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

Supplemetary Information

CS_2 capture in the ionic liquid 1-alkyl-3-methylimidazolium acetate: reaction mechanism and free energetics

Fangyong Yan,[1] Ryohei Kakuchi,[2] Kenji Takahashi[3] and Hyung J. Kim[1]*

[1]Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA 15213, USA
[2]Division of Molecular Science, Graduate School of Science and Technology, Gunma University, 1-5-1 Tenjin-cho, Kiryu 376-8515, Gunma, Japan.
[3]Institue of Science and Engineering, Kanazawa University, Kanazawa 920-1192, Japan

Table of Contents:

1. Optimized geometries (reactant, transition state and product) by DFT and MP2.

1.1 CS_2 to COS conversion by reacting with OAc^- in the presence of an ion pair in the dielectric continuum phase (DFT).

Reac. (Coordinate units (Å); Energy (Hartree): E = -1407.8733584, ZPE = 0.2256983)

S	-7.26402	-0.23181	-1.09771
C	-6.89163	-0.58200	0.37089
S	-6.51886	-0.93189	1.83956
O	0.33669	1.71932	-1.05929
C	0.97518	2.56201	-0.36494
O	2.11571	2.36178	0.16538
C	0.35278	3.94931	-0.15141
H	-0.69656	3.97107	-0.45496
H	0.44001	4.25142	0.89711
H	0.90446	4.68615	-0.74770
H	2.78146	0.64298	-0.18247
C	3.25550	-0.33915	-0.34759
N	4.42574	-0.74331	0.17048
C	5.26329	0.05383	1.08782
H	6.29190	-0.01040	0.72439
H	4.93424	1.08954	0.98801
C	5.15507	-0.42149	2.53589
H	5.48820	-1.45803	2.64372
H	5.79103	0.20696	3.16648
H	4.12597	-0.34345	2.89816
C	4.69275	-2.02917	-0.26882
H	5.58602	-2.56185	0.01617
C	3.65376	-2.39788	-1.07213
H	3.47199	-3.31037	-1.61730
N	2.77130	-1.33204	-1.10652
C	1.50884	-1.27602	-1.85553
H	1.71717	-1.39439	-2.92087
H	0.85568	-2.08308	-1.51752
H	1.04269	-0.30532	-1.66433

TS 1 (Coordinate units (Å); Energy (Hartree): E = -1407.846552, ZPE = 0.225996025)

S	-3.89785	-0.91330	-1.14036
C	-3.31854	-0.35281	0.24900
S	-3.55783	-0.15621	1.82510
O	-1.53653	0.24577	-0.10384
C	-1.25404	1.46476	-0.44899
O	-0.07159	1.82064	-0.65102
C	-2.38620	2.46400	-0.60735
H	-3.09343	2.11442	-1.36570
H	-2.93809	2.56063	0.33263

H	-1.98904	3.43688	-0.89890
H	1.27964	0.42022	-0.35922
C	2.10315	-0.28981	-0.23782
N	3.40818	0.01879	-0.22587
C	3.95922	1.38488	-0.32926
H	4.78367	1.34470	-1.04514
H	3.17203	2.00820	-0.75669
C	4.42130	1.92815	1.02212
H	5.21511	1.31044	1.45230
H	4.81498	2.93945	0.88363
H	3.58964	1.97621	1.73099
C	4.14109	-1.14389	-0.06052
H	5.21874	-1.14409	-0.02506
C	3.24629	-2.16996	0.02560
H	3.39678	-3.23051	0.14895
N	1.98340	-1.61556	-0.08586
C	0.71271	-2.35150	-0.05921
H	0.66840	-3.02805	-0.91489
H	0.64999	-2.92372	0.86794
H	-0.10346	-1.62950	-0.10708

Int 1 (Coordinate units (Å); Energy (Hartree): E = -1407.857127, ZPE = 0.2281297)

S	-3.74092	-1.03129	-1.13644
C	-3.03879	-0.30060	0.18800
S	-3.56304	-0.13651	1.76223
O	-1.69558	0.20024	-0.05211
C	-1.42369	1.46860	-0.42572
O	-0.24802	1.77052	-0.58627
C	-2.56724	2.42399	-0.62308
H	-3.25895	2.03385	-1.37523
H	-3.12634	2.53667	0.31013
H	-2.17348	3.38850	-0.94115
H	1.27223	0.38769	-0.31284
C	2.11842	-0.28709	-0.20918
N	3.41095	0.06603	-0.24347
C	3.91496	1.44793	-0.38298
H	4.74676	1.41335	-1.09032
H	3.11247	2.03155	-0.83742
C	4.34576	2.04528	0.95567
H	5.15421	1.46547	1.41041
H	4.70863	3.06395	0.79022
H	3.50635	2.08790	1.65561
C	4.18542	-1.06948	-0.08094
H	5.26313	-1.03417	-0.07818
C	3.32822	-2.12278	0.04972
H	3.51715	-3.17569	0.18595
N	2.04501	-1.61256	-0.03205
C	0.80313	-2.39215	0.04642
H	0.76319	-3.09506	-0.78744

H	0.77932	-2.93552	0.99228
H	-0.04142	-1.70627	-0.00624

TS 2 (Coordinate units (Å); Energy (Hartree): E = -1407.8406051, ZPE = 0.2270256)

S	2.69836	1.84167	1.50539
C	2.37731	0.51284	0.54920
S	2.47153	-1.17836	0.96469
O	1.99314	0.55579	-0.70343
C	1.88630	-1.13363	-0.99904
O	0.73821	-1.49068	-1.26501
C	3.07257	-1.43316	-1.89146
H	3.98563	-0.95049	-1.54247
H	3.22338	-2.51710	-1.91142
H	2.83847	-1.09371	-2.90631
H	-0.86473	-0.39407	-0.73402
C	-1.78154	0.15222	-0.51855
N	-2.92862	-0.38962	-0.08574
C	-3.13459	-1.82092	0.21675
H	-4.06709	-2.12045	-0.26769
H	-2.31748	-2.36250	-0.26276
C	-3.17452	-2.09467	1.71908
H	-3.99666	-1.55771	2.20111
H	-3.32651	-3.16573	1.88165
H	-2.23500	-1.80272	2.19681
C	-3.86659	0.61657	0.06623
H	-4.86984	0.42057	0.40902
C	-3.25932	1.78504	-0.28987
H	-3.63433	2.79540	-0.31967
N	-1.95992	1.47366	-0.64848
C	-0.94930	2.42531	-1.12841
H	-1.20257	2.74721	-2.14055
H	-0.92856	3.28676	-0.45986
H	0.02409	1.93481	-1.12169

Int 2 (Coordinate units (Å); Energy (Hartree): E = -1407.8690977, ZPE = 0.2268022)

S	-4.53337	-1.65530	0.15322
C	-3.96543	-0.05719	0.00573
S	-2.07555	-0.07643	0.07666
O	-4.56406	1.00031	-0.12739
C	-1.37661	1.55593	-0.08469
O	-0.14720	1.62213	-0.06380
C	-2.23682	2.78151	-0.23458
H	-2.88878	2.68822	-1.10652
H	-2.89440	2.89248	0.63171
H	-1.58514	3.65242	-0.33258
H	1.38387	0.20112	-0.03533
C	2.29231	-0.39043	-0.09861
N	3.52658	0.09919	-0.27925

C	3.86836	1.53377	-0.37755
H	4.56416	1.63953	-1.21303
H	2.94710	2.05726	-0.63874
C	4.46521	2.07805	0.91915
H	5.39267	1.56100	1.18184
H	4.69369	3.13959	0.78624
H	3.75935	1.97886	1.74874
C	4.42070	-0.95630	-0.31893
H	5.47909	-0.80880	-0.46223
C	3.69571	-2.10087	-0.15976
H	4.00246	-3.13439	-0.13847
N	2.37120	-1.72546	-0.02317
C	1.23870	-2.63991	0.16710
H	1.18347	-3.32734	-0.67829
H	1.37718	-3.19917	1.09377
H	0.32089	-2.05621	0.22407

TS 3 (Coordinate units (Å); Energy (Hartree): E = -1407.8629718, ZPE = 0.2257953)

S	-4.60048	-1.65650	0.39635
C	-4.33272	-0.10057	0.02046
S	-1.93519	0.04210	0.12361
O	-4.77777	0.95984	-0.27936
C	-1.19949	1.59433	-0.18960
O	0.03497	1.73023	-0.24534
C	-2.09016	2.80899	-0.36389
H	-3.11546	2.54037	-0.61969
H	-2.10554	3.36223	0.58356
H	-1.66127	3.46645	-1.12652
H	1.39882	0.24635	-0.16888
C	2.28554	-0.38758	-0.18078
N	3.55085	0.05325	-0.22224
C	3.95477	1.47433	-0.22169
H	4.70639	1.59444	-1.00556
H	3.07236	2.04846	-0.50934
C	4.48852	1.92455	1.13716
H	5.37616	1.35515	1.42844
H	4.76725	2.98072	1.07728
H	3.72729	1.81265	1.91474
C	4.40275	-1.03749	-0.22982
H	5.47512	-0.93061	-0.26461
C	3.62063	-2.15462	-0.19488
H	3.88269	-3.20057	-0.19445
N	2.30486	-1.72706	-0.16405
C	1.12098	-2.59498	-0.13531
H	1.09151	-3.19767	-1.04476
H	1.17233	-3.24501	0.73954
H	0.23046	-1.96827	-0.07744

Prod (Coordinate units (Å); Energy (Hartree): E = -1407.877274, ZPE = 0.2257765)

S	-7.85095	-1.33431	0.73267
C	-8.25180	-0.14016	-0.18680
S	-0.72392	0.60319	0.26296
O	-8.55245	0.75427	-0.87558
C	0.23307	1.97060	-0.19840
O	1.46995	1.93495	-0.38353
C	-0.47346	3.31457	-0.35896
H	-1.46235	3.19917	-0.80825
H	-0.61334	3.76171	0.63289
H	0.13853	3.99425	-0.96006
H	2.42657	0.22621	-0.25110
C	3.18678	-0.56017	-0.24174
N	4.50957	-0.35060	-0.17497
C	5.15060	0.97452	-0.05515
H	5.98300	0.99367	-0.76276
H	4.41089	1.70753	-0.38151
C	5.62274	1.26317	1.36890
H	6.36253	0.52956	1.70262
H	6.08869	2.25264	1.39606
H	4.78227	1.25894	2.06901
C	5.15805	-1.57326	-0.19451
H	6.23227	-1.65534	-0.15299
C	4.19335	-2.53413	-0.27868
H	4.26848	-3.60871	-0.32542
N	2.97324	-1.88139	-0.30520
C	1.65615	-2.52075	-0.41255
H	1.56346	-3.00174	-1.38829
H	1.55406	-3.26516	0.37879
H	0.89037	-1.75091	-0.29761

1.2 COS to CO_2 conversion by reacting with OAc^- in the presence of an ion pair in the dielectric continuum phase (DFT)

Reac. (Coordinate units (Å); Energy (Hartree): E = -1084.879449, ZPE = 0.227858919)

N	2.00626	-1.61351	0.09061
N	3.90794	-0.64299	-0.30387
O	-0.58923	1.27908	0.15648
O	1.39115	2.30076	-0.17674
O	-6.25862	-2.17536	-0.21035
H	5.14663	-2.41378	-0.34864
H	2.71351	-3.65297	0.15164
H	2.09784	0.55539	-0.12007
H	0.08655	-0.82541	0.30505
H	0.43051	-2.27074	1.31155
H	0.15901	-2.45384	-0.44314
H	4.36471	1.30543	-0.83484
H	5.53093	0.09273	-1.37565
H	5.14276	1.01313	1.54506

H	6.48728	1.47081	0.48162
H	6.31965	-0.21024	1.01429
H	-0.25386	4.22953	-0.96305
H	-0.25084	4.26697	0.79899
H	-1.65237	3.58177	-0.05878
C	4.15822	-2.00221	-0.22124
C	2.96291	-2.61155	0.02516
C	2.59752	-0.42746	-0.11021
C	4.91393	0.41231	-0.53212
C	5.76441	0.68151	0.70830
C	0.57028	-1.80582	0.33347
C	-0.56399	3.67654	-0.07018
C	0.12606	2.30547	-0.02942
C	-6.70944	-1.10609	-0.07480
S	-7.31173	0.32092	0.10624

TS 1 (Coordinate units (Å); Energy (Hartree): E = -1084.8632244, ZPE = 0.2286833)

N	1.75427	-1.58053	-0.28622
N	3.15783	0.07480	-0.18636
O	-1.81385	0.19653	-0.22361
O	-0.35082	1.85759	-0.43797
O	-4.03215	-0.35120	-1.23881
H	4.98043	-1.08300	-0.09259
H	3.18543	-3.19580	-0.22519
H	1.02583	0.46453	-0.31402
H	-0.33063	-1.61400	-0.37097
H	0.41268	-3.00506	0.46974
H	0.48393	-2.90134	-1.31151
H	2.90134	2.11167	-0.46755
H	4.52692	1.51032	-0.80909
H	3.27925	1.77660	2.00236
H	4.50691	2.84980	1.30347
H	4.91736	1.16688	1.67309
H	-2.28938	3.47182	-0.43881
H	-3.33949	2.33060	0.44491
H	-3.27879	2.27763	-1.31731
C	3.90388	-1.09083	-0.15243
C	3.02241	-2.12993	-0.21722
C	1.85782	-0.24495	-0.26602
C	3.69088	1.44968	-0.10802
C	4.12334	1.82523	1.30836
C	0.49389	-2.32813	-0.38248
C	-2.67855	2.45325	-0.41920
C	-1.53303	1.45471	-0.35882
C	-3.60454	-0.44384	-0.13535
S	-3.84053	-0.93219	1.39698

Int 1 (Coordinate units (Å); Energy (Hartree): E = -1084.8689556, ZPE = 0.2304429)

N	1.71606	-1.61720	-0.07956
N	3.08116	0.06096	-0.30024
O	-1.92132	0.27646	-0.04857
O	-0.45314	1.91867	0.00652
O	-3.86808	0.26369	-1.25539
H	4.92241	-1.06411	-0.41213
H	3.17741	-3.20484	-0.13532
H	0.95595	0.40992	-0.11768
H	-0.36476	-1.69915	0.12237
H	0.52790	-2.98113	0.98418
H	0.35744	-3.05017	-0.79256
H	2.74912	2.06526	-0.71486
H	4.34289	1.46108	-1.17548
H	3.38946	1.93417	1.72302
H	4.50813	2.96974	0.81575
H	4.99934	1.32925	1.26926
H	-3.26461	2.70286	-0.81275
H	-2.34031	3.54394	0.46152
H	-3.50373	2.24626	0.87243
C	3.84960	-1.09002	-0.30661
C	2.99271	-2.14299	-0.17003
C	1.79325	-0.28275	-0.15963
C	3.58647	1.44652	-0.38747
C	4.15459	1.94210	0.94140
C	0.47590	-2.39019	0.06843
C	-2.75816	2.58706	0.14871
C	-1.63496	1.59214	0.01431
C	-3.28427	-0.24079	-0.30941
S	-3.69673	-1.49790	0.74451

TS 2 (Coordinate units (Å); Energy (Hartree): E = -1084.848634, ZPE = 0.2295445)

N	1.88935	1.56085	0.25267
N	2.73556	-0.44124	0.22013
O	-2.07892	0.96990	0.28892
O	-1.03274	-1.10137	1.18861
O	-2.66506	1.55324	-1.82841
H	4.78146	0.10623	-0.21051
H	3.69994	2.66084	-0.16182
H	0.62722	-0.16585	0.61689
H	-0.07777	2.24003	0.44855
H	1.00455	3.31470	-0.47571
H	1.14954	3.22463	1.30214
H	1.96307	-2.27536	0.80110
H	3.72533	-2.16000	0.84103
H	2.00805	-2.28292	-1.72184
H	2.97288	-3.61329	-1.05389
H	3.78316	-2.17333	-1.69226
H	-2.95780	-0.14355	2.78404
H	-3.57692	-1.66916	2.11291

H	-4.17382	-0.11855	1.47409
C	3.77075	0.44026	-0.03868
C	3.23986	1.69662	-0.01573
C	1.60527	0.25910	0.39263
C	2.83643	-1.91472	0.25511
C	2.90450	-2.52513	-1.14382
C	0.92657	2.66084	0.39408
C	-3.30043	-0.63806	1.86887
C	-2.15196	-0.67411	0.87845
C	-2.51137	0.73169	-0.93213
S	-2.81295	-1.02342	-0.97001

Int 2 (Coordinate units (Å); Energy (Hartree): E = -1084.874151, ZPE = 0.2288056)

N	-2.21624	1.68598	-0.14198
N	-3.17876	-0.26206	-0.22145
O	4.95897	-0.33840	-0.16564
O	0.53323	-1.45181	-0.36582
O	4.46294	1.75735	0.59317
H	-5.22979	0.41687	-0.19996
H	-3.99904	2.90253	-0.10360
H	-1.02538	-0.12431	-0.21596
H	-0.20114	2.23728	-0.08451
H	-1.30598	3.33693	0.77986
H	-1.25566	3.34200	-1.00642
H	-2.40571	-2.15499	-0.55701
H	-4.09647	-1.94509	-1.02731
H	-3.05672	-2.06874	1.87718
H	-3.91924	-3.36509	1.02653
H	-4.76202	-1.85712	1.41735
H	2.25534	-3.19034	-0.99932
H	3.01422	-2.77105	0.55577
H	3.65160	-2.04481	-0.91186
C	-4.18596	0.68625	-0.18439
C	-3.58199	1.90870	-0.13623
C	-1.99556	0.36592	-0.19386
C	-3.36156	-1.72816	-0.24852
C	-3.80266	-2.28029	1.10568
C	-1.17667	2.72195	-0.11196
C	2.73433	-2.38802	-0.43312
C	1.74859	-1.26308	-0.25007
C	4.26393	0.60484	0.20090
S	2.28783	0.36330	0.18807

TS 3 (Coordinate units (Å); Energy (Hartree): E = -1084.8724979, ZPE = 0.228392)

N	2.17754	-1.70155	-0.09790
N	3.20217	0.21166	-0.21607
O	-5.12130	0.41885	0.04782
O	-0.41647	1.51121	-0.44255

O	-4.58956	-1.79749	0.45475
H	5.23007	-0.52752	-0.11515
H	3.92003	-2.96977	0.03010
H	1.04410	0.14471	-0.26579
H	0.14542	-2.18515	-0.06656
H	1.19798	-3.29761	0.84868
H	1.18232	-3.35007	-0.93727
H	2.49620	2.11509	-0.62828
H	4.18972	1.83889	-1.05431
H	3.09081	2.08966	1.81990
H	4.01623	3.32809	0.94912
H	4.79781	1.80624	1.40788
H	-2.34177	3.11768	-1.12062
H	-2.48407	3.01485	0.63822
H	-3.63937	2.12366	-0.37492
C	4.17826	-0.76470	-0.11933
C	3.53504	-1.96562	-0.04696
C	1.99862	-0.37783	-0.20025
C	3.43164	1.66930	-0.28585
C	3.86084	2.25091	1.05989
C	1.10496	-2.70323	-0.06163
C	-2.60290	2.44885	-0.29417
C	-1.62746	1.28792	-0.26909
C	-4.55105	-0.62051	0.22343
S	-2.21578	-0.32692	0.03440

Prod (Coordinate units (Å); Energy (Hartree): E = 1084.8794197, ZPE = 0.2283996)

N	-2.15561	1.74883	-0.14276
N	-3.33597	-0.07432	-0.20817
O	5.81061	-0.36202	-0.11171
O	0.10418	-1.69123	-0.40822
O	5.21884	1.81781	0.49743
H	-5.29608	0.83664	-0.16315
H	-3.78655	3.16264	-0.08552
H	-1.17816	-0.19613	-0.23050
H	-0.09231	2.05810	-0.06840
H	-1.07444	3.31386	0.73965
H	-0.99941	3.25349	-1.04421
H	-2.78092	-2.04193	-0.53312
H	-4.43676	-1.64590	-1.01223
H	-3.42794	-1.87611	1.89655
H	-4.42981	-3.06853	1.04662
H	-5.09654	-1.47316	1.43001
H	1.83161	-3.43572	-0.99789
H	2.46794	-3.07301	0.61888
H	3.24639	-2.35153	-0.79206
C	-4.22790	0.98310	-0.16095
C	-3.48654	2.12754	-0.12180
C	-2.08624	0.41172	-0.19520

C	-3.68444	-1.50943	-0.23147
C	-4.19054	-2.00373	1.12268
C	-1.00281	2.65774	-0.12940
C	2.28254	-2.65429	-0.37816
C	1.32485	-1.47322	-0.24248
C	5.49552	0.72276	0.19256
S	1.99239	0.07038	0.16857

1.3 CS_2/COS/CO_2 capture in the gas and continuum phases by EMI carbene (DFT)

EMI-CS_2 reactant (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -1178.7155215, ZPE = 0.1620663)

H	4.29892	0.78229	-0.59453
C	3.45094	0.14012	-0.40800
C	3.37542	-1.21225	-0.29068
H	4.14305	-1.96867	-0.35991
N	2.03425	-1.50435	-0.05819
C	1.51191	-2.85096	0.12056
H	1.69621	-3.46098	-0.77038
H	0.43754	-2.76875	0.28492
H	1.97522	-3.33503	0.98708
C	1.24483	-0.38602	-0.02463
S	-3.46509	-0.39344	1.47187
C	-3.49053	0.01930	-0.02591
S	-3.51512	0.43217	-1.52459
N	2.15237	0.61531	-0.24675
C	1.78480	2.03051	-0.26182
H	0.70657	2.06102	-0.43131
H	2.27554	2.50745	-1.11882
C	2.14632	2.75385	1.03793
H	1.83943	3.80412	0.98226
H	1.63731	2.28859	1.88755
H	3.22501	2.72608	1.22654

EMI-CS_2 TS (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -1178.6955749, ZPE = 0.1626582)

H	3.60410	-0.25857	0.49657
C	2.65129	0.22379	0.33908
C	2.33251	1.53943	0.21609
H	2.95145	2.42290	0.25579
N	0.95497	1.59149	0.02040
C	0.19199	2.82783	-0.12241
H	0.17267	3.37784	0.82355
H	-0.82561	2.57118	-0.41392

H	0.64046	3.45573	-0.89756
C	0.40327	0.35007	0.02347
S	-2.39044	0.18814	-1.37131
C	-1.82674	-0.16716	0.07533
S	-2.04385	-0.69792	1.56267
N	1.45805	-0.48314	0.22295
C	1.35159	-1.94640	0.24134
H	0.35337	-2.18513	0.61293
H	2.07745	-2.32105	0.97086
C	1.58785	-2.57128	-1.13518
H	1.49749	-3.66073	-1.06976
H	0.84828	-2.20739	-1.85431
H	2.58716	-2.33428	-1.51572

EMI-CS_2 Prod (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -1178.7426398, ZPE = 0.1659787)

H	3.12476	1.27208	0.50670
C	2.06883	1.26137	0.28895
C	1.23027	2.26052	-0.09549
H	1.41378	3.30785	-0.27411
N	-0.03032	1.70061	-0.24262
C	-1.25698	2.40691	-0.61030
H	-1.90902	2.49775	0.26176
H	-1.77259	1.84571	-1.39187
H	-0.98699	3.39539	-0.98308
C	0.03081	0.38392	0.05328
S	-1.32364	-1.33639	-1.43768
C	-1.11367	-0.56386	0.03277
S	-1.94066	-0.62393	1.48667
N	1.31120	0.10220	0.37892
C	1.82480	-1.23195	0.72955
H	0.97029	-1.81576	1.07583
H	2.50348	-1.09939	1.57779
C	2.52150	-1.91368	-0.44854
H	2.87857	-2.90039	-0.13696
H	1.82339	-2.04297	-1.27991
H	3.38362	-1.33422	-0.79547

EMI-CS_2 react. (continuum) (Coordinate units (Å); Energy (Hartree):
E = -1178.7250967, ZPE = 0.1620382)

H	-4.07638	0.66602	1.88648
C	-3.64397	0.07869	1.09034
C	-3.80995	-1.23147	0.76474
H	-4.41056	-2.00255	1.22344
N	-3.00505	-1.45908	-0.34704
C	-2.89008	-2.75359	-1.00947
H	-2.52786	-3.51231	-0.30925
H	-2.17965	-2.65234	-1.82966

H	-3.85916	-3.06984	-1.40732
C	-2.32790	-0.33805	-0.74353
S	5.18500	0.31333	-1.35448
C	4.78406	-0.03633	0.10671
S	4.38280	-0.38605	1.56790
N	-2.74198	0.59725	0.16612
C	-2.31402	1.99869	0.13931
H	-1.39782	2.03117	-0.45383
H	-2.06292	2.29989	1.16201
C	-3.37148	2.93399	-0.45121
H	-2.99735	3.96322	-0.45330
H	-3.60699	2.65041	-1.48195
H	-4.29685	2.91123	0.13368

EMI-CS_2 TS (continuum) (Coordinate units (Å); Energy (Hartree):
E = -1178.7039988, ZPE = 0.1621747)

H	3.55883	-0.03045	0.71959
C	2.60889	0.37742	0.40893
C	2.25074	1.64887	0.08621
H	2.82521	2.56251	0.06710
N	0.89987	1.60244	-0.24750
C	0.11453	2.77236	-0.63170
H	0.04017	3.47359	0.20429
H	-0.88347	2.43969	-0.91404
H	0.58123	3.27558	-1.48255
C	0.40014	0.34207	-0.14109
S	-2.44732	-0.53379	-1.37140
C	-1.91911	-0.22884	0.09371
S	-2.09724	-0.08653	1.66615
N	1.46400	-0.40193	0.26611
C	1.42271	-1.85392	0.47536
H	0.37686	-2.11810	0.64141
H	1.97355	-2.07678	1.39465
C	1.99968	-2.63790	-0.70476
H	1.94238	-3.71152	-0.49797
H	1.43597	-2.43235	-1.62012
H	3.04963	-2.38111	-0.87859

EMI-CS_2 Prod2 (continuum) (Coordinate units (Å); Energy (Hartree):
E = -1178.7633463, ZPE = 0.1661391)

H	3.17254	1.14207	0.50700
C	2.11632	1.17761	0.29321
C	1.31722	2.21393	-0.07681
H	1.54016	3.25533	-0.24450
N	0.03519	1.70757	-0.22736
C	-1.15260	2.49261	-0.57442
H	-1.68315	2.79155	0.33224
H	-1.80811	1.89268	-1.20557

H	-0.83057	3.37679	-1.12362
C	0.04849	0.38864	0.05288
S	-1.41960	-1.27391	-1.44291
C	-1.13600	-0.51895	0.02821
S	-1.97533	-0.60632	1.47898
N	1.31394	0.04872	0.37085
C	1.79208	-1.30586	0.70698
H	0.92056	-1.88514	1.01425
H	2.44744	-1.20337	1.57542
C	2.51729	-1.97123	-0.46224
H	2.85584	-2.96488	-0.15368
H	1.84951	-2.08297	-1.32079
H	3.39387	-1.39278	-0.76911

EMI-COS react. (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -855.7224183, ZPE = 0.1646898)

S	-3.61539	0.64309	0.12442
O	-2.37399	-1.73489	-0.36741
C	-2.88637	-0.70887	-0.15545
C	0.57301	0.41658	-0.02440
N	1.25410	1.60260	0.04538
C	0.60328	2.88075	0.29209
H	0.98308	3.33841	1.21195
H	-0.46515	2.69273	0.39752
H	0.76898	3.56884	-0.54392
C	2.62355	1.45076	-0.15192
H	3.31867	2.27711	-0.14179
C	2.82924	0.12192	-0.35285
H	3.73937	-0.42585	-0.54727
N	1.57713	-0.48037	-0.27405
C	1.34773	-1.92061	-0.39485
H	0.28397	-2.04400	-0.60487
H	1.90986	-2.28803	-1.26180
C	1.73928	-2.69244	0.86778
H	1.53837	-3.76078	0.73210
H	2.80363	-2.57428	1.09863
H	1.16046	-2.33853	1.72640

EMI-COS TS (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -855.711077, ZPE = 0.1652839)

S	-2.93465	-0.39775	-0.41411
O	-1.06684	-2.09496	0.57163
C	-1.62055	-1.14193	0.14122
C	0.09697	0.32615	0.01718
N	0.15843	1.67583	0.17409
C	-0.95850	2.50954	0.61147
H	-0.78736	2.86928	1.63088
H	-1.86693	1.90969	0.58082

H	-1.06840	3.36518	-0.06082
C	1.43230	2.16602	-0.09017
H	1.67980	3.21453	-0.02354
C	2.19308	1.09143	-0.42742
H	3.23066	1.02560	-0.71762
N	1.35920	-0.01900	-0.35850
C	1.81071	-1.39431	-0.61304
H	0.94112	-1.96621	-0.93606
H	2.51986	-1.35543	-1.44669
C	2.44664	-2.04093	0.61835
H	2.78276	-3.05383	0.37264
H	3.31297	-1.46956	0.96860
H	1.71736	-2.10921	1.42992

EMI-COS Prod (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -855.7378329, ZPE = 0.1680073)

S	-2.11912	-1.36586	-0.73959
O	-0.31748	-1.80164	1.20528
C	-0.82646	-1.10573	0.31230
C	-0.12385	0.21821	0.05496
N	-0.60954	1.46444	0.23955
C	-1.97624	1.78206	0.65958
H	-2.22050	1.23128	1.56923
H	-2.67466	1.49013	-0.12765
H	-2.03107	2.85398	0.85393
C	0.36314	2.38904	-0.10942
H	0.18793	3.45133	-0.05012
C	1.46219	1.68743	-0.49897
H	2.42545	2.02284	-0.84907
N	1.14822	0.34237	-0.38231
C	2.06454	-0.77821	-0.66277
H	1.44799	-1.62824	-0.95989
H	2.66666	-0.48046	-1.52644
C	2.93743	-1.13175	0.54097
H	3.60742	-1.95453	0.27162
H	3.55190	-0.28070	0.85357
H	2.30936	-1.45280	1.37549

EMI-COS react. (continuum) (Coordinate units (Å); Energy (Hartree):
E = -855.731147, ZPE = 0.1643363)

S	-4.74894	-0.82054	-0.66761
O	-4.74001	1.41134	0.90063
C	-4.74320	0.45545	0.22917
C	1.51330	0.45570	0.37605
N	2.32716	1.49114	0.00471
C	2.06756	2.88715	0.33856
H	1.15803	2.92840	0.93758
H	1.92927	3.48132	-0.56990

H	2.89905	3.30480	0.91414
C	3.42405	1.06770	-0.73919
H	4.16941	1.74608	-1.12636
C	3.31030	-0.28355	-0.84577
H	3.94171	-1.00610	-1.34081
N	2.14641	-0.63001	-0.16617
C	1.67414	-2.00780	-0.00335
H	0.61727	-1.94342	0.26333
H	1.74596	-2.51152	-0.97328
C	2.45272	-2.78194	1.06258
H	2.05741	-3.79983	1.14587
H	3.51568	-2.85089	0.80910
H	2.36101	-2.29509	2.03877

EMI-COS TS (continuum) (Coordinate units (Å); Energy (Hartree):
E = -855.7197868, ZPE = 0.1647043)

S	-2.60123	-0.76978	-0.88935
O	-2.30098	0.70775	1.37108
C	-2.14730	0.09709	0.37472
C	0.23704	0.36273	0.08951
N	0.87125	1.56390	-0.01657
C	0.23819	2.85850	0.22529
H	-0.73563	2.68857	0.68126
H	0.11053	3.40417	-0.71424
H	0.85508	3.45352	0.90361
C	2.19305	1.41742	-0.42502
H	2.85484	2.25713	-0.57349
C	2.40008	0.08205	-0.57543
H	3.28156	-0.46604	-0.87148
N	1.19582	-0.53979	-0.26127
C	1.00929	-1.99550	-0.23213
H	-0.05938	-2.17950	-0.35226
H	1.52237	-2.41489	-1.10327
C	1.52924	-2.63225	1.05827
H	1.36221	-3.71402	1.02955
H	2.60260	-2.45734	1.18520
H	1.00621	-2.22605	1.92971

EMI-COS Prod (continuum) (Coordinate units (Å); Energy (Hartree):
E = -855.7626941, ZPE = 0.1682213)

S	-1.38544	-1.96862	-0.89528
O	-1.44218	-0.93072	1.56059
C	-1.04812	-0.90138	0.38082
C	-0.17811	0.29107	0.01698
N	-0.59822	1.57259	0.02838
C	-1.97075	2.02427	0.28556
H	-2.45152	1.32622	0.96843
H	-2.52751	2.07679	-0.65273

H	-1.92868	3.01168	0.74487
C	0.45309	2.39763	-0.33428
H	0.33829	3.46689	-0.41207
C	1.53327	1.59719	-0.54543
H	2.54692	1.83666	-0.82443
N	1.12580	0.29141	-0.32719
C	2.01827	-0.88377	-0.38701
H	1.40450	-1.73205	-0.69299
H	2.73835	-0.68196	-1.18308
C	2.72211	-1.14769	0.94400
H	3.37662	-2.01768	0.83457
H	3.33555	-0.29398	1.24740
H	2.00022	-1.36084	1.73769

EMI-CO_2 react. (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -532.7366469, ZPE = 0.1673638)

O	2.49793	-1.70019	-0.26358
C	2.80188	-0.58946	-0.05302
O	3.21775	0.48421	0.15907
C	-0.02503	0.35320	-0.09815
N	-1.16762	-0.37179	-0.29911
C	-1.17256	-1.82583	-0.46861
H	-1.84844	-2.07235	-1.29581
H	-0.15967	-2.10309	-0.76496
C	-1.58244	-2.57056	0.80361
H	-1.56412	-3.65144	0.62751
H	-2.59344	-2.29596	1.12325
H	-0.89004	-2.34243	1.61943
C	-2.31196	0.41882	-0.27803
H	-3.30664	0.02438	-0.42178
C	-1.88888	1.69249	-0.06156
H	-2.44423	2.61515	0.01529
N	-0.50353	1.62639	0.04534
C	0.35364	2.78201	0.27450
H	0.24817	3.50757	-0.53883
H	1.38439	2.43163	0.31403
H	0.09872	3.26811	1.22194

EMI-CO_2 TS (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -532.7244292, ZPE = 0.167863)

O	-0.35378	2.64005	-0.26998
C	-1.28387	1.93029	-0.06666
O	-2.41945	1.65550	0.14668
C	-0.29677	-0.14890	-0.10963
N	1.01920	-0.44613	-0.30026
C	2.07606	0.55796	-0.48119
H	2.75795	0.18443	-1.25298
H	1.59268	1.45970	-0.85595

C	2.83142	0.85516	0.81558
H	3.61151	1.60053	0.62791
H	3.30954	-0.04354	1.22025
H	2.15026	1.25664	1.57151
C	1.24924	-1.81584	-0.25650
H	2.22882	-2.24961	-0.38890
C	0.04170	-2.40151	-0.03815
H	-0.23267	-3.44149	0.05346
N	-0.88326	-1.36808	0.04851
C	-2.31328	-1.57265	0.26968
H	-2.74023	-2.16206	-0.54770
H	-2.79532	-0.59762	0.30686
H	-2.47535	-2.09896	1.21534

EMI-CO_2 prod. (gas phase) (Coordinate units (Å); Energy (Hartree):
E = -532.7500566, ZPE = 0.1702759)

O	0.66416	2.19713	0.16504
C	-0.43013	1.65706	-0.07951
O	-1.56758	2.10280	-0.31835
C	-0.34576	0.09157	-0.09348
N	0.76975	-0.64355	-0.31344
C	2.13910	-0.13752	-0.56302
H	2.59298	-0.83693	-1.27180
H	2.03933	0.84170	-1.02675
C	2.95422	-0.03029	0.72328
H	3.96626	0.30799	0.47907
H	3.03187	-0.99435	1.23763
H	2.49740	0.70654	1.38732
C	0.45558	-1.98777	-0.25414
H	1.19542	-2.75592	-0.41428
C	-0.87696	-2.07755	0.00999
H	-1.51634	-2.93693	0.13554
N	-1.35905	-0.78575	0.09825
C	-2.76024	-0.45087	0.39387
H	-3.40488	-1.08958	-0.21348
H	-2.90474	0.59996	0.14299
H	-2.95963	-0.62466	1.45456

EMI-CO_2 react. (continuum) (Coordinate units (Å); Energy (Hartree):
E = -532.743236, ZPE = 0.1669933)

O	2.66016	-1.69140	-0.25951
C	2.95618	-0.57782	-0.05725
O	3.32975	0.51252	0.14381
C	-0.06069	0.34868	-0.05038
N	-1.19190	-0.38438	-0.28988
C	-1.19493	-1.84193	-0.44350
H	-1.80709	-2.09357	-1.31624
H	-0.16484	-2.13048	-0.65959

C	-1.70928	-2.57022	0.79962
H	-1.68052	-3.65229	0.63441
H	-2.74265	-2.29033	1.02875
H	-1.08711	-2.33745	1.66963
C	-2.33828	0.40281	-0.32960
H	-3.32389	0.00119	-0.51034
C	-1.92877	1.68130	-0.11240
H	-2.48798	2.60381	-0.07079
N	-0.54917	1.62271	0.05472
C	0.28525	2.79243	0.30722
H	0.20428	3.50721	-0.51722
H	1.31816	2.45782	0.39480
H	-0.01695	3.28537	1.23601

EMI-CO_2 TS (continuum) (Coordinate units (Å); Energy (Hartree):
E = -532.7320553, ZPE = 0.1672101)

O	1.30604	-2.44286	-0.31221
C	1.97423	-1.50311	-0.05806
O	2.90589	-0.82700	0.20604
C	0.20698	0.26435	-0.11967
N	-1.13757	0.10657	-0.29895
C	-1.80172	-1.19110	-0.47396
H	-2.56122	-1.07509	-1.25380
H	-1.04464	-1.88544	-0.83843
C	-2.43287	-1.71084	0.81924
H	-2.91394	-2.67690	0.63367
H	-3.19303	-1.02049	1.19938
H	-1.67188	-1.84858	1.59385
C	-1.81628	1.31893	-0.25006
H	-2.88580	1.39695	-0.37358
C	-0.87409	2.27657	-0.03901
H	-0.96334	3.34839	0.05295
N	0.34517	1.61314	0.03744
C	1.62037	2.29461	0.24844
H	1.81065	3.00160	-0.56430
H	2.40950	1.54571	0.27118
H	1.60541	2.83820	1.19748

EMI-CO_2 Prod (continuum) (Coordinate units (Å); Energy (Hartree):
E = -532.7774218, ZPE = 0.1706461)

O	0.35756	2.19338	-0.92796
C	-0.39590	1.62472	-0.10494
O	-1.19742	2.11144	0.72571
C	-0.32459	0.08632	-0.11647
N	0.78727	-0.66288	-0.28810
C	2.17683	-0.17148	-0.41908
H	2.69865	-0.90070	-1.04235
H	2.12395	0.77602	-0.95259

C	2.86351	-0.01410	0.93698
H	3.89015	0.32948	0.77838
H	2.90029	-0.96306	1.48054
H	2.34919	0.72600	1.55695
C	0.44666	-2.00055	-0.23375
H	1.18287	-2.78202	-0.33309
C	-0.89995	-2.06546	-0.04238
H	-1.56260	-2.91246	0.03506
N	-1.36132	-0.76614	0.03824
C	-2.78093	-0.41208	0.17883
H	-3.28353	-0.53366	-0.78318
H	-2.84500	0.61915	0.51635
H	-3.23048	-1.07840	0.91573

1.4 CS_2/COS/CO_2 capture in the gas and continuum phases by EMI carbene (MP2)

EMI-CS2 Reac. (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.5451263, ZPE = 0.1657972)

H	1.86499	0.21193	-2.13615
C	1.59991	-0.20597	-1.17806
C	1.61152	-1.50418	-0.73334
H	1.88590	-2.41855	-1.23466
N	1.18125	-1.45627	0.57947
C	0.97943	-2.63384	1.41064
H	0.13397	-3.21638	1.04296
H	0.77223	-2.28564	2.41830
H	1.87776	-3.25066	1.40881
C	0.87692	-0.18851	1.01085
S	-2.61235	1.27731	0.73048
C	-2.19191	0.08585	-0.18169
S	-1.76964	-1.10261	-1.09952
N	1.15085	0.55295	-0.11468
C	1.05103	2.00899	-0.13338
H	0.38913	2.27108	0.69020
H	0.57282	2.30557	-1.07016
C	2.41270	2.67088	0.02601
H	2.30558	3.75672	0.03232
H	2.86718	2.35750	0.96531
H	3.08002	2.39714	-0.79202

EMI-CS2 TS (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.5278839, ZPE = 0.1659744)

H	-2.74539	1.45005	1.34953
C	-2.20372	0.79262	0.68893
C	-2.57021	-0.40358	0.11306
H	-3.48999	-0.96200	0.17838
N	-1.51836	-0.77636	-0.69258

C	-1.41608	-2.05838	-1.37516
H	-1.18584	-2.84201	-0.65260
H	-0.61171	-1.98265	-2.10154
H	-2.35351	-2.27997	-1.88310
C	-0.47445	0.10455	-0.62879
S	2.67510	-0.18222	-0.64479
C	1.43648	-0.70990	0.19413
S	0.80086	-1.51523	1.41712
N	-0.94585	1.07856	0.20918
C	-0.12280	2.21720	0.62570
H	0.68866	1.83580	1.24962
H	-0.75623	2.85514	1.24386
C	0.42053	2.97262	-0.57590
H	1.02145	3.81865	-0.23889
H	1.04509	2.31393	-1.17719
H	-0.39682	3.34608	-1.19338

EMI-CS2 Prod (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.5818082, ZPE = 0.1692505)

H	3.01759	1.49488	0.54371
C	1.97429	1.40209	0.29450
C	1.07452	2.33237	-0.16552
H	1.19313	3.37943	-0.38580
N	-0.12988	1.67991	-0.32522
C	-1.40343	2.27053	-0.73329
H	-2.02650	2.42867	0.14479
H	-1.89864	1.58418	-1.41673
H	-1.19336	3.21127	-1.23580
C	0.00896	0.38404	0.03102
S	-1.06913	-1.61111	-1.32272
C	-1.06409	-0.63405	0.03019
S	-2.03246	-0.54987	1.38633
N	1.29424	0.20698	0.40899
C	1.86475	-1.08236	0.82046
H	1.02749	-1.69317	1.15611
H	2.50985	-0.88145	1.67690
C	2.61798	-1.74252	-0.32432
H	3.01716	-2.70076	0.00981
H	1.93992	-1.91523	-1.15898
H	3.45047	-1.12104	-0.65640

EMI-CS2 Reac. (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.5547525, ZPE = 0.1658846)

H	-1.59055	0.43944	2.18931
C	-1.46775	-0.04164	1.23223
C	-1.62075	-1.35411	0.86098
H	-1.89692	-2.22366	1.43536
N	-1.34389	-1.39990	-0.49199

C	-1.32369	-2.63588	-1.26574
H	-0.46464	-3.24328	-0.98165
H	-1.25134	-2.36889	-2.31581
H	-2.24062	-3.19559	-1.08978
C	-1.00488	-0.17771	-1.01665
S	2.65213	1.27281	-0.58278
C	2.21421	-0.05314	0.11429
S	1.77828	-1.37502	0.81488
N	-1.09316	0.63521	0.08820
C	-0.90536	2.08419	0.02932
H	-0.33787	2.27862	-0.87894
H	-0.29628	2.38098	0.88524
C	-2.23467	2.82538	0.01755
H	-2.06096	3.90030	-0.04543
H	-2.82804	2.51628	-0.84288
H	-2.80249	2.62161	0.92559

EMI-CS2 TS (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.536069, ZPE = 0.1656181)

H	2.79700	0.76301	1.37274
C	1.96112	0.87118	0.69993
C	1.34322	2.00507	0.21041
H	1.54926	3.04867	0.38701
N	0.38378	1.56851	-0.66752
C	-0.60500	2.43815	-1.29502
H	-1.36763	2.71313	-0.56602
H	-1.05936	1.89268	-2.11703
H	-0.11419	3.33303	-1.67161
C	0.31684	0.19919	-0.73334
S	-2.35243	-1.53372	-0.73709
C	-1.61155	-0.50143	0.21904
S	-1.49125	0.32824	1.57344
N	1.33221	-0.19219	0.10424
C	1.66520	-1.59756	0.34354
H	0.77384	-2.16837	0.08592
H	1.85753	-1.71531	1.41089
C	2.86057	-2.03976	-0.48781
H	3.07274	-3.09259	-0.29899
H	2.64801	-1.91073	-1.54882
H	3.74736	-1.45913	-0.23328

EMI-CS2 Prod (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -1176.6038634, ZPE = 0.1692146)

H	3.09385	1.33633	0.54698
C	2.04681	1.30090	0.29935
C	1.19494	2.28099	-0.14830
H	1.36502	3.32264	-0.36024

N	-0.04278	1.69628	-0.30711
C	-1.27198	2.37833	-0.71757
H	-1.84992	2.64916	0.16294
H	-1.84698	1.70924	-1.35228
H	-0.99041	3.26579	-1.27639
C	0.03291	0.39133	0.03376
S	-1.17850	-1.55635	-1.32301
C	-1.09368	-0.57607	0.02759
S	-2.07815	-0.49240	1.37596
N	1.30822	0.14123	0.40422
C	1.83027	-1.17356	0.80861
H	0.97548	-1.75724	1.14662
H	2.48637	-0.99950	1.66074
C	2.55986	-1.85495	-0.33837
H	2.92467	-2.82596	-0.00299
H	1.88269	-2.00430	-1.17810
H	3.41297	-1.26068	-0.66476

EMI-COS Reac. (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.8620033, ZPE = 0.1680685)

S	2.46233	-0.67827	0.51776
O	0.88778	-2.53986	-0.73852
C	1.55822	-1.72567	-0.20804
C	-0.49920	0.64294	-0.95694
N	0.10912	1.70300	-0.33158
C	0.97612	2.63394	-1.03800
H	0.85079	2.44886	-2.10077
H	2.01722	2.46934	-0.75801
H	0.69159	3.65947	-0.80400
C	-0.11321	1.74056	1.03233
H	0.29796	2.49889	1.67904
C	-0.91629	0.66397	1.31053
H	-1.33382	0.31923	2.24293
N	-1.12225	0.02445	0.10204
C	-2.01243	-1.11951	-0.07681
H	-1.71142	-1.58988	-1.01085
H	-1.83022	-1.82303	0.73892
C	-3.47309	-0.69292	-0.12132
H	-4.11456	-1.56190	-0.27576
H	-3.76850	-0.20923	0.81036
H	-3.62749	0.00724	-0.94161

EMI-COS TS (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.8496246, ZPE = 0.1682964)

S	-2.67818	-0.54217	-0.51192
O	-0.82116	-2.31989	0.38689
C	-1.40993	-1.33220	0.06374

C	0.14029	0.26710	0.30093
N	-0.04412	1.62007	0.31577
C	-1.22914	2.26256	0.87327
H	-1.72043	1.54848	1.52605
H	-1.91323	2.54916	0.07579
H	-0.92470	3.13980	1.44208
C	0.99421	2.29978	-0.28791
H	1.02777	3.37431	-0.36172
C	1.88453	1.34187	-0.70614
H	2.82995	1.43155	-1.21543
N	1.33875	0.12658	-0.34285
C	1.99272	-1.17060	-0.54605
H	1.27422	-1.83813	-1.01919
H	2.81494	-1.00099	-1.24245
C	2.48567	-1.75193	0.76943
H	2.99204	-2.70165	0.59079
H	3.18580	-1.06891	1.25180
H	1.64122	-1.92571	1.43379

EMI-COS Prod (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.8818418, ZPE= 0.1713869)

S	-2.21719	-1.30389	-0.60801
O	-0.11360	-1.96919	0.92936
C	-0.77399	-1.15576	0.23250
C	-0.11876	0.19062	0.04431
N	-0.64221	1.42496	0.23586
C	-2.01663	1.71011	0.65591
H	-2.30734	1.00346	1.42720
H	-2.68353	1.59634	-0.19462
H	-2.03321	2.72569	1.04520
C	0.30015	2.37922	-0.07769
H	0.09469	3.43297	0.00222
C	1.43603	1.71162	-0.46546
H	2.39195	2.07993	-0.79711
N	1.15887	0.36597	-0.37394
C	2.11373	-0.71751	-0.65913
H	1.52891	-1.58487	-0.95681
H	2.70731	-0.38180	-1.51031
C	2.97621	-1.02738	0.55391
H	3.68568	-1.81568	0.30008
H	3.53903	-0.14801	0.86959
H	2.34334	-1.37431	1.36814

EMI-COS Reac. (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.8717883, ZPE = 0.1679921)

S	2.39842	-0.67421	0.62511
O	1.01491	-2.51019	-0.87037

C	1.60573	-1.71177	-0.23073
C	-0.50182	0.65053	-0.97993
N	0.09122	1.71967	-0.35649
C	0.95594	2.66930	-1.04701
H	0.84130	2.50663	-2.11447
H	1.99493	2.50797	-0.76089
H	0.66177	3.68670	-0.79515
C	-0.14008	1.75318	1.00507
H	0.25885	2.51834	1.65119
C	-0.92968	0.66544	1.28025
H	-1.34804	0.31484	2.20999
N	-1.12390	0.02230	0.07296
C	-1.98560	-1.14833	-0.09171
H	-1.71405	-1.59201	-1.04750
H	-1.74424	-1.85989	0.70013
C	-3.45991	-0.77210	-0.05888
H	-4.07419	-1.66171	-0.20291
H	-3.72619	-0.32200	0.89756
H	-3.68293	-0.06132	-0.85448

EMI-COS TS (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.8578752, ZPE = 0.1677202)

S	-2.41442	-0.56458	-0.91369
O	-1.33861	-2.18976	0.99584
C	-1.59032	-1.30865	0.23542
C	0.13408	0.21045	0.49628
N	-0.08664	1.55824	0.42729
C	-1.23590	2.21418	1.04081
H	-1.64872	1.53855	1.78416
H	-1.98958	2.43085	0.28479
H	-0.91499	3.13666	1.52036
C	0.83189	2.20279	-0.37609
H	0.81690	3.26697	-0.54625
C	1.69061	1.23124	-0.83011
H	2.55944	1.29781	-1.46456
N	1.24244	0.04233	-0.28912
C	1.91485	-1.24701	-0.46331
H	1.16065	-2.01517	-0.30209
H	2.25260	-1.30632	-1.49852
C	3.07536	-1.40958	0.50745
H	3.54881	-2.38090	0.36029
H	3.82454	-0.63365	0.34980
H	2.71590	-1.34791	1.53439

EMI-COS Prod (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -853.9079892, ZPE = 0.171532)

S	-2.28681	-1.26988	-0.59312

O	-0.21443	-1.96384	0.93862
C	-0.81991	-1.11955	0.22802
C	-0.11369	0.19425	0.03271
N	-0.60115	1.44635	0.20774
C	-1.95656	1.79984	0.64533
H	-2.28937	1.08312	1.38874
H	-2.62946	1.78292	-0.20702
H	-1.90750	2.79410	1.07982
C	0.38060	2.36311	-0.08714
H	0.21310	3.42344	-0.00709
C	1.49865	1.65473	-0.45555
H	2.47108	1.98892	-0.77463
N	1.17659	0.32127	-0.36532
C	2.10993	-0.78267	-0.65254
H	1.51020	-1.64578	-0.92975
H	2.69186	-0.46868	-1.51800
C	2.99544	-1.07984	0.54657
H	3.67789	-1.89155	0.29410
H	3.58707	-0.20617	0.81927
H	2.38476	-1.38427	1.39414

EMI-CO_2 Reac. (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.1759411, ZPE = 0.1703346)

O	-2.68248	1.09869	-0.15110
C	-2.75327	-0.07473	-0.01884
O	-2.92919	-1.23462	0.12999
C	0.13663	-0.37876	-0.27922
N	1.05607	0.63778	-0.34318
C	0.66903	2.03081	-0.55488
H	1.43464	2.49988	-1.17646
H	-0.26495	2.00600	-1.11246
C	0.49427	2.77408	0.76185
H	0.19992	3.80780	0.57408
H	1.42237	2.77838	1.33470
H	-0.28251	2.29369	1.35529
C	2.34980	0.21982	-0.09176
H	3.19882	0.88390	-0.10248
C	2.27119	-1.13054	0.13478
H	3.03932	-1.85510	0.35065
N	0.93244	-1.45595	0.01803
C	0.40418	-2.80653	0.15646
H	0.78068	-3.44392	-0.64332
H	-0.67784	-2.73804	0.09342
H	0.69247	-3.22285	1.12123

EMI-CO_2 TS (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.1709142, ZPE = 0.1707112)

O	0.72970	2.46534	-0.20806
C	-0.42469	2.16073	-0.07064
O	-1.59211	2.38321	0.10612
C	-0.34332	-0.03442	-0.18829
N	0.77562	-0.80743	-0.32197
C	2.12461	-0.26667	-0.51989
H	2.67550	-0.99902	-1.11243
H	2.01738	0.64665	-1.09835
C	2.81606	0.00961	0.80655
H	3.82162	0.39287	0.62785
H	2.89384	-0.90007	1.40339
H	2.25640	0.75752	1.36536
C	0.50263	-2.15196	-0.17004
H	1.26015	-2.91466	-0.24594
C	-0.84620	-2.24548	0.06224
H	-1.47806	-3.10365	0.22134
N	-1.32754	-0.95196	0.04897
C	-2.73757	-0.60537	0.21374
H	-3.30947	-0.97338	-0.63704
H	-2.80865	0.47561	0.26862
H	-3.11501	-1.05316	1.13170

EMI-CO_2 Prod (gas phase) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.190237, ZPE = 0.1734466)

O	0.72946	2.19590	-0.02715
C	-0.39502	1.63767	-0.09931
O	-1.57590	2.06239	-0.17205
C	-0.31749	0.09682	-0.09725
N	0.77874	-0.67635	-0.31561
C	2.16001	-0.20263	-0.53205
H	2.63968	-0.97146	-1.13914
H	2.09332	0.72759	-1.08723
C	2.87879	0.00876	0.78987
H	3.90923	0.30835	0.59573
H	2.89216	-0.90791	1.38141
H	2.38633	0.80439	1.34461
C	0.43350	-2.00524	-0.25100
H	1.15315	-2.79197	-0.40141
C	-0.91393	-2.05703	0.01091
H	-1.57533	-2.89709	0.13645
N	-1.35539	-0.75861	0.09864
C	-2.75314	-0.38107	0.35249
H	-3.16940	0.08647	-0.53347
H	-2.79197	0.33185	1.16834
H	-3.28537	-1.29542	0.60516

EMI-CO_2 Reac. (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.1845191, ZPE = 0.1703015)

O	0.56427	2.87334	-0.61329
C	0.04804	2.33234	0.30200
O	-0.46298	1.81447	1.23336
C	-0.36287	-0.53299	-1.04624
N	0.57886	-1.16300	-0.26854
C	1.99677	-1.23295	-0.62385
H	2.34128	-2.25011	-0.43111
H	2.05109	-1.04799	-1.69488
C	2.82896	-0.22027	0.14966
H	3.87936	-0.31291	-0.12908
H	2.74383	-0.38201	1.22439
H	2.50085	0.79263	-0.08156
C	0.05585	-1.68645	0.89900
H	0.64825	-2.22310	1.62222
C	-1.28281	-1.38902	0.87892
H	-2.06758	-1.61687	1.58171
N	-1.50203	-0.70281	-0.29926
C	-2.79990	-0.15904	-0.68135
H	-3.55542	-0.94190	-0.64433
H	-2.71441	0.22091	-1.69497
H	-3.07958	0.64972	-0.00726

EMI-CO_2 TS (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.179201, ZPE = 0.1701642)

O	0.60599	2.58148	-0.35870
C	-0.50282	2.26176	-0.04809
O	-1.63675	2.37793	0.31260
C	-0.34752	-0.07590	-0.25188
N	0.80599	-0.81002	-0.32407
C	2.13569	-0.22278	-0.51246
H	2.72252	-0.93311	-1.09558
H	1.99981	0.68190	-1.09887
C	2.80552	0.08245	0.81905
H	3.79218	0.51474	0.64780
H	2.92494	-0.82610	1.40989
H	2.20656	0.79533	1.38472
C	0.59053	-2.15718	-0.10963
H	1.38352	-2.88679	-0.12867
C	-0.75779	-2.29852	0.10120
H	-1.35657	-3.17455	0.28902
N	-1.29353	-1.02887	0.01408
C	-2.72392	-0.74795	0.11769
H	-3.24165	-1.12475	-0.76283
H	-2.84782	0.32701	0.18893
H	-3.12278	-1.22806	1.00902

EMI-CO_2 Prod (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -531.2187306, ZPE = 0.17382)

O	0.70167	2.11239	-0.81852
C	-0.23920	1.61143	-0.13942
O	-1.14921	2.16671	0.53949
C	-0.29397	0.09196	-0.13342
N	0.74494	-0.77007	-0.28270
C	2.17174	-0.41047	-0.39416
H	2.66670	-1.29523	-0.79086
H	2.24177	0.39992	-1.11231
C	2.73911	-0.01189	0.95873
H	3.80088	0.21038	0.85174
H	2.62513	-0.82077	1.68035
H	2.23798	0.87821	1.33627
C	0.28646	-2.06222	-0.20081
H	0.94606	-2.90922	-0.28087
C	-1.07395	-1.99641	-0.01772
H	-1.81195	-2.77514	0.07033
N	-1.40935	-0.66584	0.02457
C	-2.78203	-0.17114	0.19282
H	-2.96729	0.62181	-0.52276
H	-2.90954	0.21058	1.20047
H	-3.44762	-1.00947	0.01068

1.5 CS_2/COS/CO_2 in the gas and continuum phases (DFT)

CS_2 (gas) (Coordinate units (Å); Energy (Hartree):
E = -834.5819747, ZPE = 0.0069265)

C	0.00000	0.00000	0.00000
S	0.00000	0.00000	1.55465
S	0.00000	0.00000	-1.55465

CS_2 (continuum) (Coordinate units (Å);
Energy (Hartree): E = -834.582407, ZPE = 0.0068086)

C	0.00000	0.00000	0.00000
S	0.00000	0.00000	1.55510
S	0.00000	0.00000	-1.55510

COS (gas) (Coordinate units (Å); Energy (Hartree):
E = -511.5870752, ZPE = 0.0092126)

C	0.00000	0.00000	-0.52163
S	0.00000	0.00000	1.03969
O	0.00000	0.00000	-1.68816

COS (continuum) (Coordinate units (Å); Energy (Hartree):
E = -511.5884224, ZPE = 0.0090919)

C	0.00000	0.00000	-0.52030

S	0.00000	0.00000	1.03931
O	0.00000	0.00000	-1.68839

CO_2 (gas) (Coordinate units (Å); Energy (Hartree):
E = -188.587438, ZPE = 0.0115856)

C	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.16976
O	0.00000	0.00000	-1.16976

CO_2 (continuum) (Coordinate units (Å); Energy (Hartree):
E = -188.5900737, ZPE = 0.0114909)

C	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.16959
O	0.00000	0.00000	-1.16958

1.6 CS_2/COS/CO_2 in the gas and continuum phases (MP2)

CS_2 (gas) (Coordinate units (Å); Energy (Hartree):
MP2 = -833.4799374, ZPE = 0.0070271)

C	0.00000	0.00000	0.00000
S	0.00000	0.00000	1.55862
S	0.00000	0.00000	-1.55862

CS_2 (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -833.4802844, ZPE = 0.0069587)

C	0.00000	0.00000	0.00000
S	0.00000	0.00000	1.55892
S	0.00000	0.00000	-1.55892

COS (gas) (Coordinate units (Å); Energy (Hartree):
MP2 = -510.7973087, ZPE = 0.0091676).

C	0.00000	0.00000	-0.51851
S	0.00000	0.00000	1.04394
O	0.00000	0.00000	-1.69899

COS (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -510.7982029, ZPE = 0.0090992)

C	0.00000	0.00000	-0.51812
S	0.00000	0.00000	1.04357
O	0.00000	0.00000	-1.69856

CO_2 (gas) (Coordinate units (Å); Energy (Hartree):

MP2 = -188.1179592, ZPE = 0.0113989)

C	0.00000	0.00000	-0.00000
O	0.00000	0.00000	1.18087
O	0.00000	0.00000	-1.18087

CO_2 (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -188.1202079, ZPE = 0.0113481)

C	0.00000	0.00000	-0.00000
O	0.00000	0.00000	1.18019
O	0.00000	0.00000	-1.18019

1.7 EMI carbene in the gas and continuum phases (DFT)

EMI carbene (gas) (Coordinate units (Å); Energy (Hartree):
E = -344.1402673, ZPE = 0.1549831)

H	-0.77185	2.18283	-0.12898
C	-0.13514	1.31110	-0.10451
C	1.20032	1.19918	0.12262
H	1.94449	1.95400	0.32836
N	1.49439	-0.15811	0.02935
C	2.82695	-0.71740	0.19989
H	3.51663	-0.31380	-0.54911
H	2.74987	-1.79716	0.07384
H	3.21529	-0.49571	1.19960
C	0.39392	-0.92209	-0.25281
N	-0.59837	0.01825	-0.33182
C	-1.99821	-0.32406	-0.57863
H	-1.99158	-1.31688	-1.03281
H	-2.40292	0.38158	-1.31389
C	-2.84546	-0.32096	0.69571
H	-3.88022	-0.59323	0.46073
H	-2.45184	-1.04385	1.41656
H	-2.85431	0.66655	1.16933

EMI carbene (continuum) (Coordinate units (Å); Energy (Hartree):
E = -344.1493534, ZPE = 0.1550457)

H	-0.78716	2.16163	-0.15121
C	-0.14270	1.29623	-0.11751
C	1.19444	1.19595	0.10883
H	1.93544	1.95566	0.30657
N	1.50006	-0.15897	0.02983
C	2.84460	-0.69575	0.20706
H	3.52523	-0.28375	-0.54389
H	2.79454	-1.77821	0.09240
H	3.22557	-0.45474	1.20382

C	0.40257	-0.92942	-0.24157
N	-0.59921	-0.00108	-0.32915
C	-2.00283	-0.34475	-0.57252
H	-2.00459	-1.35074	-0.99672
H	-2.39753	0.34048	-1.33029
C	-2.85698	-0.29267	0.69542
H	-3.89112	-0.56321	0.45810
H	-2.47957	-0.99520	1.44515
H	-2.86135	0.71089	1.13299

1.8 EMI carbene in the gas and continuum phases (MP2)

EMI carbene (gas) (Coordinate units (Å); Energy (Hartree):
MP2 = -343.0687686, ZPE = 0.1580937)

H	-0.78216	2.18334	-0.12485
C	-0.14665	1.31366	-0.10337
C	1.19614	1.19349	0.13942
H	1.94127	1.93966	0.35947
N	1.47986	-0.15567	0.03160
C	2.81038	-0.72102	0.19523
H	3.48218	-0.33767	-0.57190
H	2.71518	-1.79747	0.09417
H	3.20423	-0.47610	1.18080
C	0.38287	-0.92202	-0.27423
N	-0.60153	0.03182	-0.35319
C	-2.00177	-0.30783	-0.58288
H	-1.99626	-1.28335	-1.06427
H	-2.41883	0.42167	-1.28001
C	-2.79407	-0.34282	0.71590
H	-3.83060	-0.61899	0.51865
H	-2.35866	-1.07603	1.39318
H	-2.78608	0.63104	1.20545

EMI carbene (continuum) (Coordinate units (Å); Energy (Hartree):
MP2 = -343.0787604, ZPE = 0.1581818)

H	-0.80866	2.14852	-0.16918
C	-0.16040	1.28906	-0.13066
C	1.18497	1.19206	0.11126
H	1.92199	1.95107	0.31341
N	1.48881	-0.15393	0.03558
C	2.83600	-0.68502	0.20872
H	3.48866	-0.31819	-0.58119
H	2.77157	-1.76707	0.15790
H	3.23139	-0.38493	1.17696
C	0.39877	-0.93737	-0.24842
N	-0.60162	-0.00292	-0.34735
C	-2.00356	-0.35331	-0.57187
H	-2.00098	-1.36101	-0.98148

H	-2.40566	0.32525	-1.32520
C	-2.81439	-0.28556	0.71344
H	-3.84722	-0.57420	0.51763
H	-2.39703	-0.96488	1.45587
H	-2.81268	0.72419	1.12277

2. Tables

Table S1 SCRF/DFT results[1)] for COS-to-CO_2 conversion via S/O exchange with OAc^- in 1-pentanol ($\varepsilon = 15.13$) and in ethanol ($\varepsilon = 24.85$)

States[2)]	1-pentanol[3)]	ethanol
Reac	0	0
TS1	10.70	10.68
Int1	8.21	7.92
TS2	20.39	20.31
Int2	3.92	3.65
TS3	4.70	4.60
Prod	0.36	0.27

[1)] Units for energy: kcal/mol
[2)] Structures of the reactant, product, transition and intermediate states in 1-pentanol are exhibited in Figure 3.
[3)] Results in 1-pentanol are also presented in Figure 4b.

Table S2 Dipole moments (units: Debye) of the reactant, product and transition states for capture of CS_2, COS and CO_2 by EMI carbene[1)]

System	Reactant	Transition State	Product
EMI-CS_2 (gas phase)	2.58 (2.49)	5.92 (4.24)	8.58 (9.23)
EMI-COS (gas phase)	2.52 (2.98)	5.96 (5.22)	9.22 (10.08)
EMI-CO_2 (gas phase)	3.25 (2.99)	5.47 (5.79)	9.52 (10.21)
EMI-CS_2 (continuum)	3.47 (3.52)	6.84 (5.47)	11.81 (12.25)
EMI-COS (continuum)	4.01 (4.26)	6.52 (5.78)	12.69 (13.34)
EMI-CO_2 (continuum)	3.93 (3.52)	5.72 (5.90)	12.59 (13.14)

[1)] Calculations are performed at the B3LYP and MP2 levels using the MQZVP basis set for sulfur and 6-31+G(d,p) for other atom types with the Chelpg method. MP2 results are given in parentheses.

Table S3 Partial charges for linear CS_2/COS/CO_2, and Cc atom of EMI carbene.[1)]

System	Cc	O	S	C2
CS_2 (gas phase)	-0.002 (0.026)		0.001 (-0.013)	
COS (gas phase)	0.346 (0.428)	-0.251 (-0.309)	-0.095 (-0.119)	
CO_2 (gas phase)	0.82 (0.95)	-0.41 (0.475)		
carbene (gas phase)				-0.781 (-0.746)
CS_2 (continuum)	-0.016 (0.015)		0.008 (-0.0075)	
COS (continuum)	0.357 (0.445)	-0.276 (-0.337)	-0.081 (-0.108)	
CO_2 (continuum)	0.86 (1.0)	-0.43 (-0.5)		
carbene (continuum)				-0.910 (-0.86)

[1)] MP2 results are given in parentheses.