Electronic Supplementary Material (ESI) for Faraday Discussions
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Infrared driven CO oxidation reactions on isolated platinum cluster oxides, $Pt_nO_m^+$

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Electronic Supplementary Information

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Table S1: Structures, spin states and relative energies of the 10 lowest energy $Pt_4O_2CO^+$ structures identified based on dissociated O_2 (see Table S2 for coordinate files)

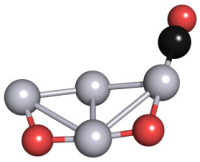
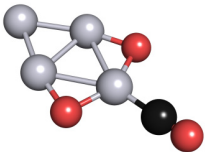
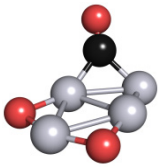
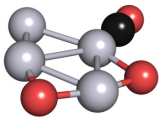
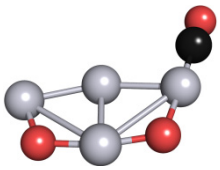
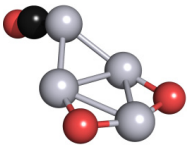
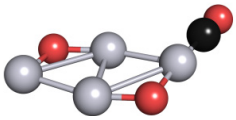
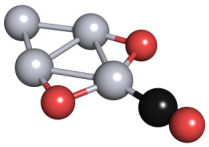
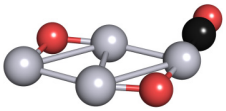
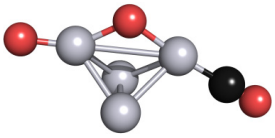
Structure Number	Structure	2S+1	Relative Energy /eV
1		2	0.00
2		2	0.07
3		2	0.11
4		2	0.11
5		4	0.22
6		2	0.23
7		2	0.27
8		4	0.31
9		4	0.33
10		2	0.37

Table S2: Coordinates for the structures in Table S1 in xyz format.

8				8			
Structure 1				**Structure 2**			
Pt	0.93061	0.77264	1.65984	Pt	-3.32120	1.83109	0.21248
Pt	-1.01579	0.13788	0.28900	Pt	-1.09301	1.38715	1.15561
Pt	-1.83070	2.15953	1.54907	Pt	0.57506	-0.32157	-0.02896
Pt	0.90557	-0.99324	-0.93423	Pt	-1.86658	0.22722	-0.95574
O	1.94870	-0.39648	0.64210	O	0.67479	0.78306	1.55172
O	-0.22876	1.96827	2.51765	O	-0.45847	-0.91692	-1.54799
C	-0.05933	-1.62714	-2.41522	C	2.24596	-1.22684	-0.15207
O	-0.65030	-2.02145	-3.30821	O	3.24346	-1.76320	-0.23504
8				8			
Structure 3				**Structure 4**			
Pt	-2.23744	0.20087	-0.48652	Pt	-1.36220	0.46373	-1.92198
Pt	-0.10740	-0.00257	0.98734	Pt	-2.10899	-0.62305	0.14425
Pt	1.94638	-1.36924	-0.04649	Pt	-0.40173	-0.97377	1.93070
Pt	-0.09785	-0.71869	-1.54926	Pt	0.48215	0.27117	-0.22219
O	1.59378	-0.65994	1.65779	O	-2.20988	-1.49681	1.89477
O	1.51700	-1.72407	-1.82703	O	1.28509	-0.29883	1.50132
C	-1.26314	1.56614	0.52494	C	1.77038	1.08909	-1.32163
O	-1.35132	2.70749	0.73923	O	2.54519	1.56847	-2.00524
8				8			
Structure 5				**Structure 6**			
Pt	1.56148	1.44099	-0.12240	Pt	-1.09931	-0.68641	-1.10906
Pt	-0.06534	-0.21909	-0.89492	Pt	-0.60868	0.01284	1.27910
Pt	-0.59565	-0.25683	1.56630	Pt	0.88467	2.19932	1.47722
Pt	0.99132	0.33052	-3.06799	Pt	0.97236	0.72637	-0.72809
O	2.00837	1.48340	-1.96989	O	-0.37571	1.39619	2.59182
O	0.83688	1.10337	1.56755	O	1.78051	2.37021	-0.14850
C	-1.95520	-1.54925	1.49504	C	-0.88205	-2.45971	-1.56852
O	-2.78185	-2.33311	1.42632	O	-0.67180	-3.55881	-1.79397
8				8			
Structure 7				**Structure 7**			
Pt	-2.06608	2.63430	1.30467	Pt	-3.32146	1.85218	0.20184
Pt	0.28092	0.89182	0.19040	Pt	-1.07646	1.39965	1.17355
Pt	-2.11475	0.33179	0.36720	Pt	0.58060	-0.32798	-0.02684
Pt	0.32586	-1.51961	-0.48788	Pt	-1.86686	0.21374	-0.97832
O	-1.60591	-1.38654	-0.21176	O	0.67911	0.79727	1.57522
O	-0.26305	2.61600	0.79675	O	-0.46852	-0.92496	-1.57172
C	2.16768	-1.72315	-0.85969	C	2.23865	-1.23416	-0.14607
O	3.27534	-1.84459	-1.09968	O	3.23494	-1.77573	-0.22766
8				8			
Structure 9				**Structure 10**			
Pt	-1.02452	0.00313	3.41340	Pt	0.65136	0.73108	2.00862
Pt	0.50632	0.16208	0.68664	Pt	-0.95029	-1.01529	1.02693
Pt	-1.86832	-0.39013	1.12781	Pt	-1.03600	1.38572	0.18814
Pt	-0.23891	-0.17272	-1.70792	Pt	0.45437	-0.35954	-1.08139
O	-1.90988	-0.53598	-0.73795	O	1.54939	0.22007	0.42309
O	0.63241	0.32667	2.59570	O	0.79173	1.28930	3.64646
C	1.43589	0.19184	-2.47172	C	-0.45592	-0.94961	-2.63800
O	2.46702	0.41511	-2.90595	O	-1.00463	-1.30173	-3.57385

Table S3: Structures, spin states and relative energies of the 10 lowest energy $Pt_4O_2CO^+$ structures identified with peroxo motifs.

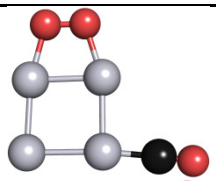
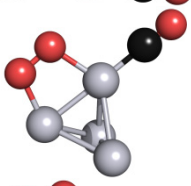
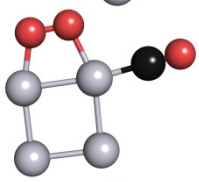
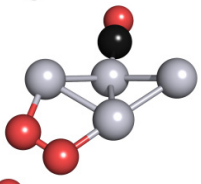
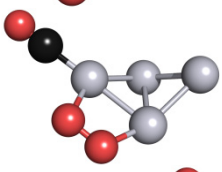
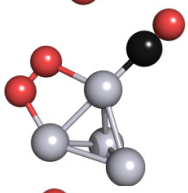
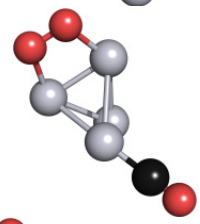
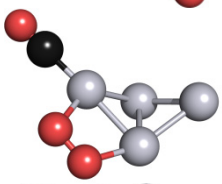
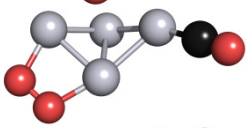
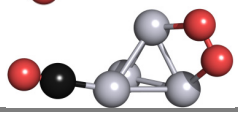
Structure Number	Structure	2S+1	Energy relative to Structure 1 /eV	Energy relative to Structure 11 /eV
11		2	1.39	0.00
12		2	1.52	0.12
13		2	1.52	0.13
14		2	1.58	0.19
15		2	1.61	0.22
16		4	1.62	0.23
17		2	1.70	0.31
18		4	1.75	0.36
19		4	1.76	0.37
20		4	1.78	0.38

Table S4: Coordinates for the structures in Table S3 in xyz format.

8			
Structure 11			
Pt	-0.99586	-1.34073	-0.09633
Pt	-0.80267	2.10125	-0.12754
Pt	0.84750	0.34284	0.11402
Pt	-2.69544	0.54048	-0.33166
O	0.92543	2.98972	0.10203
O	1.83460	2.00563	0.23424
C	0.12195	-2.84850	0.02145
O	0.76451	-3.79069	0.08379

8			
Structure 12			
Pt	-0.56007	-1.08716	1.70216
Pt	0.90939	-2.38589	-0.02117
Pt	0.12473	0.16901	-0.26805
Pt	-1.49049	-1.96003	-0.56018
C	0.65039	1.19753	-1.79776
O	0.96450	1.78133	-2.72444
O	-0.11514	1.52531	1.31809
O	-0.48332	0.75991	2.35135

8			
Structure 13			
Pt	-1.29037	-2.09094	0.00391
Pt	-1.64996	1.33525	-0.00969
Pt	0.31683	-0.15505	0.00100
Pt	-3.19684	-0.59158	-0.00434
O	-0.12112	2.50551	0.00132
O	0.98798	1.75760	0.00789
C	1.97778	-1.10545	0.00276
O	2.97569	-1.65534	-0.00284

8			
Structure 14			
Pt	0.27152	-2.49746	-0.47773
Pt	0.54545	1.56040	-0.61504
Pt	1.67477	-0.54222	0.07373
Pt	-0.90979	-0.40559	0.32530
O	2.21305	2.13355	0.14266
O	2.83569	0.99341	0.56389
C	-2.75520	-0.55959	0.08782
O	-3.87549	-0.68251	-0.10062

8			
Structure 15			
Pt	-0.82750	-3.04449	-0.96201
Pt	-0.17637	0.46515	0.02610
Pt	0.83036	-1.79322	0.35989
Pt	-1.80797	-1.40349	0.64674
O	1.83739	0.77358	0.17990
O	2.28908	-0.45505	0.45571
C	-0.86168	2.20680	-0.26279
O	-1.28330	3.25072	-0.44354

8			
Structure 16			
Pt	-0.20268	-1.15349	1.78920
Pt	0.81431	-2.48210	-0.23564
Pt	0.39391	0.13354	-0.21309
Pt	-1.57080	-1.64387	-0.36028
C	0.74054	1.14070	-1.80147
O	0.95541	1.73209	-2.75170
O	-0.40804	1.52081	1.27706
O	-0.72266	0.75231	2.29591

8			
Structure 17			
Pt	-1.47108	0.72236	0.93660
Pt	0.06007	-1.14181	-0.01636
Pt	0.32757	1.67741	-0.32787
Pt	-1.41885	0.09479	-1.62328
C	0.93633	-2.44692	-1.03639
O	1.43750	-3.24390	-1.68250
O	0.55615	2.43546	1.50193
O	-0.42769	1.90262	2.24787

8			
Structure 18			
Pt	-0.91607	-3.00985	-0.96249
Pt	-0.16172	0.42591	-0.07303
Pt	0.88485	-1.81828	0.25657
Pt	-1.75285	-1.39978	0.73479
O	1.79456	0.80545	0.26170
O	2.32081	-0.40938	0.49387
C	-0.87177	2.17859	-0.29095
O	-1.29780	3.22734	-0.42047

8			
Structure 19			
Pt	-0.96878	-1.48425	-0.18217
Pt	-0.59251	2.09065	-0.98844
Pt	0.49233	0.45414	0.49220
Pt	-2.18582	0.69165	0.37978
O	0.92176	3.07118	-0.12714
O	1.48182	2.18143	0.71421
C	0.09466	-3.03795	-0.17503
O	0.75653	-3.96685	-0.11341

8			
Structure 20			
Pt	-0.30882	-0.65427	1.90706
Pt	1.20879	-2.07490	0.32209
Pt	1.33911	0.54218	0.64063
Pt	-0.64811	-0.56933	-0.70211
C	-0.65971	-0.36048	-2.58700
O	-0.60503	-0.24782	-3.72062
O	0.27998	2.02281	1.72080
O	-0.60621	1.34180	2.41915