

Supporting Table A4MULLIKAN CHARGES (a.u.) and ELECTROSTATIC POTENTIAL(a.u.)
OF ATOMS OF 1CH4@512

ATOM ID	ATOM TYPE	MULLIKAN CHARGES	ELECTROSTATIC POTENTIAL
1	O	-0.837596	-22.256328
2	O	-0.839126	-22.216384
3	O	-0.848754	-22.212497
4	O	-0.834746	-22.23221
5	O	-0.838105	-22.324592
6	O	-0.845872	-22.259058
8	O	-0.852166	-22.230558
9	O	-0.825501	-22.365387
10	O	-0.839354	-22.367556
11	O	-0.838666	-22.328575
12	O	-0.814707	-22.25897
13	O	-0.809011	-22.323964
14	O	-0.834993	-22.26088
15	O	-0.837834	-22.32923
16	O	-0.850887	-22.303216
17	O	-0.840727	-22.318209
18	O	-0.845881	-22.270424
19	O	-0.833797	-22.357626
20	O	-0.841817	-22.350203
21	H	0.433676	-1.067561
22	H	0.424427	-1.069097
23	H	0.425671	-1.028323
24	H	0.442422	-1.028257
25	H	0.401137	-0.96425
26	H	0.451034	-0.966313
27	H	0.396209	-0.935837
28	H	0.462396	-0.939951
29	H	0.434889	-0.985519
30	H	0.450603	-0.988207
31	H	0.452997	-0.943277
32	H	0.39845	-0.935534
33	H	0.458005	-0.964498
34	H	0.403488	-0.96194
35	H	0.435877	-1.025007
36	H	0.419025	-1.02491
37	H	0.452837	-1.057286
38	H	0.429206	-1.053923
39	H	0.43985	-1.068564
40	H	0.44268	-1.071284
41	H	0.427251	-1.024411
42	H	0.42289	-1.024423
43	H	0.43083	-1.059327
44	H	0.433369	-1.060647
45	H	0.472238	-0.962796
46	H	0.400063	-0.961324
47	H	0.430189	-1.029483

48 H	0.428941	-1.029364
49 H	0.389857	-0.920496
50 H	0.491375	-0.925744
51 H	0.450902	-0.98164
52 H	0.403717	-0.974806
53 H	0.472101	-0.923275
54 H	0.396967	-0.917233
55 H	0.443835	-1.023969
56 H	0.425088	-1.020831
57 H	0.462797	-0.960503
58 H	0.404722	-0.959268
59 H	0.402008	-1.006977
60 H	0.456169	-1.014122
61 C	-0.25912	-14.76536
62 H	-0.190946	-1.126532
63 H	0.132795	-1.135621
64 H	0.01933	-1.132721
65 H	-0.259245	-1.126795

Supporting Table A5

MULLIKAN CHARGES (a.u.) and ELECTROSTATIC POTENTIAL(a.u.)

OF ATOMS OF 1CH4@512-METHANOL

ATOM ID	ATOM TYPE	MULLIKAN CHARGES	ELECTROSTATIC POTENTIAL
1 O		-0.860957	-22.278626
2 O		-0.834245	-22.240009
3 O		-0.822286	-22.293562
4 O		-0.83968	-22.24058
5 O		-0.832667	-22.330541
6 O		-0.836548	-22.265941
7 O		-0.846957	-22.294502
8 O		-0.842498	-22.256375
9 O		-0.793698	-22.287549
10 O		-0.850003	-22.350935
11 O		-0.824645	-22.304743
12 O		-0.854	-22.260006
13 O		-0.828698	-22.32414
14 O		-0.841026	-22.252692
15 O		-0.827703	-22.3139
16 O		-0.835945	-22.292844
17 O		-0.833313	-22.30997
18 O		-0.858467	-22.27327
19 O		-0.861934	-22.330423
20 O		-0.813629	-22.345579
21 H		0.429972	-0.995317
22 H		0.390318	-0.999625
23 H		0.438184	-1.007694
24 H		0.415255	-1.010002
25 H		0.398935	-0.956469
26 H		0.457998	-0.959906
27 H		0.393553	-0.944269

28 H	0.47638	-0.949376
29 H	0.432322	-0.997148
30 H	0.448797	-0.999384
31 H	0.449704	-0.967354
32 H	0.395387	-0.96065
33 H	0.49039	-0.972865
34 H	0.396329	-0.969055
35 H	0.435333	-1.032461
36 H	0.43894	-1.031304
37 H	0.430688	-1.047206
38 H	0.427881	-1.048898
39 H	0.429712	-1.052963
40 H	0.441853	-1.05436
41 H	0.421	-1.02504
42 H	0.440206	-1.026513
43 H	0.457696	-1.031189
44 H	0.413852	-1.029915
45 H	0.460397	-0.971606
46 H	0.398227	-0.963933
47 H	0.428331	-1.016392
48 H	0.432496	-1.020654
49 H	0.402546	-0.944087
50 H	0.481152	-0.950157
51 H	0.452447	-0.984117
52 H	0.401606	-0.977364
53 H	0.428341	-0.996278
54 H	0.431411	-0.9974
55 H	0.42739	-1.013483
56 H	0.447391	-1.013272
57 H	0.451988	-0.986721
58 H	0.4052	-0.982125
59 H	0.460368	-1.001274
60 H	0.404497	-0.996104
61 C	-0.298775	-14.769589
62 H	-0.091303	-1.133956
63 H	-0.254692	-1.130638
64 H	-0.030901	-1.135025
65 H	0.123298	-1.137221
66 C	-0.248333	-14.707408
67 H	0.124322	-1.133442
68 H	0.123619	-1.132566
69 H	0.153364	-1.131153
70 O	-0.582467	-22.318286
71 H	0.456297	-1.023714

Supporting Table A6

MULLICAN CHARGES OF ATOMS OF 1CH4@512-METHANOL-Na+

ATOM ID	ATOM TYPE	MULLIKAN CHARGES
1	O	-0.851413
2	O	-0.852158

3 O	-0.831375
4 O	-0.850014
5 O	-0.818564
6 O	-0.851183
7 O	-0.825361
8 O	-0.864079
9 O	-0.814992
10 O	-0.834851
11 O	-0.822023
12 O	-0.831772
13 O	-0.82158
14 O	-0.854482
15 O	-0.825323
16 O	-0.8595
17 O	-0.826376
18 O	-0.850692
19 O	-0.827647
20 O	-0.901202
21 H	0.416052
22 H	0.493772
23 H	0.446432
24 H	0.443479
25 H	0.404619
26 H	0.467643
27 H	0.407666
28 H	0.467209
29 H	0.428897
30 H	0.44125
31 H	0.459247
32 H	0.40211
33 H	0.474188
34 H	0.410016
35 H	0.443812
36 H	0.426435
37 H	0.471765
38 H	0.46253
39 H	0.464805
40 H	0.422315
41 H	0.431402
42 H	0.440263
43 H	0.515625
44 H	0.405706
45 H	0.459638
46 H	0.405886
47 H	0.443355
48 H	0.442875
49 H	0.405206
50 H	0.47472
51 H	0.450216
52 H	0.405679

53 H	0.424274
54 H	0.436472
55 H	0.441237
56 H	0.442817
57 H	0.445374
58 H	0.413411
59 H	0.451264
60 H	0.407249
61 C	-0.205164
62 H	-0.111329
63 H	-0.129575
64 H	-0.172342
65 H	-0.111158
66 C	-0.26457
67 H	0.105189
68 H	0.16607
69 H	0.133729
70 O	-0.625912
71 H	0.529577
72 Na	0.903161