

Supplementary Sheet 2 | Index, chemical formula, number of electron transfer per carbon atom (#e/C), number of carbon (#C), simplified molecular-input line-entry system name (SMILES), formation energy on Cu(100) ($E_f^{\text{Cu}(100)}$) and Cu(111) ($E_f^{\text{Cu}(111)}$). Species dissociated after optimization for all initial structures are labeled with NA. All the formation energies are in eV.

index	formula	#e/C	#C	SMILES	$E_f^{\text{Cu}(100)}$	$E_f^{\text{Cu}(111)}$
1	H	0.0	0	[H]	-0.04	-0.08
2	O	0.0	0	[O]	0.45	1.10
3	H ₂	0.0	0	[H][H]	0.00	0.00
4	HO	0.0	0	[H][O]	-0.05	0.24
5	H ₂ O	0.0	0	[H]O[H]	0.00	0.00
6	CO	0.0	1	[C][O]	0.73	0.73
7	CHO	1.0	1	[H][C][O]	0.71	1.03
8	CHO	1.0	1	[H]O[C]	0.92	1.21
9	C	2.0	1	[C]	0.77	2.14
10	CH ₂ O	2.0	1	[H][C]([H])[O]	0.16	0.67
11	CH ₂ O	2.0	1	[H][C]O[H]	0.83	1.07
12	CH	3.0	1	[H][C]	0.15	0.95
13	CH ₃ O	3.0	1	[H]C([H])([H])[O]	-0.43	-0.14
14	CH ₃ O	3.0	1	[H]O[C]([H])[H]	0.14	0.43
15	CH ₂	4.0	1	[H][C][H]	0.03	0.38
16	CH ₄ O	4.0	1	[H]OC([H])([H])[H]	-0.39	-0.39
17	CH ₃	5.0	1	[H][C]([H])[H]	-0.69	-0.68
18	CH ₄	6.0	1	[H]C([H])([H])[H]	-1.75	-1.75
19	C ₂ O ₂	0.0	2	[O][C][C][O]	1.14	2.17
20	C ₂ HO ₂	0.5	2	[H][C]([O])[C][O]	0.90	1.53
21	C ₂ HO ₂	0.5	2	[H]O[C][C][O]	1.23	1.59

22	C ₂ O	1.0	2	[C][C][O]	-0.29	0.52
23	C ₂ H ₂ O ₂	1.0	2	[H]C([H])([O])[C][O]	1.37	NA
24	C ₂ H ₂ O ₂	1.0	2	[H][C]([O])[C]([H])[O]	1.28	1.28
25	C ₂ H ₂ O ₂	1.0	2	[H]O[C]([H])[C][O]	0.24	1.11
26	C ₂ H ₂ O ₂	1.0	2	[H]O[C][C]([H])[O]	0.63	1.28
27	C ₂ H ₂ O ₂	1.0	2	[H]O[C][C]O[H]	0.47	1.07
28	C ₂ HO	1.5	2	[H][C]([C])[O]	0.30	1.11
29	C ₂ HO	1.5	2	[H][C][C][O]	-0.05	0.23
30	C ₂ HO	1.5	2	[H]O[C][C]	0.86	1.09
31	C ₂ H ₃ O ₂	1.5	2	[H][C]([O])C([H])([H])[O]	NA	NA
32	C ₂ H ₃ O ₂	1.5	2	[H]OC([H])([H])[C][O]	0.43	0.59
33	C ₂ H ₃ O ₂	1.5	2	[H]O[C]C([H])([H])[O]	1.69	2.04
34	C ₂ H ₃ O ₂	1.5	2	[H]O[C]([H])[C]([H])[O]	-0.14	0.40
35	C ₂ H ₃ O ₂	1.5	2	[H]O[C][C]([H])O[H]	0.49	0.75
36	C ₂	2.0	2	[C][C]	1.35	1.17
37	C ₂ H ₂ O	2.0	2	[H]C([H])([C])[O]	1.11	1.85
38	C ₂ H ₂ O	2.0	2	[H][C]([H])[C][O]	-0.24	0.44
39	C ₂ H ₂ O	2.0	2	[H][C][C]([H])[O]	0.02	0.54
40	C ₂ H ₂ O	2.0	2	[H]O[C]([H])[C]	-0.05	0.44
41	C ₂ H ₂ O	2.0	2	[H][C][C]O[H]	-0.03	0.30
42	C ₂ H ₄ O ₂	2.0	2	[H]C([H])([O])C([H])([H])[O]	-0.45	0.06
43	C ₂ H ₄ O ₂	2.0	2	[H]OC([H])([H])[C]([H])[O]	0.16	0.16
44	C ₂ H ₄ O ₂	2.0	2	[H]O[C]([H])C([H])([H])[O]	NA	NA
45	C ₂ H ₄ O ₂	2.0	2	[H]O[C]C([H])([H])O[H]	0.74	0.95
46	C ₂ H ₄ O ₂	2.0	2	[H]O[C]([H])[C]([H])O[H]	0.04	0.10

47	C ₂ H	2.5	2	[H][C][C]	0.33	0.44
48	C ₂ H ₃ O	2.5	2	[H]C([H])([H])[C][O]	-0.66	-0.39
49	C ₂ H ₃ O	2.5	2	[H][C]C([H])([H])[O]	1.35	NA
50	C ₂ H ₃ O	2.5	2	[H][C]([H])[C]([H])[O]	-0.98	-0.45
51	C ₂ H ₃ O	2.5	2	[H]OC([H])([H])[C]	0.18	0.72
52	C ₂ H ₃ O	2.5	2	[H]O[C][C]([H])[H]	-0.03	0.19
53	C ₂ H ₃ O	2.5	2	[H][C][C]([H])O[H]	-0.30	-0.15
54	C ₂ H ₅ O ₂	2.5	2	[H]OC([H])([H])C([H])([H])[O]	-0.51	-0.35
55	C ₂ H ₅ O ₂	2.5	2	[H]O[C]([H])C([H])([H])O[H]	-0.02	0.34
56	C ₂ H ₂	3.0	2	[H][C]([H])[C]	-0.26	0.04
57	C ₂ H ₂	3.0	2	[H][C][C][H]	0.52	0.52
58	C ₂ H ₄ O	3.0	2	[H][C]([O])C([H])([H])[H]	-0.73	-0.73
59	C ₂ H ₄ O	3.0	2	[H][C]([H])C([H])([H])[O]	0.29	1.10
60	C ₂ H ₄ O	3.0	2	[H]O[C]C([H])([H])[H]	-0.32	-0.12
61	C ₂ H ₄ O	3.0	2	[H][C]C([H])([H])O[H]	0.13	0.36
62	C ₂ H ₄ O	3.0	2	[H]O[C]([H])[C]([H])[H]	-0.85	-0.72
63	C ₂ H ₆ O ₂	3.0	2	[H]OC([H])([H])C([H])([H])O[H]	-0.51	-0.51
64	C ₂ H ₃	3.5	2	[H]C([H])([H])[C]	-0.70	-0.25
65	C ₂ H ₃	3.5	2	[H][C][C]([H])[H]	-0.59	-0.49
66	C ₂ H ₅ O	3.5	2	[H]C([H])([H])C([H])([H])[O]	-1.46	-1.30
67	C ₂ H ₅ O	3.5	2	[H]O[C]([H])C([H])([H])[H]	-0.85	-0.52
68	C ₂ H ₅ O	3.5	2	[H]OC([H])([H])[C]([H])[H]	-0.74	-0.53
69	C ₂ H ₄	4.0	2	[H][C]C([H])([H])[H]	-0.78	-0.53
70	C ₂ H ₄	4.0	2	[H][C]([H])[C]([H])[H]	-1.30	-1.30

71	C ₂ H ₆ O	4.0	2	[H]OC([H])([H])C([H])([H])[H]	-1.49	-1.49
72	C ₂ H ₅	4.5	2	[H][C]([H])C([H])([H])[H]	-1.61	-1.44
73	C ₂ H ₆	5.0	2	[H]C([H])([H])C([H])([H])[H]	-2.68	-2.68
74	C ₃ O ₃	0.0	3	[O][C][C]([O])[C][O]	1.76	2.49
75	C ₃ HO ₃	0.3	3	[H]C([O])([C][O])[C][O]	NA	NA
76	C ₃ HO ₃	0.3	3	[H][C]([O])[C]([O])[C][O]	1.16	2.11
77	C ₃ HO ₃	0.3	3	[H]O[C]([C][O])[C][O]	1.84	2.12
78	C ₃ HO ₃	0.3	3	[H]O[C][C]([O])[C][O]	1.86	2.46
79	C ₃ O ₂	0.7	3	[C][C]([O])[C][O]	NA	2.51
80	C ₃ O ₂	0.7	3	[O][C][C][C][O]	0.63	1.17
81	C ₃ H ₂ O ₃	0.7	3	[H]C([H])([O])[C]([O])[C][O]	2.34	2.85
82	C ₃ H ₂ O ₃	0.7	3	[H][C]([O])C([H])([O])[C][O]	0.81	1.49
83	C ₃ H ₂ O ₃	0.7	3	[H][C]([O])[C]([O])[C]([H])[O]	0.35	1.10
84	C ₃ H ₂ O ₃	0.7	3	[H]OC([H])([C][O])[C][O]	NA	2.70
85	C ₃ H ₂ O ₃	0.7	3	[H]O[C]C([H])([O])[C][O]	3.04	3.56
86	C ₃ H ₂ O ₃	0.7	3	[H]O[C]([H])[C]([O])[C][O]	0.58	1.31
87	C ₃ H ₂ O ₃	0.7	3	[H]O[C]([C][O])[C]([H])[O]	0.95	1.54
88	C ₃ H ₂ O ₃	0.7	3	[H]O[C][C]([O])[C]([H])[O]	0.64	1.47
89	C ₃ H ₂ O ₃	0.7	3	[H]O[C][C]([C][O])O[H]	2.30	2.60
90	C ₃ H ₂ O ₃	0.7	3	[H]O[C][C]([O])[C]O[H]	2.76	3.62
91	C ₃ HO ₂	1.0	3	[H]C([C])([O])[C][O]	NA	NA
92	C ₃ HO ₂	1.0	3	[H][C]([C][O])[C][O]	0.76	1.13
93	C ₃ HO ₂	1.0	3	[H][C]([O])[C]([C])[O]	0.75	1.57
94	C ₃ HO ₂	1.0	3	[H][C]([O])[C][C][O]	0.37	0.75
95	C ₃ HO ₂	1.0	3	[H][C][C]([O])[C][O]	NA	NA

96	C ₃ H ₃ O ₂	1.0	3	[H]O[C]([C])[C][O]	1.46	1.80
97	C ₃ H ₃ O ₂	1.0	3	[H]O[C][C]([C])[O]	1.54	2.20
98	C ₃ H ₃ O ₂	1.0	3	[H]O[C][C][C][O]	0.54	1.10
99	C ₃ H ₃ O ₃	1.0	3	[H]C([H])([O])C([H])([O])[C][O]]	NA	NA
100	C ₃ H ₃ O ₃	1.0	3	[H][C]([O])[C]([O])C([H])([H]) [O]	1.16	NA
101	C ₃ H ₃ O ₃	1.0	3	[H][C]([O])C([H])([O])[C]([H]) [O]	NA	NA
102	C ₃ H ₃ O ₃	1.0	3	[H]OC([H])([H])[C]([O])[C][O]	0.54	1.24
103	C ₃ H ₃ O ₃	1.0	3	[H]O[C]([C][O])C([H])([H])[O]	2.19	3.38
104	C ₃ H ₃ O ₃	1.0	3	[H]O[C][C]([O])C([H])([H])[O]	NA	NA
105	C ₃ H ₃ O ₃	1.0	3	[H]OC([H])([C][O])[C]([H])[O]	1.07	1.31
106	C ₃ H ₃ O ₃	1.0	3	[H]O[C]([H])C([H])([O])[C][O]	NA	NA
107	C ₃ H ₃ O ₃	1.0	3	[H]O[C]C([H])([O])[C]([H])[O]	0.98	1.72
108	C ₃ H ₃ O ₃	1.0	3	[H]O[C]([H])[C]([O])[C]([H])[O]]	0.23	0.76
109	C ₃ H ₃ O ₃	1.0	3	[H]O[C]([C]([H])[O])[C]([H])[O]]	0.12	0.62
110	C ₃ H ₃ O ₃	1.0	3	[H]O[C]C([H])([C][O])O[H]	NA	NA
111	C ₃ H ₃ O ₃	1.0	3	[H]O[C]C([H])([O])[C]O[H]	3.04	2.55
112	C ₃ H ₃ O ₃	1.0	3	[H]O[C]([H])[C]([C][O])O[H]	0.70	0.91
113	C ₃ H ₃ O ₃	1.0	3	[H]O[C][C]([O])[C]([H])O[H]	0.67	1.39
114	C ₃ H ₃ O ₃	1.0	3	[H]O[C][C](O[H])[C]([H])[O]	0.70	1.26
115	C ₃ H ₃ O ₃	1.0	3	[H]O[C][C]([C]O[H])O[H]	NA	NA
116	C ₃ O	1.3	3	[C][C]([C])[O]	NA	NA
117	C ₃ O	1.3	3	[C][C][C][O]	0.92	1.19

118	C ₃ H ₂ O ₂	1.3	3	[H]C([H])([C][O])[C][O]	NA	NA
119	C ₃ H ₂ O ₂	1.3	3	[H]C([H])([O])[C]([C])[O]	0.27	1.45
120	C ₃ H ₂ O ₂	1.3	3	[H]C([H])([O])[C][C][O]	1.07	2.24
121	C ₃ H ₂ O ₂	1.3	3	[H][C]([H])[C]([O])[C][O]	0.08	0.75
122	C ₃ H ₂ O ₂	1.3	3	[H][C]([O])C([H])([C])[O]	1.29	2.49
123	C ₃ H ₂ O ₂	1.3	3	[H][C]C([H])([O])[C][O]	NA	NA
124	C ₃ H ₂ O ₂	1.3	3	[H][C]([O])[C]([H])[C][O]	0.17	0.89
125	C ₃ H ₂ O ₂	1.3	3	[H][C][C]([O])[C]([H])[O]	0.01	0.70
126	C ₃ H ₂ O ₂	1.3	3	[H][C]([O])[C][C]([H])[O]	-0.35	0.40
127	C ₃ H ₂ O ₂	1.3	3	[H]OC([H])([C])[C][O]	NA	NA
128	C ₃ H ₂ O ₂	1.3	3	[H]O[C]C([H])([C])[O]	NA	NA
129	C ₃ H ₂ O ₂	1.3	3	[H]O[C][C]([H])[C][O]	1.16	1.24
130	C ₃ H ₂ O ₂	1.3	3	[H]O[C]([H])[C]([C])[O]	1.24	1.81
131	C ₃ H ₂ O ₂	1.3	3	[H]O[C]([C])[C]([H])[O]	0.37	0.74
132	C ₃ H ₂ O ₂	1.3	3	[H]O[C]([H])[C][C][O]	0.65	0.64
133	C ₃ H ₂ O ₂	1.3	3	[H]O[C][C][C]([H])[O]	0.36	0.74
134	C ₃ H ₂ O ₂	1.3	3	[H][C][C]([C][O])O[H]	2.34	2.85
135	C ₃ H ₂ O ₂	1.3	3	[H][C][C]([O])[C]O[H]	NA	3.42
136	C ₃ H ₂ O ₂	1.3	3	[H]O[C][C]([C])O[H]	0.87	1.55
137	C ₃ H ₂ O ₂	1.3	3	[H]O[C][C][C]O[H]	NA	1.62
138	C ₃ H ₄ O ₃	1.3	3	[H][C]([O])C([H])([O])C([H])([H])[O]	NA	NA
139	C ₃ H ₄ O ₃	1.3	3	[H]C([H])([O])[C]([O])C([H])([H])[O]	NA	NA
140	C ₃ H ₄ O ₃	1.3	3	[H]OC([H])([H])C([H])([O])[C][O]	0.07	0.64

141	C ₃ H ₄ O ₃	1.3	3	[H]OC([H])([C][O])C([H])([H])[O]	NA	NA
142	C ₃ H ₄ O ₃	1.3	3	[H]O[C]C([H])([O])C([H])([H])[O]	NA	NA
143	C ₃ H ₄ O ₃	1.3	3	[H]OC([H])([H])[C]([O])[C]([H])[O]	-0.27	0.52
144	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([C]([H])[O])C([H])([H])[O]	0.94	NA
145	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([H])[C]([O])C([H])([H])[O]	0.82	1.74
146	C ₃ H ₄ O ₃	1.3	3	[H]OC([H])([C]([H])[O])[C]([H])[O]	0.73	0.98
147	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([H])C([H])([O])[C]([H])[O]	0.58	1.26
148	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([C][O])C([H])([H])O[H]	0.39	1.07
149	C ₃ H ₄ O ₃	1.3	3	[H]O[C][C]([O])C([H])([H])O[H]	0.22	0.80
150	C ₃ H ₄ O ₃	1.3	3	[H]O[C][C](O[H])C([H])([H])O[H]	NA	NA
151	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([H])C([H])([C][O])O[H]	NA	NA
152	C ₃ H ₄ O ₃	1.3	3	[H]O[C]C([H])(O[H])[C]([H])O[H]	1.38	1.75
153	C ₃ H ₄ O ₃	1.3	3	[H]O[C]C([H])([O])[C]([H])O[H]	2.20	2.30
154	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([H])[C](O[H])[C]([H])O	0.17	0.34
155	C ₃ H ₄ O ₃	1.3	3	[H]O[C]([H])[C]([O])[C]([H])O[H]	0.06	0.90
156	C ₃ H ₄ O ₃	1.3	3	[H]O[C]C([H])([C]O[H])O[H]	NA	NA

157	C ₃ H ₄ O ₃	1.3	3	[H]O[C][C](O[H])[C]([H])O[H]	1.27	1.34
158	C ₃ HO	1.7	3	[H]C([C])([C])[O]	NA	NA
159	C ₃ HO	1.7	3	[H][C]([C])[C][O]	0.66	1.06
160	C ₃ HO	1.7	3	[H][C]([O])[C][C]	0.78	0.98
161	C ₃ HO	1.7	3	[H][C][C]([C])[O]	NA	NA
162	C ₃ HO	1.7	3	[H][C][C][C][O]	0.26	0.63
163	C ₃ HO	1.7	3	[H]O[C]([C])[C]	NA	NA
164	C ₃ HO	1.7	3	[H]O[C][C][C]	1.61	2.02
165	C ₃ H ₃ O ₂	1.7	3	[H]C([H])([H])[C]([O])[C][O]	-0.54	0.05
166	C ₃ H ₃ O ₂	1.7	3	[H][C]([O])C([H])([H])[C][O]	0.29	0.53
167	C ₃ H ₃ O ₂	1.7	3	[H]C([H])([O])C([H])([C])[O]	1.17	NA
168	C ₃ H ₃ O ₂	1.7	3	[H][C]([C][O])C([H])([H])[O]	1.53	0.72
169	C ₃ H ₃ O ₂	1.7	3	[H][C][C]([O])C([H])([H])[O]	1.09	1.99
170	C ₃ H ₃ O ₂	1.7	3	[H][C]([O])[C]C([H])([H])[O]	0.65	2.18
171	C ₃ H ₃ O ₂	1.7	3	[H][C]([H])C([H])([O])[C][O]	NA	NA
172	C ₃ H ₃ O ₂	1.7	3	[H][C]([H])[C]([O])[C]([H])[O]	-0.53	0.07
173	C ₃ H ₃ O ₂	1.7	3	[H][C]C([H])([O])[C]([H])[O]	NA	NA
174	C ₃ H ₃ O ₂	1.7	3	[H][C]([O])[C]([H])[C]([H])[O]	-0.74	-0.14
175	C ₃ H ₃ O ₂	1.7	3	[H]O[C]C([H])([H])[C][O]	1.96	2.28
176	C ₃ H ₃ O ₂	1.7	3	[H]OC([H])([H])[C]([C])[O]	0.10	0.72
177	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([C])C([H])([H])[O]	-0.16	0.87
178	C ₃ H ₃ O ₂	1.7	3	[H]OC([H])([H])[C][C][O]	0.16	0.40
179	C ₃ H ₃ O ₂	1.7	3	[H]O[C][C]C([H])([H])[O]	1.21	1.85
180	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([C][O])[C]([H])[H]	0.20	0.41
181	C ₃ H ₃ O ₂	1.7	3	[H]O[C][C]([O])[C]([H])[H]	0.13	0.83

182	C ₃ H ₃ O ₂	1.7	3	[H]OC([H])([C])[C]([H])[O]	NA	NA
183	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([H])C([H])([C])[O]	NA	NA
184	C ₃ H ₃ O ₂	1.7	3	[H][C]C([H])([C][O])O[H]	NA	NA
185	C ₃ H ₃ O ₂	1.7	3	[H][C]C([H])([O])[C]O[H]	NA	NA
186	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([H])[C]([H])[C][O]	-0.25	0.12
187	C ₃ H ₃ O ₂	1.7	3	[H]O[C][C]([H])[C]([H])[O]	NA	NA
188	C ₃ H ₃ O ₂	1.7	3	[H][C][C]([O])[C]([H])O[H]	0.08	0.75
189	C ₃ H ₃ O ₂	1.7	3	[H][C][C](O[H])[C]([H])[O]	0.12	0.55
190	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([H])[C][C]([H])[O]	-0.33	0.16
191	C ₃ H ₃ O ₂	1.7	3	[H]O[C]C([H])([C])O[H]	1.65	2.16
192	C ₃ H ₃ O ₂	1.7	3	[H]O[C][C]([H])[C]O[H]	2.20	2.61
193	C ₃ H ₃ O ₂	1.7	3	[H]O[C]([H])[C]([C])O[H]	0.41	0.80
194	C ₃ H ₃ O ₂	1.7	3	[H]O[C][C][C]([H])O[H]	0.19	0.72
195	C ₃ H ₃ O ₂	1.7	3	[H][C][C]([C]O[H])O[H]	NA	NA
196	C ₃ H ₅ O ₃	1.7	3	[H]C([H])([O])C([H])([O])C([H]) ([H])[O]	-0.50	0.65
197	C ₃ H ₅ O ₃	1.7	3	[H]OC([H])([H])C([H])([O])[C] ([H])[O]	0.19	0.42
198	C ₃ H ₅ O ₃	1.7	3	[H]OC([H])([C]([H])[O])C([H]) ([H])[O]	NA	NA
199	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])C([H])([O])C([H]) ([H])[O]	NA	NA
200	C ₃ H ₅ O ₃	1.7	3	[H]OC([H])([H])[C]([O])C([H]) ([H])[O]	-0.13	0.23
201	C ₃ H ₅ O ₃	1.7	3	[H]O[C](C([H])([H])[O])C([H]) ([H])[O]	1.46	NA
202	C ₃ H ₅ O ₃	1.7	3	[H]OC([H])([H])C([H])([C][O]) O[H]	0.10	0.43

203	C ₃ H ₅ O ₃	1.7	3	[H]O[C]C([H])([O])C([H])([H]) O[H]	0.22	0.92
204	C ₃ H ₅ O ₃	1.7	3	[H]O[C]C([H])(O[H])C([H])([H])][O]	NA	NA
205	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([C]([H])[O])C([H])([H]))O[H]	-0.26	0.20
206	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])[C]([O])C([H])([H]))O[H]	-0.29	0.25
207	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])[C](O[H])C([H])([H])][O]	0.84	NA
208	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])C([H])(O[H])[C]([H])][O]	0.73	1.08
209	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])C([H])([O])[C]([H]))O[H]	1.03	NA
210	C ₃ H ₅ O ₃	1.7	3	[H]O[C][C](O[H])C([H])([H])O[H]	0.71	0.72
211	C ₃ H ₅ O ₃	1.7	3	[H]O[C]C([H])(O[H])[C]([H])O[H]	NA	NA
212	C ₃ H ₅ O ₃	1.7	3	[H]O[C]([H])[C](O[H])[C]([H]) O[H]	0.33	0.68
213	C ₃	2.0	3	[C][C][C]	2.39	3.01
214	C ₃ H ₂ O	2.0	3	[H]C([H])([C])[C][O]	1.15	NA
215	C ₃ H ₂ O	2.0	3	[H]C([H])([O])[C][C]	-0.31	2.21
216	C ₃ H ₂ O	2.0	3	[H][C]([H])[C]([C])[O]	0.67	1.31
217	C ₃ H ₂ O	2.0	3	[H][C]([H])[C][C][O]	-0.40	0.21
218	C ₃ H ₂ O	2.0	3	[H][C]C([H])([C])[O]	NA	NA
219	C ₃ H ₂ O	2.0	3	[H][C]([C])[C]([H])[O]	-0.22	0.15
220	C ₃ H ₂ O	2.0	3	[H][C][C]([H])[C][O]	2.08	2.30
221	C ₃ H ₂ O	2.0	3	[H][C][C][C]([H])[O]	0.04	0.07

222	C ₃ H ₂ O	2.0	3	[H][C][C]([O])[C][H]	1.99	2.85
223	C ₃ H ₂ O	2.0	3	[H]OC([H])([C])[C]	NA	NA
224	C ₃ H ₂ O	2.0	3	[H]O[C][C]([H])[C]	0.35	2.28
225	C ₃ H ₂ O	2.0	3	[H]O[C]([H])[C][C]	0.52	0.71
226	C ₃ H ₂ O	2.0	3	[H][C][C]([C])O[H]	NA	NA
227	C ₃ H ₂ O	2.0	3	[H][C][C][C]O[H]	0.59	0.98
228	C ₃ H ₄ O ₂	2.0	3	[H]C([H])([H])C([H])([O])[C][O]	-0.95	-0.39
229	C ₃ H ₄ O ₂	2.0	3	[H][C]([O])[C]([O])C([H])([H])[H]	-0.68	-0.12
230	C ₃ H ₄ O ₂	2.0	3	[H]C([H])([O])C([H])([H])[C][O]	1.37	1.51
231	C ₃ H ₄ O ₂	2.0	3	[H][C]([O])C([H])([H])[C]([H])[O]	0.04	0.15
232	C ₃ H ₄ O ₂	2.0	3	[H][C]C([H])([O])C([H])([H])[O]	NA	NA
233	C ₃ H ₄ O ₂	2.0	3	[H][C]([O])[C]([H])C([H])([H])[O]	0.24	1.08
234	C ₃ H ₄ O ₂	2.0	3	[H][C]([H])[C]([O])C([H])([H])[O]	NA	NA
235	C ₃ H ₄ O ₂	2.0	3	[H]C([H])([O])[C]C([H])([H])[O]	1.08	2.13
236	C ₃ H ₄ O ₂	2.0	3	[H][C]([H])C([H])([O])[C]([H])[O]	NA	NA
237	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([C][O])C([H])([H])[H]	-0.71	-0.01
238	C ₃ H ₄ O ₂	2.0	3	[H]O[C][C]([O])C([H])([H])[H]	-0.85	-0.22
239	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])C([H])([H])[C][O]	NA	NA
240	C ₃ H ₄ O ₂	2.0	3	[H]O[C]C([H])([H])[C]([H])[O]	0.48	0.75
241	C ₃ H ₄ O ₂	2.0	3	[H]OC([H])([H])C([H])([C])[O]	NA	NA

242	C ₃ H ₄ O ₂	2.0	3	[H]OC([H])([C])C([H])([H])[O]	NA	NA
243	C ₃ H ₄ O ₂	2.0	3	[H]OC([H])([H])[C]([H])[C][O]	-0.30	0.09
244	C ₃ H ₄ O ₂	2.0	3	[H]O[C][C]([H])C([H])([H])[O]	NA	NA
245	C ₃ H ₄ O ₂	2.0	3	[H][C][C]([O])C([H])([H])O[H]	-0.74	-0.12
246	C ₃ H ₄ O ₂	2.0	3	[H][C][C](O[H])C([H])([H])[O]	0.97	1.44
247	C ₃ H ₄ O ₂	2.0	3	[H]OC([H])([H])[C][C]([H])[O]	-0.44	-0.14
248	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])[C]C([H])([H])[O]	0.47	1.28
249	C ₃ H ₄ O ₂	2.0	3	[H]OC([H])([C][O])[C]([H])[H]	NA	NA
250	C ₃ H ₄ O ₂	2.0	3	[H]O[C]C([H])([O])[C]([H])[H]	1.86	NA
251	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([C]([H])[H])[C]([H])[O]	-0.79	-0.22
252	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])[C]([O])[C]([H])[H]	-1.04	-0.04
253	C ₃ H ₄ O ₂	2.0	3	[H][C]C([H])(O[H])[C]([H])[O]	0.14	0.66
254	C ₃ H ₄ O ₂	2.0	3	[H][C]C([H])([O])[C]([H])O[H]	NA	NA
255	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])[C]([H])[C]([H])[O]	-0.57	-0.38
256	C ₃ H ₄ O ₂	2.0	3	[H]O[C]C([H])([H])[C]O[H]	2.73	2.83
257	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([C])C([H])([H])O[H]	-0.24	0.29
258	C ₃ H ₄ O ₂	2.0	3	[H]O[C][C]C([H])([H])O[H]	-0.07	0.19
259	C ₃ H ₄ O ₂	2.0	3	[H]O[C][C](O[H])[C]([H])[H]	0.16	0.70
260	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])C([H])([C])O[H]	0.85	1.86
261	C ₃ H ₄ O ₂	2.0	3	[H][C]C([H])([C]O[H])O[H]	NA	NA
262	C ₃ H ₄ O ₂	2.0	3	[H]O[C][C]([H])[C]([H])O[H]	0.52	0.36
263	C ₃ H ₄ O ₂	2.0	3	[H][C][C](O[H])[C]([H])O[H]	0.16	0.60
264	C ₃ H ₄ O ₂	2.0	3	[H]O[C]([H])[C][C]([H])O[H]	NA	NA

265	C ₃ H ₆ O ₃	2.0	3	[H]OC([H])([H])C([H])([O])C([H])([H])[O]	-0.75	-0.10
266	C ₃ H ₆ O ₃	2.0	3	[H]OC([H])(C([H])([H])[O])C([H])([H])[O]	-0.81	-0.10
267	C ₃ H ₆ O ₃	2.0	3	[H]OC([H])([H])C([H])(O[H])[C]([H])[O]	-0.06	0.18
268	C ₃ H ₆ O ₃	2.0	3	[H]O[C]([H])C([H])([O])C([H])([H])O[H]	0.04	0.67
269	C ₃ H ₆ O ₃	2.0	3	[H]O[C]([H])C([H])(O[H])C([H])([H])[O]	NA	NA
270	C ₃ H ₆ O ₃	2.0	3	[H]O[C](C([H])([H])[O])C([H])([H])O[H]	-0.09	0.67
271	C ₃ H ₆ O ₃	2.0	3	[H]OC([H])([H])[C]([O])C([H])([H])O[H]	-0.26	-0.03
272	C ₃ H ₆ O ₃	2.0	3	[H]O[C]C([H])(O[H])C([H])([H])O[H]	0.50	0.84
273	C ₃ H ₆ O ₃	2.0	3	[H]O[C]([H])[C](O[H])C([H])([H])O[H]	-0.13	-0.00
274	C ₃ H ₆ O ₃	2.0	3	[H]O[C]([H])C([H])(O[H])[C]([H])O[H]	1.60	1.44
275	C ₃ H	2.3	3	[H][C]([C])[C]	NA	NA
276	C ₃ H	2.3	3	[H][C][C][C]	0.63	1.24
277	C ₃ H ₃ O	2.3	3	[H]C([H])([H])[C]([C])[O]	-0.85	-0.06
278	C ₃ H ₃ O	2.3	3	[H]C([H])([H])[C][C][O]	-0.94	-0.58
279	C ₃ H ₃ O	2.3	3	[H][C]([O])C([H])([H])[C]	-0.12	0.32
280	C ₃ H ₃ O	2.3	3	[H][C]C([H])([H])[C][O]	NA	NA
281	C ₃ H ₃ O	2.3	3	[H][C]([C])C([H])([H])[O]	-0.42	0.44
282	C ₃ H ₃ O	2.3	3	[H][C][C]C([H])([H])[O]	0.69	1.15
283	C ₃ H ₃ O	2.3	3	[H][C]([H])C([H])([C])[O]	NA	NA

284	C ₃ H ₃ O	2.3	3	[H][C]([H])[C]([H])[C][O]	-0.48	-0.10
285	C ₃ H ₃ O	2.3	3	[H][C][C]([O])[C]([H])[H]	-0.49	0.31
286	C ₃ H ₃ O	2.3	3	[H][C]([H])[C][C]([H])[O]	-0.15	0.06
287	C ₃ H ₃ O	2.3	3	[H][C]C([H])([O])[C][H]	NA	NA
288	C ₃ H ₃ O	2.3	3	[H][C][C]([H])[C]([H])[O]	-0.14	-0.02
289	C ₃ H ₃ O	2.3	3	[H]O[C]C([H])([H])[C]	0.94	2.43
290	C ₃ H ₃ O	2.3	3	[H]OC([H])([H])[C][C]	0.16	0.25
291	C ₃ H ₃ O	2.3	3	[H]O[C]([C])[C]([H])[H]	-0.22	0.36
292	C ₃ H ₃ O	2.3	3	[H]O[C][C][C]([H])[H]	-0.10	0.15
293	C ₃ H ₃ O	2.3	3	[H][C]C([H])([C])O[H]	NA	NA
294	C ₃ H ₃ O	2.3	3	[H]O[C]([H])[C]([H])[C]	-0.32	0.03
295	C ₃ H ₃ O	2.3	3	[H][C][C]([H])[C]O[H]	2.40	2.63
296	C ₃ H ₃ O	2.3	3	[H][C][C][C]([H])O[H]	-0.23	0.07
297	C ₃ H ₃ O	2.3	3	[H][C][C]([C][H])O[H]	NA	NA
298	C ₃ H ₅ O ₂	2.3	3	[H][C]([O])C([H])([O])C([H])([H])[H]	-0.90	-0.82
299	C ₃ H ₅ O ₂	2.3	3	[H]C([H])([H])[C]([O])C([H])([H])[O]	NA	NA
300	C ₃ H ₅ O ₂	2.3	3	[H][C]([O])C([H])([H])C([H])([H])[O]	NA	NA
301	C ₃ H ₅ O ₂	2.3	3	[H][C]([H])C([H])([O])C([H])([H])[O]	NA	NA
302	C ₃ H ₅ O ₂	2.3	3	[H][C](C([H])([H])[O])C([H])([H])[O]	NA	NA
303	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([C][O])C([H])([H])[H]	-0.84	-0.61
304	C ₃ H ₅ O ₂	2.3	3	[H]O[C]C([H])([O])C([H])([H])[H]	-0.76	-0.09

305	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([C]([H])[O])C([H])([H]) [H]	-1.32	-0.85
306	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])[C]([O])C([H])([H]) [H]	-1.22	-0.67
307	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([H])C([H])([H])[C] [O]	-0.23	-0.32
308	C ₃ H ₅ O ₂	2.3	3	[H]O[C]C([H])([H])C([H])([H]) [O]	NA	NA
309	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])C([H])([H])[C]([H] [O])	-0.13	0.16
310	C ₃ H ₅ O ₂	2.3	3	[H][C]C([H])([O])C([H])([H])O [H]	NA	NA
311	C ₃ H ₅ O ₂	2.3	3	[H][C]C([H])(O[H])C([H])([H]) [O]	NA	NA
312	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([H])[C]([H])[C]([H] [O])	-1.11	-0.54
313	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])[C]([H])C([H])([H] [O])	0.22	0.63
314	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([H])[C]([O])[C]([H] [H])	-1.33	-0.77
315	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([C]([H])[H])C([H])([H] [O])	0.05	NA
316	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([H])[C]C([H])([H]) [O]	-0.12	0.95
317	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([C]([H])[H])[C]([H] [O])	NA	NA
318	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])C([H])([O])[C]([H] [H])	NA	NA
319	C ₃ H ₅ O ₂	2.3	3	[H]O[C][C](O[H])C([H])([H])[H]]	-0.63	-0.29
320	C ₃ H ₅ O ₂	2.3	3	[H]O[C]C([H])([H])[C]([H])O[H]]	1.09	1.44

321	C ₃ H ₅ O ₂	2.3	3	[H]OC([H])([H])C([H])([C])O[H]	-0.19	NA
322	C ₃ H ₅ O ₂	2.3	3	[H]O[C][C]([H])C([H])([H])O[H]	0.22	0.07
323	C ₃ H ₅ O ₂	2.3	3	[H][C][C](O[H])C([H])([H])O[H]	-0.35	-0.21
324	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])[C]C([H])([H])O[H]	0.01	-0.04
325	C ₃ H ₅ O ₂	2.3	3	[H]O[C]C([H])(O[H])[C]([H])[H]	NA	NA
326	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])[C](O[H])[C]([H])[H]	-0.68	-0.33
327	C ₃ H ₅ O ₂	2.3	3	[H][C]C([H])(O[H])[C]([H])O[H]	NA	NA
328	C ₃ H ₅ O ₂	2.3	3	[H]O[C]([H])[C]([H])[C]([H])O[H]	-0.45	-0.10
329	C ₃ H ₇ O ₃	2.3	3	[H]OC([H])([H])C([H])(O[H])C([H])([H])[O]	-0.93	-0.60
330	C ₃ H ₇ O ₃	2.3	3	[H]OC([H])([H])C([H])([O])C([H])([H])O[H]	-1.01	-0.67
331	C ₃ H ₇ O ₃	2.3	3	[H]O[C]([H])C([H])(O[H])C([H])([H])O[H]	-0.20	0.29
332	C ₃ H ₇ O ₃	2.3	3	[H]O[C](C([H])([H])O[H])C([H])([H])O[H]	-0.40	0.06
333	C ₃ H ₂	2.7	3	[H]C([H])([C])[C]	NA	NA
334	C ₃ H ₂	2.7	3	[H][C]([H])[C][C]	-0.35	0.12
335	C ₃ H ₂	2.7	3	[H][C][C]([H])[C]	-0.34	NA
336	C ₃ H ₂	2.7	3	[H][C][C][C][H]	-0.48	0.07
337	C ₃ H ₄ O	2.7	3	[H]C([H])([H])C([H])([C])[O]	-0.22	NA
338	C ₃ H ₄ O	2.7	3	[H][C]([C][O])C([H])([H])[H]	-1.34	-0.66

339	C ₃ H ₄ O	2.7	3	[H][C][C]([O])C([H])([H])[H]	-1.79	-1.14
340	C ₃ H ₄ O	2.7	3	[H][C]([O])[C]C([H])([H])[H]	-0.97	-0.35
341	C ₃ H ₄ O	2.7	3	[H]C([H])([C])C([H])([H])[O]	-0.50	0.31
342	C ₃ H ₄ O	2.7	3	[H][C]([H])C([H])([H])[C][O]	0.74	1.18
343	C ₃ H ₄ O	2.7	3	[H][C]C([H])([H])[C]([H])[O]	-0.20	0.13
344	C ₃ H ₄ O	2.7	3	[H][C][C]([H])C([H])([H])[O]	0.83	0.23
345	C ₃ H ₄ O	2.7	3	[H][C]([H])[C]C([H])([H])[O]	0.22	1.06
346	C ₃ H ₄ O	2.7	3	[H][C]C([H])([O])[C]([H])[H]	NA	NA
347	C ₃ H ₄ O	2.7	3	[H][C]([H])[C]([H])[C]([H])[O]	-1.25	-0.83
348	C ₃ H ₄ O	2.7	3	[H][C]([H])[C]([O])[C]([H])[H]	-2.00	-1.04
349	C ₃ H ₄ O	2.7	3	[H]O[C]([C])C([H])([H])[H]	-1.29	-0.78
350	C ₃ H ₄ O	2.7	3	[H]O[C][C]C([H])([H])[H]	-1.16	-0.82
351	C ₃ H ₄ O	2.7	3	[H]O[C]([H])C([H])([H])[C]	NA	0.80
352	C ₃ H ₄ O	2.7	3	[H][C]C([H])([H])[C]O[H]	3.26	3.60
353	C ₃ H ₄ O	2.7	3	[H]OC([H])([H])[C]([H])[C]	-0.53	-0.16
354	C ₃ H ₄ O	2.7	3	[H][C][C]C([H])([H])O[H]	-0.54	-0.55
355	C ₃ H ₄ O	2.7	3	[H]OC([H])([C])[C]([H])[H]	NA	NA
356	C ₃ H ₄ O	2.7	3	[H]O[C][C]([H])[C]([H])[H]	-0.30	0.10
357	C ₃ H ₄ O	2.7	3	[H][C][C](O[H])[C]([H])[H]	-0.64	-0.22
358	C ₃ H ₄ O	2.7	3	[H]O[C]([H])[C][C]([H])[H]	-0.00	-0.25
359	C ₃ H ₄ O	2.7	3	[H][C]C([H])([C][H])O[H]	NA	NA
360	C ₃ H ₄ O	2.7	3	[H][C][C]([H])[C]([H])O[H]	-0.33	-0.19
361	C ₃ H ₆ O ₂	2.7	3	[H]C([H])([H])C([H])([O])C([H] D)([H])[O]	-1.75	-1.01
362	C ₃ H ₆ O ₂	2.7	3	[H]C([H])([O])C([H])([H])C([H] D)([H])[O]	-1.62	0.36

363	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([C]([H])[O])C([H]) ([H])[H]	-1.13	-0.97
364	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])C([H])([O])C([H]) ([H])[H]	-0.98	-0.35
365	C ₃ H ₆ O ₂	2.7	3	[H]O[C](C([H])([H])[H])C([H]) ([H])[O]	0.16	NA
366	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([H])[C]([O])C([H]) ([H])[H]	-1.06	-1.06
367	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([H])C([H])([H])[C] ([H])[O]	-0.85	-0.66
368	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])C([H])([H])C([H]) ([H])[O]	NA	NA
369	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([H])C([H])([O])[C] ([H])[H]	-1.06	-0.29
370	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([C]([H])[H])C([H]) ([H])[O]	NA	NA
371	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([H])[C]([H])C([H]) ([H])[O]	-0.81	-0.28
372	C ₃ H ₆ O ₂	2.7	3	[H]O[C]C([H])(O[H])C([H])([H]) [H]	-0.58	-0.21
373	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])[C](O[H])C([H])([H]) [H]	-1.20	-1.07
374	C ₃ H ₆ O ₂	2.7	3	[H]O[C]C([H])([H])C([H])([H]) O[H]	0.73	-0.10
375	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])C([H])([H])[C]([H]) O[H]	0.31	0.47
376	C ₃ H ₆ O ₂	2.7	3	[H][C]C([H])(O[H])C([H])([H]) O[H]	-0.14	0.14
377	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])[C]([H])C([H])([H]) O[H]	-0.89	-0.71
378	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([C]([H])[H])C([H])([H]) O[H]	-0.96	-0.87

379	C ₃ H ₆ O ₂	2.7	3	[H]OC([H])([H])[C]C([H])([H]) O[H]	-0.06	0.28
380	C ₃ H ₆ O ₂	2.7	3	[H]O[C]([H])C([H])(O[H])[C]([H]) [H]	NA	NA
381	C ₃ H ₈ O ₃	2.7	3	[H]OC([H])([H])C([H])(O[H])C ([H])([H])O[H]	-0.52	-0.52
382	C ₃ H ₃	3.0	3	[H]C([H])([H])[C][C]	-1.09	-0.93
383	C ₃ H ₃	3.0	3	[H][C]C([H])([H])[C]	NA	NA
384	C ₃ H ₃	3.0	3	[H][C]([H])[C]([H])[C]	-0.78	-0.24
385	C ₃ H ₃	3.0	3	[H][C][C][C]([H])[H]	-1.00	-0.72
386	C ₃ H ₃	3.0	3	[H][C][C]([H])[C][H]	1.92	2.12
387	C ₃ H ₅ O	3.0	3	[H]C([H])([H])C([H])([H])[C] O]	-1.41	-1.32
388	C ₃ H ₅ O	3.0	3	[H][C]C([H])([O])C([H])([H])[H]	-0.59	-0.46
389	C ₃ H ₅ O	3.0	3	[H][C]([O])[C]([H])C([H])([H]) [H]	-2.02	-1.49
390	C ₃ H ₅ O	3.0	3	[H][C]([H])[C]([O])C([H])([H]) [H]	-2.19	-1.68
391	C ₃ H ₅ O	3.0	3	[H]C([H])([H])[C]C([H])([H])[O]	0.29	0.91
392	C ₃ H ₅ O	3.0	3	[H][C]C([H])([H])C([H])([H])[O]	1.24	NA
393	C ₃ H ₅ O	3.0	3	[H][C]([H])C([H])([H])[C]([H]) [O]	NA	NA
394	C ₃ H ₅ O	3.0	3	[H][C]([H])[C]([H])C([H])([H]) [O]	-0.41	0.06
395	C ₃ H ₅ O	3.0	3	[H][C]([H])C([H])([O])[C]([H]) [H]	NA	NA
396	C ₃ H ₅ O	3.0	3	[H]OC([H])([C])C([H])([H])[H]	NA	NA

397	C ₃ H ₅ O	3.0	3	[H]O[C][C]([H])C([H])([H])[H]	-1.14	-0.85
398	C ₃ H ₅ O	3.0	3	[H][C][C](O[H])C([H])([H])[H]	-1.58	-1.25
399	C ₃ H ₅ O	3.0	3	[H]O[C]([H])[C]C([H])([H])[H]	-1.23	-0.95
400	C ₃ H ₅ O	3.0	3	[H]OC([H])([H])C([H])([H])[C]	-0.53	-0.36
401	C ₃ H ₅ O	3.0	3	[H]O[C]C([H])([H])[C]([H])[H]	0.96	1.18
402	C ₃ H ₅ O	3.0	3	[H][C]C([H])([H])[C]([H])O[H]	0.59	0.76
403	C ₃ H ₅ O	3.0	3	[H][C][C]([H])C([H])([H])O[H]	-0.68	-0.66
404	C ₃ H ₅ O	3.0	3	[H]OC([H])([H])[C][C]([H])[H]	-0.65	-0.49
405	C ₃ H ₅ O	3.0	3	[H][C]C([H])(O[H])[C]([H])[H]	NA	NA
406	C ₃ H ₅ O	3.0	3	[H]O[C]([H])[C]([H])[C]([H])[H]	-1.48	-1.14
407	C ₃ H ₅ O	3.0	3	[H]O[C]([C]([H])[H])[C]([H])[H]	-1.71	-1.33
408	C ₃ H ₇ O ₂	3.0	3	[H]OC([H])(C([H])([H])[H])C([H])([H])[O]	-1.71	-1.44
409	C ₃ H ₇ O ₂	3.0	3	[H]OC([H])([H])C([H])([O])C([H])([H])[H]	-1.81	-1.52
410	C ₃ H ₇ O ₂	3.0	3	[H]OC([H])([H])C([H])([H])C([H])([H])[O]	-1.47	-1.32
411	C ₃ H ₇ O ₂	3.0	3	[H]O[C]([H])C([H])(O[H])C([H])([H])[H]	-1.26	-0.75
412	C ₃ H ₇ O ₂	3.0	3	[H]O[C](C([H])([H])[H])C([H]) ([H])O[H]	-1.06	-0.68
413	C ₃ H ₇ O ₂	3.0	3	[H]O[C]([H])C([H])([H])C([H]) ([H])O[H]	-0.78	-0.53
414	C ₃ H ₇ O ₂	3.0	3	[H]OC([H])([H])C([H])(O[H])[C]([H])[H]	-1.06	-0.71
415	C ₃ H ₇ O ₂	3.0	3	[H]OC([H])([H])[C]([H])C([H]) ([H])O[H]	-1.04	-0.71

416	C ₃ H ₄	3.3	3	[H][C]([C])C([H])([H])[H]	-1.51	-1.17
417	C ₃ H ₄	3.3	3	[H][C][C]C([H])([H])[H]	-1.55	-1.51
418	C ₃ H ₄	3.3	3	[H][C]([H])C([H])([H])[C]	0.63	1.08
419	C ₃ H ₄	3.3	3	[H][C]C([H])([H])[C][H]	2.82	3.02
420	C ₃ H ₄	3.3	3	[H][C][C]([H])[C]([H])[H]	-0.85	-0.64
421	C ₃ H ₄	3.3	3	[H][C]([H])[C][C]([H])[H]	-0.43	-0.83
422	C ₃ H ₆ O	3.3	3	[H][C]([O])C([H])([H])C([H])([H])[H]	-1.91	-1.91
423	C ₃ H ₆ O	3.3	3	[H][C]([H])C([H])([O])C([H])([H])[H]	-2.01	-1.33
424	C ₃ H ₆ O	3.3	3	[H][C](C([H])([H])[H])C([H])([H])[O]	-0.57	NA
425	C ₃ H ₆ O	3.3	3	[H]C([H])([H])[C]([O])C([H])([H])[H]	-2.21	-2.21
426	C ₃ H ₆ O	3.3	3	[H][C]([H])C([H])([H])C([H])([H])[O]	0.28	NA
427	C ₃ H ₆ O	3.3	3	[H]O[C]C([H])([H])C([H])([H])[H]	-1.10	-1.02
428	C ₃ H ₆ O	3.3	3	[H][C]C([H])(O[H])C([H])([H])[H]	NA	NA
429	C ₃ H ₆ O	3.3	3	[H]O[C]([H])[C]([H])C([H])([H])[H]	-1.85	-1.75
430	C ₃ H ₆ O	3.3	3	[H]O[C]([C]([H])[H])C([H])([H])[H]	-2.05	-1.98
431	C ₃ H ₆ O	3.3	3	[H]OC([H])([H])[C]C([H])([H])[H]	-0.79	-0.44
432	C ₃ H ₆ O	3.3	3	[H][C]C([H])([H])C([H])([H])O[H]	-0.87	-0.66
433	C ₃ H ₆ O	3.3	3	[H]O[C]([H])C([H])([H])[C]([H])[H]	NA	NA

434	C ₃ H ₆ O	3.3	3	[H]OC([H])([H])[C]([H])[C]([H]) [H]	-1.25	-1.25
435	C ₃ H ₆ O	3.3	3	[H]OC([H])([C]([H])[H])[C]([H]) [H]	NA	NA
436	C ₃ H ₈ O ₂	3.3	3	[H]OC([H])([H])C([H])(O[H])C ([H])([H])[H]	-1.56	-1.56
437	C ₃ H ₈ O ₂	3.3	3	[H]OC([H])([H])C([H])([H])C([H]) ([H])O[H]	-1.43	-1.43
438	C ₃ H ₅	3.7	3	[H]C([H])([H])C([H])([H])[C]	-1.60	-1.29
439	C ₃ H ₅	3.7	3	[H][C][C]([H])C([H])([H])[H]	-1.77	-1.66
440	C ₃ H ₅	3.7	3	[H][C]([H])[C]C([H])([H])[H]	-1.70	-1.42
441	C ₃ H ₅	3.7	3	[H][C]C([H])([H])[C]([H])[H]	0.65	0.76
442	C ₃ H ₅	3.7	3	[H][C]([H])[C]([H])[C]([H])[H]	-2.26	-1.86
443	C ₃ H ₇ O	3.7	3	[H]C([H])([H])C([H])([H])C([H]) ([H])O	-2.44	-2.26
444	C ₃ H ₇ O	3.7	3	[H]C([H])([H])C([H])(O)C([H]) ([H])[H]	-2.77	-2.44
445	C ₃ H ₇ O	3.7	3	[H]O[C]([H])C([H])([H])C([H]) ([H])[H]	-1.76	-1.53
446	C ₃ H ₇ O	3.7	3	[H]OC([H])([C]([H])[H])C([H]) ([H])[H]	-2.07	-1.82
447	C ₃ H ₇ O	3.7	3	[H]OC([H])([H])[C]([H])C([H]) ([H])[H]	-1.60	-1.39
448	C ₃ H ₇ O	3.7	3	[H]O[C](C([H])([H])[H])C([H]) ([H])[H]	-1.95	-1.61
449	C ₃ H ₇ O	3.7	3	[H]OC([H])([H])C([H])([H])[C] ([H])[H]	-1.33	-1.42
450	C ₃ H ₆	4.0	3	[H][C]C([H])([H])C([H])([H])[H]	-1.64	-1.62
451	C ₃ H ₆	4.0	3	[H][C]([H])[C]([H])C([H])([H])	-2.53	-2.42

				[H]		
452	C ₃ H ₆	4.0	3	[H]C([H])([H])[C]C([H])([H])[H]	-1.66	-1.39
453	C ₃ H ₆	4.0	3	[H][C]([H])C([H])([H])[C]([H])[H]	-0.35	0.00
454	C ₃ H ₈ O	4.0	3	[H]OC([H])([H])C([H])([H])C([H])([H])[H]	-2.46	-2.46
455	C ₃ H ₈ O	4.0	3	[H]OC([H])(C([H])([H])[H])C([H])([H])[H]	-2.57	-2.57
456	C ₃ H ₇	4.3	3	[H][C]([H])C([H])([H])C([H])([H])[H]	-2.47	-2.40
457	C ₃ H ₇	4.3	3	[H][C](C([H])([H])[H])C([H])([H])[H]	-2.52	-2.27
458	C ₃ H ₈	4.7	3	[H]C([H])([H])C([H])([H])C([H])([H])[H]	-3.68	-3.68