1.839516
H	-6.075137	1.661638	-1.738288
H	-5.979066	1.414947	0.737041
C	3.127700	1.330022	0.113698
N	2.283076	2.241393	0.978462
C	2.380813	1.767945	2.388891
H	1.890399	2.500403	3.041558
H	1.871337	0.799685	2.467715
H	3.440459	1.669905	2.651597
C	2.799644	3.634541	0.894842
H	3.809248	3.660685	1.320137
H	2.827355	3.945213	-0.155255
H	2.132568	4.293203	1.463439
C	0.846609	2.222740	0.561347
H	0.520666	1.181135	0.455162

H	0.259985	2.738136	1.331400
H	0.746095	2.744639	-0.396479
C	2.770691	1.313119	-1.372903
H	3.030141	0.306720	0.501890
H	4.168898	1.656091	0.238049
O	3.753689	0.625816	-2.067893
H	2.722229	2.340556	-1.775347
H	1.767649	0.862421	-1.495609
H	3.733229	-0.321326	-1.753653
S	3.197566	-2.198390	-0.924275

[R, Approximation: A Orientation: Downward]

C	2.439681	3.016020	-1.891221
C	1.660946	1.887660	-1.352588
H	3.419734	3.223403	-1.456433
H	2.123195	1.343364	-0.524594
S	0.574618	-2.556885	-1.170314
C	2.029885	-2.359283	-0.406145
S	3.313599	-1.354030	-0.699694
Cl	2.236789	-3.439617	1.094237
H	2.342681	3.250200	-2.954880
C	0.780287	1.056204	-2.241618
H	0.534126	1.626007	-3.158038
H	1.323295	0.131712	-2.517021
O	-0.396239	0.732192	-1.542018
C	-1.344104	0.073815	-2.354764
H	-0.900875	-0.832053	-2.799666
H	-1.648730	0.749609	-3.177981
C	-2.535332	-0.285629	-1.508887
C	-2.922711	-1.615903	-1.330130
C	-3.239902	0.724851	-0.842415
C	-3.994962	-1.934571	-0.494183
H	-2.367250	-2.410106	-1.833451
C	-4.307623	0.409514	-0.004542
H	-2.937973	1.765799	-0.984504
C	-4.685704	-0.924025	0.173166
H	-4.286143	-2.977756	-0.360953
H	-4.854060	1.204878	0.506411
H	-5.523985	-1.172986	0.826323
H	1.303877	3.172852	1.429486
O	1.047968	2.883831	2.322957
C	-0.339190	2.713290	2.350231
H	-0.649179	2.735637	3.405458
H	-0.871982	3.546880	1.857345
C	-0.854134	1.442778	1.684725
H	-1.935181	1.364471	1.871114
H	-0.697097	1.445329	0.595006
N	-0.234997	0.157083	2.177257
C	-1.110463	-0.974418	1.750286
H	-1.274556	-0.888315	0.669434
H	-0.588957	-1.916949	1.958083
H	-2.059832	-0.916444	2.296321
C	-0.082438	0.147914	3.654330
H	-1.051423	0.371664	4.117467
H	0.255127	-0.850573	3.955423
H	0.666139	0.895868	3.938887
C	1.100664	-0.048060	1.531923
H	0.925793	-0.131024	0.453324
H	1.740218	0.803125	1.779424
H	1.526397	-0.985480	1.908710
S	1.006970	3.530644	-0.892494

[TS, Approximation: A Orientation: Downward]

C	-2.493311	-2.271721	-1.568512
C	-1.643439	-1.188953	-1.063194
H	-3.194507	-2.677520	-0.828651
H	-1.172915	-1.365155	-0.101620
S	-1.302619	2.498172	0.040296
C	-2.743067	1.751838	0.310567
S	-3.252269	0.167952	0.005478
Cl	-4.046790	2.737649	1.053852
H	-3.014674	-2.030610	-2.504338
C	-0.934641	-0.253841	-2.006093
H	-0.852191	-0.735797	-2.996051
H	-1.508030	0.683457	-2.119741
O	0.337096	0.030066	-1.480102
C	1.018022	1.023371	-2.207981
H	0.414165	1.947451	-2.243738
H	1.179397	0.680947	-3.248328
C	2.336264	1.285884	-1.532230
C	2.603553	2.512211	-0.918780
C	3.291194	0.263498	-1.457711
C	3.806373	2.716963	-0.238569
H	1.859567	3.310663	-0.968028
C	4.490283	0.463914	-0.777466
H	3.082948	-0.695211	-1.939557
C	4.749049	1.692592	-0.163650
H	4.005359	3.680187	0.234358
H	5.231498	-0.336440	-0.731703
H	5.690694	1.852762	0.364559
H	-0.693589	-3.440901	0.309578
O	-0.346535	-3.290881	1.227680
C	1.038396	-3.191519	1.112042
H	1.511295	-3.693813	1.972362
H	1.408440	-3.709320	0.209147
C	1.558937	-1.766790	0.987603
H	2.657796	-1.789222	0.949277
H	1.184553	-1.282825	0.072971
N	1.201589	-0.836913	2.130361
C	2.091944	0.355724	2.037207
H	1.992521	0.781659	1.031114
H	1.777623	1.088745	2.789470
H	3.126527	0.041235	2.217399
C	1.391096	-1.499928	3.446121
H	2.407657	-1.908633	3.498623
H	1.245624	-0.750756	4.233218
H	0.649659	-2.299573	3.552103
C	-0.216125	-0.369298	2.011825
H	-0.320377	0.162708	1.056554
H	-0.871279	-1.243990	2.054936
H	-0.418559	0.317713	2.842806
S	-1.006771	-3.311534	-1.817176

[P, Approximation: A Orientation: Downward]

C	1.717366	1.583515	-2.080374
C	1.876444	0.449541	-1.068341
H	2.277801	2.459718	-1.715371
H	1.470690	0.751297	-0.094080
S	2.536228	-1.208521	1.608705
C	3.751050	-0.686067	0.668438
S	3.686232	0.220767	-0.799040
Cl	5.432034	-1.011102	1.078509
H	2.195458	1.278013	-3.028178
C	1.231955	-0.872508	-1.492729

H	1.080702	-0.863323	-2.588584
H	1.890148	-1.725751	-1.244348
O	-0.004310	-1.035791	-0.843783
C	-0.597493	-2.277565	-1.121762
H	-0.115947	-3.084675	-0.537282
H	-0.466174	-2.523976	-2.192856
C	-2.068312	-2.197364	-0.812307
C	-2.690704	-3.092441	0.060176
C	-2.825850	-1.183137	-1.413111
C	-4.057123	-2.981535	0.330496
H	-2.101461	-3.880546	0.534810
C	-4.188342	-1.072864	-1.145069
H	-2.320622	-0.476876	-2.079345
C	-4.806814	-1.971442	-0.270476
H	-4.535303	-3.686651	1.012660
H	-4.773815	-0.284712	-1.622850
H	-5.875229	-1.886753	-0.063726
H	-0.265939	3.120789	-0.608307
O	-0.691232	3.517296	0.214172
C	-2.034245	3.193596	0.075322
H	-2.635626	3.865690	0.708973
H	-2.388572	3.343470	-0.962181
C	-2.347984	1.736971	0.386604
H	-3.429764	1.559336	0.304005
H	-1.806797	1.088582	-0.319701
N	-1.937178	1.274623	1.772327
C	-2.734462	0.064085	2.112024
H	-2.610631	-0.670071	1.306526
H	-2.365676	-0.346360	3.059646
H	-3.789713	0.347324	2.204336
C	-2.169228	2.328915	2.793633
H	-3.215672	2.653228	2.744852
H	-1.953415	1.904333	3.781251
H	-1.495153	3.167245	2.586615
C	-0.487332	0.901878	1.770968
H	-0.341479	0.079732	1.057604
H	0.078672	1.783699	1.455360
H	-0.212492	0.595154	2.787886
S	-0.030431	2.006813	-2.369210

[R, Approximation: B Orientation: Upward]

C	-1.511744	-1.374921	0.794414
C	-0.774278	-1.959082	1.932608
H	0.300438	-2.138949	1.810004
S	2.782278	-1.182859	1.471192
C	2.952708	-1.981460	0.013597
Cl	4.299344	-1.291281	-1.060947
S	2.135296	-3.256326	-0.629900
H	-2.561395	-1.659928	0.679147
C	-0.739382	-1.084460	-0.471277
H	-0.861295	-1.915933	-1.187904
H	0.328694	-1.013109	-0.215788
O	-1.089198	0.136886	-1.095234
C	-2.221483	0.117112	-1.944262
H	-2.127160	-0.708866	-2.669956
H	-2.181235	1.064012	-2.503643
C	-3.529604	0.010526	-1.196042
C	-4.445994	-1.002112	-1.485666
C	-3.815180	0.921219	-0.171102
C	-5.633724	-1.110354	-0.759553
H	-4.224314	-1.719724	-2.279515
C	-4.994588	0.809094	0.559702

H	-3.095861	1.712303	0.058836
C	-5.906162	-0.208394	0.267136
H	-6.342364	-1.907225	-0.991226
H	-5.204974	1.516576	1.363413
H	-6.829604	-0.296458	0.841883
H	-1.306896	-2.655814	2.584026
C	1.911447	1.407647	-1.301920
H	0.852301	1.553273	-1.528772
H	2.092335	0.397591	-0.916311
N	2.322391	2.385831	-0.247327
C	2.206239	3.766906	-0.786727
H	2.452453	4.481770	0.007566
H	2.915798	3.870811	-1.615671
H	1.181482	3.919339	-1.142281
C	3.745308	2.110525	0.115119
H	4.347830	2.136751	-0.800212
H	4.082242	2.882419	0.816726
H	3.798077	1.113049	0.573189
C	1.471756	2.201328	0.993624
H	2.532693	1.579751	-2.188900
C	0.127721	2.913306	0.977971
H	2.062017	2.575628	1.841798
H	1.347421	1.115093	1.119779
O	-0.665605	2.640875	-0.137204
H	-0.362020	2.627801	1.926337
H	0.271016	4.003651	1.016905
H	-0.828223	1.678800	-0.218899
S	-1.230379	-0.211129	2.159998

[TS, Approximation: B Orientation: Upward]

C	1.202184	-1.331308	-0.387591
C	0.233057	-2.258981	-0.953367
H	-0.434267	-2.831359	-0.297970
S	-2.090212	-1.391058	-1.411328
C	-2.926443	-2.132670	-0.156961
Cl	-4.291961	-1.126452	0.517176
S	-2.637874	-3.573763	0.580143
H	2.245426	-1.656385	-0.525718
C	0.868363	-0.962986	1.055645
H	1.258220	-1.742080	1.738755
H	-0.229605	-0.957991	1.155784
O	1.310898	0.307679	1.463997
C	2.608210	0.365355	2.014820
H	2.678858	-0.308300	2.888395
H	2.724194	1.398393	2.374653
C	3.700688	0.033622	1.024797
C	4.581436	-1.027456	1.249755
C	3.808449	0.773448	-0.159148
C	5.557922	-1.350762	0.306327
H	4.496592	-1.611673	2.169641
C	4.774384	0.445036	-1.106732
H	3.113414	1.596116	-0.340972
C	5.650402	-0.617803	-0.876106
H	6.240495	-2.182080	0.490945
H	4.840218	1.016891	-2.033753
H	6.405912	-0.874423	-1.620744
H	0.484290	-2.738226	-1.901546
C	-1.766793	1.423005	1.112033
H	-0.714921	1.569799	1.375382
H	-1.897310	0.493251	0.544612
N	-2.222407	2.550932	0.237016
C	-2.077088	3.837194	0.967078

H	-2.362785	4.660300	0.300788
H	-2.739582	3.815840	1.840330
H	-1.034270	3.938763	1.286504
C	-3.655408	2.319332	-0.100919
H	-4.226157	2.228873	0.830942
H	-4.021525	3.165838	-0.693267
H	-3.727079	1.383917	-0.668886
C	-1.441714	2.560931	-1.059067
H	-2.401291	1.413211	2.006641
C	-0.053658	3.186680	-0.973051
H	-2.043377	3.125290	-1.785370
H	-1.379579	1.509811	-1.374852
O	0.730521	2.729064	0.083526
H	0.413122	2.999201	-1.957731
H	-0.138435	4.279145	-0.866338
H	0.895319	1.771074	-0.044700
S	0.813024	-0.037667	-1.635559

[P, Approximation: B Orientation: Upward]

C	0.850468	-1.072327	-0.674549
C	-0.020539	-2.212381	-1.202788
H	0.013437	-3.130285	-0.596427
S	-1.773190	-1.711814	-1.345904
C	-2.556229	-2.510864	-0.031336
Cl	-4.272336	-2.059220	-0.075656
S	-1.987919	-3.479903	1.137830
H	1.892700	-1.414670	-0.794786
C	0.567325	-0.879860	0.819668
H	0.911291	-1.769033	1.385227
H	-0.523842	-0.815476	0.963907
O	1.105864	0.288788	1.388333
C	2.376692	0.168986	1.976426
H	2.362386	-0.607096	2.765235
H	2.562789	1.138059	2.463899
C	3.490654	-0.131168	0.998715
C	4.292570	-1.264912	1.149351
C	3.709344	0.721518	-0.090491
C	5.304014	-1.548257	0.229647
H	4.118847	-1.937898	1.993117
C	4.712134	0.435875	-1.013308
H	3.066340	1.593610	-0.223369
C	5.511382	-0.698812	-0.855726
H	5.923554	-2.437836	0.356696
H	4.864571	1.097584	-1.867622
H	6.294846	-0.920885	-1.582584
H	0.269529	-2.446282	-2.235142
C	-1.801780	1.542256	0.929939
H	-0.744556	1.565849	1.214507
H	-1.955595	0.775312	0.161204
N	-2.187097	2.868273	0.347425
C	-1.944993	3.934951	1.355512
H	-2.191805	4.907638	0.913118
H	-2.587959	3.741649	2.222470
H	-0.890477	3.896150	1.648652
C	-3.635099	2.820716	0.007995
H	-4.201709	2.566367	0.911399
H	-3.946336	3.799880	-0.373540
H	-3.786748	2.049985	-0.756946
C	-1.416701	3.134635	-0.930305
H	-2.447006	1.358800	1.798798
C	0.013930	3.631865	-0.728401

H	-1.989930	3.887169	-1.490066
H	-1.409522	2.180246	-1.474463
O	0.757983	2.892488	0.180391
H	0.460365	3.634615	-1.741238
H	0.001875	4.679950	-0.388212
H	0.855090	1.977646	-0.210497
S	0.597823	0.421359	-1.691991

[R, Approximation: B Orientation: Downward]

C	0.550677	-2.275469	-0.602532
C	1.406049	-2.748838	0.498515
H	2.255629	-2.115088	0.773581
H	1.525507	-3.825188	0.640640
S	4.354782	-1.217986	-0.880068
C	4.295555	-0.026987	0.276467
Cl	5.821659	0.973445	0.415607
S	3.090898	0.417183	1.340259
H	0.041173	-3.042432	-1.196313
C	0.896565	-1.015291	-1.342326
H	1.504823	-1.272877	-2.228345
H	1.509651	-0.366849	-0.694185
O	-0.309280	-0.387796	-1.737860
C	-0.179867	0.950285	-2.154036
H	-0.796538	1.092425	-3.056102
H	0.864471	1.161136	-2.446034
C	-0.613660	1.939459	-1.089665
C	-1.321435	3.091467	-1.445286
C	-0.292487	1.731622	0.259176
C	-1.687334	4.032882	-0.480447
H	-1.581914	3.259962	-2.493542
C	-0.654684	2.672970	1.222887
H	0.257303	0.836707	0.562236
C	-1.351524	3.827374	0.857129
H	-2.232006	4.931079	-0.777239
H	-0.375195	2.507151	2.265196
H	-1.625460	4.566247	1.612144
N	-4.002601	-0.162143	0.482524
C	-3.497946	-0.530980	1.840422
H	-3.377269	-1.616965	1.880397
H	-4.228345	-0.191680	2.584593
H	-2.535938	-0.026868	1.996800
C	-4.110970	1.323554	0.409492
H	-3.103706	1.749177	0.498322
H	-4.745896	1.670461	1.233145
H	-4.553221	1.598902	-0.554377
C	-5.341059	-0.774844	0.267441
H	-5.261263	-1.855880	0.425397
H	-5.671557	-0.555398	-0.754848
H	-6.040708	-0.338227	0.989176
C	-3.012188	-0.606115	-0.571741
C	-3.100617	-2.067612	-0.986489
H	-2.017142	-0.354965	-0.185562
H	-3.186642	0.018775	-1.459523
O	-3.086913	-2.989169	0.067028
H	-2.260719	-2.207870	-1.689057
H	-4.025003	-2.242953	-1.556603
H	-2.180533	-3.052280	0.417488
S	-0.186330	-2.065771	1.063698

[TS, Approximation: B Orientation: Downward]

C	1.138352	-1.267834	0.033300
C	2.183482	-1.580010	1.002036

H	2.542651	-0.798280	1.671827
H	2.412278	-2.619129	1.225894
S	4.266848	-1.419610	-0.258685
C	4.769388	0.154844	0.080880
Cl	6.292562	0.592101	-0.778439
S	4.109272	1.311512	1.047638
H	1.011573	-2.030119	-0.746792
C	1.120747	0.126662	-0.535254
H	1.973927	0.250219	-1.230265
H	1.239195	0.860649	0.279649
O	-0.101033	0.304177	-1.221067
C	-0.418255	1.627011	-1.562299
H	-0.821028	1.632238	-2.588186
H	0.493811	2.251423	-1.580042
C	-1.438041	2.248251	-0.626355
C	-2.324875	3.217996	-1.105505
C	-1.504293	1.877759	0.723189
C	-3.253185	3.819720	-0.254796
H	-2.287632	3.506790	-2.159201
C	-2.429222	2.484080	1.575662
H	-0.842514	1.095911	1.107463
C	-3.306067	3.456161	1.091138
H	-3.936723	4.575811	-0.645350
H	-2.460799	2.193708	2.627843
H	-4.026044	3.930462	1.760141
N	-3.999584	-1.173255	-0.120286
C	-3.692244	-1.298644	1.337273
H	-3.146333	-2.232848	1.492603
H	-4.639016	-1.297357	1.890920
H	-3.071119	-0.443912	1.630965
C	-4.693603	0.125743	-0.351479
H	-3.994265	0.941477	-0.128144
H	-5.566764	0.182162	0.309222
H	-5.007583	0.174223	-1.400624
C	-4.887244	-2.292667	-0.534467
H	-4.398535	-3.238511	-0.276446
H	-5.059778	-2.226854	-1.615289
H	-5.837958	-2.195571	0.002841
C	-2.709450	-1.161359	-0.913468
C	-2.117309	-2.529855	-1.220577
H	-1.998803	-0.554433	-0.340247
H	-2.920385	-0.643845	-1.860217
O	-1.965591	-3.367894	-0.115895
H	-1.159466	-2.309638	-1.725847
H	-2.744854	-3.059435	-1.953807
H	-1.255951	-2.991095	0.452802
S	0.025727	-1.538426	1.469409

[P, Approximation: B Orientation: Downward]

C	1.240784	-1.161466	0.324305
C	2.585698	-1.371786	1.018292
H	2.758092	-0.625383	1.806415
H	2.600884	-2.369403	1.474963
S	4.045589	-1.371098	-0.090161
C	4.698718	0.227449	0.038852
Cl	6.113694	0.336440	-1.008939
S	4.213750	1.488014	0.929657
H	1.161698	-1.892499	-0.499645
C	1.144029	0.222880	-0.297015
H	2.020348	0.424549	-0.946168
H	1.135247	0.984203	0.504032
O	-0.028193	0.294636	-1.081610

C	-0.401291	1.579259	-1.490543
H	-0.804920	1.506773	-2.513955
H	0.483077	2.241781	-1.551709
C	-1.447007	2.218607	-0.594094
C	-2.281761	3.218350	-1.106273
C	-1.595927	1.828815	0.742774
C	-3.242109	3.829048	-0.299547
H	-2.180419	3.521281	-2.152039
C	-2.552285	2.447362	1.551317
H	-0.985484	1.013035	1.146975
C	-3.378243	3.447023	1.035951
H	-3.886283	4.605970	-0.715515
H	-2.651574	2.138677	2.594298
H	-4.124833	3.927369	1.670834
N	-3.951099	-1.243671	-0.202790
C	-3.686441	-1.371474	1.263492
H	-3.127642	-2.295630	1.430380
H	-4.651469	-1.384632	1.784936
H	-3.078882	-0.515188	1.578129
C	-4.676244	0.034754	-0.444209
H	-4.011623	0.868034	-0.182357
H	-5.576017	0.055200	0.182123
H	-4.951197	0.089725	-1.503998
C	-4.788397	-2.387253	-0.650611
H	-4.269782	-3.316589	-0.390284
H	-4.935973	-2.316532	-1.734975
H	-5.755001	-2.331648	-0.135893
C	-2.639035	-1.184860	-0.959900
C	-1.985459	-2.531547	-1.240691
H	-1.960445	-0.571010	-0.355889
H	-2.845798	-0.673896	-1.911558
O	-1.834405	-3.347558	-0.125468
H	-1.020621	-2.267269	-1.713749
H	-2.564115	-3.088106	-1.996243
H	-1.194011	-2.880826	0.488620
S	-0.067323	-1.473751	1.567866

4. Optimized geometries

The current section gathers the energetically minimized geometries of the different stationary points found across the computational studies for the transformation of **(R)-1a/(S)-1a** to **(R)-2a/(S)-2a**. All values are reported, as XYZ Cartesian coordinates, in Angstroms.

[CS_2ClLi]

C	0.026058	-0.000301	0.003157
S	-0.714650	1.508126	0.007361
Cl	1.785779	-0.000974	-0.006500
Li	-2.537424	0.001420	-0.048004
S	-0.716744	-1.507245	0.007361

[CSOClLi]

C	0.000000	0.311590	0.000000
S	-1.343371	-0.730351	0.000000
Cl	1.623290	-0.423061	0.000000
Li	-1.926908	1.572707	0.000000
O	-0.040159	1.536250	0.000000

[LiCl]

Cl	0.000000	0.000000	0.308267
Li	0.000000	0.000000	-1.746846

[1D]

C	-1.053341	-0.215288	1.571349
C	0.255350	0.511042	1.151635
H	0.114745	1.546037	0.813172
H	0.969321	0.484207	1.984782
O	-0.814334	-1.522146	1.807607
C	-2.149100	0.039869	0.524741
C	-2.766825	-1.035751	-0.113843
C	-2.559717	1.339274	0.199358
C	-3.760661	-0.822982	-1.071516
H	-2.460445	-2.042919	0.170504
C	-3.550987	1.556834	-0.754617
H	-2.104309	2.195194	0.706028
C	-4.153479	0.473281	-1.397942
H	-4.234825	-1.675659	-1.561867
H	-3.858802	2.575916	-0.996538
H	-4.930649	0.641733	-2.145448
S	0.959142	-0.473389	-0.218922
C	2.615625	0.025255	-0.419473
Cl	3.119202	1.418265	0.512274
S	3.618146	-0.732092	-1.438184
Li	0.290493	-2.647334	1.250723
H	-1.376066	0.342652	2.483226

[R1A]

C	-1.606400	0.578760	-0.223970
C	-2.568750	0.019180	0.742360
O	-2.462830	-0.484630	-0.566420
H	-3.490370	0.565950	0.969490
H	-2.189870	-0.635950	1.535160
C	-0.150040	0.270120	-0.127580
C	0.784660	1.307200	-0.057530
C	0.290690	-1.056700	-0.091690
C	2.143900	1.022040	0.062850
H	0.444361	2.344530	-0.099610
C	1.649890	-1.340160	0.026260
H	-0.444730	-1.859500	-0.172260

C	2.579440	-0.302380	0.106610
H	2.866851	1.837720	0.117960
H	1.987100	-2.377880	0.049680
H	3.643660	-0.525980	0.196890
H	-1.854730	1.539810	-0.689800

[TS-R1A]

C	-1.606400	0.578760	-0.223970
C	-2.568750	0.019180	0.742360
O	-2.462830	-0.484630	-0.566420
H	-3.490370	0.565950	0.969490
H	-2.189870	-0.635950	1.535160
C	-0.150040	0.270120	-0.127580
C	0.784660	1.307200	-0.057530
C	0.290690	-1.056700	-0.091690
C	2.143900	1.022040	0.062850
H	0.444361	2.344530	-0.099610
C	1.649890	-1.340160	0.026260
H	-0.444730	-1.859500	-0.172260
C	2.579440	-0.302380	0.106610
H	2.866851	1.837720	0.117960
H	1.987100	-2.377880	0.049680
H	3.643660	-0.525980	0.196890
H	-1.854730	1.539810	-0.689800

[TS-R1B]

C	0.034127	2.424296	0.040867
C	-0.633180	1.420731	-0.805190
O	-1.241127	2.624286	0.536782
H	0.803022	2.099583	0.761595
S	1.568524	0.390417	-1.401706
C	1.967045	-0.246321	0.102772
Cl	3.600432	-0.944369	0.149068
S	1.126597	-0.372920	1.543363
Li	-1.038554	1.151512	1.689784
H	0.445211	3.250923	-0.562875
C	-1.494035	0.210325	-0.464065
C	-1.151600	-1.114041	-0.784179
C	-2.781560	0.432262	0.067627
C	-2.024665	-2.166002	-0.523845
H	-0.188314	-1.334173	-1.237324
C	-3.648813	-0.628457	0.339302
H	-3.109396	1.454722	0.250199
C	-3.272739	-1.935976	0.052563
H	-1.714207	-3.181974	-0.772100
H	-4.632062	-0.415347	0.761997
H	-3.948011	-2.766776	0.261994
H	-0.908319	1.837637	-1.782887

[TS-R1C]

C	-0.683129	-0.133768	0.162301
C	-0.066512	0.078698	-1.155040
O	-0.247046	-1.432374	0.232813
H	-0.235305	0.539300	0.923475
C	-2.189742	0.051417	0.144354
C	-2.760699	1.320235	0.288790
C	-3.009322	-1.061512	-0.046007
C	-4.144409	1.473060	0.240337
H	-2.118068	2.189850	0.450185
C	-4.395577	-0.907776	-0.085773
H	-2.537615	-2.040055	-0.145997
C	-4.964225	0.357942	0.053396

H	-4.587287	2.463655	0.357004
H	-5.035747	-1.780695	-0.225892
H	-6.048460	0.477435	0.021009
H	0.605700	0.903141	-1.402504
H	-0.469101	-0.521298	-1.974225
S	2.390548	-0.922608	-1.290077
C	2.760503	0.044374	0.055747
S	2.847839	-0.432751	1.637361
Cl	3.015670	1.759439	-0.298808
Li	1.346786	-2.111027	0.569672

[TS-R1D]

C	-1.287047	0.974822	-1.129908
C	0.086676	0.750514	-0.636164
O	-0.969793	2.241740	-0.659897
H	0.885735	1.142007	-1.259851
H	0.182494	0.684709	0.445137
S	1.448674	-1.152726	-0.593112
C	2.704362	-0.278051	0.110418
Cl	4.148121	-1.258526	0.410386
S	2.848301	1.326971	0.576175
Li	0.585637	2.812198	0.089447
C	-2.402045	0.251869	-0.421319
C	-2.791942	-1.019913	-0.853562
C	-3.034554	0.831095	0.678772
C	-3.800762	-1.708534	-0.184541
H	-2.299454	-1.472370	-1.718319
C	-4.049677	0.142778	1.345005
H	-2.726753	1.828766	0.994689
C	-4.432640	-1.127161	0.916780
H	-4.098688	-2.701865	-0.524394
H	-4.545803	0.602300	2.201777
H	-5.225968	-1.665189	1.438270
H	-1.394018	0.913634	-2.224929

[1A]

C	-0.322804	0.302499	0.700951
C	0.181035	-0.887621	1.571919
H	1.109340	-0.522134	2.074043
H	-0.575986	-0.954642	2.390444
O	0.356025	-2.038343	0.887463
C	-1.773000	0.229077	0.278157
C	-2.455995	1.395068	-0.089446
C	-2.446502	-0.999248	0.243251
C	-3.793105	1.340110	-0.477226
H	-1.932959	2.354640	-0.066015
C	-3.785935	-1.050058	-0.141345
H	-1.896529	-1.900952	0.521434
C	-4.461031	0.115411	-0.503966
H	-4.316684	2.256371	-0.755163
H	-4.306332	-2.009313	-0.158686
H	-5.508777	0.070440	-0.806005
S	0.624993	0.289441	-0.903231
C	2.296170	0.281209	-0.375275
Cl	2.725333	1.495080	0.787906
S	3.399270	-0.743964	-0.988565
Li	1.116596	-2.253891	-0.616196
H	-0.121925	1.271332	1.181060

[1B]

C	-0.162526	1.126392	0.360887
C	-0.412237	2.620897	0.012376

H	-0.754615	2.647488	-1.050639
H	-1.315154	2.888332	0.610341
O	0.657590	3.396069	0.254543
C	-1.354399	0.256804	0.059719
C	-1.732276	-0.034804	-1.256514
C	-2.161099	-0.198047	1.108739
C	-2.888809	-0.767679	-1.515880
H	-1.106104	0.304527	-2.084887
C	-3.318922	-0.930351	0.851083
H	-1.870348	0.020216	2.139219
C	-3.685980	-1.217490	-0.463090
H	-3.167575	-0.990751	-2.547172
H	-3.933997	-1.282189	1.681138
H	-4.589205	-1.794870	-0.667098
S	1.342798	0.672689	-0.588328
C	1.851958	-0.885875	-0.031638
Cl	1.070299	-1.506501	1.411588
S	3.039223	-1.712063	-0.765654
Li	2.083074	4.129814	0.456949
H	0.105366	1.070671	1.424525

[1C]

C	-0.990930	0.991701	0.574757
C	0.104028	-0.080247	0.316102
H	0.048053	-0.947572	0.987417
H	0.052238	-0.409384	-0.731041
O	-0.747607	2.101790	-0.155515
C	-2.334593	0.324127	0.273537
C	-2.840996	-0.697619	1.085236
C	-3.067046	0.728135	-0.842969
C	-4.054199	-1.311441	0.779205
H	-2.283665	-1.009626	1.973414
C	-4.283148	0.116531	-1.151273
H	-2.661549	1.540315	-1.447266
C	-4.778836	-0.906458	-0.343629
H	-4.440175	-2.105189	1.421712
H	-4.850502	0.442892	-2.025335
H	-5.730716	-1.383925	-0.582743
S	1.700454	0.769260	0.569702
C	2.955689	-0.273622	-0.036353
Cl	2.445096	-1.862515	-0.557819
S	4.504184	0.191807	-0.088060
Li	0.576782	2.937428	-0.726213
H	-0.983831	1.184927	1.675558

[S1a]

C	1.606420	0.578899	-0.223713
C	2.568757	0.018851	0.742293
O	2.462784	-0.484336	-0.566745
H	2.190012	-0.636560	1.534908
H	3.490414	0.565431	0.969730
C	0.150047	0.270162	-0.127449
C	-0.784677	1.307192	-0.057436
C	-0.290654	-1.056681	-0.091603
C	-2.143945	1.021995	0.062827
H	-0.444442	2.344537	-0.099468
C	-1.649837	-1.340182	0.026190
H	0.444782	-1.859468	-0.172130
C	-2.579438	-0.302426	0.106533
H	-2.866902	1.837649	0.117912
H	-1.987031	-2.377896	0.049558
H	-3.643646	-0.526069	0.196724

H	1.854510	1.540212	-0.689116

[TS-1A]

C	0.005791	1.504338	1.238727
C	0.598290	0.164797	0.939570
O	0.008259	2.133120	0.029086
H	-1.000254	1.355923	1.687807
H	0.019713	-0.747232	1.123948
S	-1.163690	-0.706427	-1.399349
C	-2.430831	-0.351156	-0.352149
S	-3.354239	1.030196	-0.284712
Cl	-2.790145	-1.609952	0.862706
Li	-1.177454	1.752490	-1.216298
C	1.902521	-0.020604	0.414287
C	2.376219	-1.343292	0.245593
C	2.765032	1.075301	0.154126
C	3.691694	-1.568929	-0.130457
H	1.692163	-2.177315	0.418018
C	4.074566	0.838567	-0.222710
H	2.354640	2.083526	0.222421
C	4.535787	-0.478731	-0.360425
H	4.063637	-2.586182	-0.253529
H	4.746491	1.673185	-0.424566
H	5.569674	-0.655235	-0.663292
H	0.625151	1.998038	2.024996

[TS-1B]

C	-0.247697	1.792599	-0.946148
C	-0.549273	0.692586	-0.028488
O	-0.687872	2.616014	0.083921
H	0.816934	1.882891	-1.233368
S	1.049461	-1.025136	-0.797545
C	2.385720	-0.366206	-0.038022
Cl	3.861586	-1.330299	-0.232600
S	2.612905	1.021286	0.889080
Li	0.796877	2.784026	1.070531
H	-0.866639	1.810221	-1.858370
H	0.091276	0.586854	0.843539
C	-1.879443	0.067503	0.059838
C	-2.048252	-1.063956	0.870575
C	-2.979631	0.584097	-0.637769
C	-3.289557	-1.685695	0.961251
H	-1.189267	-1.466790	1.412069
C	-4.224258	-0.029981	-0.531086
H	-2.867772	1.493318	-1.229496
C	-4.379924	-1.169088	0.259883
H	-3.408152	-2.573900	1.583333
H	-5.079514	0.384919	-1.066333
H	-5.355457	-1.652172	0.335094

[TS-1C]

C	1.286988	0.975065	-1.129276
C	-0.086660	0.750576	-0.635418
O	0.969676	2.241850	-0.658944
H	-0.182521	0.684632	0.445873
H	-0.885713	1.142063	-1.259095
S	-1.448548	-1.152698	-0.592855
C	-2.704585	-0.278151	0.110218
Cl	-4.147982	-1.259031	0.410601
S	-2.849140	1.327031	0.575243
Li	-0.586489	2.812471	0.088820
C	2.402178	0.252051	-0.421075

C	3.034680	0.830927	0.679203
C	2.792282	-1.019466	-0.853914
C	4.050023	0.142525	1.345013
H	2.726701	1.828393	0.995589
C	3.801313	-1.708177	-0.185307
H	2.299785	-1.471640	-1.718815
C	4.433198	-1.127149	0.916191
H	4.546159	0.601773	2.201927
H	4.099401	-2.701298	-0.525630
H	5.226701	-1.665239	1.437351
H	1.393756	0.914102	-2.224331

[TS-1D]

C	-1.141341	-0.947131	0.786769
C	-0.140853	-1.099729	-0.278818
O	-0.362687	-0.107660	1.535602
H	0.086072	-0.202893	-0.862172
H	0.236021	-2.056093	-0.644242
S	2.388470	-1.376086	0.537391
C	2.837035	0.142041	-0.089167
S	2.693763	1.605364	0.668724
Cl	3.496080	0.124880	-1.722156
Li	1.266633	0.166890	2.067410
C	-2.434844	-0.346611	0.261899
C	-3.433162	-1.159132	-0.286151
C	-2.610748	1.037192	0.303371
C	-4.599650	-0.588968	-0.790839
H	-3.299964	-2.244063	-0.306830
C	-3.782605	1.605950	-0.196116
H	-1.821950	1.648274	0.744591
C	-4.775758	0.795637	-0.745967
H	-5.378721	-1.225681	-1.213519
H	-3.922188	2.687682	-0.155411
H	-5.691719	1.241951	-1.136733
H	-1.363492	-1.915466	1.276181

[1A']

C	0.049714	-0.753438	1.702409
H	0.728292	-1.598259	1.977592
C	0.407452	-0.475300	0.212732
H	0.107255	-1.333753	-0.401872
O	-1.249647	-1.011698	1.897776
C	1.863129	-0.161318	-0.008417
C	2.664503	-1.031838	-0.755705
C	2.452640	0.968744	0.574935
C	4.026437	-0.782271	-0.915928
H	2.213151	-1.914866	-1.213509
C	3.813011	1.221919	0.409234
H	1.840955	1.659890	1.160087
C	4.603758	0.346083	-0.334548
H	4.638682	-1.471574	-1.499786
H	4.257795	2.107863	0.865350
H	5.669292	0.543837	-0.461998
S	-0.585249	0.970414	-0.356345
C	-2.215114	0.419033	-0.416141
Cl	-2.466814	-1.281204	-0.962937
S	-3.510182	1.369896	-0.206205
Li	-2.805066	-1.398675	1.555980
H	0.426508	0.122314	2.283284

[1B']

C	0.273556	2.374341	0.010112

H	-0.609117	3.050404	-0.107489
C	-0.221264	1.262098	0.965032
O	0.755801	1.910098	-1.155154
C	-1.424478	0.465518	0.506206
C	-2.067877	0.764930	-0.699541
C	-1.937111	-0.562502	1.306379
C	-3.195234	0.045177	-1.096382
H	-1.661742	1.547331	-1.341346
C	-3.060603	-1.282972	0.909448
H	-1.437258	-0.811010	2.245984
C	-3.693578	-0.982281	-0.297275
H	-3.684995	0.287654	-2.041348
H	-3.443521	-2.083408	1.544866
H	-4.572599	-1.547217	-0.611874
S	1.233257	0.246240	1.477894
C	1.860923	-0.567179	0.087840
Cl	0.674884	-1.246179	-1.078729
S	3.427180	-0.923861	-0.093357
Li	1.187474	0.837061	-2.315296
H	1.013908	2.970294	0.591374
H	-0.459525	1.718182	1.941826

[1C']

C	-0.627039	-0.487884	0.665566
C	0.007239	-0.926059	-0.686648
H	-0.495844	-1.798781	-1.129072
H	-0.010256	-0.103227	-1.414705
O	0.042170	0.539480	1.211991
C	-2.101101	-0.193358	0.361156
C	-3.021697	-1.231640	0.179178
C	-2.539959	1.125115	0.232528
C	-4.352838	-0.957616	-0.130096
H	-2.692220	-2.268721	0.292993
C	-3.871297	1.404768	-0.078107
H	-1.818201	1.926653	0.395100
C	-4.781774	0.364418	-0.261482
H	-5.061274	-1.777629	-0.262291
H	-4.202588	2.440942	-0.172501
H	-5.824558	0.581701	-0.499260
S	1.715272	-1.495868	-0.443366
C	2.665680	-0.088564	-0.154469
Cl	2.134256	1.425898	-0.965768
S	4.064973	-0.099225	0.656746
Li	1.119782	1.770034	1.341244
H	-0.621336	-1.400742	1.308306

[1D']

C	-0.572419	-1.354163	-0.536499
C	0.167243	-1.501942	0.827510
H	-0.497528	-1.827138	1.641516
H	1.000057	-2.212946	0.746653
O	0.246478	-0.870883	-1.486466
C	-1.842357	-0.522628	-0.339386
C	-1.876944	0.802555	-0.776850
C	-2.968683	-1.055145	0.296215
C	-3.014362	1.585466	-0.577718
H	-0.991244	1.198680	-1.276363
C	-4.108527	-0.277177	0.495593
H	-2.957076	-2.096875	0.631278
C	-4.133461	1.048263	0.058660
H	-3.028992	2.621556	-0.921941
H	-4.983164	-0.707369	0.987395

H	-5.025187	1.658914	0.211127
S	0.805810	0.101828	1.394312
C	2.121197	0.474907	0.346770
Cl	3.117779	-0.922689	-0.225428
S	2.615582	1.975942	0.010742
Li	1.684442	-0.676488	-2.266713
H	-0.916645	-2.397722	-0.742150

[2A]

C	0.210388	0.154664	1.461019
C	-0.442083	0.561389	0.119100
H	-0.310749	1.640038	-0.032753
O	1.528551	-0.349446	1.229056
S	0.568677	-0.294139	-1.147827
C	2.025624	-0.092086	-0.074301
Cl	2.491037	1.716613	-0.054004
S	3.401710	-1.143536	-0.451258
Li	2.806731	-1.654869	1.681342
H	-0.358104	-0.647357	1.950204
H	0.269735	1.022705	2.132864
C	-1.909031	0.216807	0.029629
C	-2.858028	1.236045	-0.086644
C	-2.344680	-1.114199	0.079492
C	-4.219467	0.934964	-0.144970
H	-2.525700	2.275323	-0.134201
C	-3.702376	-1.415488	0.020556
H	-1.607469	-1.918006	0.148042
C	-4.644393	-0.390426	-0.090194
H	-4.948797	1.741463	-0.236424
H	-4.028661	-2.456189	0.055479
H	-5.708406	-0.627449	-0.138396

[2B]

C	0.258494	0.700058	-1.376115
C	-0.463170	1.067868	-0.065738
H	-0.538056	2.160045	0.020205
O	1.656914	0.673315	-1.124030
S	0.683827	0.512412	1.266186
C	1.962848	-0.032345	0.064393
Cl	1.661748	-1.833498	-0.339458
S	3.643296	0.253107	0.555613
Li	3.385906	1.390237	-1.395568
H	0.078077	1.442212	-2.163108
C	-1.847306	0.468773	0.011380
C	-2.971501	1.297430	-0.017013
C	-2.023641	-0.919680	0.078392
C	-4.255975	0.751326	0.014579
H	-2.840114	2.381184	-0.060891
C	-3.303913	-1.464211	0.107094
H	-1.143495	-1.567362	0.120838
C	-4.424234	-0.629837	0.074765
H	-5.126003	1.409799	-0.004584
H	-3.430053	-2.546742	0.161686
H	-5.427165	-1.058927	0.102423
H	-0.059510	-0.292574	-1.726040

[2C]

C	0.354170	0.961974	0.256086
C	-0.187665	1.381078	-1.112096
H	0.190953	2.369314	-1.401490
H	0.065211	0.643250	-1.886581
O	-0.583476	0.013661	0.805014

C	1.739815	0.368974	0.212516
C	2.840933	1.159738	0.549942
C	1.938942	-0.950724	-0.208162
C	4.133031	0.641687	0.460974
H	2.685638	2.187767	0.886420
C	3.229797	-1.468318	-0.289483
H	1.073061	-1.564129	-0.467706
C	4.328630	-0.673452	0.042377
H	4.988066	1.265842	0.725524
H	3.379683	-2.498770	-0.615766
H	5.338537	-1.081429	-0.023441
S	-1.982838	1.433510	-0.857987
C	-1.827105	-0.096579	0.119113
Cl	-1.574071	-1.513126	-1.087065
S	-3.154141	-0.426917	1.248601
Li	-1.251256	-0.533835	2.489014
H	0.348008	1.841757	0.918579

[2D]

C	-0.300560	-1.037008	-0.392897
C	0.280657	-1.600804	0.920421
H	-0.514003	-1.905989	1.612370
H	0.943843	-2.451961	0.718975
O	0.589344	-0.011184	-0.858730
C	-1.677730	-0.431960	-0.246456
C	-1.839720	0.833391	0.335789
C	-2.804934	-1.139950	-0.671230
C	-3.115562	1.375114	0.490075
H	-0.962791	1.381193	0.694967
C	-4.080031	-0.597728	-0.512105
H	-2.681973	-2.121688	-1.134706
C	-4.237162	0.660833	0.067334
H	-3.233620	2.357985	0.949216
H	-4.953599	-1.157828	-0.849375
H	-5.234435	1.086511	0.188630
S	1.240842	-0.236453	1.630564
C	1.739652	0.230805	-0.062661
Cl	2.998851	-1.002887	-0.655657
S	2.273440	1.914373	-0.248136
Li	0.415764	1.727611	-1.567858
H	-0.322103	-1.835389	-1.148977

[TS-2A]

C	0.076280	-0.054360	1.700951
C	-0.417636	0.386383	0.288779
H	-0.166389	1.441350	0.121169
O	1.421738	-0.046620	1.801218
S	0.577447	-0.599815	-0.893304
C	2.163189	-0.074020	-0.420846
Cl	2.418608	1.668400	-0.353562
S	3.492746	-1.070648	-0.531462
Li	2.971679	-0.693215	1.840428
H	-0.379806	-1.049538	1.899837
H	-0.415231	0.659282	2.399206
C	-1.886955	0.160931	0.057828
C	-2.430736	-1.131090	0.070076
C	-2.742328	1.252620	-0.126741
C	-3.799512	-1.323904	-0.103369
H	-1.774690	-1.994005	0.208584
C	-4.113119	1.060404	-0.293733
H	-2.326737	2.262548	-0.139376
C	-4.644598	-0.228388	-0.283439

H	-4.208526	-2.335547	-0.097299
H	-4.767686	1.921889	-0.435629
H	-5.716797	-0.380226	-0.417756

[TS-2B]

C	0.475652	1.572494	-1.480036
C	-0.259316	1.534402	-0.119902
H	-0.529399	2.559566	0.180714
O	1.142177	0.419325	-1.727931
S	1.060924	1.139333	1.102714
C	1.749055	-0.313522	0.422445
Cl	0.681138	-1.702250	0.260158
S	3.391292	-0.578552	0.435550
Li	2.541826	-0.512500	-1.883886
H	1.132753	2.467956	-1.463275
H	-0.311120	1.777913	-2.239172
C	-1.497436	0.670009	-0.050134
C	-2.337076	0.752444	1.066565
C	-1.845980	-0.191728	-1.095760
C	-3.501525	-0.008058	1.140423
H	-2.069527	1.417418	1.891976
C	-3.014099	-0.949777	-1.024822
H	-1.173045	-0.290869	-1.948909
C	-3.844824	-0.861559	0.091307
H	-4.144578	0.067083	2.018958
H	-3.272366	-1.620699	-1.846115
H	-4.757126	-1.457954	0.145486

[TS-2C]

C	0.471842	-0.833881	-0.545820
C	-0.060688	-1.226152	0.872641
H	0.376540	-2.165056	1.239991
H	0.130720	-0.431373	1.605748
O	-0.353361	0.067199	-1.134156
C	1.892425	-0.312233	-0.348657
C	2.978066	-1.189252	-0.279692
C	2.110113	1.058520	-0.188631
C	4.266095	-0.704211	-0.050856
H	2.814585	-2.262143	-0.414872
C	3.396429	1.544888	0.040240
H	1.251540	1.729406	-0.254757
C	4.477932	0.664990	0.110258
H	5.108134	-1.397310	-0.003967
H	3.558715	2.617669	0.161870
H	5.485279	1.046516	0.285659
S	-1.840748	-1.487733	0.720819
C	-2.275151	0.096326	0.139318
Cl	-1.672529	1.459986	1.067143
S	-3.585322	0.324927	-0.865146
Li	-1.577276	0.434123	-2.251906
H	0.540931	-1.786510	-1.115725

[TS-2D]

C	-0.432406	-1.143519	-0.655395
C	0.205697	-1.630874	0.687680
H	-0.529796	-2.057619	1.383646
H	0.999331	-2.365194	0.498135
O	0.451129	-0.385683	-1.338391
C	-1.757287	-0.437131	-0.378001
C	-1.793704	0.949542	-0.203703
C	-2.947365	-1.162692	-0.270105
C	-2.996402	1.597307	0.077341

H	-0.862578	1.517646	-0.276225
C	-4.152834	-0.518349	0.007890
H	-2.930553	-2.246729	-0.415047
C	-4.179739	0.865447	0.182192
H	-3.010400	2.679864	0.217182
H	-5.075418	-1.097122	0.081644
H	-5.121679	1.372934	0.397366
S	0.915466	-0.179353	1.503350
C	2.022957	0.307908	0.255003
Cl	3.135583	-0.935075	-0.327062
S	2.377535	1.903965	-0.036254
Li	1.262404	0.903619	-2.041531
H	-0.671575	-2.092525	-1.185872

[3A]

C	0.253978	0.066909	1.021573
C	-0.388158	-0.417788	-0.274200
H	0.042216	0.182399	-1.094206
O	1.683074	-0.246742	1.000480
S	-0.032281	-2.193227	-0.578978
C	2.563718	0.387623	0.263292
Cl	2.241841	2.058866	-0.041069
S	3.889316	-0.379772	-0.296614
Li	2.062261	-2.144229	0.277806
H	0.138593	1.145137	1.195375
C	-1.863671	-0.065745	-0.187693
C	-2.295376	1.197343	-0.611143
C	-2.797460	-0.945217	0.369904
C	-3.632136	1.573822	-0.487248
H	-1.573076	1.891136	-1.050826
C	-4.133412	-0.568198	0.499882
H	-2.461087	-1.937683	0.675534
C	-4.555622	0.690694	0.071516
H	-3.953965	2.557962	-0.832591
H	-4.852445	-1.266780	0.931785
H	-5.603516	0.980477	0.166489
H	-0.123113	-0.495405	1.883531

[3B]

C	-0.902797	0.830373	1.600038
C	-0.144203	1.771103	0.664417
H	0.256009	2.552371	1.331258
O	-1.689927	-0.107864	0.801861
S	-1.281183	2.574911	-0.532101
C	-1.261301	-1.218240	0.247689
Cl	0.013391	-2.046184	1.057108
S	-1.984897	-1.784210	-1.103944
Li	-2.611890	0.748861	-0.789863
H	-0.254873	0.251459	2.271821
C	1.047061	1.025490	0.072047
C	2.138187	0.736682	0.905377
C	1.059514	0.533448	-1.234565
C	3.194382	-0.050968	0.457667
H	2.152492	1.129851	1.926245
C	2.112017	-0.267371	-1.684263
H	0.235450	0.800204	-1.898361
C	3.177585	-0.568526	-0.839828
H	4.034349	-0.264022	1.121476
H	2.098778	-0.651902	-2.705770
H	4.000399	-1.192673	-1.192608
H	-1.660572	1.372993	2.175045

[3C]

C	0.050570	0.972877	-0.579355
C	0.719544	1.840253	0.468784
H	0.116896	2.758566	0.538716
H	0.664258	1.347843	1.453291
O	0.925440	-0.205579	-0.847278
C	-1.384634	0.544002	-0.370903
C	-2.150097	1.033269	0.689579
C	-1.967984	-0.339425	-1.286971
C	-3.480269	0.638346	0.835120
H	-1.710908	1.720971	1.413263
C	-3.291835	-0.741345	-1.134884
H	-1.374113	-0.723107	-2.120141
C	-4.052048	-0.251844	-0.071436
H	-4.069885	1.026723	1.666961
H	-3.734285	-1.435870	-1.850710
H	-5.090919	-0.563375	0.047728
S	2.446462	2.280312	0.040809
C	1.262311	-1.149814	-0.003007
Cl	0.164427	-1.509820	1.276058
S	2.674927	-1.955612	-0.190132
Li	2.897124	0.407201	-1.136265
H	0.133225	1.485098	-1.547472

[3D]

C	-0.131214	0.011718	0.806862
C	0.210170	1.414179	1.285697
H	-0.520783	1.669410	2.069423
H	1.189594	1.357949	1.788866
O	0.764860	-0.287710	-0.341159
C	-1.531770	-0.257592	0.309592
C	-1.850338	-1.560524	-0.092846
C	-2.517977	0.731580	0.276627
C	-3.135434	-1.873362	-0.527055
H	-1.080885	-2.336652	-0.062077
C	-3.808678	0.413471	-0.148537
H	-2.265519	1.756073	0.551627
C	-4.119367	-0.883576	-0.552531
H	-3.372465	-2.891778	-0.838734
H	-4.573715	1.191141	-0.170556
H	-5.129388	-1.125255	-0.887738
S	0.242526	2.708039	-0.013358
C	2.034637	-0.595941	-0.243208
Cl	2.503889	-1.471772	1.174235
S	3.083846	-0.199362	-1.426799
Li	0.944788	1.297277	-1.636565
H	0.111674	-0.729471	1.581074

[TS-3A]

C	0.175046	-0.619216	-1.050881
C	-0.423293	-0.300819	0.347248
H	-0.272527	-1.183479	0.984952
O	1.472553	-0.028169	-1.242742
S	0.494103	1.055425	1.139653
C	2.399948	-0.108857	-0.279550
Cl	2.464049	-1.648374	0.541520
S	3.717406	0.898932	-0.355058
Li	1.547512	1.998018	-0.721211
H	0.256603	-1.703068	-1.216227
H	-0.428641	-0.178376	-1.852921
C	-1.923162	-0.116576	0.188404
C	-2.525280	1.142188	0.102185

C	-2.727209	-1.256429	0.057946
C	-3.897207	1.258301	-0.120493
H	-1.908064	2.032204	0.236430
C	-4.098520	-1.142293	-0.165940
H	-2.272287	-2.247162	0.141099
C	-4.688108	0.118062	-0.258984
H	-4.352979	2.248533	-0.177172
H	-4.709302	-2.041839	-0.260816
H	-5.762034	0.210970	-0.428719

[TS-3B]

C	0.175046	-0.619216	-1.050881
C	-0.423293	-0.300819	0.347248
H	-0.272527	-1.183479	0.984952
O	1.472553	-0.028169	-1.242742
S	0.494103	1.055425	1.139653
C	2.399948	-0.108857	-0.279550
Cl	2.464049	-1.648374	0.541520
S	3.717406	0.898932	-0.355058
Li	1.547512	1.998018	-0.721211
H	0.256603	-1.703068	-1.216227
H	-0.428641	-0.178376	-1.852921
C	-1.923162	-0.116576	0.188404
C	-2.525280	1.142188	0.102185
C	-2.727209	-1.256429	0.057946
C	-3.897207	1.258301	-0.120493
H	-1.908064	2.032204	0.236430
C	-4.098520	-1.142293	-0.165940
H	-2.272287	-2.247162	0.141099
C	-4.688108	0.118062	-0.258984
H	-4.352979	2.248533	-0.177172
H	-4.709302	-2.041839	-0.260816
H	-5.762034	0.210970	-0.428719

[TS-3C]

C	0.153900	-0.827745	-0.827250
C	-0.413972	-1.916310	0.102960
H	-0.065990	-2.886378	-0.280198
H	-0.008269	-1.798025	1.117664
O	-0.788602	0.268307	-0.985063
C	1.533252	-0.312545	-0.469424
C	2.486889	-1.195657	0.047128
C	1.890647	1.020907	-0.694560
C	3.777151	-0.751871	0.334026
H	2.226717	-2.239914	0.228949
C	3.178201	1.464061	-0.398195
H	1.154233	1.719897	-1.094230
C	4.126204	0.579580	0.115079
H	4.510707	-1.451999	0.736958
H	3.440651	2.509296	-0.569526
H	5.134005	0.928015	0.346026
S	-2.225080	-1.868554	0.188142
C	-1.522642	0.732991	0.032887
Cl	-0.706585	0.851104	1.563143
S	-2.866596	1.644948	-0.314404
Li	-2.683324	-0.450559	-1.587413
H	0.187716	-1.227214	-1.852054

[TS-3D]

C	0.236920	-0.106795	-0.907300
C	-0.300434	1.290811	-1.283941
H	0.557792	1.914003	-1.572142

H	-0.945024	1.208321	-2.169271
O	-0.518917	-0.658100	0.216276
C	1.673715	-0.142539	-0.437271
C	2.247344	0.947881	0.229262
C	2.426599	-1.306329	-0.617809
C	3.555556	0.869658	0.705979
H	1.669711	1.865932	0.367976
C	3.735604	-1.382518	-0.144543
H	1.981453	-2.158607	-1.136330
C	4.301092	-0.294620	0.519820
H	3.996724	1.725823	1.218797
H	4.316074	-2.293682	-0.296884
H	5.326362	-0.352015	0.888799
S	-1.261157	2.055457	0.053774
C	-1.850888	-0.565938	0.274555
Cl	-2.667475	-0.792606	-1.249059
S	-2.607004	-0.816378	1.727670
Li	-0.589957	0.651983	1.803055
H	0.102717	-0.809560	-1.741953

[TS-4A]

C	-0.137513	0.757505	1.095284
C	0.921825	-0.201710	1.268753
H	1.169532	-0.166866	2.348840
O	-1.361130	0.280612	-0.676723
S	0.017183	-1.825635	1.148058
C	-2.596054	0.265052	-0.538425
Cl	-3.287517	1.743597	0.184762
S	-3.604533	-1.006810	-0.930258
Li	-1.199100	-1.627287	-0.823821
H	-0.961710	0.762267	1.812913
C	2.163306	0.017924	0.432435
C	2.739829	1.294772	0.403624
C	2.768471	-1.014403	-0.286892
C	3.888022	1.539715	-0.345542
H	2.290532	2.108797	0.979830
C	3.921843	-0.770430	-1.033697
H	2.323104	-2.009210	-0.253976
C	4.481981	0.504886	-1.069107
H	4.322660	2.540473	-0.361001
H	4.384053	-1.585795	-1.592671
H	5.382002	0.693741	-1.656384
H	-0.048700	1.611671	0.423337

[TS-4B]

C	0.571535	-1.453275	1.638184
C	-0.157460	-1.939707	0.497383
H	-0.601489	-2.901212	0.828753
O	1.996337	0.106315	0.870837
S	1.188451	-2.508477	-0.653623
C	1.532874	1.120989	0.324016
Cl	0.299861	2.000832	1.270121
S	1.949586	1.691870	-1.192927
Li	2.608617	-0.658319	-0.779360
H	0.317390	-0.519839	2.143850
C	-1.224956	-0.991904	-0.004278
C	-1.167470	-0.397597	-1.264535
C	-2.270322	-0.654339	0.865334
C	-2.128208	0.542909	-1.640103
H	-0.357033	-0.669021	-1.941637
C	-3.232157	0.278172	0.488088
H	-2.328188	-1.123218	1.852187

C	-3.158183	0.884765	-0.767159
H	-2.063911	1.013737	-2.622261
H	-4.040072	0.534967	1.175117
H	-3.905981	1.622086	-1.063391
H	1.282577	-2.121568	2.129950

[TS-4C]

C	0.252268	1.102850	0.592237
C	-0.279212	2.391459	0.171305
H	0.262852	3.016990	0.926224
H	0.129505	2.715884	-0.797224
O	-1.040771	-0.139823	-0.701529
C	1.537148	0.569021	0.238127
C	2.236100	0.990514	-0.912794
C	2.117440	-0.389178	1.094367
C	3.492036	0.471393	-1.185690
H	1.780848	1.704955	-1.598930
C	3.381028	-0.895772	0.821560
H	1.565358	-0.722701	1.974638
C	4.063847	-0.466468	-0.317969
H	4.031321	0.787626	-2.078949
H	3.832995	-1.630126	1.488614
H	5.052620	-0.871966	-0.539610
S	-2.050208	2.721679	0.383567
C	-1.565651	-1.195790	-0.322437
Cl	-0.428828	-2.436075	0.292456
S	-3.202042	-1.543903	-0.324704
Li	-2.725657	0.853229	-0.738707
H	-0.236293	0.658932	1.467796

[TS-4D]

C	-0.868387	0.281878	-1.363179
C	-2.340924	0.257401	-1.302354
H	-2.589892	1.215795	-1.810996
H	-2.695864	-0.531085	-1.980200
O	-0.580476	-1.582922	-0.477829
C	0.033681	1.138001	-0.636854
C	-0.342853	1.881006	0.505379
C	1.359673	1.235409	-1.118787
C	0.583679	2.711213	1.122625
H	-1.362655	1.788472	0.882105
C	2.280608	2.057245	-0.486436
H	1.650744	0.660662	-2.000139
C	1.889994	2.794413	0.634557
H	0.290696	3.290154	1.998995
H	3.301113	2.128767	-0.863340
H	2.614348	3.439707	1.135025
S	-3.222575	0.204949	0.298020
C	0.471361	-1.747844	0.175613
Cl	1.917532	-2.074577	-0.807587
S	0.610354	-1.667894	1.831535
Li	-1.775491	-1.392273	1.072442
H	-0.441720	-0.129679	-2.283446

[R5A]

C	0.176580	0.894357	-0.266676
C	0.197144	2.402456	0.027807
H	0.434480	2.562888	1.092917
H	1.054347	2.798796	-0.537839
S	-1.307125	3.312098	-0.471031
C	1.509506	0.226927	-0.026114
C	2.043689	0.111969	1.262747

C	2.265730	-0.214319	-1.116270
C	3.309397	-0.435837	1.456198
H	1.460409	0.445935	2.124487
C	3.534015	-0.761247	-0.923528
H	1.854589	-0.129625	-2.124872
C	4.058364	-0.873626	0.362958
H	3.713072	-0.522563	2.466241
H	4.112566	-1.103161	-1.783227
H	5.049138	-1.304585	0.515326
S	-1.153815	0.179402	0.800570
C	-1.720175	-1.304334	0.061481
Cl	-0.806594	-1.882284	-1.300022
S	-3.003650	-2.092613	0.647000
Li	-2.874695	1.946779	0.331548
H	-0.154488	0.750539	-1.303552

[R5C]

C	0.722098	0.922751	0.933389
H	1.001790	1.598404	1.760242
C	-0.245007	-0.078236	1.570679
H	0.221484	-0.713812	2.336852
H	-1.088939	0.446344	2.032592
S	-0.143129	1.966431	-0.311852
C	2.012512	0.293289	0.421441
C	2.358475	-1.045359	0.646658
C	2.921853	1.093072	-0.290384
C	3.565131	-1.569804	0.173265
H	1.696732	-1.712120	1.202554
C	4.129620	0.578110	-0.749147
H	2.649415	2.130179	-0.492503
C	4.456998	-0.761397	-0.523267
H	3.803388	-2.618787	0.358186
H	4.819921	1.225071	-1.293672
H	5.400187	-1.169164	-0.890430
S	-0.932803	-1.223887	0.319717
C	-2.420609	-0.466208	-0.217000
Cl	-3.427184	0.257299	0.982158
S	-2.915195	-0.623039	-1.768799
Li	-0.463418	0.243468	-1.776449

[S5A]

C	0.357001	-0.200177	0.700320
C	-0.132695	1.093911	1.358672
H	-1.085137	0.865814	1.861107
H	0.588873	1.308036	2.164503
S	-0.335379	2.598354	0.331044
C	1.809198	-0.275687	0.271828
C	2.372418	-1.536522	0.027927
C	2.605956	0.865448	0.131274
C	3.706824	-1.658190	-0.347860
H	1.755353	-2.432400	0.138532
C	3.945565	0.739398	-0.240835
H	2.165514	1.850204	0.296477
C	4.498330	-0.516317	-0.483140
H	4.132150	-2.646460	-0.529746
H	4.559259	1.635809	-0.344050
H	5.545535	-0.607804	-0.776252
S	-0.620203	-0.580170	-0.841899
C	-2.282668	-0.607882	-0.286955
Cl	-2.594495	-1.496810	1.164799
S	-3.473676	0.102056	-1.136939
Li	-1.373047	1.724409	-1.468528

H	0.152572	-1.048390	1.370740

[S5C]

C	-0.762776	-0.934481	0.048136
C	-0.030773	-0.306995	-1.156537
H	-0.493166	-0.608186	-2.109114
H	-0.034073	0.789761	-1.108766
S	0.116133	-0.661113	1.633731
C	-2.169630	-0.363307	0.051087
C	-3.247121	-1.129450	-0.402452
C	-2.404444	0.957157	0.456706
C	-4.535533	-0.592969	-0.447893
H	-3.076773	-2.162132	-0.717337
C	-3.686528	1.496458	0.404941
H	-1.566872	1.547052	0.837014
C	-4.758134	0.722317	-0.047267
H	-5.367241	-1.208241	-0.795974
H	-3.854711	2.525778	0.726996
H	-5.764151	1.143932	-0.080991
S	1.699951	-0.853326	-1.285027
C	2.600262	0.259791	-0.272746
Cl	2.146212	1.922999	-0.315033
S	3.959174	-0.236572	0.498749
Li	2.027755	-1.780058	1.129886
H	-0.847956	-2.013718	-0.149017

[TS-R5A]

C	-1.720777	1.814959	0.501381
C	-0.653832	1.584482	-0.455458
H	-1.455453	1.517567	1.526502
H	-0.924991	1.732081	-1.507198
S	-0.959854	-1.335467	-1.541245
C	-0.242739	-1.681990	-0.061738
S	-0.967811	-1.688972	1.441212
Cl	1.491446	-2.033761	-0.110177
Li	-2.814482	-0.915720	-0.025187
C	0.715815	1.351672	-0.167280
C	1.635527	1.336834	-1.246696
C	1.192117	1.172396	1.155856
C	2.989916	1.190459	-1.007276
H	1.257083	1.443300	-2.265109
C	2.551731	1.028888	1.384515
H	0.494211	1.147187	1.992052
C	3.444637	1.042307	0.308665
H	3.698065	1.183695	-1.835987
H	2.922677	0.894220	2.400593
H	4.513274	0.923225	0.497256
H	-1.727489	2.933784	0.503559
S	-3.395015	1.306064	-0.014649

[TS-R5B]

C	0.253656	1.616019	-1.031835
C	0.541593	0.601262	-0.017423
H	0.821486	1.508626	-1.962244
S	-1.034974	-1.154146	-0.712045
C	-2.433080	-0.529960	-0.050632
Cl	-3.848963	-1.575711	-0.244798
S	-2.762409	0.891475	0.788915
Li	-1.212115	2.771757	0.947188
H	-0.813387	1.727446	-1.266019
H	-0.080148	0.579409	0.875820
C	1.812497	-0.136422	0.072364

C	2.832685	0.005266	-0.879003
C	1.987324	-1.036337	1.134129
C	4.002210	-0.739867	-0.766138
H	2.725738	0.716838	-1.698760
C	3.154484	-1.784978	1.241488
H	1.188616	-1.153809	1.870189
C	4.164710	-1.637978	0.290013
H	4.793707	-0.618639	-1.506967
H	3.277233	-2.485623	2.068480
H	5.082049	-2.223070	0.372217
S	0.933443	2.905084	0.086225

[TS-R5C]

C	-1.121063	0.768183	-1.001402
C	-0.055509	-0.154864	-1.344149
H	0.781996	0.217936	-1.938094
H	-0.245414	-1.227469	-1.385392
S	1.443117	-1.323173	0.415277
C	2.835113	-0.355456	0.233831
S	3.248261	0.917654	1.193919
Cl	3.853308	-0.740628	-1.145117
Li	0.881355	0.559045	1.782239
C	-2.396159	0.189438	-0.460161
C	-3.621659	0.766512	-0.805497
C	-2.386063	-0.905179	0.413222
C	-4.814858	0.259587	-0.291697
H	-3.639448	1.624065	-1.481987
C	-3.577348	-1.415069	0.924066
H	-1.436913	-1.364791	0.702566
C	-4.796418	-0.833261	0.573286
H	-5.763652	0.720579	-0.571141
H	-3.553944	-2.271223	1.600335
H	-5.729517	-1.232333	0.973832
H	-1.316656	1.421850	-1.866367
S	-0.169063	1.849617	0.180649

[TS-R5D]

C	-1.273483	0.957008	-0.799280
C	0.104063	0.880018	-0.335098
H	0.857092	1.429328	-0.894517
H	0.280681	0.584408	0.698026
S	1.462191	-0.984486	-0.852039
C	2.798626	-0.361331	-0.049287
Cl	4.210953	-1.417349	-0.110512
S	3.046056	1.070283	0.793866
Li	1.028564	2.548853	0.903223
C	-2.290656	-0.016632	-0.284545
C	-1.949518	-1.095557	0.535475
C	-3.631901	0.164351	-0.647122
C	-2.935102	-1.972629	0.993109
H	-0.907788	-1.276167	0.807261
C	-4.612804	-0.709860	-0.192006
H	-3.902807	1.010266	-1.283284
C	-4.266456	-1.782418	0.633410
H	-2.654092	-2.813078	1.629775
H	-5.653760	-0.555331	-0.480682
H	-5.034908	-2.469545	0.990993
H	-1.365725	1.133067	-1.876954
S	-1.254947	2.603436	0.086329

[R2a]

C	-0.211798	-1.204693	-0.608040

H	-0.514318	-2.020356	-1.280049
C	0.404457	-1.828383	0.648187
H	-0.374736	-2.124596	1.363759
H	1.014166	-2.705576	0.391186
S	1.154796	-0.333790	-1.462334
C	-1.415289	-0.328932	-0.319698
C	-2.678324	-0.932681	-0.306671
C	-1.311917	1.031868	-0.012478
C	-3.817089	-0.195753	0.012419
H	-2.770086	-1.993692	-0.553015
C	-2.451381	1.768629	0.308705
H	-0.340533	1.529630	-0.034495
C	-3.705101	1.158929	0.322941
H	-4.794638	-0.680439	0.011925
H	-2.356093	2.829561	0.544731
H	-4.594653	1.740526	0.569747
S	1.473540	-0.595070	1.451086
C	2.024117	0.176138	-0.022952
S	3.228217	1.275999	-0.060518

[S2a]

C	0.379261	1.434837	0.572093
C	-0.195581	0.467591	-0.457461
H	-0.083950	0.896706	-1.463427
S	2.188275	1.472802	0.381442
C	-1.647090	0.130004	-0.209127
C	-2.620457	0.548834	-1.120417
C	-2.042500	-0.565592	0.940847
C	-3.969850	0.283949	-0.885406
H	-2.318138	1.086189	-2.022066
C	-3.389110	-0.830321	1.174625
H	-1.288233	-0.913371	1.650907
C	-4.356442	-0.404837	0.262281
H	-4.719936	0.615429	-1.605054
H	-3.685263	-1.375820	2.071964
H	-5.411195	-0.615378	0.445795
S	0.867936	-1.035493	-0.407758
C	2.377957	-0.218547	-0.052659
S	3.829002	-0.958351	-0.125759
H	0.135327	1.117394	1.596081
H	-0.009147	2.450029	0.410332

[TS-R6A]

C	0.307757	2.230453	0.624938
C	-0.224056	0.965505	1.305839
S	1.179288	-0.189418	1.578295
C	1.810321	-0.622347	-0.002514
Cl	0.592919	-1.501027	-1.106413
S	3.373281	-0.918627	-0.261220
Li	-0.503935	0.444927	-1.812751
H	1.079681	2.664371	1.275102
S	1.031424	1.928775	-1.015761
H	-0.472818	1.208664	2.354353
H	-0.508269	2.969332	0.575876
C	-1.460286	0.337617	0.680285
C	-1.893640	-0.934249	1.080354
C	-2.220421	1.025618	-0.278834
C	-3.026617	-1.514749	0.519617
H	-1.312887	-1.485752	1.822259
C	-3.350740	0.433487	-0.856449
H	-1.936408	2.035026	-0.584640
C	-3.753436	-0.840343	-0.463593

H	-3.338867	-2.508645	0.844010
H	-3.921873	0.984563	-1.605811
H	-4.633564	-1.302493	-0.912778

[TS-R6C]

C	-0.646436	1.243052	0.224156
C	0.093801	1.160060	-1.128011
H	0.903163	1.900738	-1.193928
S	0.791851	-0.480296	-1.431882
C	2.030708	-0.594685	-0.214398
Cl	3.262596	0.910133	-0.336302
S	2.635740	-1.957977	0.384119
Li	2.318364	1.949958	1.470159
H	-0.891115	2.308849	0.352665
S	0.429964	0.710898	1.596835
C	-1.956341	0.476734	0.173313
C	-3.122114	1.143134	-0.221415
C	-2.026413	-0.893462	0.451008
C	-4.332663	0.460331	-0.339389
H	-3.081968	2.214987	-0.434038
C	-3.234059	-1.578581	0.327660
H	-1.124882	-1.414974	0.777721
C	-4.390764	-0.905541	-0.067184
H	-5.233153	0.999010	-0.639950
H	-3.272219	-2.647002	0.547448
H	-5.336128	-1.443535	-0.156038
H	-0.598103	1.331536	-1.966817

[TS-S6A]

C	0.126717	-1.713371	0.457168
C	0.499971	-0.382151	-0.213021
S	-0.409051	0.999419	0.582042
C	-2.066133	0.684015	0.164458
Cl	-2.272660	0.442488	-1.750063
S	-3.356887	1.226993	0.952697
Li	-2.479546	-1.840042	-1.522393
H	0.539401	-1.723773	1.476269
S	-1.657010	-2.029382	0.569515
H	0.197461	-0.384213	-1.269159
H	0.638270	-2.510411	-0.105949
C	1.977907	-0.076283	-0.124578
C	2.741198	0.046280	-1.289818
C	2.608696	0.064820	1.118776
C	4.110771	0.298040	-1.217290
H	2.256100	-0.056580	-2.263163
C	3.975847	0.322221	1.191221
H	2.024051	-0.020250	2.038342
C	4.730868	0.436724	0.023386
H	4.694350	0.388690	-2.134872
H	4.454278	0.433955	2.165502
H	5.802057	0.636158	0.081412

[TS-S6C]

C	-0.604431	-1.156297	-0.157533
C	0.202754	-0.768084	-1.421073
H	0.043872	0.273807	-1.720720
S	1.983111	-1.019358	-1.273375
C	2.424331	0.118943	-0.029899
Cl	1.586789	1.812962	-0.245693
S	3.799520	0.083459	0.802822
Li	-0.193976	1.397384	1.305567
H	-0.761017	-2.242836	-0.193660

S	0.268239	-0.819720	1.427550
C	-1.963254	-0.482558	-0.147304
C	-3.095409	-1.203144	0.251326
C	-2.120319	0.883251	-0.440154
C	-4.337747	-0.582681	0.367127
H	-2.991437	-2.264291	0.487922
C	-3.363246	1.508096	-0.319220
H	-1.272594	1.475748	-0.803057
C	-4.477906	0.777021	0.088079
H	-5.204600	-1.166711	0.681352
H	-3.460715	2.568563	-0.559122
H	-5.450696	1.261759	0.180450
H	-0.098878	-1.395904	-2.273117

[4-R]

C	-1.225862	0.743447	0.136270
C	-2.152077	0.082838	1.088194
S	-2.512082	-0.293043	-0.641993
H	-1.384549	1.813670	-0.021982
H	-2.892105	0.702091	1.601907
H	-1.752499	-0.744569	1.682297
C	0.205154	0.325524	0.045297
C	1.194564	1.304309	-0.087704
C	0.587607	-1.020179	0.120250
C	2.543247	0.949256	-0.134463
H	0.904816	2.355427	-0.153110
C	1.932582	-1.374004	0.076389
H	-0.181942	-1.792948	0.188729
C	2.916241	-0.390112	-0.049781
H	3.303852	1.724809	-0.239116
H	2.216882	-2.426058	0.134099
H	3.970120	-0.670204	-0.087649

[4-S]

C	1.225862	0.743447	0.136270
C	2.152077	0.082838	1.088194
S	2.512082	-0.293043	-0.641993
H	1.752499	-0.744569	1.682297
H	2.892105	0.702091	1.601907
C	-0.205154	0.325524	0.045297
C	-1.194564	1.304309	-0.087704
C	-0.587607	-1.020179	0.120250
C	-2.543247	0.949256	-0.134463
H	-0.904816	2.355427	-0.153110
C	-1.932582	-1.374004	0.076389
H	0.181942	-1.792948	0.188729
C	-2.916241	-0.390112	-0.049781
H	-3.303852	1.724809	-0.239116
H	-2.216882	-2.426058	0.134099
H	-3.970120	-0.670204	-0.087649
H	1.384549	1.813670	-0.021982

[TS-S5A]

C	2.766937	0.412956	1.130685
C	1.386189	-0.013700	1.377930
H	3.045312	1.203777	1.837291
H	0.857756	0.459304	2.211139
S	-0.444539	2.271175	0.591384
C	-1.401069	1.240810	-0.336524
S	-0.994687	0.519214	-1.778329
Cl	-2.998643	0.858423	0.330331
Li	1.074217	1.749673	-1.239214

C	0.683270	-1.073752	0.756304
C	-0.605081	-1.391315	1.258961
C	1.223844	-1.847143	-0.305927
C	-1.314022	-2.464470	0.745997
H	-1.035015	-0.769906	2.048324
C	0.516446	-2.931493	-0.794565
H	2.183171	-1.554232	-0.736552
C	-0.747590	-3.236277	-0.272959
H	-2.308327	-2.698850	1.126118
H	0.931655	-3.532921	-1.603464
H	-1.307572	-4.079137	-0.682444
H	3.408400	-0.463948	1.337566
S	3.122060	0.923362	-0.612765

[TS-S5B]

C	0.253506	1.615823	1.031745
C	0.541527	0.601107	0.017306
H	-0.813551	1.727300	1.265815
S	-1.035021	-1.154220	0.711950
C	-2.433127	-0.529922	0.050621
Cl	-3.849001	-1.575691	0.244714
S	-2.762510	0.891650	-0.788673
Li	-1.211704	2.771541	-0.948026
H	0.821261	1.508305	1.962184
H	-0.080096	0.579283	-0.876023
C	1.812457	-0.136563	-0.072347
C	1.987424	-1.036506	-1.134063
C	2.832626	0.005344	0.879008
C	3.154716	-1.784946	-1.241399
H	1.188734	-1.154147	-1.870117
C	4.002281	-0.739588	0.766166
H	2.725568	0.716957	1.698715
C	4.164933	-1.637710	-0.289952
H	3.277580	-2.485608	-2.068360
H	4.793770	-0.618174	1.506972
H	5.082392	-2.222613	-0.372162
S	0.933432	2.904981	-0.086127

[TS-S5C]

C	1.101209	1.523106	-0.705476
C	-0.142659	1.342082	-1.428148
H	-0.456332	0.355936	-1.779760
H	-0.536384	2.199967	-1.976114
S	-2.457843	1.095259	-0.364596
C	-2.285690	-0.526270	0.103599
S	-2.107379	-1.088652	1.652318
Cl	-2.225391	-1.695481	-1.216638
Li	-1.304777	1.254607	1.734868
C	1.939148	0.323022	-0.370729
C	3.328815	0.473373	-0.303866
C	1.382562	-0.928685	-0.088696
C	4.145400	-0.603342	0.035306
H	3.772656	1.449341	-0.514344
C	2.198136	-2.007233	0.249551
H	0.302674	-1.078983	-0.129463
C	3.582005	-1.848614	0.312926
H	5.227319	-0.468679	0.081771
H	1.744436	-2.975894	0.465281
H	4.219631	-2.693503	0.577641
H	1.699436	2.281878	-1.231763
S	0.457660	2.462433	0.784665

[TS-S5D]

C	1.276773	1.008821	-0.929903
C	-0.097790	0.929020	-0.442997
H	-0.245925	0.732861	0.618593
H	-0.891128	1.352124	-1.056061
S	-1.321625	-1.079538	-0.707809
C	-2.694475	-0.456797	0.025428
Cl	-4.036753	-1.601595	0.102394
S	-3.036303	1.045512	0.700969
Li	-1.127169	2.663291	0.570897
C	2.282237	0.083672	-0.305243
C	2.567602	0.117434	1.064105
C	2.902447	-0.878242	-1.107544
C	3.449971	-0.804567	1.620716
H	2.110157	0.891071	1.684608
C	3.790294	-1.798800	-0.550441
H	2.686930	-0.907195	-2.177997
C	4.063544	-1.765920	0.815329
H	3.667254	-0.768600	2.689552
H	4.269689	-2.543170	-1.188252
H	4.758535	-2.484390	1.252836
H	1.351744	1.024227	-2.022257
S	1.173892	2.742312	-0.267604