

An investigation of the initial steps of the electrochemical reduction mechanism of CO₂ on Pt electrodes

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This file contains

Structures and vibrational frequencies (only for Pt13 clusters) in water and acetonitrile solvent for different spin multiplicities and total charges of:

1. Pt13 and Pt20 clusters
2. CO₂ adsorbed on Pt clusters
3. Transition states for CO₂ adsorption on Pt13 clusters
4. CO₂ (2 H₂O) adsorbed on Pt13 clusters
5. COOH adsorbed on Pt clusters
6. HCO₂ adsorbed on Pt clusters
7. CO adsorbed on Pt clusters

All the structures here reported were optimized at the B3LYP/SDD-6-311+G(d,p) level of theory in the case of Pt13 clusters or at the level described in the text to computed B3LYP/SDD-6-311+G(d,p) energies for Pt20 clusters.

1. Structures and vibrational frequencies of Pt13 and Pt20 clusters

Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge 0 – Spin Multiplicity 3

Pt	-0.045324	-0.117969	0.038083
Pt	-0.056772	0.067927	2.577931
Pt	2.268810	0.028004	1.354766
Pt	1.640013	2.353580	0.357812
Pt	0.855733	4.624910	-0.714439
Pt	-0.985955	4.878660	1.013498
Pt	-0.276379	2.584818	2.080447
Pt	-2.686634	0.106906	2.495789
Pt	-2.575746	0.122424	-0.130387
Pt	-1.184558	0.097350	-2.361010
Pt	-0.208066	2.396482	-1.617875
Pt	-2.045318	2.622042	0.189943
Pt	-2.856978	2.641793	2.721533

Vibrational Frequencies (cm⁻¹)

30.2618	32.8405	45.2829
49.0518	51.2822	52.3261
58.3522	62.0180	67.9614
78.4187	88.5619	92.1283
101.7725	105.2106	112.3880
115.9633	116.8244	125.3884
128.8484	132.2032	143.3246
158.8941	160.1007	163.0700
165.5308	167.0335	173.1031
174.2246	180.5014	184.1602
191.9154	210.4870	213.7498

Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge -1 – Spin Multiplicity 2

Pt	-0.048489	-0.116524	0.041341
Pt	-0.035888	0.049224	2.582521
Pt	2.280121	0.008157	1.337203
Pt	1.635232	2.349481	0.366838
Pt	0.826399	4.625952	-0.684664
Pt	-1.025976	4.821904	1.053822
Pt	-0.222113	2.587300	2.153068
Pt	-2.665451	0.162225	2.484341
Pt	-2.578791	0.104148	-0.146168
Pt	-1.174057	0.079787	-2.369297
Pt	-0.213477	2.392464	-1.617552
Pt	-2.110240	2.627354	0.124872
Pt	-2.824443	2.715457	2.679767

Vibrational Frequencies (cm-1)

27.9604	31.1524	42.7942
46.1920	47.4636	51.9309
53.6584	59.5098	64.9279
76.8194	86.3354	88.7004
93.8301	101.0724	106.4854
109.2645	113.1534	116.3358
117.2700	129.2839	139.4918
142.2101	157.7136	157.9125
159.5739	161.2202	165.6606
171.3955	172.5241	180.3204
188.2547	197.9074	208.9200

Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge -2 – Spin Multiplicity 1

Pt	-0.014729	-0.093423	0.010250
Pt	0.062220	-0.051186	2.569613
Pt	2.337987	-0.058580	1.258534
Pt	1.687300	2.368489	0.527069
Pt	0.737703	4.540765	-0.601668
Pt	-1.152571	4.639081	1.166996
Pt	-0.238243	2.468523	2.215645
Pt	-2.526246	0.488360	2.370840
Pt	-2.560411	0.011075	-0.238511
Pt	-1.097978	0.013983	-2.420006
Pt	-0.363725	2.413268	-1.678422
Pt	-2.182907	2.520483	0.123250
Pt	-2.845573	3.146089	2.702501

Vibrational Frequencies (cm-1)

25.4725	34.8993	38.7195
42.6232	43.8712	45.2376
45.6339	55.1486	63.6098
73.9186	75.8489	78.9458
91.5545	96.2376	102.2263
107.8600	108.2885	108.9868
116.9220	117.8031	134.5547
139.1133	144.2378	151.2199
157.6928	158.7414	166.7964
172.6410	177.5134	178.8476
182.1169	205.8421	207.6877

Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge 0 – Spin Multiplicity 3

Pt	-0.045324	-0.117969	0.038083
Pt	-0.056772	0.067927	2.577931
Pt	2.268810	0.028004	1.354766
Pt	1.640013	2.353580	0.357812
Pt	0.855733	4.624910	-0.714439
Pt	-0.985955	4.878660	1.013498
Pt	-0.276379	2.584818	2.080447
Pt	-2.686634	0.106906	2.495789
Pt	-2.575746	0.122424	-0.130387
Pt	-1.184558	0.097350	-2.361010
Pt	-0.208066	2.396482	-1.617875
Pt	-2.045318	2.622042	0.189943
Pt	-2.856978	2.641793	2.721533

Vibrational Frequencies (cm-1)

30.3522	32.7820	45.3036
48.9852	51.1384	52.2122
58.5314	61.8579	68.1311
78.3755	88.5554	92.0565
101.5869	105.1604	112.3260
115.9433	116.7735	125.3827
128.7395	132.1803	143.3917
159.0015	160.0834	163.1145
165.5383	166.9677	173.1074
174.1911	180.6017	184.3384
192.0367	210.5679	213.7170

Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -1 – Spin Multiplicity 2

Pt	-0.047972	-0.117397	0.040719
Pt	-0.035892	0.049765	2.581774
Pt	2.279418	0.008528	1.337965
Pt	1.634879	2.348721	0.366746
Pt	0.824242	4.624222	-0.683769
Pt	-1.027258	4.820789	1.055467
Pt	-0.221134	2.587219	2.153293
Pt	-2.664736	0.164367	2.482338
Pt	-2.578314	0.104602	-0.147442
Pt	-1.172538	0.079273	-2.369085
Pt	-0.214889	2.392000	-1.617480
Pt	-2.110479	2.627154	0.125211
Pt	-2.822502	2.717686	2.680354

Vibrational Frequencies (cm-1)

27.7487	31.2271	42.8864
46.1316	47.3664	51.8014
54.2403	59.6882	65.4054
76.7144	86.4708	88.8055
93.8211	100.9787	106.5771
109.5231	113.3469	116.3247
117.5186	129.4121	139.8175
142.5568	157.5513	157.9320
159.9592	161.4630	166.1294
171.7288	173.2491	180.2877
188.7352	198.1387	209.1545

Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -2 – Spin Multiplicity 1

Pt	-0.014729	-0.093423	0.010250
Pt	0.062220	-0.051186	2.569613
Pt	2.337987	-0.058580	1.258534
Pt	1.687300	2.368489	0.527069
Pt	0.737703	4.540765	-0.601668
Pt	-1.152571	4.639081	1.166996
Pt	-0.238243	2.468523	2.215645
Pt	-2.526246	0.488360	2.370840
Pt	-2.560411	0.011075	-0.238511
Pt	-1.097978	0.013983	-2.420006
Pt	-0.363725	2.413268	-1.678422
Pt	-2.182907	2.520483	0.123250
Pt	-2.845573	3.146089	2.702501

Vibrational Frequencies (cm-1)

25.3558	35.0135	38.8108
42.5500	43.8991	45.3817
45.5327	55.1327	63.7779
73.7422	76.1721	78.9237
91.4583	96.3332	102.0914
107.7746	108.3278	109.0272
116.8087	117.7210	134.5250
139.1314	144.2863	151.2963
157.6901	158.9274	166.6419
172.6290	177.5544	179.1062
182.1399	205.9764	207.7720

Pt20 – B3LYP/see text – Water – Charge 0 – Spin Multiplicity 15

Pt	-2.801561	-1.429350	2.491303
Pt	-0.101213	-1.430803	2.416818
Pt	2.744267	-1.538448	2.508848
Pt	-4.184877	-1.560996	0.092233
Pt	-1.448641	-1.911027	0.113376
Pt	1.368556	-1.928220	0.194984
Pt	4.134236	-1.722780	0.117820
Pt	-2.793581	-1.746281	-2.296129
Pt	0.027479	-1.787260	-2.182483
Pt	2.752426	-1.853555	-2.277666
Pt	-2.754929	0.725033	0.749490
Pt	0.017668	0.667370	0.747322
Pt	2.792268	0.615818	0.765767
Pt	-1.364397	0.536822	-1.642505
Pt	1.412059	0.484016	-1.631619
Pt	-1.325529	3.011702	1.401498
Pt	1.448212	2.957557	1.410485
Pt	0.066076	2.824817	-0.995716
Pt	2.841357	2.770775	-0.983210
Pt	-2.710007	2.879303	-1.000388

Pt20 – B3LYP/see text – Water – Charge -1 – Spin Multiplicity 14

Pt	-2.801579	-1.429334	2.491386
Pt	-0.088472	-1.446978	2.427563
Pt	2.744302	-1.538466	2.508807
Pt	-4.184869	-1.560969	0.092022
Pt	-1.454515	-1.899917	0.119351
Pt	1.357018	-1.928200	0.190613
Pt	4.134239	-1.722717	0.117875
Pt	-2.793606	-1.746296	-2.296058
Pt	0.020928	-1.789689	-2.181549
Pt	2.752430	-1.853603	-2.277706
Pt	-2.754928	0.725025	0.749552
Pt	0.017674	0.667349	0.747344
Pt	2.792284	0.615806	0.765730
Pt	-1.364413	0.536827	-1.642450
Pt	1.412056	0.484026	-1.631614
Pt	-1.325527	3.011713	1.401470
Pt	1.448208	2.957558	1.410494
Pt	0.066082	2.824810	-0.995717
Pt	2.841352	2.770776	-0.983217
Pt	-2.710016	2.879298	-1.000385

Pt20 – B3LYP/see text – Water – Charge -2 – Spin Multiplicity 13

Pt	-2.801573	-1.429366	2.491396
Pt	-0.086403	-1.470213	2.427967
Pt	2.744287	-1.538422	2.508839
Pt	-4.184878	-1.560946	0.091976
Pt	-1.463719	-1.904402	0.123561
Pt	1.357416	-1.948958	0.192509
Pt	4.134232	-1.722797	0.117763
Pt	-2.793547	-1.746299	-2.296053
Pt	0.019704	-1.792097	-2.178439
Pt	2.752416	-1.853550	-2.277663
Pt	-2.754925	0.725023	0.749567
Pt	0.017658	0.667379	0.747386
Pt	2.792279	0.615823	0.765741
Pt	-1.364424	0.536789	-1.642418
Pt	1.412044	0.484012	-1.631596
Pt	-1.325527	3.011719	1.401456
Pt	1.448209	2.957560	1.410487
Pt	0.066092	2.824808	-0.995741
Pt	2.841361	2.770769	-0.983217
Pt	-2.710014	2.879298	-1.000389

Pt20 – B3LYP/see text – Acetonitrile – Charge 0 – Spin Multiplicity 15

Pt	-2.801561	-1.429350	2.491303
Pt	-0.101213	-1.430803	2.416818
Pt	2.744267	-1.538448	2.508848
Pt	-4.184877	-1.560996	0.092233
Pt	-1.448641	-1.911027	0.113376
Pt	1.368556	-1.928220	0.194984
Pt	4.134236	-1.722780	0.117820
Pt	-2.793581	-1.746281	-2.296129
Pt	0.027479	-1.787260	-2.182483
Pt	2.752426	-1.853555	-2.277666
Pt	-2.754929	0.725033	0.749490
Pt	0.017668	0.667370	0.747322
Pt	2.792268	0.615818	0.765767
Pt	-1.364397	0.536822	-1.642505
Pt	1.412059	0.484016	-1.631619
Pt	-1.325529	3.011702	1.401498
Pt	1.448212	2.957557	1.410485
Pt	0.066076	2.824817	-0.995716
Pt	2.841357	2.770775	-0.983210
Pt	-2.710007	2.879303	-1.000388

Pt20 – B3LYP/see text – Acetonitrile – Charge -1 – Spin Multiplicity 14

Pt	-2.801579	-1.429334	2.491386
Pt	-0.088472	-1.446978	2.427563
Pt	2.744302	-1.538466	2.508807
Pt	-4.184869	-1.560969	0.092022
Pt	-1.454515	-1.899917	0.119351
Pt	1.357018	-1.928200	0.190613
Pt	4.134239	-1.722717	0.117875
Pt	-2.793606	-1.746296	-2.296058
Pt	0.020928	-1.789689	-2.181549
Pt	2.752430	-1.853603	-2.277706
Pt	-2.754928	0.725025	0.749552
Pt	0.017674	0.667349	0.747344
Pt	2.792284	0.615806	0.765730
Pt	-1.364413	0.536827	-1.642450
Pt	1.412056	0.484026	-1.631614
Pt	-1.325527	3.011713	1.401470
Pt	1.448208	2.957558	1.410494
Pt	0.066082	2.824810	-0.995717
Pt	2.841352	2.770776	-0.983217
Pt	-2.710016	2.879298	-1.000385

Pt20 – B3LYP/see text – Acetonitrile – Charge -2 – Spin Multiplicity 13

Pt	-2.801573	-1.429366	2.491396
Pt	-0.086403	-1.470213	2.427967
Pt	2.744287	-1.538422	2.508839
Pt	-4.184878	-1.560946	0.091976
Pt	-1.463719	-1.904402	0.123561
Pt	1.357416	-1.948958	0.192509
Pt	4.134232	-1.722797	0.117763
Pt	-2.793547	-1.746299	-2.296053
Pt	0.019704	-1.792097	-2.178439
Pt	2.752416	-1.853550	-2.277663
Pt	-2.754925	0.725023	0.749567
Pt	0.017658	0.667379	0.747386
Pt	2.792279	0.615823	0.765741
Pt	-1.364424	0.536789	-1.642418
Pt	1.412044	0.484012	-1.631596
Pt	-1.325527	3.011719	1.401456
Pt	1.448209	2.957560	1.410487
Pt	0.066092	2.824808	-0.995741
Pt	2.841361	2.770769	-0.983217
Pt	-2.710014	2.879298	-1.000389

2. CO₂ adsorbed on Pt₁₃ and Pt₂₀ clusters

CO₂ on Pt₁₃ – B3LYP/SDD-6-311+G(d,p) – Water – Charge 0 – Spin Multiplicity 3 Bridge

C	0.530177	2.901543	4.130030
O	1.359759	3.910379	4.128768
Pt	-0.226958	2.635870	2.268936
Pt	1.447391	4.527002	2.014208
Pt	3.471702	2.872933	1.837373
Pt	1.624283	1.099417	1.295972
Pt	0.251883	1.635007	-1.529402
Pt	1.143522	3.810604	-2.660914
Pt	0.486337	4.997227	-0.392221
Pt	-0.549585	6.188566	1.696197
Pt	-2.244089	4.330516	2.031470
Pt	-2.100543	1.033420	1.377745
Pt	-0.293630	-0.282007	0.188100
Pt	2.390541	2.909705	-0.529426
Pt	-1.278686	3.105553	-0.094927
O	0.232670	2.242871	5.128069

Vibrational Frequencies (cm⁻¹)

19.0896	30.0047	32.8445
43.2577	43.8650	47.6207
59.5762	60.1453	73.6688
76.9831	79.9669	89.1284
92.0222	98.8639	100.0136
104.9000	113.8283	119.6680
123.3783	130.4738	136.8383
141.3072	147.9446	150.8502
156.8427	157.1454	168.2006
173.0794	174.7690	176.5402
183.7558	186.4666	194.5016
197.7424	208.8541	213.7220
328.1824	399.7686	634.4426
755.5398	1076.7631	1524.8620

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge 0 – Spin Multiplicity 3 Top

Pt	0.515535	0.624224	-0.428833
Pt	-0.540503	2.494452	-1.814604
Pt	-2.040663	2.644003	0.281983
Pt	-2.819120	2.676184	2.777515
Pt	-2.954089	0.141933	2.684944
Pt	-2.099933	0.044838	0.215829
Pt	-1.291435	0.000682	-2.255617
Pt	-0.368983	-0.073317	2.334390
Pt	-0.251763	2.526649	2.311974
Pt	-0.905102	4.837715	1.202282
Pt	0.889534	4.253709	-0.511962
Pt	1.913617	2.290943	0.900881
Pt	2.090657	-0.259850	1.508836
C	0.668794	2.928984	4.094783
O	0.329004	2.204813	5.052891
O	1.471745	3.885257	4.067948

Vibrational Frequencies (cm-1)

30.3497	32.2325	37.1725
45.3310	47.6274	52.0413
56.8797	59.4018	59.9048
65.4670	69.3102	76.5141
85.7444	89.8447	97.4275
104.0678	109.1045	112.2331
115.2816	123.2240	124.3165
129.3632	135.8736	144.6219
147.5732	159.5258	160.7996
163.8029	169.1708	172.2590
176.6184	178.0945	181.2846
195.9243	201.9988	217.6029
301.3210	303.0845	657.6455
712.5251	1191.2447	1526.9718

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge -1 – Spin Multiplicity 2 Top

C	0.312217	2.658282	4.358565
O	-0.033001	3.631254	5.065494
Pt	0.037926	2.881625	2.351876
Pt	1.788069	4.704359	1.807547
Pt	3.743052	3.017760	1.459645
Pt	1.841755	1.211419	1.500900
Pt	-0.011074	1.597023	-1.621293
Pt	1.127948	3.585900	-2.912709
Pt	0.392860	4.991943	-0.834521
Pt	-0.239010	6.285337	1.346061
Pt	-1.953516	4.560571	2.094248
Pt	-2.003835	1.296203	1.661201
Pt	-0.203006	-0.025300	0.422576
Pt	1.957277	2.780574	-0.510094
Pt	-1.283406	3.189537	-0.025477
O	0.770520	1.552121	4.725959

Vibrational Frequencies (cm-1)

31.1701	33.3747	40.9863
47.5599	49.1498	50.6330
52.6632	55.6613	58.5298
60.9221	65.9568	71.0987
73.8387	92.5019	94.2106
101.3576	103.0012	107.0697
108.4961	114.9401	119.0358
124.4032	130.9573	141.3090
146.4009	159.7470	161.3521
166.1329	167.1074	169.1459
176.1217	177.8541	181.3233
189.2779	198.9928	211.7255
305.4537	312.6126	650.8013
726.7737	1191.9450	1504.2026

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge -2 – Spin Multiplicity 1 Top

Pt	0.560573	0.633832	-0.479560
Pt	-0.576600	2.471190	-1.834039
Pt	-2.023338	2.582374	0.298474
Pt	-2.809416	2.653679	2.781910
Pt	-2.846162	0.102566	2.662704
Pt	-2.306823	0.038521	0.099232
Pt	-1.283220	-0.011158	-2.310788
Pt	-0.261419	-0.049033	2.315404
Pt	-0.224072	2.542849	2.369840
Pt	-0.996114	4.849110	1.249462
Pt	0.800375	4.252440	-0.487456
Pt	1.899154	2.306166	0.890179
Pt	2.197562	-0.240480	1.446260
C	0.669548	2.946988	4.150510
O	0.006071	2.654945	5.174356
O	1.801175	3.487227	4.096751

31.2881	32.0450	38.3773
40.1480	43.5900	45.6504
48.5232	52.3998	54.5222
61.0630	66.0894	68.8791
74.3655	91.0719	92.6903
99.9255	100.5243	101.3453
106.6764	109.5676	115.0817
121.3849	128.7844	136.8546
146.1523	157.3238	160.5799
162.0871	164.8272	166.6848
174.8914	179.4551	182.7129
182.9807	198.9196	206.6738
303.9976	307.6110	663.8744
727.0546	1188.0354	1483.8310

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge 0 – Spin Multiplicity 3 Bridge

C	0.417593	2.814053	4.267285
O	1.144932	3.824980	4.465246
Pt	-0.079007	2.666493	2.266115
Pt	1.773428	4.423053	2.160659
Pt	3.658346	2.704036	1.537291
Pt	1.679452	1.056710	1.212029
Pt	0.544554	1.648508	-1.169652
Pt	1.129509	3.562280	-2.817105
Pt	0.004110	5.124364	-1.017774
Pt	-0.209570	6.023092	1.434096
Pt	-2.058452	4.393422	2.085110
Pt	-2.075271	1.155896	1.488667
Pt	-0.362528	-0.315396	0.322721
Pt	2.036617	3.750849	-0.280582
Pt	-1.321373	3.110390	-0.098919
O	-0.037563	1.975877	5.034790

Vibrational Frequencies (cm-1)

25.8838	30.5070	35.6314
41.5292	48.5659	52.0676
54.0422	57.9136	60.6364
72.1707	75.4799	87.4372
91.4924	96.5997	101.5931
107.8332	110.7088	113.4726
116.6821	120.5943	125.3740
131.0833	134.3662	146.2024
148.6824	159.1194	160.8304
164.4340	167.1581	169.8305
175.2904	181.0090	184.4554
198.6549	204.9622	215.6747
295.4736	332.1524	639.1010
714.4182	1182.1816	1659.5719

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge 0 – Spin Multiplicity 5 Top

Pt	0.362743	0.139981	-0.297514
Pt	-0.306365	2.411832	-1.613247
Pt	-2.047586	2.654493	0.279767
Pt	-2.847893	2.671323	2.785316
Pt	-2.880831	0.142588	2.618634
Pt	-2.329336	0.091048	0.065914
Pt	-1.303330	0.105792	-2.333932
Pt	-0.287605	-0.028801	2.339175
Pt	-0.256378	2.579229	2.342507
Pt	-0.936471	4.857040	1.171545
Pt	0.925845	4.426913	-0.494601
Pt	1.742397	2.252657	0.702146
Pt	2.201338	-0.169373	1.557646
C	0.716070	2.968789	4.161167
O	0.526560	2.082380	4.993273
O	1.328136	4.035321	4.145443

Vibrational Frequencies (cm-1)

25.7103	32.6814	36.0981
42.7981	45.4381	46.5050
49.9917	55.9667	58.4126
63.3633	76.0680	78.7523
80.5075	91.4597	94.0644
96.3969	104.1936	105.7702
110.5463	116.8730	122.4619
131.4616	136.1786	144.2464
148.7563	150.1131	156.8698
161.8239	168.4379	170.9797
172.3656	177.4283	181.9524
194.3427	195.9602	209.4285
268.0070	276.1404	655.9787
672.2674	1213.7309	1722.0081

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -1 – Spin Multiplicity 2 Bridge

C	0.411822	2.795760	4.303027
O	1.140529	3.795633	4.525628
Pt	-0.071947	2.679373	2.302607
Pt	1.792283	4.427048	2.125326
Pt	3.697368	2.728211	1.517449
Pt	1.706065	1.061883	1.343414
Pt	0.446589	1.660947	-1.301040
Pt	1.170378	3.615078	-2.871159
Pt	0.017941	5.105090	-1.043665
Pt	-0.213700	5.993209	1.405917
Pt	-2.099375	4.402432	2.073961
Pt	-2.069425	1.173825	1.515041
Pt	-0.311222	-0.244465	0.335582
Pt	2.005800	3.672490	-0.302916
Pt	-1.323354	3.110012	-0.091674
O	-0.054975	1.942082	5.052479

Vibrational Frequencies (cm-1)

26.6818	34.4902	37.5287
43.2036	48.0898	50.7993
52.6535	54.5614	58.8931
60.6425	68.0338	72.9032
91.8462	93.6738	100.3654
103.2084	104.8029	107.0604
109.7974	115.2118	118.0612
124.7867	129.3582	142.2427
149.5697	159.1768	164.1827
164.4472	166.7560	168.5678
177.6000	180.6054	184.6465
190.1444	201.8941	212.3196
294.6151	326.1199	638.6110
714.9249	1191.1590	1648.4220

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -1 – Spin Multiplicity 2 Top

C	0.329076	2.637082	4.462541
O	0.578708	3.709961	5.011040
Pt	0.039229	2.838118	2.394807
Pt	1.716335	4.653615	1.537746
Pt	3.752874	3.011426	1.556422
Pt	1.856950	1.183745	1.533642
Pt	0.068914	1.631189	-1.634518
Pt	1.221868	3.655967	-2.838303
Pt	0.150792	5.128129	-0.971114
Pt	-0.319781	6.271371	1.334058
Pt	-1.975086	4.491649	2.095058
Pt	-1.966772	1.273664	1.655033
Pt	-0.160483	-0.023050	0.390229
Pt	2.000453	2.794343	-0.437411
Pt	-1.244393	3.186400	-0.045689
O	0.196094	1.474998	4.846438

Vibrational Frequencies (cm-1)

28.0373	32.1052	33.5960
38.5503	45.4266	45.8500
50.2121	51.2745	55.0297
57.7270	60.6925	64.3516
73.2443	90.6906	92.9504
98.0143	100.2794	105.4800
107.9537	115.0656	119.1459
121.7155	130.4593	139.1120
146.5081	156.1505	159.4551
162.6216	164.6122	167.0668
175.0720	178.1183	182.5916
187.1105	198.1003	213.8186
265.0419	270.0883	651.2029
667.8409	1214.0736	1716.0499

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -2 – Spin Multiplicity 1 Top

C	0.355168	2.599681	4.428472
O	0.895031	3.587424	4.941586
Pt	0.030185	2.833138	2.385046
Pt	1.848335	4.640505	1.983035
Pt	3.733911	2.882435	1.501481
Pt	1.728148	1.223713	1.270875
Pt	0.260076	1.523798	-1.368548
Pt	1.174938	3.435773	-2.906104
Pt	0.034308	5.076357	-1.206717
Pt	-0.204297	6.085443	1.207532
Pt	-2.037931	4.503746	2.078345
Pt	-2.002156	1.344512	1.641493
Pt	-0.316016	-0.212616	0.510512
Pt	2.034429	3.725295	-0.382209
Pt	-1.242217	3.146411	-0.071800
O	-0.047136	1.522995	4.876979

Vibrational Frequencies (cm-1)

21.4527	29.5294	36.5093
38.8149	40.4403	42.4335
44.3949	50.9743	53.7588
56.2069	61.2632	64.8543
71.1163	74.2331	89.7604
92.4793	94.1048	99.5320
105.0238	109.7891	114.5921
119.1150	127.9845	133.3358
145.2468	155.5929	157.9734
160.7417	163.9237	165.7336
173.6634	178.5712	182.1088
183.7107	197.7510	206.8742
275.0435	288.4948	650.1770
689.1380	1212.2487	1682.0310

CO2 on Pt20 – B3LYP/see text – Water – Charge 0 – Spin Multiplicity 15 Bridge

Pt	-2.801574	-1.429337	2.491327
Pt	-0.091280	-1.389233	2.434008
Pt	2.744288	-1.538462	2.508806
Pt	-4.184862	-1.560998	0.092146
Pt	-1.425042	-2.021851	0.115765
Pt	1.379250	-1.924341	0.206771
Pt	4.134226	-1.722703	0.117897
Pt	-2.793571	-1.746268	-2.296083
Pt	0.002142	-1.755493	-2.202156
Pt	2.752406	-1.853579	-2.277698
Pt	-2.754934	0.725037	0.749508
Pt	0.017688	0.667345	0.747322
Pt	2.792276	0.615787	0.765742
Pt	-1.364404	0.536833	-1.642476
Pt	1.412043	0.483992	-1.631625
Pt	-1.325528	3.011704	1.401491
Pt	1.448210	2.957558	1.410488
Pt	0.066082	2.824816	-0.995711
Pt	2.841354	2.770775	-0.983216
Pt	-2.710011	2.879303	-1.000383
C	-0.800567	-3.978473	0.278420
O	-1.682640	-4.817129	0.355709
O	0.457103	-4.090429	0.286529

CO2 on Pt20 – B3LYP/see text – Water – Charge -1 – Spin Multiplicity 14 Bridge

Pt	-2.801567	-1.429355	2.491305
Pt	-0.083518	-1.401807	2.435618
Pt	2.744281	-1.538445	2.508805
Pt	-4.184868	-1.560993	0.092208
Pt	-1.424614	-2.025114	0.114198
Pt	1.378373	-1.914576	0.203662
Pt	4.134225	-1.722728	0.117908
Pt	-2.793608	-1.746266	-2.296108
Pt	0.002145	-1.755712	-2.203511
Pt	2.752427	-1.853550	-2.277708
Pt	-2.754914	0.725044	0.749476
Pt	0.017702	0.667374	0.747330
Pt	2.792255	0.615782	0.765763
Pt	-1.364418	0.536803	-1.642514
Pt	1.412071	0.483984	-1.631614
Pt	-1.325528	3.011697	1.401513
Pt	1.448213	2.957560	1.410479
Pt	0.066063	2.824812	-0.995720
Pt	2.841356	2.770774	-0.983217
Pt	-2.710002	2.879310	-1.000374
C	-0.809424	-3.983801	0.272837
O	-1.695845	-4.820390	0.354119
O	0.446436	-4.103271	0.275524

CO2 on Pt20 – B3LYP/see text – Water – Charge 0 – Spin Multiplicity 14 Top

Pt	-2.801622	-1.429307	2.491328
Pt	-0.103047	-1.462037	2.390508
Pt	2.744377	-1.538536	2.508748
Pt	-4.184874	-1.560993	0.092145
Pt	-1.478692	-2.152683	0.104314
Pt	1.351162	-1.883813	0.179886
Pt	4.134230	-1.722582	0.118023
Pt	-2.793519	-1.746271	-2.296096
Pt	0.006547	-1.778203	-2.189586
Pt	2.752356	-1.853647	-2.277756
Pt	-2.754931	0.725051	0.749567
Pt	0.017640	0.667291	0.747326
Pt	2.792266	0.615798	0.765695
Pt	-1.364410	0.536861	-1.642438
Pt	1.412055	0.483978	-1.631677
Pt	-1.325536	3.011711	1.401463
Pt	1.448200	2.957549	1.410517
Pt	0.066128	2.824813	-0.995708
Pt	2.841345	2.770783	-0.983203
Pt	-2.710016	2.879301	-1.000399
C	-1.565440	-4.286882	0.203808
O	-2.722569	-4.683465	0.212470
O	-0.451213	-4.789487	0.235580

CO2 on Pt20 – B3LYP/see text – Water – Charge -2 – Spin Multiplicity 13 Bridge

Pt	-2.801577	-1.429334	2.491320
Pt	-0.034362	-1.331028	2.551164
Pt	2.744290	-1.538465	2.508808
Pt	-4.184869	-1.561001	0.092179
Pt	-1.415495	-1.985484	0.245718
Pt	1.389890	-1.899134	0.253238
Pt	4.134229	-1.722707	0.117899
Pt	-2.793573	-1.746269	-2.296099
Pt	-0.029804	-1.759970	-2.158937
Pt	2.752406	-1.853581	-2.277697
Pt	-2.754926	0.725041	0.749512
Pt	0.017686	0.667345	0.747295
Pt	2.792271	0.615791	0.765750
Pt	-1.364402	0.536831	-1.642493
Pt	1.412053	0.483996	-1.631621
Pt	-1.325528	3.011703	1.401496
Pt	1.448210	2.957556	1.410491
Pt	0.066076	2.824818	-0.995708
Pt	2.841353	2.770777	-0.983215
Pt	-2.710011	2.879303	-1.000383
C	-0.806212	-3.939078	0.379832
O	-1.685487	-4.785114	0.481425
O	0.451080	-4.070430	0.344486

CO2 on Pt20 – B3LYP/see text – Water – Charge -2 – Spin Multiplicity 13 Top

Pt	-2.801592	-1.429308	2.491308
Pt	-0.079012	-1.477095	2.385710
Pt	2.744323	-1.538525	2.508753
Pt	-4.184861	-1.561003	0.092177
Pt	-1.477391	-2.173865	0.111526
Pt	1.357814	-1.906729	0.161589
Pt	4.134219	-1.722584	0.118016
Pt	-2.793542	-1.746250	-2.296091
Pt	-0.008459	-1.777002	-2.190933
Pt	2.752411	-1.853640	-2.277726
Pt	-2.754918	0.725044	0.749560
Pt	0.017630	0.667290	0.747316
Pt	2.792263	0.615782	0.765671
Pt	-1.364409	0.536863	-1.642446
Pt	1.412037	0.483969	-1.631697
Pt	-1.325534	3.011713	1.401464
Pt	1.448206	2.957545	1.410524
Pt	0.066132	2.824819	-0.995696
Pt	2.841342	2.770784	-0.983202
Pt	-2.710019	2.879300	-1.000398
C	-1.599200	-4.297276	0.220319
O	-2.760495	-4.687707	0.185947
O	-0.496529	-4.824545	0.300432

CO2 on Pt20 – B3LYP/see text – Acetonitrile – Charge 0 – Spin Multiplicity 15 Bridge

Pt	-2.801574	-1.429337	2.491327
Pt	-0.091280	-1.389233	2.434008
Pt	2.744288	-1.538462	2.508806
Pt	-4.184862	-1.560998	0.092146
Pt	-1.425042	-2.021851	0.115765
Pt	1.379250	-1.924341	0.206771
Pt	4.134226	-1.722703	0.117897
Pt	-2.793571	-1.746268	-2.296083
Pt	0.002142	-1.755493	-2.202156
Pt	2.752406	-1.853579	-2.277698
Pt	-2.754934	0.725037	0.749508
Pt	0.017688	0.667345	0.747322
Pt	2.792276	0.615787	0.765742
Pt	-1.364404	0.536833	-1.642476
Pt	1.412043	0.483992	-1.631625
Pt	-1.325528	3.011704	1.401491
Pt	1.448210	2.957558	1.410488
Pt	0.066082	2.824816	-0.995711
Pt	2.841354	2.770775	-0.983216
Pt	-2.710011	2.879303	-1.000383
C	-0.800567	-3.978473	0.278420
O	-1.682640	-4.817129	0.355709
O	0.457103	-4.090429	0.286529

CO2 on Pt20 – B3LYP/see text – Acetonitrile – Charge -1 – Spin Multiplicity 14 Bridge

Pt	-2.801567	-1.429355	2.491305
Pt	-0.083518	-1.401807	2.435618
Pt	2.744281	-1.538445	2.508805
Pt	-4.184868	-1.560993	0.092208
Pt	-1.424614	-2.025114	0.114198
Pt	1.378373	-1.914576	0.203662
Pt	4.134225	-1.722728	0.117908
Pt	-2.793608	-1.746266	-2.296108
Pt	0.002145	-1.755712	-2.203511
Pt	2.752427	-1.853550	-2.277708
Pt	-2.754914	0.725044	0.749476
Pt	0.017702	0.667374	0.747330
Pt	2.792255	0.615782	0.765763
Pt	-1.364418	0.536803	-1.642514
Pt	1.412071	0.483984	-1.631614
Pt	-1.325528	3.011697	1.401513
Pt	1.448213	2.957560	1.410479
Pt	0.066063	2.824812	-0.995720
Pt	2.841356	2.770774	-0.983217
Pt	-2.710002	2.879310	-1.000374
C	-0.809424	-3.983801	0.272837
O	-1.695845	-4.820390	0.354119
O	0.446436	-4.103271	0.275524

CO2 on Pt20 – B3LYP/see text – Acetonitrile – Charge -1 – Spin Multiplicity 14 Top

Pt	-2.801622	-1.429307	2.491328
Pt	-0.103047	-1.462037	2.390508
Pt	2.744377	-1.538536	2.508748
Pt	-4.184874	-1.560993	0.092145
Pt	-1.478692	-2.152683	0.104314
Pt	1.351162	-1.883813	0.179886
Pt	4.134230	-1.722582	0.118023
Pt	-2.793519	-1.746271	-2.296096
Pt	0.006547	-1.778203	-2.189586
Pt	2.752356	-1.853647	-2.277756
Pt	-2.754931	0.725051	0.749567
Pt	0.017640	0.667291	0.747326
Pt	2.792266	0.615798	0.765695
Pt	-1.364410	0.536861	-1.642438
Pt	1.412055	0.483978	-1.631677
Pt	-1.325536	3.011711	1.401463
Pt	1.448200	2.957549	1.410517
Pt	0.066128	2.824813	-0.995708
Pt	2.841345	2.770783	-0.983203
Pt	-2.710016	2.879301	-1.000399
C	-1.565440	-4.286882	0.203808
O	-2.722569	-4.683465	0.212470
O	-0.451213	-4.789487	0.235580

CO2 on Pt20 – B3LYP/see text – Acetonitrile – Charge -2 – Spin Multiplicity 13 Bridge

Pt	-2.801577	-1.429334	2.491320
Pt	-0.034362	-1.331028	2.551164
Pt	2.744290	-1.538465	2.508808
Pt	-4.184869	-1.561001	0.092179
Pt	-1.415495	-1.985484	0.245718
Pt	1.389890	-1.899134	0.253238
Pt	4.134229	-1.722707	0.117899
Pt	-2.793573	-1.746269	-2.296099
Pt	-0.029804	-1.759970	-2.158937
Pt	2.752406	-1.853581	-2.277697
Pt	-2.754926	0.725041	0.749512
Pt	0.017686	0.667345	0.747295
Pt	2.792271	0.615791	0.765750
Pt	-1.364402	0.536831	-1.642493
Pt	1.412053	0.483996	-1.631621
Pt	-1.325528	3.011703	1.401496
Pt	1.448210	2.957556	1.410491
Pt	0.066076	2.824818	-0.995708
Pt	2.841353	2.770777	-0.983215
Pt	-2.710011	2.879303	-1.000383
C	-0.806212	-3.939078	0.379832
O	-1.685487	-4.785114	0.481425
O	0.451080	-4.070430	0.344486

CO2 on Pt20 – B3LYP/see text – Acetonitrile – Charge -2 – Spin Multiplicity 13 Top

Pt	-2.801592	-1.429308	2.491308
Pt	-0.079012	-1.477095	2.385710
Pt	2.744323	-1.538525	2.508753
Pt	-4.184861	-1.561003	0.092177
Pt	-1.477391	-2.173865	0.111526
Pt	1.357814	-1.906729	0.161589
Pt	4.134219	-1.722584	0.118016
Pt	-2.793542	-1.746250	-2.296091
Pt	-0.008459	-1.777002	-2.190933
Pt	2.752411	-1.853640	-2.277726
Pt	-2.754918	0.725044	0.749560
Pt	0.017630	0.667290	0.747316
Pt	2.792263	0.615782	0.765671
Pt	-1.364409	0.536863	-1.642446
Pt	1.412037	0.483969	-1.631697
Pt	-1.325534	3.011713	1.401464
Pt	1.448206	2.957545	1.410524
Pt	0.066132	2.824819	-0.995696
Pt	2.841342	2.770784	-0.983202
Pt	-2.710019	2.879300	-1.000398
C	-1.599200	-4.297276	0.220319
O	-2.760495	-4.687707	0.185947
O	-0.496529	-4.824545	0.300432

3. Transition states for CO₂ adsorption on Pt₁₃ clusters

CO₂ on Pt₁₃ – B3LYP/SDD-6-311+G(d,p) – Water – Charge 0 – Spin Multiplicity 3

C	0.429746	2.427948	4.978503
O	1.016732	3.412486	5.222882
Pt	0.009675	2.945956	2.246504
Pt	1.632951	4.778871	1.295139
Pt	3.665237	3.171662	1.560004
Pt	1.850268	1.252142	1.583322
Pt	0.084664	1.577148	-1.645602
Pt	1.221015	3.610385	-2.861926
Pt	0.218810	5.129800	-1.003291
Pt	-0.414008	6.411763	1.196613
Pt	-2.011291	4.581560	1.933235
Pt	-1.957452	1.315699	1.569450
Pt	-0.118709	-0.029940	0.427023
Pt	2.023335	2.746938	-0.479193
Pt	-1.296284	3.196585	-0.173277
O	-0.109912	1.389603	5.040591

Vibrational Frequencies (cm⁻¹)

-146.2455	28.9252	29.7615
31.4539	33.8913	41.8562
46.7158	47.7823	49.4515
55.8446	59.1793	60.9483
73.6508	85.5301	89.3102
92.3557	95.7708	102.6061
107.3957	112.9450	116.1438
120.2887	126.9342	132.1543
140.9400	144.1416	145.4051
157.8848	161.4609	164.3522
167.0819	170.8619	171.8669
174.2222	179.8966	194.4042
196.7095	214.8181	364.4089
624.2507	1295.7848	2211.5902

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Water – Charge -1 – Spin Multiplicity 2

C	0.438859	2.600077	5.078861
O	0.779273	3.704939	5.260954
Pt	0.001726	2.825830	2.241600
Pt	1.695829	4.659774	1.498786
Pt	3.725909	3.007864	1.537682
Pt	1.840807	1.170113	1.464157
Pt	0.095587	1.654071	-1.738861
Pt	1.272479	3.687755	-2.904417
Pt	0.144471	5.136946	-1.049677
Pt	-0.357190	6.255226	1.263452
Pt	-2.026300	4.455067	1.962600
Pt	-2.015315	1.285375	1.512425
Pt	-0.173146	-0.004758	0.279485
Pt	1.996256	2.811825	-0.485209
Pt	-1.313282	3.195070	-0.214601
O	0.138814	1.473432	5.182740

Vibrational Frequencies (cm-1)

-121.1315	21.8001	22.7918
25.1484	29.1345	41.7274
42.9204	44.7341	48.0992
51.4421	54.2954	55.2344
57.3288	72.4322	88.0888
90.8735	91.8215	98.9516
104.2801	107.4330	113.9981
115.9858	119.3040	129.5406
138.0499	141.6320	145.6120
157.9039	160.6009	161.1305
165.1142	167.8025	174.0409
176.4065	179.9045	185.7640
196.3860	210.9348	373.8763
623.5187	1303.9049	2228.7757

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge 0 – Spin Multiplicity 3

C	0.413304	2.537460	4.933131
O	1.018632	3.522527	5.142525
Pt	0.017825	2.869273	2.263409
Pt	1.628280	4.726059	1.329283
Pt	3.666851	3.122699	1.561139
Pt	1.857391	1.197257	1.541713
Pt	0.083428	1.605836	-1.679761
Pt	1.227304	3.667108	-2.842924
Pt	0.216727	5.143008	-0.954833
Pt	-0.416051	6.364091	1.279929
Pt	-2.001464	4.511258	1.986730
Pt	-1.956032	1.265333	1.526270
Pt	-0.114707	-0.051122	0.353759
Pt	2.026315	2.738122	-0.485937
Pt	-1.284344	3.186599	-0.158238
O	-0.138683	1.513098	5.093783

Vibrational Frequencies (cm-1)

-154.9988	25.0772	28.2555
30.7382	38.5148	42.0795
46.8106	48.5310	49.7693
51.7025	55.6021	59.1238
73.6422	85.2203	89.7052
92.3138	96.5348	101.8273
108.3700	112.9456	116.7142
120.5635	127.5860	132.3196
141.0976	144.3583	146.2016
158.1616	161.8617	166.6107
168.1876	171.9418	172.3097
177.7312	182.2932	194.4010
197.3268	215.2951	383.2634
623.9671	1292.4611	2227.7163

CO2 on Pt13 – B3LYP/SDD-6-311+G(d,p) – Acetonitrile – Charge -1 – Spin Multiplicity 2

C	0.370287	2.590676	5.021369
O	0.732502	3.682720	5.253084
Pt	0.048822	2.830777	2.276823
Pt	1.713718	4.667608	1.465122
Pt	3.752374	3.026745	1.495183
Pt	1.874860	1.180071	1.455958
Pt	0.081272	1.647615	-1.724332
Pt	1.239137	3.680516	-2.910610
Pt	0.131061	5.138169	-1.051863
Pt	-0.342752	6.262218	1.263994
Pt	-1.983645	4.455264	2.008445
Pt	-1.977308	1.288654	1.562057
Pt	-0.152970	-0.003434	0.304940
Pt	2.000580	2.809518	-0.504663
Pt	-1.289642	3.192097	-0.171440
O	0.046482	1.469391	5.145912

Vibrational Frequencies (cm-1)

-146.7514	21.6226	22.7261
27.7110	32.4806	41.7350
43.4641	45.5780	48.7432
51.4695	53.1101	56.0865
58.4122	72.6117	88.4534
90.9468	91.8726	99.4457
104.8017	108.1103	115.0470
116.2148	119.4747	129.6774
138.4710	145.7770	148.0149
158.2875	161.0271	161.4822
165.1324	173.0579	173.9653
178.1170	181.8680	185.9855
196.7808	212.7352	379.9536
621.9146	1297.4827	2239.7167

4. CO₂ (2 H₂O) adsorbed on Pt₁₃ clusters

CO₂ (2 H₂O) on Pt₁₃ – B3LYP/SDD-6-311+G(d,p) – water – Charge -1 – Spin Multiplicity 2

C	0.088395	2.572847	4.843851
Pt	-0.106587	2.862843	2.847280
Pt	1.142068	0.740355	2.011168
Pt	3.490862	1.905462	2.056866
Pt	2.116182	4.093913	2.387559
Pt	0.656130	6.204113	1.907448
Pt	-1.513172	5.050631	2.581569
Pt	-2.513746	1.974410	2.089670
Pt	-1.154959	0.192109	0.859491
Pt	-0.417114	1.698417	-1.146708
Pt	1.303786	3.273848	-2.369067
Pt	0.952699	4.808145	-0.280034
Pt	1.781443	2.227651	0.038171
Pt	-1.201528	3.571558	0.453289
O	0.456017	1.430236	5.218745
O	-0.204585	3.556309	5.566989
O	0.918668	0.658216	7.838039
O	0.365425	3.426926	8.316902
H	0.145294	3.526888	7.366531
H	0.592752	2.480756	8.377907
H	0.714009	0.917905	6.909895
H	0.192542	0.079479	8.101105

Vibrational Frequencies

20.0185	21.0930	32.3828
33.3442	34.4270	46.1711
47.5821	50.6110	52.2822
54.2935	57.6515	59.7640
63.0053	69.3442	73.2846
91.3035	93.3768	94.8362
101.9498	103.1135	107.0318
108.5166	114.8120	118.9855
124.2753	125.8056	131.1275
134.2621	147.8264	152.2005
160.5880	161.8681	166.0616
168.1799	169.5957	177.9466
179.1087	183.3401	186.5999
188.3907	202.3708	213.2803
250.6958	340.7906	350.1461
400.0586	493.1476	555.0008
635.8041	653.5395	722.5180
763.5875	1200.0177	1483.6752
1601.2553	1652.8193	3382.9551
3481.3403	3606.4206	3830.6480

CO2 (2 H2O) on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge -2 – Spin Multiplicity 2

C	0.113140	2.594315	4.861425
Pt	-0.103034	2.856132	2.869094
Pt	1.217794	0.772731	2.051026
Pt	3.528794	2.012299	2.101963
Pt	2.050634	4.163076	2.251082
Pt	0.520826	6.248242	1.885567
Pt	-1.596351	4.983711	2.556191
Pt	-2.489147	1.900546	2.109741
Pt	-1.052878	0.165290	0.874640
Pt	-0.349158	1.669336	-1.155319
Pt	1.324197	3.304692	-2.341879
Pt	0.788980	4.947119	-0.373616
Pt	1.850646	2.179119	0.027516
Pt	-1.175133	3.511544	0.446113
O	0.233605	1.407456	5.269212
O	0.081647	3.634568	5.568564
O	0.696643	0.573355	7.861367
O	0.637002	3.414103	8.302933
H	0.434998	3.536749	7.349699
H	0.671479	2.443912	8.385188
H	0.499072	0.865525	6.940578
H	-0.079174	0.069197	8.135581

Vibrational Frequencies

16.7120	23.2445	29.9713
31.9093	36.1083	40.3230
43.3165	44.5087	46.0258
50.7335	54.9347	57.8171
61.0756	66.3212	70.6821
75.2046	86.8932	92.3495
93.6250	100.5214	102.2664
105.3490	109.9687	114.9087
121.2052	127.4457	129.5544
132.2932	146.8277	150.6306
158.0688	161.4262	161.7058
164.6092	171.8011	176.7419
179.2236	180.7381	183.3541
183.6919	185.7861	201.0625
207.8825	341.3508	346.2737
407.3807	507.1576	549.7699
635.2376	652.1857	726.2280
763.4001	1197.5054	1452.0602
1601.8145	1656.2640	3368.6926
3449.8212	3621.8685	3829.0737

5. COOH adsorbed on Pt clusters

COOH on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge 0 – Spin Multiplicity 2

C	0.572456	2.985696	4.038650
O	0.957063	4.084201	4.402157
Pt	-0.317348	2.614066	2.297280
Pt	1.868368	2.246471	0.951805
Pt	2.040690	-0.285453	1.617820
Pt	-0.375889	0.034909	2.529656
Pt	-2.206072	0.094114	0.160126
Pt	-1.271185	-0.051405	-2.275935
Pt	-0.490954	2.419961	-1.814049
Pt	0.941195	4.198550	-0.539180
Pt	-0.900937	4.922643	1.068216
Pt	-2.888117	2.788541	2.721636
Pt	-2.975675	0.251043	2.653672
Pt	0.444264	0.557217	-0.339218
Pt	-2.009010	2.673260	0.256600
O	0.715373	1.941120	4.907704
H	0.391783	1.128562	4.442009

vibrational frequencies (cm⁻¹)

31.2769	34.5603	45.6950
48.2321	50.5815	54.8842
58.4669	59.5697	61.2519
64.2631	74.9234	82.7997
87.6660	93.9558	99.8859
102.2183	106.8321	109.0847
114.7764	118.5669	121.8343
129.1840	132.6007	145.1681
151.0299	162.0880	163.6558
169.0569	169.9369	170.7405
178.7192	181.3034	185.0055
189.3310	207.5938	213.0897
328.6091	339.6586	617.1188
684.2259	712.7312	983.2776
1299.7247	1621.8688	3246.2162

COOH on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge -1 – Spin Multiplicity 1

C	0.584043	2.968431	4.052984
O	0.967340	4.054889	4.457419
Pt	-0.308679	2.640085	2.307114
Pt	1.881540	2.288191	0.963904
Pt	2.075015	-0.231344	1.677188
Pt	-0.404838	0.053197	2.452255
Pt	-2.363918	0.100971	0.144134
Pt	-1.246137	-0.101145	-2.214578
Pt	-0.491514	2.381810	-1.829692
Pt	0.909420	4.197752	-0.551574
Pt	-0.929538	4.935179	1.075265
Pt	-2.888131	2.831026	2.693678
Pt	-2.998792	0.284763	2.680942
Pt	0.540184	0.575253	-0.353833
Pt	-1.986747	2.635586	0.248606
O	0.738657	1.892660	4.885989
H	0.418100	1.096192	4.389149

vibrational frequencies (cm⁻¹)

21.7374	30.5947	38.6852
41.2488	44.5107	45.6143
46.0593	51.7591	55.7133
58.4437	69.7155	71.5329
75.2018	78.3960	92.5398
96.6580	101.6318	105.2055
110.5230	112.1614	115.6153
125.9235	128.4765	143.3790
145.8188	159.2922	161.9207
163.1814	165.7746	171.4097
179.3577	181.9554	183.6418
185.2839	205.3410	207.4886
327.3631	338.4779	605.4129
675.7437	711.3751	974.7326
1299.7733	1613.8327	3222.4191

COOH on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge 0 – Spin Multiplicity 2

C	0.575240	2.981686	4.059038
O	0.944426	4.076247	4.418016
Pt	-0.314381	2.621707	2.300290
Pt	1.870452	2.249207	0.955460
Pt	2.042520	-0.281671	1.623588
Pt	-0.373576	0.044715	2.533491
Pt	-2.208158	0.094924	0.165234
Pt	-1.268364	-0.058058	-2.267707
Pt	-0.490114	2.415120	-1.815423
Pt	0.940049	4.194997	-0.539307
Pt	-0.912432	4.923890	1.054458
Pt	-2.885291	2.800353	2.716894
Pt	-2.972512	0.262206	2.660398
Pt	0.444166	0.558932	-0.332548
Pt	-2.015052	2.674191	0.249247
O	0.719038	1.923736	4.893478
H	0.399992	1.121315	4.404344

vibrational frequencies (cm-1)

32.4618	33.8208	46.3927
47.7411	51.0732	54.7054
59.0753	59.2774	61.4446
66.9446	74.3933	75.2950
87.5647	94.0381	101.1210
103.7904	106.8282	110.8782
114.8128	117.9751	122.9215
129.0344	132.8351	145.2526
150.7530	162.0838	163.9562
168.7542	170.4817	170.7349
178.5816	180.9273	185.4263
189.8174	206.7016	213.2972
327.1482	341.1348	619.8211
712.9182	721.6710	1069.3032
1317.1652	1704.8608	3209.6584

COOH on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge -1 – Spin Multiplicity 1

C	0.583963	2.966317	4.074033
O	0.955896	4.048822	4.469695
Pt	-0.299075	2.644929	2.307784
Pt	1.887924	2.285064	0.963422
Pt	2.083793	-0.236921	1.666399
Pt	-0.391322	0.060525	2.454330
Pt	-2.362237	0.101639	0.152972
Pt	-1.249018	-0.104965	-2.207364
Pt	-0.493834	2.379323	-1.831935
Pt	0.907572	4.192010	-0.548505
Pt	-0.940972	4.934649	1.067220
Pt	-2.876826	2.843955	2.690965
Pt	-2.983872	0.295927	2.691821
Pt	0.540493	0.576377	-0.354793
Pt	-1.992625	2.636118	0.242258
O	0.722194	1.882417	4.879303
H	0.403948	1.097309	4.361346

vibrational frequencies (cm⁻¹)

25.2779	31.8266	40.3743
44.5738	45.1049	46.3552
52.5476	55.6403	58.5307
61.2726	68.3497	71.0806
75.5038	86.0478	93.1505
101.0492	101.8978	107.3810
110.5930	111.8608	116.4788
125.8090	128.6237	143.0795
145.8088	159.3550	162.0740
162.9793	165.2174	172.5050
179.3713	181.9841	184.0656
185.7741	205.1799	207.8854
327.7701	341.4263	615.0012
717.9316	729.3630	1062.1660
1322.1735	1697.9355	3197.3536

COOH on Pt20 – B3LYP/see text – water – Charge 0 – Spin Multiplicity 14

Pt	-2.801560	-1.429342	2.491311
Pt	-0.078984	-1.462657	2.377909
Pt	2.744227	-1.538447	2.508831
Pt	-4.184856	-1.561005	0.092173
Pt	-1.461733	-2.091420	0.091778
Pt	1.384923	-1.931168	0.170794
Pt	4.134235	-1.722721	0.117870
Pt	-2.793594	-1.746259	-2.296084
Pt	0.020100	-1.782390	-2.198133
Pt	2.752439	-1.853573	-2.277684
Pt	-2.754914	0.725034	0.749508
Pt	0.017702	0.667348	0.747304
Pt	2.792276	0.615787	0.765727
Pt	-1.364409	0.536834	-1.642478
Pt	1.412048	0.483989	-1.631626
Pt	-1.325526	3.011705	1.401495
Pt	1.448213	2.957555	1.410496
Pt	0.066076	2.824817	-0.995715
Pt	2.841348	2.770779	-0.983212
Pt	-2.710015	2.879301	-1.000382
C	-1.462541	-4.074975	0.231885
O	-2.467753	-4.739829	0.232200
O	-0.258049	-4.670026	0.330671
H	0.439641	-3.962670	0.310358

COOH on Pt20 – B3LYP/see text – acetonitrile – Charge 0 – Spin Multiplicity 14

Pt	-2.801560	-1.429342	2.491311
Pt	-0.078984	-1.462657	2.377909
Pt	2.744227	-1.538447	2.508831
Pt	-4.184856	-1.561005	0.092173
Pt	-1.461733	-2.091420	0.091778
Pt	1.384923	-1.931168	0.170794
Pt	4.134235	-1.722721	0.117870
Pt	-2.793594	-1.746259	-2.296084
Pt	0.020100	-1.782390	-2.198133
Pt	2.752439	-1.853573	-2.277684
Pt	-2.754914	0.725034	0.749508
Pt	0.017702	0.667348	0.747304
Pt	2.792276	0.615787	0.765727
Pt	-1.364409	0.536834	-1.642478
Pt	1.412048	0.483989	-1.631626
Pt	-1.325526	3.011705	1.401495
Pt	1.448213	2.957555	1.410496
Pt	0.066076	2.824817	-0.995715
Pt	2.841348	2.770779	-0.983212
Pt	-2.710015	2.879301	-1.000382
C	-1.462541	-4.074975	0.231885
O	-2.467753	-4.739829	0.232200
O	-0.258049	-4.670026	0.330671
H	0.439641	-3.962670	0.310358

6. HCO₂ adsorbed on Pt clusters

HCOO on Pt₁₃ – B3LYP/SDD-6-311+G(d,p) – water – Charge 0 – Spin Multiplicity 2

O	0.654541	3.185438	4.319127
C	0.628095	2.818001	5.520265
Pt	-0.990165	4.468309	3.510475
Pt	-1.570590	4.758121	6.131402
Pt	0.265565	6.565237	6.473694
Pt	0.042071	6.831486	3.888200
Pt	-2.632937	8.063667	3.237488
Pt	-4.427798	8.329356	5.130985
Pt	-4.105958	5.768699	5.485556
Pt	-3.641487	3.219869	5.680308
Pt	-3.189071	2.960306	3.195406
Pt	-3.251478	5.575553	3.041031
Pt	-1.645514	5.184210	1.009510
Pt	-0.750576	7.500857	1.500301
Pt	-2.051138	7.540312	5.846043
O	-0.155740	3.193080	6.447353
H	1.373878	2.071927	5.826043

Vibrational Frequencies (cm⁻¹)

22.0779	28.7811	31.8120
35.3404	45.9858	48.3726
52.5337	59.0462	60.1057
78.1507	79.1623	83.4612
90.0665	93.4804	95.1755
101.3407	105.8598	112.2853
118.2566	121.0888	127.9999
137.8628	138.8435	142.2178
145.8122	155.4920	157.7430
163.3194	171.4636	172.5777
174.4479	179.1355	182.8882
192.8044	205.5966	207.2946
267.8822	327.6046	347.3148
772.9561	1029.2782	1310.7952
1373.3182	1480.2321	3047.9171

HCOO on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge -1 – Spin Multiplicity 1

O	0.667472	3.342084	4.194349
C	0.780528	2.716617	5.303399
Pt	-1.079440	4.531454	3.788029
Pt	-1.381157	4.746629	6.352205
Pt	0.185274	6.823357	6.650593
Pt	-0.036165	6.920426	4.052702
Pt	-2.587219	8.049073	3.098895
Pt	-4.352607	8.620384	4.930666
Pt	-4.607628	6.032711	5.201855
Pt	-3.728556	3.643443	5.825833
Pt	-3.234316	2.945390	3.416528
Pt	-3.258212	5.580448	3.066960
Pt	-1.521145	4.929818	1.222681
Pt	-0.607510	7.283125	1.536515
Pt	-2.372605	7.040296	5.950117
O	0.036889	2.788942	6.304397
H	1.648094	2.040233	5.347460

Vibrational Frequencies (cm-1)

31.4075	34.4317	40.2793
42.2052	43.8413	49.8653
51.7651	56.7546	60.5797
67.2179	72.6890	73.5959
87.0678	90.7744	91.4063
100.5834	107.0003	109.6911
114.1845	117.9519	127.9257
132.4834	136.0076	152.8235
156.8477	162.4615	164.2483
165.9643	167.5979	172.9362
179.9193	182.4859	185.8146
188.3498	201.6507	216.8994
231.9400	300.2154	344.1559
771.9232	1032.6048	1297.8886
1383.9917	1506.9456	3015.3531

HCOO on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge 0 – Spin Multiplicity 2

O	0.630039	3.183425	4.301947
C	0.615569	2.831428	5.505832
Pt	-0.987253	4.467123	3.519004
Pt	-1.570121	4.753500	6.141340
Pt	0.256370	6.573020	6.485270
Pt	0.066073	6.811138	3.893746
Pt	-2.626793	8.059281	3.243660
Pt	-4.438824	8.323041	5.122624
Pt	-4.102285	5.765369	5.484955
Pt	-3.644845	3.215942	5.678996
Pt	-3.169763	2.954278	3.199284
Pt	-3.243679	5.573949	3.043634
Pt	-1.645112	5.184671	1.011949
Pt	-0.742226	7.497960	1.512342
Pt	-2.060953	7.544186	5.847864
O	-0.151004	3.209019	6.443558
H	1.366501	2.087099	5.807179

Vibrational Frequencies (cm-1)

22.7478	28.9967	31.9434
40.9137	49.1646	51.1514
53.1466	59.4859	62.6246
80.6412	82.8426	86.9870
91.2461	94.8399	97.0484
102.7324	111.8197	112.7451
120.7383	121.5941	128.5973
137.9799	139.0682	144.1742
152.4266	157.3384	163.0728
164.5158	172.9157	173.5206
179.2525	181.4843	184.2816
192.6560	206.6867	208.9347
290.3356	350.2441	365.5957
779.5919	1029.3951	1324.8141
1384.3129	1536.2021	3036.7312

HCOO on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge -1 – Spin Multiplicity 1

O	0.652546	3.319498	4.187934
C	0.754241	2.721834	5.309981
Pt	-1.064601	4.530200	3.779560
Pt	-1.353098	4.744117	6.342593
Pt	0.196474	6.831366	6.644218
Pt	-0.043158	6.934345	4.049113
Pt	-2.593453	8.051685	3.106689
Pt	-4.366831	8.603178	4.933654
Pt	-4.596228	6.016755	5.204210
Pt	-3.703254	3.632906	5.823156
Pt	-3.222687	2.945285	3.407106
Pt	-3.250398	5.580311	3.065612
Pt	-1.513183	4.938238	1.217409
Pt	-0.614799	7.297070	1.535326
Pt	-2.362819	7.033627	5.955108
O	0.037516	2.843223	6.323509
H	1.595428	2.010789	5.358006

Vibrational Frequencies (cm⁻¹)

30.6110	34.2283	39.3279
42.0042	44.0296	49.7566
52.0476	56.5989	59.8698
67.2198	72.5313	74.5803
88.9329	91.1943	94.4631
100.3887	109.7301	113.5492
115.3393	119.0962	125.9131
132.8895	134.2463	153.2059
157.0941	161.4164	164.4144
165.6121	167.6125	171.6811
179.6869	183.4465	187.2451
188.7993	205.0405	218.8488
244.2958	310.2785	354.5860
777.7777	1028.8170	1317.4065
1390.4568	1561.2066	2992.1445

7. CO adsorbed on Pt clusters

CO on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge 0 – Spin Multiplicity 3

Pt	0.612573	0.629791	-0.451920
Pt	-0.478102	2.510802	-1.782286
Pt	-1.915134	2.560935	0.353551
Pt	-2.960530	2.607699	2.739792
Pt	-3.111976	0.073324	2.613409
Pt	-2.278071	0.014957	0.119939
Pt	-1.219167	0.035523	-2.274203
Pt	-0.506740	-0.134564	2.134840
Pt	-0.350514	2.575875	2.437194
Pt	-1.039280	4.912147	1.078126
Pt	0.918253	4.271270	-0.426953
Pt	1.830933	2.292910	1.035144
Pt	2.068853	-0.274609	1.590162
C	0.498388	2.630920	4.086292
O	0.994554	2.670804	5.120473

Vibrational Frequencies (cm-1)

27.6084	33.3115	40.1594
43.0951	49.2612	52.5866
53.1102	53.7602	58.2152
64.3219	66.3080	75.6370
81.6435	83.5260	100.3322
103.0631	108.9307	114.9379
115.9163	125.8373	128.3616
132.6730	136.6221	143.9262
150.6946	153.9639	162.4128
168.5387	170.6230	176.6500
181.6036	187.3423	189.5143
206.6732	211.7596	434.3933
467.5169	492.1856	2008.2871

CO on Pt13 – B3LYP/SDD-6-311+G(d,p) – water – Charge -1 – Spin Multiplicity 2

Pt	0.619740	0.588566	-0.554911
Pt	-0.492294	2.499549	-1.825181
Pt	-1.815170	2.496837	0.409872
Pt	-3.060196	2.557386	2.682973
Pt	-3.116613	0.021121	2.519339
Pt	-2.266495	-0.035121	0.034361
Pt	-1.263718	0.042998	-2.376479
Pt	-0.532369	-0.047761	2.114925
Pt	-0.326875	2.644625	2.643863
Pt	-1.006314	4.870622	1.130927
Pt	0.894699	4.241718	-0.444324
Pt	1.788541	2.231875	0.990564
Pt	1.992923	-0.343293	1.520389
C	0.557764	2.763186	4.252290
O	1.090420	2.845476	5.274951

Vibrational Frequencies (cm-1)

23.8810	28.9307	33.1335
35.1654	40.1253	46.3900
49.1049	51.7561	52.5796
54.7333	62.8541	71.9303
75.6178	83.4715	89.6871
99.6382	108.0678	109.7234
111.9904	113.1733	117.8274
124.4440	128.7751	134.0038
139.0337	146.8717	158.9497
160.1703	167.4067	170.7808
178.6207	184.3347	190.6767
198.6124	207.1545	393.9227
412.9517	515.5325	1948.9024

CO on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge 0 – Spin Multiplicity 3

Pt	0.375943	-0.139508	-0.483082
Pt	-0.158309	2.380940	-1.540230
Pt	-1.878517	2.540433	0.379915
Pt	-3.150713	2.549457	2.644988
Pt	-2.967893	0.021375	2.465805
Pt	-2.289926	0.028402	-0.059465
Pt	-1.304125	0.226641	-2.469533
Pt	-0.378270	0.030268	2.259941
Pt	-0.401357	2.675326	2.545649
Pt	-1.074567	4.900003	1.135366
Pt	0.892168	4.491197	-0.419782
Pt	1.541649	2.190408	0.676235
Pt	2.093655	-0.233571	1.493928
C	0.541313	2.847030	4.130715
O	1.114280	2.965208	5.121548

Vibrational Frequencies (cm-1)

21.3352	25.7259	31.1285
36.0255	38.2833	40.8881
46.2138	51.8054	52.0831
57.5370	61.6697	67.1648
79.4176	83.2806	89.0191
91.8843	99.8473	109.9303
118.3200	123.0591	129.2857
133.3112	136.8309	140.2364
146.0304	148.6770	156.3254
156.6345	170.4955	171.1559
177.5031	189.6789	192.2318
199.0513	204.8755	412.3038
419.5490	503.4817	2015.2597

CO on Pt13 – B3LYP/SDD-6-311+G(d,p) – acetonitrile – Charge -1 – Spin Multiplicity 2

Pt	0.330016	-0.283557	-0.441812
Pt	-0.144707	2.394276	-1.590351
Pt	-1.797529	2.504371	0.403271
Pt	-3.140070	2.546998	2.630963
Pt	-3.000113	0.019626	2.422251
Pt	-2.352411	0.033975	-0.116817
Pt	-1.254796	0.190356	-2.477592
Pt	-0.405646	0.032692	2.180361
Pt	-0.370816	2.702878	2.648488
Pt	-1.087925	4.892924	1.127876
Pt	0.871721	4.529559	-0.448586
Pt	1.444578	2.231303	0.646381
Pt	2.091396	-0.154138	1.485997
C	0.589089	2.862312	4.213565
O	1.182548	2.970032	5.198004

Vibrational Frequencies (cm-1)

24.9403	28.2017	31.4036
34.1356	35.4154	39.9979
41.1484	47.8882	55.5338
56.6420	61.6463	72.5538
82.7199	84.8873	88.0893
90.2161	100.1551	107.3390
110.3576	116.0329	119.0339
124.1177	130.8359	133.3108
137.8592	144.3542	151.1607
158.1097	170.2977	171.0192
177.8788	190.4866	191.6205
200.6992	201.4018	400.0001
405.6449	514.5861	1989.4732

CO on Pt20 – B3LYP/see text – water – Charge 0 – Spin Multiplicity 15

Pt	-2.801566	-1.429337	2.491332
Pt	-0.016674	-1.382382	2.450598
Pt	2.744293	-1.538461	2.508799
Pt	-4.184856	-1.560997	0.092130
Pt	-1.461048	-2.189582	0.154412
Pt	1.345286	-1.921162	0.185705
Pt	4.134219	-1.722707	0.117898
Pt	-2.793570	-1.746269	-2.296067
Pt	0.020070	-1.748805	-2.200679
Pt	2.752398	-1.853573	-2.277702
Pt	-2.754962	0.725035	0.749460
Pt	0.017695	0.667325	0.747377
Pt	2.792275	0.615788	0.765721
Pt	-1.364381	0.536855	-1.642428
Pt	1.412036	0.483986	-1.631637
Pt	-1.325525	3.011709	1.401480
Pt	1.448207	2.957558	1.410491
Pt	0.066091	2.824816	-0.995720
Pt	2.841354	2.770775	-0.983215
Pt	-2.710020	2.879299	-1.000386
C	-1.399888	-4.018202	0.191350
O	-1.369229	-5.168838	0.215679

CO on Pt20 – B3LYP/see text – acetonitrile – Charge 0 – Spin Multiplicity 15

Pt	-2.801570	-1.429393	2.491311
Pt	-0.007891	-1.385201	2.445287
Pt	2.744266	-1.538363	2.508795
Pt	-4.184870	-1.560988	0.092211
Pt	-1.462082	-2.186003	0.152964
Pt	1.352162	-1.926797	0.180248
Pt	4.134231	-1.722965	0.117967
Pt	-2.793572	-1.746307	-2.296109
Pt	0.011945	-1.747893	-2.201727
Pt	2.752415	-1.853486	-2.277713
Pt	-2.754919	0.725018	0.749525
Pt	0.017657	0.667424	0.747288
Pt	2.792296	0.615841	0.765706
Pt	-1.364408	0.536783	-1.642509
Pt	1.412044	0.484094	-1.631648
Pt	-1.325526	3.011703	1.401495
Pt	1.448214	2.957547	1.410511
Pt	0.066074	2.824815	-0.995702
Pt	2.841362	2.770770	-0.983216
Pt	-2.710005	2.879307	-1.000380
C	-1.364598	-4.015964	0.198833
O	-1.310340	-5.163200	0.246670