all lengths and distances are in angstron

Supporting Table A1 Calculated geometrical parameters using WB97XD/631++G(d) for 1CH4@512 cluster

Bond	Bond Length	Donor	Acceptor	H bond distance
O1 - H57	0.971163	H21	O11	1.9353
O1 - H58	0.961469	H22	O19	1.9786
O2 - H49	0.962239	H23	O14	1.92026
O2 - H50	0.978735	H24	O12	1.91058
O3 - H53	0.980756	H26	O4	1.99463
O3 - H54	0.961816	H28	O2	1.91787
O4 - H27	0.961205	H29	O4	1.92309
O4 - H28	0.976288	H30	O18	1.91242
O5 - H35	0.968589	H31	O7	1.89304
O5 - H36	0.968678	H33	O8	1.91165
O6 - H33	0.974013	H35	O1	1.91206
O6 - H34	0.961393	H36	O6	1.91573
O7 - H29	0.970352	H37	O10	1.89599
O7 - H30	0.976142	H38	O5	2.00839
O8 - H31	0.990528	H39	O13	1.8935
O8 - H32	0.961828	H40	O9	1.91846
O9 - H21	0.971412	H41	O12	1.97454
O9 - H22	0.975013	H42	O1	1.93046
O10 - H39	0.970404	H43	O15	1.92769
O10 - H40	0.977098	H44	O16	1.92939
O11 - H23	0.968227	H45	O2	1.92188
O11 - H24	0.967759	H47	O14	1.91636
O12 - H45	0.971382	H48	O18	1.90579
O12 - H46	0.960674	H50	O3	1.90383
O13 - H41	0.968446	H51	O17	1.957
O13 - H42	0.968458	H53	O8	1.9721
O14 - H25	0.960862	H55	O16	1.87837
O14 - H26	0.972034	H56	O6	1.92453
O15 - H47	0.968122	H57	O3	1.93188
O15 - H48	0.969301	H60	O20	1.88764
O16 - H59	0.961474			
O16 - H60	0.99			
O17 - H55	0.977053			
O17 - H56	0.969579			
O18 - H51	0.98674			
O18 - H52	0.961112			
O19 - H43	0.973077			
O19 - H44	0.970034			
O20 - H37	0.981317			
O20 - H38	0.971533			
C61 - H62	1.09439			
C61 - H63	1.09197			
C61 - H64	1.09217			
C61 - H65	1.09355			

Supporting Table A2 Calculated geometrical parameters using WB97XD/631++G(d) for 1CH4@512 cluster - methanol

Bond	Bond Length	Donor	Acceptor	H bond distance
O1 - H57	0.981909	H22	O10	2.08464
O1 - H58	0.961503	H23	O14	1.90136
O2 - H49	0.961903	H24	O9	1.91263
O2 - H50	0.982927	H26	O4	1.9818
O3 - H53	0.970603	H28	O2	1.90983
O3 - H54	0.971906	H29	O4	1.92884
O4 - H27	0.961162	H30	O18	1.90122
O4 - H28	0.978841	H31	O7	1.89545
O5 - H35	0.970785	H33	O8	1.90988
O5 - H36	0.968966	H35	O1	1.91572
O6 - H33	0.977486	H36	O6	1.93074
O6 - H34	0.961435	H37	O16	1.90057
O7 - H29	0.969684	H38	O5	1.9886
O7 - H30	0.975079	H39	O13	1.89435
O8 - H31	0.987206	H40	O20	1.90437
O8 - H32	0.961357	H41	O12	1.99838
O9 - H21	0.965993	H42	O1	1.90939
O9 - H22	0.978339	H43	O70	1.86153
O10 - H39	0.97332	H44	O16	1.9418
O10 - H40	0.976829	H45	O11	1.89978
O11 - H23	0.970395	H47	O14	1.91817
O11 - H24	0.97585	H48	O19	1.91167
O12 - H45	0.988065	H50	O12	1.89229
O12 - H46	0.961089	H51	O15	1.89789
O13 - H41	0.968434	H53	O2	1.91313
O13 - H42	0.971951	H54	O8	1.9858
O14 - H25	0.960981	H55	O18	1.99666
O14 - H26	0.974969	H56	O6	1.90131
O15 - H47	0.968823	H57	O3	1.90524
O15 - H48	0.978875	H59	O17	1.88294
O16 - H59	0.983236	H71	O9	1.81264
O16 - H60	0.961533			
O17 - H55	0.971644			
O17 - H56	0.971858			
O18 - H51	0.987586			
O18 - H52	0.960949			
O19 - H43	0.970759			
O19 - H44	0.970594			
O20 - H37	0.970482			
O20 - H38	0.974055			
C61 - H62	1.09244			
C61 - H63	1.09405			
C61 - H64	1.09287			
C61 - H65	1.09242			
C66 - H67	1.09849			
C66 - H68	1.0976			

C66 - H69	1.09199
C66 - O70	1.41441
O70 - H71	0.975462

Supporting Table A3 Calculated geometrical parameters using WB97XD/631++G(d) for 1CH4@512 cluster - methanol and sodium ion

Bond	Bond Length	Donor	Acceptor	H bond distance
O1 - H57	0.985267	H22	O10	1.93348
O1 - H58	0.962644	H23	O14	1.89652
O2 - H49	0.962721	H24	O9	1.91798
O2 - H50	0.981159	H26	O4	1.97988
O3 - H53	0.970648	H28	O2	1.91101
O3 - H54	0.971892	H29	O4	1.92777
O4 - H27	0.961784	H30	O18	1.90354
O4 - H28	0.978626	H31	O7	1.89585
O5 - H35	0.9723	H33	O8	1.90679
O5 - H36	0.970885	H35	O1	1.91307
O6 - H33	0.979494	H36	O6	1.92767
O6 - H34	0.962398	H37	O16	1.90091
O7 - H29	0.969711	H38	O5	1.99095
O7 - H30	0.973549	H39	O13	1.92039
O8 - H31	0.986781	H40	O20	2.1116
O8 - H32	0.962027	H41	O12	2.00255
O9 - H21	0.962695	H42	O1	1.90821
O9 - H22	0.977668	H44	O16	1.92383
O10 - H39	0.984348	H45	O11	1.9021
O10 - H40	0.973599	H47	O14	1.90992
O11 - H23	0.971642	H48	O19	1.92071
O11 - H24	0.97276	H50	O12	1.89506
O12 - H45	0.987352	H51	O15	1.90068
O12 - H46	0.961977	H53	O2	1.91268
O13 - H41	0.970284	H54	O8	1.98803
O13 - H42	0.973774	H55	O18	1.99968
O14 - H25	0.962103	H56	O6	1.90143
O14 - H26	0.976486	H57	O3	1.90179
O15 - H47	0.970927	H59	O17	1.87592
O15 - H48	0.9728	H71	O9	2.06701
O16 - H59	0.991348	H71	O19	2.29107
O16 - H60	0.963002			
O17 - H55	0.972745			
O17 - H56	0.973023			
O18 - H51	0.984912			
O18 - H52	0.961801			
O19 - H43	0.962205			
O19 - H44	0.976964			
O20 - H37	0.976478			
O20 - H38	0.981609			
C61 - H62	1.09306			
C61 - H63	1.09224			
C61 - H64	1.09282			

C61 - H65	1.09295
C66 - H67	1.09602
C66 - H68	1.09408
C66 - H69	1.09189
C66 - O70	1.42034
O70 - H71	0.975567