A Computational Study of Detoxification of Lewisite Warfare Agents by British Anti Lewisite: Catalytic Effects of Water, and Ammonia on Reaction Mechanism Kinetics

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Table S1: Relative free energies (ΔG , kcal/mol) calculated at M062X/GENECP level of theory in different solvent for all the species involved in the uncatalyzed detoxification reaction of BAL

Species	ΔG		
	Water	Dimethyl Sulfoxide	Cyclohexane
BAL+ LEW	0.0	0.0	0.0
URC	13.33	7.34	4.21
UTS1-SA	46.62	39.13	37.95
UINT-SA	29.69	26.21	23.62
UTS2-SB	36.36	30.47	28.04
PC	5.93	3.15	- 6.66

Table S2: Relative free energies (ΔG, kcal/mol) calculated at M062X/GENECP level of theory in different solvent for all the species involved in the H_2O catalyzed reaction of BAL

Species	ΔG		
	Water	Dimethyl Sulfoxide	Cyclohexane
BAL+ LEW+H_2O	0.00	0.00	0.00
CRC-W	18.92	15.58	7.36
CTS1-W	44.67	38.80	36.01
CINT-W	26.75	22.63	20.10
CTS2-W	28.74	22.63	6.39
PC-W	5.93	3.15	-6.66

Table S3: Relative free energies (ΔG , kcal/mol) calculated at M062X/GENECP level of theory in different solvent for all the species involved in the NH_3 catalyzed reaction of BAL

Species	ΔG		
	Water	Dimethyl Sulfoxide	Cyclohexane
BAL+ LEW+NH_3	0.0	0.0	0.0
CRC-A	14.48	11.32	6.97
CTS1-A	43.24	40.84	38.39
CINT-A	26.88	21.74	18.73
CTS2-A	37.25	31.43	26.99
PC-A	5.93	3.15	-6.66

Table S4. NBO Data [Occupation Number (ON), Orbital Energy E (in au), Second-Order perturbation Energy (Donor to Acceptor)(in Kcal/mol)

Species	ON (lp Cl)	E (lp Cl)	Lp (Cl) →σ* (S - H)	Wiberg BO (Cl-H)
UTS1-SA	1.767	-0.329	178.31	0.424
UTS1-SB	1.849	-0.327	180.21	0.421
UTS2-SB	1.899	-0.314	24.69	0.154
UTS2-SA	1.868	-0.308	27.57	0.149

Table S5. M062X/GENECP Calculated Electron Density (ρ) and Laplacian of the Electron Density ($\nabla^2\rho$) at the Bond Critical point (BCP) in au for H-Bonds

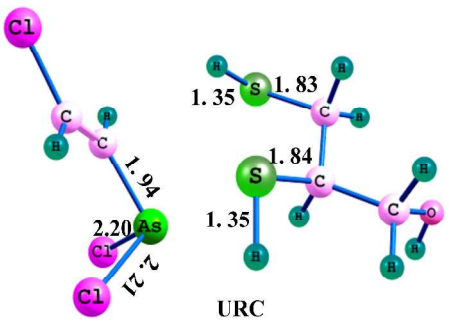
Species	Bond	ρ	$\nabla^2\rho$
UTS1-SA	Clx-H(SA)	0.0176	0.0704
UTS1-SB	Cly-H(SB)	0.0175	0.0704
UTS2-SB	Cly-H(SB)	0.0107	0.0751
UTS2-SA	Clx-H(SA)	0.0109	0.0762
CTS1-W	H(O)-Clx	0.0181	0.0620
	H(SA)-O(H_2O)	0.0116	0.0474
CTS2-W	H(H_2O)-Cly	0.0197	0.0643
	H(SB)-O(H_2O)	0.0122	0.0508
CTS1-A	H(NH_3)-Clx	0.0111	0.0397
	H(SA)-N(NH_3)	0.0115	0.0361
CTS2-A	H(NH_3)-Cly	0.0142	0.0567
	H(SB)-(NH_3)	0.0135	0.0541

Table S6. Cartesian coordinates of all optimized stationary points involved in the detoxification of BAL in gas-phase, optimized at M062X/GENECP level of theory.

URC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.871246	-1.026683	-0.266794
2	6	0	2.876750	1.079664	-0.819050
3	6	0	2.716240	-0.043117	0.195480
4	1	0	3.653966	0.790426	-1.525751
5	1	0	3.199288	2.000189	-0.330644
6	1	0	2.280615	-0.912474	-0.304021
7	16	0	1.399763	1.421244	-1.838898
8	16	0	1.549733	0.503291	1.502967
9	6	0	4.067518	-0.413598	0.806010
10	1	0	4.511233	0.468283	1.270151
11	1	0	3.928359	-1.168530	1.586310
12	8	0	4.979229	-0.855786	-0.180033
13	1	0	4.722214	-1.734682	-0.474712
14	17	0	-1.601335	-1.556587	1.754727
15	1	0	1.533110	-0.651952	2.192834
16	1	0	0.683191	2.059321	-0.895075
17	17	0	-2.387211	-2.081460	-1.486376
18	6	0	-1.741157	0.702211	-0.427711
19	6	0	-2.051979	1.462787	0.603980
20	1	0	-1.924947	1.174347	1.638273
21	1	0	-1.898238	1.034401	-1.448938
22	17	0	-2.727200	3.058473	0.423336

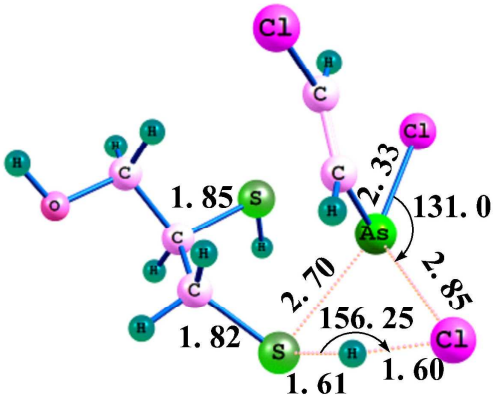


URC

UTS1-SA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.342097	-0.235741	0.521448
2	6	0	1.544697	-1.536184	-0.679843
3	6	0	2.112297	-1.056681	0.660419
4	1	0	2.267925	-2.232224	-1.100386
5	1	0	1.456631	-0.700992	-1.371684
6	1	0	2.507389	-1.907770	1.215122
7	16	0	-0.049418	-2.394410	-0.477766
8	16	0	0.879024	-0.275400	1.806224
9	6	0	3.221375	-0.029451	0.452097
10	1	0	2.795849	0.863061	-0.025399
11	1	0	3.650717	0.259093	1.416620
12	8	0	4.180140	-0.652087	-0.375966
13	1	0	4.856352	-0.013271	-0.617627
14	17	0	-2.548145	-1.130645	-1.904780
15	1	0	-1.155458	-1.800119	-1.486547
16	1	0	0.601019	-1.376149	2.530938
17	17	0	-1.865841	1.555716	1.921327
18	6	0	-0.416935	0.875098	-0.796496
19	1	0	-0.372369	0.456605	-1.793791
20	6	0	0.110603	2.056186	-0.530454
21	1	0	0.058662	2.560545	0.425060
22	17	0	0.971365	2.972018	-1.739020

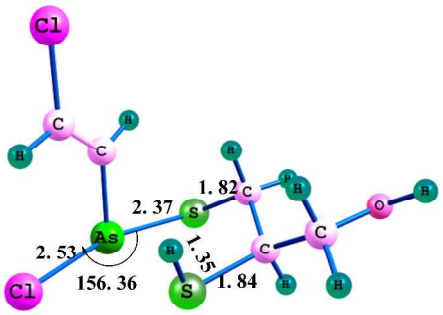


UTS1-SA

UINT-SA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	0.671918	-1.199903	0.647887
2	6	0	-1.888133	0.680768	0.985293
3	6	0	-2.365469	0.075599	-0.331280
4	1	0	-2.751418	1.101738	1.499151
5	1	0	-1.178681	1.489152	0.790991
6	1	0	-3.157967	-0.646921	-0.132248
7	16	0	-1.140331	-0.593283	2.045944
8	16	0	-1.047517	-0.916871	-1.131297
9	6	0	-2.875975	1.124687	-1.310929
10	1	0	-2.067076	1.833354	-1.532903
11	1	0	-3.190187	0.648278	-2.245411
12	8	0	-3.958106	1.766755	-0.670621
13	1	0	-4.311258	2.449871	-1.247453
14	1	0	-0.374729	0.091912	-1.720662
15	17	0	1.855165	-1.670729	-1.534443
16	6	0	1.328197	0.637387	0.673318
17	6	0	2.195725	1.160113	-0.179398
18	1	0	1.005903	1.201863	1.541846
19	1	0	2.583609	0.656624	-1.053751
20	17	0	2.825591	2.772378	0.030253

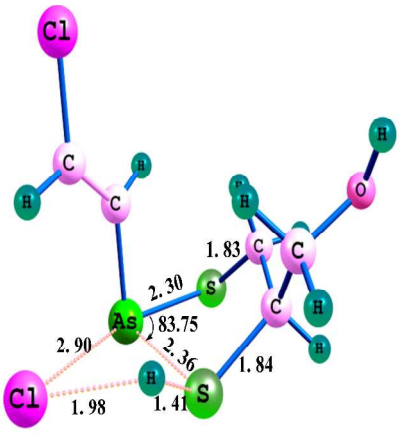


UINT-SA

UTS2-SB

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.238876	-1.368516	-0.686881
2	6	0	1.871479	0.860712	-0.918475
3	6	0	2.093741	0.561283	0.572338
4	1	0	2.767819	1.334007	-1.315950
5	1	0	1.051036	1.569119	-1.025677
6	1	0	3.145762	0.338433	0.748796
7	16	0	1.544923	-0.620460	-1.938587
8	16	0	1.226885	-0.968527	1.121506
9	6	0	1.670024	1.733684	1.446798
10	1	0	0.600835	1.921548	1.288859
11	1	0	1.835902	1.500684	2.503593
12	8	0	2.460674	2.827096	1.029591
13	1	0	2.173357	3.622656	1.486385
14	1	0	0.071966	-0.635665	1.862180
15	17	0	-1.646908	-1.633027	1.843209
16	6	0	-1.155147	0.346602	-0.862624
17	1	0	-0.867490	0.881240	-1.762447
18	6	0	-2.148026	0.808617	-0.118329
19	1	0	-2.527599	0.341439	0.779262
20	17	0	-2.964588	2.293569	-0.536126

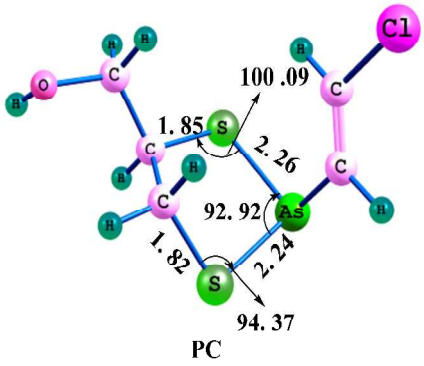


UTS2-SB

PC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	0.441555	-1.616128	-0.361840
2	6	0	-1.310171	0.267047	1.181783
3	6	0	-1.925938	0.473832	-0.190485
4	1	0	-2.032134	0.537937	1.952673
5	1	0	-0.422545	0.890020	1.303008
6	1	0	-2.876323	-0.061457	-0.244926
7	16	0	-0.863085	-1.480465	1.460595
8	16	0	-0.874734	-0.216552	-1.550505
9	6	0	-2.154633	1.959220	-0.470285
10	1	0	-1.206729	2.492627	-0.382910
11	1	0	-2.526947	2.098437	-1.489543
12	8	0	-3.030936	2.534128	0.480502
13	1	0	-3.926607	2.233270	0.300786
14	6	0	1.814601	-0.358473	0.247721
15	6	0	2.004796	0.851271	-0.244241
16	1	0	2.476112	-0.752614	1.013477
17	1	0	1.391216	1.300957	-1.013174
18	17	0	3.296076	1.900877	0.291114

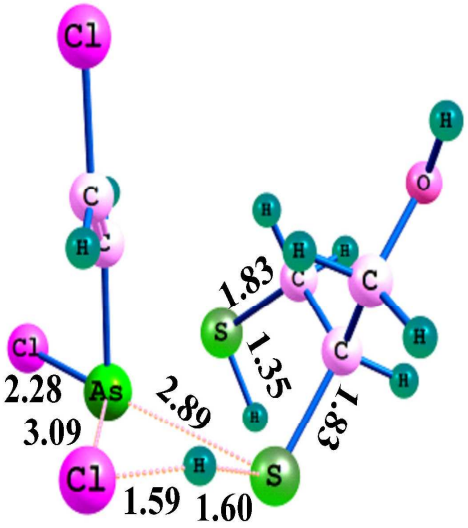


PC

UTS1-SB

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.356784	-0.385689	0.362288
2	6	0	1.293771	-1.170084	-1.516638
3	6	0	2.049099	-1.444645	-0.198359
4	1	0	1.784841	-1.660751	-2.354603
5	1	0	1.263241	-0.103399	-1.737638
6	1	0	2.617225	-2.366090	-0.331697
7	16	0	-0.466401	-1.682830	-1.580009
8	16	0	1.002575	-1.738577	1.268716
9	6	0	3.034056	-0.312780	0.050054
10	1	0	2.476993	0.602828	0.280740
11	1	0	3.662503	-0.565356	0.907418
12	8	0	3.798549	-0.164939	-1.136445
13	1	0	4.404228	0.574437	-1.035847
14	1	0	0.742580	-0.372304	2.069922
15	17	0	-0.019534	0.748213	2.910472
16	6	0	-0.601588	1.160489	-0.562714
17	1	0	-0.871541	1.215696	-1.613326
18	6	0	0.087411	2.146703	-0.012065
19	1	0	0.359969	2.216818	1.031234
20	17	0	0.642412	3.495347	-0.964948
21	1	0	-0.340345	-2.849527	-0.913365
22	17	0	-3.297554	-0.136541	-0.813040

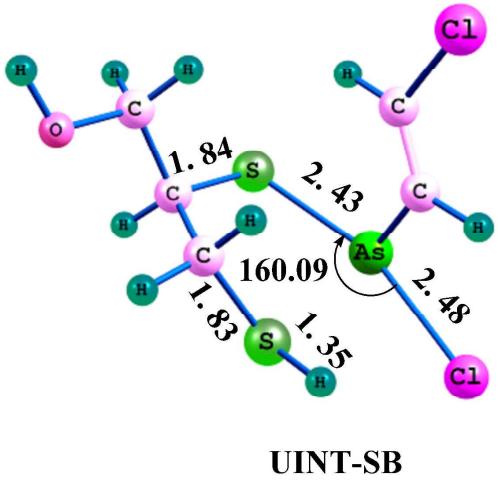


UTS1-SB

UINT-SB

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.276201	-0.368464	0.767752
2	6	0	1.256452	-1.013083	-1.161373
3	6	0	1.995805	-1.198474	0.156359
4	1	0	1.783365	-1.514039	-1.971852
5	1	0	1.126946	0.042852	-1.395877
6	1	0	2.293989	-2.243513	0.254258
7	16	0	-0.405313	-1.755387	-1.010246
8	16	0	0.961590	-0.795834	1.625023
9	6	0	3.254105	-0.344830	0.138681
10	1	0	2.972411	0.713235	0.078391
11	1	0	3.809002	-0.506011	1.066778
12	8	0	4.008251	-0.740539	-0.996446
13	1	0	4.847939	-0.273451	-1.001073
14	17	0	-3.272566	-0.470098	-0.712455
15	1	0	-1.024483	-1.125294	-2.029909
16	6	0	-0.867736	1.346146	-0.076217
17	1	0	-1.618026	1.696184	-0.775453
18	6	0	0.156742	2.104894	0.279107
19	1	0	0.916163	1.813433	0.992376
20	17	0	0.406017	3.701382	-0.372114

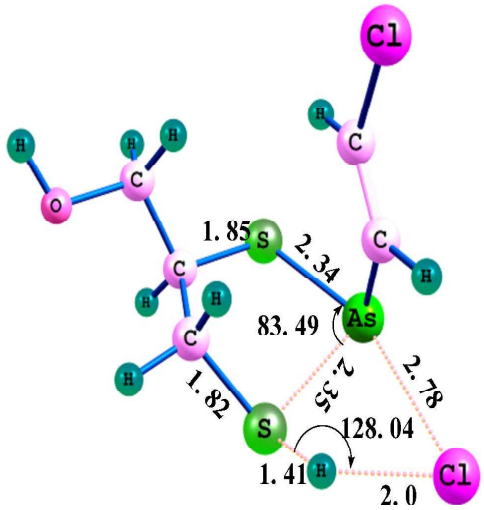


UINT-SB

UTS2-SA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.175069	-0.278229	0.900312
2	6	0	0.974353	-1.198200	-1.181138
3	6	0	1.830388	-1.322361	0.078373
4	1	0	1.398772	-1.803493	-1.980083
5	1	0	0.889907	-0.164012	-1.509674
6	1	0	2.115881	-2.366980	0.209775
7	16	0	-0.698484	-1.826256	-0.810644
8	16	0	0.964557	-0.846991	1.646462
9	6	0	3.097343	-0.498522	-0.093225
10	1	0	2.828638	0.558361	-0.205215
11	1	0	3.725129	-0.608626	0.795709
12	8	0	3.745844	-0.990590	-1.253507
13	1	0	4.565897	-0.508847	-1.391275
14	17	0	-3.256224	-0.122731	-0.945283
15	1	0	-1.610979	-1.073752	-1.574295
16	6	0	-0.659608	1.359680	-0.032382
17	1	0	-1.378724	1.715323	-0.760474
18	6	0	0.388794	2.081545	0.328276
19	1	0	1.113872	1.784897	1.073773
20	17	0	0.733714	3.641113	-0.367246

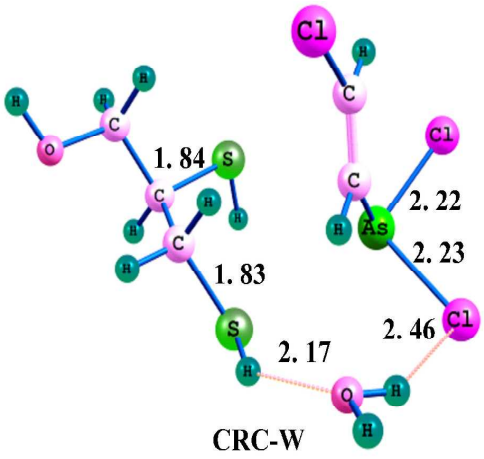


UTS2-SA

CRC-W

Standard orientation:

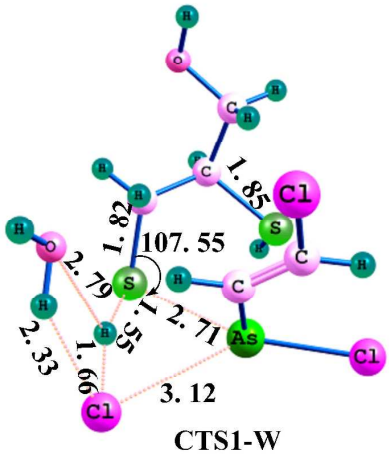
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.490145	0.094328	-0.778507
2	6	0	2.189856	1.070364	0.314492
3	6	0	2.858032	0.413333	-0.883395
4	1	0	2.951816	1.592538	0.889384
5	1	0	1.728128	0.307350	0.941462
6	1	0	3.351267	1.165229	-1.499895
7	16	0	0.920875	2.277240	-0.224206
8	16	0	1.694249	-0.517932	-1.970224
9	6	0	3.899675	-0.597875	-0.419979
10	1	0	3.396396	-1.409306	0.122210
11	1	0	4.401910	-1.020427	-1.294470
12	8	0	4.809724	0.088442	0.418860
13	1	0	5.472247	-0.530369	0.737200
14	17	0	-3.152724	1.219460	0.232516
15	1	0	0.539409	2.668597	1.008049
16	1	0	1.289069	0.533885	-2.702242
17	17	0	-2.566706	-1.785729	-1.276925
18	6	0	-0.724429	-0.519359	0.901316
19	1	0	-0.529555	0.260186	1.632064
20	6	0	-0.367265	-1.772337	1.102567
21	1	0	-0.544336	-2.587889	0.415567
22	17	0	0.468601	-2.279600	2.550596
23	1	0	-1.830874	2.249168	2.031213
24	8	0	-1.000212	2.379614	2.507384
25	1	0	-1.239895	2.579864	3.415937



CTS1-W

Standard orientation:

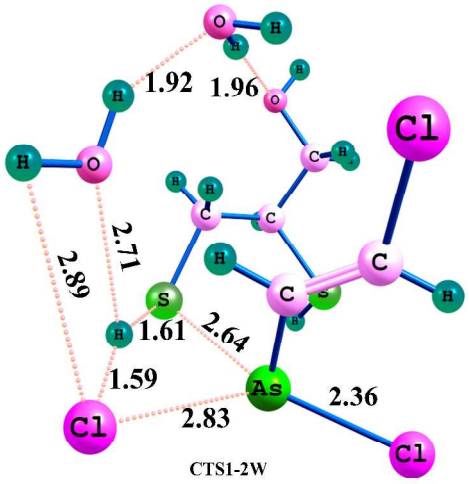
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.353003	-0.389326	-0.628087
2	6	0	1.623006	1.193892	-0.947488
3	6	0	2.088526	-0.217634	-1.321903
4	1	0	2.395390	1.885396	-1.278225
5	1	0	1.524425	1.313633	0.129472
6	1	0	2.540472	-0.210679	-2.314196
7	16	0	0.057171	1.625766	-1.769480
8	16	0	0.744249	-1.494115	-1.444626
9	6	0	3.101175	-0.753174	-0.312964
10	1	0	2.620880	-0.821301	0.671336
11	1	0	3.439037	-1.750926	-0.611032
12	8	0	4.166855	0.171508	-0.310310
13	1	0	4.750079	-0.014793	0.430538
14	17	0	-2.228120	2.479006	0.249609
15	1	0	-0.878654	2.241422	-0.698524
16	1	0	0.486244	-1.346665	-2.758844
17	17	0	-2.026690	-2.569792	-0.174321
18	6	0	-0.432506	-0.112013	1.065988
19	1	0	-0.180701	0.916532	1.298958
20	6	0	-0.146821	-1.086323	1.911701
21	1	0	-0.393769	-2.130001	1.776654
22	17	0	0.694085	-0.776988	3.408498
23	1	0	0.822245	3.316167	2.421645
24	8	0	0.602329	2.926338	1.572145
25	1	0	-0.320695	3.163472	1.393755



CTS1-2W

Standard orientation:

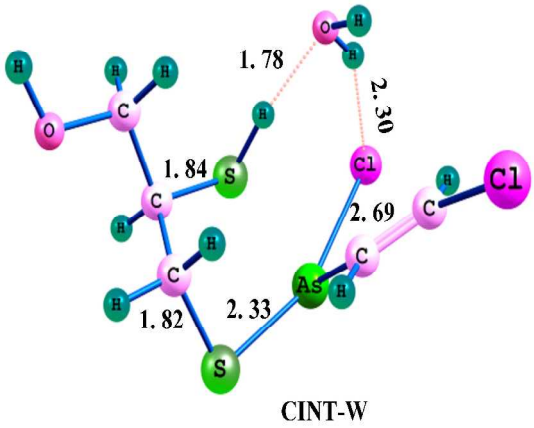
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.748668	-0.113617	-0.216713
2	6	0	1.281751	0.345159	-1.603122
3	6	0	1.326265	-1.185803	-1.659890
4	1	0	2.058200	0.725723	-2.265300
5	1	0	1.505986	0.702687	-0.603310
6	1	0	1.469381	-1.519537	-2.687301
7	16	0	-0.319873	1.014656	-2.139648
8	16	0	-0.220348	-2.033042	-1.083124
9	6	0	2.447253	-1.730470	-0.776991
10	1	0	2.197250	-1.549140	0.276283
11	1	0	2.558791	-2.805883	-0.927572
12	8	0	3.644528	-1.039382	-1.115194
13	1	0	4.397861	-1.629020	-1.022570
14	17	0	-1.934510	2.713821	-0.070556
15	1	0	-0.846546	2.116344	-1.077025
16	1	0	-0.808923	-2.136824	-2.289625
17	17	0	-2.680424	-1.835731	1.104845
18	6	0	-0.311921	0.288801	1.049044
19	1	0	0.166022	1.254740	0.906823
20	6	0	0.057292	-0.531551	2.013437
21	1	0	-0.390427	-1.487780	2.244944
22	17	0	1.378125	-0.133503	3.102473
23	1	0	2.347441	2.545817	0.456996
24	8	0	1.446381	2.796635	0.197984
25	1	0	1.262423	3.673242	0.543229
26	8	0	3.615013	1.146211	0.802130
27	1	0	3.769660	0.508128	0.089037
28	1	0	3.237018	0.642538	1.532068



CINT-W

Standard orientation:

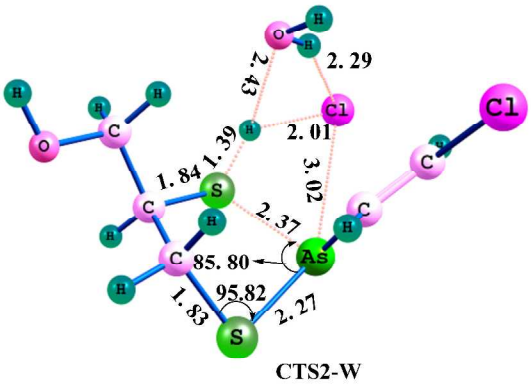
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.420855	-1.426720	-0.393276
2	6	0	2.019496	0.373154	-1.235691
3	6	0	2.462119	0.193774	0.210401
4	1	0	2.886951	0.651795	-1.832609
5	1	0	1.288399	1.182041	-1.303855
6	1	0	3.285565	-0.519362	0.253489
7	16	0	1.340229	-1.177218	-1.906638
8	16	0	1.135722	-0.559006	1.233253
9	6	0	2.890623	1.506123	0.855833
10	1	0	2.041738	2.201474	0.860553
11	1	0	3.200883	1.331906	1.891111
12	8	0	3.958451	1.997884	0.071995
13	1	0	4.292566	2.809802	0.463415
14	1	0	0.412515	0.579804	1.514357
15	17	0	-1.790072	-1.252902	1.912791
16	6	0	-1.234687	0.252771	-0.981918
17	6	0	-2.398716	0.691761	-0.530816
18	1	0	-0.762831	0.734924	-1.830218
19	1	0	-2.954379	0.247128	0.283567
20	17	0	-3.174328	2.102904	-1.208684
21	1	0	-1.389766	0.970352	2.324805
22	8	0	-0.803673	1.728100	2.139727
23	1	0	-1.305084	2.308070	1.557206



CTS2-W

Standard orientation:

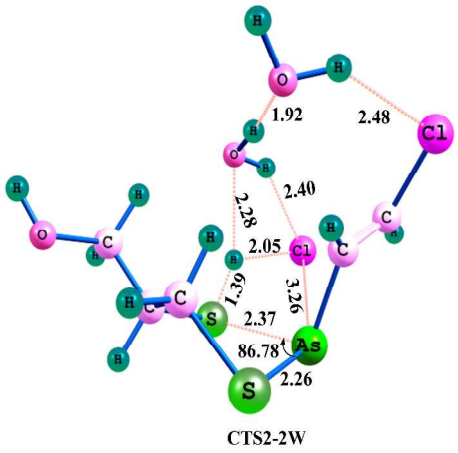
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.228438	-1.561470	0.412452
2	6	0	1.955180	-0.256263	-1.276712
3	6	0	2.389213	0.408264	0.023553
4	1	0	2.795220	-0.255881	-1.970115
5	1	0	1.141743	0.310199	-1.729879
6	1	0	3.349091	-0.002156	0.339349
7	16	0	1.465860	-2.002454	-1.025150
8	16	0	1.259617	-0.008181	1.415945
9	6	0	2.492037	1.923198	-0.107179
10	1	0	1.505047	2.334337	-0.340098
11	1	0	2.838844	2.352831	0.838548
12	8	0	3.429436	2.149131	-1.145364
13	1	0	3.455441	3.089454	-1.343182
14	1	0	0.267521	0.959576	1.476903
15	17	0	-1.596876	0.658626	2.385552
16	6	0	-1.219790	-0.489910	-0.864833
17	1	0	-0.801227	-0.358622	-1.854800
18	6	0	-2.455412	-0.099706	-0.596769
19	1	0	-2.940069	-0.183235	0.366592
20	17	0	-3.428622	0.712950	-1.792184
21	8	0	-0.751118	2.633323	0.033165
22	1	0	-1.389102	2.708376	-0.682742
23	1	0	-1.252139	2.253896	0.777763



CTS2-2W

Standard orientation:

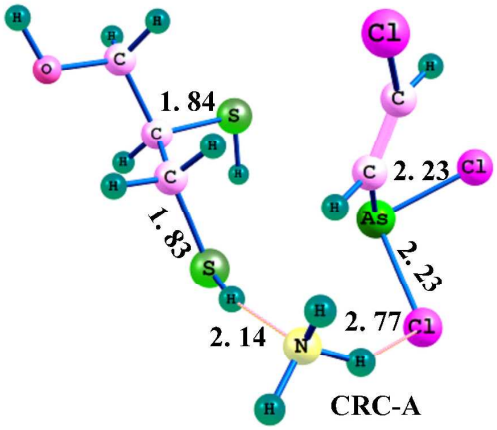
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.170247	-1.579189	-0.699790
2	6	0	1.784631	0.703142	-1.149628
3	6	0	2.487388	0.182267	0.093842
4	1	0	2.486131	1.304151	-1.727545
5	1	0	0.931691	1.327138	-0.874911
6	1	0	3.394499	-0.347848	-0.200611
7	16	0	1.256993	-0.690503	-2.217981
8	16	0	1.485857	-1.114695	0.930749
9	6	0	2.849140	1.281040	1.085682
10	1	0	1.939763	1.788677	1.414062
11	1	0	3.346181	0.838700	1.955770
12	8	0	3.729311	2.144928	0.383703
13	1	0	3.892543	2.923781	0.922325
14	1	0	0.535713	-0.501425	1.749998
15	17	0	-1.216773	-1.374725	2.381708
16	6	0	-1.339635	-0.022102	-0.735604
17	1	0	-1.047901	0.808219	-1.366787
18	6	0	-2.550121	-0.098135	-0.210574
19	1	0	-2.902988	-0.878045	0.450361
20	17	0	-3.748700	1.151710	-0.477571
21	8	0	-0.251156	1.642306	1.756532
22	1	0	-0.679553	2.119383	1.030689
23	1	0	-0.891952	0.992443	2.085843
24	8	0	-1.127110	3.102480	-0.558076
25	1	0	-2.065762	2.963564	-0.734336
26	1	0	-0.989568	4.053942	-0.545975



CRC-A

Standard orientation:

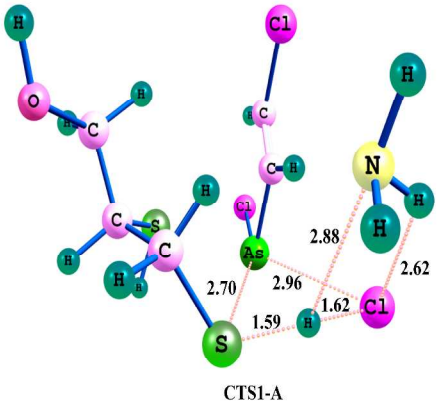
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	1.461572	-0.548044	-0.704987
2	6	0	-2.266449	-0.600523	0.738249
3	6	0	-2.968878	-0.661805	-0.608879
4	1	0	-3.013337	-0.705638	1.522936
5	1	0	-1.765665	0.363149	0.843999
6	1	0	-3.440435	-1.635714	-0.746221
7	16	0	-1.040613	-1.953630	0.900136
8	16	0	-1.844033	-0.374664	-2.039041
9	6	0	-4.046520	0.411382	-0.699307
10	1	0	-3.575772	1.401485	-0.638508
11	1	0	-4.556077	0.325251	-1.663136
12	8	0	-4.940908	0.205080	0.378622
13	1	0	-5.640482	0.862222	0.336535
14	17	0	2.872714	-1.360768	0.818157
15	1	0	-0.472085	-1.505062	2.048682
16	1	0	-1.323794	-1.612880	-2.075323
17	17	0	2.875773	0.716811	-1.870326
18	6	0	0.818342	0.866739	0.464365
19	1	0	0.458307	0.525956	1.428806
20	6	0	0.735134	2.131474	0.102974
21	1	0	1.081931	2.536868	-0.837090
22	17	0	0.030232	3.345053	1.146135
23	7	0	0.706302	-0.586202	3.587464
24	1	0	0.590660	-1.198460	4.387056
25	1	0	0.648302	0.367012	3.928755
26	1	0	1.646049	-0.725482	3.227485



CTS1-A

Standard orientation:

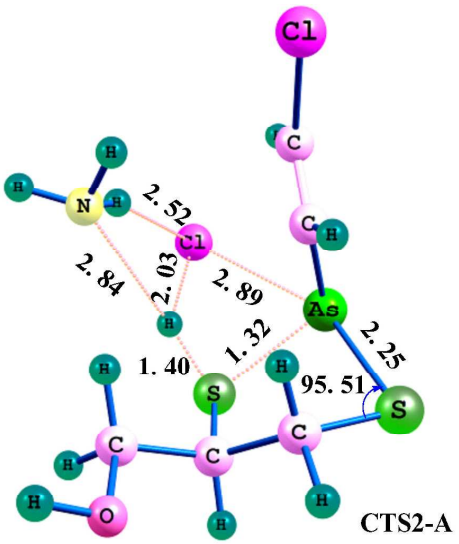
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.358568	-0.399263	-0.586682
2	6	0	1.663953	1.061340	-1.065184
3	6	0	2.083672	-0.391122	-1.326259
4	1	0	2.446308	1.696088	-1.477830
5	1	0	1.605019	1.274505	0.000694
6	1	0	2.537768	-0.476693	-2.313682
7	16	0	0.086843	1.491646	-1.869107
8	16	0	0.706104	-1.635744	-1.352764
9	6	0	3.080090	-0.871656	-0.274982
10	1	0	2.596297	-0.851371	0.709862
11	1	0	3.394300	-1.897056	-0.494115
12	8	0	4.169556	0.024902	-0.336256
13	1	0	4.757566	-0.139019	0.406065
14	17	0	-2.287081	2.351802	0.020096
15	1	0	-0.907692	2.144774	-0.803339
16	1	0	0.433026	-1.547733	-2.669042
17	17	0	-2.089567	-2.506619	0.104017
18	6	0	-0.384172	0.002457	1.053012
19	1	0	-0.041971	1.028287	1.157431
20	6	0	-0.154051	-0.880890	2.007852
21	1	0	-0.479944	-1.911332	2.009601
22	17	0	0.742827	-0.449755	3.443713
23	1	0	1.098263	3.376748	2.269239
24	1	0	-0.328911	3.321282	1.460741
25	7	0	0.671852	3.167151	1.373999
26	1	0	1.014171	3.850446	0.707171



CTS2-A

Standard orientation:

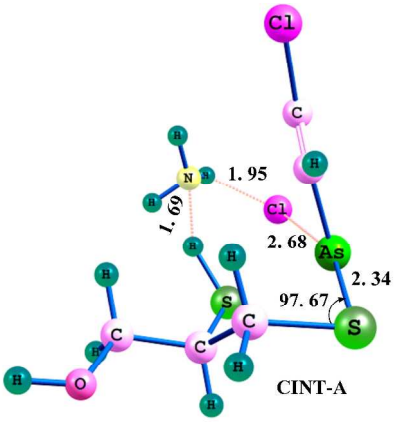
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.267149	-1.560435	0.302056
2	6	0	1.904035	-0.163677	-1.322975
3	6	0	2.416500	0.331714	0.022115
4	1	0	2.712571	-0.109404	-2.050851
5	1	0	1.090751	0.477209	-1.665031
6	1	0	3.351065	-0.176089	0.264568
7	16	0	1.362669	-1.910466	-1.239540
8	16	0	1.293789	-0.156821	1.397554
9	6	0	2.626708	1.839848	0.040681
10	1	0	1.666736	2.331910	-0.143480
11	1	0	3.007217	2.149254	1.020165
12	8	0	3.576274	2.102535	-0.979432
13	1	0	3.636949	3.052216	-1.113016
14	1	0	0.287232	0.802628	1.588642
15	17	0	-1.500299	0.408159	2.480396
16	6	0	-1.267203	-0.356767	-0.853903
17	1	0	-0.872759	-0.170155	-1.845384
18	6	0	-2.497521	0.014690	-0.537338
19	1	0	-2.960762	-0.130461	0.429060
20	17	0	-3.505595	0.881719	-1.664757
21	1	0	-1.238919	2.209279	0.787167
22	1	0	-1.242098	2.645830	-0.785036
23	7	0	-0.713900	2.720967	0.078193
24	1	0	-0.733191	3.698905	0.347902



CINT-A

Standard orientation:

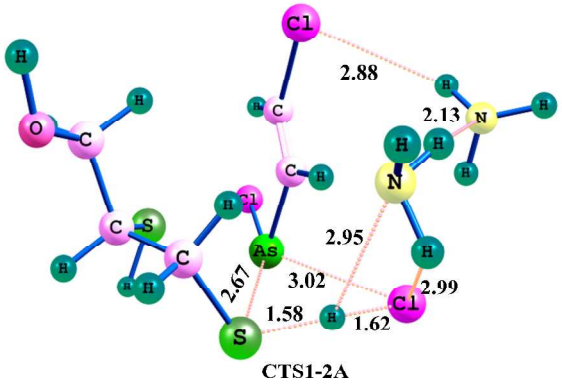
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	0.1379350	-0.683189	-1.198816
2	6	0	-2.366118	-0.974067	0.584606
3	6	0	-2.563454	0.446490	0.091825
4	1	0	-3.334246	-1.411329	0.830454
5	1	0	-1.746963	-0.985494	1.484007
6	1	0	-3.268916	0.444387	-0.739052
7	16	0	-1.626645	-2.018540	-0.716596
8	16	0	-0.995250	1.192402	-0.526751
9	6	0	-3.107501	1.342687	1.194652
10	1	0	-2.396460	1.359066	2.030517
11	1	0	-3.223786	2.363211	0.816370
12	8	0	-4.353015	0.797471	1.592368
13	1	0	-4.781974	1.398689	2.206868
14	1	0	2.355766	4.324810	-1.201146
15	17	0	1.768846	1.357969	-1.795640
16	6	0	1.071673	-0.969595	0.509563
17	6	0	2.388159	-0.899585	0.552763
18	1	0	0.492411	-1.183432	1.402060
19	1	0	3.032101	-0.683253	-0.288932
20	17	0	3.287441	-1.050155	2.060666
21	7	0	2.40045728	3.789751	-0.328648
22	1	0	1.491835	3.769173	0.124201
23	1	0	0.581549	1.925120	-0.992408
24	1	0	2.727782	2.843824	-0.517898



CTS1-2A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.292174	-1.552398	-0.194435
2	6	0	1.487423	1.025077	-1.461828
3	6	0	2.578985	0.436307	-0.560709
4	1	0	1.985125	1.673537	-2.180894
5	1	0	0.786484	1.643036	-0.902510
6	1	0	3.458110	0.182131	-1.153163
7	16	0	0.576452	-0.259157	-2.374706
8	16	0	2.137872	-1.150800	0.296617
9	6	0	2.980468	1.426198	0.528832
10	1	0	2.104800	1.642356	1.153333
11	1	0	3.768406	0.999599	1.157758
12	8	0	3.432525	2.579426	-0.149079
13	1	0	3.513110	3.305939	0.474819
14	17	0	-2.528470	-0.428273	-1.893754
15	1	0	-0.985304	-0.024332	-2.200043
16	1	0	2.613503	-1.985543	-0.648431
17	17	0	-0.243112	-2.768473	1.809128
18	6	0	-0.646392	0.171607	0.647745
19	1	0	-0.939096	0.973003	-0.027382
20	6	0	-0.530033	0.385402	1.946521
21	1	0	-0.268001	-0.356069	2.688367
22	17	0	-0.800391	1.967482	2.638556
23	1	0	-2.163039	2.721024	-0.656915
24	1	0	-1.689989	2.436083	-2.191697
25	7	0	-1.357998	2.756135	-1.287389
26	1	0	-1.079447	3.724919	-1.390679
27	7	0	-3.668388	1.792876	0.531765
28	1	0	-3.416111	1.565243	1.486755
29	1	0	-3.617139	0.938452	-0.016887
30	1	0	-4.633491	2.100512	0.535184

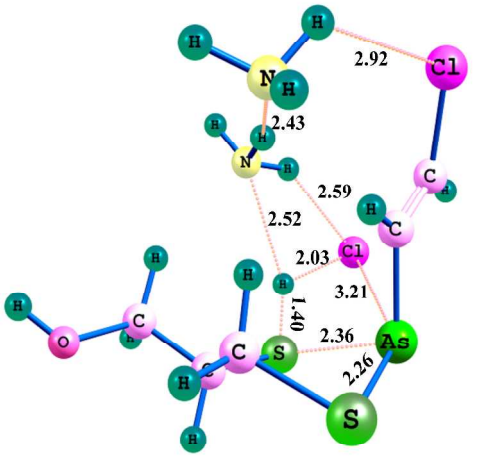


CTS1-2A

CTS2-2A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-0.201884	-1.385012	-1.039219
2	6	0	1.815289	0.902057	-0.889543
3	6	0	2.466445	0.074697	0.206431
4	1	0	2.556347	1.590434	-1.295294
5	1	0	0.981667	1.484766	-0.491599
6	1	0	3.370690	-0.395188	-0.184372
7	16	0	1.267629	-0.171480	-2.271289
8	16	0	1.418689	-1.362443	0.686632
9	6	0	2.816493	0.894161	1.440760
10	1	0	1.899139	1.325519	1.849003
11	1	0	3.279341	0.246221	2.192987
12	8	0	3.730115	1.884187	0.992318
13	1	0	3.927274	2.476938	1.722365
14	1	0	0.428141	-0.981136	1.607577
15	17	0	-1.280792	-2.048294	1.914238
16	6	0	-1.317942	0.157438	-0.658738
17	1	0	-0.976531	1.133968	-0.979684
18	6	0	-2.542641	-0.014299	-0.191156
19	1	0	-2.944527	-0.941876	0.192905
20	17	0	-3.664286	1.319749	-0.057821
21	1	0	-1.105522	0.525342	2.196815
22	1	0	-0.785991	1.896618	1.342055
23	7	0	-0.473341	1.319866	2.118676
24	1	0	-0.566471	1.864828	2.968317
25	7	0	-0.786365	3.501061	-0.493926
26	1	0	-1.793119	3.546956	-0.373172
27	1	0	-0.593697	3.704574	-1.468714
28	1	0	-0.378159	4.251150	0.052162



CTS2-2A

Table S7: Data for Arrhenius plot (ln k vs 1/T) obtained by numerical integration			
1/T	*ln* k_{uc}	l*n* k_A	*ln* k_W
0.006666667	-87.0582032	-79.12237303	-79.46786709
0.00625	-79.7058621	-72.26602136	-72.58992205
0.005882353	-73.2185024	-66.2162993	-66.52114701
0.005555556	-67.4519604	-60.83876859	-61.12668031
0.005263158	-62.2924228	-56.02729373	-56.3000522
0.005	-57.648839	-51.69696636	-51.95608691
0.004761905	-53.4475012	-47.77905113	-48.0258326
0.004545455	-49.6281033	-44.21731	-44.45287414
0.004347826	-46.1408269	-40.9652855	-41.19060771
0.004166667	-42.9441569	-37.98426303	-38.20019682
0.004	-40.0032204	-35.24172237	-35.44901881
0.003846154	-37.2885099	-32.71014637	-32.90946987
0.003703704	-34.774889	-30.36609452	-30.55803567
0.003571429	-32.4408125	-28.18947494	-28.37456106
0.003448276	-30.2677068	-26.16296706	-26.34167092
0.003333333	-28.2394748	-24.2715597	-24.44430679
0.003225806	-26.3420964	-22.50217863	-22.66935327
0.003125	-24.5633042	-20.84338387	-21.00533437
0.003030303	-22.8923176	-19.28512213	-19.44216514
0.002941176	-21.3196244	-17.81852284	-17.97094709
0.002857143	-19.8367993	-16.43572923	-16.58379872
0.002777778	-18.4363534	-15.12975748	-15.27371425
0.002702703	-17.1116072	-13.8943788	-14.03444529
0.002631579	-15.8565846	-12.72402005	-12.86040118
0.002564103	-14.6659221	-11.6136797	-11.74656469
0.0025	-13.5347927	-10.55885637	-10.6884203
0.002439024	-12.4588403	-9.555487833	-9.681893066
0.002380952	-11.4341238	-8.599898751	-8.723296129
0.002325581	-10.4570685	-7.688755672	-7.80928562
0.002272727	-9.52442483	-6.819028188	-6.936821673
0.002222222	-8.63323197	-5.987955259	-6.10313465
0.002173913	-7.78078663	-5.193015935	-5.30569577
0.00212766	-6.96461557	-4.431903817	-4.542191488
0.002083333	-6.18245163	-3.702504704	-3.810501073
0.002040816	-5.43221274	-3.002876983	-3.108676939
0.002	-4.71198342	-2.331234371	-2.434927327
0.001960784	-4.01999838	-1.685930684	-1.787601029

0.001923077	-3.35462815	-1.065446371	-1.165173877
0.001886792	-2.71436624	-0.468376559	-0.566236756
0.001851852	-2.09781772	0.106579555	0.010515047
0.001818182	-1.50368916	0.660628174	0.566291336
0.001785714	-0.93077947	1.194889343	1.102215479
0.001754386	-0.37797188	1.710404506	1.619331988
0.001724138	0.155773386	2.208143284	2.118613321
0.001694915	0.671425587	2.689009561	2.600965983
0.001666667	1.169889381	3.153846962	3.06723603
0.001639344	1.652010098	3.603443793	3.518214016
0.001612903	2.118578534	4.0385375	3.954639476
0.001587302	2.570335272	4.459818708	4.37720497
0.0015625	3.007974611	4.867934878	4.78655976
0.001538462	3.432148123	5.263493628	5.183313135
0.001515152	3.843467892	5.64706575	5.568037444
0.001492537	4.242509457	6.019187957	5.941270849
0.001470588	4.629814504	6.380365393	6.303519847
0.001449275	5.005893316	6.731073918	6.655261558
0.001428571	5.371227019	7.0717622	6.996945826
0.001408451	5.726269629	7.402853628	7.328997143
0.001388889	6.071449944	7.724748073	7.651816408
0.001369863	6.407173261	8.037823491	7.965782545
0.001351351	6.733822975	8.342437412	8.271253988
0.001333333	7.051762027	8.638928295	8.568570047
0.001315789	7.36133426	8.927616786	8.858052168
0.001298701	7.662865655	9.208806875	9.140005094
0.001282051	7.956665473	9.482786961	9.414717935
0.001265823	8.24302732	9.749830843	9.68246516
0.00125	8.522230118	10.01019863	9.94350751
0.001234568	8.794539018	10.26413758	10.19809285
0.001219512	9.060206236	10.5118829	10.44645695
0.001204819	9.319471831	10.75365845	10.68882422
0.001190476	9.572564435	10.98967744	10.92540838
0.001176471	9.819701916	11.22014304	11.15641309
0.001162791	10.06109201	11.44524898	11.38203255
0.001149425	10.29693291	11.66518006	11.60245202
0.001136364	10.52741378	11.88011272	11.81784835
0.001123596	10.7527153	12.09021543	12.02839044
0.001111111	10.97301013	12.29564918	12.23423968
0.001098901	11.1884633	12.49656791	12.43555038
0.001086957	11.39923271	12.69311884	12.63247014

0.001075269	11.60546944	12.88544287	12.82514021
0.00106383	11.80731815	13.0736749	13.01369584
0.001052632	12.00491742	13.25794415	13.19826659
0.001041667	12.19840003	13.43837446	13.37897662
0.001030928	12.3878933	13.61508456	13.55594498
0.001020408	12.57351936	13.78818832	13.72928586
0.001010101	12.7553954	13.95779504	13.89910885
0.001	12.93363391	14.12400963	14.06551916

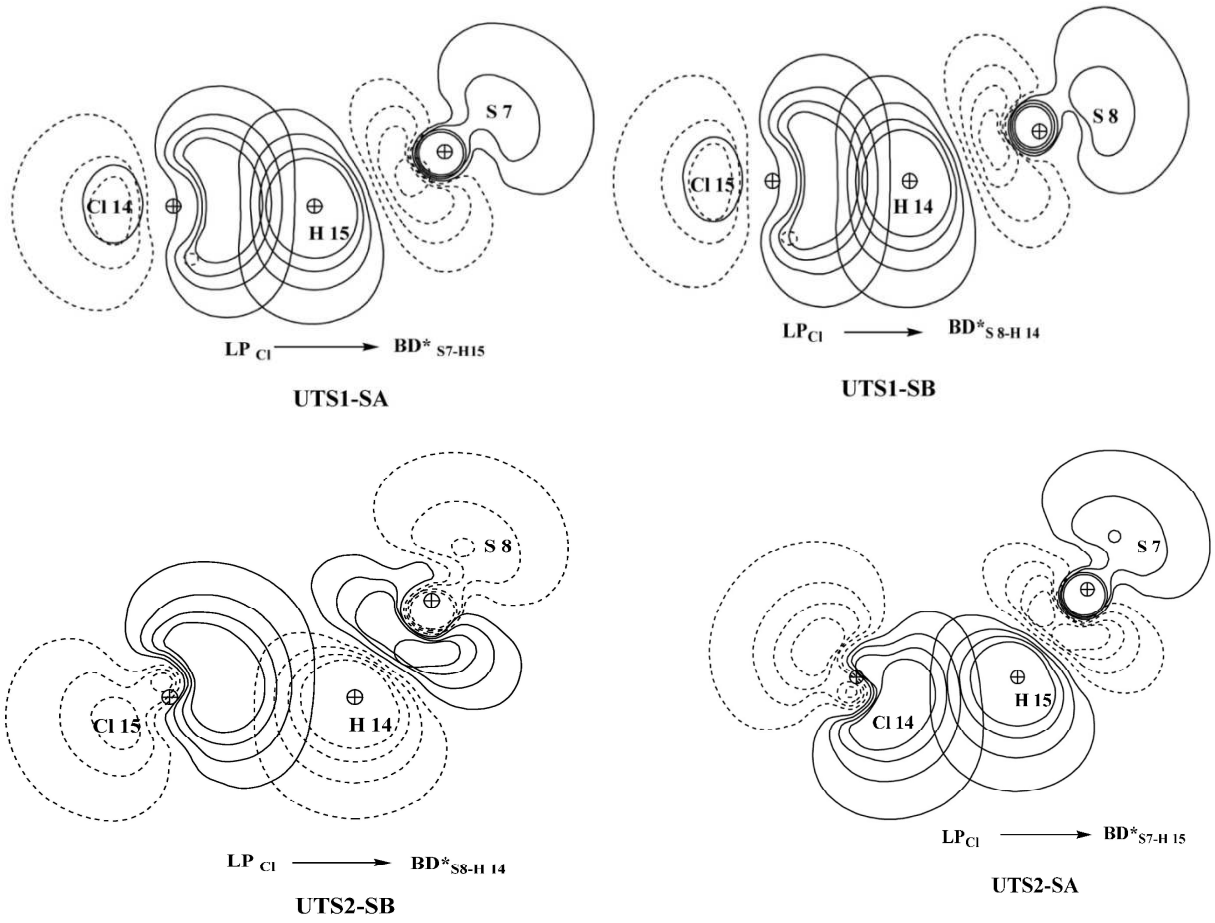


Figure S1. Contour plot of orbital overlap for UTS1-SA, UTS1-SB, UTS2-SB and UTS2-SA

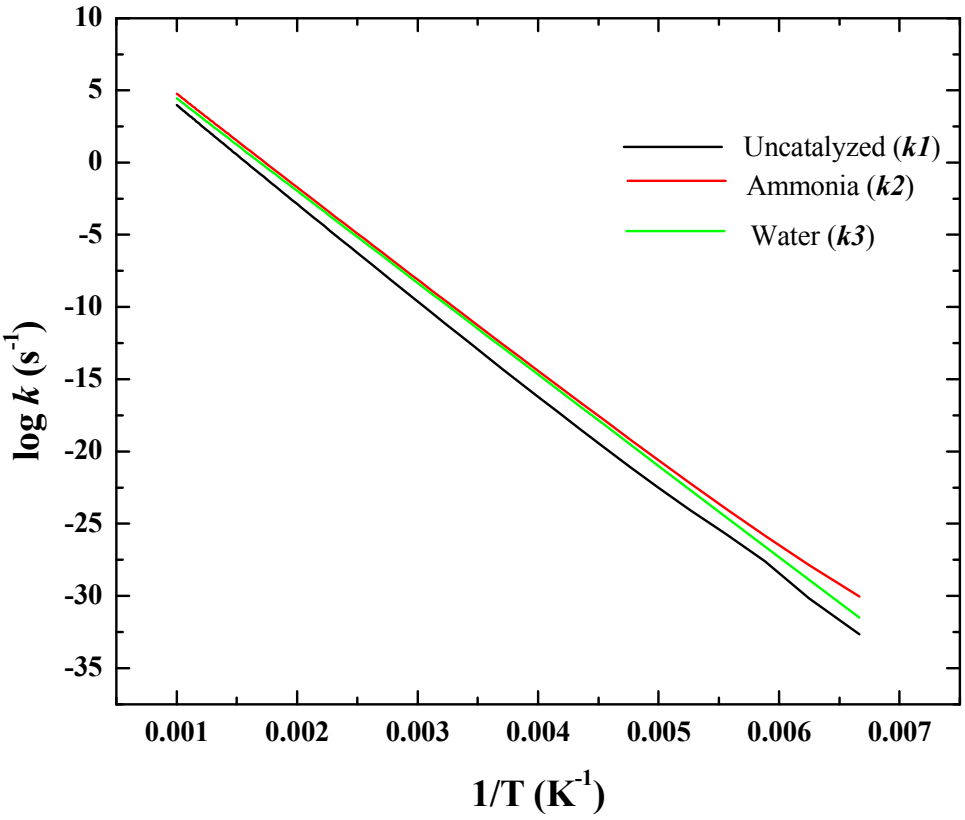


Figure S2. Arrhenius plots of the calculated rate constants for three channels for the detoxification of Lewisite by BAL.

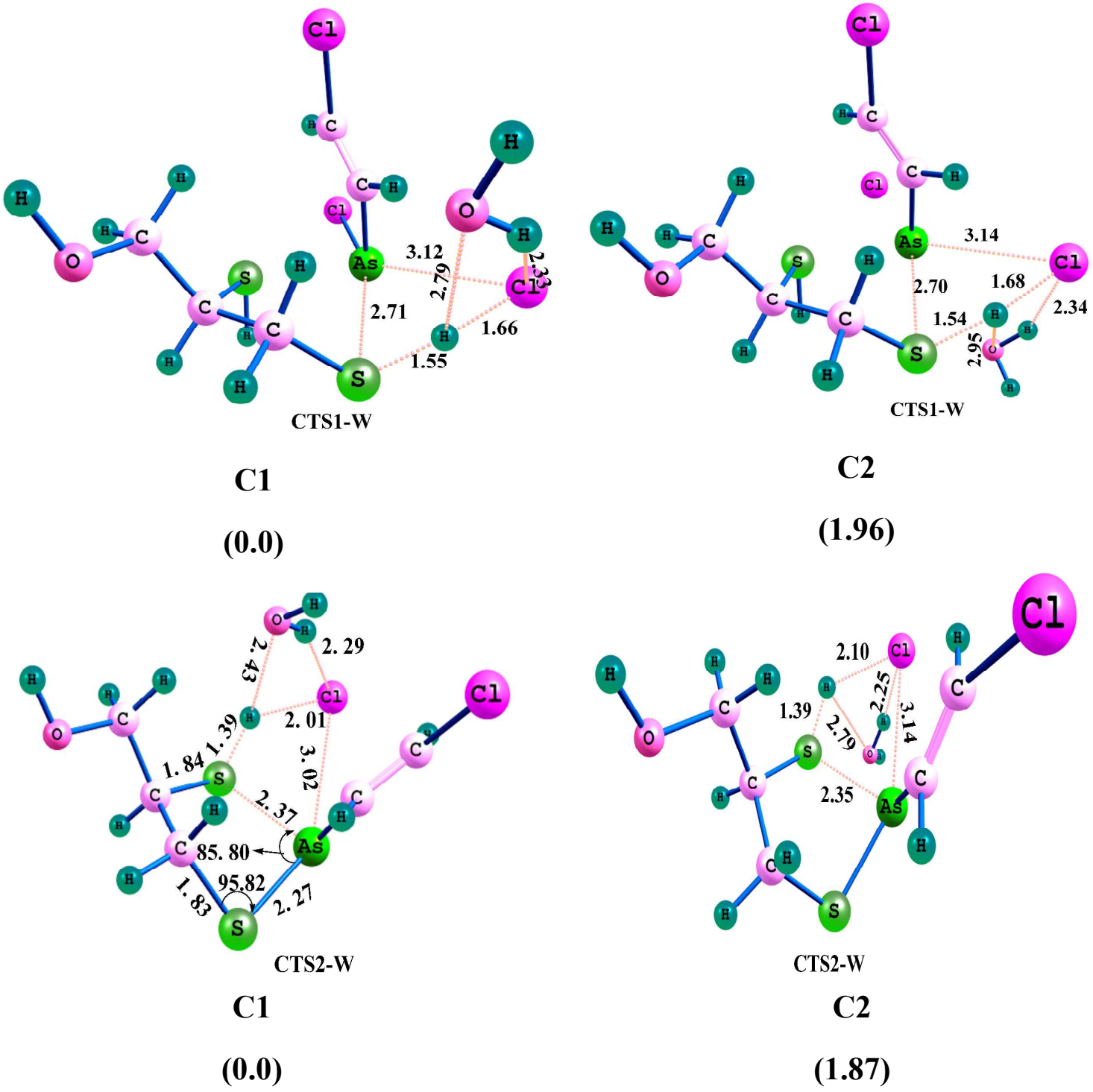


Figure S3. Conformational search for TS with important geometrical parameters for H_2O catalyzed reaction at M062X/TZVP level in gas phase [(Relative energies are given the parenthesis)].

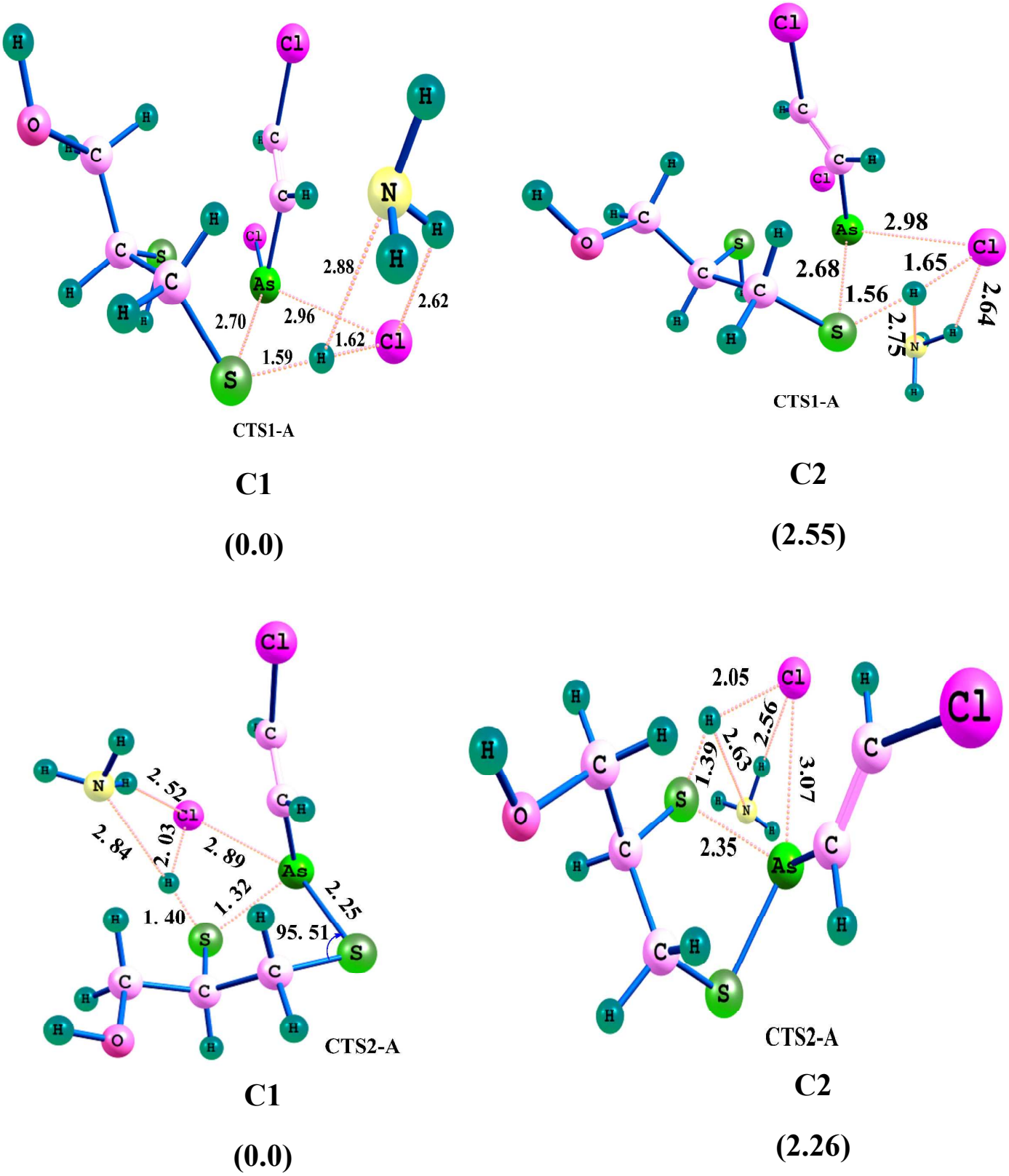


Figure S4. Conformational search for TS with important geometrical parameters for NH_3 catalyzed reaction at M062X/TZVP level in gas phase [(Relative energies are given the parenthesis)].