Activation of *β*-Diketones for CO_2 Capturing and Utilization

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Electronic supplementary information (ESI)

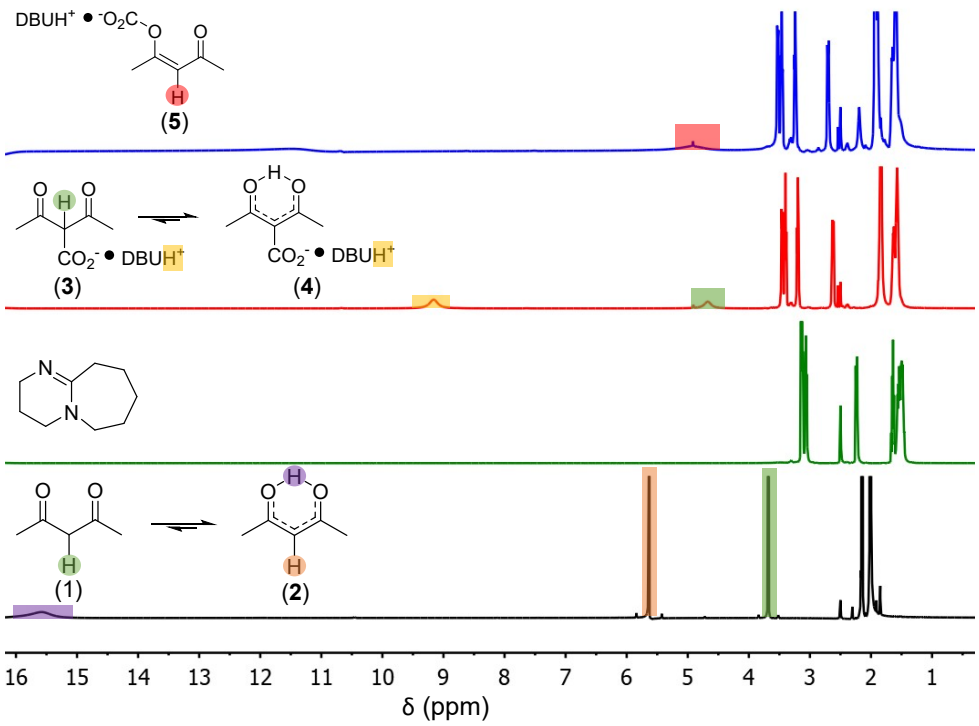


Figure S1. ^{1}H NMR spectra of **ACAC** (black), **DBU** (green), **ACAC/DBU** mixture dissolved in DMSO-d_6 before (red) and after (blue) bubbling CO_2.

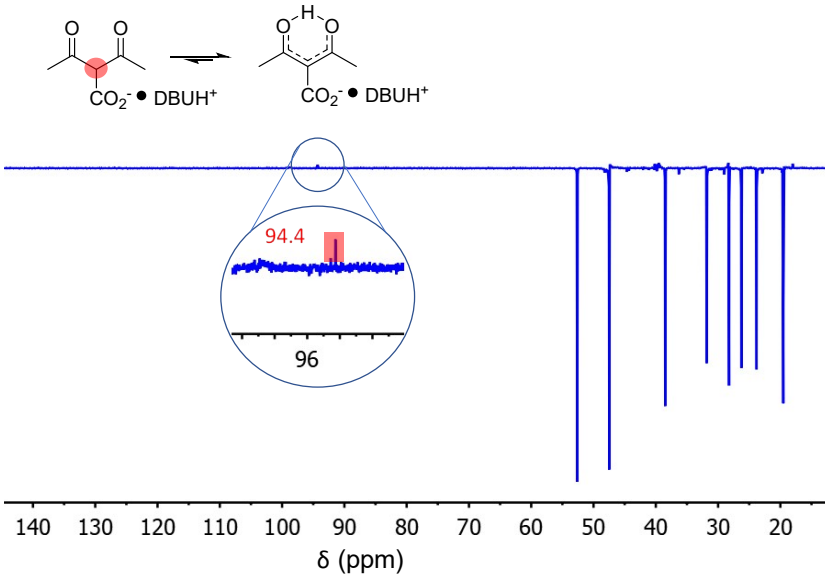


Figure S2. DEPT-135 spectrum of **ACAC/DBU** mixture before bubbling CO_2 (the adduct was formed in the presence of atmospheric CO_2). The peak labelled in red designates the α-carbon.

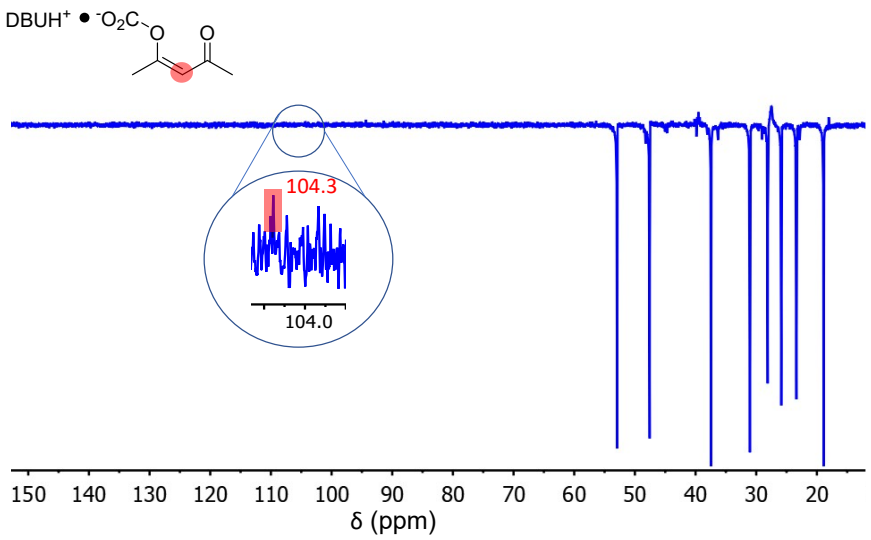


Figure S3. DEPT-135 spectrum of **ACAC**/**DBU** mixture after bubbling CO_2. The peak labelled in red designates the *enol* carbon.

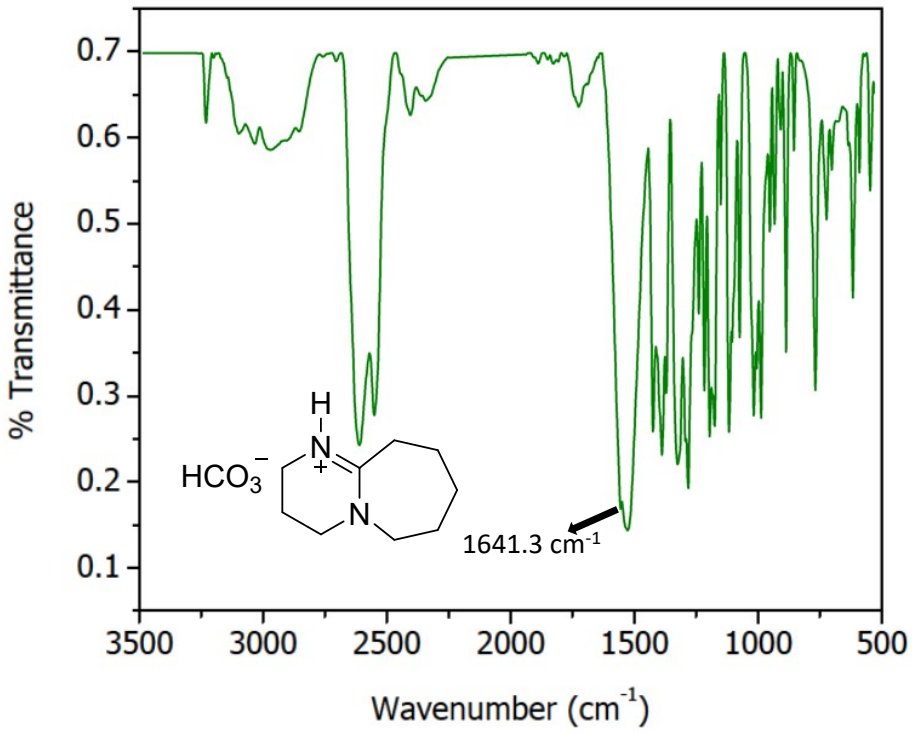


Figure S4. ATR-FTIR spectrum of the **DBU**-CO_2 adduct.

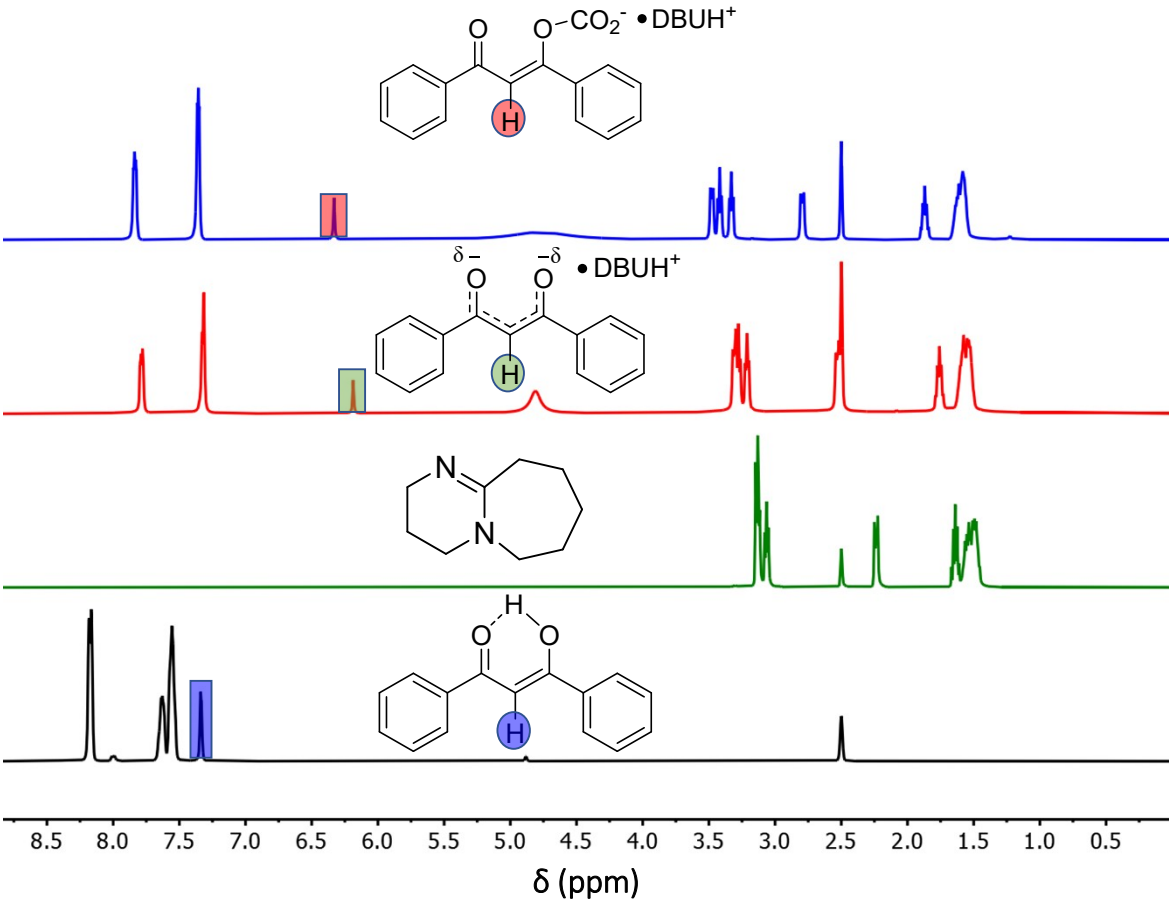


Figure S5. ^{1}H NMR spectra of **DBM** (black), **DBU** (green) and **DBM**/**DBU** mixture dissolved in DMSO-d_6 before (red) and after (blue) bubbling CO_2.

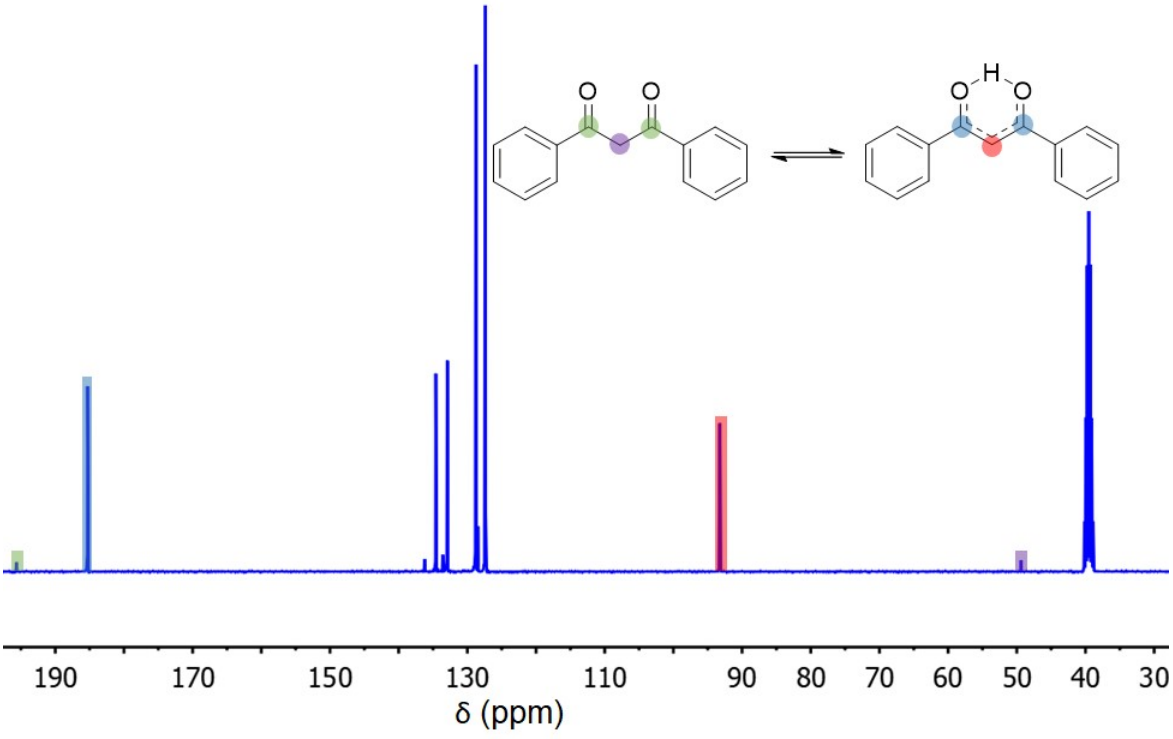


Figure S6. ^{13}C NMR spectrum of **DBM** dissolved in DMSO-d_6.

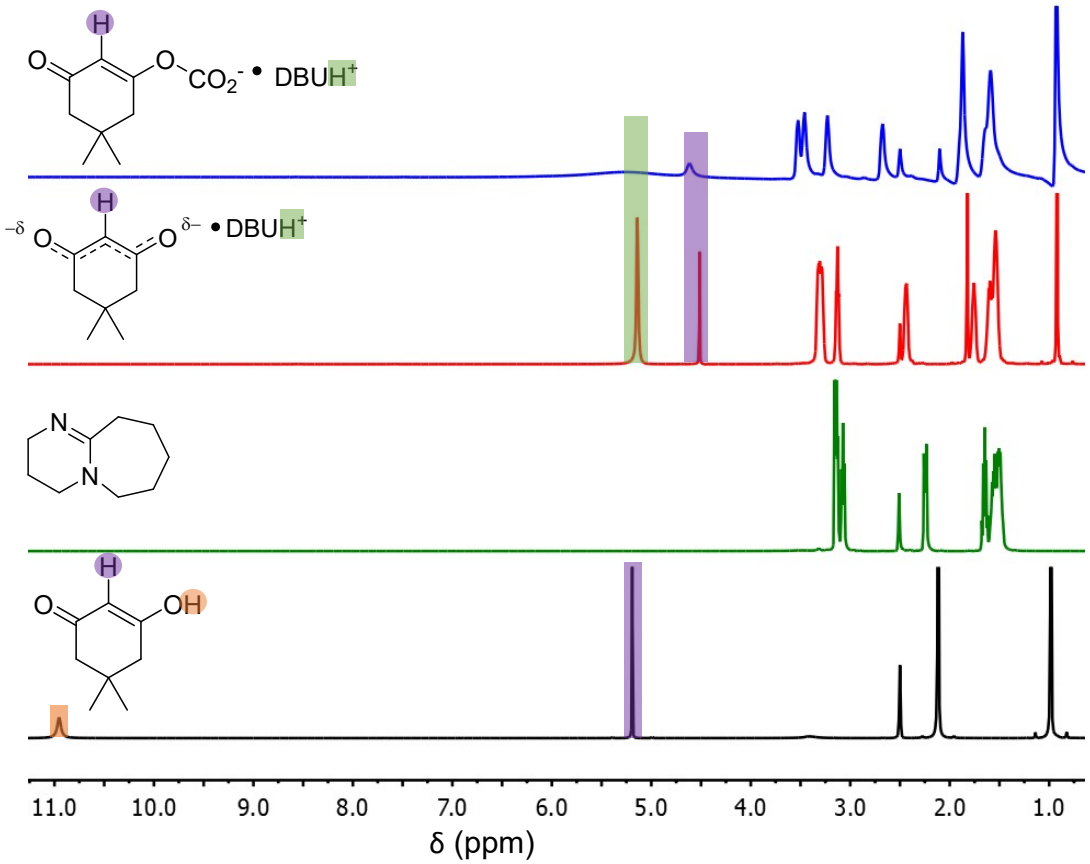


Figure S7. ^{1}H NMR spectra of **DMD** (black), **DBU** (green) and dimedone/**DBU** mixture dissolved in DMSO-d_6 before (red) and after (blue) bubbling CO_2.

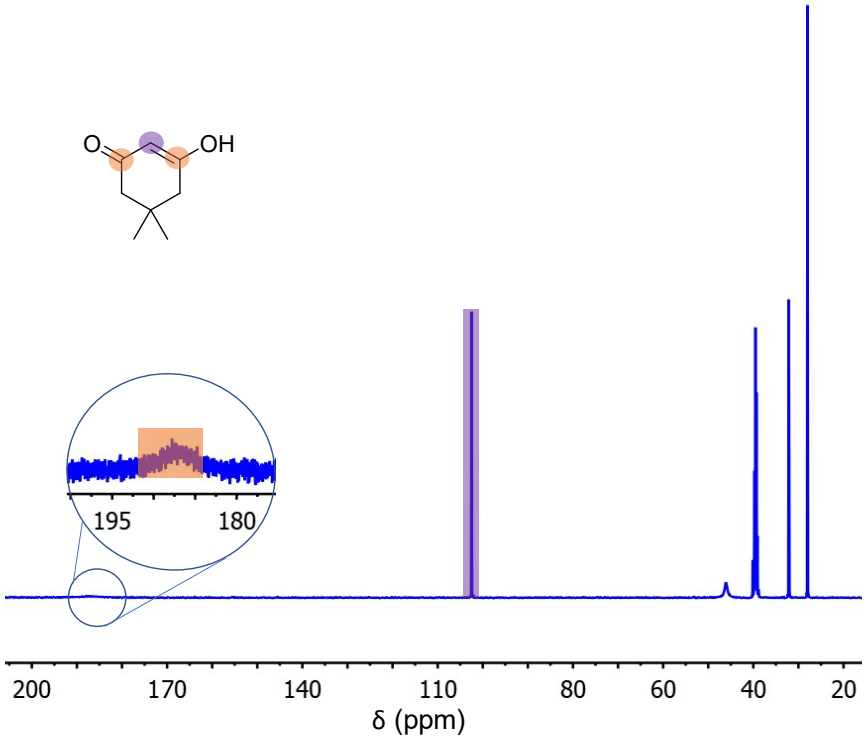


Figure S8. ^{13}C NMR spectrum of **DMD** dissolved in DMSO-d_6.

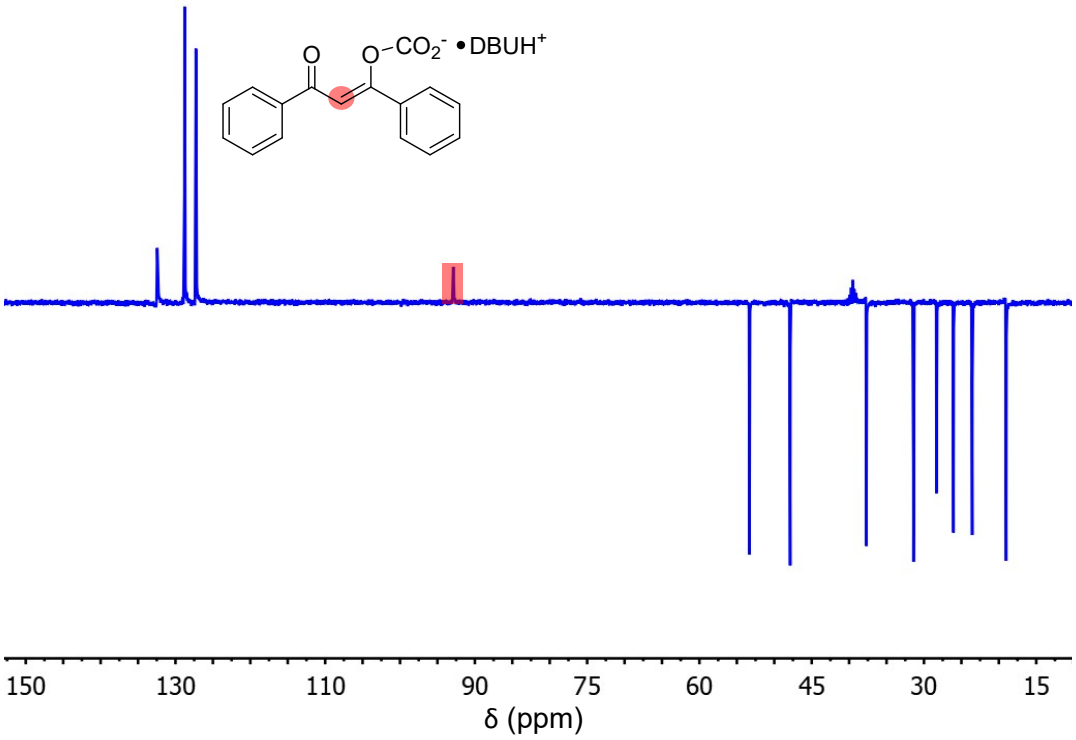


Figure S9. DEPT-135 spectrum of **DBM**/**DBU** mixture after bubbling CO_2. The peak labelled in **red** designates the *enol* carbon.

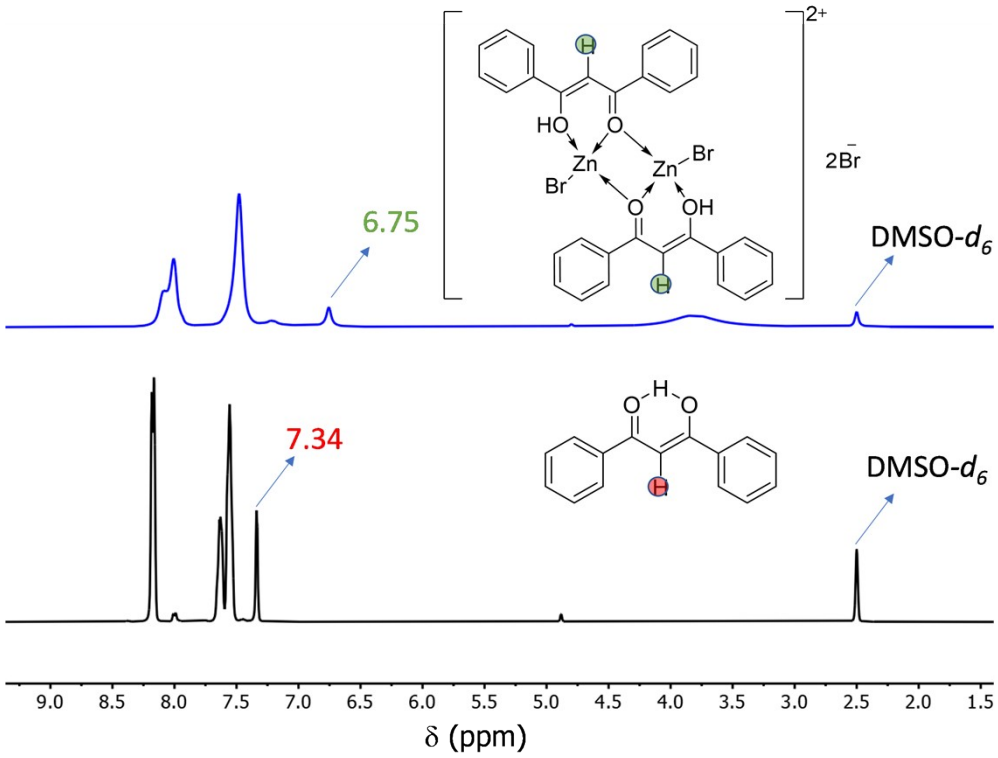


Figure S10. ^{1}H NMR spectra of **DBM** (black) and Zn-**DBM** (blue) mixture dissolved in DMSO-d_6.

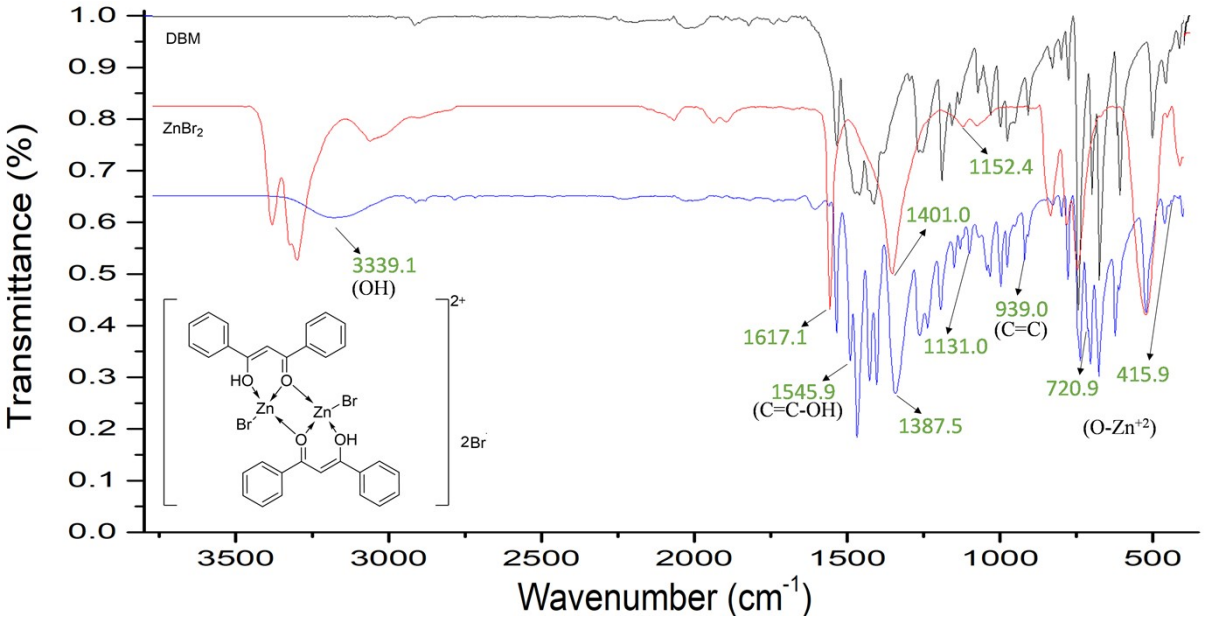


Figure S11. ATR-FTIR spectra of **DBM** (black), $ZnBr_2$ (red) and Zn-**DBM** (blue).

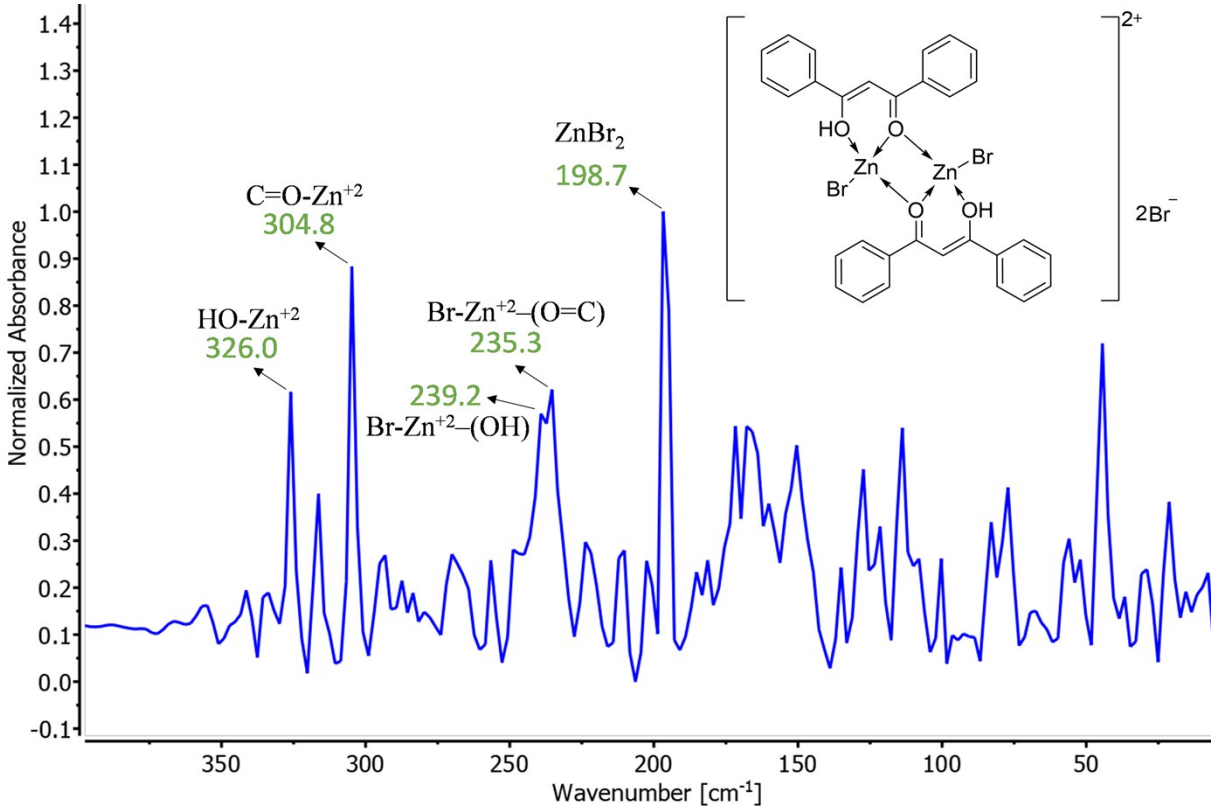


Figure S12. Far-IR spectrum of Zn-**DBM**.

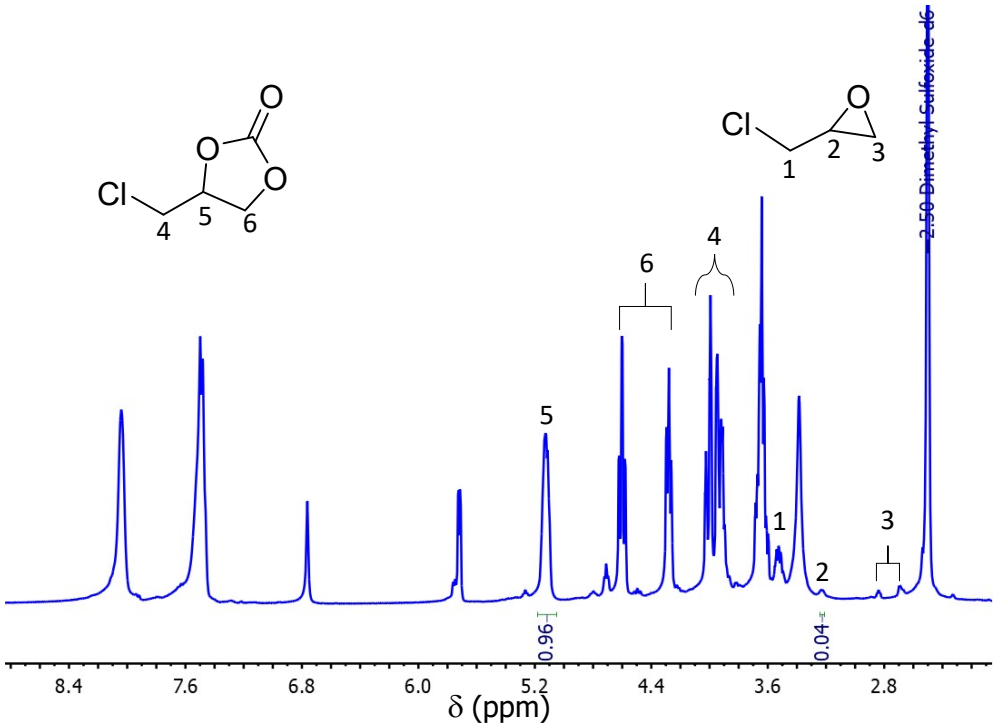


Figure S13. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 15 mol% catalyst loading; Table 2, entry 1).

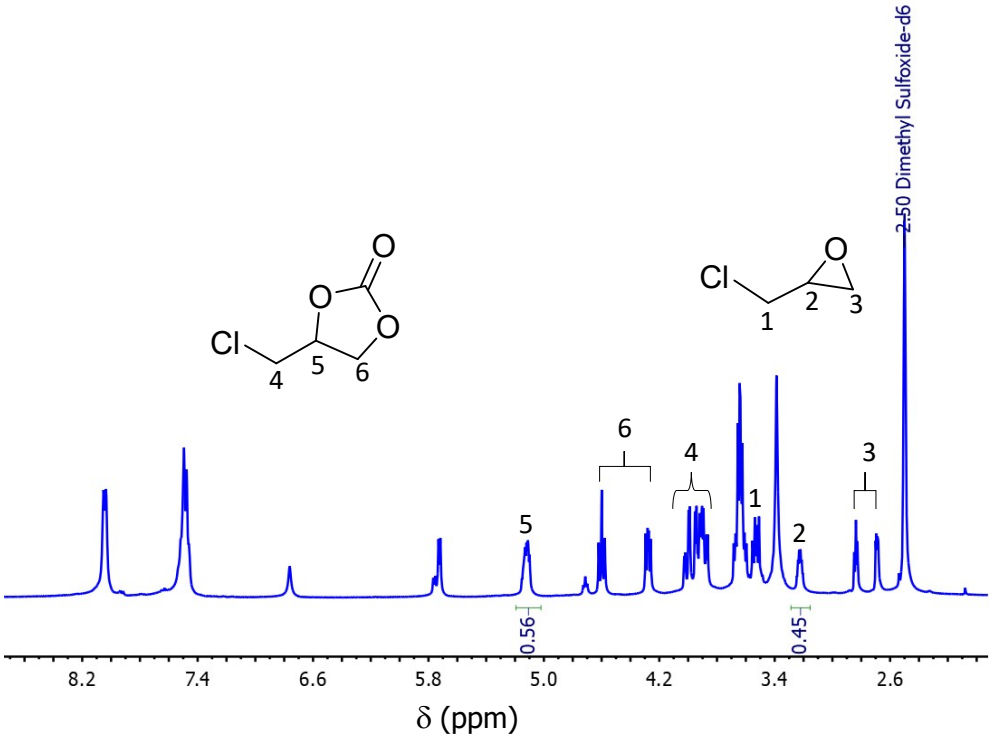


Figure S14. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 40 ºC and 15 mol% catalyst loading; Table 2, entry 2).

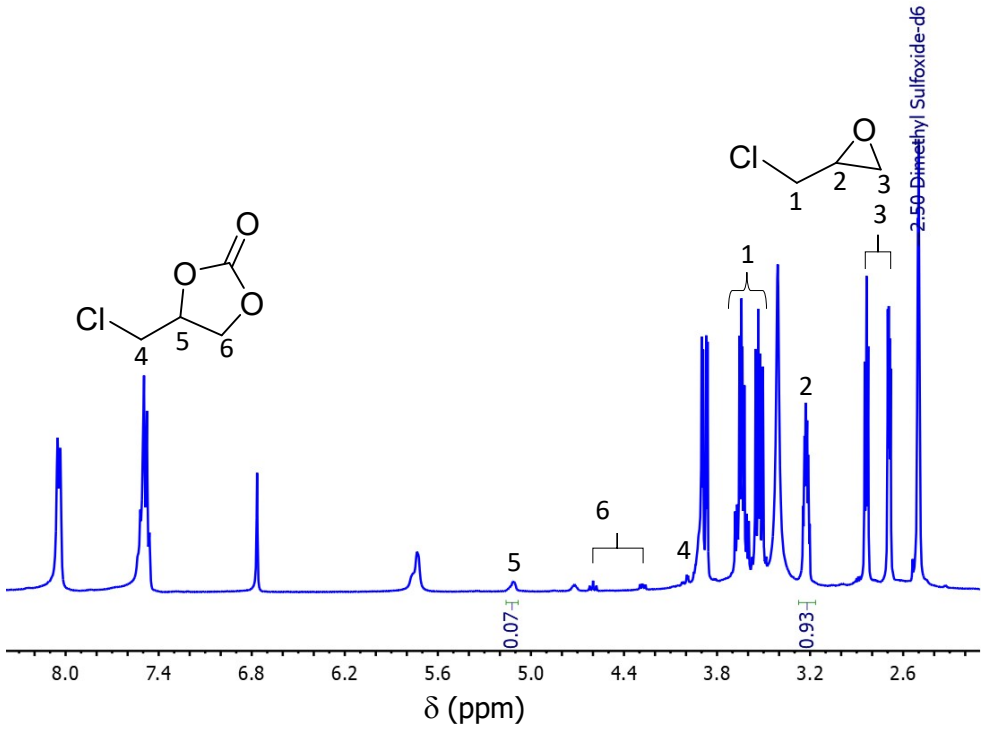


Figure S15. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 20 ºC and 15 mol% catalyst loading; Table 2, entry 3).

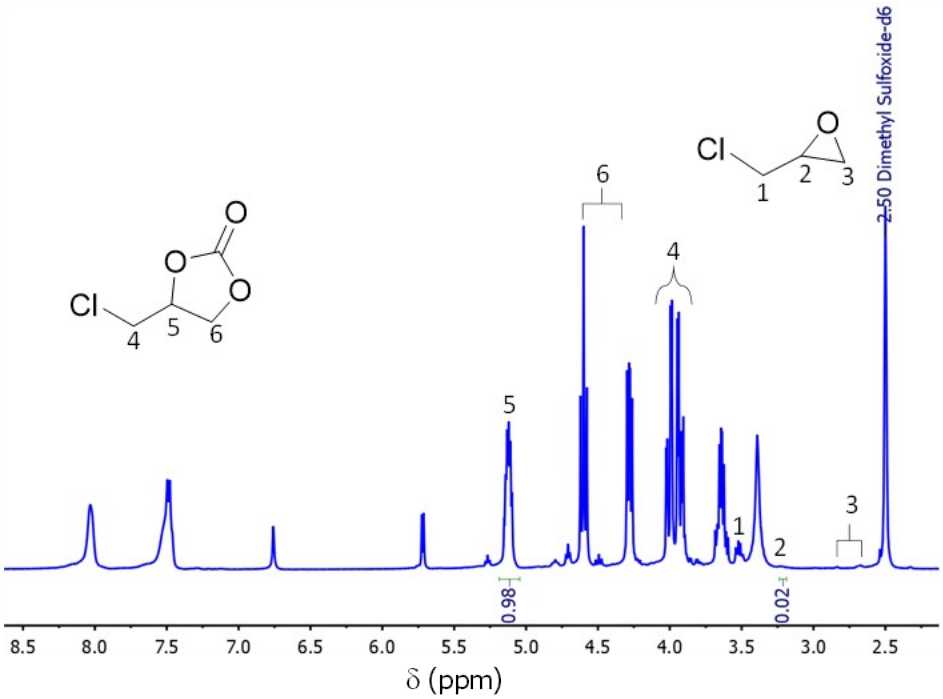


Figure S16. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 10 mol% catalyst loading; Table 2, entry 4).

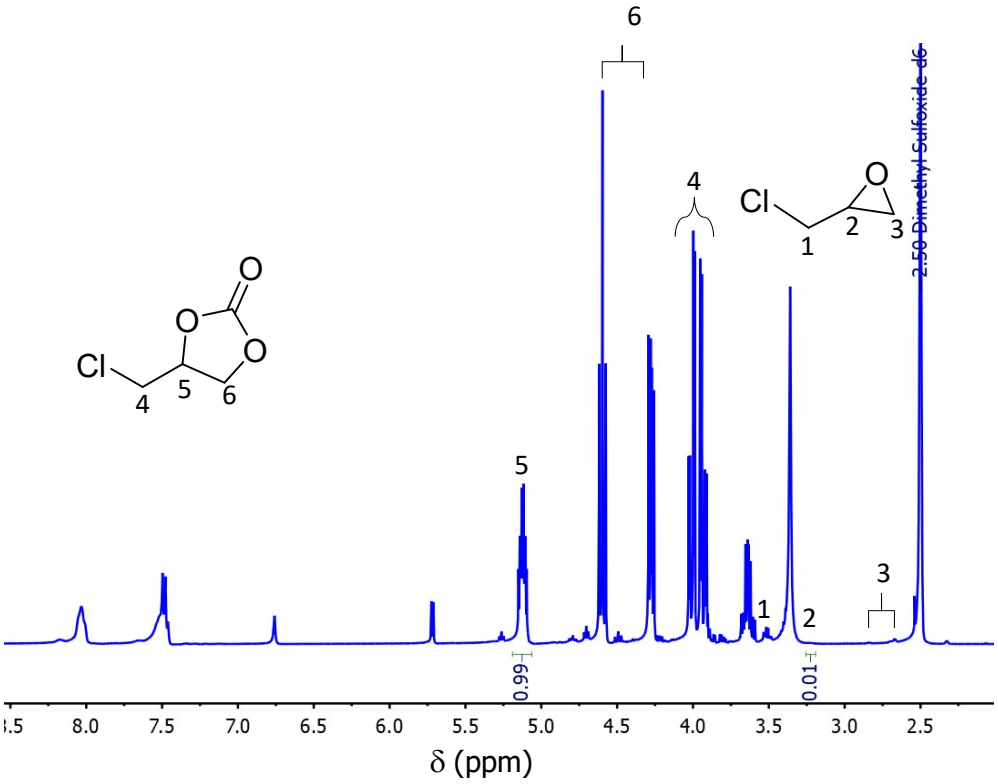


Figure S17. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 5 mol% catalyst loading; Table 2, entry 5).

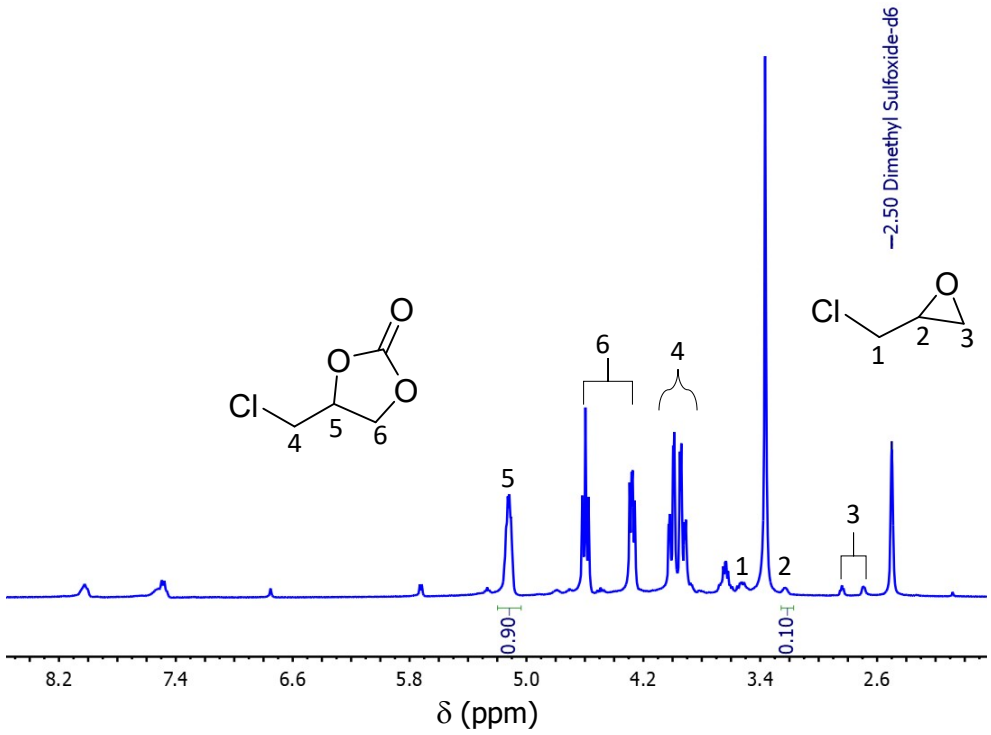


Figure S18. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 2.5 mol% catalyst loading; Table 2, entry 6).

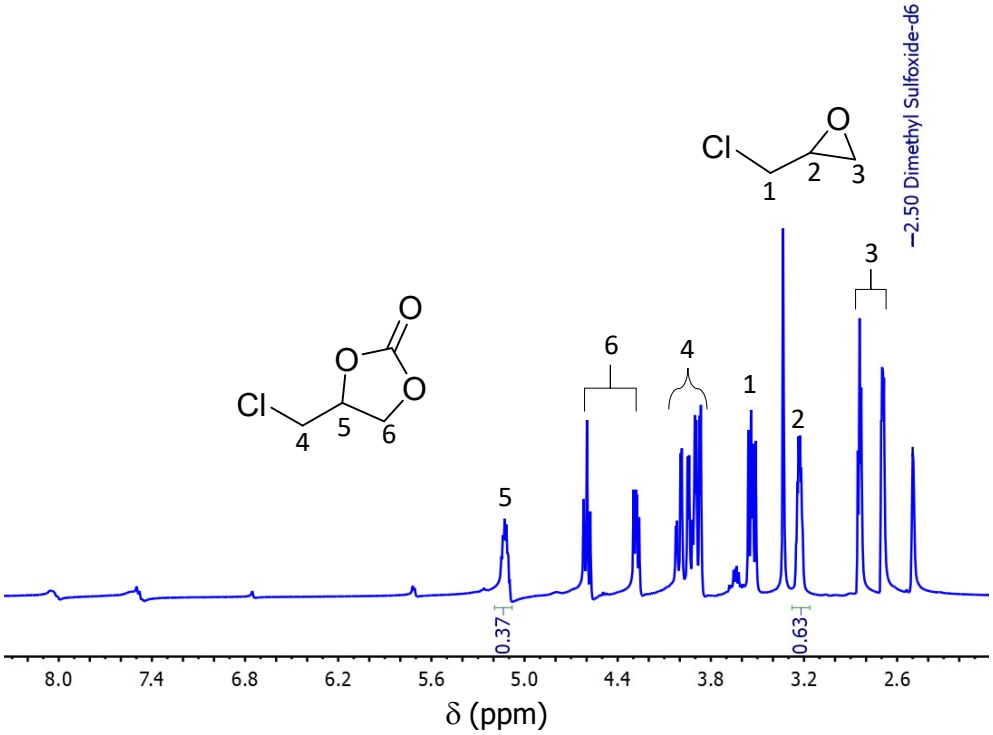


Figure S19. ^{1}H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 1 mol% catalyst loading; Table 2, entry 7).

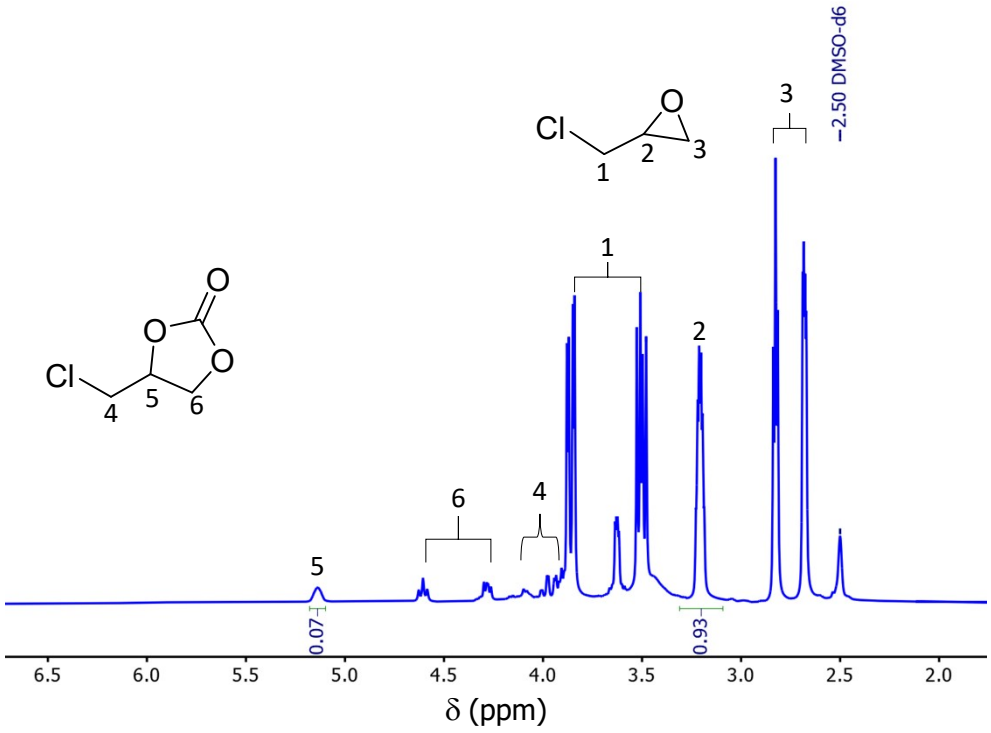


Figure S20. ^{1}H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by $ZnBr_2$ (Reaction conditions: 16 h, 60 ºC and 10 mol% catalyst loading; Table 2, entry 8).

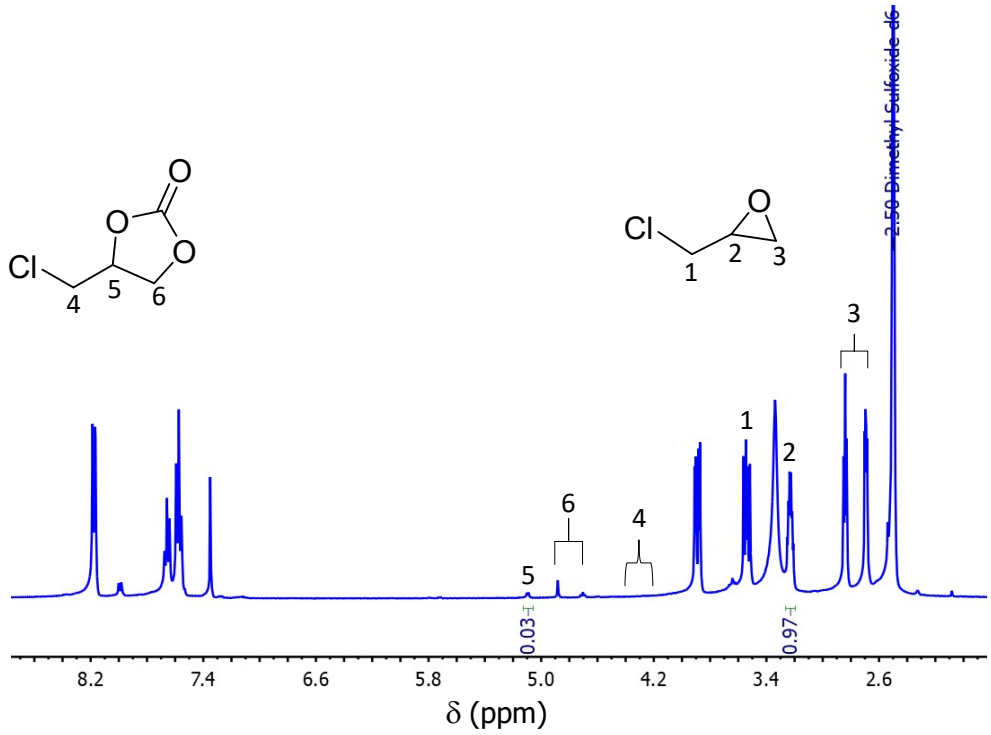


Figure S21. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by **DBM** (Reaction conditions: 16 h, 60 ºC and 5 mol% catalyst loading; Table 2, entry 9).

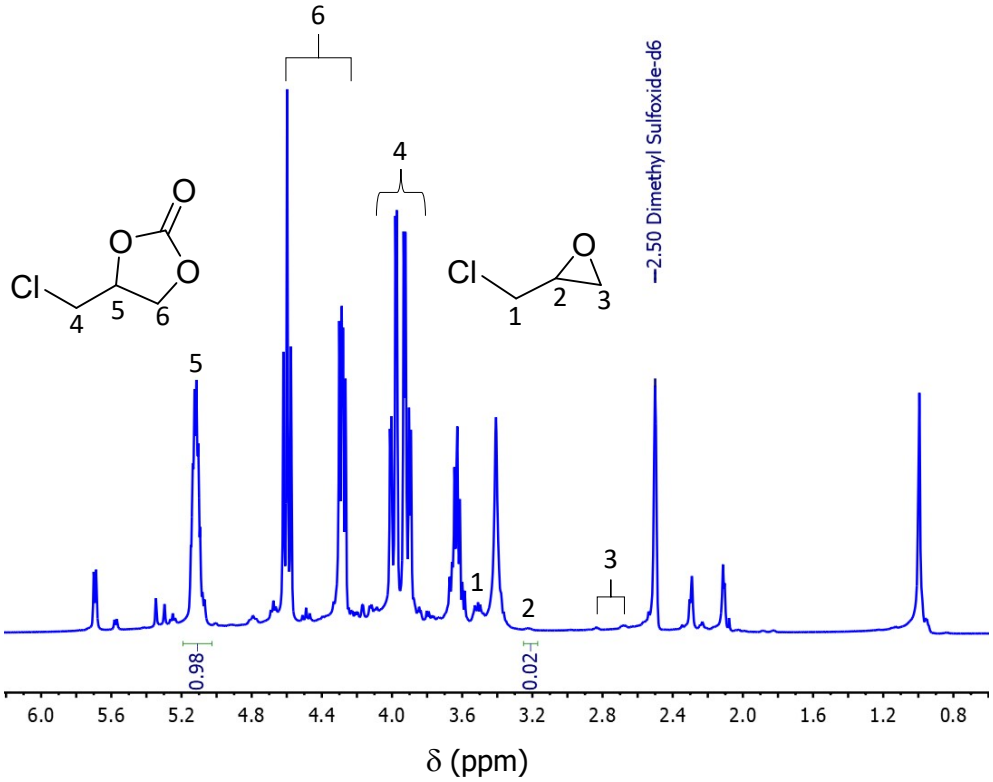


Figure S22. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DMD** (Reaction conditions: 16 h, 60 ºC and 5 mol% catalyst loading; Table 2, entry 10).

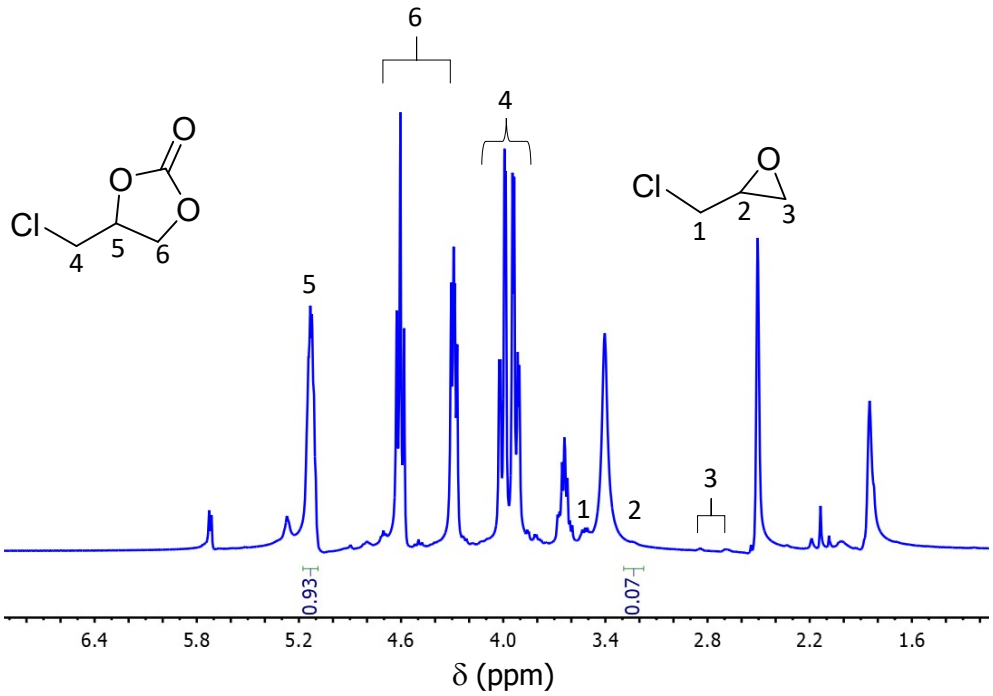


Figure S23. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**ACAC** (Reaction conditions: 16 h, 60 ºC and 5 mol% catalyst loading; Table 2, entry 11).

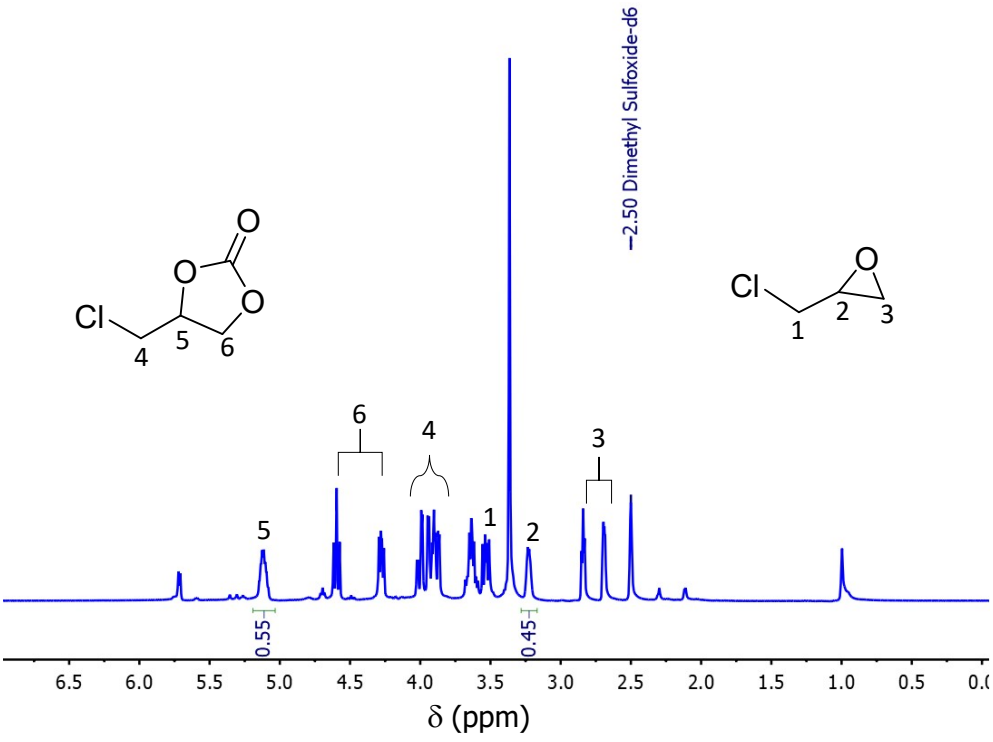


Figure S24. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DMD** (Reaction conditions: 16 h, 60 ºC and 2.5 mol% catalyst loading; Table 2, entry 12).

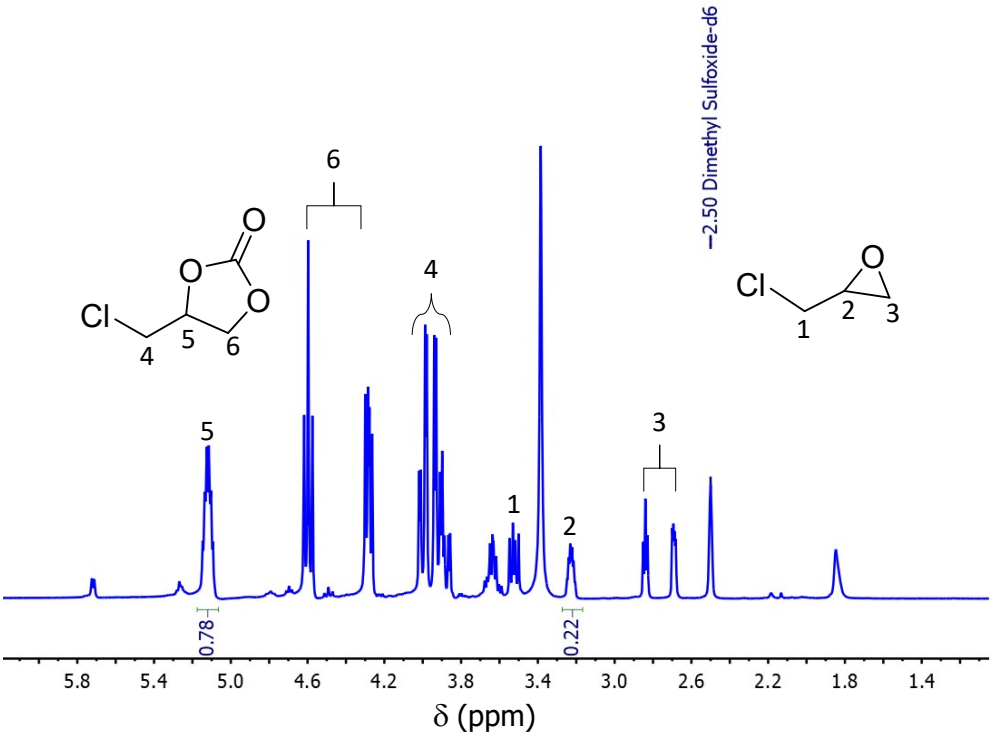


Figure S25. [1]H NMR spectrum of epichlorohydrin conversion (in DMSO-d_6) catalyzed by Zn-**ACAC** (Reaction conditions: 16 h, 60 ºC and 2.5 mol% catalyst loading; Table 2, entry 13).

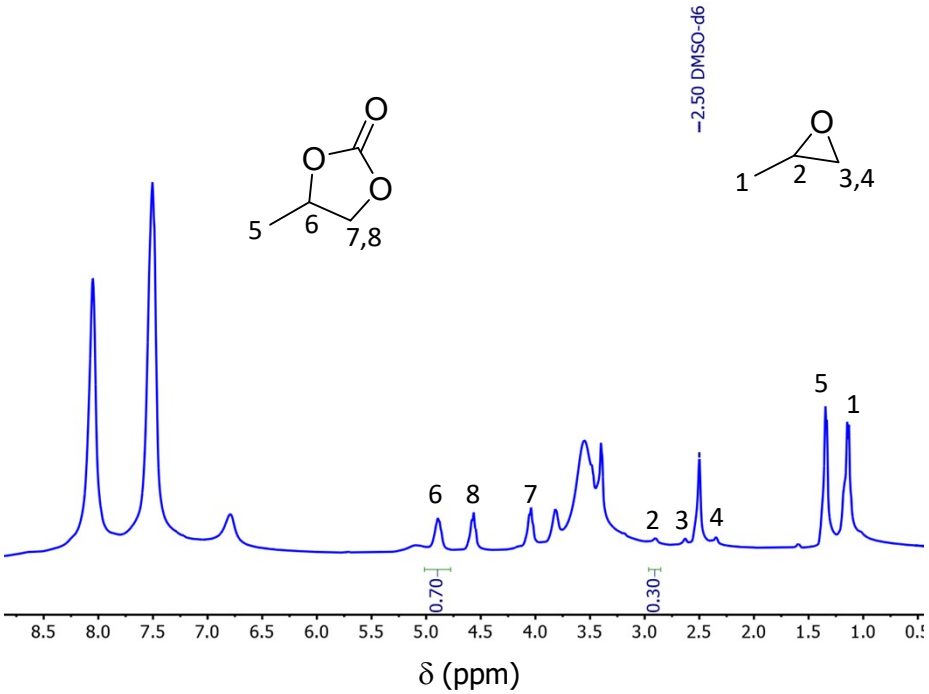


Figure S26. [1]H NMR spectrum of propylene oxide conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 20 ºC and 15 mol% catalyst loading; Table 3, entry 1).

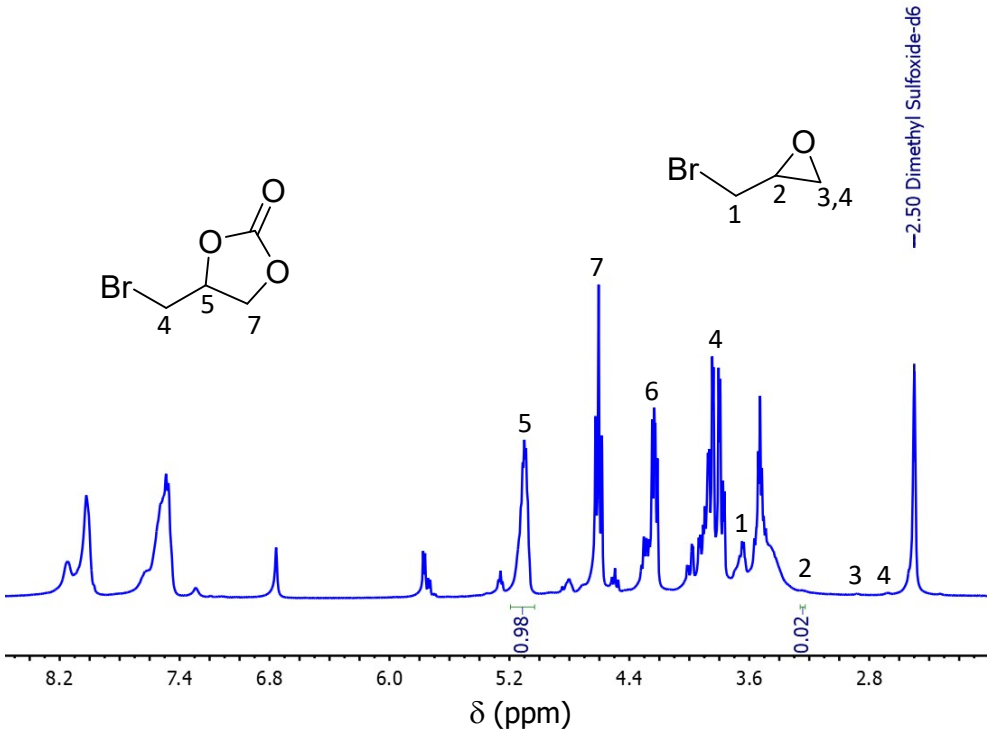


Figure S27. [1]H NMR spectrum of epibromohydrin conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 15 mol% catalyst loading; Table 2, entry 3)

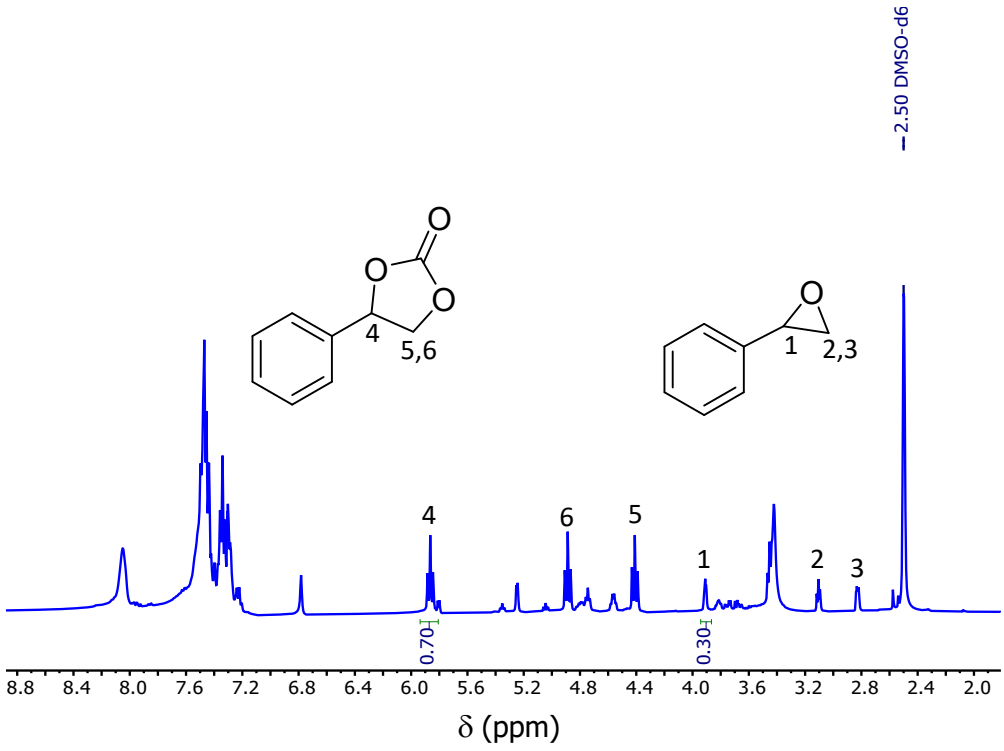


Figure S28. [1]H NMR spectrum of styrene oxide conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 16 h, 60 ºC and 15 mol% catalyst loading; Table 2, entry 4)

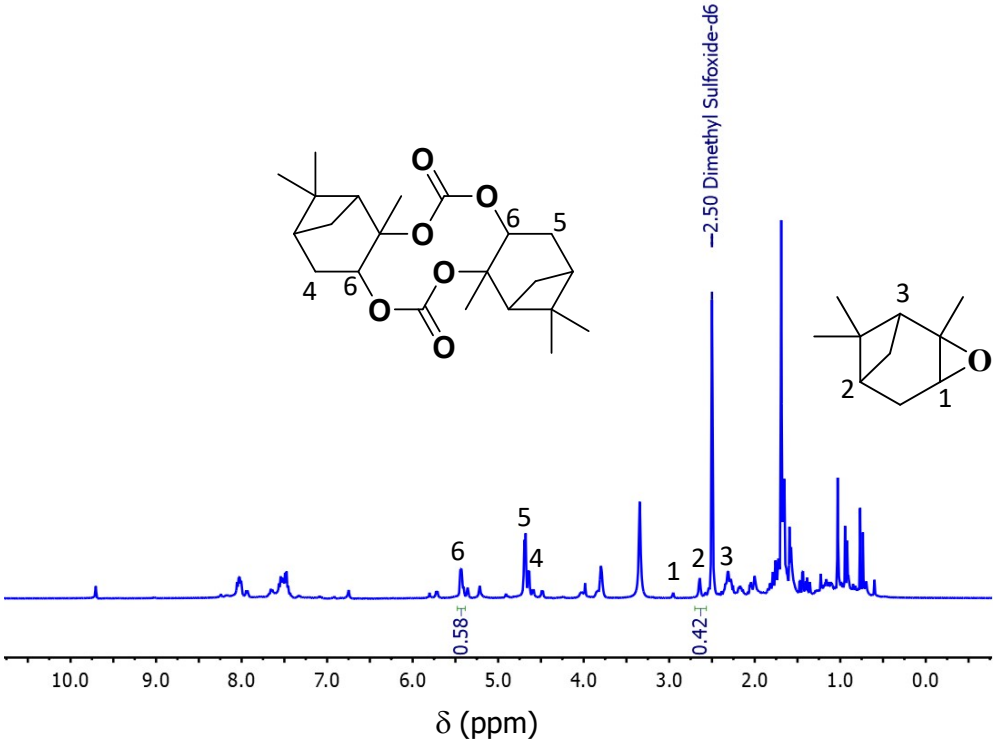


Figure S29. ^{1}H NMR spectrum of pinene oxide conversion (in DMSO-d_6) catalyzed by Zn-**DBM** (Reaction conditions: 90 h, 60 ºC and 15 mol% catalyst loading; Table 2, entry 5)

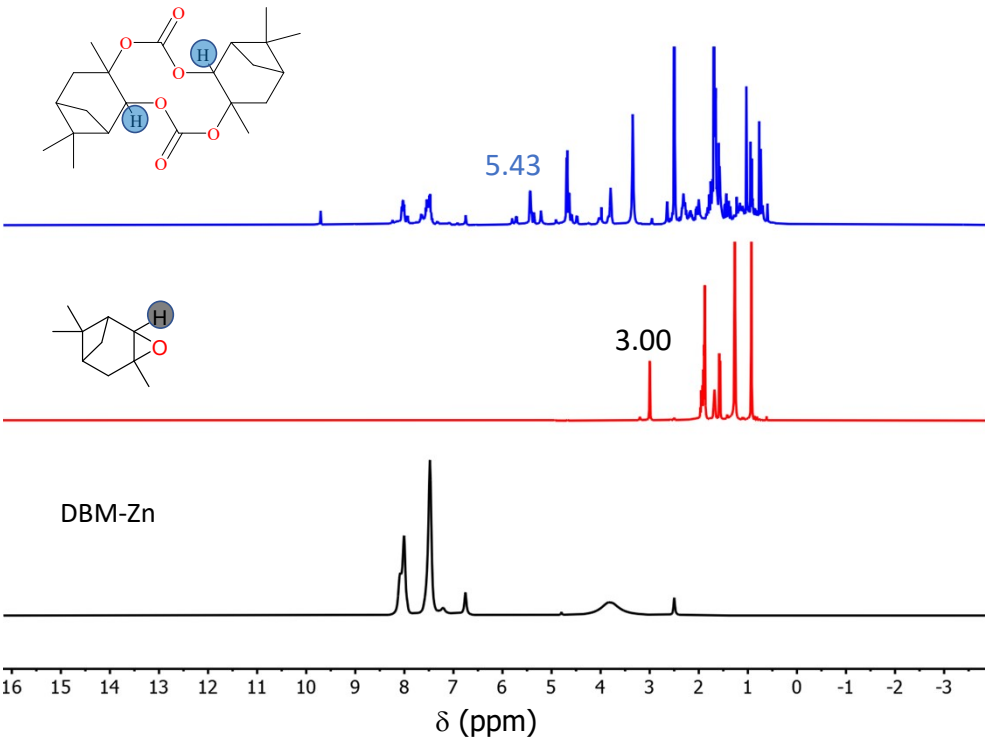


Figure S30. ^{1}H NMR spectra (in DMSO-d_6) of **PiC** (blue trace), **PiO** (red trace) and Zn-**DBM** (black trace)

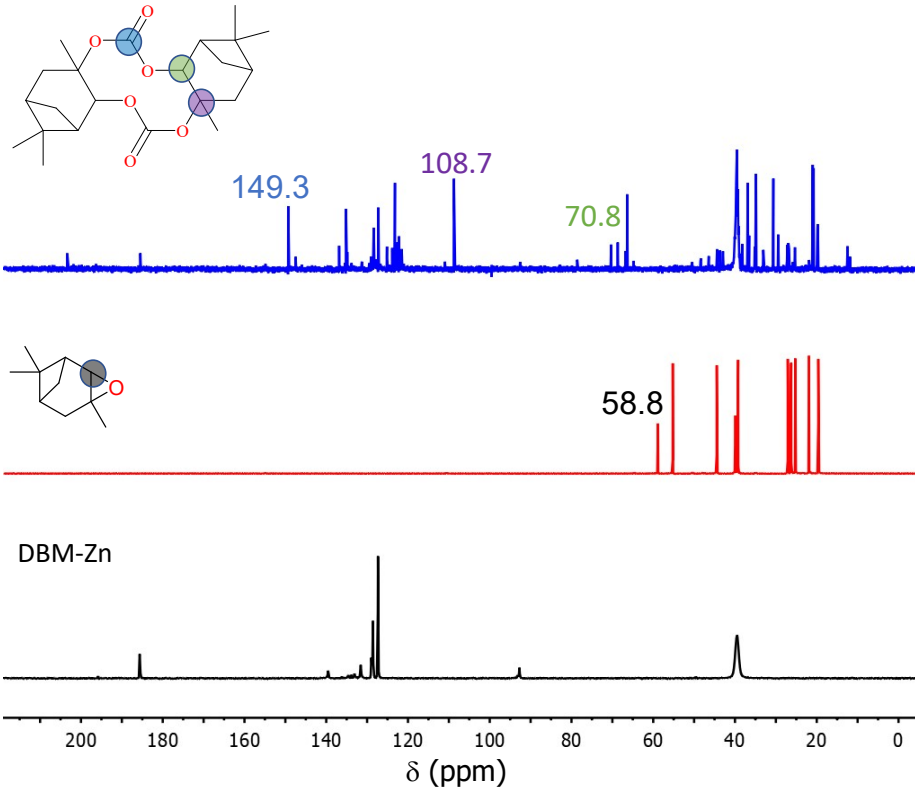


Figure S31. ^{13}C NMR spectra (in DMSO-d_6) of **PiC** (blue trace), **PiO** (red trace) and Zn-**DBM** (**black** trace)

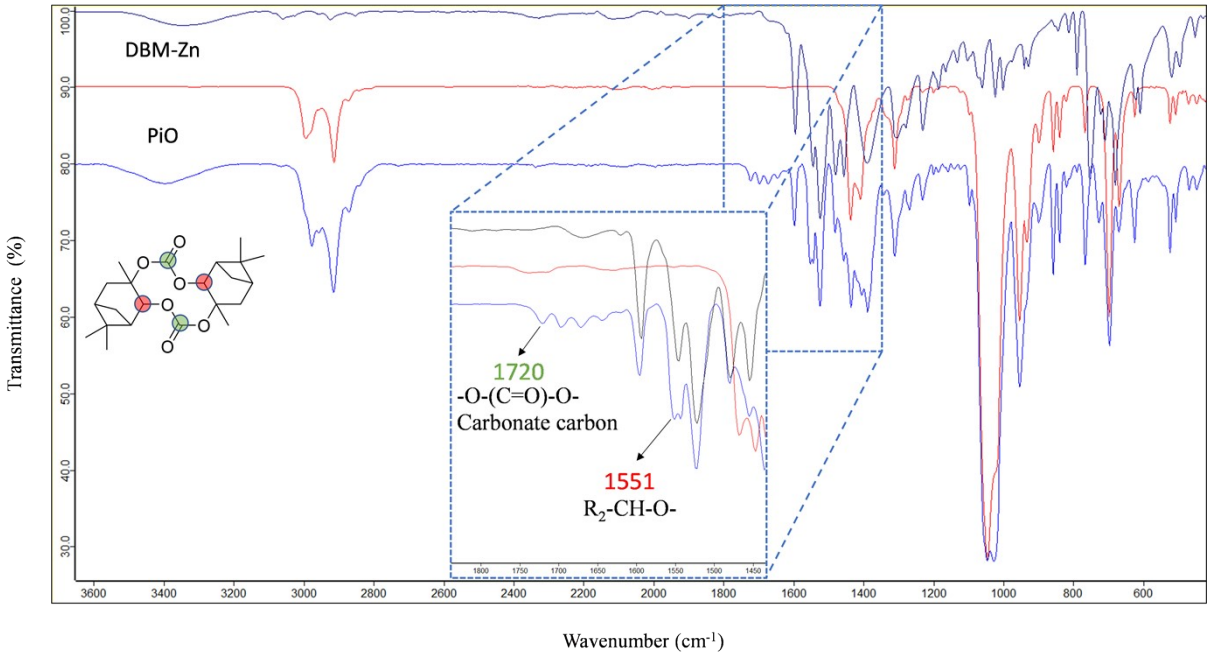
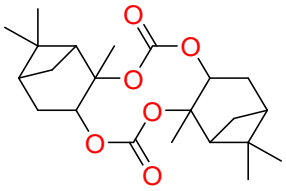


Figure S32. ATR-FTIR spectra (in DMSO) of **PiC** (blue trace), **PiO** (red trace) and solid Zn-**DBM** (**black** trace)

Table S1. High resolution mass spectrometry (**HRMS**) for Zn-DBM, PiC.

Molecule	Chemical formula	m/z (calc.)	m/z (found)
PiC	 $C_{22}H_{32}O_6$ = M	415.20966 $[M+Na]^+$	415.20911

Ionic Conductivity Measurements

Ionic conductivity measurements were conducted to verify the presence of free ions in solution upon complexation. While the conductivity of the zinc precursor and **DBM** dissolved in acetonitrile were 5.82 and 2.1 μS, respectively; the value was increased significantly up to 22.6 μS for Zn-**DBM**.

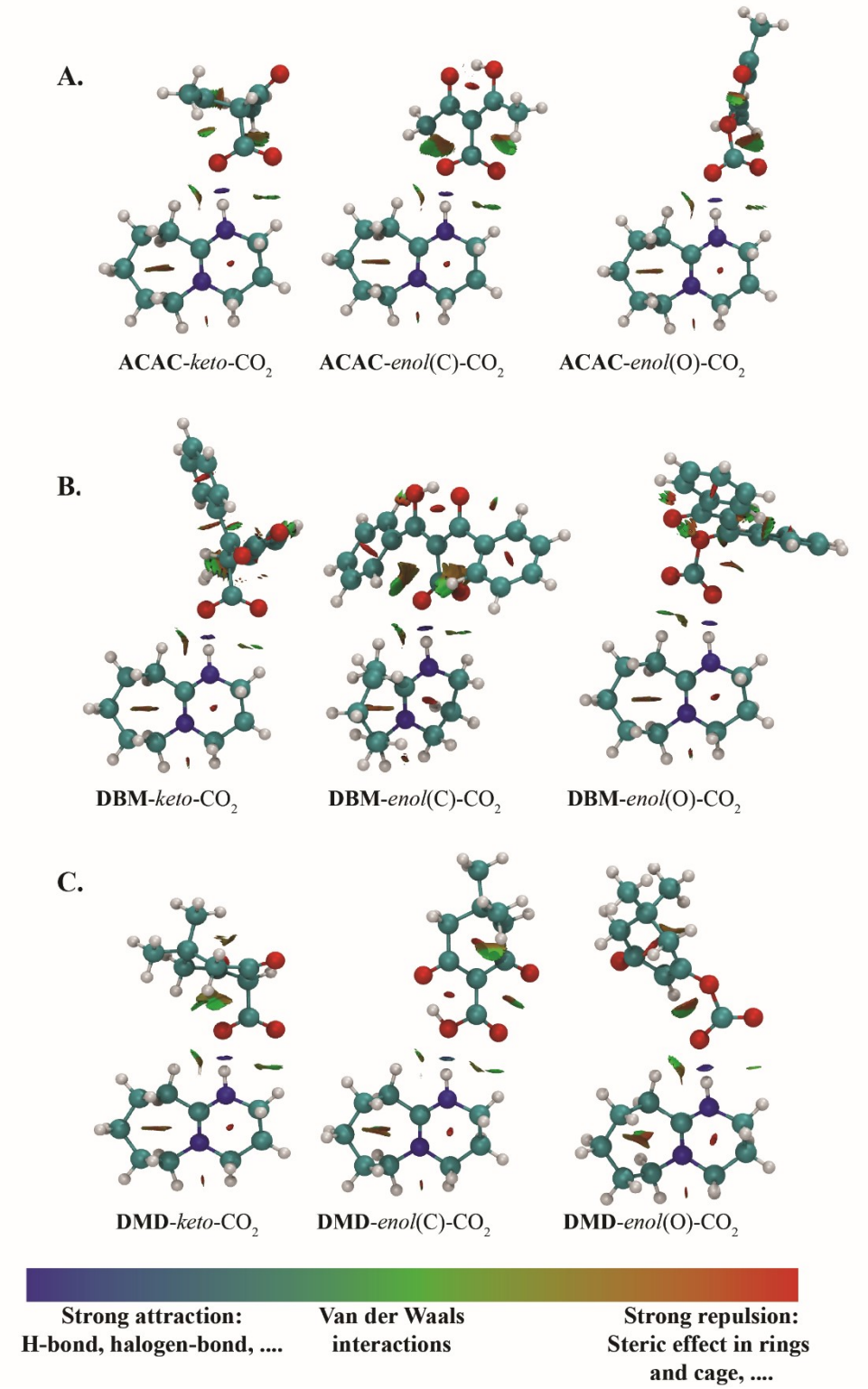


Figure S33. Gradient isosurface plots of different $[DBUH]^+$ $[diketone\text{-}CO_2]^-$ evidencing non-covalent interactions (NCI) obtained from the M06-2X/6-311++G** densities.

DFT-Optimized Coordinates

ACAC-*keto*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002991	0.000003902	-0.000015911
2	6	-0.000013906	-0.000009358	0.000004036
3	1	0.000004667	-0.000000897	0.000001385
4	1	-0.000000312	-0.000000659	-0.000005907
5	1	0.000004086	-0.000000023	-0.000003598
6	6	-0.000012697	-0.000000568	-0.000002605
7	6	0.000006493	0.000011864	0.000010694
8	1	0.000003488	0.000001208	0.000002062
9	1	-0.000003646	0.000004919	0.000000303
10	6	0.000001168	-0.000007521	0.000000706
11	1	0.000000986	0.000001298	0.000006469
12	1	0.000001553	-0.000000390	0.000005974
13	1	0.000002679	-0.000000888	0.000003209
14	8	0.000008072	0.000000397	-0.000003137
15	8	-0.000005622	-0.000003284	-0.000003680

ACAC-*enol*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000003476	0.000001581	-0.000001053
2	6	-0.000000434	-0.000001634	-0.000000451
3	1	-0.000000492	0.000001235	-0.000005068
4	1	-0.000000345	0.000001498	-0.000002518
5	1	-0.000002223	0.000000278	-0.000002880
6	6	-0.000000143	0.000000001	-0.000000005
7	6	0.000001126	0.000000271	0.000000182
8	6	-0.000001009	-0.000000866	0.000000962
9	1	-0.000000586	-0.000000844	0.000000704
10	1	-0.000000964	-0.000001760	0.000002891
11	1	0.000000661	0.000000216	0.000002558
12	8	0.000000408	0.000001413	0.000000434
13	8	0.000000271	-0.000001467	0.000003467
14	1	-0.000000594	-0.000000071	-0.000001618
15	1	0.000000848	0.000000148	0.000002394

DBM-*keto*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001218	0.000001320	0.000001872
2	6	0.000005094	-0.000002885	-0.000008797
3	6	0.000009108	0.000018560	-0.000007214
4	6	-0.000012842	0.000001706	0.000006244
5	6	0.000001312	-0.000007273	0.000003409
6	8	0.000001773	0.000005945	0.000000709
7	8	0.000002087	-0.000005349	-0.000002745
8	6	-0.000002571	0.000003786	-0.000002339
9	6	0.000002797	-0.000003401	-0.000005247
10	6	-0.000003437	-0.000001364	-0.000004122
11	6	0.000004247	0.000000184	-0.000000045
12	6	-0.000003144	-0.000005503	0.000002940
13	1	-0.000001612	-0.000004608	-0.000004558
14	1	-0.000001493	-0.000006758	-0.000003253
15	1	-0.000001393	-0.000003283	0.000000025

16	1	0.000000804	0.000002153	0.000001962
17	1	-0.000000713	0.000000890	0.000003062
18	6	-0.000000087	0.000003285	-0.000001491
19	6	-0.000000292	0.000000712	0.000002107
20	6	-0.000003556	-0.000001288	0.000003789
21	6	0.000001579	0.000002312	0.000002151
22	6	0.000000558	-0.000002458	0.000002073
23	1	0.000002402	0.000004103	-0.000002318
24	1	-0.000000942	-0.000000087	0.000003414
25	1	-0.000002258	-0.000002847	0.000005441
26	1	0.000000450	0.000001512	-0.000000439
27	1	-0.000002097	-0.000001265	0.000003965
28	1	0.000000627	0.000001072	0.000001757
29	1	0.000002380	0.000000829	-0.000002350

DBM-*enol*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002181	0.000007529	-0.000000307
2	6	-0.000020634	-0.000015056	0.000005183
3	6	0.000009400	-0.000003396	-0.000001702
4	6	0.000005481	0.000020677	0.000019480
5	6	-0.000013763	-0.000009163	-0.000007486
6	8	0.000006159	0.000004938	0.000001836
7	8	0.000007488	-0.000022214	-0.000003178
8	1	-0.000002162	-0.000000620	-0.000003942
9	1	-0.000008024	0.000007828	0.000006070
10	6	0.000001343	0.000017647	-0.000003572
11	6	-0.000000615	-0.000003516	0.000000580
12	6	0.000005892	0.000004641	0.000003502
13	6	-0.000004507	-0.000001568	-0.000002634
14	6	0.000007086	-0.000001739	-0.000001911
15	1	0.000002415	-0.000003660	0.000004005
16	1	-0.000005379	0.000001115	0.000000551
17	1	-0.000001934	-0.000001458	-0.000003155
18	1	0.000002059	-0.000006739	-0.000004222
19	1	-0.000002637	0.000003556	-0.000006256
20	6	0.000009903	-0.000000150	0.000002651
21	6	0.000016961	0.000008432	-0.000000925
22	6	-0.000005708	-0.000006571	-0.000003714
23	6	-0.000003789	0.000003605	0.000002254
24	6	-0.000000835	-0.000001758	-0.000002240
25	1	-0.000006532	-0.000004677	0.000005245
26	1	-0.000003184	-0.000000696	-0.000001864
27	1	0.000003076	0.000004013	-0.000004933
28	1	0.000003285	-0.000001754	0.000002147
29	1	0.000001338	0.000000756	-0.000001464

DMD-*keto*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004772	-0.000013902	-0.000008014
2	6	-0.000007767	-0.000007602	-0.000000854
3	6	-0.000003223	-0.000010383	0.000002086
4	1	-0.000004349	-0.000006536	0.000006301
5	1	-0.000002381	0.000015308	0.000009212
6	6	0.000005375	0.000023537	0.000004494
7	6	-0.000003031	0.000024732	-0.000001223
8	6	-0.000005084	-0.000000824	0.000013421
9	1	0.000004696	-0.000005871	-0.000008147
10	1	0.000012170	-0.000004456	0.000001250

11	1	0.000002381	-0.000005247	-0.000009015
12	1	-0.000007179	-0.000000901	-0.000009182
13	1	0.000002838	0.000001953	-0.000005453
14	1	0.000001504	0.000000173	-0.000001996
15	8	-0.000000728	-0.000003716	0.000002952
16	8	0.000000007	-0.000006265	0.000004166

DMD-*enol*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000096581	-0.000095910	0.000073086
2	6	0.000041520	0.000046466	0.000017156
3	6	0.000102761	0.000114992	-0.000070216
4	6	-0.000002642	-0.000010511	0.000016840
5	6	-0.000040669	-0.000003288	-0.000011156
6	6	0.000017850	-0.000014129	0.000011238
7	1	0.000002700	0.000019577	0.000000756
8	1	0.000005331	0.000001014	-0.000000090
9	1	0.000020767	-0.000016536	0.000002124
10	1	-0.000012221	-0.000012001	-0.000008981
11	1	-0.000009024	0.000005048	0.000017731
12	1	-0.000000343	0.000008117	0.000018043
13	8	-0.000018443	-0.000090274	0.000025201
14	8	-0.000007999	0.000010420	-0.000009843
15	1	0.000020603	0.000041551	-0.000041330
16	1	-0.000023610	-0.000004536	-0.000040558

ACAC-*keto*-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000177	0.000000056	0.000000722
2	6	0.000002672	-0.000001115	0.000003385
3	1	0.000000407	0.000000337	-0.000003008
4	1	0.000001730	0.000001463	-0.000002293
5	1	0.000001365	0.000000599	-0.000002838
6	6	-0.000007119	0.000006349	-0.000001415
7	6	-0.000009532	-0.000000003	-0.000003831
8	6	0.000014338	-0.000000165	0.000003074
9	1	0.000002496	-0.000001079	-0.000001173
10	6	-0.000000188	0.000001492	-0.000001041
11	1	-0.000000640	0.000003075	0.000000065
12	1	-0.000001564	0.000002778	0.000000084
13	1	-0.000000095	0.000002337	-0.000000389
14	8	0.000000171	0.000000028	-0.000005276
15	8	0.000005666	0.000004859	0.000002373
16	8	-0.000003491	0.000003762	-0.000001724
17	8	-0.000001411	-0.000005547	-0.000005669
18	6	0.000000152	-0.000001011	0.000000488
19	6	-0.000000851	-0.000000878	0.000000668
20	7	0.000003750	-0.000002252	0.000003437
21	1	-0.000000204	-0.000000305	0.000000683
22	1	-0.000000391	-0.000001070	0.000001264
23	6	-0.000003812	-0.000002904	0.000002310
24	6	0.000000739	-0.000001229	-0.000000324
25	1	0.000000489	-0.000001838	0.000000462
26	1	0.000000401	-0.000001593	0.000000453
27	6	-0.000001203	0.000000212	0.000002222
28	7	0.000006240	0.000004529	-0.000004746
29	6	-0.000002516	-0.000000631	0.000001337
30	1	-0.000000658	-0.000000884	0.000000999
31	1	-0.000000966	-0.000002074	0.000001032
32	6	0.000000896	-0.000003893	0.000002516

33	1	-0.000001007	-0.000000132	0.000001876
34	1	-0.000000988	-0.000001099	0.000002230
35	1	-0.000001557	-0.000000082	0.000001520
36	1	-0.000000732	-0.000001283	0.000001218
37	6	0.000000638	0.000000966	-0.000001307
38	6	0.000000215	-0.000000734	-0.000000204
39	1	0.000001182	-0.000001430	-0.000000616
40	1	0.000000568	-0.000000603	-0.000000457
41	1	0.000000116	-0.000000015	0.000000119
42	1	0.000000311	0.000000214	-0.000000355
43	1	0.000000973	-0.000000347	-0.000000998
44	1	0.000000909	-0.000001139	-0.000000313
45	1	-0.000007679	0.000002277	0.000003437

ACAC-*enol*(C)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000005653	-0.000004630	0.000010674
2	6	0.000006755	0.000006232	0.000010132
3	1	-0.000003005	-0.000006661	0.000008826
4	1	-0.000004522	-0.000005733	0.000015396
5	1	-0.000001682	-0.000000861	0.000011945
6	6	-0.000006116	-0.000003184	0.000005419
7	6	0.000002496	0.000003577	0.000008472
8	6	0.000002754	0.000009864	-0.000004205
9	1	0.000003162	0.000007678	-0.000002861
10	1	0.000004609	0.000011795	0.000001127
11	1	0.000002250	0.000007200	-0.000001169
12	8	-0.000006996	-0.000003100	0.000011994
13	8	-0.000000171	0.000008753	0.000004791
14	6	0.000009598	0.000015211	-0.000000870
15	1	-0.000000470	0.000005670	0.000011697
16	8	0.000000636	0.000001349	0.000001149
17	8	-0.000001675	-0.000008038	-0.000001198
18	6	-0.000000982	0.000000113	-0.000002804
19	6	0.000001266	-0.000007610	-0.000002382
20	7	-0.000002482	-0.000000596	-0.000007133
21	1	-0.000002622	-0.000007571	-0.000001240
22	1	-0.000000889	-0.000006722	-0.000006929
23	6	0.000003987	-0.000000088	-0.000001613
24	6	0.000000137	0.000000702	0.000004597
25	1	0.000001368	0.000002796	-0.000003608
26	1	-0.000000156	-0.000001756	-0.000001425
27	6	0.000002572	-0.000011237	-0.000009590
28	7	0.000001479	-0.000002690	-0.000004602
29	6	-0.000004941	-0.000001753	-0.000011991
30	1	-0.000000088	-0.000006227	-0.000012750
31	1	0.000001243	0.000000148	-0.000012545
32	6	0.000003864	0.000001414	-0.000012592
33	1	-0.000000648	-0.000008160	-0.000011331
34	1	0.000003365	-0.000004299	-0.000017028
35	1	-0.000000405	-0.000000362	-0.000008792
36	1	0.000001356	0.000004184	-0.000010793
37	6	-0.000001691	-0.000001850	0.000003405
38	6	-0.000000563	0.000002649	0.000005404
39	1	0.000000406	0.000004103	0.000005812
40	1	-0.000002375	-0.000002592	0.000006769
41	1	-0.000002337	-0.000005665	0.000004534
42	1	-0.000001396	-0.000000356	0.000004924
43	1	-0.000000579	0.000003151	0.000009340
44	1	0.000001248	0.000005557	0.000003273
45	1	-0.000002107	-0.000000405	-0.000000229

ACAC-*enol*(O)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001749	-0.000002070	-0.000001984
2	6	-0.000001251	-0.000004554	-0.000005286
3	1	-0.000000125	-0.000001202	-0.000003417
4	1	-0.000000603	-0.000002577	-0.000001561
5	1	0.000000371	-0.000000508	-0.000001293
6	6	-0.000000761	0.000003027	-0.000000580
7	6	0.000006112	0.000000741	0.000002647
8	6	0.000002875	0.000003164	-0.000005624
9	1	0.000001579	0.000003038	-0.000002596
10	1	0.000001259	0.000002459	-0.000001142
11	1	-0.000000069	0.000001410	-0.000003246
12	8	0.000002772	-0.000001693	-0.000000134
13	8	-0.000020369	0.000009765	0.000000155
14	1	0.000000650	0.000002198	-0.000003022
15	6	0.000016963	-0.000012527	-0.000000738
16	8	0.000000374	-0.000002551	-0.000002775
17	8	-0.000001438	0.000005219	-0.000002998
18	6	-0.000000888	-0.000001536	0.000003045
19	6	0.000001658	0.000001825	0.000003310
20	7	-0.000003475	0.000000139	-0.000000659
21	1	0.000001307	0.000002069	0.000002190
22	1	-0.000000121	0.000001183	0.000001881
23	6	0.000003497	0.000001739	-0.000000119
24	6	-0.000000341	0.000000507	0.000004596
25	1	-0.000000552	-0.000001442	0.000003547
26	1	0.000000279	-0.000000231	0.000004041
27	6	-0.000000613	-0.000001845	-0.000001741
28	7	-0.000006307	-0.000015035	0.000007467
29	6	0.000007230	0.000000513	-0.000002830
30	1	-0.000000018	-0.000000388	-0.000001410
31	1	0.000000312	-0.000001734	-0.000000901
32	6	-0.000001203	0.000010939	-0.000003818
33	1	-0.000000589	0.000001041	-0.000003103
34	1	-0.000002739	-0.000001780	-0.000002909
35	1	-0.000000120	-0.000002862	-0.000004358
36	1	-0.000000872	-0.000003555	-0.000002031
37	6	-0.000000181	0.000000019	-0.000000902
38	6	-0.000000120	0.000000403	0.000005458
39	1	0.000000297	-0.000001021	0.000006039
40	1	0.000000259	0.000001472	0.000005502
41	1	0.000000010	0.000002139	0.000003242
42	1	0.000000215	0.000000744	0.000001055
43	1	-0.000000103	0.000000400	0.000005874
44	1	-0.000000374	-0.000000964	0.000003731
45	1	-0.000003041	0.000003924	-0.000002604

DBM-*keto*-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001604	0.000001047	-0.000001641
2	6	-0.000000662	0.000000278	0.000001550
3	6	0.000011409	0.000003594	0.000000182
4	6	-0.000007376	-0.000001462	-0.000008630
5	6	0.000000527	0.000000775	0.000002831
6	8	-0.000000663	0.000002329	-0.000001808
7	8	-0.000000944	0.000002337	0.000002852
8	6	0.000001114	0.000000862	-0.000001949
9	6	0.000001455	0.000000813	-0.000001039
10	6	0.000001155	0.000000844	-0.000001207
11	6	0.000001057	-0.000000250	-0.000000732
12	6	0.000001342	0.000000702	-0.000000530
13	1	0.000000688	0.000001531	-0.000000967

14	1	0.000001672	0.000001088	-0.000001202
15	1	0.000001632	0.000000517	-0.000001019
16	1	0.000000396	0.000000335	0.000000339
17	1	0.000000915	0.000000266	-0.000000638
18	6	-0.000000450	0.000002828	0.000000582
19	6	0.000000047	0.000000723	-0.000000603
20	6	-0.000002005	-0.000000504	-0.000000209
21	6	-0.000001713	0.000001426	-0.000001002
22	6	0.000000529	0.000002344	0.000000061
23	1	-0.000001957	0.000001779	-0.000001387
24	1	-0.000001179	-0.000000480	0.000000961
25	1	0.000000291	0.000000577	0.000000542
26	1	-0.000000941	0.000002955	-0.000000692
27	1	-0.000000756	0.000002004	-0.000000454
28	1	-0.000001940	0.000004010	0.000000691
29	6	0.000004512	0.000002116	0.000009086
30	8	-0.000007020	-0.000004986	-0.000004019
31	8	-0.000003751	-0.000003192	-0.000004795
32	6	-0.000001367	-0.000002010	0.000000094
33	6	-0.000001352	-0.000000193	0.000001878
34	7	0.000002229	-0.000002333	0.000002245
35	1	0.000000591	-0.000001838	0.000000719
36	1	-0.000000034	-0.000002087	0.000000478
37	6	-0.000000360	0.000003898	-0.000002377
38	6	0.000000391	-0.000001145	0.000001469
39	1	-0.000000216	-0.000001475	0.000000581
40	1	-0.000000330	-0.000002008	0.000001132
41	6	-0.000001768	-0.000000459	-0.000001877
42	7	-0.000002344	-0.000007503	0.000001709
43	6	-0.000000285	0.000000165	-0.000000297
44	1	-0.000000025	-0.000001350	0.000000983
45	1	-0.000000234	-0.000001314	0.000000887
46	6	-0.000001029	-0.000001060	0.000009543
47	1	0.000000323	-0.000000871	0.000000501
48	1	0.000000192	-0.000000828	-0.000000096
49	1	0.000002540	0.000001116	-0.000002470
50	1	0.000000645	0.000001389	-0.000002350
51	6	-0.000000221	-0.000001423	-0.000000216
52	6	-0.000000230	-0.000000776	0.000000070
53	1	-0.000000439	-0.000001359	0.000001031
54	1	-0.000000099	-0.000002152	0.000000549
55	1	0.000000289	-0.000000907	0.000000990
56	1	0.000001090	-0.000001012	0.000000454
57	1	0.000000160	-0.000001000	0.000001221
58	1	-0.000001059	-0.000000928	0.000000744
59	1	0.000007163	0.000002258	-0.000002746

DBM-*enol*(C)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000014875	0.000006505	-0.000002460
2	6	-0.000006758	-0.000017759	0.000001370
3	6	0.000004404	-0.000005629	-0.000009644
4	6	0.000008877	0.000023085	0.000007574
5	6	0.000001029	-0.000010049	0.000003584
6	8	0.000013678	0.000006775	0.000028121
7	8	-0.000000190	-0.000034910	0.000025858
8	6	-0.000040438	0.000020211	-0.000007080
9	1	-0.000003865	0.000012768	-0.000054440
10	6	-0.000000369	0.000000342	-0.000001439
11	6	0.000001828	-0.000002736	-0.000001095
12	6	-0.000000122	0.000000192	-0.000000987
13	6	0.000000297	-0.000001249	0.000001818
14	6	-0.000001662	-0.000000203	-0.000000251
15	1	0.000000968	-0.000003713	0.000000873

16	1	-0.000000555	-0.000004103	0.000000009
17	1	-0.000001454	-0.000001125	-0.000000067
18	1	0.000001202	0.000000458	-0.000001391
19	1	-0.000000568	0.000000665	0.000000967
20	6	0.000000277	-0.000003662	0.000004173
21	6	-0.000002542	-0.000003279	-0.000000549
22	6	0.000001627	-0.000000692	0.000002750
23	6	0.000002824	-0.000001444	0.000000076
24	6	0.000005274	-0.000000822	0.000000495
25	1	0.000005339	-0.000000999	0.000001031
26	1	0.000003248	0.000000273	-0.000001028
27	1	0.000003662	0.000002134	-0.000001052
28	1	0.000003921	-0.000002819	0.000001306
29	1	0.000003963	-0.000000495	0.000000403
30	8	0.000076885	0.000020328	-0.000225904
31	8	0.000018001	-0.000014785	0.000004711
32	6	-0.000005178	0.000003867	-0.000002389
33	6	0.000000165	0.000003525	0.000002419
34	7	-0.000015717	-0.000005597	-0.000001442
35	1	-0.000002949	0.000001947	-0.000003859
36	1	-0.000005418	0.000002297	-0.000001932
37	6	0.000023903	0.000008320	0.000001973
38	6	-0.000000173	0.000003692	-0.000000554
39	1	-0.000001865	0.000002138	0.000003110
40	1	-0.000000800	0.000004951	-0.000001056
41	6	0.000002020	-0.000002812	0.000000794
42	7	0.000049414	0.000061052	-0.000376005
43	6	-0.000008189	0.000001101	0.000000335
44	1	-0.000004858	0.000003389	-0.000002776
45	1	-0.000001817	0.000002605	0.000003140
46	6	0.000010776	-0.000006327	-0.000010805
47	1	-0.000004237	0.000000230	-0.000001405
48	1	-0.000004178	-0.000000752	0.000003186
49	1	-0.000008991	0.000003813	0.000006438
50	1	-0.000000980	0.000000975	0.000007102
51	6	-0.000008130	0.000002144	0.000001120
52	6	-0.000000440	0.000002580	-0.000000762
53	1	0.000001192	0.000003376	0.000000419
54	1	-0.000001733	0.000004550	-0.000004316
55	1	0.000000430	0.000002803	-0.000005396
56	1	-0.000001363	-0.000000389	-0.000000132
57	1	0.000000315	0.000002551	-0.000001697
58	1	-0.000001330	0.000001737	0.000002792
59	1	-0.000123521	-0.000091030	0.000603963

DBM-*enol*(O)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002746	0.000001891	-0.000002063
2	6	-0.000001884	-0.000000291	-0.000001606
3	6	0.000002504	-0.000001176	-0.000000113
4	6	-0.000001354	0.000006629	-0.000005057
5	6	-0.000000433	-0.000002036	0.000001586
6	8	0.000001332	0.000001640	-0.000001048
7	8	0.000005259	-0.000007818	0.000002869
8	1	0.000000830	0.000000726	-0.000000725
9	6	0.000001337	0.000001163	0.000000490
10	6	-0.000000561	-0.000000810	0.000000157
11	6	-0.000000156	-0.000000205	0.000000952
12	6	-0.000000125	-0.000000859	0.000000226
13	6	0.000000507	-0.000001451	0.000001968
14	1	-0.000000778	-0.000001384	-0.000002023
15	1	-0.000000809	-0.000001147	0.000001090
16	1	0.000000215	-0.000000906	0.000001551
17	1	0.000001185	0.000000036	0.000000296

18	1	0.000001382	-0.000000414	0.000001331
19	6	-0.000000554	0.000001812	-0.000002207
20	6	0.000001171	0.000001059	-0.000000319
21	6	0.000001402	0.000001783	-0.000001877
22	6	0.000001513	0.000001615	-0.000001854
23	6	0.000002323	0.000002415	-0.000002619
24	1	0.000000425	0.000001836	-0.000002414
25	1	0.000001654	0.000001271	-0.000001038
26	1	0.000002570	0.000001732	-0.000001297
27	1	0.000001186	0.000002360	-0.000002969
28	1	0.000002214	0.000002398	-0.000002301
29	6	-0.000012166	0.000007358	0.000000161
30	8	0.000000632	-0.000001697	-0.000000481
31	8	0.000005240	-0.000003824	-0.000001240
32	6	-0.000000814	-0.000000797	0.000000218
33	6	-0.000001191	-0.000000644	0.000000599
34	7	0.000000898	-0.000001189	0.000000988
35	1	-0.000001526	-0.000001195	0.000000872
36	1	-0.000000599	-0.000001152	0.000001382
37	6	-0.000001587	0.000001356	-0.000000398
38	6	-0.000001394	-0.000000242	-0.000000174
39	1	-0.000000553	-0.000000261	0.000000243
40	1	-0.000001356	-0.000000692	0.000000246
41	6	-0.000000863	-0.000001652	0.000001793
42	7	0.000000915	-0.000003036	0.000000438
43	6	0.000000183	-0.000000453	0.000001490
44	1	0.000000084	-0.000001071	0.000001540
45	1	0.000000409	-0.000000660	0.000001030
46	6	0.000000865	-0.000000621	0.000000588
47	1	0.000000078	-0.000001257	0.000001763
48	1	0.000000923	-0.000000987	0.000001793
49	1	0.000000619	-0.000000709	0.000001330
50	1	0.000000665	-0.000000318	0.000001017
51	6	-0.000002175	0.000001174	-0.000003206
52	6	-0.000001111	0.000000102	-0.000000209
53	1	-0.000001493	-0.000000036	-0.000000567
54	1	-0.000001902	-0.000000481	-0.000000146
55	1	-0.000001595	-0.000000637	0.000000584
56	1	-0.000000988	-0.000003335	0.000005934
57	1	-0.000001563	-0.000000111	-0.000000623
58	1	-0.000000828	0.000000063	-0.000000371
59	1	-0.000002908	0.000005137	0.000002421

DMD-*keto*-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000021535	-0.000010104	0.000003243
2	6	0.000004590	0.000011490	0.000007727
3	6	-0.000015381	0.000003471	-0.000002805
4	1	-0.000002371	0.000003781	0.000005511
5	6	-0.000026120	-0.000014391	0.000010918
6	6	0.000006196	-0.000003253	0.000002991
7	6	-0.000001921	0.000004079	0.000000162
8	6	-0.000002116	-0.000002804	-0.000004086
9	1	0.000000784	0.000003685	-0.000002818
10	1	-0.000000025	0.000001022	-0.000002341
11	1	-0.000000230	-0.000003865	0.000000077
12	1	0.000000640	-0.000000333	0.000001478
13	6	-0.000005067	0.000006781	-0.000005329
14	6	-0.000002899	0.000003981	-0.000002669
15	8	0.000002134	0.000001055	0.000006128
16	8	-0.000001005	0.000006175	-0.000003125
17	8	0.000001312	0.000006846	0.000004154
18	8	0.000020921	0.000009811	-0.000002915
19	6	0.000000840	-0.000002120	-0.000004289

20	6	-0.000002176	-0.000002595	-0.000001907
21	7	0.000004954	-0.000000903	0.000002775
22	1	0.000001042	0.000002208	-0.000001894
23	1	-0.000000106	-0.000001149	-0.000000157
24	6	-0.000004146	0.000000174	-0.000003744
25	6	0.000000325	-0.000000747	-0.000004926
26	1	0.000000062	-0.000003273	-0.000003217
27	1	0.000000897	-0.000002438	-0.000004066
28	6	-0.000002161	0.000000522	0.000002412
29	7	0.000007805	-0.000005775	0.000006574
30	6	0.000000326	-0.000001083	0.000005041
31	1	-0.000000300	-0.000001145	0.000003548
32	1	-0.000000600	-0.000004069	0.000002922
33	6	-0.000002188	0.000003521	0.000006973
34	1	-0.000000955	0.000000786	0.000005605
35	1	-0.000001377	-0.000002198	0.000006824
36	1	-0.000003131	0.000000136	0.000004425
37	1	-0.000001250	-0.000003932	0.000003477
38	6	0.000001548	-0.000002433	-0.000000567
39	6	0.000002005	-0.000001058	-0.000004853
40	1	0.000000749	-0.000002749	-0.000006823
41	1	0.000001273	0.000000566	-0.000006080
42	1	-0.000000593	0.000003370	-0.000002253
43	1	0.000000277	0.000001903	-0.000000819
44	1	0.000000780	-0.000000270	-0.000005928
45	1	0.000000183	-0.000002886	-0.000003629
46	1	-0.000017508	0.000002748	0.000002479
47	1	0.000000188	-0.000004669	-0.000003057
48	1	0.000002182	-0.000003712	-0.000004115
49	1	0.000002335	-0.000001189	-0.000004624
50	1	0.000001284	0.000001894	-0.000000401
51	1	0.000003796	0.000003407	-0.000002354
52	1	0.000002661	0.000001729	0.000000344

DMD-*enol*(C)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000004894	-0.000004311	-0.000003102
2	6	0.000001192	0.000007981	0.000007595
3	6	-0.000000134	0.000002041	-0.000006006
4	6	0.000000435	0.000004480	-0.000002749
5	6	-0.000001452	0.000002692	0.000000502
6	6	-0.000007807	-0.000001635	0.000007734
7	1	0.000001057	-0.000000606	0.000000229
8	1	0.000000381	-0.000003713	-0.000001569
9	1	0.000001073	0.000001398	-0.000005333
10	1	0.000000313	-0.000001709	-0.000003856
11	6	0.000002283	-0.000001469	0.000005497
12	6	-0.000000575	0.000005078	-0.000006657
13	8	0.000005654	0.000002627	0.000002004
14	8	0.000001187	-0.000008492	-0.000002520
15	6	0.000014397	0.000008049	0.000004140
16	1	-0.000009926	0.000001864	-0.000004898
17	8	-0.000001590	-0.000003583	-0.000000233
18	8	-0.000016085	0.000005066	0.000004244
19	6	-0.000000670	-0.000000661	-0.000000924
20	6	0.000001767	-0.000001321	0.000000848
21	7	-0.000004731	0.000000558	0.000002546
22	1	-0.000000317	-0.000003130	0.000000634
23	1	0.000000311	-0.000001998	0.000001773
24	6	0.000006453	0.000002668	0.000003421
25	6	0.000000675	-0.000000697	-0.000001965
26	1	-0.000000078	0.000000677	-0.000000040
27	1	0.000000114	-0.000000819	-0.000000656
28	6	0.000000170	-0.000001901	0.000003150

29	7	-0.000008480	-0.000002890	0.000000101
30	6	0.000001024	-0.000000430	0.000004230
31	1	-0.000000094	-0.000001104	0.000003605
32	1	-0.000000159	0.000001339	0.000003190
33	6	-0.000002931	0.000002267	0.000004407
34	1	-0.000000494	-0.000001539	0.000004714
35	1	-0.000000241	0.000000243	0.000005516
36	1	0.000000034	0.000000028	0.000002929
37	1	-0.000000144	0.000002472	0.000002833
38	6	-0.000000053	-0.000001233	-0.000001646
39	6	0.000000274	-0.000000836	-0.000001801
40	1	0.000000001	0.000000288	-0.000002965
41	1	0.000000416	-0.000002023	-0.000002478
42	1	0.000000704	-0.000002052	-0.000001260
43	1	0.000000139	-0.000001156	-0.000000980
44	1	0.000000150	-0.000000650	-0.000003691
45	1	-0.000000094	0.000000971	-0.000001715
46	1	0.000017843	-0.000011666	0.000000437
47	1	0.000002613	0.000004622	-0.000007436
48	1	0.000002330	-0.000003025	-0.000000306
49	1	0.000000326	-0.000001864	-0.000004742
50	1	0.000001681	0.000004921	-0.000002239
51	1	-0.000000439	0.000000402	-0.000001510
52	1	-0.000003611	0.000003783	-0.000003004

DMD-*enol*(O)-CO_2/DBUH

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000004532	-0.000004885	-0.000002893
2	6	0.000003199	0.000009541	-0.000000780
3	6	0.000001208	0.000006913	0.000008810
4	6	0.000003487	0.000009012	-0.000001589
5	6	-0.000002319	0.000001766	-0.000004272
6	6	0.000013757	-0.000054242	-0.000075947
7	1	0.000000319	-0.000000464	-0.000002068
8	1	-0.000000480	-0.000001020	-0.000000919
9	1	-0.000000621	0.000000593	-0.000000418
10	1	0.000000376	0.000000476	-0.000000473
11	6	-0.000044877	0.000032489	0.000049805
12	6	0.000013494	0.000010167	0.000024126
13	8	-0.000000844	0.000001682	0.000000748
14	8	-0.000001555	-0.000003551	-0.000001162
15	1	-0.000000129	-0.000000857	-0.000001195
16	6	-0.000007195	-0.000000659	0.000004957
17	8	0.000005572	-0.000006276	0.000003252
18	8	0.000001026	0.000000043	0.000001869
19	6	0.000000065	-0.000000330	-0.000002767
20	6	-0.000002259	-0.000000396	0.000002347
21	7	0.000003921	-0.000003617	-0.000001130
22	1	0.000000727	-0.000002768	-0.000001273
23	1	0.000000571	-0.000000748	0.000000597
24	6	0.000001259	0.000003199	-0.000006673
25	6	0.000001133	0.000001488	-0.000001537
26	1	0.000000425	0.000000073	-0.000000774
27	1	0.000000450	-0.000000100	-0.000001868
28	6	-0.000002915	0.000001272	0.000001215
29	7	-0.000005146	-0.000012274	0.000015609
30	6	0.000000350	-0.000000078	0.000001252
31	1	-0.000000289	-0.000002537	0.000001851
32	1	-0.000000486	-0.000000831	0.000002020
33	6	0.000004742	-0.000003734	0.000000766
34	1	-0.000000272	-0.000001675	0.000002626
35	1	-0.000000629	-0.000000815	0.000003556
36	1	0.000000252	-0.000000632	0.000003113
37	1	-0.000000616	0.000000866	0.000002145

38	6	-0.000001599	-0.000001109	-0.000003910
39	6	-0.000002912	0.000000767	0.000000849
40	1	0.000000874	0.000000623	-0.000002935
41	1	0.000000705	-0.000000169	-0.000002373
42	1	0.000001906	-0.000001890	-0.000000724
43	1	0.000000739	-0.000000413	0.000000406
44	1	0.000000810	0.000000796	-0.000001645
45	1	-0.000000035	0.000001289	-0.000000615
46	1	-0.000002120	0.000013069	-0.000004245
47	1	-0.000000531	0.000007758	0.000007707
48	1	-0.000000608	0.000004831	0.000009116
49	1	0.000005105	0.000006173	0.000009808
50	1	0.000008733	-0.000006264	-0.000008826
51	1	0.000007091	0.000000777	-0.000008749
52	1	0.000000671	-0.000003330	-0.000016790
