

Computational study of CO reactivity with Nb₃X heteronuclear clusters

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Nb₃X

-334.1206594

0, 3

11	-0.005644	-0.014733	2.636782
41	-1.288350	-0.655640	-0.240379
41	0.000304	1.314946	-0.230047
41	1.289560	-0.655352	-0.237003

-333.9248186

1, 2

11	0.004642	1.294211	2.532148
41	1.235463	-0.736349	0.031287
41	0.002134	1.120232	-0.743111
41	-1.238842	-0.731110	0.032467

-334.166641

-1, 4

11	-0.002096	-0.061717	2.624161
41	-1.262186	-0.663875	-0.247129
41	-0.000734	1.342875	-0.211084
41	1.263482	-0.662442	-0.245830

-414.318329

0, 3

13	-0.000224	-0.571486	2.031267
41	-1.272745	-0.617531	-0.315569
41	1.276056	-0.612376	-0.314672
41	-0.003241	1.411110	-0.013819

-414.0842499

1, 2

13	-0.135274	-0.000371	2.081418
41	-1.464902	-0.001193	-0.264476
41	0.755023	-1.221514	-0.197820
41	0.752771	1.222825	-0.197666

-414.391314

-1, 4

13	-0.001549	0.000613	2.101898
41	-0.187187	1.402688	-0.222434
41	-1.121174	-0.863666	-0.222448
41	1.308851	-0.539217	-0.221574

-218.621052

0,3

21	-0.000162	0.002546	1.980827
41	-0.140738	1.414625	-0.339610
41	-1.155143	-0.829863	-0.337436
41	1.295964	-0.586065	-0.337524

-218.416996

1,2

21	0.005287	-0.337632	1.949230
41	-0.016357	1.466910	-0.146098
41	1.255836	-0.633482	-0.426885
41	-1.242187	-0.660494	-0.425403

-218.680794

-1,4

21	0.000384	-0.002573	2.049308
41	0.976109	-1.015871	-0.351115
41	-1.368362	-0.336741	-0.350023
41	0.392057	1.353930	-0.348507

-202.565447

0,2

38	2.312739	-0.000674	0.266159
41	-0.518773	-1.287528	-0.725149
41	-0.520170	1.294261	-0.715613
41	-1.104572	-0.006108	1.194078

-202.377502

1,3

38	2.237963	-0.000260	0.110660
41	-0.840617	-0.001332	1.308155
41	-0.616646	1.302336	-0.704254
41	-0.616946	-1.300763	-0.706465

-202.624220

-1,3

38	-2.373186	-0.251177	0.153489
41	1.027617	-0.213985	1.210962
41	0.824012	-1.025029	-0.915775
41	0.347909	1.471813	-0.437444

-210.192746

0,3

39	1.921867	-0.000099	0.000232
41	-0.609642	-0.118165	1.418965
41	-0.609315	-1.169985	-0.811938
41	-0.609160	1.288245	-0.607248

-209.985868

1,2

39	-1.937548	-0.148593	0.000072
41	0.695500	-0.693120	-1.188342
41	0.695630	-0.692963	1.188374
41	0.451903	1.527428	-0.000101

-210.255628

-1,4
39 1.986826 -0.000760 0.000445
41 -0.630599 -0.174131 1.400308
41 -0.628942 1.300300 -0.549361
41 -0.630366 -1.125446 -0.851371

-218.937176
0,2
40 -1.655744 -0.097629 0.472707
41 1.058427 -0.039177 1.155867
41 0.217848 1.334756 -0.730027
41 0.339085 -1.200331 -0.887018

-218.728957
1,3
40 -1.683640 -0.424573 0.010102
41 0.772869 -0.587786 -1.221997
41 0.100992 1.517647 -0.043799
41 0.768715 -0.515643 1.255940

-218.994501
-1,1
40 -2.089748 -0.000205 0.000015
41 0.056799 1.337909 -0.000016
41 0.057107 -1.337701 -0.000016
41 1.924873 -0.000009 0.000017

-228.912715
0,1
41 0.801548 0.561080 1.195506
41 -1.322396 -0.615515 0.509591
41 -0.312597 1.142240 -0.991876
41 0.833445 -1.087806 -0.713221

-228.693538
1,2
41 0.000807 1.286354 -0.842926
41 0.000947 -1.286337 -0.842949
41 1.334598 0.000058 0.844044
41 -1.336352 -0.000076 0.841831

-228.953748
-1,2
41 0.868904 -0.298136 1.240010
41 -1.310026 -0.876946 0.000404
41 -0.427500 1.473990 -0.000409
41 0.868622 -0.298909 -1.240005

-240.174228
0,2
42 -0.667415 -0.004287 1.287150
41 -1.196444 -0.009042 -0.992050
41 0.929243 1.224953 -0.163709
41 0.950895 -1.211521 -0.162785

-239.976481
1,1
42 -0.000129 0.000756 1.450365

41	-1.267289	-0.742121	-0.495002
41	1.276436	-0.726437	-0.494807
41	-0.009014	1.467784	-0.495931

-240.230900

-1,3

42	0.019733	-0.788577	1.201667
41	-1.301490	-0.386022	-0.748539
41	-0.026294	1.535001	0.275655
41	1.307570	-0.341168	-0.758092

-252.817991

0,1

43	0.918949	-0.013861	1.130530
41	1.103963	0.009443	-1.083104
41	-1.030344	1.165725	-0.039714
41	-1.037395	-1.160630	-0.062860

-252.613761

1,2

43	-0.088053	0.008152	1.473151
41	0.448656	1.375616	-0.497834
41	1.013744	-1.054119	-0.451082
41	-1.370052	-0.330047	-0.596095

-252.875908

-1,2

43	-0.408430	-0.078938	1.320304
41	-1.332673	0.006982	-0.808245
41	0.916970	-1.213677	-0.342883
41	0.844056	1.289484	-0.233582

-266.945213

0,2

44	1.128473	0.003998	-1.009783
41	-1.061786	1.146668	-0.053653
41	0.914433	-0.005860	1.200979
41	-1.063691	-1.145099	-0.063656

-266.735884

1,3

44	-1.260317	-0.001411	-0.826224
41	1.427903	0.000144	-0.739694
41	-0.038498	1.267235	0.812295
41	-0.036870	-1.265865	0.814078

-267.000816

-1,3

44	-1.166393	-0.727477	-0.680108
41	1.044324	-0.905892	0.725773
41	-0.851441	0.916314	0.844686
41	1.058856	0.770285	-0.840586

-282.649676

0,3

45	-1.616563	0.010220	-0.019590
41	0.603440	-0.792580	-1.139173
41	0.565786	-0.602146	1.263296

41	0.605050	1.383509	-0.102621
-282.434817			
1,2			
45	-1.477873	0.001383	0.558557
41	0.206068	1.240503	-0.814828
41	0.201352	-1.238764	-0.817968
41	1.214636	-0.003257	1.019746
-282.702625			
-1,4			
45	-1.571922	-0.292410	0.002071
41	0.738681	-0.601361	-1.177948
41	0.247239	1.508133	-0.009053
41	0.739360	-0.585835	1.184727
-300.022835			
0,2			
46	1.713800	-0.009750	0.199514
41	-0.907538	0.000417	1.243620
41	-0.517524	-1.231324	-0.737527
41	-0.497738	1.241846	-0.729938
-299.810960			
1,3			
46	1.682477	-0.000270	0.000791
41	-0.628580	-0.759679	-1.175752
41	-0.630241	-0.638214	1.245273
41	-0.628837	1.398197	-0.070408
-300.077158			
-1,3			
46	1.707703	-0.001270	0.182193
41	-0.515414	-1.280429	-0.711555
41	-0.887462	-0.000480	1.216984
41	-0.513083	1.282334	-0.709840
-319.105337			
0,3			
47	2.203469	-0.000309	-0.394267
41	-0.222986	1.154622	0.521133
41	-0.223368	-1.154043	0.521630
41	-2.079575	-0.000225	-0.590799
-318.890036			
1,2			
47	1.845552	-0.040928	0.000024
41	-0.732675	-0.710780	1.158507
41	-0.732638	-0.711414	-1.158190
41	-0.650320	1.469112	-0.000345
-319.168635			
-1,4			
47	2.323013	-0.000068	-0.228615
41	-2.200274	-0.000067	-0.339994
41	-0.231373	-1.213187	0.301067
41	-0.231318	1.213331	0.300998

-339.896494
0,2
48 2.464677 -0.000127 -0.000717
41 -2.389118 -0.000585 -0.001064
41 -0.248548 1.153830 0.000952
41 -0.247810 -1.153097 0.000953

-339.667336
1,3
48 2.482900 -0.000229 -0.199481
41 -0.297764 -1.191911 0.278765
41 -0.299741 1.193723 0.277879
41 -2.309305 -0.001544 -0.323106

-339.959132
-1,3
48 -2.269814 -0.000809 0.256549
41 2.060207 -0.000024 0.437896
41 0.297634 1.279419 -0.368884
41 0.299502 -1.278448 -0.369363

Nb₃X-CO

-447.74863
0,1
11 -1.420816 0.327276 2.150199
41 -0.728290 -0.993568 -0.574959
41 0.436740 1.395593 -0.330687
41 1.371071 -0.667293 0.367559
6 -1.487545 1.006262 -0.379449
8 -2.463263 0.154799 0.085760

-527.93033
0,3
13 0.565279 0.029213 2.105968
41 -0.018671 1.489718 -0.088497
41 1.449161 -0.492574 -0.501764
41 -0.801993 -1.093950 0.095627
6 -1.838803 0.746720 -0.394161
8 -2.760525 -0.111384 -0.591580

-332.27089
0,1
21 -0.357518 -0.214140 1.913767
41 -0.210090 -1.106789 -0.884833
41 -0.609593 1.374596 -0.418550
41 1.583889 0.099179 0.135740
6 -1.852129 -0.006877 0.202068
8 -1.588977 -1.313528 0.808982

-316.18658
0,2
38 -1.870216 -1.111413 0.018845
41 1.238837 -0.422726 1.141286
41 1.227148 -0.526868 -1.108700
41 0.123248 1.581924 -0.054197
6 -1.821293 1.425543 -0.008345

8 -3.020321 0.969364 0.027501
-323.83664
0,1
39 1.864426 0.417948 -0.038269
41 -0.455901 -1.021900 -1.218256
41 -0.773854 1.425955 -0.307608
41 -0.871341 -0.346415 1.246405
6 0.622533 -1.695514 0.259631
8 1.212138 -1.061268 1.424067

-332.56756
0,2
40 -1.138725 -1.139144 -0.133015
41 1.365948 -0.313464 -1.045387
41 -0.319523 1.504035 -0.157734
41 0.979665 -0.174887 1.315447
6 -2.172856 0.826506 -0.042647
8 -3.060445 -0.129543 0.121386

-342.52693
0,1
41 1.126667 -0.159193 1.230005
41 1.127163 -0.165446 -1.228952
41 -0.854130 -1.158878 0.002162
41 -0.474271 1.488947 -0.003282
6 -2.230683 0.533455 -0.000671
8 -3.069814 -0.427916 0.000846

-353.78080
0,2
42 0.040661 1.439435 -0.289774
41 -1.648394 -0.130736 -0.411520
41 0.064485 -0.270776 1.481224
41 0.719190 -1.338249 -0.646753
6 1.894446 0.283516 -0.424718
8 2.797382 1.146608 -0.327774

-366.43733
0,3
43 1.046473 -0.245091 -1.077507
41 1.252853 -0.041125 1.143957
41 -0.565954 1.501628 -0.128492
41 -0.876655 -1.173587 0.000078
6 -2.246260 0.501083 0.157145
8 -2.967599 -0.528896 0.469082

-380.56399
0,2
44 1.358012 -0.117864 -0.994375
41 1.046161 -0.160485 1.208481
41 -0.605290 1.442071 -0.025553
41 -0.943051 -1.124550 -0.085706
6 -2.355943 0.499457 -0.048713
8 -3.128436 -0.531149 -0.117668

-396.26264
0,3

45	1.392842	-0.120417	-1.018824
41	-0.490077	1.470633	0.012730
41	-0.893765	-1.121843	-0.111227
41	0.772576	-0.215807	1.364435
6	-2.220746	0.556146	-0.321107
8	-3.036440	-0.421303	-0.516218

-413.63742

0,2			
46	-1.401723	-0.994504	-0.600109
41	-0.797112	1.322742	0.639554
41	0.647287	-0.785972	1.101248
41	0.742818	0.784933	-0.928807
6	2.284865	-0.648657	-0.012362
8	3.307170	-0.568834	-0.701578

-432.72162

0,3			
47	-2.639543	0.162473	-0.041714
41	2.171751	-0.522539	-0.035249
41	-0.138893	-1.263480	0.040537
41	0.065119	1.084456	0.057793
6	1.988849	1.615816	-0.010775
8	3.263545	1.429120	-0.070141

-453.51401

0,2			
48	2.095377	-0.113444	-0.164933
41	-0.558157	1.380740	-0.566829
41	-0.619495	-1.130783	-0.636723
41	-0.403416	-0.005044	1.513764
6	-2.198495	0.332272	-0.284297
8	-2.820414	-0.823721	-0.387013

Nb₃X-C-O

-447.83051

0,1			
11	-0.378161	-1.043532	2.272836
41	0.145362	1.421459	0.077521
41	1.480963	-0.498366	-0.204848
41	-1.241197	-0.459366	-0.664115
6	0.067579	-1.830225	-0.122985
8	-1.504498	0.430925	1.023230

-528.00743

0,1			
13	-0.273167	-0.652628	2.068381
41	1.329336	-0.760836	-0.078154
41	-0.106100	1.423235	0.008868
41	-1.242138	-0.706936	-0.597310
6	-1.598860	0.429302	0.975628
8	1.739910	0.966796	-0.676536

-332.37293

0,1

21	-1.844460	1.016900	0.782431
41	-0.677733	-1.118393	-0.608925
41	0.735108	1.328657	-0.336926
41	1.408093	-0.684340	0.532880
6	-1.010198	0.760177	-1.159141
8	-1.911165	-0.809861	0.931951

-316.30442
0,2

38	2.227292	-0.534988	-0.504066
41	0.009519	1.367243	0.670530
41	-1.669588	0.231441	-0.879720
41	-0.776703	-1.359995	0.548492
6	0.580827	-0.326445	1.508360
8	1.473197	1.562744	-0.475879

-323.93851
0,1

39	2.088407	-0.386423	-0.448968
41	-0.064543	1.351043	0.634876
41	-0.580317	-1.435494	0.428976
41	-1.724337	0.204306	-0.706562
6	0.749171	-0.288736	1.410380
8	1.399273	1.486103	-0.700175

-332.66386
0,2

40	-1.673248	-0.001673	-0.480387
41	0.368285	-0.019141	1.459833
41	0.657006	-1.436122	-0.646126
41	0.638435	1.461453	-0.609222
6	1.897396	0.014918	-0.176814
8	-1.583402	-0.034549	1.486561

-342.60443
0,3

41	-0.129193	1.613584	0.222964
41	-0.193197	-0.676079	1.310087
41	-1.517874	-0.387037	-0.802377
41	1.570362	-0.569296	-0.445800
6	-0.036737	-1.689119	-0.783496
8	1.410797	1.363331	-0.872361

-353.86401
0,2

42	-0.960419	-0.302533	-1.192494
41	-0.942019	-0.422152	1.151032
41	0.439047	1.464118	-0.257640
41	1.568789	-0.741853	0.120011
6	0.124483	-1.813344	-0.612652
8	-0.513477	1.410225	1.526390

-366.52252
0,3

43	-0.166210	-0.514717	1.301573
41	1.459008	-0.744919	-0.481664
41	-1.351766	-0.706215	-0.696646
41	-0.071229	1.599737	0.145776

6	-1.266192	1.150464	-1.284603
8	1.658453	1.142164	-0.740766

-380.65242

0,2			
44	0.798524	1.115687	-0.713700
41	1.467393	-0.736593	0.499134
41	-1.003876	0.758045	0.851097
41	-0.823378	-1.094490	-0.729631
6	-0.204611	-0.976757	1.500341
8	-2.394139	0.095609	-0.380480

-396.34563

0,1			
45	-1.329041	-0.705494	0.733046
41	1.146676	0.537502	0.942595
41	-0.854558	1.046228	-0.873329
41	0.669399	-1.077805	-0.816144
6	0.234277	2.130581	0.238703
8	2.372375	-0.222398	-0.474660

-413.71722

0,2			
46	1.583422	-0.758741	-0.225591
41	0.334308	1.638663	0.153696
41	-1.036232	-0.451638	-1.083191
41	-0.535912	-0.445168	1.307807
6	-0.627933	1.414727	-1.475676
8	-2.289821	-0.500302	0.465060

-432.80397

0,3			
47	-2.310255	-0.029664	-0.447721
41	2.103301	-0.111312	-0.633241
41	-0.031650	1.162772	0.649759
41	0.126371	-1.312250	0.439977
6	1.436499	-0.151013	1.370578
8	1.230511	1.624080	-0.737106

-453.57524

0,2			
48	-2.575418	-0.017435	0.260507
41	2.241659	-0.210527	0.471349
41	0.088750	1.186827	-0.349986
41	0.208250	-1.261310	-0.506033
6	0.522308	0.221205	1.333139
8	2.050144	1.399382	-0.591458