

## Supporting Information

# **Difference for SO<sub>2</sub> and CO<sub>2</sub> in TMGL Ionic Liquids: A Theoretical Investigation**

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### **Cartesian Coordinates**

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### 1) TMG

C 0	1.172183	-1.841275	0.284262
N 0	1.172183	-0.369073	0.284262
C 0	2.502186	0.258680	0.284262
C 0	-1.339793	-0.869977	-1.128618
N 0	-1.154788	-0.078338	0.098761
C 0	-2.392247	0.426355	0.712737
C 0	0.055684	0.351264	0.503241
N 0	0.152399	1.534764	1.144900
H 0	0.201371	-2.221713	0.597291
H 0	1.924479	-2.185886	0.999879
H 0	1.421864	-2.236932	-0.704493
H 0	2.435218	1.292683	-0.056242
H 0	3.138775	-0.290116	-0.413118
H 0	2.967550	0.219926	1.276768
H 0	-0.405432	-0.935568	-1.683473
H 0	-2.078915	-0.364134	-1.756820
H 0	-1.703993	-1.875685	-0.899636
H 0	-2.219226	0.690069	1.756820
H 0	-3.138775	-0.370158	0.680737
H 0	-2.790082	1.291450	0.168247
H 0	-0.567188	2.236932	1.061394
H 0	0.947148	1.752294	1.727029

HF=-363.033168

### 2) LAC

C 0	0.319838	-1.235191	0.534890
C 0	0.319838	0.294865	0.534890
O 0	1.657430	0.796644	0.534890
C 0	-0.449889	0.880247	-0.698435
O 0	-1.657430	0.566944	-0.816143
O 0	0.262722	1.622969	-1.442019
H 0	-0.708921	-1.608960	0.543166
H 0	0.855653	-1.622969	1.411253
H 0	0.822346	-1.611144	-0.364668
H 0	-0.195777	0.649893	1.442019
H 0	1.635674	1.347475	-0.285836

HF= -343.1028678

### 3) SO<sub>2</sub>

S	0	0.642830	-0.380984	0.000000
O	0	0.642830	1.084640	0.000000
O	0	-0.642830	-1.084640	0.000000

HF= -548.5993578

### 4)CO<sub>2</sub>

C	0	0.000000	0.000000	0.000000
O	0	0.000000	1.169378	0.000000
O	0	0.000000	-1.169378	0.000000

HF= -188.5903926

### 5) TMG-CO<sub>2</sub>(B3LYP/6-31++G\*\*)

C	0	-0.176472	-3.578395	-0.452849
O	0	-0.176472	-2.402234	-0.452849
O	0	-0.178614	-4.739907	-0.452849
C	0	0.456489	4.154869	-0.156557
N	0	0.914629	2.787049	0.135011
C	0	2.338519	2.662085	0.476315
C	0	-1.871747	2.560600	0.979667
N	0	-1.182973	1.737863	-0.027267
C	0	-2.031821	0.763423	-0.728133
C	0	0.159733	1.701679	-0.132096
N	0	0.761705	0.558311	-0.511393
H	0	-0.491233	4.132534	-0.691893
H	0	1.200862	4.640763	-0.794547
H	0	0.346800	4.739907	0.761298
H	0	2.523439	1.722940	0.999352
H	0	2.603122	3.483303	1.146004
H	0	2.976711	2.726952	-0.413790
H	0	-1.151017	3.018153	1.655220
H	0	-2.529674	1.911698	1.565526
H	0	-2.478428	3.338794	0.507121
H	0	-1.555811	0.442342	-1.655220
H	0	-2.976711	1.251380	-0.977114
H	0	-2.245792	-0.109752	-0.100906
H	0	0.306765	-0.342132	-0.432353
H	0	1.695427	0.569388	-0.892991

HF= -551.6299471

**6) TMG-2CO2(B3LYP/6-31++G\*\*)**

C 0	-1.527023	-3.543613	0.056536
O 0	-1.527023	-2.367724	0.056536
O 0	-1.528642	-4.705510	0.056536
C 0	-0.911619	4.147503	0.758733
N 0	-0.433509	2.770409	0.952643
C 0	0.971831	2.646299	1.363248
C 0	-3.250298	2.406347	1.628839
N 0	-2.492484	1.699066	0.585740
C 0	-3.280363	0.781878	-0.249115
C 0	-1.143815	1.696410	0.549890
N 0	-0.496641	0.604826	0.105101
H 0	-1.830132	4.153012	0.174150
H 0	-0.148956	4.705510	0.206877
H 0	-1.083954	4.646117	1.717348
H 0	1.153642	1.662299	1.796525
H 0	1.172961	3.401919	2.126055
H 0	1.655003	2.810115	0.521855
H 0	-2.575589	2.811961	2.380953
H 0	-3.919961	1.691456	2.116749
H 0	-3.852624	3.214247	1.202506
H 0	-2.746861	0.559567	-1.173777
H 0	-4.221589	1.274507	-0.503478
H 0	-3.507194	-0.151639	0.278706
H 0	-0.940875	-0.304029	0.094675
H 0	0.455251	0.657378	-0.233434
C 0	3.313004	0.065117	-1.757325
O 0	2.394355	0.439028	-1.125666
O 0	4.221589	-0.303079	-2.380953

HF= -740.2261939

**7)TMG-SO2(B3LYP/6-31++G\*\*)**

S 0	2.150813	-3.463332	0.283372
O 0	2.150813	-1.986219	0.283372
O 0	0.848050	-4.122747	0.283372
C 0	-1.301905	3.462760	-0.116564
N 0	-1.034480	2.065752	-0.493078
C 0	-2.145478	1.372461	-1.158638
C 0	1.678077	3.134269	-0.640978
N 0	1.215056	2.009603	0.186042
C 0	2.225495	1.433739	1.085581
C 0	0.039661	1.388484	-0.034724

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N 0	-0.065354	0.069633	0.208560
H 0	-0.584459	3.799446	0.629933
H 0	-2.303996	3.519551	0.319449
H 0	-1.261655	4.122747	-0.988243
H 0	-1.779750	0.497531	-1.697694
H 0	-2.592082	2.057366	-1.882791
H 0	-2.923776	1.073105	-0.445386
H 0	1.003003	3.293249	-1.480323
H 0	2.668100	2.888239	-1.036606
H 0	1.755389	4.053585	-0.052765
H 0	1.742659	0.867753	1.882791
H 0	2.787139	2.255224	1.535599
H 0	2.923776	0.784043	0.546257
H 0	0.743908	-0.544495	0.241574
H 0	-0.970291	-0.356448	0.340690

HF= -911.645393

**8)TMGSO2-TS(B3LYP/6-31++G\*\*)**

S 0	-1.819217	-0.285749	-3.024858
O 0	-1.819217	1.290241	-3.024858
O 0	-3.177042	-0.812121	-3.024858
H 0	-1.305157	1.440715	-2.106893
C 0	2.456433	0.820816	0.281551
N 0	1.312524	0.349080	-0.514557
C 0	1.556010	0.257466	-1.956711
C 0	0.749035	-0.854697	2.070399
N 0	-0.140971	0.022916	1.293853
C 0	-1.396300	0.381370	1.968523
C 0	0.054776	0.293493	-0.020255
N 0	-0.989608	0.540724	-0.857680
H 0	2.116331	1.237222	1.228067
H 0	2.957582	1.614127	-0.280886
H 0	3.177042	0.019135	0.469410
H 0	0.910135	-0.497067	-2.404338
H 0	2.590192	-0.056021	-2.109899
H 0	1.407135	1.222869	-2.455454
H 0	1.454219	-1.359832	1.412370
H 0	0.132786	-1.614127	2.561071
H 0	1.295416	-0.300852	2.839900
H 0	-1.806388	1.307312	1.561681
H 0	-1.178939	0.553046	3.024858
H 0	-2.139520	-0.422860	1.899022

H 0 -1.867916 0.380583 -0.364593  
HF= -911.5652092

**9)TMGSO2(B3LYP /6-31++G\*\*)**

N 0 1.047052 -1.231750 -0.546915  
N 0 1.047052 1.120480 -0.546915  
C 0 0.242684 -2.465323 -0.546915  
C 0 2.479481 -1.422556 -0.829786  
C 0 0.999506 2.341410 0.278860  
C 0 1.650331 1.291337 -1.877310  
C 0 0.547214 -0.054377 -0.125775  
N 0 -0.493585 -0.044585 0.757964  
S 0 -2.037628 0.869836 0.458968  
O 0 -3.050251 -0.156052 0.759901  
O 0 -1.974774 1.918318 1.720397  
H 0 -0.820120 -2.234694 -0.622133  
H 0 0.526239 -3.057576 -1.420101  
H 0 0.432622 -3.063269 0.351976  
H 0 3.050251 -0.557293 -0.496822  
H 0 2.823534 -2.298846 -0.273033  
H 0 2.654819 -1.593617 -1.895921  
H 0 1.995260 2.793877 0.278131  
H 0 0.287787 3.063269 -0.132644  
H 0 0.717872 2.095758 1.300701  
H 0 1.227899 2.194363 -2.326403  
H 0 2.736246 1.410943 -1.814234  
H 0 1.409599 0.442029 -2.515327  
H 0 -0.684035 -0.910258 1.259777  
H 0 -2.397973 1.534877 2.515327  
HF= -911.6088834

**10)TMGCO2-TS(B3LYP /6-31++G\*\*)**

N 0 -0.049401 -1.154976 0.039392  
C 0 -0.049401 0.212836 0.039392  
N 0 0.867636 0.892299 0.767393  
N 0 -0.934605 0.890060 -0.721037  
C 0 0.592560 2.208514 1.368215  
C 0 2.102443 0.247717 1.235920  
C 0 -2.170421 0.269120 -1.211288  
C 0 -0.594809 2.169796 -1.368220  
H 0 0.550292 -1.503228 0.784998  
H 0 0.819486 2.148017 2.436830

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H 0	1.212788	2.992435	0.923655
H 0	-0.459430	2.465332	1.257418
H 0	2.870336	1.017265	1.338203
H 0	1.967146	-0.230491	2.214351
H 0	2.458555	-0.482503	0.507355
H 0	-1.995724	-0.334775	-2.109457
H 0	-2.636341	-0.332081	-0.431159
H 0	-2.870336	1.066229	-1.467195
H 0	-1.187210	2.995227	-0.962943
H 0	0.465319	2.386964	-1.251873
H 0	-0.809752	2.077409	-2.436830
C 0	-1.533051	-2.554521	0.039392
O 0	-2.313652	-2.596131	0.894447
O 0	-1.011481	-2.995227	-1.011361
H 0	-0.249480	-2.207329	-1.031565

HF= -551.5230164

**11)TMGCO2 (B3LYP /6-31++G\*\*)**

N 0	-0.026468	-1.032177	-0.067629
C 0	-0.026468	0.340059	-0.067629
C 0	-1.111356	-1.969586	-0.067629
N 0	-0.990651	1.000139	0.602804
N 0	0.949629	0.966527	-0.738676
C 0	-1.472163	2.332198	0.196165
C 0	-1.575403	0.481739	1.859304
C 0	1.668567	0.322079	-1.854459
C 0	1.501900	2.264671	-0.310983
O 0	-0.899311	-3.116684	0.201590
O 0	-2.319875	-1.496384	-0.402374
H 0	0.870247	-1.507451	-0.053418
H 0	-2.564114	2.328545	0.255750
H 0	-1.094842	3.116684	0.858482
H 0	-1.178128	2.544585	-0.831095
H 0	-1.022808	-0.390229	2.206268
H 0	-1.503623	1.268001	2.615742
H 0	-2.626217	0.216165	1.719641
H 0	2.626217	-0.089006	-1.517160
H 0	1.061822	-0.468039	-2.295512
H 0	1.865099	1.080487	-2.615742
H 0	1.226507	3.061956	-1.006879
H 0	1.159985	2.511726	0.692409
H 0	2.591358	2.176472	-0.292686

H 0 -2.307088 -0.585314 -0.731831  
HF= -551.5862245

**12) 1 (B3LYP/6-31++G\*\*)**

C 0 0.300101 -2.589997 0.021498  
C 0 -0.816343 -1.543638 0.021498  
O 0 -1.423105 -1.468849 1.310330  
C 0 -0.284118 -0.158119 -0.437975  
O 0 0.217921 -0.053611 -1.564498  
O 0 -0.443934 0.765355 0.451266  
H 0 0.738422 -2.674860 -0.977225  
H 0 -0.099615 -3.563617 0.327759  
H 0 1.085729 -2.303576 0.729535  
H 0 -1.582589 -1.838477 -0.711892  
H 0 -1.313845 -0.531817 1.564498  
S 0 0.300101 2.824169 0.021498  
O 0 -0.790053 3.563617 0.707610  
O 0 1.582589 2.785423 0.767276  
HF= -891.7378344

**13) 2 (B3LYP/6-31++G\*\*)**

C 0 1.543981 -1.231359 1.474209  
C 0 1.543981 0.298248 1.474209  
O 0 2.876249 0.801982 1.474209  
C 0 0.786670 0.877337 0.247121  
O 0 -0.443738 0.538460 0.165605  
O 0 1.439758 1.610308 -0.523728  
H 0 0.518452 -1.610308 1.506810  
H 0 2.098390 -1.605607 2.342534  
H 0 2.029830 -1.609922 0.567958  
H 0 1.024725 0.658809 2.375012  
H 0 2.896147 1.352841 0.662428  
S 0 -1.630375 1.233932 -1.576116  
O 0 -1.640517 -0.018279 -2.375012  
O 0 -2.896147 1.510147 -0.848371  
HF= -891.7399322

**14) 3 (B3LYP/6-31++G\*\*)**

C 0 -0.308820 -1.956835 -0.481587  
C 0 -0.308820 -0.433382 -0.481587  
O 0 1.038974 0.075696 -0.481587  
C 0 -0.986974 0.197753 -1.747606



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O	0	-2.144027	-0.158312	-2.031774
O	0	-0.220544	1.031451	-2.334443
H	0	-1.339613	-2.318517	-0.534866
H	0	0.163467	-2.348963	0.426921
H	0	0.238917	-2.337525	-1.351076
H	0	-0.826949	-0.056983	0.412083
H	0	0.934870	0.732344	-1.265146
S	0	1.860492	0.945226	1.500752
O	0	2.144027	2.348963	1.129605
O	0	0.656305	0.726580	2.334443

HF=-891.7268275

**15) 4 (B3LYP/6-31++G\*\*)**

C	0	1.559960	-2.662831	1.854077
C	0	1.559960	-1.132436	1.854077
O	0	2.892191	-0.633390	1.854077
C	0	0.768809	-0.571986	0.646102
O	0	-0.455475	-0.866829	0.590101
O	0	1.441961	0.132009	-0.166287
H	0	0.535782	-3.044311	1.890315
H	0	2.116271	-3.030778	2.722991
H	0	2.046909	-3.041958	0.949130
H	0	1.044968	-0.772450	2.757176
H	0	2.942385	-0.076465	1.053823
S	0	-1.674658	-0.996126	-1.426162
O	0	-1.683176	-2.468939	-1.552634
O	0	-2.942385	-0.391062	-0.965659
S	0	0.559574	1.937538	-1.472515
O	0	1.228654	1.650640	-2.757176
O	0	1.139349	3.044311	-0.684760

HF=-1440.3599072

**16) 5 (B3LYP/6-31++G\*\*)**

C	0	1.056853	-2.289045	0.974337
C	0	1.056853	-0.766935	0.974337
O	0	2.408140	-0.278563	0.974337
C	0	0.309557	-0.169149	-0.250192
O	0	-0.875902	-0.529702	-0.395750
O	0	1.005536	0.618746	-0.949754
H	0	0.031212	-2.660976	0.978430
H	0	1.574557	-2.666729	1.860024
H	0	1.565622	-2.672459	0.085575

H 0	0.555575	-0.395228	1.875807
H 0	2.438662	0.361857	0.230850
S 0	-2.497580	-0.153543	-2.163314
O 0	-3.502724	-1.090172	-1.641976
O 0	-2.808974	1.272844	-1.991806
S 0	3.401561	0.432434	3.106306
O 0	3.502724	1.884999	2.936537
O 0	2.308744	-0.054344	3.956060
S 0	0.595540	2.031197	-2.902086
O 0	1.916791	2.672459	-2.883123
O 0	0.392231	1.028127	-3.956060

HF=-1989.2488071

**16) 6 (B3LYP/6-311+G\*)**

C 0	1.157769	-4.062801	-1.815497
N 0	1.157769	-2.599078	-1.815497
C 0	2.481967	-1.978306	-1.815497
C 0	-1.469357	-2.972903	-2.972636
N 0	-1.165672	-2.327536	-1.697336
C 0	-2.324896	-1.907560	-0.900507
C 0	0.075118	-1.891292	-1.389917
N 0	0.260094	-0.767802	-0.713306
H 0	0.190903	-4.444209	-1.498309
H 0	1.910591	-4.425570	-1.109340
H 0	1.393325	-4.458379	-2.807601
H 0	2.402604	-0.927405	-2.088287
H 0	3.101806	-2.485443	-2.557036
H 0	2.972801	-2.056544	-0.838904
H 0	-0.584157	-3.011694	-3.603269
H 0	-2.237003	-2.392905	-3.493580
H 0	-1.848957	-3.988281	-2.825759
H 0	-2.034570	-1.778238	0.139254
H 0	-3.075146	-2.698346	-0.956631
H 0	-2.761273	-0.977682	-1.276418
H 0	-0.524117	-0.171859	-0.400987
H 0	1.043874	-0.715537	-0.063979
C 0	-1.521436	3.604486	2.696903
C 0	-2.378102	2.488012	2.101285
O 0	-3.101806	2.964108	0.977079
C 0	-1.526669	1.261463	1.709530
O 0	-0.887445	0.721378	2.665878
O 0	-1.545918	0.913479	0.507475

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H 0	-1.016701	3.265286	3.603269
H 0	-2.157121	4.458379	2.941870
H 0	-0.768706	3.938335	1.977235
H 0	-3.095121	2.142872	2.857394
H 0	-2.828627	2.407226	0.229678
S 0	0.304646	-1.141108	2.699903
O 0	1.474549	-0.790471	1.851824
O 0	-0.601507	-2.119505	2.062766

HF= -1255.1047111

**16) 7 (B3LYP/6-311+G\*)**

C 0	-0.041679	-3.786080	-0.967149
N 0	-0.041679	-2.325106	-0.967149
C 0	1.280080	-1.684759	-0.967149
C 0	-2.518142	-2.696154	-2.434023
N 0	-2.363833	-2.057461	-1.126599
C 0	-3.593804	-1.520370	-0.547327
C 0	-1.152934	-1.605902	-0.694571
N 0	-1.087111	-0.488682	0.009795
H 0	-1.026131	-4.170072	-0.709577
H 0	0.672940	-4.144774	-0.220280
H 0	0.253778	-4.185077	-1.942054
H 0	1.195072	-0.656829	-1.311998
H 0	1.918591	-2.234683	-1.661187
H 0	1.737621	-1.694701	0.025622
H 0	-1.554767	-2.791226	-2.928053
H 0	-3.162821	-2.078885	-3.067124
H 0	-2.972116	-3.686772	-2.339402
H 0	-3.450182	-1.316862	0.512428
H 0	-4.383082	-2.266628	-0.655271
H 0	-3.916729	-0.599476	-1.046274
H 0	-1.733989	0.268513	-0.198635
H 0	-0.207709	-0.143075	0.442438
C 0	3.699649	1.808602	2.008613
C 0	2.355106	2.530731	2.074025
O 0	2.545800	3.923204	1.879841
C 0	1.346242	1.939912	1.066278
O 0	1.078174	0.727246	1.146923
O 0	0.867338	2.789020	0.238744
H 0	3.581333	0.746109	2.229448
H 0	4.383082	2.248467	2.738591
H 0	4.147499	1.919523	1.017164

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H 0 1.911984 2.370529 3.067124  
H 0 1.947884 4.185077 1.162491  
S 0 -0.423384 2.492038 -1.572680  
O 0 -1.725091 2.111013 -0.970592  
O 0 0.253794 1.378222 -2.264085  
HF=-1255.1037718

**16) 8 (B3LYP/6-311+G\*)**

C 0 0.114751 -3.390901 -2.012834  
N 0 0.114751 -1.925845 -2.012834  
C 0 1.442959 -1.304957 -2.012834  
C 0 -2.452593 -2.336744 -3.308599  
N 0 -2.211738 -1.648236 -2.043580  
C 0 -3.402194 -1.206850 -1.318063  
C 0 -0.981461 -1.211582 -1.676683  
N 0 -0.847537 -0.069140 -1.016816  
H 0 -0.849880 -3.770835 -1.687131  
H 0 0.868935 -3.739866 -1.304784  
H 0 0.347564 -3.785528 -3.006439  
H 0 1.357262 -0.242786 -2.232655  
H 0 2.041676 -1.779831 -2.793154  
H 0 1.945848 -1.437557 -1.052344  
H 0 -1.537850 -2.383958 -3.894404  
H 0 -3.199904 -1.782912 -3.885085  
H 0 -2.825728 -3.352530 -3.148093  
H 0 -3.153778 -1.011117 -0.276861  
H 0 -4.143584 -2.007597 -1.347880  
H 0 -3.846128 -0.308654 -1.762309  
H 0 -1.615467 0.584418 -0.924495  
H 0 -0.119889 0.046924 -0.293767  
C 0 3.468380 0.494091 2.578730  
C 0 2.072684 0.869273 3.085975  
O 0 2.129963 2.030004 3.894404  
C 0 1.096413 1.062341 1.911550  
O 0 0.815311 0.046303 1.199500  
O 0 0.666381 2.223461 1.725931  
H 0 3.451998 -0.448247 2.026937  
H 0 4.143584 0.390920 3.430751  
H 0 3.863045 1.279094 1.927927  
H 0 1.683129 0.048251 3.702371  
H 0 1.650912 2.724112 3.414039  
S 0 -1.101861 3.335670 0.417245

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O O -2.056533 2.245237 0.135019  
O O -0.310484 3.785528 -0.726475  
S O 0.558209 -2.245771 1.920940  
O O -0.747321 -2.416382 1.266908  
O O 1.699085 -2.824599 1.198954  
HF=-1803.7846963

**16) 9 (B3LYP/6-311+G\*)**

C O 0.753282 -3.072847 -3.477690  
N O 0.753282 -1.607212 -3.477690  
C O 2.085020 -0.995223 -3.477690  
C O -1.864881 -1.985257 -4.674119  
N O -1.572268 -1.327414 -3.401835  
C O -2.736284 -0.858695 -2.652679  
C O -0.323767 -0.896430 -3.080946  
N O -0.152739 0.233966 -2.408978  
H O -0.222057 -3.456258 -3.190423  
H O 1.479656 -3.421484 -2.741363  
H O 1.020064 -3.461963 -4.464309  
H O 2.007947 0.066445 -3.703697  
H O 2.681649 -1.478404 -4.253894  
H O 2.583593 -1.126995 -2.515126  
H O -0.966018 -2.052855 -5.281685  
H O -2.607276 -1.398013 -5.223626  
H O -2.266892 -2.990673 -4.520218  
H O -2.469142 -0.668995 -1.614395  
H O -3.498981 -1.639277 -2.669317  
H O -3.168639 0.050315 -3.087996  
H O -0.922448 0.862049 -2.227130  
H O 0.599572 0.350506 -1.701472  
C O 2.123744 2.540917 2.078185  
C O 0.767514 1.873157 1.868373  
O O -0.283918 2.732748 2.320182  
C O 0.502313 1.509193 0.398273  
O O 1.313005 0.693466 -0.160926  
O O -0.482104 2.033540 -0.156997  
H O 2.931623 1.872294 1.775088  
H O 2.252072 2.793421 3.132652  
H O 2.194585 3.461963 1.493962  
H O 0.714033 0.947106 2.455622  
H O -0.827495 2.900797 1.524026  
S O -1.722615 1.656757 4.099987

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O O -1.170733 0.318094 3.859731  
O O -1.239413 2.369258 5.281685  
S O 2.051329 -1.445389 0.679987  
O O 1.366576 -2.173395 -0.404186  
O O 3.498981 -1.298294 0.517174  
HF=-1803.7776655

**16) 10 (B3LYP /6-311+G\*)**

C O -0.533822 -3.953311 -2.579246  
N O -0.533822 -2.487785 -2.579246  
C O 0.794685 -1.871555 -2.579246  
C O -3.174037 -2.884202 -3.718271  
N O -2.857272 -2.214228 -2.459112  
C O -4.004498 -1.780062 -1.660703  
C O -1.608326 -1.780793 -2.164542  
N O -1.431374 -0.640351 -1.506996  
H O -1.500360 -4.335246 -2.264775  
H O 0.209023 -4.306979 -1.861556  
H O -0.289774 -4.342395 -3.571646  
H O 0.721180 -0.823827 -2.865622  
H O 1.412396 -2.392706 -3.312334  
H O 1.273257 -1.938629 -1.598025  
H O -2.295256 -2.928051 -4.357086  
H O -3.950512 -2.317881 -4.241455  
H O -3.543938 -3.899708 -3.550117  
H O -3.705142 -1.609037 -0.628608  
H O -4.751546 -2.575732 -1.672166  
H O -4.463268 -0.869188 -2.061535  
H O -2.210449 -0.023578 -1.303232  
H O -0.647026 -0.527489 -0.851649  
C O 2.719837 1.564352 0.279281  
C O 1.936273 1.251345 1.550459  
O O 1.852585 2.422548 2.364347  
C O 0.527478 0.703263 1.257176  
O O 0.444253 -0.342355 0.559581  
O O -0.427849 1.355603 1.762727  
H O 2.845070 0.664056 -0.324937  
H O 3.705749 1.947680 0.547730  
H O 2.205369 2.325634 -0.313174  
H O 2.459272 0.469486 2.115990  
H O 0.908469 2.575910 2.542750  
S O -2.762618 1.041284 1.509241

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O	O	-2.913296	1.273057	0.057112
O	O	-2.940300	-0.358158	1.917789
S	O	3.606073	2.915523	4.201125
O	O	4.751546	2.536175	3.373765
O	O	3.331373	4.342395	4.357086
S	O	-0.422681	-2.521829	1.714342
O	O	-0.896401	-3.126474	0.460522
O	O	0.846030	-3.031381	2.231538

HF=-2352.4607469

**17) LAC-CO2 (B3LYP /6-31++G\*\*)**

C	O	1.561829	-2.036697	0.350052
C	O	1.227661	-0.792800	1.175766
O	O	2.389800	0.016418	1.355530
C	O	0.103210	0.060974	0.512177
O	O	-1.006104	-0.499710	0.321014
O	O	0.434280	1.251877	0.236877
H	O	0.670151	-2.660202	0.232864
H	O	2.352692	-2.620010	0.838272
H	O	1.918381	-1.743942	-0.644577
H	O	0.856262	-1.109711	2.163330
H	O	2.083664	0.871246	0.972519
C	O	-2.397812	1.352127	-0.749069
O	O	-2.836288	1.761169	0.259857
O	O	-2.120911	1.076096	-1.855698

**18) TMGLCO2-TS (B3LYP /6-31++G\*\*)**

N	O	-0.458160	0.847977	-0.467270
C	O	-0.458160	2.152115	-0.467270
N	O	0.690735	2.935959	-0.467270
N	O	-1.648972	2.846039	-0.477768
C	O	0.807922	4.085632	0.429657
C	O	1.965027	2.311172	-0.804779
C	O	-2.883865	2.177475	-0.084641
C	O	-1.835388	4.044403	-1.289978
H	O	0.441925	0.438614	-0.221359
H	O	1.418106	3.829544	1.308533
H	O	1.285553	4.927490	-0.085098
H	O	-0.176361	4.397095	0.776794
H	O	2.663528	3.093933	-1.116440
H	O	2.409241	1.765457	0.040070
H	O	1.832794	1.615555	-1.635483

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H 0	-3.413055	1.755890	-0.947800
H 0	-2.653976	1.371002	0.611389
H 0	-3.536728	2.907898	0.407349
H 0	-2.276886	4.854904	-0.696365
H 0	-0.880737	4.379333	-1.693726
H 0	-2.509644	3.826950	-2.129623
C 0	-1.417221	-0.404480	-1.962189
O 0	-2.052002	0.365707	-2.591202
O 0	-0.965240	-1.463776	-1.657822
C 0	2.885193	-4.297256	1.146057
C 0	2.368332	-2.997086	1.773041
O 0	3.441925	-2.233856	2.293045
C 0	1.580322	-2.156693	0.773895
O 0	0.506683	-2.774994	0.296265
O 0	1.923386	-1.022034	0.466248
H 0	2.056259	-4.927505	0.813110
H 0	3.469330	-4.840088	1.893677
H 0	3.536728	-4.079590	0.293961
H 0	1.675690	-3.245590	2.591217
H 0	3.413803	-1.368347	1.851807
H 0	0.028320	-2.206955	-0.352127

HF= -894.8702248

**19) TMGLCO2 (B3LYP /6-31++G\*\*)**

N 0	-0.479706	0.637527	-0.785156
C 0	-0.479706	1.976974	-0.785156
N 0	0.707200	2.640488	-0.785156
N 0	-1.630157	2.683990	-0.749161
C 0	0.902725	3.894669	-0.058502
C 0	1.930130	2.002502	-1.283844
C 0	-2.871689	2.109436	-0.225357
C 0	-1.801270	3.917358	-1.518143
C 0	-1.385681	-0.235779	-1.596298
O 0	-2.146057	0.329132	-2.376740
O 0	-1.197479	-1.460983	-1.359390
H 0	0.329910	0.156525	-0.367310
H 0	1.742706	3.777542	0.635391
H 0	1.129852	4.722992	-0.739548
H 0	0.009720	4.138672	0.516296
H 0	2.556854	2.772369	-1.743393
H 0	2.490204	1.514800	-0.478546
H 0	1.678986	1.257095	-2.038345



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H 0	-3.492508	1.722488	-1.037521
H 0	-2.639740	1.293991	0.459641
H 0	-3.403412	2.894882	0.321823
H 0	-2.060608	4.758728	-0.865585
H 0	-0.890823	4.152390	-2.067688
H 0	-2.610748	3.767258	-2.240723
C 0	2.833542	-4.098877	0.791733
C 0	2.251740	-2.901245	1.549576
O 0	3.292236	-2.096085	2.080200
C 0	1.337250	-2.057053	0.663055
O 0	0.313354	-2.691147	0.176880
O 0	1.598938	-0.857285	0.467117
H 0	2.036713	-4.758743	0.439041
H 0	3.492523	-4.657547	1.461807
H 0	3.423996	-3.759460	-0.065323
H 0	1.627640	-3.271530	2.376755
H 0	3.147842	-1.200226	1.731857
H 0	-0.304749	-2.102753	-0.457138

HF= -894.885066

**20) TMGL-2SCO2 (B3LYP/6-311+G\*)**

C 0	0.378616	-3.698242	-0.271835
N 0	0.390167	-2.354187	0.296524
C 0	1.716782	-1.757721	0.471252
C 0	-2.171066	-2.138657	-1.079376
N 0	-1.934067	-2.120605	0.365555
C 0	-3.134766	-1.902206	1.170364
C 0	-0.710266	-1.809143	0.869370
N 0	-0.601898	-1.015289	1.920303
H 0	-0.596008	-4.161377	-0.137833
H 0	1.127518	-4.311676	0.238815
H 0	0.621170	-3.682648	-1.339157
H 0	1.635132	-0.690125	0.662094
H 0	2.281509	-1.908813	-0.452408
H 0	2.257278	-2.221619	1.300003
H 0	-1.230988	-2.088760	-1.621948
H 0	-2.766327	-1.264542	-1.355316
H 0	-2.704132	-3.048508	-1.369888
H 0	-2.921677	-2.091049	2.221130
H 0	-3.902100	-2.605484	0.838882
H 0	-3.510010	-0.883209	1.052139
H 0	-1.318359	-0.315384	2.120743

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H 0	0.256683	-0.971619	2.486694
C 0	3.890121	-2.509857	4.830658
C 0	3.379364	-1.133774	5.245422
O 0	4.470490	-0.332932	5.672134
C 0	2.564224	-0.458328	4.121109
O 0	1.625946	-1.081512	3.607849
O 0	2.953323	0.733887	3.840118
H 0	3.060043	-3.166107	4.563446
H 0	4.443039	-2.958374	5.659210
H 0	4.569931	-2.426010	3.978043
H 0	2.673508	-1.252670	6.081360
H 0	4.357712	0.534882	5.255417
S 0	1.885605	2.168732	2.605820
O 0	0.548157	2.170502	3.244446
O 0	1.911453	1.537567	1.266174
C 0	0.638351	3.564255	-4.878494
N 0	0.317871	2.618332	-3.811722
C 0	-1.110825	2.500061	-3.548065
C 0	2.959091	1.483002	-4.139740
N 0	2.533234	2.380722	-3.068237
C 0	3.508240	2.521286	-1.995500
C 0	1.181808	2.470367	-2.736252
N 0	0.720123	2.431259	-1.530746
H 0	1.712280	3.712662	-4.953583
H 0	0.171555	4.540878	-4.688766
H 0	0.266251	3.191055	-5.836884
H 0	-1.300568	1.691452	-2.845581
H 0	-1.622253	2.286789	-4.490250
H 0	-1.532440	3.423294	-3.128357
H 0	2.144836	1.311264	-4.838974
H 0	3.275131	0.510162	-3.736740
H 0	3.804871	1.914200	-4.683304
H 0	3.240097	3.356155	-1.348755
H 0	4.484772	2.731110	-2.437271
H 0	3.600922	1.618774	-1.375717
H 0	1.392715	2.127441	-0.831116
C 0	-4.149400	2.186050	1.867798
C 0	-2.638306	2.333740	1.863113
O 0	-2.075867	1.362732	2.756042
C 0	-2.033600	2.099304	0.467529
O 0	-1.249893	3.087296	0.082657
O 0	-2.235809	1.076874	-0.167145

H 0	-4.613861	2.931274	1.215836
H 0	-4.530823	2.323364	2.881516
H 0	-4.443176	1.195786	1.514755
H 0	-2.353668	3.335785	2.194611
H 0	-1.190369	1.671936	3.030930
H 0	-0.625549	2.827850	-0.689835

**Table S1** The thermochemical parameters for the interaction between the LAC anion and the SO<sub>2</sub> (kJ mol<sup>-1</sup>)

Complexes	HF/6-31G*		B3LYP/6-31G*		B3LYP/6-311+G*	
	$\Delta E$	$\Delta H$	$\Delta E$	$\Delta H$	$\Delta E$	$\Delta H$
1	-89.32	-91.80	-99.14	-101.62	-87.15	-89.63
2	-93.30	-95.78	-106.11	-108.59	-91.244	-93.72
3	-46.32	-48.80	-74.026	-76.50	-59.34	-61.81
4	-142.51	-147.47	-158.35	-163.31	-139.80	-144.75
5	-173.87	-181.30	-199.28	-206.71	-175.45	-182.9
LAC-CO <sub>2</sub>	-34.04	-36.52	-40.77	-43.25	-24.89	-27.37
TMG-SO <sub>2</sub>	-28.93	-31.41	-33.21	-35.69	-27.32	-29.79
TMG-CO <sub>2</sub>	-8.59	-11.07	-14.68	-17.16	-10.51	-12.99
TMG-2CO <sub>2</sub>	-15.51	-20.46	-27.57	-32.52	-19.26	-24.22