Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Reactivity of silica supported zirconium hydride with N_2O and CO_2 probe molecules: a computational point of view.

Mahboubeh Poor Kalhor,[a] Raphael Wischert,[b†1] Christophe Copéret,[b,*] Henry Chermette,[a,*]

[a] University of Lyon; Université Lyon 1(UCBL) and UMR CNRS 5280 Institut Sciences Analytiques, F-69622 Villeurbanne Cedex, France

[b] Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir Prelog Weg 2, CH-8093 Zürich, Switzerland.

Cartesian coordinates of the structures

[1] †Present address: Eco-Efficient Products and Processes Laboratory (E2P2L), UMI 3464 CNRS – Solvay, 3966 Jin Du Road, Xin Zhuang Ind. Zone, 201108 Shanghai, China.

1-H

1.Zr	0.009288	0.001839	0.005833
2.O	1.996687	-0.000383	0.000026
3.O	-0.258514	1.968450	0.021483
4.O	-0.253513	-0.322320	1.949716
5.H	-0.934846	-1.048521	-1.250713
6.Si	0.627573	0.632498	3.001160
7.Si	0.602851	2.826722	1.152953
8.Si	2.765379	0.944577	1.143389
9.O	2.238912	0.459838	2.643830
10.O	0.224155	2.213746	2.657655
11.O	2.224605	2.506469	0.927006
12.O	0.237620	4.408349	0.997326
13.O	0.391325	0.244816	4.568021
14.O	4.390322	0.835849	1.079334
15.H	0.697243	5.016134	1.599364
16.H	4.757430	0.500205	0.246614
17.H	-0.484271	-0.115551	4.780898

2-H

1.Zr	0.009904	0.012785	0.003305
2.O	1.971450	-0.006736	-0.005078
3.O	-0.292212	1.946908	-0.012990
4.Si	3.076406	1.221381	-0.113143
5.O	2.319962	2.684160	-0.050964
6.Si	0.766144	3.220646	0.040831
7.O	4.107712	1.239020	1.171714
8.O	3.839730	0.981898	-1.554328
9.H	4.396371	1.718772	-1.854852
10.H	4.736870	0.499844	1.198678
11.O	0.597719	4.214147	-1.262343
12.O	0.452673	3.968280	1.475813
13.H	1.086996	4.658469	1.729419
14.H	-0.242137	4.699682	-1.301580
15.H	-0.671062	-0.753505	-1.567616
16.H	-0.652412	-0.752171	1.583263

N2O

1.N	0.000371	0.000000	0.000000
2.N	1.139008	0.000000	0.000000
3.O	-1.197713	0.000000	0.000000

TS1 (= 1-H…ONN)

1.Zr	-0.670482	0.152090	0.142630
2.O	1.261385	-0.366508	-0.133679
3.Si	2.383821	0.850378	-0.289564

4.O	2.299600	1.772943	1.099493
5.Si	0.866296	2.560497	1.416628
6.O	0.494130	3.423665	0.039643
7.Si	0.475757	2.624962	-1.423062
8.O	1.932855	1.837833	-1.547065
9.O	-0.726793	1.473999	-1.353075
10.O	-0.987464	-2.026760	0.208598
11.N	0.046710	-3.008760	0.112259
12.N	0.394950	-4.079036	0.133245
13.H	-2.318101	-0.911124	0.377901
14.O	-0.311516	1.411051	1.632328
15.O	3.895396	0.308825	-0.590163
16.O	0.933365	3.499375	2.749356
17.O	0.287297	3.668450	-2.664722
18.H	1.547908	4.250308	2.708108
19.H	-0.561013	3.597337	-3.130611
20.H	4.144836	-0.510574	-0.134430

1-OH

1.Zr	-0.023841	-0.017842	-0.037813
2.O	1.978656	-0.015442	-0.021070
3.O	-0.263750	1.957248	0.002564
4.O	-0.273030	-0.330798	1.925175
5.O	-0.951912	-1.203990	-1.320802
6.Si	0.586822	0.639951	2.970186
7.Si	0.589060	2.824675	1.129887
8.Si	2.735422	0.940702	1.112144
9.O	2.203442	0.473368	2.618823
10.O	0.202026	2.226443	2.636172
11.O	2.209223	2.506262	0.900569
12.O	0.225870	4.407541	0.966427
13.O	0.291499	0.298127	4.541561
14.O	4.365441	0.858732	1.025026
15.H	0.640889	5.005243	1.609604
16.H	4.703710	0.236526	0.361288
17.H	-0.318138	-0.442971	4.685748
18.H	-1.548624	-1.193875	-2.084266

2-H.N2O (= 2-H…ONN)

1.Zr	-0.103715	0.133093	-0.009565
2.O	1.869277	-0.041920	-0.007288
3.O	-0.211525	2.096530	-0.017904
4.Si	3.069570	1.086040	-0.121543
5.O	2.450643	2.608986	-0.068769
6.Si	0.945378	3.272203	0.020453
7.O	4.106759	1.019747	1.158786
8.O	3.815413	0.770238	-1.559147
9.H	4.427968	1.459627	-1.864016
10.H	4.688656	0.242259	1.166196
11.O	0.870350	4.269756	-1.289534

12.O	0.710526	4.062541	1.447517
13.H	1.405883	4.698092	1.683435
14.H	0.069682	4.817120	-1.336817
15.H	-0.909389	-0.391085	-1.618151
16.H	-0.881371	-0.456627	1.591309
17.O	0.205981	-2.484799	-0.141008
18.N	1.313133	-2.957218	-0.067288
19.N	2.352298	-3.403739	-0.006398

TS2

1.Zr	-0.015824	0.027492	-0.071845
2.O	1.950627	-0.013709	0.046084
3.Si	3.033017	1.234440	0.028599
4.O	2.260348	2.686801	0.109176
5.Si	0.703319	3.225036	0.137377
6.O	-0.360067	1.965667	0.035792
7.O	0.601540	4.229173	-1.166561
8.O	0.342567	3.977380	1.558576
9.O	4.015248	1.224496	1.351853
10.O	3.859533	1.060578	-1.387605
11.O	-1.317831	-1.582898	-0.899786
12.N	-2.085618	-2.621379	-0.319770
13.N	-2.765593	-3.516113	-0.428223
14.H	-0.483820	-0.432937	-1.903588
15.H	-0.660114	-0.711571	1.517133
16.H	4.409266	1.821009	-1.638335
17.H	4.654648	0.493765	1.374385
18.H	0.989822	4.640695	1.848808
19.H	-0.221260	4.742665	-1.216247

2-(H)(OH)

1.Zr	0.023106	0.019067	-0.004867
2.O	1.999601	0.001876	-0.029576
3.Si	3.090424	1.243881	-0.008105
4.O	2.358625	2.662596	0.408268
5.Si	0.815986	3.236807	0.334139
6.O	-0.233819	1.952448	0.330798
7.O	0.458861	4.237895	1.591846
8.H	0.118542	3.793532	2.385452
9.H	-0.016383	4.720085	-1.112333
10.O	0.747008	4.123196	-1.051361
11.H	4.846957	0.290112	0.987355
12.O	3.712048	1.294706	-1.538564
13.H	4.203144	2.105370	-1.751747
14.O	-0.856099	-0.642954	-1.625117
15.H	-0.836026	-0.585509	-2.592452
16.H	-0.604671	-0.954206	1.469869
17.O	4.245521	1.035119	1.149084

TS3

1.H	0.088238	-0.093554	0.017209
2.O	1.831054	0.112559	-0.019030
3.Zr	0.474950	1.828196	0.018929
4.O	-0.526438	2.459676	-1.566334
5.Si	-0.168318	3.455048	-2.828636
6.O	-1.208353	4.728941	-2.673927
7.O	2.168097	2.844036	-0.404767
8.Si	2.629819	3.752736	-1.685781
9.O	3.901461	2.939211	-2.364815
10.O	1.402661	3.937670	-2.773931
11.O	-0.306839	2.694888	-4.286493
12.O	3.027869	5.302908	-1.274673
13.N	3.234133	0.237100	-0.225639
14.N	4.227819	-0.189300	-0.538720
15.H	3.800470	5.376464	-0.691221
16.H	4.225281	3.319541	-3.197948
17.H	-1.215068	2.449249	-4.526345
18.H	-1.022561	5.477999	-3.263550
19.O	-0.210880	2.413442	1.763488
20.H	-0.751481	3.132473	2.125533

2-(OH)2

1.Zr	-0.009865	-0.008916	0.063952
2.O	1.978547	-0.013603	0.044357
3.Si	3.067062	1.221783	0.002758
4.O	2.352605	2.660340	0.365834
5.Si	0.803959	3.225422	0.336432
6.O	-0.235745	1.943573	0.410121
7.O	0.500159	4.271277	1.575425
8.H	0.188362	3.852120	2.393874
9.H	-0.062426	4.705452	-1.088187
10.O	0.679436	4.079404	-1.067076
11.H	4.816768	0.292250	1.030266
12.O	3.668122	1.206318	-1.539083
13.H	4.221545	1.973102	-1.762326
14.O	-0.787592	-0.556603	-1.658245
15.H	-0.597305	-0.423079	-2.599451
16.O	-0.741017	-1.091901	1.549164
17.O	4.243672	1.066663	1.150924
18.H	-1.387227	-1.815332	1.562806

1-H.CO2

1.Zr	0.064869	-0.053299	-0.025290
2.O	2.050926	0.005290	-0.006899
3.Si	2.828529	1.465143	0.013829
4.O	-0.132899	1.210872	-1.555733
5.Si	0.700058	2.639984	-1.473603

6.O	-0.172396	1.227616	1.483011
7.Si	0.649166	2.663939	1.400536
8.O	0.277241	3.405055	-0.048556
9.O	2.330127	2.305114	-1.340153
10.O	2.282746	2.321836	1.337209
11.O	0.248010	3.577876	2.695255
12.O	4.444228	1.229393	0.057340
13.O	0.354249	3.531897	-2.797344
14.H	4.985299	2.009833	0.258150
15.H	0.870502	4.346901	-2.904535
16.H	0.607002	4.479209	2.708756
17.H	-0.588986	-1.847694	-0.010857
18.C	-3.027230	-1.144136	-0.003668
19.O	-2.540308	-0.064322	-0.051890
20.O	-3.587369	-2.165014	0.042030

TS4

1.Zr	-0.013138	0.029133	-0.027041
2.O	1.974457	-0.003348	-0.014941
3.Si	2.829379	1.411487	-0.004058
4.O	-0.150360	1.317838	-1.535186
5.Si	0.744680	2.710954	-1.451231
6.O	-0.158966	1.309394	1.489439
7.Si	0.729570	2.706177	1.420729
8.O	0.374925	3.481578	-0.015984
9.O	2.356503	2.291396	-1.341568
10.O	2.344574	2.290916	1.329468
11.O	0.382450	3.614217	2.731695
12.O	4.426461	1.078430	0.008003
13.O	0.416627	3.622954	-2.764127
14.H	5.023777	1.835366	0.119379
15.H	0.906751	4.457347	-2.839528
16.H	0.830277	4.473361	2.788912
17.H	-0.735074	-1.763933	-0.035838
18.C	-2.724161	-1.263005	0.017961
19.O	-2.502909	-0.084886	0.023212
20.O	-3.220041	-2.321602	0.020878

1-\eta1-O2CH

1.Zr	0.061781	-0.149192	-0.089680
2.O	2.042708	-0.026362	-0.033815
3.O	-0.293242	1.804019	-0.005536
4.O	-0.083128	-0.290196	-2.062228
5.O	2.369992	0.678991	-2.601733
6.Si	0.754200	0.783250	-3.009581
7.H	0.917784	0.980866	-5.234626
8.O	0.272629	2.323326	-2.584620
9.Si	0.548897	2.815640	-1.013342
10.O	0.076709	4.350729	-0.735251
11.H	0.489498	5.041085	-1.278952

12.O	2.177506	2.572992	-0.735476
13.Si	2.805909	1.055812	-1.034960
14.O	4.413827	0.977006	-0.781881
15.H	4.950596	1.669622	-1.199060
16.O	-0.987667	-1.477445	0.991732
17.C	-1.532249	-2.426769	1.786039
18.O	-1.692308	-2.319291	2.978628
19.H	-1.819728	-3.323235	1.205166
20.O	0.471852	0.424031	-4.575195

TS5

1.Zr	-0.036673	0.028750	0.067480
2.O	1.947174	0.024719	0.046494
3.Si	2.759594	1.472002	0.035420
4.O	2.239089	2.351270	-1.285614
5.Si	0.618882	2.756137	-1.348739
6.O	0.277056	3.518521	0.094765
7.Si	0.658715	2.725298	1.514009
8.O	2.270823	2.316164	1.386783
9.O	-0.258123	1.349586	-1.397856
10.O	-0.216445	1.317499	1.568365
11.O	-0.951616	-1.759226	0.020170
12.C	-1.587179	-2.949957	0.100708
13.H	-0.880350	-3.794879	-0.026958
14.O	-2.774747	-3.088602	0.263512
15.O	4.367376	1.202108	0.007900
16.O	0.242909	3.658048	-2.653362
17.O	0.323141	3.610909	2.840250
18.H	4.907795	1.887800	-0.416558
19.H	0.780995	4.451777	-2.802714
20.H	0.698491	4.505616	2.869945

1-\eta2-O2CH

1.Zr	0.061781	-0.149192	-0.089680
2.O	2.042708	-0.026362	-0.033815
3.O	-0.293242	1.804019	-0.005536
4.O	-0.083128	-0.290196	-2.062228
5.O	2.369992	0.678991	-2.601733
6.Si	0.754200	0.783250	-3.009581
7.H	0.917784	0.980866	-5.234626
8.O	0.272629	2.323326	-2.584620
9.Si	0.548897	2.815640	-1.013342
10.O	0.076709	4.350729	-0.735251
11.H	0.489498	5.041085	-1.278952
12.O	2.177506	2.572992	-0.735476
13.Si	2.805909	1.055812	-1.034960
14.O	4.413827	0.977006	-0.781881
15.H	4.950596	1.669622	-1.199060
16.O	-0.987667	-1.477445	0.991732
17.C	-1.532249	-2.426769	1.786039

18.O	-1.692308	-2.319291	2.978628
19.H	-1.819728	-3.323235	1.205166
20.O	0.471852	0.424031	-4.575195

2-H.CO2

1.Si	0.061735	-0.036747	-0.027211
2.O	1.704658	-0.031275	-0.179234
3.O	-0.560987	1.489473	0.064232
4.O	-0.446963	-0.795078	1.347515
5.O	-0.469260	-0.808036	-1.382334
6.Si	-1.486172	-0.436293	-2.623156
7.O	-2.159434	1.054438	-2.392686
8.Zr	-1.865486	2.459283	-1.052151
9.O	-0.685800	-0.337203	-4.061689
10.O	-2.616977	-1.636413	-2.599563
11.H	-3.552125	2.720188	-0.238934
12.H	-1.096081	3.888916	-1.986281
13.H	-3.238157	-1.622913	-3.345767
14.H	-0.103863	-1.088938	-4.259680
15.H	2.181811	0.289111	0.603232
16.H	-0.287999	-1.752835	1.368389
17.O	-1.693019	4.363317	0.751998
18.C	-2.696088	4.680398	1.292220
19.O	-3.669496	4.988676	1.852916

TS6

1.Zr	-0.045457	0.048510	0.004643
2.O	1.922453	-0.005369	0.010107
3.O	-0.252303	2.003103	0.036462
4.Si	3.064855	1.181636	-0.108207
5.O	2.363472	2.669335	-0.171528
6.Si	0.837430	3.243695	0.062855
7.O	4.039187	1.242596	1.220536
8.O	3.887852	0.842197	-1.495029
9.H	4.536122	1.513601	-1.763901
10.H	4.577391	0.448024	1.368728
11.O	0.612344	4.299736	-1.180697
12.O	0.655836	3.943621	1.544120
13.H	1.362870	4.559474	1.797056
14.H	-0.181744	4.852938	-1.102538
15.H	-0.835956	-0.454367	-1.654642
16.H	-0.784906	-0.525162	1.622470
17.O	-0.128113	-2.439318	-0.325322
18.C	-0.573912	-2.589442	-1.423529
19.O	-0.978814	-2.961676	-2.453224

2-(H)(\eta1-O2CH)

1.Si	-0.000035	0.000043	0.000011
2.O	1.642856	0.000071	0.000053

3.O	-0.615587	1.541376	-0.000046
4.O	-0.667160	-0.712743	1.322895
5.O	-0.404729	-0.770696	-1.397031
6.Si	-1.441567	-0.487498	-2.642921
7.O	-2.076583	1.042705	-2.535581
8.Zr	-1.764931	2.489600	-1.260800
9.O	-0.675526	-0.519548	-4.095653
10.O	-2.611538	-1.631848	-2.478100
11.H	-3.393236	2.783840	-0.399525
12.O	-0.666360	4.054644	-2.128328
13.H	-3.298020	-1.628738	-3.165247
14.H	-0.111821	-1.293355	-4.259067
15.H	2.059642	0.373872	0.793388
16.H	-0.580305	-1.678839	1.370172
17.C	-1.530102	5.050095	-2.046354
18.O	-1.424955	6.202540	-2.400779
19.H	-2.517438	4.739069	-1.536418

TS7

1.Si	0.186281	-0.023869	-0.171429
2.O	1.814245	-0.115733	-0.376280
3.O	-0.344732	1.547281	-0.113825
4.O	-0.342690	-0.694789	1.234711
5.O	-0.436326	-0.775562	-1.496448
6.Si	-1.661232	-0.473870	-2.552226
7.O	-2.214523	1.076858	-2.350714
8.Zr	-1.658295	2.531916	-1.171342
9.O	-1.161559	-0.537946	-4.116690
10.O	-2.810946	-1.590331	-2.178555
11.H	-3.097711	2.876841	-0.036635
12.O	-0.713366	4.071636	-2.213642
13.H	-3.575576	-1.617612	-2.776513
14.H	-0.699217	-1.350445	-4.380100
15.H	2.342161	0.147161	0.395488
16.H	-0.289863	-1.663629	1.279893
17.C	-1.536856	5.094716	-2.028029
18.O	-1.432363	6.230995	-2.430597
19.H	-2.451442	4.816583	-1.392189

2-(H)(\eta2-O2CH)

1.Si	0.001879	0.001671	-0.000838
2.O	1.649943	-0.002635	-0.007303
3.O	-0.606402	1.540286	-0.004552
4.O	-0.641860	-0.713058	1.335036
5.O	-0.410836	-0.792189	-1.383098
6.Si	-1.251704	-0.445517	-2.755505
7.O	-1.943480	1.054826	-2.659867
8.Zr	-1.759452	2.458593	-1.301352
9.O	-0.267032	-0.364431	-4.074597

10.O	-2.375962	-1.644031	-2.854372
11.H	-3.409030	2.390547	-0.452397
12.O	-0.492808	4.089086	-2.145950
13.H	-2.907527	-1.638056	-3.667023
14.H	0.336148	-1.117576	-4.185768
15.H	2.059080	0.309385	0.816213
16.H	-0.531435	-1.676703	1.382629
17.C	-1.381811	4.991811	-1.923031
18.H	-1.165977	6.037804	-2.202594
19.O	-2.485783	4.678168	-1.391314

2-(H)(\eta2-O2CH).CO2

1.Si	0.000002	-0.016642	0.000550
2.O	1.649491	-0.027630	-0.006112
3.O	-0.613334	1.512370	0.003000
4.O	-0.637917	-0.754509	1.332419
5.O	-0.418485	-0.800259	-1.388844
6.Si	-1.381330	-0.413789	-2.665743
7.O	-2.142726	1.026713	-2.400368
8.Zr	-2.011606	2.437032	-1.042304
9.O	-0.519109	-0.195541	-4.054586
10.O	-2.452147	-1.664399	-2.763985
11.C	-4.405687	2.812613	-0.034180
12.H	-1.076012	3.836239	-1.893927
13.H	-3.009499	-1.658030	-3.559149
14.H	0.111251	-0.904654	-4.261176
15.H	2.058282	0.235682	0.834048
16.H	-0.521067	-1.718255	1.361297
17.O	-4.164583	3.175304	-1.234239
18.O	-3.484301	2.311083	0.688938
19.H	-5.419135	2.937173	0.383118
20.O	-1.708477	4.586375	0.472661
21.C	-1.133288	5.430774	-0.129287
22.O	-0.579692	6.326716	-0.629072

2-(H)(\eta2-O2CH)(\eta1-O2CH)

1.Zr	0.089964	-0.012050	-0.492643
2.O	2.064114	0.024030	-0.480802
3.Si	3.212816	1.192455	-0.303948
4.O	2.523630	2.573626	0.288517
5.Si	0.975948	3.010886	0.656588
6.O	-0.073884	1.833671	0.169468
7.O	3.838824	1.415313	-1.813717
8.H	4.480351	2.140243	-1.889206
9.O	4.353782	0.795621	0.817539
10.H	4.912714	0.036436	0.584020
11.O	0.733850	3.153252	2.283205
12.H	1.394126	3.691420	2.749519
13.O	0.738459	4.428516	-0.150161

14.H	-0.072652	4.902892	0.094817
15.O	-1.780232	0.236797	-1.799888
16.C	-1.165810	-0.321188	-2.764613
17.H	-1.669603	-0.475195	-3.732436
18.O	0.052273	-0.704396	-2.623140
19.O	-0.521091	-1.340385	0.847998
20.C	-0.925610	-1.860038	2.031738
21.O	-0.846263	-3.027305	2.323502
22.H	-1.343407	-1.082789	2.702779

2-(\eta2-O2CH)2

1.Si	0.058834	0.018922	-0.060906
2.O	1.709144	0.044359	-0.057666
3.O	-0.582657	1.537660	-0.102896
4.O	-0.574272	-0.688385	1.288477
5.O	-0.335225	-0.814619	-1.425554
6.Si	-1.227552	-0.447206	-2.761282
7.O	-1.972128	1.011691	-2.580509
8.Zr	-1.937346	2.436681	-1.215889
9.O	-0.289920	-0.300950	-4.111775
10.O	-2.312784	-1.685885	-2.870944
11.C	-4.334790	2.439918	-0.193954
12.O	-0.573491	3.844829	-2.248258
13.H	-2.830581	-1.691551	-3.692449
14.H	0.377056	-0.998278	-4.219533
15.H	2.103989	0.423320	0.744416
16.H	-0.406885	-1.641710	1.367678
17.C	-1.198714	4.877023	-1.805789
18.H	-0.833497	5.881055	-2.076138
19.O	-2.222358	4.737785	-1.071594
20.O	-4.197034	2.492636	-1.459167
21.O	-3.307787	2.393361	0.565213
22.H	-5.348319	2.429143	0.239759

1-H…NNO

1.Zr	-0.010781	0.043300	-0.023209
2.O	2.035489	0.063980	-0.035047
3.SI	2.794790	1.532717	-0.018035
4.O	2.280537	2.343622	1.354402
5.SI	0.665765	2.725760	1.466517
6.O	0.277402	3.543266	0.066247
7.SI	0.663216	2.815684	-1.382717
8.O	2.274653	2.433333	-1.317371
9.O	-0.215599	1.395238	-1.462198
10.N	0.860015	-2.419149	0.096040
11.N	1.239812	-3.488687	0.147994
12.O	1.636546	-4.611583	0.201417
13.H	-1.364330	-1.293528	-0.060257
14.O	-0.205530	1.308746	1.479325

15.O	4.426867	1.446909	-0.097778
16.O	0.293540	3.564039	2.817150
17.O	0.370393	3.808050	-2.647558
18.H	0.693555	4.445470	2.892540
19.H	-0.368856	3.539203	-3.215409
20.H	4.825489	0.701011	0.377687

2-H…NNO

1.Zr	0.248024	-0.166787	-0.110963
2.O	2.199189	0.074709	0.012613
3.Si	3.109879	1.448489	0.048871
4.O	2.159163	2.775323	0.278842
5.Si	0.544435	3.076114	0.369824
6.O	-0.326883	1.675576	0.264812
7.O	0.250459	4.091265	-0.896625
8.O	0.120787	3.727863	1.823222
9.O	4.148842	1.477043	1.328822
10.O	3.884087	1.495331	-1.406020
11.N	-1.673751	-1.674325	-0.476761
12.N	-2.533436	-2.416019	-0.555035
13.O	-3.429953	-3.199147	-0.612788
14.H	-0.016817	-0.501952	-1.941613
15.H	-0.140681	-1.293937	1.347198
16.H	4.325678	2.336071	-1.608939
17.H	4.859829	0.817191	1.284569
18.H	0.654692	4.489587	2.102599
19.H	-0.657783	4.432466	-0.940751