

Electronic Supporting Information

Density Functional Theory modelling of protection agents for carbonate stones: case study of oxalate and oxamate inorganic salts

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Figure S1. Isosurface of selected virtual Kohn-Sham Molecular Orbitals calculated for MeOx⁻ (LUMO) and MeOxam⁻ (LUMO+1) at the optimised geometries at DFT level (functional PBE0, Basis Set def2-SVP). Cutoff value = 0.100 |e|.

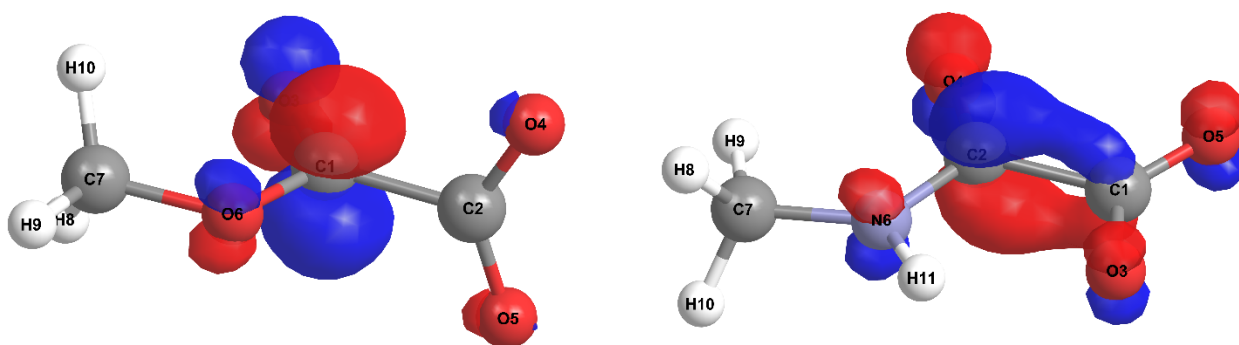


Table S1. DFT-Optimised geometry calculated in the gas phase for Ox^{2-} in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	0.78032	0.00011	-0.00016
C	-0.78038	-0.00004	-0.00020
O	1.35200	0.55880	0.97410
O	-1.35180	-0.97446	0.55846
O	-1.35306	0.97382	-0.55839
O	1.35291	-0.55821	-0.97390

Table S2. DFT-Optimised geometry calculated in the gas phase for Oxam⁻ in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	-0.86073	-0.00561	0.00071
C	0.70873	0.20458	-0.00121
O	-1.19485	-1.2116	0.09953
O	1.29262	1.26813	0.08696
O	-1.54875	1.01123	-0.08654
N	1.35085	-0.98894	-0.12333
H	2.33663	-1.03612	0.06615
H	0.72729	-1.77717	0.00059

Table S3. DFT-Optimised geometry calculated in the gas phase for MeOx⁻ in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	-0.1719	0.33700	-0.00035
C	1.30861	-0.09767	0.00012
O	-0.60734	1.46383	-0.0021
O	1.79302	-0.23275	1.13314
O	1.79218	-0.23665	-1.13279
O	-1.01132	-0.73533	0.00122
C	-2.38581	-0.41377	0.00067
H	-2.65833	0.16756	-0.88468
H	-2.92106	-1.36437	0.00233
H	-2.65832	0.17072	0.88393

Table S4. DFT-Optimised geometry calculated in the gas phase for MeOxam[−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	-1.30089	-0.19427	0.00000
C	0.15015	0.43820	-0.00001
O	-1.29190	-1.45056	0.00002
O	0.42002	1.62744	0.00001
O	-2.24295	0.59689	-0.00001
N	1.08785	-0.54153	-0.00003
C	2.49140	-0.29531	0.00001
H	2.98801	-0.71008	-0.88707
H	2.63013	0.78858	-0.00010
H	2.98795	-0.70991	0.88722
H	0.65362	-1.45964	-0.00006

Table S5. DFT-Optimised geometry calculated in the gas phase for PhOx[−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	1.46207	-0.27975	0.33797
C	2.87774	0.12335	-0.12309
O	1.14497	-1.09548	1.15649
O	3.40151	1.01562	0.55416
O	3.26773	-0.52823	-1.10180
O	0.50590	0.46229	-0.35692
C	-0.82208	0.22175	-0.18507
C	-1.65072	1.33002	-0.05124
C	-1.37376	-1.05579	-0.21679
C	-3.02366	1.16648	0.04297
H	-1.19460	2.31281	-0.02844
C	-2.74777	-1.20732	-0.11467
H	-0.72325	-1.91316	-0.31671
C	-3.58099	-0.10413	0.01556
H	-3.66088	2.03923	0.14208
H	-3.17230	-2.20570	-0.13923
H	-4.65485	-0.23445	0.09305

Table S6. DFT-Optimised geometry calculated in the gas phase for PhOxam[−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-TZVP).

C	-2.89851	0.28825	0.00014
C	-1.53037	-0.50875	-0.00010
O	-3.92146	-0.38976	0.00005
O	-1.40338	-1.71512	-0.00013
O	-2.73680	1.53505	0.00038
N	-0.49269	0.39155	-0.00034
C	0.86595	0.19208	-0.00035
C	1.70785	1.31387	-0.00027
C	1.45352	-1.08106	-0.00002
C	3.08283	1.17120	0.00004
H	1.26094	2.30292	-0.00048
C	2.83323	-1.20498	0.00024
H	0.80410	-1.94518	-0.00009
C	3.66270	-0.09139	0.00025
H	3.70892	2.05801	0.00007
H	3.26808	-2.19984	0.00046
H	4.74119	-0.20393	0.00045
H	-0.90444	1.33058	-0.00006

Table S7. DFT-Optimised geometry calculated for [Ox·calcite]²⁻ in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	1.01098	2.54980	1.29226
C	-2.68861	6.99386	-1.50708
C	0.20855	7.47383	1.27840
C	1.81344	-2.37422	1.30612
C	-0.28131	-7.77822	-1.46549
C	2.61585	-7.29825	1.31998
C	-1.08374	-2.85419	-1.47935
C	-1.88618	2.06984	-1.49322
C	3.36894	5.45715	-0.24745
C	5.72691	8.36449	-1.78716
C	8.62406	8.84446	0.99832
C	4.17138	0.53312	-0.23359
C	7.33177	-1.48356	-1.75944
C	11.03136	-5.92762	1.03990
C	4.97381	-4.39091	-0.21973
C	8.13421	-6.40759	-1.74558
C	6.52934	3.44047	-1.77330
C	9.42649	3.92043	1.01218
C	-3.44173	-5.76154	0.06038
C	-5.79967	-8.66888	1.60007
C	-4.24414	-0.83752	0.04648
C	-7.40453	1.17918	1.57235
C	-11.10412	5.62323	-1.22699
C	-5.04656	4.08653	0.03264
C	-8.20697	6.10320	1.55849
C	-6.60210	-3.74485	1.58621
C	-8.69682	-9.14885	-1.18541
C	-10.30169	0.69920	-1.21313
C	-9.49926	-4.22482	-1.19927
C	10.22893	-1.00359	1.02604
C	-1.65909	-0.41025	2.78649
C	-2.01100	0.57134	3.95973
Ca	-0.83881	4.77183	-0.10740
Ca	-1.64125	9.69586	-0.12126
Ca	-0.03649	-0.15222	-0.09350
Ca	0.76604	-5.07624	-0.07967
Ca	1.56849	-10.00024	-0.06582
Ca	2.32159	2.75514	-1.63326
Ca	4.41631	8.15914	1.13836
Ca	6.77427	11.06649	-0.40135
Ca	6.02117	-1.68891	1.16608
Ca	9.18157	-3.70559	-0.35977
Ca	3.12404	-2.16884	-1.61939
Ca	6.82361	-6.61292	1.17994

Ca	9.98400	-8.62962	-0.34591
Ca	5.21873	3.23512	1.15222
Ca	7.57670	6.14246	-0.38749
Ca	-2.39437	-3.05934	1.44614
Ca	-4.48906	-8.46353	-1.32545
Ca	-6.09393	1.38451	-1.35318
Ca	-9.25433	3.40120	0.17268
Ca	-3.19665	1.86434	1.43221
Ca	-6.89637	6.30855	-1.36703
Ca	-10.05676	8.32523	0.15882
Ca	-5.29147	-3.53948	-1.33934
Ca	-7.64946	-6.44685	0.20040
Ca	-3.99921	6.78852	1.41845
Ca	-8.45190	-1.52283	0.18654
Ca	-1.59190	-7.98356	1.46003
Ca	3.92644	-7.09293	-1.60553
Ca	8.37913	1.21844	-0.37363
Ca	1.51914	7.67918	-1.64711
O	0.00048	8.75058	1.27481
O	2.75568	-7.92764	2.44147
O	-0.87568	-4.13096	-1.47576
O	-2.02601	2.69923	-2.61470
O	1.07920	1.90245	0.17437
O	1.15081	1.92041	2.41375
O	8.55583	9.49182	2.11621
O	0.80292	3.82655	1.28866
O	11.23943	-7.20437	1.04349
O	4.03154	1.16251	-1.35507
O	4.37944	-0.74364	-0.22999
O	4.10315	1.18048	0.88431
O	9.35827	4.56780	2.13007
O	1.60533	-1.09748	1.30253
O	1.88163	-3.02159	0.18821
O	1.95324	-3.00361	2.42761
O	-1.15197	-2.20684	-0.36147
O	-1.22358	-2.22480	-2.60084
O	-5.59160	-9.94563	1.60366
O	-11.31219	6.89998	-1.23058
O	-4.17591	-1.48487	-1.07139
O	-4.45222	0.43924	0.04292
O	-4.10428	-1.46687	1.16798
O	-8.62859	-9.79621	-2.30330
O	-1.67812	0.79307	-1.48962
O	-1.95439	2.71720	-0.37531
O	-2.48055	5.71711	-1.50347
O	-2.75684	7.64122	-0.38918
O	-2.82844	7.62325	-2.62856

O	-4.97834	3.43915	-1.08526
O	-4.90677	3.45711	1.15419
O	-5.25464	5.36327	0.02904
O	-7.19647	-0.09758	1.57594
O	-7.54437	1.80856	0.45086
O	-7.47276	1.82654	2.69024
O	-10.50975	1.97596	-1.21672
O	-9.43102	-4.87218	-2.31716
O	-3.64975	-4.48478	0.05675
O	-3.37348	-6.40890	-1.05754
O	-3.30187	-6.39093	1.18185
O	-0.34953	-7.13086	-0.34758
O	-0.42114	-7.14883	-2.58698
O	-0.07324	-9.05497	-1.46190
O	2.40779	-6.02149	1.31639
O	2.68409	-7.94560	0.20210
O	4.90558	-3.74354	0.89817
O	4.83398	-3.76151	-1.34122
O	5.18187	-5.66765	-0.21614
O	7.12371	-0.20681	-1.76303
O	7.47161	-2.11295	-0.63795
O	7.40000	-2.13092	-2.87733
O	10.43699	-2.28034	1.02963
O	3.57700	4.18040	-0.24385
O	3.30071	6.10451	0.87045
O	3.22911	6.08653	-1.36894
O	0.27677	6.82647	0.16051
O	0.34838	6.84444	2.39989
O	6.66917	2.81107	-0.65181
O	6.59757	2.79310	-2.89119
O	6.32128	4.71722	-1.77689
O	9.63456	2.64368	1.01577
O	9.28666	4.54983	-0.10931
O	5.86674	7.73510	-0.66567
O	5.79514	7.71713	-2.90505
O	5.51884	9.64124	-1.79075
O	8.83212	7.56771	1.00191
O	8.48423	9.47385	-0.12317
O	10.08910	-0.37420	-0.09545
O	10.16070	-0.35623	2.14393
O	7.92614	-5.13084	-1.74917
O	8.27404	-7.03698	-0.62409
O	8.20244	-7.05495	-2.86347
O	10.89153	-5.29823	-0.08159
O	10.96313	-5.28026	2.15779
O	-6.74193	-3.11546	0.46472
O	-6.67033	-3.09749	2.70410

O	-6.39404	-5.02161	1.58980
O	-9.70732	-2.94807	-1.20286
O	-9.35942	-4.85421	-0.07778
O	-5.93950	-8.03949	0.47858
O	-5.86789	-8.02151	2.71796
O	-8.90489	-7.87209	-1.18900
O	-8.55699	-9.77824	-0.06392
O	-10.16186	0.06981	-0.09164
O	-10.23346	0.05184	-2.33102
O	-7.99891	4.82645	1.56208
O	-8.34680	6.73259	0.43700
O	-8.27520	6.75056	2.67638
O	-10.96429	4.99384	-0.10550
O	-11.03590	4.97587	-2.34488
O	-2.61514	1.62216	3.54149
O	-1.54911	0.13131	1.63823
O	-1.57374	-1.64112	2.97790
O	-1.71482	0.25645	5.09211

Table S8. DFT-Optimised geometry calculated for [Oxam·calcite][−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	-1.80427	0.59571	3.91368
C	-1.60494	-0.44594	2.80162
C	-4.24783	-0.83572	0.04291
C	-1.88958	2.07090	-1.49766
C	-1.08872	-2.85349	-1.48419
C	1.00886	2.54973	1.28677
C	-5.04866	4.08859	0.02950
C	-0.28799	-7.77776	-1.47073
C	2.61042	-7.29882	1.31358
C	1.80969	-2.37454	1.30024
C	-2.69028	6.99515	-1.51099
C	4.16805	0.53199	-0.24037
C	4.96877	-4.39229	-0.22692
C	3.36722	5.45626	-0.25383
C	0.20814	7.47400	1.27332
C	-7.40698	1.18199	1.57012
C	-10.30540	0.70304	-1.21430
C	-6.60626	-3.74228	1.58357
C	-9.50467	-4.22123	-1.20085
C	-5.80553	-8.66666	1.59692
C	-3.44735	-5.76005	0.05660
C	-8.70384	-9.14550	-1.18739
C	-8.20771	6.10626	1.55666
C	5.72568	8.36289	-1.79434
C	6.52640	3.43862	-1.78088
C	9.42482	3.91746	1.00344
C	10.22554	-1.00681	1.01689
C	7.32713	-1.48576	-1.76752
C	8.12786	-6.41003	-1.75407
C	11.02627	-5.93108	1.03025
C	8.62399	8.84174	0.98998
C	-11.10613	5.62742	-1.22765
Ca	-3.19818	1.86439	1.42790
Ca	-2.39920	-3.05681	1.44141
Ca	-0.04003	-0.15131	-0.09814
Ca	-6.09749	1.38715	-1.35589
Ca	-0.84073	4.77244	-0.11213
Ca	-6.89815	6.31129	-1.36937
Ca	0.76082	-5.07614	-0.08529
Ca	1.56152	-10.00043	-0.07185
Ca	2.31845	2.75463	-1.63926
Ca	3.11894	-2.16976	-1.62593
Ca	5.21684	3.23360	1.14506
Ca	6.01757	-1.69066	1.15850

Ca	3.91990	-7.09387	-1.61235
Ca	6.81829	-6.61496	1.17197
Ca	4.41612	8.15786	1.13170
Ca	1.51770	7.67903	-1.65271
Ca	-3.99973	6.79013	1.41505
Ca	-1.64138	9.69676	-0.12556
Ca	-9.25651	3.40464	0.17124
Ca	-8.45577	-1.51964	0.18468
Ca	-7.65505	-6.44390	0.19803
Ca	-4.49597	-8.46163	-1.32902
Ca	-1.59756	-7.98279	1.45529
Ca	7.57519	6.14013	-0.39545
Ca	8.37592	1.21585	-0.38199
Ca	9.17665	-3.70842	-0.36864
Ca	9.97748	-8.63269	-0.35518
Ca	6.77447	11.06450	-0.40890
Ca	-5.29666	-3.53734	-1.34261
Ca	-10.05733	8.32903	0.15777
H	-0.82528	-0.60660	5.20250
H	-1.37499	0.92759	5.87021
N	-1.31665	0.27368	5.09992
O	-1.61818	0.05554	1.65185
O	-2.41643	1.63686	3.64959
O	-1.53045	-1.65126	3.09793
O	-4.45567	0.44118	0.03959
O	-4.18029	-1.48304	-1.07497
O	-4.10778	-1.46526	1.16439
O	-1.95706	2.71821	-0.37968
O	-2.02960	2.70025	-2.61897
O	-1.68188	0.79400	-1.49417
O	-1.15633	-2.20610	-0.36624
O	-0.88115	-4.13026	-1.48070
O	-1.22877	-2.22402	-2.60561
O	0.80130	3.82660	1.28329
O	1.14891	1.92026	2.40820
O	1.07652	1.90241	0.16883
O	-4.98104	3.44124	-1.08840
O	-4.90853	3.45910	1.15109
O	-5.25620	5.36539	0.02603
O	-0.35561	-7.13036	-0.35280
O	-0.42804	-7.14829	-2.59216
O	-0.08042	-9.05463	-1.46725
O	2.67793	-7.94622	0.19573
O	2.75047	-7.92829	2.43501
O	2.40275	-6.02205	1.31010
O	1.87724	-3.02193	0.18233
O	1.60203	-1.09782	1.29671

O	1.94974	-3.00402	2.42166
O	-2.48261	5.71829	-1.50750
O	-2.75779	7.64245	-0.39305
O	-2.83032	7.62463	-2.63242
O	4.02800	1.16146	-1.36181
O	4.37561	-0.74477	-0.23691
O	4.10043	1.17938	0.87757
O	4.90116	-3.74489	0.89102
O	4.82878	-3.76275	-1.34832
O	5.17634	-5.66917	-0.22342
O	3.57488	4.17950	-0.25034
O	3.29970	6.10366	0.86411
O	3.22717	6.08573	-1.37526
O	0.27581	6.82668	0.15540
O	0.00057	8.75087	1.26983
O	0.34819	6.84453	2.39475
O	-7.54704	1.81143	0.44869
O	-7.19932	-0.09478	1.57360
O	-7.47450	1.82939	2.68806
O	-10.51296	1.97991	-1.21778
O	-10.16535	0.07367	-0.09287
O	-10.23778	0.05575	-2.33224
O	-6.74631	-3.11282	0.46214
O	-6.67378	-3.09499	2.70151
O	-6.39859	-5.01915	1.58705
O	-9.71224	-2.94436	-1.20433
O	-9.43705	-4.86853	-2.31879
O	-9.36462	-4.85071	-0.07942
O	-5.94558	-8.03718	0.47549
O	-5.59786	-9.94343	1.60041
O	-5.87305	-8.01926	2.71486
O	-3.37956	-6.40742	-1.06153
O	-3.65407	-4.48398	0.05308
O	-3.30702	-6.38950	1.17784
O	-8.91151	-7.86873	-1.19088
O	-8.63632	-9.79290	-2.30534
O	-8.56379	-9.77498	-0.06597
O	-8.00005	4.82949	1.56015
O	-8.27533	6.75366	2.67460
O	-8.34776	6.73574	0.43523
O	5.86573	7.73342	-0.67291
O	5.79320	7.71549	-2.91228
O	5.51801	9.63966	-1.79782
O	6.31874	4.71539	-1.78436
O	6.59392	2.79122	-2.89882
O	6.66645	2.80915	-0.65955
O	9.28477	4.54694	-0.11799

O	9.35720	4.56486	2.12138
O	9.63238	2.64070	1.00692
O	10.08549	-0.37733	-0.10454
O	10.43311	-2.28368	1.02038
O	10.15793	-0.35951	2.13483
O	7.46718	-2.11523	-0.64610
O	7.11946	-0.20888	-1.77101
O	7.39465	-2.13305	-2.88547
O	7.92019	-5.13326	-1.75755
O	8.26791	-7.03950	-0.63264
O	8.19548	-7.05743	-2.87201
O	11.23394	-7.20795	1.03373
O	10.88622	-5.30171	-0.09108
O	10.95865	-5.28378	2.14819
O	8.83165	7.56497	0.99347
O	8.55647	9.48914	2.10792
O	8.48394	9.47121	-0.13145
O	-11.31379	6.90419	-1.23114
O	-10.96608	4.99794	-0.10623
O	-11.03851	4.98002	-2.34560

Table S9. DFT-Optimised geometry calculated for [MeOx·calcite][−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	0.58413	-0.13352	4.65252
C	-1.43018	0.73150	3.77084
C	-1.47963	-0.39802	2.72707
C	-1.90319	2.06829	-1.51576
C	-4.25917	-0.83791	0.02910
C	-1.10223	-2.85608	-1.50200
C	0.99927	2.54801	1.26429
C	-5.06011	4.08638	0.01539
C	-2.70402	6.99254	-1.52940
C	-7.41612	1.18020	1.56031
C	-0.30141	-7.78033	-1.48826
C	2.60105	-7.30051	1.29169
C	1.80022	-2.37625	1.27804
C	4.15627	0.52986	-0.26686
C	4.95710	-4.39439	-0.25312
C	3.35533	5.45412	-0.28061
C	-10.31859	0.70038	-1.21973
C	-8.21696	6.10446	1.54657
C	-6.61529	-3.74405	1.57406
C	-9.51775	-4.22387	-1.20599
C	-5.81445	-8.66841	1.58770
C	-3.45847	-5.76220	0.04297
C	-8.71682	-9.14813	-1.19224
C	0.19845	7.47226	1.25055
C	5.71149	8.36034	-1.82542
C	6.51232	3.43608	-1.81167
C	9.41478	3.91580	0.96828
C	10.21562	-1.00845	0.98202
C	7.31315	-1.48828	-1.79802
C	8.61385	8.84006	0.95453
C	8.11399	-6.41253	-1.78427
C	11.01645	-5.93271	0.99567
C	-11.11942	5.62474	-1.23338
Ca	-0.05172	-0.15378	-0.11869
Ca	-3.20781	1.86316	1.41196
Ca	-2.40791	-3.05920	1.42586
Ca	-0.85234	4.77023	-0.13257
Ca	-6.11088	1.38445	-1.36767
Ca	-9.26773	3.40241	0.16347
Ca	-6.91167	6.30864	-1.38144
Ca	0.74935	-5.07829	-0.10515
Ca	1.55018	-10.00254	-0.09141
Ca	2.30461	2.75205	-1.66370
Ca	5.20703	3.23191	1.11624

Ca	3.10539	-2.17209	-1.64997
Ca	6.00786	-1.69235	1.12998
Ca	3.90624	-7.09642	-1.63622
Ca	6.80870	-6.61661	1.14373
Ca	4.40620	8.15616	1.10259
Ca	1.50374	7.67643	-1.67746
Ca	-4.00921	6.78836	1.39861
Ca	-8.46688	-1.52185	0.17721
Ca	-7.66605	-6.44609	0.19086
Ca	-4.50917	-8.46423	-1.34020
Ca	-1.60671	-7.98451	1.43974
Ca	-1.65315	9.69458	-0.14630
Ca	-5.30998	-3.53997	-1.35407
Ca	7.56309	6.13802	-0.42857
Ca	8.36392	1.21376	-0.41482
Ca	9.16475	-3.71049	-0.40118
Ca	6.76225	11.06237	-0.44232
Ca	9.96569	-8.63475	-0.38743
Ca	-10.06865	8.32677	0.14972
H	1.11629	0.09879	3.71749
H	1.19263	0.13657	5.52206
H	0.29935	-1.19143	4.69076
O	-0.58530	0.71162	4.74509
O	-1.61718	0.06300	1.56194
O	-2.25944	1.62545	3.62972
O	-1.50088	-1.59332	3.05237
O	-1.69548	0.79142	-1.51219
O	-2.04488	2.69732	-2.63706
O	-1.96909	2.71594	-0.39789
O	-4.46700	0.43899	0.02569
O	-4.19324	-1.48556	-1.08869
O	-4.11747	-1.46711	1.15055
O	-1.16826	-2.20834	-0.38416
O	-0.89465	-4.13284	-1.49844
O	-1.24394	-2.22694	-2.62341
O	1.06531	1.90036	0.14645
O	1.14097	1.91886	2.38570
O	0.79168	3.82488	1.26074
O	-4.99409	3.43870	-1.10243
O	-4.91832	3.45724	1.13695
O	-5.26767	5.36319	0.01185
O	-2.49632	5.71567	-1.52584
O	-2.76992	7.64016	-0.41155
O	-2.84571	7.62168	-2.65081
O	-7.55782	1.80932	0.43891
O	-7.20843	-0.09656	1.56387
O	-7.48202	1.82793	2.67816

O	-0.36741	-7.13260	-0.37041
O	-0.44311	-7.15119	-2.60967
O	-0.09382	-9.05720	-1.48470
O	2.66694	-7.94824	0.17394
O	2.74274	-7.92964	2.41310
O	2.39336	-6.02374	1.28813
O	1.86612	-3.02398	0.16020
O	1.59250	-1.09951	1.27448
O	1.94191	-3.00539	2.39945
O	4.01457	1.15900	-1.38827
O	4.36386	-0.74690	-0.26331
O	4.09027	1.17759	0.85098
O	4.89110	-3.74666	0.86473
O	4.81540	-3.76526	-1.37453
O	5.16469	-5.67126	-0.24955
O	3.56302	4.17736	-0.27705
O	3.28943	6.10185	0.83724
O	3.21364	6.08326	-1.40201
O	-10.52618	1.97725	-1.22329
O	-10.17689	0.07134	-0.09832
O	-10.25259	0.05275	-2.33758
O	-8.00926	4.82769	1.55013
O	-8.28296	6.75219	2.66441
O	-8.35865	6.73360	0.42516
O	-6.75699	-3.11492	0.45265
O	-6.68119	-3.09642	2.69191
O	-6.40759	-5.02092	1.57762
O	-9.72535	-2.94701	-1.20955
O	-9.45175	-4.87150	-2.32383
O	-9.37606	-4.85301	-0.08458
O	-5.95615	-8.03927	0.46629
O	-5.60676	-9.94517	1.59126
O	-5.88035	-8.02068	2.70555
O	-3.39240	-6.40991	-1.07495
O	-3.66572	-4.48574	0.03942
O	-3.31661	-6.39133	1.16431
O	-8.92451	-7.87136	-1.19580
O	-8.65092	-9.79586	-2.31009
O	-8.57512	-9.77727	-0.07083
O	0.26446	6.82463	0.13270
O	-0.00915	8.74913	1.24699
O	0.34014	6.84312	2.37196
O	5.85318	7.73120	-0.70401
O	5.77739	7.71261	-2.94326
O	5.50380	9.63710	-1.82898
O	6.30463	4.71285	-1.81523
O	6.57822	2.78835	-2.92951

O	6.65402	2.80694	-0.69036
O	9.27309	4.54494	-0.15313
O	9.34878	4.56353	2.08612
O	9.62238	2.63904	0.97184
O	10.07392	-0.37931	-0.13939
O	10.42321	-2.28532	0.98558
O	10.14962	-0.36082	2.09987
O	7.45485	-2.11741	-0.67661
O	7.10546	-0.21141	-1.80158
O	7.37905	-2.13590	-2.91587
O	8.47216	9.46920	-0.16688
O	8.54795	9.48779	2.07238
O	8.82154	7.56329	0.95809
O	7.90630	-5.13577	-1.78783
O	8.25568	-7.04167	-0.66286
O	8.17999	-7.06026	-2.90212
O	11.22414	-7.20957	0.99923
O	10.87476	-5.30367	-0.12564
O	10.95045	-5.28508	2.11352
O	-11.32711	6.90150	-1.23694
O	-10.97772	4.99560	-0.11197
O	-11.05342	4.97701	-2.35123

Table S10. DFT-Optimised geometry calculated for [MeOxam·calcite][−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	0.99839	2.54749	1.26468
C	-1.90485	2.06803	-1.51460
C	-1.39563	0.73533	3.71759
C	-1.50165	-0.42702	2.72606
C	-4.26092	-0.83765	0.03108
C	-1.10470	-2.85647	-1.50065
C	-0.30470	-7.78085	-1.48672
C	1.79852	-2.37690	1.27862
C	2.59854	-7.30128	1.29246
C	-2.70486	6.99242	-1.52843
C	4.15467	0.52870	-0.26711
C	4.95469	-4.39568	-0.25317
C	3.35455	5.45309	-0.28104
C	-5.06105	4.08677	0.01717
C	0.19838	7.47188	1.25074
C	6.51082	3.43441	-1.81273
C	5.71080	8.35880	-1.82667
C	9.41405	3.91387	0.96644
C	10.21407	-1.01052	0.98038
C	7.31083	-1.49008	-1.79889
C	8.61393	8.83826	0.95251
C	8.11086	-6.41447	-1.78496
C	11.01409	-5.93490	0.99422
C	-8.21718	6.10550	1.54899
C	-7.41716	1.18111	1.56292
C	-10.32040	0.70155	-1.21636
C	-6.61714	-3.74328	1.57685
C	-5.81711	-8.66777	1.59069
C	-3.46104	-5.76207	0.04514
C	-9.52037	-4.22284	-1.20242
C	-8.72025	-9.14723	-1.18849
C	-11.12042	5.62603	-1.23019
C	0.72817	-0.11162	4.65312
Ca	-0.85320	4.76991	-0.13189
Ca	-3.20877	1.86336	1.41345
Ca	-2.40968	-3.05914	1.42755
Ca	-0.05340	-0.15423	-0.11782
Ca	-6.11262	1.38490	-1.36540
Ca	0.74686	-5.07887	-0.10410
Ca	1.54688	-10.00326	-0.09017
Ca	2.30303	2.75109	-1.66365
Ca	3.10299	-2.17319	-1.64973
Ca	5.20622	3.23068	1.11552
Ca	6.00625	-1.69371	1.12945

Ca	3.90303	-7.09765	-1.63579
Ca	6.80626	-6.61810	1.14339
Ca	4.40621	8.15507	1.10168
Ca	1.50297	7.67560	-1.67761
Ca	-4.00935	6.78869	1.39991
Ca	-6.91259	6.30922	-1.37936
Ca	-1.65320	9.69439	-0.14582
Ca	7.56238	6.13628	-0.43011
Ca	8.36239	1.21189	-0.41618
Ca	9.16241	-3.71249	-0.40234
Ca	6.76236	11.06077	-0.44405
Ca	9.96253	-8.63688	-0.38840
Ca	-9.26874	3.40351	0.16637
Ca	-8.46871	-1.52088	0.18029
Ca	-7.66869	-6.44526	0.19413
Ca	-4.51253	-8.46404	-1.33756
Ca	-1.60929	-7.98457	1.44162
Ca	-5.31253	-3.53964	-1.35161
Ca	-10.06886	8.32801	0.15243
H	-0.38252	1.62413	5.12691
H	1.52415	0.39066	4.08377
H	1.02812	-0.29810	5.69376
H	0.53069	-1.07119	4.16180
N	-0.45428	0.73345	4.64175
O	0.79101	3.82440	1.26108
O	1.06404	1.89975	0.14688
O	1.14027	1.91842	2.38611
O	-1.97036	2.71578	-0.39677
O	-1.69735	0.79113	-1.51099
O	-2.04671	2.69700	-2.63592
O	-2.21313	1.66526	3.55165
O	-1.52595	-1.61920	3.06835
O	-1.64529	0.00845	1.54982
O	-4.11905	-1.46678	1.15254
O	-4.46854	0.43928	0.02762
O	-4.19538	-1.48540	-1.08668
O	-1.17035	-2.20863	-0.38285
O	-1.24659	-2.22739	-2.62208
O	-0.89734	-4.13326	-1.49705
O	-0.37031	-7.13302	-0.36891
O	-0.09731	-9.05775	-1.48311
O	-0.44657	-7.15177	-2.60814
O	1.86404	-3.02472	0.16082
O	1.94039	-3.00597	2.40004
O	1.59102	-1.10012	1.27501
O	2.66405	-7.94911	0.17474
O	2.39106	-6.02448	1.28885

O	2.74041	-7.93036	2.41388
O	-2.49738	5.71551	-1.52482
O	-2.84673	7.62149	-2.64986
O	-2.77037	7.64014	-0.41062
O	4.01280	1.15778	-1.38853
O	4.08906	1.17653	0.85071
O	4.36205	-0.74809	-0.26350
O	4.88908	-3.74785	0.86464
O	5.16207	-5.67259	-0.24955
O	4.81280	-3.76662	-1.37460
O	3.56202	4.17630	-0.27743
O	3.21268	6.08217	-1.40246
O	3.28904	6.10092	0.83677
O	-5.26839	5.36361	0.01358
O	-4.91908	3.45770	1.13875
O	-4.99541	3.43899	-1.10061
O	0.26400	6.82414	0.13293
O	0.34025	6.84281	2.37217
O	-0.00900	8.74878	1.24714
O	6.65269	2.80533	-0.69141
O	6.30333	4.71121	-1.81634
O	6.57633	2.78658	-2.93055
O	5.85267	7.72972	-0.70525
O	5.50331	9.63559	-1.83028
O	5.77631	7.71097	-2.94448
O	9.27218	4.54294	-0.15498
O	9.62144	2.63707	0.97006
O	9.34844	4.56170	2.08426
O	10.07220	-0.38144	-0.14104
O	10.14846	-0.36279	2.09820
O	10.42146	-2.28742	0.98399
O	7.45271	-2.11915	-0.67747
O	7.37635	-2.13781	-2.91671
O	7.10335	-0.21318	-1.80251
O	8.47206	9.46733	-0.16892
O	8.82142	7.56146	0.95612
O	8.54842	9.48608	2.07032
O	7.90337	-5.13767	-1.78857
O	8.17647	-7.06230	-2.90277
O	8.25273	-7.04354	-0.66353
O	11.22158	-7.21181	0.99783
O	10.94848	-5.28718	2.11203
O	10.87222	-5.30593	-0.12710
O	-8.35905	6.73457	0.42756
O	-8.28279	6.75332	2.66680
O	-8.00970	4.82869	1.55259
O	-7.55903	1.81016	0.44150

O	-7.48267	1.82893	2.68073
O	-7.20967	-0.09569	1.56653
O	-10.52778	1.97845	-1.21997
O	-10.25479	0.05382	-2.33417
O	-10.17852	0.07257	-0.09494
O	-6.75901	-3.11421	0.45543
O	-6.40965	-5.02018	1.58047
O	-6.68265	-3.09555	2.69467
O	-5.95899	-8.03869	0.46927
O	-5.88262	-8.01994	2.70850
O	-5.60963	-9.94457	1.59430
O	-3.39535	-6.40989	-1.07275
O	-3.31899	-6.39114	1.16649
O	-3.66808	-4.48558	0.04154
O	-9.37850	-4.85191	-0.08100
O	-9.72776	-2.94594	-1.20603
O	-9.45476	-4.87057	-2.32024
O	-8.92774	-7.87043	-1.19210
O	-8.57838	-9.77630	-0.06706
O	-8.65474	-9.79505	-2.30630
O	-11.32790	6.90283	-1.23380
O	-11.05481	4.97821	-2.34801
O	-10.97855	4.99696	-0.10877

Table S11. DFT-Optimised geometry calculated for [PhOx-calcite][−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	-0.36969	-1.02840	6.48539
C	-0.20924	-0.34109	5.28696
C	0.89751	-0.49858	4.46394
C	1.85223	-1.44153	4.84635
C	1.72027	-2.14940	6.03920
C	0.61428	-1.93649	6.86411
C	-1.75328	0.68048	3.79541
C	-1.59320	-0.40327	2.69811
C	1.80474	-2.34200	1.13085
C	-4.26513	-0.82820	-0.09706
C	-1.92772	2.10164	-1.62541
C	-1.09983	-2.81823	-1.64760
C	0.97686	2.57776	1.15304
C	-0.27207	-7.73799	-1.66978
C	2.63250	-7.26177	1.10858
C	-5.09300	4.09162	-0.07485
C	-2.75549	7.02141	-1.60314
C	4.14220	0.58774	-0.39755
C	4.96997	-4.33203	-0.41974
C	3.31432	5.50751	-0.37538
C	0.14909	7.49753	1.17522
C	-7.43042	1.16182	1.45359
C	-10.33499	0.68560	-1.32487
C	-6.60265	-3.75795	1.43141
C	-9.50722	-4.23416	-1.34705
C	-5.77487	-8.67782	1.40913
C	-3.43741	-5.74797	-0.11919
C	-8.67934	-9.15393	-1.36923
C	-8.25819	6.08158	1.47577
C	5.65189	8.43735	-1.90369
C	6.47966	3.51759	-1.92587
C	9.38423	3.99370	0.85249
C	10.21201	-0.92607	0.83031
C	7.30743	-1.40228	-1.94815
C	8.13521	-6.32205	-1.97033
C	11.03978	-5.84584	0.80803
C	8.55636	8.91347	0.87467
C	-11.16276	5.60547	-1.30259
Ca	-3.22633	1.86921	1.30294
Ca	-2.39899	-3.04952	1.28107
Ca	-0.06175	-0.12004	-0.24707
Ca	-6.13133	1.39369	-1.47509
Ca	-0.88924	4.79951	-0.22506
Ca	0.76628	-5.04001	-0.26950

Ca	1.59406	-9.95976	-0.29169
Ca	-6.95908	6.31344	-1.45292
Ca	2.27602	2.80949	-1.77564
Ca	3.10374	-2.11016	-1.79784
Ca	5.18054	3.28574	1.00272
Ca	6.00831	-1.63404	0.98054
Ca	3.93151	-7.03003	-1.82000
Ca	6.83609	-6.55380	0.95835
Ca	4.35277	8.20550	1.02500
Ca	1.44821	7.72938	-1.75347
Ca	-4.05451	6.78956	1.32554
Ca	-1.71704	9.71941	-0.20288
Ca	-9.29655	3.38358	0.07550
Ca	-8.46876	-1.53618	0.05331
Ca	-7.64100	-6.45594	0.03104
Ca	-4.47575	-8.44596	-1.51946
Ca	-1.57118	-7.96984	1.25890
Ca	7.51801	6.21548	-0.52560
Ca	8.34578	1.29571	-0.54778
Ca	9.17356	-3.62406	-0.57006
Ca	10.00143	-8.54383	-0.59224
Ca	6.69024	11.13534	-0.50342
Ca	-5.30354	-3.52623	-1.49736
Ca	-10.12442	8.30346	0.09768
H	1.02356	0.08632	3.54195
H	2.67108	-1.65214	4.15919
H	2.47688	-2.88523	6.32275
H	0.50659	-2.49038	7.80006
H	-1.25894	-0.85082	7.09277
O	-1.20999	0.58219	4.97334
O	-2.47762	1.62921	3.53079
O	-1.62977	-1.60699	2.97800
O	-1.57892	0.10988	1.54828
O	1.95179	-2.97821	2.24758
O	1.59002	-1.06641	1.13664
O	1.87224	-2.98150	0.00837
O	-4.11801	-1.46440	1.01971
O	-4.19756	-1.46761	-1.21949
O	-4.47991	0.44754	-0.09116
O	-1.99524	2.74104	-0.50295
O	-1.71302	0.82595	-1.63119
O	-2.07477	2.73775	-2.74205
O	-1.16748	-2.17871	-0.52514
O	-1.24690	-2.18202	-2.76433
O	-0.88527	-4.09383	-1.65336
O	0.76227	3.85347	1.15880
O	1.04447	1.93836	0.03057

O	1.12392	1.94156	2.26976
O	-0.33968	-7.09849	-0.54730
O	-0.05749	-9.01369	-1.67554
O	-0.41913	-7.10179	-2.78651
O	2.70003	-7.90127	-0.01379
O	2.41783	-5.98616	1.11433
O	2.77956	-7.89797	2.22530
O	-5.02535	3.45217	-1.19729
O	-5.30753	5.36727	-0.06907
O	-4.94585	3.45541	1.04204
O	-2.54081	5.74571	-1.60890
O	-2.90255	7.65761	-2.71987
O	-2.82300	7.66081	-0.48067
O	3.99514	1.22395	-1.51427
O	4.07458	1.22724	0.72492
O	4.35677	-0.68786	-0.40331
O	4.90235	-3.69253	0.70274
O	5.18454	-5.60773	-0.42550
O	4.82289	-3.69584	-1.53646
O	3.52899	4.23192	-0.38113
O	3.16726	6.14371	-1.49210
O	3.24681	6.14701	0.74710
O	0.21668	6.85814	0.05273
O	0.29615	6.86133	2.29194
O	-0.06549	8.77323	1.18097
O	-7.57748	1.79800	0.33687
O	-7.49794	1.80132	2.57607
O	-7.21574	-0.11378	1.44783
O	-10.54957	1.96131	-1.31912
O	-10.26737	0.04620	-2.44735
O	-10.18793	0.04950	-0.20815
O	-6.74971	-3.12174	0.31468
O	-6.38797	-5.03365	1.42565
O	-6.67016	-3.11855	2.55389
O	-9.72180	-2.95846	-1.34130
O	-9.36016	-4.87037	-0.23033
O	-9.43960	-4.87357	-2.46953
O	-5.92193	-8.04161	0.29240
O	-5.84239	-8.03832	2.53160
O	-5.56019	-9.95342	1.40337
O	-3.36979	-6.38747	-1.24167
O	-3.29025	-6.38417	0.99753
O	-3.65196	-4.47237	-0.11344
O	-8.89402	-7.87833	-1.36348
O	-8.53228	-9.79013	-0.25251
O	-8.61182	-9.79343	-2.49171
O	-8.04352	4.80598	1.47001

O	-8.40525	6.71779	0.35904
O	-8.32581	6.72109	2.59825
O	5.79895	7.80115	-0.78697
O	5.43721	9.71295	-1.89794
O	5.71941	7.79785	-3.02617
O	6.26499	4.79319	-1.92012
O	6.62672	2.88138	-0.80925
O	6.54718	2.87808	-3.04835
O	9.23717	4.62990	-0.26423
O	9.59881	2.71810	0.84674
O	9.31662	4.63320	1.97497
O	10.06494	-0.28986	-0.28641
O	10.14439	-0.28667	1.95279
O	10.42658	-2.20177	0.82456
O	7.45450	-2.03848	-0.83143
O	7.37495	-2.04168	-3.07063
O	7.09276	-0.12658	-1.94240
O	7.92053	-5.04645	-1.96457
O	8.20283	-6.96155	-3.09281
O	8.28227	-6.95825	-0.85360
O	11.25445	-7.12154	0.80228
O	10.97216	-5.20643	1.93051
O	10.89272	-5.20974	-0.30859
O	8.77104	7.63787	0.86892
O	8.40930	9.54967	-0.24205
O	8.48884	9.55297	1.99715
O	-11.37744	6.88107	-1.29684
O	-11.09514	4.96597	-2.42507
O	-11.01570	4.96927	-0.18587

Table S12. DFT-Optimised geometry calculated for [PhOxam-calcite][−] in orthogonal Cartesian format (Å; functional PBE0, Basis Set def2-SVP).

C	-0.10727	-0.34256	5.38244
C	-1.68262	0.68804	3.75086
C	-1.57302	-0.40455	2.66882
C	-4.26699	-0.83184	-0.09988
C	-1.93315	2.10026	-1.62934
C	-1.10087	-2.81887	-1.65259
C	0.97271	2.57866	1.14737
C	-5.09925	4.08723	-0.07660
C	-0.26872	-7.73788	-1.67584
C	2.63713	-7.25938	1.10078
C	1.80498	-2.34036	1.12412
C	-2.76530	7.01928	-1.60601
C	4.13887	0.59165	-0.40540
C	4.97103	-4.32737	-0.42864
C	3.30661	5.51067	-0.38216
C	0.14055	7.49769	1.17061
C	-7.43311	1.15517	1.45295
C	-10.33896	0.67667	-1.32377
C	-6.60095	-3.76386	1.42970
C	-9.50680	-4.24236	-1.34702
C	-5.76879	-8.68298	1.40636
C	-3.43489	-5.75087	-0.12306
C	-8.67454	-9.16138	-1.37027
C	-8.26527	6.07419	1.47619
C	5.64062	8.44278	-1.91159
C	6.47278	3.52376	-1.93483
C	9.37863	4.00216	0.84179
C	10.21079	-0.91686	0.81855
C	7.30493	-1.39536	-1.95817
C	8.13709	-6.31439	-1.98141
C	11.04295	-5.83589	0.79521
C	8.54637	8.92118	0.86504
C	-11.17112	5.59579	-1.30043
C	0.88581	-0.84536	4.54135
C	1.77100	-1.79880	5.04287
C	1.71103	-2.19486	6.37783
C	0.74352	-1.65040	7.22359
C	-0.17698	-0.73532	6.72362
Ca	-3.22983	1.86646	1.29986
Ca	-2.39801	-3.05170	1.27687
Ca	-0.06431	-0.11998	-0.25248
Ca	-6.13602	1.38850	-1.47651
Ca	-0.89623	4.79891	-0.22932
Ca	-6.96816	6.30754	-1.45327

Ca	0.76807	-5.03913	-0.27590
Ca	1.60023	-9.95814	-0.29915
Ca	2.26985	2.81189	-1.78208
Ca	3.10198	-2.10700	-1.80533
Ca	5.17567	3.29042	0.99454
Ca	6.00783	-1.62861	0.97129
Ca	3.93413	-7.02614	-1.82858
Ca	6.83999	-6.54763	0.94805
Ca	4.34351	8.20944	1.01788
Ca	1.43766	7.73103	-1.75885
Ca	-4.06231	6.78594	1.32345
Ca	-1.72840	9.71805	-0.20608
Ca	-9.30207	3.37542	0.07626
Ca	-8.46990	-1.54360	0.05301
Ca	-7.63775	-6.46262	0.02967
Ca	-4.47168	-8.44963	-1.52300
Ca	-1.56583	-7.97123	1.25362
Ca	7.50957	6.22242	-0.53489
Ca	8.34173	1.30340	-0.55814
Ca	9.17389	-3.61563	-0.58148
Ca	10.00615	-8.53465	-0.60472
Ca	6.67741	11.14154	-0.51165
Ca	-5.30385	-3.53064	-1.49985
Ca	-10.13433	8.29455	0.09950
H	-1.29795	1.36071	5.55198
H	0.99359	-0.50652	3.50485
H	2.47225	-2.24611	4.33565
H	2.41558	-2.93733	6.76190
H	0.68773	-1.95525	8.27166
H	-0.96590	-0.33404	7.36556
N	-1.06546	0.59549	4.92352
O	-1.59210	0.09180	1.51052
O	-2.42630	1.64871	3.48209
O	-1.60372	-1.61002	2.95311
O	-4.48290	0.44370	-0.09370
O	-4.19955	-1.47106	-1.22242
O	-4.11863	-1.46805	1.01673
O	-2.00055	2.73949	-0.50676
O	-2.08146	2.73636	-2.74581
O	-1.71731	0.82475	-1.63540
O	-1.16840	-2.17954	-0.53002
O	-0.88517	-4.09427	-1.65863
O	-1.24920	-2.18266	-2.76916
O	0.75699	3.85418	1.15341
O	1.12103	1.94247	2.26393
O	1.04021	1.93945	0.02478
O	-5.03172	3.44797	-1.19916

O	-4.95085	3.45103	1.04011
O	-5.31492	5.36269	-0.07055
O	-0.33622	-7.09857	-0.55325
O	-0.41704	-7.10169	-2.79240
O	-0.05301	-9.01339	-1.68187
O	2.70453	-7.89869	-0.02171
O	2.78545	-7.89557	2.21734
O	2.42132	-5.98397	1.10681
O	1.87237	-2.97967	0.00153
O	1.58913	-1.06496	1.13017
O	1.95329	-2.97655	2.24069
O	-2.54949	5.74378	-1.61204
O	-2.83270	7.65850	-0.48341
O	-2.91362	7.65548	-2.72257
O	3.99056	1.22785	-1.52195
O	4.35459	-0.68376	-0.41143
O	4.07137	1.23096	0.71719
O	4.90353	-3.68806	0.69395
O	4.82270	-3.69119	-1.54521
O	5.18675	-5.60288	-0.43468
O	3.52242	4.23527	-0.38819
O	3.23922	6.14999	0.74044
O	3.15830	6.14687	-1.49871
O	0.20804	6.85848	0.04802
O	-0.07516	8.77320	1.17665
O	0.28887	6.86149	2.28717
O	-7.58143	1.79135	0.33639
O	-7.21729	-0.12024	1.44692
O	-7.50051	1.79448	2.57554
O	-10.55468	1.95218	-1.31774
O	-10.19065	0.04057	-0.20721
O	-10.27147	0.03745	-2.44637
O	-6.74927	-3.12766	0.31314
O	-6.66835	-3.12464	2.55229
O	-6.38513	-5.03937	1.42367
O	-9.72252	-2.96685	-1.34099
O	-9.43931	-4.88157	-2.46961
O	-9.35848	-4.87855	-0.23046
O	-5.91711	-8.04678	0.28980
O	-5.55297	-9.95839	1.40033
O	-5.83619	-8.04366	2.52895
O	-3.36739	-6.39018	-1.24566
O	-3.65058	-4.47547	-0.11704
O	-3.28647	-6.38706	0.99349
O	-8.89036	-7.88597	-1.36423
O	-8.60715	-9.80069	-2.49286
O	-8.52623	-9.79757	-0.25371

O	-8.04945	4.79878	1.47016
O	-8.33277	6.71350	2.59879
O	-8.41359	6.71038	0.35963
O	5.78894	7.80659	-0.79502
O	5.70801	7.80347	-3.03418
O	5.42480	9.71819	-1.90555
O	6.25696	4.79917	-1.92880
O	6.54017	2.88444	-3.05742
O	6.62109	2.88756	-0.81837
O	9.23031	4.63836	-0.27477
O	9.31113	4.64147	1.96439
O	9.59435	2.72675	0.83577
O	10.06247	-0.28067	-0.29801
O	10.42651	-2.19237	0.81252
O	10.14329	-0.27765	1.94114
O	7.45325	-2.03156	-0.84161
O	7.08912	-0.11986	-1.95214
O	7.37233	-2.03458	-3.08076
O	7.92128	-5.03898	-1.97538
O	8.28541	-6.95058	-0.86485
O	8.20459	-6.95370	-3.10401
O	11.25877	-7.11139	0.78918
O	10.89463	-5.19979	-0.32125
O	10.97545	-5.19667	1.91780
O	8.76219	7.64577	0.85901
O	8.47898	9.56050	1.98763
O	8.39805	9.55738	-0.25152
O	-11.38694	6.87120	-1.29440
O	-11.02280	4.95959	-0.18387
O	-11.10363	4.95647	-2.42302

Table S13. Wiberg bond indexes WBI (in parenthesis the relative variations with respect to the corresponding indexes in the gas-phase) and anion-to-lattice charge transfer (ΔQ_s , |e|) calculated upon interaction of the anions Ox^{2-} , MeOx^- , PhOx^- , Oxam^- , MeOxam^- , and PhOxam^- with the modelled calcite surface portion (Calcite = $\text{Ca}_{30}\text{C}_{30}\text{O}_{90}$) at PBE0/def2-SVP level.

	$[\text{Ox}\cdot\text{Calcite}]^{2-}$	$[\text{Ox}\cdot\text{Calcite}]^{2- \text{ } ^a}$	$[\text{MeOx}\cdot\text{Calcite}]^-$	$[\text{PhOx}\cdot\text{Calcite}]^-$	$[\text{Oxam}\cdot\text{Calcite}]^-$	$[\text{MeOxam}\cdot\text{Calcite}]^-$	$[\text{PhOxam}\cdot\text{Calcite}]^-$
WBI($\text{C}_1\text{-C}_2$)	0.871 (-0.026)	0.858 (-0.038)	0.901 (-0.026)	0.897 (-0.025)	0.903 (-0.038)	0.906 (-0.039)	0.903 (-0.036)
WBI($\text{C}_1\text{-O}_1$)	1.438 (0.008)	1.279 (-0.151)	1.331 (-0.151)	1.344 (-0.142)	1.365 (-0.044)	1.331 (-0.073)	1.342 (-0.050)
WBI($\text{C}_1\text{-O}_2$)	1.305 (-0.125)	1.249 (-0.181)	1.487 (0.035)	1.490 (0.004)	1.460 (-0.080)	1.482 (-0.061)	1.482 (-0.075)
WBI($\text{C}_2\text{-O}_3$)	1.645 (0.215)	1.283 (-0.147)	1.556 (-0.142)	1.577 (-0.153)	1.500 (-0.154)	1.439 (-0.197)	1.464 (-0.214)
ΔQ_s	0.368	0.643	0.380	0.083	0.118	0.106	0.093

^a Data calculated at DFT-D3 level (PBE0/def2-SVP).