Supporting Information

Theoretical investigation of defective MXenes as potential electrocatalysts for CO reduction toward C_2 products

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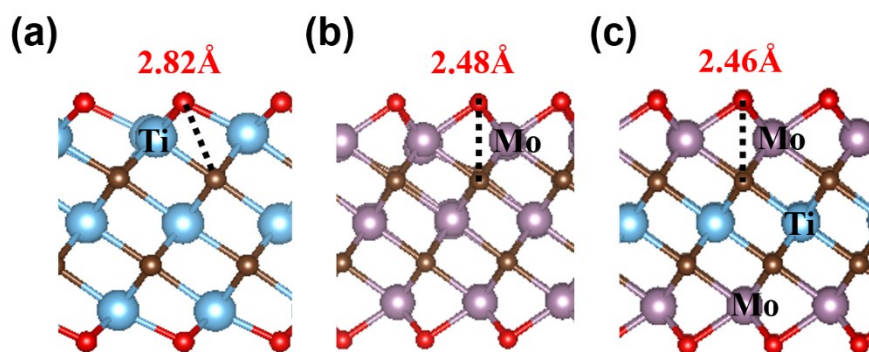Email: tianziqi@nimte.ac.cn; czhan021@ucr.edu; chenliang@nimte.ac.cn

Figure S1. The most stable configurations of the terminal oxygen in (a)Ti_3C_2(b)Mo_3C_2(c)Mo_2TiC_2.
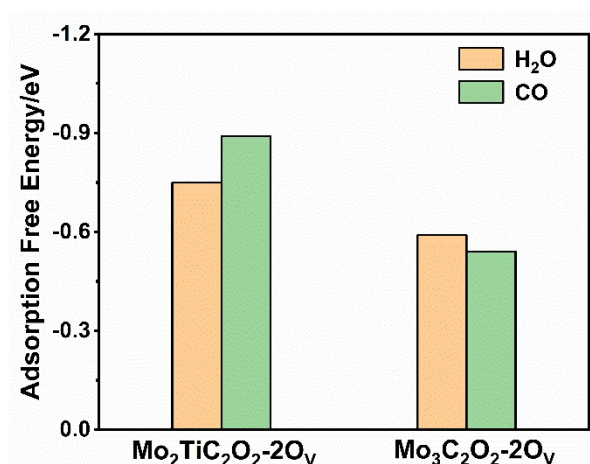

Figure S2. Comparison adsorption free energies of H_2O and CO on selected candidates.

Table S1 Calculated ZPE and TS energies for different species, where the label * denotes the status of adsorption.

Adsorbed species	$Mo_3C_2O_2$-$2O_V$		$Mo_2TiC_2O_2$-$2O_V$	
	E_{ZPE} (eV)	E_{TS} (eV)	E_{ZPE} (eV)	E_{TS} (eV)
*CO	0.22	0.09	0.21	0.07
*COH	0.52	0.08	0.49	0.10
*CHO	0.51	0.08	0.49	0.10
*H_2O	0.68	0.09	0.65	0.11
*OCCO	0.44	0.15	0.44	0.14
*OCCOH	0.76	0.17	0.77	0.19
*CO-*CO	0.43	0.24	0.41	0.19
*CO-*COH	0.70	0.18	0.71	0.22

2*COH	0.99	0.23	1.02	0.19
***COH-*COH**	1.05	0.23	1.09	0.19
***CCOH**	0.66	0.13	0.67	0.11
***CHCOH**	0.98	0.11	0.98	0.11
***CCH**	0.50	0.09	0.50	0.09
***CHCH**	0.83	0.07	0.82	0.08
***CH₂CH**	1.08	0.09	1.08	0.11
***CH₂CH₂**	1.40	0.13	1.40	0.16
***CH₃CH₂**	1.68	0.15	1.70	0.17
***CH₃CH₃**	1.99	0.20	2.01	0.23
***CHCHOH**	1.26	0.13	1.26	0.16
***CH₂COH**	1.24	0.13	1.22	0.12
***CH₂CHOH**	1.56	0.17	1.57	0.20
***CH₂CH₂OH**	1.86	0.21	1.86	0.17
***CH₃CH₂OH**	2.11	0.23	2.17	0.27

The atomic coordinates of all the optimized key intermediates on the Mo$_3$C$_2$O$_2$-2O$_V$ and Mo$_2$TiC$_2$O$_2$-2O$_V$ at the DFT-D3 computational level.

		a	b
Slab/Mo$_3$C$_2$O$_2$-2O$_V$		**9.13230**	**9.13230**

Mo1	1.0	0.111183	0.222375	0.369955
Mo2	1.0	0.222442	0.111089	0.629836
Mo3	1.0	0.000566	-0.000676	0.498403
Mo4	1.0	0.444664	0.221893	0.370963
Mo5	1.0	0.554719	0.111240	0.629807
Mo6	1.0	0.334140	0.002164	0.497991
Mo7	1.0	0.778608	0.222283	0.369977
Mo8	1.0	0.889612	0.113154	0.629322
Mo9	1.0	0.664994	-0.000750	0.498415
Mo10	1.0	0.110578	0.553429	0.372488
Mo11	1.0	0.207457	0.433630	0.623502
Mo12	1.0	0.001632	0.336584	0.501391
Mo13	1.0	0.444935	0.553842	0.372136
Mo14	1.0	0.544080	0.422061	0.618018
Mo15	1.0	0.336908	0.338797	0.502984
Mo16	1.0	0.776600	0.553881	0.372131
Mo17	1.0	0.892289	0.433641	0.623556
Mo18	1.0	0.668080	0.338635	0.502992

Mo19	1.0	0.109550	0.887572	0.372089
Mo20	1.0	0.224247	0.782418	0.628980
Mo21	1.0	-0.000748	0.669582	0.501949
Mo22	1.0	0.445002	0.887494	0.372106
Mo23	1.0	0.563789	0.799368	0.624769
Mo24	1.0	0.336671	0.669697	0.501975
Mo25	1.0	0.777275	0.887432	0.371068
Mo26	1.0	0.901391	0.799218	0.624667
Mo27	1.0	0.665222	0.664424	0.507518
C1	1.0	0.108522	0.216364	0.564290
C2	1.0	0.223312	0.116438	0.434698
C3	1.0	0.437099	0.208276	0.563952
C4	1.0	0.559740	0.116381	0.434700
C5	1.0	0.774220	0.216433	0.564238
C6	1.0	0.890383	0.114013	0.434513
C7	1.0	0.114747	0.563540	0.563163
C8	1.0	0.223185	0.443034	0.436095
C9	1.0	0.444142	0.561815	0.573933
C10	1.0	0.555999	0.445097	0.436561
C11	1.0	0.783615	0.561557	0.573853
C12	1.0	0.886792	0.442940	0.436156
C13	1.0	0.118265	0.894046	0.565202
C14	1.0	0.220526	0.774367	0.435488
C15	1.0	0.441859	0.894148	0.565219
C16	1.0	0.558056	0.775756	0.435714
C17	1.0	0.781183	0.896461	0.563786
C18	1.0	0.884381	0.775708	0.435709
O1	1.0	0.113599	0.226610	0.688507
O2	1.0	0.221202	0.107915	0.312011
O3	1.0	0.446195	0.226422	0.688710
O4	1.0	0.553903	0.107304	0.311986
O5	1.0	0.778943	0.226535	0.688513
O6	1.0	0.888635	0.110079	0.311194
O7	1.0	0.107468	0.548413	0.685870
O8	1.0	0.224415	0.446182	0.312319
O9	1.0	0.555873	0.443293	0.312494
O10	1.0	0.890873	0.446037	0.312367
O11	1.0	0.112078	0.891703	0.689250
O12	1.0	0.221318	0.775626	0.313244
O13	1.0	0.445922	0.892168	0.689198
O14	1.0	0.554375	0.774079	0.312524
O15	1.0	0.779973	0.893991	0.687386
O16	1.0	0.887053	0.774178	0.312509

		a	b
*CO/Mo₃C₂O₂-2O_V		9.13230	9.13230

Mo1	1.0	0.115019	0.227108	0.369881
Mo2	1.0	0.223357	0.115291	0.627714
Mo3	1.0	0.002575	0.001511	0.497706
Mo4	1.0	0.448439	0.227257	0.370237
Mo5	1.0	0.555854	0.115079	0.627795
Mo6	1.0	0.335251	0.003094	0.497292
Mo7	1.0	0.782057	0.227194	0.369745
Mo8	1.0	0.890151	0.116594	0.627375
Mo9	1.0	0.665286	0.000834	0.497645
Mo10	1.0	0.114017	0.558667	0.370282
Mo11	1.0	0.210510	0.440067	0.623967
Mo12	1.0	0.003721	0.340966	0.501073
Mo13	1.0	0.447898	0.559553	0.371293
Mo14	1.0	0.557606	0.448000	0.628177
Mo15	1.0	0.334976	0.337336	0.501420
Mo16	1.0	0.780887	0.559896	0.371451
Mo17	1.0	0.893915	0.439261	0.623627
Mo18	1.0	0.667993	0.336030	0.500877
Mo19	1.0	0.114739	0.893145	0.370935
Mo20	1.0	0.224278	0.783464	0.627855
Mo21	1.0	0.002042	0.670864	0.500080
Mo22	1.0	0.448413	0.892770	0.370739
Mo23	1.0	0.564891	0.797878	0.624265
Mo24	1.0	0.336148	0.670719	0.500064
Mo25	1.0	0.781280	0.892765	0.370820
Mo26	1.0	0.897462	0.798114	0.623789
Mo27	1.0	0.665961	0.665451	0.504435
C1	1.0	0.110918	0.221340	0.563578
C2	1.0	0.225594	0.119394	0.433640
C3	1.0	0.441752	0.218149	0.562573
C4	1.0	0.562252	0.119185	0.433365
C5	1.0	0.775456	0.220532	0.563340
C6	1.0	0.893194	0.118206	0.434178
C7	1.0	0.116504	0.566360	0.562983
C8	1.0	0.224297	0.448301	0.434612
C9	1.0	0.445200	0.561852	0.571290
C10	1.0	0.557984	0.448507	0.435854
C11	1.0	0.782711	0.561518	0.570724
C12	1.0	0.891743	0.448202	0.434611
C13	1.0	0.119009	0.895721	0.563639
C14	1.0	0.223410	0.778261	0.433842

C15	1.0	0.442686	0.895496	0.563779
C16	1.0	0.559806	0.779557	0.434629
C17	1.0	0.782025	0.898462	0.562441
C18	1.0	0.888361	0.779968	0.434886
C19	1.0	0.618910	0.547831	0.721988
O1	1.0	0.111261	0.228600	0.686923
O2	1.0	0.226663	0.114644	0.310925
O3	1.0	0.442500	0.222258	0.686164
O4	1.0	0.559735	0.114634	0.310818
O5	1.0	0.779605	0.228313	0.686839
O6	1.0	0.893255	0.114752	0.310792
O7	1.0	0.108024	0.551944	0.685912
O8	1.0	0.226776	0.449158	0.311172
O9	1.0	0.559673	0.449870	0.312006
O10	1.0	0.892192	0.450133	0.311311
O11	1.0	0.110292	0.894044	0.687166
O12	1.0	0.226259	0.781456	0.311319
O13	1.0	0.447162	0.893973	0.687482
O14	1.0	0.559996	0.781613	0.311553
O15	1.0	0.780409	0.898736	0.686404
O16	1.0	0.892657	0.782103	0.311838
O17	1.0	0.644760	0.583381	0.778194

	a	b
2*CO/Mo$_3$C$_2$O$_2$-2O$_V$	9.13230	9.13230

Mo1	1.0	0.112879	0.228844	0.348323
Mo2	1.0	0.224079	0.115837	0.589721
Mo3	1.0	0.999460	0.999917	0.468091
Mo4	1.0	0.446912	0.228697	0.348568
Mo5	1.0	0.557419	0.116738	0.590678
Mo6	1.0	0.334055	0.002518	0.467598
Mo7	1.0	0.779314	0.228259	0.347930
Mo8	1.0	0.890520	0.118733	0.590365
Mo9	1.0	0.665343	0.002126	0.468738
Mo10	1.0	0.111273	0.559783	0.348250
Mo11	1.0	0.210363	0.441585	0.586231
Mo12	1.0	0.001385	0.341645	0.471634
Mo13	1.0	0.445909	0.561416	0.348925
Mo14	1.0	0.548375	0.447411	0.591338
Mo15	1.0	0.334421	0.338191	0.471684
Mo16	1.0	0.778100	0.560618	0.348970
Mo17	1.0	0.894476	0.451283	0.595589
Mo18	1.0	0.670629	0.343495	0.473162

Mo19	1.0	0.112555	0.894846	0.348866
Mo20	1.0	0.228599	0.786172	0.590612
Mo21	1.0	0.997348	0.667811	0.471086
Mo22	1.0	0.446099	0.894554	0.348555
Mo23	1.0	0.565228	0.799825	0.586953
Mo24	1.0	0.333852	0.670872	0.470132
Mo25	1.0	0.778257	0.894648	0.348592
Mo26	1.0	0.898288	0.799685	0.587350
Mo27	1.0	0.664234	0.667988	0.473606
C1	1.0	0.108580	0.221736	0.529402
C2	1.0	0.223493	0.119486	0.408307
C3	1.0	0.441171	0.218747	0.529064
C4	1.0	0.560258	0.120493	0.408329
C5	1.0	0.776115	0.225852	0.530951
C6	1.0	0.890685	0.118322	0.408541
C7	1.0	0.112613	0.567708	0.530770
C8	1.0	0.223577	0.449499	0.408901
C9	1.0	0.443241	0.565250	0.535573
C10	1.0	0.556832	0.449695	0.409690
C11	1.0	0.780164	0.563574	0.538220
C12	1.0	0.889339	0.448300	0.408754
C13	1.0	0.117651	0.895836	0.529811
C14	1.0	0.219571	0.779183	0.407952
C15	1.0	0.443633	0.897892	0.529969
C16	1.0	0.557060	0.781882	0.408338
C17	1.0	0.781147	0.899959	0.529389
C18	1.0	0.885519	0.779754	0.408681
C19	1.0	0.542329	0.549250	0.675976
C20	1.0	0.851143	0.540015	0.679022
O1	1.0	0.113424	0.228263	0.645764
O2	1.0	0.224442	0.117097	0.292584
O3	1.0	0.440942	0.221784	0.645912
O4	1.0	0.557217	0.117128	0.292420
O5	1.0	0.779235	0.222168	0.647760
O6	1.0	0.891004	0.117150	0.292417
O7	1.0	0.127963	0.561071	0.647182
O8	1.0	0.224335	0.450849	0.292539
O9	1.0	0.557067	0.450980	0.292990
O10	1.0	0.889543	0.450714	0.292423
O11	1.0	0.114983	0.897919	0.646139
O12	1.0	0.223549	0.783581	0.292629
O13	1.0	0.449447	0.896080	0.646967
O14	1.0	0.557736	0.783744	0.292525
O15	1.0	0.783001	0.902293	0.646185

O16	1.0	0.890661	0.784062	0.292974
O17	1.0	0.532926	0.588697	0.727399
O18	1.0	0.852906	0.576541	0.731474

	a	b
2*COH/Mo$_3$C$_2$O$_2$-2O$_V$	9.13230	9.13230

Mo1	1.0	0.116536	0.231882	0.350313
Mo2	1.0	0.226752	0.111457	0.592984
Mo3	1.0	0.005077	0.005012	0.471170
Mo4	1.0	0.450023	0.231835	0.350337
Mo5	1.0	0.559729	0.111328	0.592847
Mo6	1.0	0.337875	0.004686	0.471017
Mo7	1.0	0.783424	0.231880	0.350327
Mo8	1.0	0.892903	0.110935	0.591905
Mo9	1.0	0.671175	0.005330	0.470856
Mo10	1.0	0.116758	0.565053	0.350332
Mo11	1.0	0.221915	0.442835	0.591418
Mo12	1.0	0.005282	0.340124	0.472725
Mo13	1.0	0.449843	0.564519	0.350966
Mo14	1.0	0.559302	0.442776	0.594773
Mo15	1.0	0.338559	0.338980	0.472908
Mo16	1.0	0.783171	0.564757	0.350955
Mo17	1.0	0.896916	0.442832	0.591064
Mo18	1.0	0.671651	0.338940	0.472981
Mo19	1.0	0.116751	0.898376	0.350459
Mo20	1.0	0.228825	0.781996	0.593371
Mo21	1.0	0.004124	0.672840	0.472670
Mo22	1.0	0.449801	0.898349	0.350509
Mo23	1.0	0.560224	0.782760	0.592514
Mo24	1.0	0.339812	0.671993	0.472818
Mo25	1.0	0.783397	0.898239	0.350284
Mo26	1.0	0.897784	0.782829	0.592432
Mo27	1.0	0.671189	0.670229	0.473806
C1	1.0	0.114839	0.221202	0.532599
C2	1.0	0.227471	0.119541	0.409952
C3	1.0	0.445561	0.218300	0.532149
C4	1.0	0.561798	0.119755	0.409848
C5	1.0	0.779629	0.220873	0.532542
C6	1.0	0.894852	0.119941	0.410312
C7	1.0	0.119398	0.564647	0.532871
C8	1.0	0.226736	0.451585	0.410722
C9	1.0	0.448438	0.559658	0.535468
C10	1.0	0.560553	0.451006	0.411022

C11	1.0	0.785708	0.559952	0.535424
C12	1.0	0.894645	0.451596	0.410772
C13	1.0	0.121005	0.894430	0.533406
C14	1.0	0.226548	0.782601	0.409930
C15	1.0	0.446962	0.894365	0.533101
C16	1.0	0.561800	0.784045	0.410519
C17	1.0	0.783427	0.894469	0.531801
C18	1.0	0.892671	0.784201	0.410441
C19	1.0	0.465739	0.565988	0.653977
C20	1.0	0.775227	0.565447	0.653841
O1	1.0	0.114305	0.221813	0.648714
O2	1.0	0.228278	0.122593	0.294258
O3	1.0	0.446521	0.217486	0.649907
O4	1.0	0.561315	0.122399	0.294222
O5	1.0	0.784000	0.222927	0.648724
O6	1.0	0.894683	0.122280	0.294201
O7	1.0	0.115596	0.555710	0.649198
O8	1.0	0.228483	0.456009	0.294465
O9	1.0	0.561901	0.456343	0.294655
O10	1.0	0.894920	0.456037	0.294503
O11	1.0	0.117130	0.889320	0.650679
O12	1.0	0.228024	0.788993	0.294245
O13	1.0	0.449708	0.889920	0.650589
O14	1.0	0.561191	0.788413	0.294616
O15	1.0	0.784987	0.893520	0.649037
O16	1.0	0.894425	0.788645	0.294535
O17	1.0	0.453422	0.563788	0.716615
O18	1.0	0.790550	0.561408	0.716073
H1	1.0	0.903559	0.649466	0.729894
H2	1.0	0.437559	0.656966	0.731482

	a	b
*COH-*COH/Mo$_3$C$_2$O$_2$-2O$_V$	9.13230	9.13230

Mo1	1.0	0.119703	0.232664	0.349894
Mo2	1.0	0.230449	0.113772	0.593865
Mo3	1.0	0.012899	0.008632	0.471171
Mo4	1.0	0.453037	0.232516	0.350340
Mo5	1.0	0.565748	0.114771	0.594171
Mo6	1.0	0.343118	0.007393	0.471112
Mo7	1.0	0.786710	0.232812	0.349805
Mo8	1.0	0.900721	0.119025	0.593126
Mo9	1.0	0.674948	0.009717	0.471198
Mo10	1.0	0.119230	0.565051	0.351062

Mo11	1.0	0.219218	0.440857	0.586947
Mo12	1.0	0.011054	0.343753	0.473566
Mo13	1.0	0.452657	0.564666	0.351244
Mo14	1.0	0.563043	0.446497	0.587874
Mo15	1.0	0.345130	0.339420	0.474092
Mo16	1.0	0.785685	0.564725	0.351257
Mo17	1.0	0.904109	0.440623	0.588514
Mo18	1.0	0.674680	0.339930	0.474428
Mo19	1.0	0.119572	0.899207	0.350860
Mo20	1.0	0.234428	0.787301	0.593605
Mo21	1.0	0.005999	0.673834	0.474184
Mo22	1.0	0.453329	0.899418	0.350881
Mo23	1.0	0.576490	0.791067	0.595830
Mo24	1.0	0.345828	0.674777	0.473705
Mo25	1.0	0.786046	0.898235	0.350702
Mo26	1.0	0.892560	0.789033	0.596673
Mo27	1.0	0.676928	0.674987	0.474623
C1	1.0	0.119326	0.221052	0.532333
C2	1.0	0.231120	0.122949	0.410099
C3	1.0	0.449929	0.218872	0.532772
C4	1.0	0.567501	0.122505	0.410062
C5	1.0	0.782922	0.222129	0.532916
C6	1.0	0.898737	0.122304	0.410712
C7	1.0	0.124693	0.571024	0.531450
C8	1.0	0.230796	0.451949	0.411256
C9	1.0	0.452990	0.564725	0.537423
C10	1.0	0.564841	0.453384	0.411691
C11	1.0	0.791933	0.563731	0.538501
C12	1.0	0.897168	0.451816	0.411223
C13	1.0	0.123342	0.896518	0.533740
C14	1.0	0.230157	0.784591	0.411063
C15	1.0	0.453124	0.897239	0.533699
C16	1.0	0.565809	0.785432	0.411194
C17	1.0	0.789645	0.896913	0.534656
C18	1.0	0.895675	0.785259	0.411021
C19	1.0	0.564305	0.620946	0.672431
C20	1.0	0.713355	0.609753	0.671898
O1	1.0	0.125021	0.232546	0.648962
O2	1.0	0.230622	0.121868	0.294270
O3	1.0	0.455304	0.228755	0.648763
O4	1.0	0.563282	0.122335	0.294306
O5	1.0	0.791207	0.231874	0.649315
O6	1.0	0.897031	0.121469	0.294327
O7	1.0	0.123155	0.555434	0.647479

O8	1.0	0.230513	0.456509	0.294768
O9	1.0	0.563661	0.456060	0.294905
O10	1.0	0.897375	0.456455	0.294728
O11	1.0	0.121665	0.895507	0.651037
O12	1.0	0.229951	0.788103	0.295103
O13	1.0	0.456933	0.895518	0.651293
O14	1.0	0.562914	0.787993	0.295123
O15	1.0	0.799734	0.919235	0.651476
O16	1.0	0.897029	0.787888	0.295016
O17	1.0	0.471743	0.576543	0.726267
O18	1.0	0.767534	0.556344	0.721530
H1	1.0	0.696950	0.540537	0.758807
H2	1.0	0.369037	0.584080	0.721616

	a	b
Slab /$Mo_2TiC_2O_2$-$2O_V$	9.08280	9.08280

Mo1	1.0	0.112299	0.223749	0.371585
Mo2	1.0	0.225063	0.113550	0.628489
Mo3	1.0	0.445329	0.223549	0.371215
Mo4	1.0	0.556920	0.112769	0.628633
Mo5	1.0	0.778974	0.223468	0.371216
Mo6	1.0	0.889599	0.113422	0.628460
Mo7	1.0	0.112468	0.556955	0.371775
Mo8	1.0	0.218719	0.436349	0.627212
Mo9	1.0	0.445470	0.556994	0.371763
Mo10	1.0	0.558727	0.441225	0.628208
Mo11	1.0	0.778983	0.557060	0.371421
Mo12	1.0	0.883736	0.441348	0.628243
Mo13	1.0	0.111987	0.889722	0.371428
Mo14	1.0	0.226627	0.784041	0.627876
Mo15	1.0	0.445158	0.889471	0.371482
Mo16	1.0	0.558202	0.783931	0.627815
Mo17	1.0	0.778749	0.889838	0.371407
Mo18	1.0	0.888540	0.776113	0.628195
Ti1	1.0	0.002254	0.001785	0.498936
Ti2	1.0	0.335158	0.002138	0.498902
Ti3	1.0	0.669196	0.001934	0.498806
Ti4	1.0	0.003145	0.337389	0.501268
Ti5	1.0	0.336311	0.337455	0.501280
Ti6	1.0	0.668854	0.334906	0.498706
Ti7	1.0	0.003120	0.667003	0.500778
Ti8	1.0	0.334443	0.666439	0.502970
Ti9	1.0	0.666279	0.667305	0.500397

C1	1.0	0.111768	0.221922	0.563503
C2	1.0	0.224072	0.113483	0.435821
C3	1.0	0.446764	0.223177	0.563681
C4	1.0	0.556800	0.112464	0.435456
C5	1.0	0.777942	0.223113	0.563767
C6	1.0	0.890864	0.113486	0.435841
C7	1.0	0.111269	0.556161	0.569219
C8	1.0	0.224021	0.446598	0.436556
C9	1.0	0.446258	0.556006	0.569234
C10	1.0	0.556607	0.446167	0.435966
C11	1.0	0.777915	0.554344	0.563320
C12	1.0	0.891021	0.446197	0.435957
C13	1.0	0.112999	0.891100	0.563812
C14	1.0	0.223783	0.778167	0.436309
C15	1.0	0.446893	0.892190	0.563378
C16	1.0	0.555845	0.778293	0.436229
C17	1.0	0.779597	0.891034	0.563726
C18	1.0	0.890068	0.778440	0.436026
O1	1.0	0.115656	0.229302	0.688051
O2	1.0	0.222753	0.112036	0.311824
O3	1.0	0.445814	0.226369	0.688245
O4	1.0	0.556155	0.111875	0.311731
O5	1.0	0.781724	0.226374	0.688201
O6	1.0	0.889998	0.112300	0.311841
O7	1.0	0.223680	0.446418	0.312209
O8	1.0	0.556702	0.446003	0.311886
O9	1.0	0.777415	0.553415	0.687889
O10	1.0	0.890099	0.445873	0.311892
O11	1.0	0.111592	0.885113	0.687728
O12	1.0	0.222920	0.778544	0.311900
O13	1.0	0.442128	0.883336	0.687855
O14	1.0	0.556397	0.778761	0.311928
O15	1.0	0.773833	0.884628	0.687589
O16	1.0	0.889838	0.778963	0.311847

	a	b
$^{*}CO/Mo_2TiC_2O_2-2O_V$	9.08280	9.08280

Mo1	1.0	0.113859	0.226089	0.371439
Mo2	1.0	0.222921	0.112394	0.627928
Mo3	1.0	0.446777	0.225932	0.371121
Mo4	1.0	0.558238	0.116029	0.627958
Mo5	1.0	0.780602	0.225808	0.371148
Mo6	1.0	0.889792	0.112294	0.627913

Mo7	1.0	0.114196	0.559001	0.371803
Mo8	1.0	0.221424	0.442554	0.629117
Mo9	1.0	0.446655	0.559016	0.371752
Mo10	1.0	0.560004	0.443586	0.628229
Mo11	1.0	0.780425	0.559113	0.371124
Mo12	1.0	0.884114	0.443821	0.628211
Mo13	1.0	0.113461	0.891928	0.371217
Mo14	1.0	0.228035	0.787413	0.627228
Mo15	1.0	0.446786	0.891868	0.371426
Mo16	1.0	0.559396	0.787327	0.627234
Mo17	1.0	0.780162	0.891874	0.371211
Mo18	1.0	0.888614	0.776995	0.627752
Ti1	1.0	0.002095	0.002389	0.498241
Ti2	1.0	0.335954	0.003080	0.498658
Ti3	1.0	0.668969	0.002783	0.498579
Ti4	1.0	0.002955	0.336945	0.501340
Ti5	1.0	0.335147	0.336928	0.501426
Ti6	1.0	0.669201	0.336554	0.498825
Ti7	1.0	0.003139	0.668500	0.500016
Ti8	1.0	0.334054	0.666737	0.503323
Ti9	1.0	0.666853	0.667861	0.500025
C1	1.0	0.109937	0.219017	0.562662
C2	1.0	0.224907	0.115279	0.435586
C3	1.0	0.446714	0.224432	0.563380
C4	1.0	0.557844	0.114682	0.435307
C5	1.0	0.778781	0.224336	0.563376
C6	1.0	0.891534	0.115182	0.435579
C7	1.0	0.112126	0.559146	0.569238
C8	1.0	0.224974	0.448176	0.436492
C9	1.0	0.447516	0.559023	0.569272
C10	1.0	0.557124	0.447565	0.435864
C11	1.0	0.778487	0.555959	0.563128
C12	1.0	0.891949	0.447582	0.435910
C13	1.0	0.112868	0.891616	0.563127
C14	1.0	0.224832	0.779885	0.436179
C15	1.0	0.447801	0.894615	0.562830
C16	1.0	0.556620	0.779693	0.436158
C17	1.0	0.779656	0.891398	0.563128
C18	1.0	0.890181	0.778809	0.435645
C19	1.0	0.268277	0.541979	0.724515
O1	1.0	0.107433	0.214672	0.687068
O2	1.0	0.225024	0.115050	0.311707
O3	1.0	0.445849	0.227698	0.687603
O4	1.0	0.558495	0.114998	0.311650

O5	1.0	0.782040	0.227730	0.687587
O6	1.0	0.892031	0.114850	0.311720
O7	1.0	0.225542	0.448879	0.312128
O8	1.0	0.558199	0.448837	0.311813
O9	1.0	0.777507	0.554923	0.688117
O10	1.0	0.892685	0.448665	0.311936
O11	1.0	0.111832	0.886214	0.687301
O12	1.0	0.225348	0.781698	0.311967
O13	1.0	0.446690	0.893552	0.687023
O14	1.0	0.558589	0.781730	0.311930
O15	1.0	0.774347	0.886202	0.687290
O16	1.0	0.891982	0.781674	0.311546
O17	1.0	0.283315	0.576867	0.781473

	a	b
$2^*CO/Mo_2TiC_2O_2\text{-}2O_V$	9.08280	9.08280

Mo1	1.0	0.111511	0.229672	0.372152
Mo2	1.0	0.218817	0.117819	0.628373
Mo3	1.0	0.444572	0.229388	0.371859
Mo4	1.0	0.555117	0.119972	0.628522
Mo5	1.0	0.778335	0.229553	0.371952
Mo6	1.0	0.886298	0.115882	0.628887
Mo7	1.0	0.111457	0.562443	0.372474
Mo8	1.0	0.223866	0.447785	0.630966
Mo9	1.0	0.444191	0.562367	0.372206
Mo10	1.0	0.556782	0.447999	0.628160
Mo11	1.0	0.778044	0.562530	0.371921
Mo12	1.0	0.882000	0.449284	0.629667
Mo13	1.0	0.111286	0.895613	0.371988
Mo14	1.0	0.229727	0.793300	0.627211
Mo15	1.0	0.444321	0.895548	0.372044
Mo16	1.0	0.556191	0.794736	0.626271
Mo17	1.0	0.777877	0.895763	0.371924
Mo18	1.0	0.884195	0.783697	0.628540
Ti1	1.0	0.000110	0.006633	0.499117
Ti2	1.0	0.332525	0.005391	0.499937
Ti3	1.0	0.666127	0.006256	0.499419
Ti4	1.0	0.000100	0.339495	0.502464
Ti5	1.0	0.333165	0.341453	0.501288
Ti6	1.0	0.666485	0.339970	0.499389
Ti7	1.0	-0.000100	0.671969	0.500971
Ti8	1.0	0.333053	0.671246	0.502366
Ti9	1.0	0.665532	0.672692	0.500005

C1	1.0	0.106756	0.223976	0.563537
C2	1.0	0.223094	0.118943	0.436312
C3	1.0	0.443712	0.228785	0.563359
C4	1.0	0.556013	0.118633	0.436124
C5	1.0	0.777052	0.226456	0.564135
C6	1.0	0.889676	0.119143	0.436355
C7	1.0	0.112677	0.564584	0.568963
C8	1.0	0.222317	0.451699	0.437018
C9	1.0	0.445908	0.564095	0.567989
C10	1.0	0.555228	0.451287	0.436453
C11	1.0	0.776655	0.564700	0.563591
C12	1.0	0.889777	0.451237	0.436801
C13	1.0	0.108470	0.895079	0.563957
C14	1.0	0.222508	0.783659	0.436782
C15	1.0	0.445570	0.898860	0.562756
C16	1.0	0.554431	0.783736	0.436495
C17	1.0	0.777274	0.896231	0.563440
C18	1.0	0.888770	0.783388	0.436276
C19	1.0	0.349398	0.545612	0.719840
C20	1.0	0.054999	0.538626	0.711322
O1	1.0	0.105706	0.220132	0.688656
O2	1.0	0.222234	0.118082	0.312545
O3	1.0	0.443290	0.233134	0.687384
O4	1.0	0.555703	0.118197	0.312500
O5	1.0	0.770567	0.224697	0.688238
O6	1.0	0.889101	0.118153	0.312567
O7	1.0	0.222470	0.451622	0.312736
O8	1.0	0.555683	0.451530	0.312531
O9	1.0	0.765128	0.560052	0.688163
O10	1.0	0.889777	0.451876	0.312763
O11	1.0	0.111735	0.896285	0.687275
O12	1.0	0.222391	0.784812	0.312672
O13	1.0	0.447295	0.903993	0.688677
O14	1.0	0.555739	0.784755	0.312593
O15	1.0	0.773374	0.893856	0.687809
O16	1.0	0.889045	0.784861	0.312518
O17	1.0	0.400828	0.580124	0.774860
O18	1.0	0.067857	0.564544	0.769806

	a	b
2*COH/Mo$_2$TiC$_2$O$_2$-2O$_V$	9.08280	9.08280

Mo1	1.0	0.109920	0.232334	0.373400
Mo2	1.0	0.216349	0.119669	0.630317

Mo3	1.0	0.442976	0.232213	0.373397
Mo4	1.0	0.551318	0.119448	0.630068
Mo5	1.0	0.776634	0.232216	0.373405
Mo6	1.0	0.886383	0.119742	0.630352
Mo7	1.0	0.109991	0.565407	0.373644
Mo8	1.0	0.215510	0.449197	0.629560
Mo9	1.0	0.443037	0.565422	0.373635
Mo10	1.0	0.555466	0.452092	0.629990
Mo11	1.0	0.776335	0.565167	0.373438
Mo12	1.0	0.880157	0.451803	0.629452
Mo13	1.0	0.109828	0.898612	0.373341
Mo14	1.0	0.219511	0.791664	0.629564
Mo15	1.0	0.443057	0.898574	0.373541
Mo16	1.0	0.555359	0.791280	0.630745
Mo17	1.0	0.776298	0.898640	0.373338
Mo18	1.0	0.885566	0.788533	0.629915
Ti1	1.0	0.995437	0.007651	0.500686
Ti2	1.0	0.329750	0.008598	0.501555
Ti3	1.0	0.662656	0.008765	0.501572
Ti4	1.0	0.996475	0.341253	0.502220
Ti5	1.0	0.329177	0.341799	0.502298
Ti6	1.0	0.663073	0.342395	0.501950
Ti7	1.0	0.996535	0.675309	0.501850
Ti8	1.0	0.330143	0.674585	0.503374
Ti9	1.0	0.662916	0.675507	0.502054
C1	1.0	0.103467	0.223722	0.564728
C2	1.0	0.220487	0.121228	0.437644
C3	1.0	0.438731	0.229418	0.565570
C4	1.0	0.553452	0.120798	0.437786
C5	1.0	0.773690	0.229065	0.565330
C6	1.0	0.886837	0.121187	0.437584
C7	1.0	0.106127	0.566460	0.567039
C8	1.0	0.220344	0.454257	0.438240
C9	1.0	0.444149	0.566553	0.567747
C10	1.0	0.553159	0.453945	0.438010
C11	1.0	0.774959	0.566706	0.564842
C12	1.0	0.887053	0.453815	0.437982
C13	1.0	0.104428	0.898377	0.565708
C14	1.0	0.220410	0.786612	0.438039
C15	1.0	0.441795	0.899064	0.565133
C16	1.0	0.552810	0.786692	0.438020
C17	1.0	0.776632	0.898225	0.565706
C18	1.0	0.886345	0.786394	0.437447
C19	1.0	0.425919	0.570458	0.695033

C20	1.0	0.123604	0.572803	0.693918
O1	1.0	0.106515	0.228489	0.691356
O2	1.0	0.221652	0.121225	0.313920
O3	1.0	0.441852	0.233059	0.689425
O4	1.0	0.554952	0.121299	0.314115
O5	1.0	0.773690	0.232833	0.689110
O6	1.0	0.888193	0.121279	0.313914
O7	1.0	0.221792	0.454873	0.314212
O8	1.0	0.554879	0.454585	0.314097
O9	1.0	0.772956	0.561283	0.689260
O10	1.0	0.888365	0.454417	0.314134
O11	1.0	0.107507	0.899352	0.691079
O12	1.0	0.221703	0.787725	0.314164
O13	1.0	0.441706	0.901915	0.689920
O14	1.0	0.554880	0.787836	0.314121
O15	1.0	0.776732	0.901571	0.690648
O16	1.0	0.888233	0.787801	0.313922
O17	1.0	0.439042	0.562300	0.761463
O18	1.0	0.105325	0.563818	0.761065
H1	1.0	0.336604	0.463864	0.780221
H2	1.0	0.090394	0.657271	0.778134

	a	b
*COH-*COH/Mo$_2$TiC$_2$O$_2$-2O$_V$	9.08280	9.08280

Mo1	1.0	0.122023	0.230796	0.374731
Mo2	1.0	0.233362	0.117813	0.630747
Mo3	1.0	0.455297	0.230579	0.374247
Mo4	1.0	0.569126	0.118809	0.631056
Mo5	1.0	0.789136	0.230789	0.374553
Mo6	1.0	0.899726	0.117261	0.631673
Mo7	1.0	0.122138	0.563835	0.375108
Mo8	1.0	0.239077	0.446547	0.629781
Mo9	1.0	0.455084	0.563939	0.374859
Mo10	1.0	0.567441	0.447551	0.630665
Mo11	1.0	0.788915	0.563893	0.374622
Mo12	1.0	0.895227	0.451749	0.633018
Mo13	1.0	0.121913	0.896684	0.374578
Mo14	1.0	0.237165	0.789544	0.632821
Mo15	1.0	0.454932	0.896626	0.374691
Mo16	1.0	0.570811	0.792286	0.630981
Mo17	1.0	0.788544	0.896777	0.374670
Mo18	1.0	0.897266	0.785750	0.630972
Ti1	1.0	0.010924	0.005152	0.501759

Ti2	1.0	0.344206	0.005441	0.502302
Ti3	1.0	0.678117	0.006922	0.501768
Ti4	1.0	0.011591	0.340011	0.505339
Ti5	1.0	0.344870	0.340293	0.502532
Ti6	1.0	0.678675	0.339829	0.501479
Ti7	1.0	0.010589	0.671741	0.504295
Ti8	1.0	0.343265	0.671070	0.505985
Ti9	1.0	0.674189	0.671404	0.504224
C1	1.0	0.118775	0.223068	0.565382
C2	1.0	0.233338	0.118490	0.438785
C3	1.0	0.457631	0.229041	0.565940
C4	1.0	0.566275	0.118408	0.438619
C5	1.0	0.789267	0.227377	0.566844
C6	1.0	0.900471	0.119423	0.438979
C7	1.0	0.122853	0.561445	0.572847
C8	1.0	0.232938	0.452298	0.439673
C9	1.0	0.459318	0.564336	0.571105
C10	1.0	0.566352	0.451934	0.438920
C11	1.0	0.788341	0.562510	0.566849
C12	1.0	0.900893	0.452151	0.439350
C13	1.0	0.121328	0.894839	0.567039
C14	1.0	0.232619	0.783781	0.439672
C15	1.0	0.458337	0.896967	0.566567
C16	1.0	0.564647	0.783696	0.439390
C17	1.0	0.788968	0.897025	0.566671
C18	1.0	0.899113	0.783136	0.439132
C19	1.0	0.215245	0.560105	0.719064
C20	1.0	0.066277	0.569075	0.718414
O1	1.0	0.125489	0.223897	0.690027
O2	1.0	0.233091	0.120517	0.314988
O3	1.0	0.455122	0.231417	0.690184
O4	1.0	0.566801	0.120436	0.314931
O5	1.0	0.786086	0.225563	0.691456
O6	1.0	0.899899	0.120069	0.315162
O7	1.0	0.232908	0.453887	0.315334
O8	1.0	0.566439	0.453954	0.314992
O9	1.0	0.775661	0.562022	0.691841
O10	1.0	0.900040	0.453707	0.315137
O11	1.0	0.123999	0.901050	0.690964
O12	1.0	0.233205	0.786644	0.315236
O13	1.0	0.460264	0.901446	0.691596
O14	1.0	0.566417	0.786998	0.315222
O15	1.0	0.785653	0.892753	0.691358
O16	1.0	0.899922	0.787242	0.315077

O17	1.0	0.309157	0.587397	0.774911
O18	1.0	0.016570	0.603804	0.777787
H1	1.0	0.256988	0.614495	0.813047
H2	1.0	-0.092246	0.600879	0.770231