

Supporting Information for

Revisiting Formic Acid Decomposition by a Graph-Theoretical Approach

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Figure S1. Unimolecular HCOOH decomposition including the oxygen atoms with a formal charge of -2. To compare with Figure 3, the nodes added to Figure 3 are shown by yellow circles in this figure. 127 possible molecular graphs were reduced to 40 graphs in the reduction step.

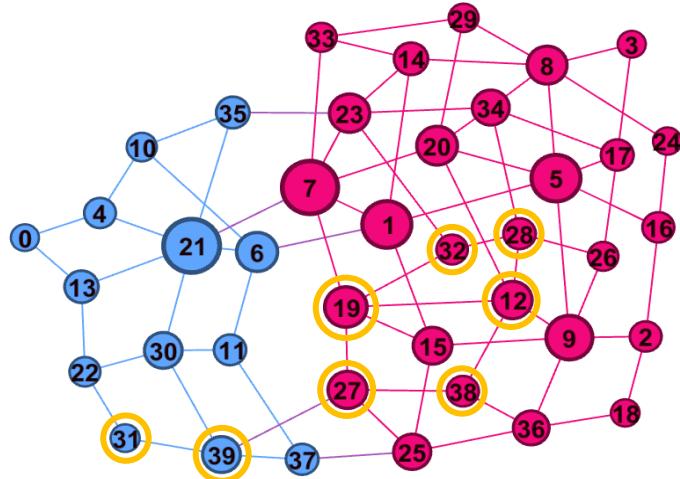


Table S1. Chemical formulae and connected information (CI) in the chemical reaction network of unimolecular HCOOH decomposition including the oxygen atoms with a formal charge of -2 . Formal charges (\oplus and \ominus) are indicated on the right of the corresponding atom in the chemical formula.

No.	Chemical formula	CI
0	CO_2, H_2	4, 13
1	$\text{HC}(=\text{O})\text{OH}$	5, 6, 7, 14, 15
2	$\text{CO}, \text{H}_2\text{O}$	9, 16, 18
3	$\text{C}(\text{OH})_2$	8, 17
4	$\text{CO}_2, \text{H}^\oplus, \text{H}^\ominus$	0, 10, 21
5	$\text{C}^\ominus(=\text{O})\text{OH}, \text{H}^\oplus$	1, 8, 9, 16, 17, 20
6	$\text{C}^\oplus(=\text{O})\text{OH}, \text{H}^\ominus$	1, 10, 11, 21
7	$\text{HC}(=\text{O})\text{O}^\ominus, \text{H}^\oplus$	1, 19, 20, 21, 23, 33
8	$\text{C}(\text{OH})\text{O}^\ominus, \text{H}^\oplus$	3, 5, 14, 24, 29, 34
9	$\text{CO}, \text{O}^\ominus\text{H}, \text{H}^\oplus$	2, 5, 12, 15, 26, 36
10	$\text{C}(=\text{O}^\oplus\text{H})=\text{O}, \text{H}^\ominus$	4, 6, 35
11	$\text{C}(=\text{O}^\oplus)\text{OH}, \text{H}^\ominus$	6, 30, 37
12	$\text{CO}, \text{O}^{2\ominus}, 2\text{H}^\oplus$	9, 19, 20, 28, 38
13	$\text{C}^\oplus(=\text{O})\text{O}^\ominus, \text{H}_2$	0, 21, 22
14	$\text{HC}^\oplus(\text{OH})\text{O}^\ominus$	1, 8, 23, 33
15	$\text{HC}^\oplus=\text{O}, \text{O}^\ominus\text{H}$	1, 9, 19, 25
16	$\text{C}^\ominus(=\text{O})\text{O}^\oplus\text{H}_2$	2, 5, 24
17	$\text{C}^\ominus(=\text{O}^\oplus\text{H})\text{OH}$	3, 5, 26, 34
18	$\text{C}^\ominus\equiv\text{O}^\oplus, \text{H}_2\text{O}$	2, 36
19	$\text{HC}^\oplus=\text{O}, \text{O}^{2\ominus}, \text{H}^\oplus$	7, 12, 15, 27, 32
20	$\text{C}^\ominus(=\text{O})\text{O}^\ominus, 2\text{H}^\oplus$	5, 7, 12, 29, 34
21	$\text{C}^\oplus(=\text{O})\text{O}^\ominus, \text{H}^\oplus, \text{H}^\ominus$	4, 6, 7, 13, 30, 35
22	$\text{C}(=\text{O}^\oplus)\text{O}^\ominus, \text{H}_2$	13, 30, 31
23	$\text{HC}(=\text{O}^\oplus\text{H})\text{O}^\ominus$	7, 14, 32, 34, 35
24	$\text{C}(\text{O}^\oplus\text{H}_2)\text{O}^\ominus$	8, 16
25	$\text{HC}\equiv\text{O}^\oplus, \text{O}^\ominus\text{H}$	15, 27, 36, 37
26	$\text{C}=\text{O}^\oplus\text{H}, \text{O}^\ominus\text{H}$	9, 17, 28
27	$\text{HC}\equiv\text{O}^\oplus, \text{O}^{2\ominus}, \text{H}^\oplus$	19, 25, 38, 39
28	$\text{C}=\text{O}^\oplus\text{H}, \text{O}^{2\ominus}, \text{H}^\oplus$	12, 26, 32, 34
29	$\text{C}(\text{O}^\ominus)_2, 2\text{H}^\oplus$	8, 20, 33
30	$\text{C}(=\text{O}^\oplus)\text{O}^\ominus, \text{H}^\oplus, \text{H}^\ominus$	11, 21, 22, 39
31	$\text{C}^\ominus\equiv\text{O}^\oplus, \text{O}^{2\ominus}, \text{H}_2$	22, 39
32	$\text{HC}^\oplus=\text{O}^\oplus\text{H}, \text{O}^{2\ominus}$	19, 23, 28
33	$\text{HC}^\oplus(\text{O}^\ominus)_2, \text{H}^\oplus$	7, 14, 29

34	$C^\ominus(=O^\oplus H)O^\ominus, H^\oplus$	8, 17, 20, 23, 28
35	$C^\oplus(=O^\oplus H)O^\ominus, H^\ominus$	10, 21, 23
36	$C^\ominus\equiv O^\oplus, O^\ominus H, H^\oplus$	9, 18, 25, 38
37	$C^\oplus\equiv O^\oplus, O^\ominus H, H^\ominus$	11, 25, 39
38	$C^\ominus\equiv O^\oplus, O^{2\ominus}, 2H^\oplus$	12, 27, 36
39	$C^\oplus\equiv O^\oplus, O^{2\ominus}, H^\oplus, H^\ominus$	27, 30, 31, 37

Table S2. Chemical formulae, connected information (CI), and betweenness centrality (BC) values of molecular graphs in the chemical reaction network of HCOOH+H₂O. Formal charges \oplus and \ominus are indicated on the right of the corresponding atom in the chemical formula. BC-c and BC-h are the BC values in the separation network for the decarboxylation and the dehydration groups, respectively.

No.	Chemical formula	CI	BC	BC-c	BC-h
0	CO ₂ , H ₂ O, H ₂	6, 16, 27	20.9	15.6	
1	C(=O)(OH) ₂ , H ₂	7, 12, 28, 30	105.6	62.6	
2	HC(=O)OH, H ₂ O	8, 9, 13, 17, 29, 31	669.0		143.9
3	CO, 2H ₂ O	18, 34, 37	66.8		44.1
4	HC(OH) ₃	10, 11, 14, 32	115.0		14.3
5	C(OH) ₂ , H ₂ O	15, 19, 35, 36	74.2		55.3
6	CO ₂ , H ₂ O, H \oplus , H \ominus	0, 20, 22, 26, 39	146.9	69.2	
7	C(=O)(OH) ₂ , H \oplus , H \ominus	1, 21, 23, 25, 41, 43	336.5	145.1	
8	C \ominus (=O)OH, H ₂ O, H \oplus	2, 15, 18, 33, 34, 36, 38, 42	667.2		338.6
9	C \oplus (=O)OH, H ₂ O, H \ominus	2, 21, 22, 24, 39, 43	505.6	107.5	
10	C \ominus (OH) ₃ , H \oplus	4, 19, 35, 40	68.5		32.2
11	C \oplus (OH) ₃ , H \ominus	4, 23, 41	63.7	2.5	
12	C(=O)(OH)O \ominus , H ₂ , H \oplus	1, 25, 44, 46, 60, 72, 74	292.7	188.1	
13	HC(=O)O \ominus , H ₂ O, H \oplus	2, 38, 39, 45, 50, 63, 73	668.5		113.1
14	HC(OH) ₂ O \ominus , H \oplus	4, 40, 41, 47, 61, 75	423.9		84.2
15	C(OH)O \ominus , H ₂ O, H \oplus	5, 8, 29, 48, 51, 62, 64, 78, 80	563.2		349.6
16	CO ₂ , O \ominus H, H ₂ , H \oplus	0, 26, 52, 74	41.2	31.6	
17	HC(=O)OH, O \ominus H, H \oplus	2, 42, 43, 53, 56, 63, 75, 82	956.3		201.8
18	CO, H ₂ O, O \ominus H, H \oplus	3, 8, 31, 54, 59, 68, 83, 87	514.0		304.3
19	C(OH) ₂ , O \ominus H, H \oplus	5, 10, 32, 57, 64, 85	169.6		106.7
20	CO ₂ , H ₃ O \oplus , H \ominus	6, 77	7.1	3.2	
21	C(=O)(O \oplus H ₂)OH, H \ominus	7, 9, 65, 79, 84	225.7	92.0	
22	C(=O \oplus H)=O, H ₂ O, H \ominus	6, 9, 69, 81	83.6	35.4	
23	C(=O \oplus H)(OH) ₂ , H \ominus	7, 11, 66, 86	100.2	43.7	
24	C(\equiv O \oplus)OH, H ₂ O, H \ominus	9, 67, 70, 88	167.0	64.0	
25	C(=O)(OH)O \ominus , 2H \oplus , H \ominus	7, 12, 65, 66, 71, 90, 92	491.6	229.9	
26	CO ₂ , O \ominus H, 2H \oplus , H \ominus	6, 16, 69, 92	91.3	43.9	
27	C \oplus (=O)O \ominus , H ₂ O, H ₂	0, 39, 44, 49, 74	204.5	98.3	

28	$\text{C}^{\oplus}(\text{OH})_2\text{O}^{\ominus}, \text{H}_2$	1, 41, 46, 72	85.1	31.5	
29	$\text{HC}^{\oplus}(\text{OH})\text{O}^{\ominus}, \text{H}_2\text{O}$	2, 15, 47, 50, 73, 75	350.0		147.5
30	$\text{C}^{\oplus}(=\text{O})\text{OH}, \text{O}^{\ominus}\text{H}, \text{H}_2$	1, 43, 52, 55, 74	243.8	111.6	
31	$\text{HC}^{\oplus}=\text{O}, \text{H}_2\text{O}, \text{O}^{\ominus}\text{H}$	2, 18, 53, 58, 82	301.8		117.5
32	$\text{HC}^{\oplus}(\text{OH})_2, \text{O}^{\ominus}\text{H}$	4, 19, 56, 75	128.0		54.1
33	$\text{C}^{\ominus}(=\text{O})\text{OH}, \text{H}_3\text{O}^{\oplus}$	8, 48, 54, 76	130.2		82.5
34	$\text{C}^{\ominus}(=\text{O})\text{O}^{\oplus}\text{H}_2, \text{H}_2\text{O}$	3, 8, 51, 83	111.2		68.6
35	$\text{C}^{\ominus}(\text{OH})_2\text{O}^{\oplus}\text{H}_2,$	5, 10, 57, 78	51.8		33.1
36	$\text{C}^{\ominus}(=\text{O}^{\oplus}\text{H})\text{OH}, \text{H}_2\text{O}$	5, 8, 59, 80, 85	144.6		91.5
37	$\text{C}^{\ominus}\equiv\text{O}^{\oplus}, 2\text{H}_2\text{O}$	3, 87	5.1		3.1
38	$\text{C}^{\ominus}(=\text{O})\text{O}^{\ominus}, \text{H}_2\text{O}, 2\text{H}^{\oplus}$	8, 13, 62, 76, 80, 91	303.7		133.7
39	$\text{C}^{\oplus}(=\text{O})\text{O}^{\ominus}, \text{H}_2\text{O}, \text{H}^{\oplus}, \text{H}^{\ominus}$	6, 9, 13, 27, 65, 67, 77, 81, 92	932.3	267.8	
40	$\text{C}^{\ominus}(\text{OH})_2\text{O}^{\ominus}, 2\text{H}^{\oplus}$	10, 14, 64, 78, 89	198.2		99.7
41	$\text{C}^{\oplus}(\text{OH})_2\text{O}^{\ominus}, \text{H}^{\oplus}, \text{H}^{\ominus}$	7, 11, 14, 28, 66, 79, 90	437.2	89.3	
42	$\text{C}^{\ominus}(=\text{O})\text{OH}, \text{O}^{\ominus}\text{H}, 2\text{H}^{\oplus}$	8, 17, 64, 68, 83, 85, 91	478.2		240.5
43	$\text{C}^{\oplus}(=\text{O})\text{OH}, \text{O}^{\ominus}\text{H}, \text{H}^{\oplus}, \text{H}^{\ominus}$	7, 9, 17, 30, 69, 70, 84, 86, 92	1051.1	266.4	
44	$\text{C}(=\text{O})(\text{O}^{\oplus}\text{H}_2)\text{O}^{\ominus}, \text{H}_2$	12, 27, 65, 109	101.0	66.2	
45	$\text{HC}(=\text{O})\text{O}^{\ominus}, \text{H}_3\text{O}^{\oplus}$	13, 76, 77, 110	178.7		18.8
46	$\text{C}(=\text{O}^{\oplus}\text{H})(\text{OH})\text{O}^{\ominus}, \text{H}_2$	12, 28, 66, 93, 111	111.1	65.8	
47	$\text{HC}(\text{O}^{\oplus}\text{H}_2)(\text{OH})\text{O}^{\ominus}$	14, 29, 78, 79, 94, 112	368.9		76.5
48	$\text{C}(\text{OH})\text{O}^{\ominus}, \text{H}_3\text{O}^{\oplus}$	15, 33, 95, 113	74.0		59.1
49	$\text{C}(\equiv\text{O}^{\oplus})\text{O}^{\ominus}, \text{H}_2\text{O}, \text{H}_2$	27, 67, 96	27.4	19.8	
50	$\text{HC}(=\text{O}^{\oplus}\text{H})\text{O}^{\ominus}, \text{H}_2\text{O}$	13, 29, 80, 81, 97	262.7		35.8
51	$\text{C}(\text{O}^{\oplus}\text{H}_2)\text{O}^{\ominus}, \text{H}_2\text{O}$	15, 34, 98, 114	79.6		57.8
52	$\text{C}(=\text{O}^{\oplus}\text{H})=\text{O}, \text{O}^{\ominus}\text{H}, \text{H}_2$	16, 30, 69, 111	47.6	31.2	
53	$\text{HC}(=\text{O})\text{O}^{\oplus}\text{H}_2, \text{O}^{\ominus}\text{H}$	17, 31, 83, 84, 112	302.7		58.6
54	$\text{CO}, \text{H}_3\text{O}^{\oplus}, \text{O}^{\ominus}\text{H}$	18, 33, 117	81.6		55.3
55	$\text{C}(\equiv\text{O}^{\oplus})\text{OH}, \text{O}^{\ominus}\text{H}, \text{H}_2$	30, 70, 96, 115	116.9	69.3	
56	$\text{HC}(=\text{O}^{\oplus}\text{H})\text{OH}, \text{O}^{\ominus}\text{H}$	17, 32, 85, 86, 97, 116	390.0		80.0
57	$\text{C}(\text{O}^{\oplus}\text{H}_2)\text{OH}, \text{O}^{\ominus}\text{H}$	19, 35, 98, 118	47.7		36.7
58	$\text{HC}\equiv\text{O}^{\oplus}, \text{H}_2\text{O}, \text{O}^{\ominus}\text{H}$	31, 87, 88, 101	166.3		22.2
59	$\text{C}=\text{O}^{\oplus}\text{H}, \text{H}_2\text{O}, \text{O}^{\ominus}\text{H}$	18, 36, 102, 118	58.2		47.9
60	$\text{C}(=\text{O})(\text{O}^{\ominus})_2, \text{H}_2, 2\text{H}^{\oplus}$	12, 71, 93, 119	46.2	33.1	
61	$\text{HC}(\text{O}^{\ominus})_2\text{OH}, 2\text{H}^{\oplus}$	14, 89, 90, 94, 105, 120	411.8		91.1
62	$\text{C}(\text{O}^{\ominus})_2, \text{H}_2\text{O}, 2\text{H}^{\oplus}$	15, 38, 73, 95, 106, 121	225.7		140.9

63	$\text{HC}(\text{=O})\text{O}^\ominus, \text{O}^\ominus\text{H}, 2\text{H}^\oplus$	13, 17, 91, 92, 97, 120	515.4		73.4
64	$\text{C}(\text{OH})\text{O}^\ominus, \text{O}^\ominus\text{H}, 2\text{H}^\oplus$	15, 19, 40, 42, 75, 98, 106, 123	430.4		272.0
65	$\text{C}(\text{=O})(\text{O}^\oplus\text{H}_2)\text{O}^\ominus, \text{H}^\oplus, \text{H}^\ominus$	21, 25, 39, 44, 100, 122	313.6	149.5	
66	$\text{C}(\text{=O}^\oplus\text{H})(\text{OH})\text{O}^\ominus, \text{H}^\oplus, \text{H}^\ominus$	23, 25, 41, 46, 100, 107, 124	319.8	140.8	
67	$\text{C}(\equiv\text{O}^\oplus)\text{O}^\ominus, \text{H}_2\text{O}, \text{H}^\oplus, \text{H}^\ominus$	24, 39, 49, 99, 108	189.0	87.9	
68	$\text{CO}, 2\text{O}^\ominus\text{H}, 2\text{H}^\oplus$	18, 42, 82, 102, 125	194.6		120.4
69	$\text{C}(\text{=O}^\oplus\text{H})=\text{O}, \text{O}^\ominus\text{H}, \text{H}^\oplus, \text{H}^\ominus$	22, 26, 43, 52, 104, 124	198.4	92.1	
70	$\text{C}(\equiv\text{O}^\oplus)\text{OH}, \text{O}^\ominus\text{H}, \text{H}^\oplus, \text{H}^\ominus$	24, 43, 55, 103, 108, 126	325.3	141.3	
71	$\text{C}(\text{=O})(\text{O}^\ominus)_2, 3\text{H}^\oplus, \text{H}^\ominus$	25, 60, 107, 128	88.6	41.3	
72	$\text{C}^\oplus(\text{O}^\ominus)_2\text{OH}, \text{H}_2, \text{H}^\oplus$	12, 28, 90, 93, 109, 119	165.6	77.0	
73	$\text{HC}^\oplus(\text{O}^\ominus)_2, \text{H}_2\text{O}, \text{H}^\oplus$	13, 29, 62, 94, 110, 120	299.3		119.1
74	$\text{C}^\oplus(\text{=O})\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}_2, \text{H}^\oplus$	12, 16, 27, 30, 92, 96, 111	348.0	194.4	
75	$\text{HC}^\oplus(\text{OH})\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}^\oplus$	14, 17, 29, 32, 64, 97, 112, 120	538.9		227.7
76	$\text{C}^\ominus(\text{=O})\text{O}^\ominus, \text{H}_3\text{O}^\oplus, \text{H}^\oplus$	33, 38, 45, 95, 113	132.2		57.0
77	$\text{C}^\oplus(\text{=O})\text{O}^\ominus, \text{H}_3\text{O}^\oplus, \text{H}^\ominus$	20, 39, 45, 99	175.6	36.4	
78	$\text{C}^\ominus(\text{O}^\oplus\text{H}_2)(\text{OH})\text{O}^\ominus, \text{H}^\oplus$	15, 35, 40, 47, 98, 114, 121	343.6		170.3
79	$\text{C}^\oplus(\text{O}^\oplus\text{H}_2)(\text{OH})\text{O}^\ominus, \text{H}^\ominus$	21, 41, 47, 100, 122	231.6	33.1	
80	$\text{C}^\ominus(\text{=O}^\oplus\text{H})\text{O}^\ominus, \text{H}_2\text{O}, \text{H}^\oplus$	15, 36, 38, 50, 113, 123	239.9		109.4
81	$\text{C}^\oplus(\text{=O}^\oplus\text{H})\text{O}^\ominus, \text{H}_2\text{O}, \text{H}^\ominus$	22, 39, 50, 100, 124	225.3	49.2	
82	$\text{HC}^\oplus=\text{O}, 2\text{O}^\ominus\text{H}, \text{H}^\oplus$	17, 31, 68, 101, 116	256.1		100.3
83	$\text{C}^\ominus(\text{=O})\text{O}^\oplus\text{H}_2, \text{O}^\ominus\text{H}, \text{H}^\oplus$	18, 34, 42, 53, 98, 118	275.4		144.1
84	$\text{C}^\oplus(\text{=O})\text{O}^\oplus\text{H}_2, \text{O}^\ominus\text{H}, \text{H}^\ominus$	21, 43, 53, 103	222.9	42.4	
85	$\text{C}^\ominus(\text{=O}^\oplus\text{H})\text{OH}, \text{O}^\ominus\text{H}, \text{H}^\oplus$	19, 36, 42, 56, 102, 118, 123	298.7		145.4
86	$\text{C}^\oplus(\text{=O}^\oplus\text{H})\text{OH}, \text{O}^\ominus\text{H}, \text{H}^\ominus$	23, 43, 56, 104, 124	276.1	50.8	
87	$\text{C}^\ominus\equiv\text{O}^\oplus, \text{H}_2\text{O}, \text{O}^\ominus\text{H}, \text{H}^\oplus$	18, 37, 58, 117, 125	185.9		85.5
88	$\text{C}^\oplus\equiv\text{O}^\oplus, \text{H}_2\text{O}, \text{O}^\ominus\text{H}, \text{H}^\ominus$	24, 58, 103, 126	119.4	10.7	
89	$\text{C}^\ominus(\text{O}^\ominus)_2\text{OH}, 3\text{H}^\oplus$	40, 61, 106, 121, 127	187.1		103.3
90	$\text{C}^\oplus(\text{O}^\ominus)_2\text{OH}, 2\text{H}^\oplus, \text{H}^\ominus$	25, 41, 61, 72, 107, 122, 128	449.8	93.4	
91	$\text{C}^\ominus(\text{=O})\text{O}^\ominus, \text{O}^\ominus\text{H}, 3\text{H}^\oplus$	38, 42, 63, 106, 123	184.7		79.7
92	$\text{C}^\oplus(\text{=O})\text{O}^\ominus, \text{O}^\ominus\text{H}, 2\text{H}^\oplus, \text{H}^\ominus$	25, 26, 39, 43, 63, 74, 108, 124	844.9	247.6	
93	$\text{C}(\text{=O}^\oplus\text{H})(\text{O}^\ominus)_2, \text{H}_2, \text{H}^\oplus$	46, 60, 72, 107	27.0	17.0	
94	$\text{HC}(\text{O}^\ominus)_2\text{O}^\oplus\text{H}_2, \text{H}^\oplus$	47, 61, 73, 121, 122	251.7		40.7
95	$\text{C}(\text{O}^\ominus)_2, \text{H}_3\text{O}^\oplus, \text{H}^\oplus$	48, 62, 76, 110	50.9		36.9
96	$\text{C}(\equiv\text{O}^\oplus)\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}_2, \text{H}^\oplus$	49, 55, 74, 108	68.4	50.1	
97	$\text{HC}(\text{=O}^\oplus\text{H})\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}^\oplus$	50, 56, 63, 75, 123, 124	381.5		56.0

98	$\text{C}(\text{O}^\oplus\text{H}_2)\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}^\oplus$	51, 57, 64, 78, 83, 112	208.6		130.7
99	$\text{C}(\equiv\text{O}^\oplus)\text{O}^\ominus, \text{H}_3\text{O}^\oplus, \text{H}^\ominus$	67, 77	10.4	4.8	
100	$\text{C}(\equiv\text{O}^\oplus\text{H})(\text{O}^\oplus\text{H}_2)\text{O}^\ominus, \text{H}^\ominus$	65, 66, 79, 81	92.8	41.3	
101	$\text{HC}\equiv\text{O}^\oplus, 2\text{O}^\ominus\text{H}, \text{H}^\oplus$	58, 82, 125, 126	137.2		14.1
102	$\text{C}=\text{O}^\oplus\text{H}, 2\text{O}^\ominus\text{H}, \text{H}^\oplus$	59, 68, 85, 116	55.4		38.5
103	$\text{C}(\equiv\text{O}^\oplus)\text{O}^\oplus\text{H}_2, \text{O}^\ominus\text{H}, \text{H}^\ominus$	70, 84, 88	51.8	20.3	
104	$\text{C}(\equiv\text{O}^\oplus\text{H})_2, \text{O}^\ominus\text{H}, \text{H}^\ominus$	69, 86	6.7	2.5	
105	$\text{HC}(\text{O}^\ominus)_3, 3\text{H}^\oplus$	61, 127, 128	78.9		5.7
106	$\text{C}(\text{O}^\ominus)_2, \text{O}^\ominus\text{H}, 3\text{H}^\oplus$	62, 64, 89, 91, 120	172.2		108.9
107	$\text{C}(\equiv\text{O}^\oplus\text{H})(\text{O}^\ominus)_2, 2\text{H}^\oplus, \text{H}^\ominus$	66, 71, 90, 93	74.5	26.4	
108	$\text{C}(\equiv\text{O}^\oplus)\text{O}^\ominus, \text{O}^\ominus\text{H}, 2\text{H}^\oplus, \text{H}^\ominus$	67, 70, 92, 96	133.6	65.5	
109	$\text{C}^\oplus(\text{O}^\ominus)_2\text{O}^\oplus\text{H}_2, \text{H}_2$	44, 72, 122	43.1	16.6	
110	$\text{HC}^\oplus(\text{O}^\ominus)_2, \text{H}_3\text{O}^\oplus$	45, 73, 95	47.5		16.5
111	$\text{C}^\oplus(\equiv\text{O}^\oplus\text{H})\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}_2$	46, 52, 74, 124	106.6	50.4	
112	$\text{HC}^\oplus(\text{O}^\oplus\text{H}_2)\text{O}^\ominus, \text{O}^\ominus\text{H}$	47, 53, 75, 98	142.0		56.2
113	$\text{C}^\ominus(\equiv\text{O}^\oplus\text{H})\text{O}^\ominus, \text{H}_3\text{O}^\oplus$	48, 76, 80	23.3		13.4
114	$\text{C}^\ominus(\text{O}^\oplus\text{H}_2)_2\text{O}^\ominus$	51, 78	8.6		4.5
115	$\text{C}^\oplus\equiv\text{O}^\oplus, 2\text{O}^\ominus\text{H}, \text{H}_2$	55, 126	15.4	5.0	
116	$\text{HC}^\oplus\equiv\text{O}^\oplus\text{H}, 2\text{O}^\ominus\text{H}$	56, 82, 102	53.3		18.4
117	$\text{C}^\ominus\equiv\text{O}^\oplus, \text{H}_3\text{O}^\oplus, \text{O}^\ominus\text{H}$	54, 87	7.6		5.1
118	$\text{C}^\ominus(\equiv\text{O}^\oplus\text{H})\text{O}^\oplus\text{H}_2, \text{O}^\ominus\text{H}$	57, 59, 83, 85	65.7		42.2
119	$\text{C}^\oplus(\text{O}^\ominus)_3, \text{H}_2, 2\text{H}^\oplus$	60, 72, 128	17.7	7.1	
120	$\text{HC}^\oplus(\text{O}^\ominus)_2, \text{O}^\ominus\text{H}, 2\text{H}^\oplus$	61, 63, 73, 75, 106	257.8		98.4
121	$\text{C}^\ominus(\text{O}^\ominus)_2\text{O}^\oplus\text{H}_2, 2\text{H}^\oplus$	62, 78, 89, 94	111.3		55.6
122	$\text{C}^\oplus(\text{O}^\ominus)_2\text{O}^\oplus\text{H}_2, \text{H}^\oplus, \text{H}^\ominus$	65, 79, 90, 94, 109	235.5	38.8	
123	$\text{C}^\ominus(\equiv\text{O}^\oplus\text{H})\text{O}^\ominus, \text{O}^\ominus\text{H}, 2\text{H}^\oplus$	64, 80, 85, 91, 97	158.2		68.7
124	$\text{C}^\oplus(\equiv\text{O}^\oplus\text{H})\text{O}^\ominus, \text{O}^\ominus\text{H}, \text{H}^\oplus, \text{H}^\ominus$	66, 69, 81, 86, 92, 97, 111	481.6	118.1	
125	$\text{C}^\ominus\equiv\text{O}^\oplus, 2\text{O}^\ominus\text{H}, 2\text{H}^\oplus$	68, 87, 101	48.6		22.0
126	$\text{C}^\oplus\equiv\text{O}^\oplus, 2\text{O}^\ominus\text{H}, \text{H}^\oplus, \text{H}^\ominus$	70, 88, 101, 115	143.5	19.3	
127	$\text{C}^\ominus(\text{O}^\ominus)_3, 4\text{H}^\oplus$	89, 105	15.6		8.7
128	$\text{C}^\oplus(\text{O}^\ominus)_3, 3\text{H}^\oplus, \text{H}^\ominus$	71, 90, 105, 119	102.6	11.1	