Electronic Supplementary Information

Photoelectron spectroscopy of solvated dicarboxylate and alkali metal ion clusters, $M^+[O_2C(CH_2)_2CO_2]^{2-}$ $[H_2O]_n$ (M = Na, K, n = 1-6)

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Contents

0

1

0A, 0.0   0B, +0.6 (+0.4,+0.1)   0C, +26.2 (+25.4,+24.8)

1A, 0.0   1B, +1.1 (+1.2,+1.1)   1C, +2.0 (+1.6,+1.5)   1D, +5.6 (+4.6,+4.2)

1E, +8.1   1F, +29.9   1G, +30.8

Figure S1. B3LYP/6-31++G(d, p) optimized structures of Na$^+$(DC$_2$$^{2-}$)(H$_2$O)$_n$ (n = 0-1). Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. Na in green, C in light blue, H in gray, O of DC$_2$$^{2-}$ in red and O of H$_2$O in purple are used for all the structures.

[1A+W2]
2A, 0.0

[1B+W2]
2B, +4.0 (+3.4,+3.5)

(1B+W2)
2C+4.0(+3.2,+3.2)

[1D+W2]
2D, +5.7 (+5.2,+5.2)

2E, +7.4

2F, +7.5

2G, +32.0

2H, +33.8

2I, +35.1

2J, +35.9

2K, +39.8
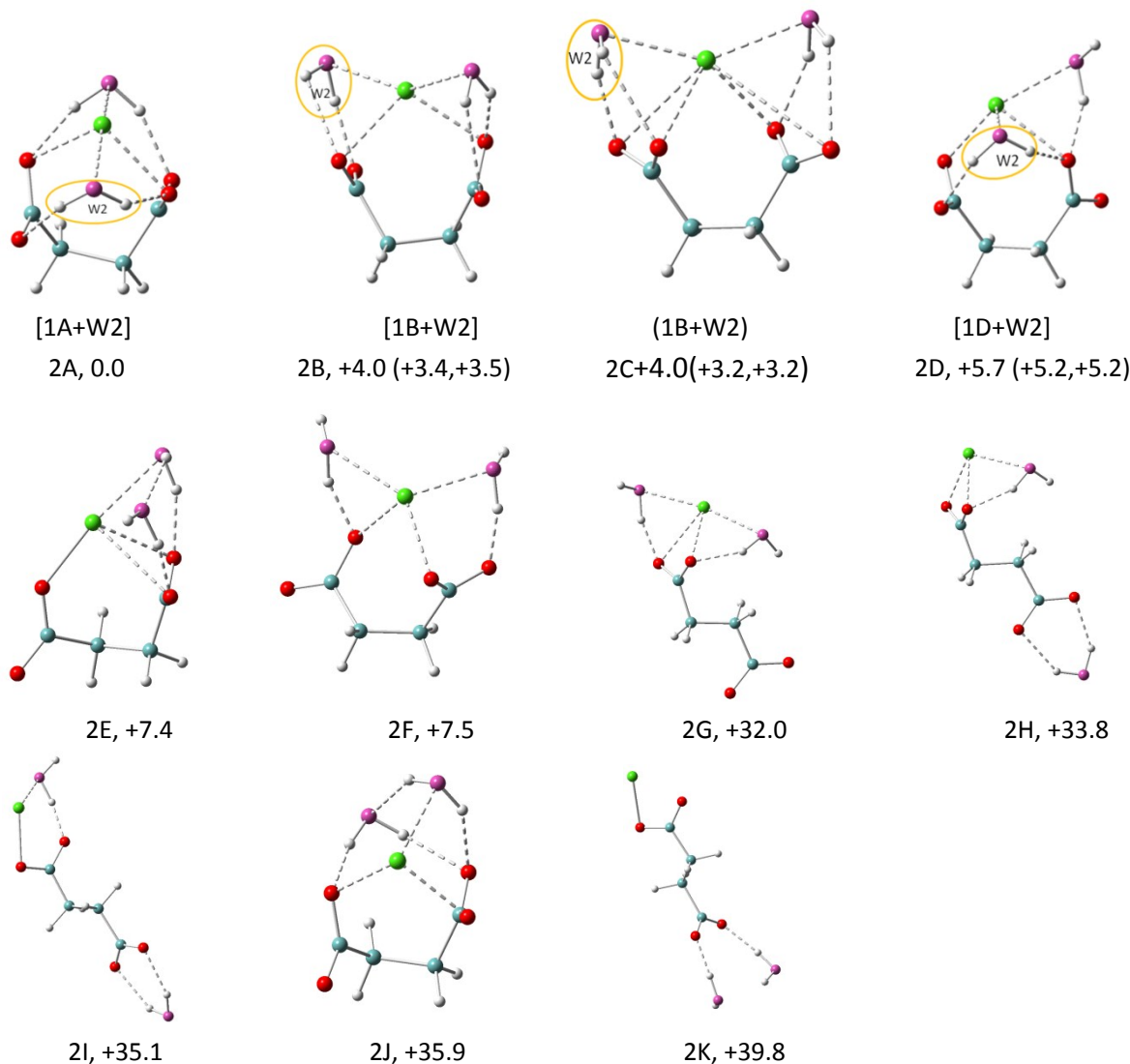
Figure S2. B3LYP/6-31++G(d, p) optimized structures of $Na^+(DC_2^{2-})(H_2O)_2$. Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. The growth pattern of solvated clusters with n waters from the (n-1) clusters is noted in brackets with the *n*-th water circled. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures.

3

[2A+W3]

3A, 0.0

[2A+W3]

3B, +0.2 (+0.1,+0.1)

3C, +1.3 (+0.9,+0.8)

3D, +2.6 (+1.9,+1.8)

3E, +4.9 (+3.4, +3.4)

3F, +9.9

3G, +13.1

3H, +14.3

3I, +33.2

3J, +35.5

3K, +39.2
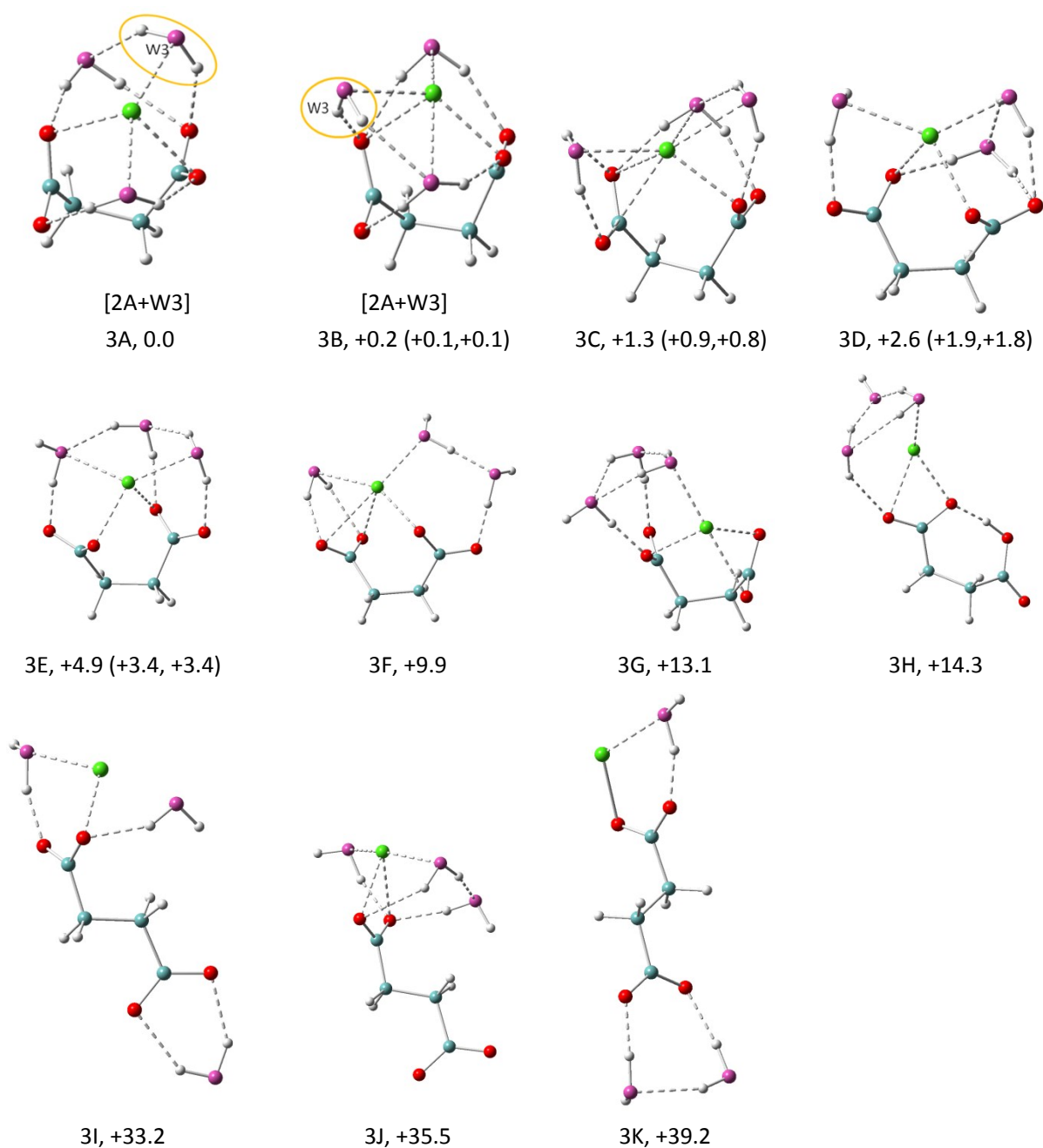
Figure S3. B3LYP/6-31++G(d, p) optimized structures of $Na^+(DC_2^{2-})(H_2O)_3$. Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. The growth pattern of solvated clusters with n waters from the (n-1) clusters is noted in brackets with the *n*-th water circled. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures.

4
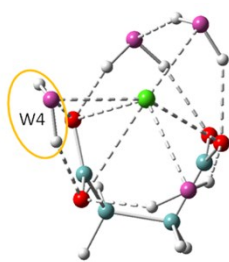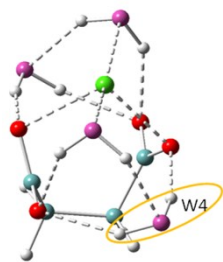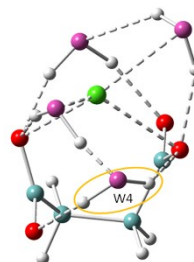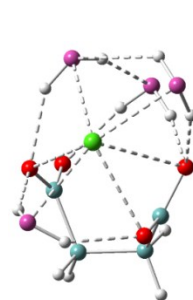
[3A+W4]   [3A+W4]   [3C+W4]
4A,0.0   4B, +0.1 (+0.2,+0.3)   4C, +0.4 (+0.0,+0.0)   4D, +1.5 (+1.7, +1.7)
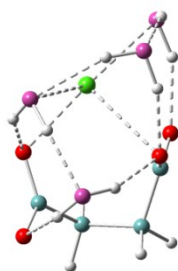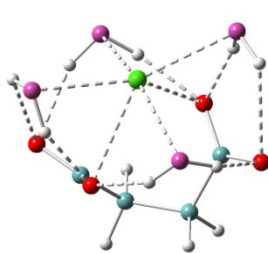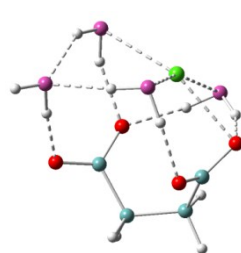
4E, +2.5 (+3.0, +3.1)   4F, +2.6 (+1.3, +1.2)   4G, +4.3 (+3.3, +3.4)   4H, +5.4 (+4.6, +4.6)
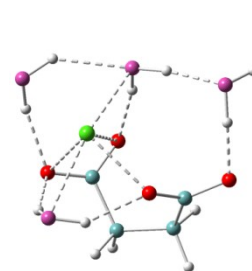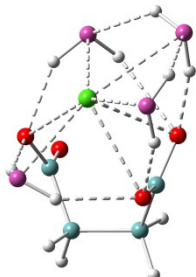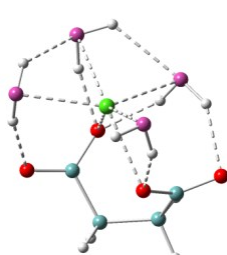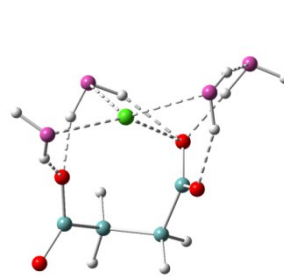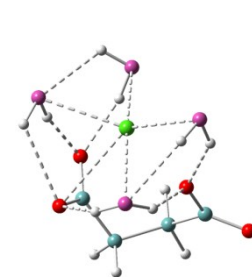
4I, +6.0 (+5.5, +5.5)   4J, +6.1   4K, +9.4   4L, +9.9
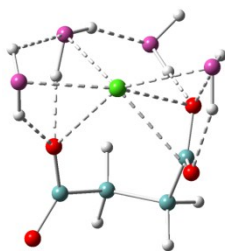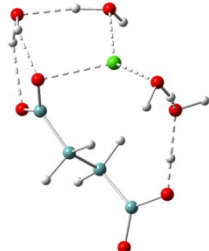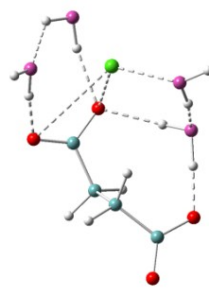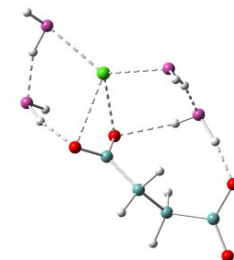
4M, +10.3   4N, +21.6   4O, +22.8   4P, +25.5
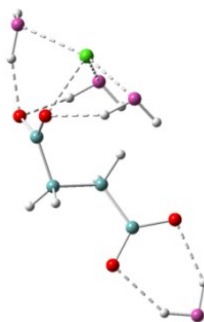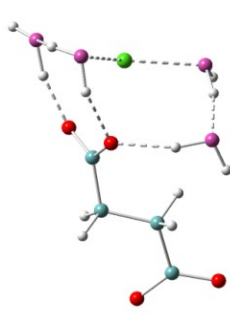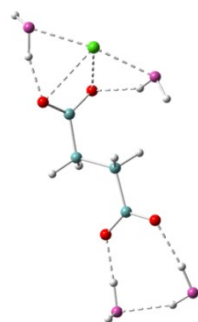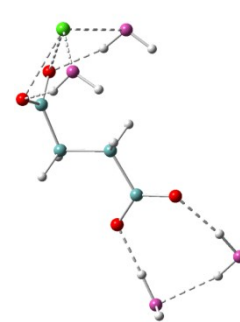
4Q, +32.4   4R, +36.7   4S, +36.9   4T, +37.7

Figure S4. B3LYP/6-31++G(d, p) optimized structures of $Na^+(DC_2^{2-})(H_2O)_4$. Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. The growth pattern of solvated clusters with n waters from the (n-1) clusters is noted in brackets with the *n*-th water circled. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures.

5

[4B+W5]
5A, 0.0

[4C+W5]
5B, +1.6 (+1.7,+1.6)

5C, +3.0 (+2.7,+2.6)

5D, +3.3 (+2.6, +2.6)

5E, +3.9 (+2.8, +2.7)

5F, +4.0 (+3.3, +3.3)

5G, +4.8 (+2.2, +1.8)

5H, +6.4

5I, +6.6

5J, +9.3

5K, +10.4

5L, +12.2

5M, +32.3
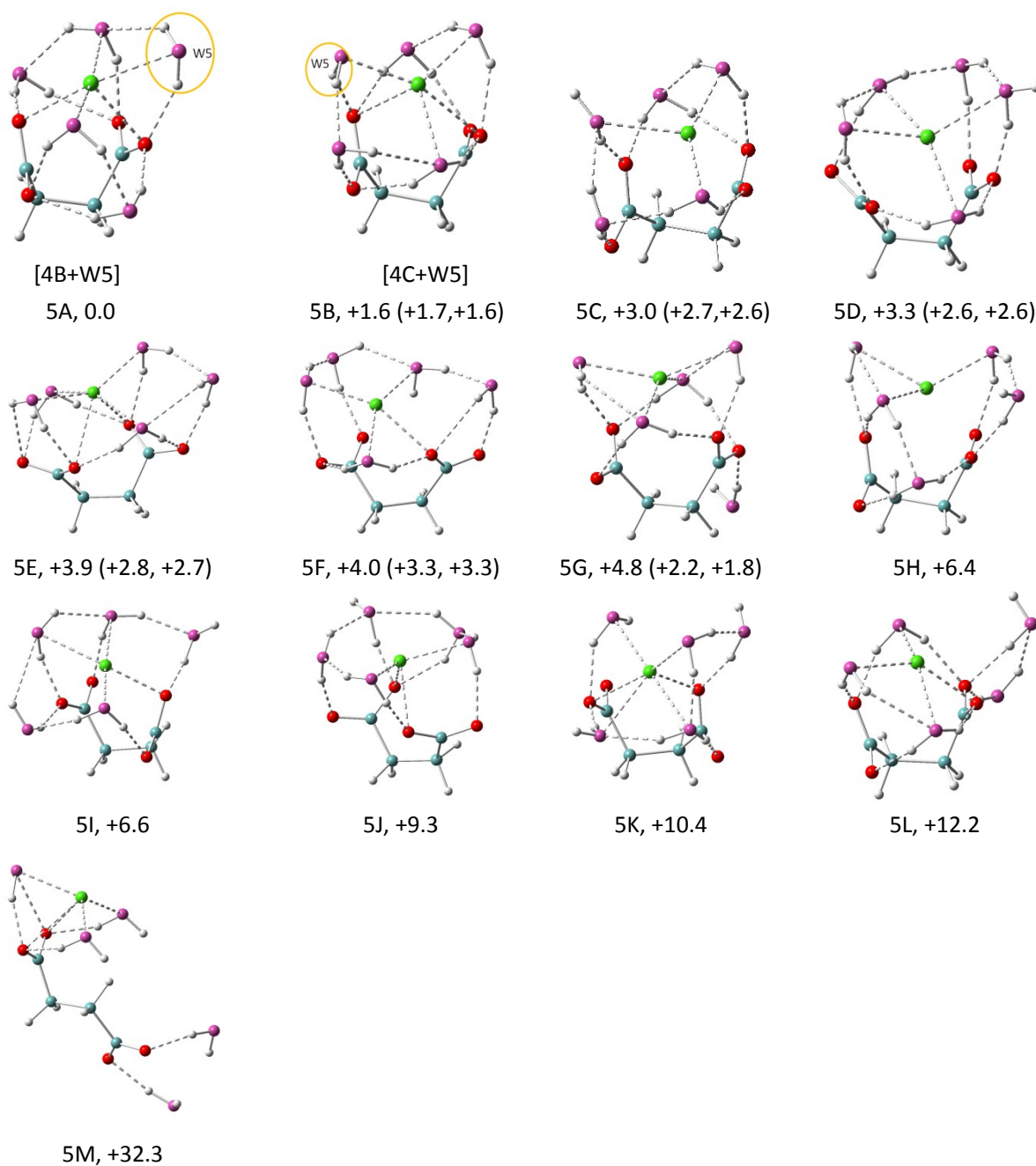
Figure S5. B3LYP/6-31++G(d, p) optimized structures of $Na^+(DC_2^{2-})(H_2O)_5$. Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. The growth pattern of solvated clusters with n waters from the (n-1) clusters is noted in brackets with the *n*-th water circled. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures.

6

[5A+W6]

6A, 0.0   6B+1.9 (0.0,0.0)   6C, +2.7 (+2.2,+2.2)   6D, +5.1 (+4.8,+4.6)

6E, +6.3   6F, +6.3   6G, +7.0   6H, +7.7

6I, +7.8   6J, +8.4   6K, +8.6   6L, +8.8

6M, +8.8   6N, +9.3   6O, +9.7   6P, +10.7

Figure S6. B3LYP/6-31++G(d, p) optimized structures of $Na^+(DC_2^{2-})(H_2O)_6$. Relative energies (kcal/mol) including zero-point energy and free energy correction (at 100 K) (first and second numbers in parenthesis, respectively) are shown. The lowest isomers in the energy range of 0-6 kcal/mol are real minima based on frequency calculations. The growth pattern of solvated clusters with n waters from the (n-1) clusters is noted in brackets with the *n*-th water circled. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures.

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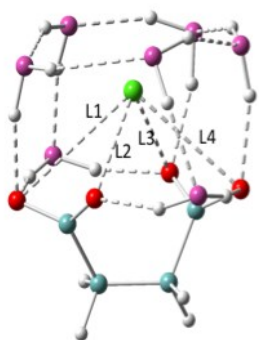
7A, +0.0
L1=3.30, L2=2.49
L3=2.45, L4=3.01
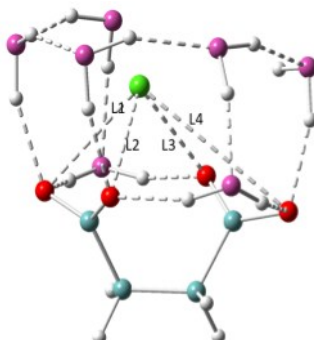
7B, +0.6 (+0.4)
L1=2.74, L2=2.59
L3=2.39, L4=3.81
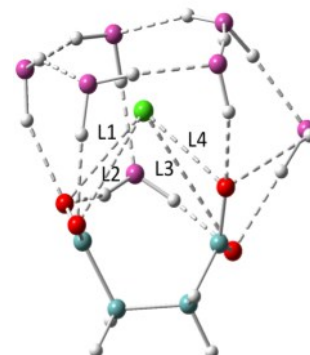
7C, +2.3 (+1.6)
L1=2.45, L2=3.30
L3=3.50, L4=2.38
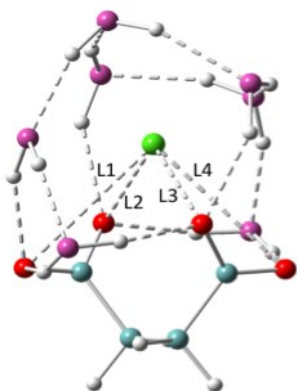
7D, +3.4 (+3.6)
L1=3.29, L2=2.30
L3=2.36, L4=3.35
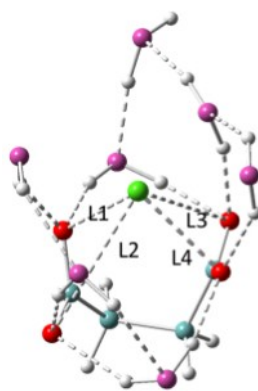
7E, +4.8 (+3.5)
L1=2.48, L2=3.51
L3=3.38, L4=2.46
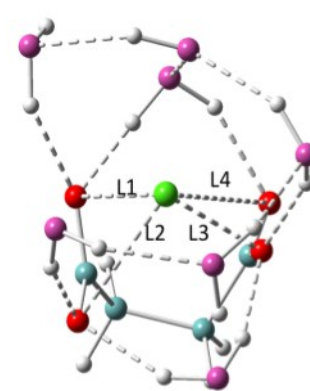
7F, +5.5 (+5.1)
L1=2.46, L2=2.76
L3=2.40, L4=4.00
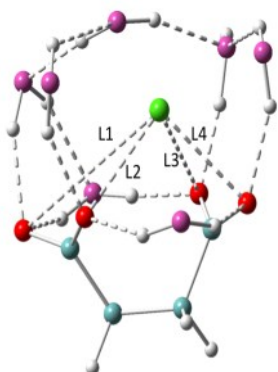
7G, +7.1 (+5.7)
L1=4.23, L2=2.48
L3=3.36, L4=2.62
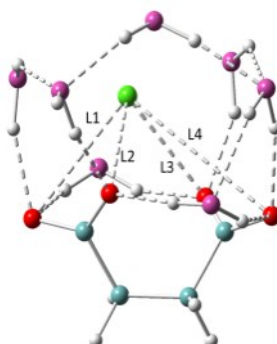
7H, +7.4 (+5.6)
L1=3.15, L2=2.67
L3=2.65, L4=4.03
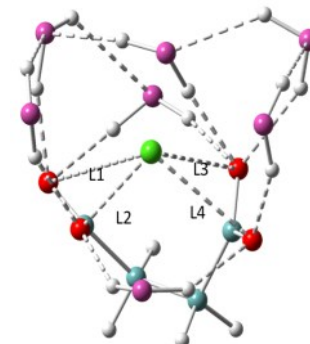
7I, +7.6 (+6.3)
L1=4.25, L2=2.58
L3=3.30, L4=2.68

n=7
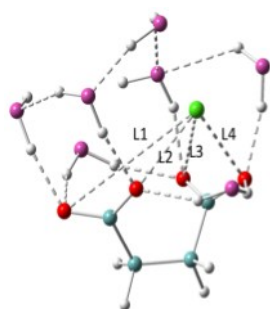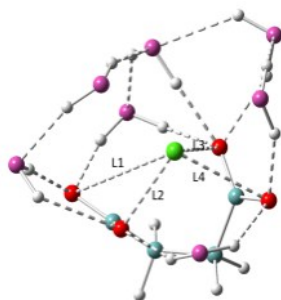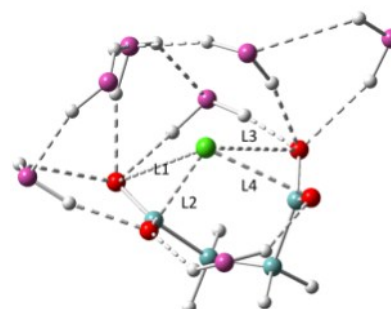
7J, +9.0 (+6.9)	7K, +9.4 (+8.4)	7L, +13.0 (+10.7)
L1=4.37, L2=2.50	L1=3.92, L2=2.45	L1=3.85, L2=2.47
L3=3.37, L4=2.44	L3=2.91, L4=2.76	L3=3.38, L4=2.48

Figure S7. Typical low-lying isomers of Na^+-$DC_2^{2-}(H_2O)_7$ clusters. L1, L2 indicate the distances between Na^+ and O atoms of the first carboxylate, L3, L4 indicate the distances between Na^+ and O atoms of the second one. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures. The bond distances are in angstrom and the energies are in kcal/mol. The relative energies in the parentheses include the zero-point correction.

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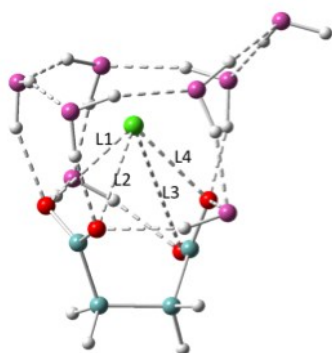
8A, +0.0
L1=2.56, L2=2.71
L3=4.00, L4=2.41
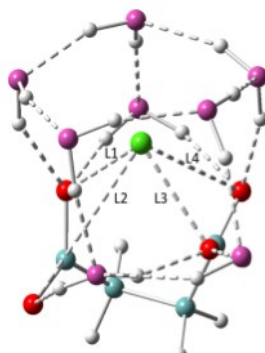
8B, +0.3 (+1.1)
L1=2.40, L2=2.83
L3=2.39, L4=3.02
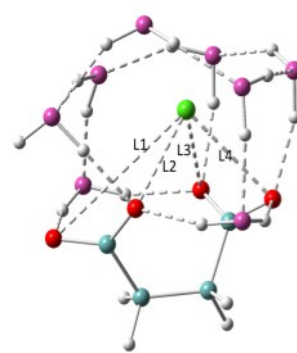
8C, +0.4 (+0.5)
L1=4.02, L2=2.46
L3=2.66, L4=2.74
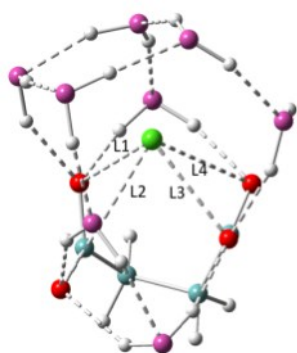
8D, +0.7 (+0.5)
L1=2.38, L2=3.58
L3=2.51, L4=3.17
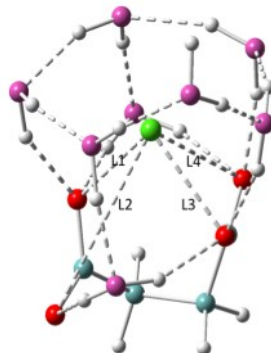
8E, +1.1 (+0.9)
L1=2.44, L2=4.01
L3=2.45, L4=2.82
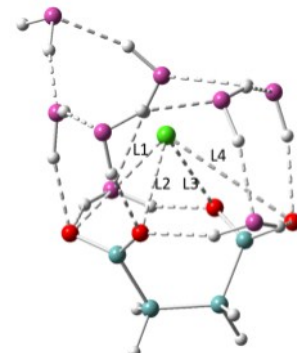
8F, +1.5 (+0.7)
L1=3.01, L2=2.51
L3=2.47, L4=3.37
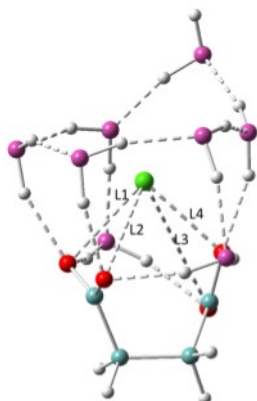
8G, +1.9 (+1.6)
L1=2.52, L2=2.80
L3=3.93, L4=2.38
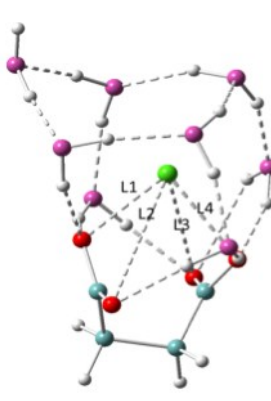
8H, +3.7 (+2.7)
L1=2.38, L2=3.82
L3=3.35, L4=2.46
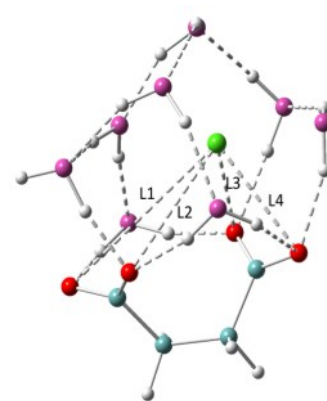
8I, +5.1 (+3.6)
L1=4.48, L2=3.39
L3=2.42, L4=2.89
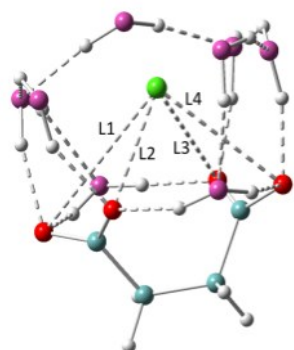
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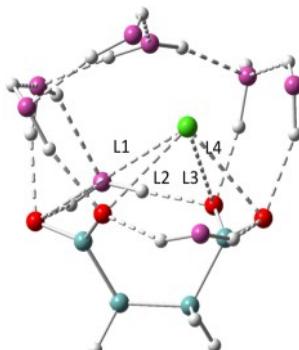
8K, +6.2 (+4.7)
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L3=3.48, L4=2.63
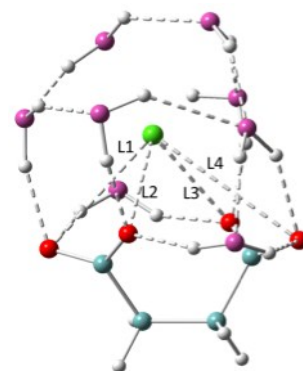
8L, +7.2 (+5.7)
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L3=2.56, L4=3.75
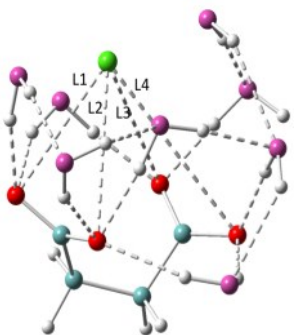
8M, +10.6 (+8.7)
L1=3.29, L2=3.66
L3=3.59, L4=4.61
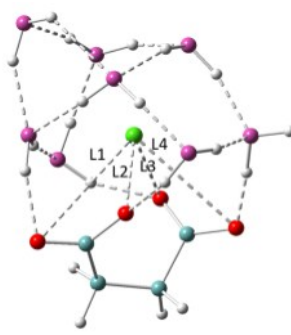
8N, +12.3 (+10.8)
L1=3.78, L2=2.34
L3=2.31, L4=3.41

Figure S8. Typical low-lying isomers of $Na^+\text{-}DC_2^{2-}(H_2O)_8$ clusters. L1, L2 indicate the distances between Na^+ and O atoms of the first carboxylate, L3, L4 indicate the distances between Na^+ and O atoms of the second one. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures. The relative energies in the parentheses include the zero-point correction. The isomers in bold are solvent separated ion pair (SSIP). The bond distances are in angstrom and the energies are in kcal/mol.

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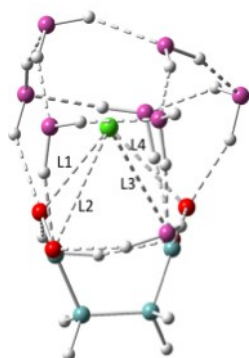
9A, +0.0 kcal/mol
L1=2.42, L2=3.32
L3=3.46, L4=2.45
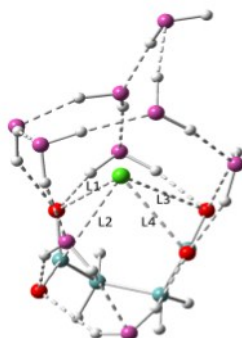
9B, +3.2 (+3.1)
L1=2.46, L2=3.63
L3=3.19, L4=2.54
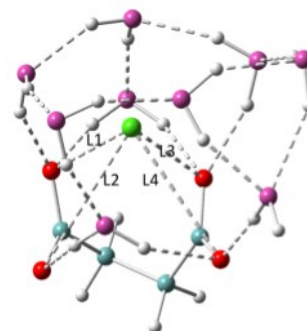
9C, +4.4 (+3.7)
L1=2.54, L2=3.64
L3=2.42, L4=3.35
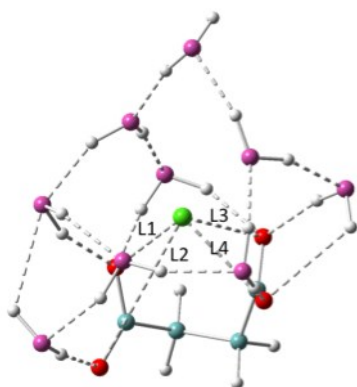
9D, +5.8 (+5.1)
L1=2.46, L2=4.10
L3=2.67, L4=2.58
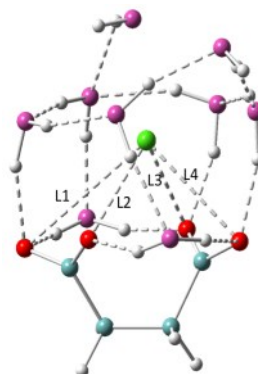
9E, +6.0 (+4.9)
L1=3.60, L2=4.55
L3=2.55, L4=2.95
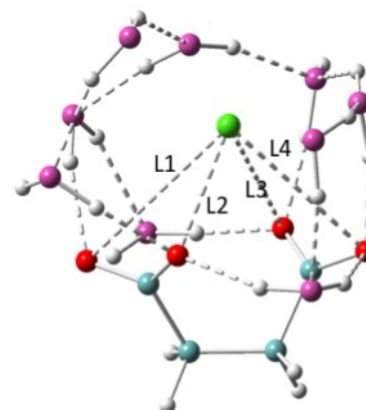
9F, +7.1 (+6.2)
L1=3.96, L2=2.44
L3=3.81, L4=3.61
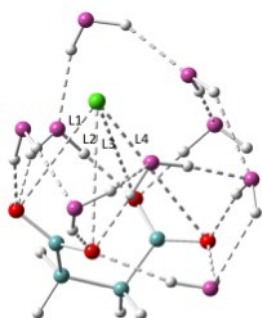
9G, +9.45 (+7.9)
L1=3.34, L2=3.73
L3=4.02, L4=4.87
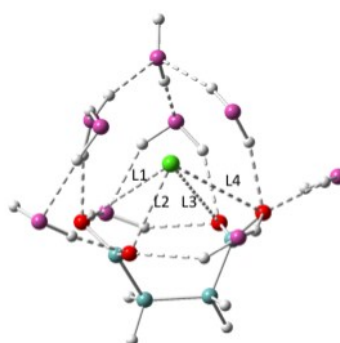
9H, +9.9 (+8.6)
L1=3.51, L2=2.47
L3=4.69, L4=3.41
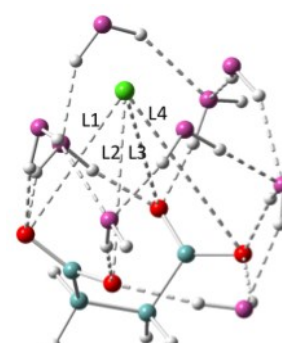
9I, +11.1 (+9.0)
L1=3.74, L2=4.23
L3=3.86, L4=4.71
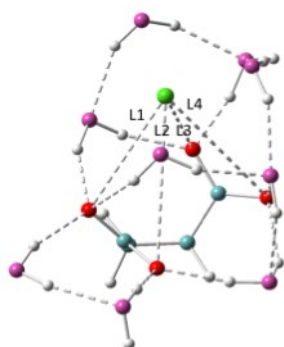
9J, +16.9 (+14.1)
L1=3.45, L2=4.38
L3=2.57, L4=4.04
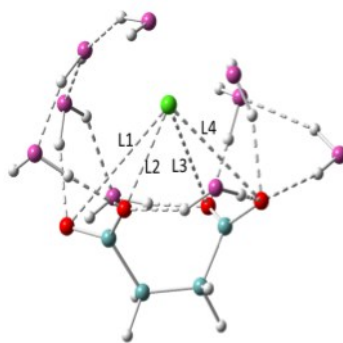
9K, +17.1 (+14.8)
L1=4.12, L2=2.50
L3=3.96, L4=3.43

Figure S9. Typical low-lying isomers of Na^+-$DC_2{}^{2-}(H_2O)_9$ clusters. L1, L2 indicate the distances between Na^+ and O atoms of the first carboxylate, L3, L4 indicate the distances between Na^+ and O atoms of the second one. Na in green, C in light blue, H in gray, O of $DC_2{}^{2-}$ in red and O of H_2O in purple are used for all the structures. The relative energies in the parentheses include the zero-point correction. The isomers in bold are solvent separated ion pair (SSIP). The bond distances are in angstrom and the energies are in kcal/mol.

n=10
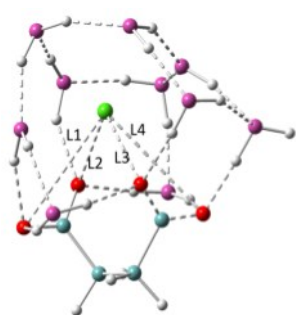
10A, +0.0
L1=3.63, L2=2.44
L3=2.46, L4=3.65
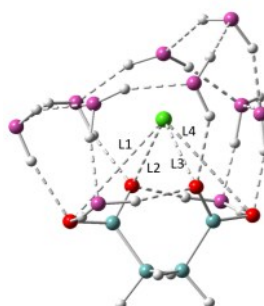
10B, +0.1(+0.5)
L1=3.60, L2=2.44
L3=2.42, L4=3.40
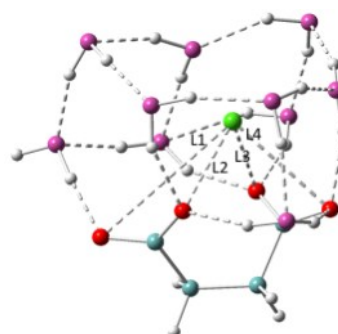
10C, +1.0 (+0.8)
L1=3.99, L2=2.44
L3=2.50, L4=3.00
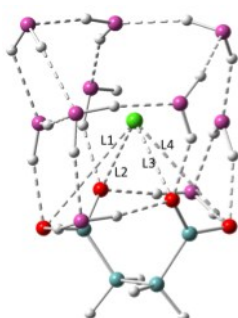
10D, +2.4 (+2.2)
L1=3.55, L2=2.54
L3=2.48, L4=3.61
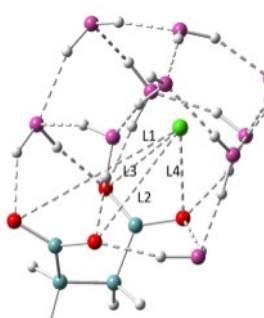
10E, +3.2 (+3.1)
L1=5.03, L2=3.93
L3=2.96, L4=2.45
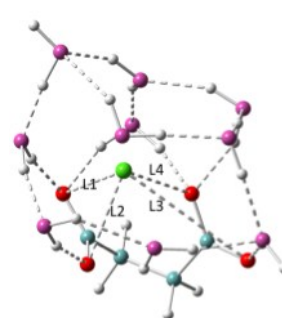
10F, +5.1 (+3.6)
L1=2.68, L2=2.70
L3=4.12, L4=2.47
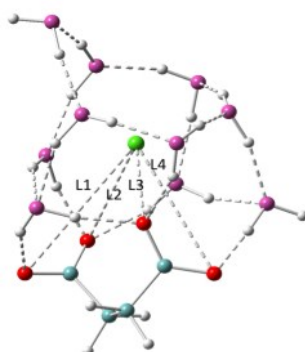
10G, +6.0 (+4.5)
L1=4.48, L2=3.45
L3=2.47, L4=4.07
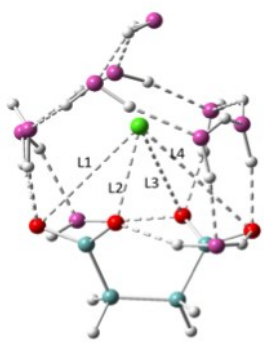
10H, +7.1 (+6.1)
L1=3.61, L2=2.38
L3=3.80, L4=3.87
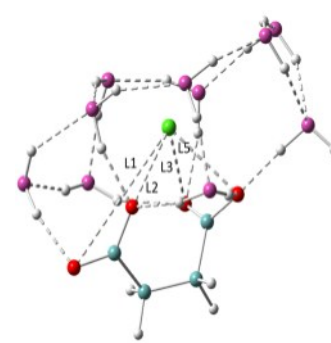
10I, +8.3 (+7.2)
L1=4.49, L2=2.44
L3=2.59, L4=2.57

n=10
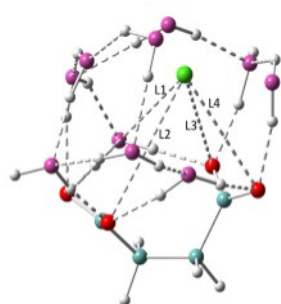
10J, +9.4 (+7.4)
L1=4.97, L2=4.12
L3=4.18, L4=3.71
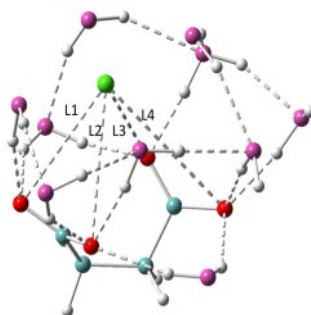
10K, +10.8 (+9.1)
L1=3.43, L2=3.65
L3=2.68, L4=4.28
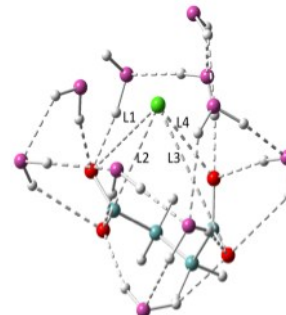
10L, +11.9 (+10.4)
L1=3.61, L2=3.59
L3=4.21, L4=2.58
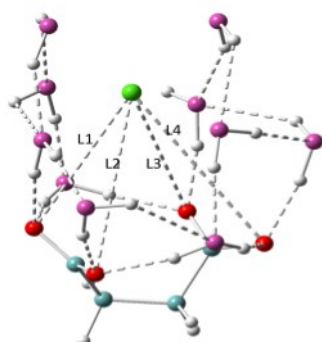
10M, +13.3 (+11.1)
L1=3.92, L2=4.55
L3=3.84, L4=4.69
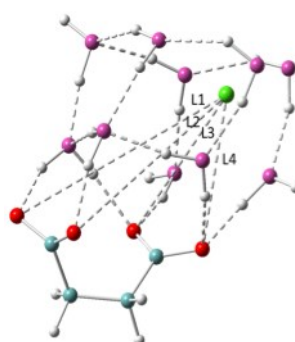
10N, +22.9 (+19.6)
L1=6.33, L2=5.72
L3=4.34, L4=3.81

Figure S10. Typical low-lying isomers of Na^+-$DC_2^{2-}$$(H_2O)_{10}$ clusters. L1, L2 indicate the distances between Na^+ and O atoms of the first carboxylate, L3, L4 indicate the distances between Na^+ and O atoms of the second one. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures. The relative energies in the parentheses include the zero-point correction. The isomers in bold are solvent separated ion pair (SSIP). The bond distances are in angstrom and the energies are in kcal/mol.
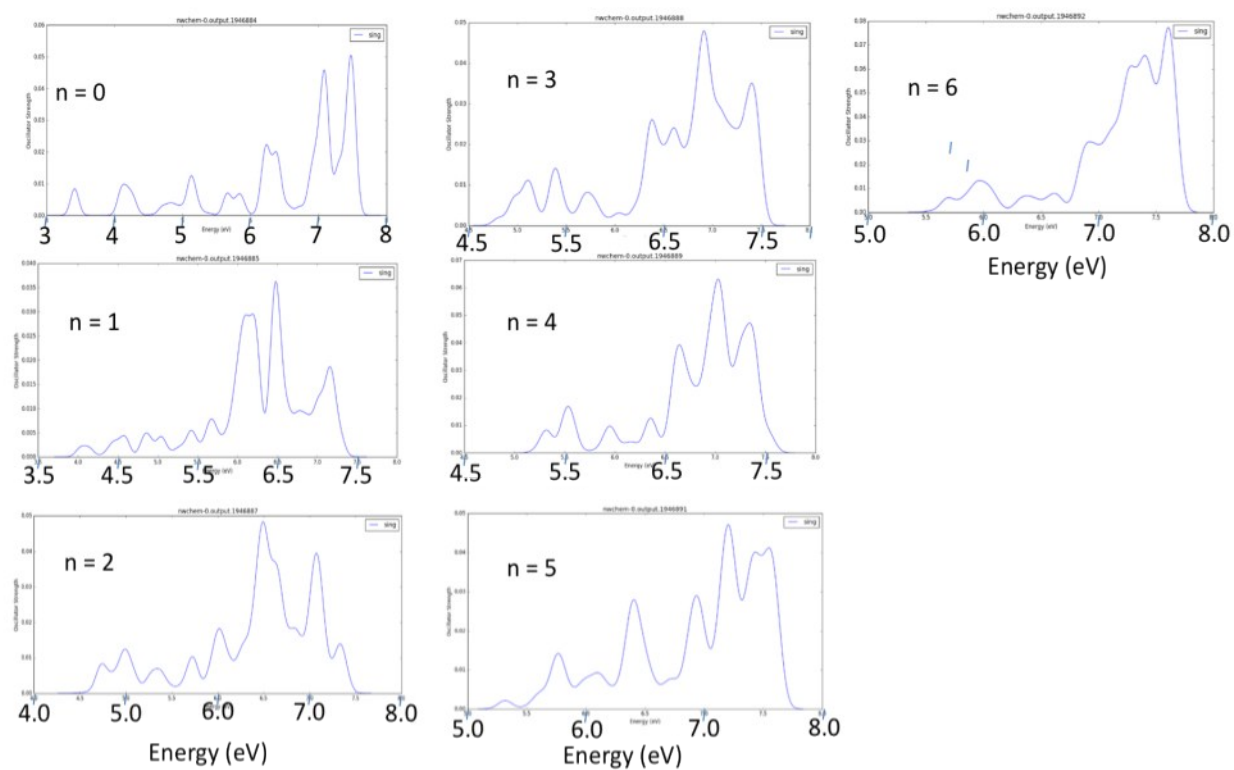
Figure S11. Excitation Curves of $Na^+\text{-}(DC_2)^{2-}(H_2O)_n$ (n = 0-6) with TD-B3LYP method
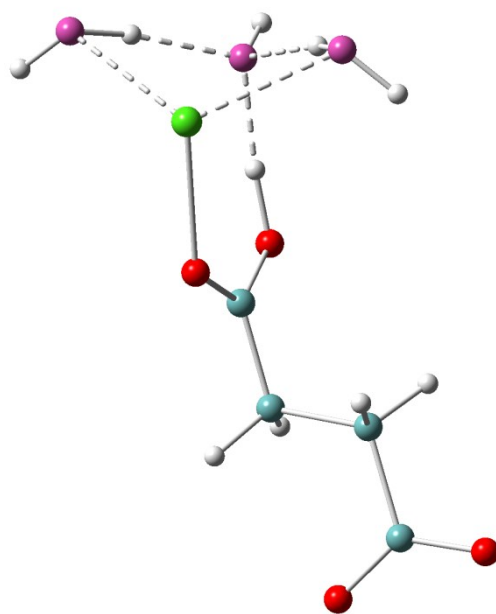
3A′

Figure S12. Structure of $Na^+(HDC_2)^-(OH)^-(H_2O)_2$. Na in green, C in light blue, H in gray, O of DC_2^{2-} in red and O of H_2O in purple are used for all the structures. The structure is real minima based on the frequency calculation.

Table S1. Relative energies of the low energy isomers of Na^+-$(DC_2^{2-})(H_2O)_n$ (n = 0-6) with the zero-point energy (ZPE) and free energy (at 100 K and 50K) correction.

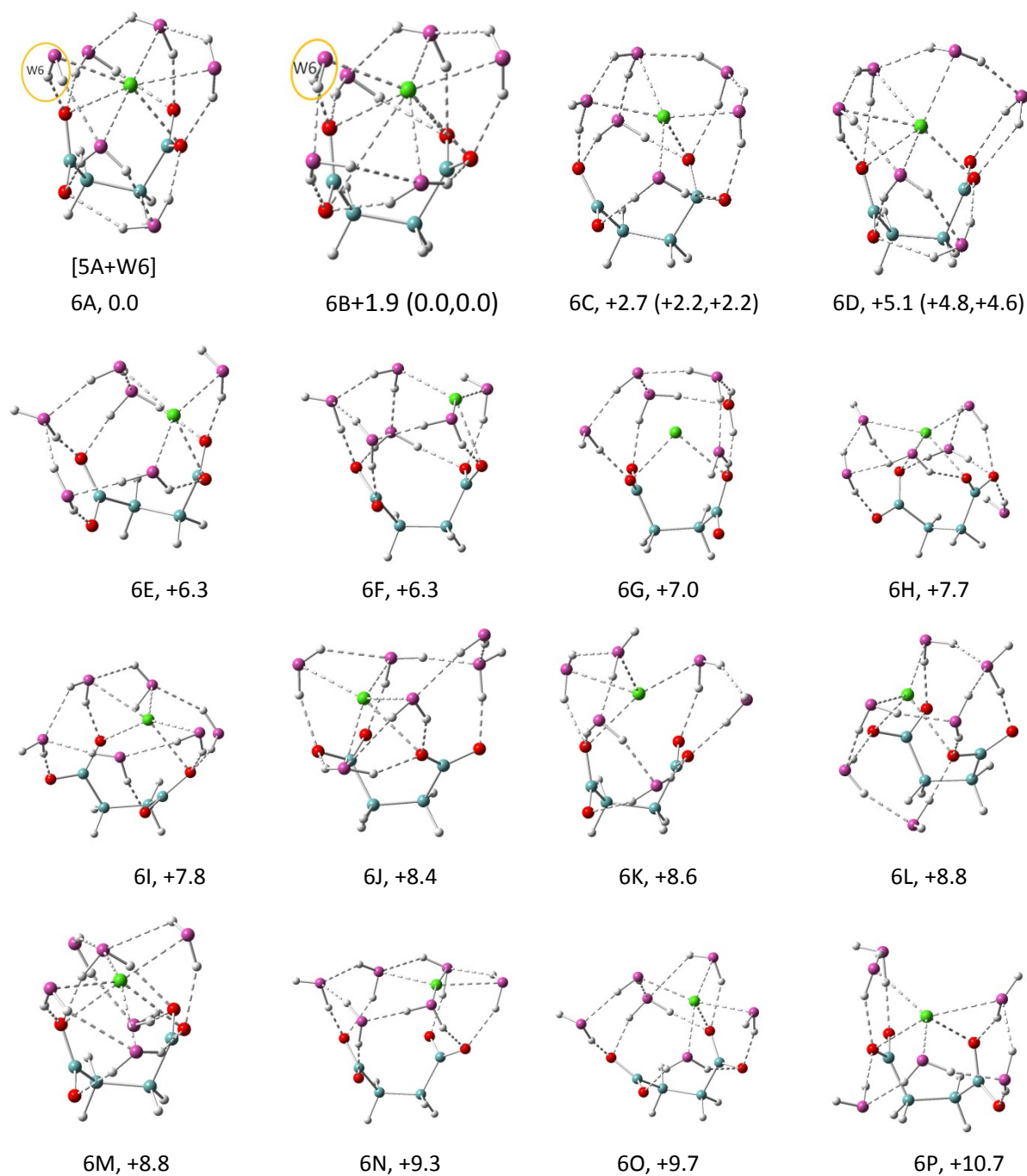| Name	ZPE Correction (kcal/mol)	Free Energy Correction (kcal/mol)		ΔE* (kcal/mol)	ΔE* With ZPE (kcal/mol)	ΔE* With Free Energy (kcal/mol)	
		100K	50K			100K	50K
0A	51.6	46.1	49.2	0.0	0.0	0.0	0.0
0B	51.3	45.6	48.8	0.6	0.4	0.1	0.2
0C	50.3	44.7	47.9	26.2	25.0	24.8	24.9
1A	67.8	62.1	65.3	0.0	0.0	0.0	0.0
1B	67.9	62.1	65.4	1.1	1.2	1.1	1.1
1C	67.4	61.6	64.9	2.0	1.6	1.5	1.6
1D	66.8	60.7	64.2	5.6	4.6	4.2	4.5
2A	84.4	78.4	81.9	0.0	0.0	0.0	0.0
2B	83.8	77.9	81.3	4.0	3.4	3.5	3.5
2C	83.6	77.6	81.0	4.0	3.2	3.2	3.2
2D	83.9	77.9	81.3	5.7	5.2	5.2	5.2
3A	101.3	95.3	98.7	0.0	0.0	0.0	0.0
3B	101.2	95.2	98.6	0.2	0.1	0.1	0.1
3C	100.8	94.8	98.3	1.3	0.9	0.8	0.8
3D	100.5	94.5	98.0	2.6	1.9	1.8	1.9
3E	99.8	93.8	97.2	4.9	3.4	3.4	3.4
4A	117.6	111.4	115.0	0.0	0.0	0.0	0.0
4B	117.7	111.7	115.2	0.1	0.2	0.3	0.3
4C	117.2	111.0	114.6	0.4	0.0	0.0	0.0
4D	117.8	111.7	115.2	1.5	1.7	1.7	1.7
4E	118.1	112.0	115.5	2.5	3.0	3.1	3.0
4F	116.3	110.1	113.6	2.6	1.3	1.2	1.2
4G	116.6	110.5	114.0	4.3	3.3	3.4	3.3
4H	116.8	110.6	114.2	5.4	4.6	4.6	4.6
4I	117.1	110.9	114.5	6.0	5.5	5.5	5.5
5A	134.0	127.7	131.3	0.0	0.0	0.0	0.0
5B	134.1	127.7	131.4	1.6	1.7	1.6	1.7
5C	133.6	127.3	130.9	3.0	2.7	2.6	2.6
5D	133.3	127.0	130.7	3.3	2.6	2.6	2.6
5E	132.9	126.5	130.2	3.9	2.8	2.7	2.8
5F	133.3	127.0	130.7	4.0	3.3	3.3	3.3
5G	131.4	124.7	128.6	4.8	2.2	1.8	2.1
6A	150.1	143.7	147.4	0.0	0.0	0.0	0.0
6B	143.7	150.2	147.5	1.9	0.0	0.0	0.0
6C	149.7	143.2	147.0	2.7	2.2	2.2	2.2

| 6D | 149.8 | 143.2 | 147.0 | 5.1 | 4.7 | 4.6 | 4.7 |

Table S2. The Cartesian atomic coordinates of the typical low-lying isomers of Na^+-DC_2^{2-} using B3LYP exchange-correlation functional with dispersion correction.

0A

C	-0.82649805	-0.67127215	0.49759645
C	0.00974340	-0.85453519	-0.80637983
C	-0.33894750	0.16300908	-1.93579525
O	-0.82448919	-0.27018786	-2.99598266
C	0.00827426	-0.78181858	1.81017407
O	-0.23636121	-1.71775176	2.59228997
O	0.89432396	0.14141757	1.97017833
O	-0.07370876	1.39430297	-1.65910984
H	-1.29105807	0.32789356	0.48139543
H	-1.63980398	-1.40077752	0.52405790
H	1.07673211	-0.72778909	-0.56173781
H	-0.11161714	-1.87196780	-1.18663285
Na	0.80539063	1.50628949	0.30495512

0B

C	-0.92354306	-1.27744170	0.30627338
H	-1.82893913	-0.67618700	0.16442615
H	-1.20457068	-2.30857596	0.55248557
C	-0.15360911	-1.29300917	-1.04400997
H	0.78146926	-1.85208489	-0.93538450
H	-0.78866275	-1.78792711	-1.79180226
C	-0.10486570	-0.71462495	1.50349922
O	0.54039996	-1.52868373	2.19375042
O	-0.17031311	0.55715404	1.69209981
C	0.14568470	0.13854205	-1.51082658
O	-0.85260541	0.89100727	-1.75044139
O	1.35040503	0.54105241	-1.46785648
Na	0.24617505	1.92718918	0.11236370

0C

C	-0.02749897	0.18077837	1.17788030
H	0.01637450	1.27101105	1.05317915
H	-1.09039478	-0.08927093	1.23691609
C	0.62175875	-0.51162534	-0.03850235
H	1.67516552	-0.22404327	-0.08726868
H	0.55919952	-1.59442038	0.09750259
C	0.63058814	-0.16843647	2.55877532
O	0.09152882	0.40780505	3.54381620
O	1.60459637	-0.96781065	2.54568730
C	-0.08286017	-0.10984902	-1.31685939
O	-1.09454052	-0.79389508	-1.71419426
O	0.31718057	0.93415563	-1.94881927
Na	-1.42296313	0.72144376	-3.25715623

Table S3. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)$ using B3LYP exchange-correlation functional with dispersion correction.

1A

C	-1.21733302	-1.48107418	0.40941240
C	-0.60890806	-1.54969048	-1.01927969
C	-0.32373600	-0.13459784	-1.55559077
O	-1.30041093	0.66059307	-1.66999574
C	-0.32259010	-0.65072010	1.35681637
O	0.79938147	-1.13404484	1.67154680
O	-0.74428188	0.50972030	1.67594044
O	0.89693098	0.20065172	-1.71444797
H	-2.20802166	-1.02086668	0.35487675
H	-1.30340309	-2.50396532	0.79960579
H	0.32427575	-2.11956413	-0.99215184
H	-1.32683865	-2.05199081	-1.68202736
Na	0.11842112	1.76831504	0.05928048
O	2.30241079	0.95293680	0.56417100
H	2.12700274	0.52938982	-0.30278084
H	1.94585331	0.28208085	1.19373809

1B

C	-0.92973471	-1.53108917	0.31457919
C	-0.40733813	-1.58061355	-1.14571830
C	-0.63735261	-0.26029194	-1.93243388
O	-1.67097680	-0.17318269	-2.62388547
C	-0.10193277	-0.58110316	1.18360338
O	-0.65446717	0.47623722	1.62379781
O	1.13815040	-0.85081646	1.32322416
O	0.27021427	0.64024792	-1.80043680
H	-1.97878041	-1.21880467	0.32770662
H	-0.84931196	-2.53969158	0.74276788
H	0.66335662	-1.81294478	-1.11221292
H	-0.93792970	-2.38276728	-1.67173454
Na	1.07273063	1.35216838	0.02987343
O	1.81107461	1.59809856	2.30367160
H	1.91299950	0.62653589	2.14124774
H	0.84029962	1.58383426	2.44130757

1C

C	0.53346905	-1.90341485	-0.68724618
H	0.05515612	-1.90479522	-1.67164111
H	1.09814918	-2.83521743	-0.54907940
C	-0.55134330	-1.82240282	0.42171986
H	-0.05162899	-1.87323106	1.39425667
H	-1.23190208	-2.67549827	0.30857627
C	1.48460316	-0.70134430	-0.57572907
O	1.37538965	0.21488277	-1.45062468
O	2.20295316	-0.61795642	0.46781998
C	-1.38632501	-0.52647102	0.33959217
O	-1.00801605	0.43067250	1.12663453
O	-2.33159305	-0.46299765	-0.46645638
Na	0.90699565	1.46854453	0.47517522
O	-1.07329754	2.85575910	0.25104891
H	-1.39713173	2.83009789	-0.65811281
H	-1.32721066	1.94428536	0.61705618

1D

C	-1.01713909	-0.91890760	0.23024784
C	-0.28068959	-1.19922648	-1.10908403
C	-0.65314869	-0.21517291	-2.25930672
O	-1.15626606	-0.68103900	-3.29815129
C	-0.13532356	-1.00777910	1.50172084
O	-0.52164470	-1.67354757	2.47194611
O	0.95850673	-0.31023006	1.44083787
O	-0.37865186	1.01967842	-2.02226765
H	-1.41679364	0.10824096	0.20188787
H	-1.87675630	-1.58411743	0.34609351
H	0.80166855	-1.10772756	-0.93398580
H	-0.47269579	-2.22530681	-1.43522850
Na	0.70064240	1.25366183	-0.16212710
O	1.44025603	2.15054942	1.96979808
H	1.29083761	1.15906475	2.06133004
H	2.24619495	2.35751046	2.45355071

1E

C	-1.06387723	-0.57216975	-0.07397596
C	-0.20467988	-0.75113368	-1.36321939
C	-0.53407790	0.28169238	-2.48557252
O	-1.00324017	-0.13823937	-3.55691637
C	-0.25619212	-0.70191743	1.23981449
O	-0.49644663	-1.64556935	2.01438513
O	0.63021957	0.22299081	1.43118760
O	-0.27132040	1.50731116	-2.18516952
H	-1.51686039	0.43149760	-0.08669383
H	-1.88249622	-1.29569113	-0.06476501
H	0.85897777	-0.63225916	-1.10185941
H	-0.32526302	-1.76457483	-1.75338344
Na	0.60937750	1.61006112	-0.22709212
O	1.54298682	-0.64863890	3.93083295
H	1.41250653	-0.15495039	3.09270955
H	0.88641469	-1.34839014	3.78187736

1F

C	1.14015911	0.33285246	1.17403070
H	1.20534987	-0.76309282	1.18870521
H	1.92687139	0.68915007	0.49561307
C	-0.24405943	0.76847688	0.64785062
H	-1.01012027	0.39839071	1.33441846
H	-0.28624842	1.86052622	0.63010718
C	1.47915652	0.85327681	2.61601793
O	0.59798423	1.54005266	3.19876897
O	2.62113197	0.51087448	3.02773233
C	-0.48080240	0.22171772	-0.73940298
O	-0.97630583	-0.96646414	-0.85700468
O	-0.13958252	0.91177010	-1.75635764
Na	-0.51652417	-0.69711346	-3.18989082
O	-2.57567856	-1.67373312	-2.76396668
H	-2.14285955	-1.44802026	-1.87609519
H	-3.49065960	-1.37724711	-2.71860487

1G

C	-0.26285124	0.45048119	0.20606135
C	-1.77958363	0.35585054	0.53182517
C	1.81838228	-0.60820744	-0.69572953
C	0.34039021	-0.81550368	-0.43305949
H	0.19524817	-1.65869981	0.24709429
H	-0.11787281	1.31250336	-0.45781884
H	0.26252515	0.68056532	1.14217980
H	-0.17930979	-1.02502028	-1.37152938
O	2.65758841	-0.86935094	0.23847290
O	-2.28156710	1.41351574	1.01437562
O	-2.36430799	-0.73867255	0.29788466
O	2.18797660	-0.12591978	-1.82549590
Na	4.22036494	0.01506096	-1.01700221
O	-4.85147292	0.28474357	1.25086705
H	-4.27578793	-0.40988044	0.87302852
H	-4.15729402	0.97518950	1.31903404

Table S4. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_2$ using B3LYP exchange-correlation functional with dispersion correction.

2A

C	-1.07388893	-1.72529799	0.39868518
C	-0.45032831	-1.74245796	-1.02341142
C	-0.33747138	-0.30916964	-1.57160992
O	-1.40416838	0.26273344	-1.92061222
C	-0.19517413	-0.89872140	1.35353656
O	0.90072084	-1.40428863	1.71471408
O	-0.59314308	0.28081305	1.64040766
O	0.81776102	0.23585704	-1.54852842
H	-2.07835990	-1.29449316	0.34157994
H	-1.13258766	-2.75632329	0.76906919
H	0.53975167	-2.20594352	-0.97213927
H	-1.10007633	-2.32839293	-1.68512705
Na	0.69902793	1.58557817	0.28680496
O	2.69587511	0.31302822	0.52069562
H	2.32725993	0.02559888	-0.34093658
H	2.24301087	-0.30018389	1.14799331
O	-1.54727636	2.28961370	-0.05896429
H	-1.61780836	1.59174689	0.62550695
H	-1.59664839	1.76077732	-0.89121325

2B

C	0.27555289	-1.99736930	-0.81864117
H	-0.06230625	-1.82110022	-1.84388000
H	0.75478784	-2.98262611	-0.74897775
C	-0.94439137	-1.97145293	0.13893190
H	-0.60421323	-2.19334665	1.15459215
H	-1.66028232	-2.73580645	-0.18861724
C	1.29042107	-0.91551337	-0.42678562
O	1.38864812	0.10541117	-1.17839599
O	1.88967091	-1.05187654	0.68630844
C	-1.64769473	-0.60074900	0.11751410
O	-1.43685609	0.15950267	1.13839992
O	-2.31943361	-0.28416478	-0.88824704
Na	0.40434057	1.38927635	0.54825092
O	-1.67911801	2.54090328	-0.01619264
H	-1.91725984	2.15378382	-0.87354748
H	-1.87834978	1.75756267	0.56756937
O	2.75807491	1.46215812	0.99949405
H	2.58947452	0.47722220	1.07215711
H	2.85102608	1.52034594	0.03481291

2C

C	-0.77770213	-1.66163667	1.25195166
C	-0.31861400	-2.23138798	-0.09976361
C	-0.36999713	-1.22414473	-1.26749754
O	0.37396340	-1.42643263	-2.25560482
C	-0.02635401	-0.37590258	1.63137819
O	-0.67776069	0.53367854	2.23728273
O	1.17881991	-0.25776295	1.24549209
O	-1.16474756	-0.22011375	-1.13596688
H	-1.84590115	-1.42918191	1.23742681
H	-0.60270845	-2.40863841	2.04111711
H	0.71288409	-2.58813112	-0.03323350
H	-0.94921087	-3.09021382	-0.37428774
Na	0.27306292	1.39502064	-0.27525981
O	0.93133734	2.59425242	1.69340774
H	1.69098379	1.98984210	1.72144905
H	0.23971406	1.97726540	2.07613331
O	0.17585905	1.46521376	-2.70812890
H	-0.58571384	0.92038108	-2.37110940
H	0.75263098	0.73036964	-2.97849822

2D

C	-1.42518056	-1.70716477	0.44347686
C	-0.72138367	-1.72325998	-0.93934641
C	-0.64841944	-0.32541909	-1.58133837
O	-1.56221169	0.04793891	-2.33115155
C	-0.57825271	-0.95677767	1.48561373
O	0.52142340	-1.48682958	1.81582053
O	-1.00130134	0.17795132	1.87753891
O	0.39056564	0.38736326	-1.25853338
H	-2.41141440	-1.24049315	0.35159682
H	-1.54519174	-2.74667860	0.77534860
H	0.28719706	-2.12893911	-0.80169790
H	-1.28799010	-2.37298798	-1.61597167
Na	0.44580375	1.48249703	0.83333366
O	2.40071367	0.13152312	0.66311643
H	1.93713621	0.00545971	-0.19256084
H	1.92874572	-0.51601507	1.24065847
O	0.53600092	2.96834909	-1.04810069
H	1.36795848	3.25978192	-1.43714828
H	0.38987327	2.03143294	-1.39958585

2E

C	-0.56058546	-1.85215168	0.90531014
C	0.10978282	-2.28931566	-0.42119342
C	-0.45324203	-1.56000447	-1.67291774
O	-1.24974682	-2.18702466	-2.39980867
C	-0.22172715	-0.41040211	1.28129232
O	-1.18062897	0.42063918	1.38156980
O	1.00626144	-0.11201003	1.41159149
O	-0.04098372	-0.35900830	-1.85028916
H	-1.64744540	-1.96234349	0.83635347
H	-0.18967504	-2.50194666	1.71048054
H	1.18472864	-2.08961807	-0.33432004
H	-0.04904046	-3.36567433	-0.55141982
Na	0.65208367	1.23883309	-0.63012392
O	2.04040264	2.37130647	1.04452685
H	1.75106428	1.49897651	1.41708298
H	1.25669248	2.93387517	1.15192956
O	-0.73286537	2.81676816	0.60721886
H	-0.94735721	1.91406672	1.04179420
H	-1.56943127	3.15805399	0.27332480

2F

C	0.34233917	-2.11220717	-0.53618214
H	-0.00796035	-2.09170790	-1.57350246
H	0.87399235	-3.06438171	-0.38572203
C	-0.83721332	-2.05633349	0.45074509
H	-0.42049596	-1.97349729	1.46370184
H	-1.41921521	-2.98341693	0.40093803
C	1.36934372	-0.98601360	-0.35015418
O	1.85736705	-0.46658759	-1.40831029
O	1.64618313	-0.61156790	0.82566031
C	-1.82192448	-0.87734349	0.28317061
O	-1.29620504	0.25974417	-0.02908854
O	-3.03024664	-1.07993028	0.49600722
Na	0.58757704	1.41284814	0.45421536
O	-1.47426600	2.60981945	0.93424900
H	-2.00796073	3.23889809	0.43833769
H	-1.70289068	1.69116321	0.56852445
O	2.26106992	2.06835991	-1.05439482
H	2.27850345	1.05853241	-1.20205895
H	1.98505061	2.43243571	-1.90321024

2G

C	0.84793558	0.35945554	1.28734093
H	0.95534093	-0.72795900	1.15766779
H	1.49221007	0.84567923	0.54344038
C	-0.61845357	0.77624792	1.04623488
H	-1.24473544	0.39176881	1.85334388
H	-0.67519506	1.86941082	1.04680587
C	1.45107123	0.71584373	2.69152605
O	0.71287232	1.34711550	3.48837653
O	2.63893982	0.31672893	2.83679775
C	-1.07171610	0.22720100	-0.28960062
O	-1.84432571	-0.79350701	-0.30831592
O	-0.57074088	0.71946783	-1.36142662
Na	-0.28922157	-1.38345704	-2.25147973
O	-2.53878043	-1.83253328	-2.58490226
H	-2.46141602	-1.38403505	-1.67489684
H	-3.11091728	-1.26533587	-3.11370754
O	1.80921394	-0.48168251	-1.76590959
H	1.18304002	0.24799590	-1.53158827
H	2.30234099	-0.63128800	-0.94710644

2H

C	-0.51886519	0.09935002	0.16545508
C	-2.02224071	0.06815738	0.56107581
C	1.52920700	-0.99676680	-0.67446909
C	0.05001965	-1.20707107	-0.42787454
H	-0.11322572	-2.02731792	0.27415783
H	-0.39613700	0.91703185	-0.55742772
H	0.04592948	0.37615240	1.06728472
H	-0.47014635	-1.42788909	-1.36432625
O	2.37595464	-1.39155305	0.18900883
O	-2.45179885	1.15734642	1.04337886
O	-2.65683740	-1.00354763	0.37177471
O	1.87874098	-0.28996991	-1.69559329
Na	3.68955802	0.32247784	-0.41224024
O	2.24791203	2.16479497	-0.71434303
H	1.83939484	1.42518827	-1.23740083
H	1.55130219	2.44447302	-0.10589408
O	-5.05334272	0.14587475	1.45804335
H	-4.54514806	-0.58857033	1.06257404
H	-4.32366926	0.80155602	1.46182976

2I

C	-0.91023517	0.47382784	0.32742262
C	-2.44498986	0.27685620	0.47943442
C	1.26528865	-0.25580892	-0.66261772
C	-0.22313172	-0.52448883	-0.62573546
H	-0.41591622	-1.53971955	-0.26976869
H	-0.73791061	1.50246283	-0.01471101
H	-0.46734654	0.39464195	1.32892346
H	-0.64587911	-0.41470982	-1.62762740
O	1.99744033	-0.78582503	0.25201860
O	-3.01687643	1.14497821	1.20162491
O	-2.97108413	-0.70882865	-0.10824565
O	1.73481568	0.53479809	-1.54673285
Na	3.69758961	0.78812370	-0.65520408
O	4.55742012	-0.99529227	0.45051873
H	3.54928069	-1.11685282	0.45622341
H	4.90878267	-1.38155152	1.25848477
O	-5.56220908	-0.02112783	0.87525796
H	-4.89877871	0.62403950	1.20131871
H	-4.93642057	-0.57368929	0.36602433

2J

C	0.31730	-1.94220	-0.77031
H	1.32255	-2.12474	-1.16209
H	-0.34291	-2.77489	-1.04471
C	0.38546	-1.86012	0.77941
H	-0.62872	-1.74446	1.17567
H	0.81218	-2.79789	1.15392
C	-0.23204	-0.64353	-1.37798
O	-1.47447	-0.40617	-1.24670
O	0.60252	0.15999	-1.89438
C	1.27949	-0.69254	1.25433
O	2.50918	-0.86065	1.29447
O	0.65956	0.41039	1.53423
Na	0.53230	1.68182	-0.24364
O	-2.04855	0.48195	1.37959
H	-1.07884	0.42203	1.59014
H	-2.10767	-0.06377	0.57038
O	-1.65172	2.32153	-0.68818
H	-1.67295	1.49088	-1.22245
H	-1.97863	1.97892	0.17217

2K

C	0.26776692	0.40414754	0.26043507
C	-1.27187459	0.39299120	0.41338236
C	2.33892782	-0.57149763	-0.74618894
C	0.83077637	-0.69928810	-0.65412773
H	0.56368850	-1.67676367	-0.24465029
H	0.55436598	1.39130236	-0.12467999
H	0.70154595	0.32048343	1.26494186
H	0.38608656	-0.59869205	-1.64744007
O	3.06829172	-1.20390927	0.09665691
O	-1.72972145	1.27584346	1.20155123
O	-1.92901743	-0.45835684	-0.24289512
O	2.84039765	0.20834548	-1.63139606
Na	4.80690254	-0.14569983	-0.72435257
O	-4.37491618	1.66512437	1.20250282
H	-3.38208815	1.52148154	1.25188189
H	-4.56861183	1.51345187	0.26875545
O	-4.44059666	-1.23577171	0.70553905
H	-4.62649951	-0.42087739	1.20061058
H	-3.54830456	-1.04305752	0.33163373

Table S5. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_3$ using B3LYP exchange-correlation functional with dispersion correction.

3A

C	0.05156	-2.11766	-0.72554
H	1.05630	-2.30990	-1.11378
H	-0.61361	-2.94668	-0.99658
C	0.12130	-2.02257	0.82359
H	-0.89069	-1.93180	1.22975
H	0.58641	-2.93811	1.20712
C	-0.48977	-0.81743	-1.34134
O	-1.72768	-0.57660	-1.22340
O	0.34939	-0.02198	-1.86885
C	0.97290	-0.81182	1.24032
O	2.21928	-0.90349	1.12802
O	0.33867	0.24803	1.58449
Na	0.41197	1.62227	-0.20721
O	2.67346	1.08138	-0.74828
H	2.75301	0.48443	0.03183
H	2.15821	0.53041	-1.37169
O	-2.38601	0.27454	1.40327
H	-1.42204	0.23375	1.62651
H	-2.41949	-0.24559	0.57655
O	-1.81912	2.15586	-0.61049
H	-1.85152	1.34199	-1.16549
H	-2.18543	1.80764	0.23008

3B

C	-0.89217609	-2.04493880	0.63715316
H	-1.93014354	-1.71639990	0.52328967
H	-0.87104177	-3.05348919	1.06690285
C	-0.21462316	-2.08890407	-0.75877695
H	0.82817083	-2.39833323	-0.63877303
H	-0.74554188	-2.81604219	-1.38463835
C	-0.12249157	-1.09470884	1.56969731
O	1.00177980	-1.47816292	1.98124262
O	-0.63548533	0.05627086	1.79219736
C	-0.29297585	-0.71499302	-1.44012004
O	-1.41046724	-0.34230745	-1.87756302
O	0.77202073	-0.00101463	-1.45037202
Na	0.55919306	1.46854997	0.46298320
O	0.32312978	2.71442596	-1.58812174
H	0.47396554	1.77538268	-1.85929659
H	-0.61049184	2.71620923	-1.32175286
O	-1.95045634	1.62394469	-0.01469439
H	-1.96700504	1.01420835	-0.78624132
H	-1.75963298	1.01063265	0.73303220
O	2.62645063	0.31556868	0.65305947
H	2.27971754	-0.01436596	-0.20073725
H	2.24635646	-0.32132910	1.30155710

3C

C	-1.10443548	-1.92210608	0.79397882
H	-2.10956064	-1.49075726	0.80554400
H	-1.09871164	-2.85807917	1.36678394
C	-0.69156052	-2.23066288	-0.66898171
H	0.29686279	-2.69857633	-0.67200602
H	-1.43135354	-2.91480199	-1.10224470
C	-0.11919952	-0.94348046	1.44394984
O	1.06915498	-1.33924909	1.62289308
O	-0.52163444	0.24448816	1.68634337
C	-0.66059566	-0.93678702	-1.50064227
O	-1.76197308	-0.39787473	-1.78543048
O	0.49240135	-0.45559212	-1.76730244
Na	1.07179262	0.97636754	-0.05340368
O	0.89978149	2.22009710	-2.14598466
H	0.08986934	2.51558552	-1.69453690
H	0.69434003	1.27167584	-2.33824827
O	2.25617106	1.04209111	2.03604676
H	2.03210903	0.07137524	1.99007335
H	1.43186218	1.37200150	2.42718579
O	-1.33005976	1.91304857	-0.34757350
H	-1.29254276	1.40269993	0.49044655
H	-1.64048216	1.23500300	-0.99353583

3D

C	0.32028208	-2.19855480	-0.24550827
H	0.13723104	-2.14323037	-1.32286998
H	0.75528121	-3.18834687	-0.04457992
C	-0.99161154	-2.04409709	0.53836907
H	-0.84816559	-2.30232590	1.59075406
H	-1.74991449	-2.72604840	0.12566552
C	1.38147881	-1.13490188	0.10944682
O	2.22190719	-0.83887006	-0.79547589
O	1.31827634	-0.59203724	1.25060908
C	-1.56142731	-0.61847055	0.49832405
O	-1.32576049	0.10241380	-0.52963328
O	-2.18917944	-0.20681920	1.51544863
Na	0.26696642	1.36972700	0.79119308
O	-1.83726479	2.42809594	1.20697503
H	-2.12182728	1.50165682	1.46004145
H	-2.00385519	2.39912932	0.25304463
O	1.84613894	1.91312548	-0.83720102
H	2.29923647	1.05204953	-0.67709155
H	1.32281792	1.69060239	-1.63487386
O	0.42185678	0.27294897	-2.67232475
H	-0.29763218	0.12972803	-2.01651935
H	1.13914786	-0.29170380	-2.31930900

3E

C	-0.45799270	-2.05706117	1.43799508
C	-0.39519372	-2.45274603	-0.04962704
C	-0.62479674	-1.25692852	-0.99234403
O	-0.03257873	-1.25505140	-2.10782414
C	0.40466210	-0.82007093	1.74894786
O	-0.03263084	-0.00272609	2.61966634
O	1.46852342	-0.66263818	1.07939162
O	-1.34927695	-0.30920628	-0.54429020
H	-1.48415277	-1.82772136	1.73629658
H	-0.10193172	-2.89579873	2.05477031
H	0.57990371	-2.88013420	-0.29816533
H	-1.16041014	-3.21402842	-0.26244714
Na	0.84579722	0.92415740	-0.39181298
O	0.31349920	2.31125325	1.51196380
H	0.99753431	2.81779107	1.96186460
H	0.20392971	1.44803919	2.05060951
O	0.79215117	1.26643730	-2.73578018
H	0.04119055	1.83133834	-2.48049348
H	0.42690460	0.34201388	-2.70778562
O	-1.24050064	2.32171272	-0.97468429
H	-1.47274854	1.35786687	-0.89332524
H	-0.98823362	2.58965940	-0.07485505

3F

C	-0.02043066	-2.02665304	-1.24819155
H	-0.26059234	-1.53555212	-2.19703756
H	0.38533820	-3.01826560	-1.49300939
C	-1.28844682	-2.15853520	-0.39523694
H	-1.08405783	-2.69966201	0.53316859
H	-2.04486386	-2.72594265	-0.95837065
C	1.11233483	-1.20539333	-0.60281512
O	2.13461193	-0.99576721	-1.33045924
O	0.96799696	-0.77835417	0.57586761
C	-1.89759731	-0.79840849	-0.02100870
O	-1.80758884	0.14430150	-0.86867721
O	-2.39262270	-0.67520484	1.14478867
Na	-0.29750363	1.00253918	0.96312979
O	-2.51392673	2.02408095	1.11001706
H	-2.69800991	1.08777088	1.38306946
H	-2.47253047	1.85859198	0.14842030
O	3.35202796	1.14070263	-0.54002857
H	2.91496079	0.23898820	-0.76585361
H	3.57560113	1.51289898	-1.40116185
O	1.45868720	2.49085828	0.79119835
H	2.18115084	1.98354937	0.31875379
H	1.38975547	3.34011794	0.34305885

3G				**3H**		
O	2.89897954	0.90389866	0.67223724	O	0.20900739	-1.29883107	-3.88224447
H	3.18010254	1.47640278	1.39395335	H	0.04630130	-1.03398674	-4.79003594
C	-2.85392894	0.21276212	-0.11002572	C	0.64059426	1.51730845	1.57109868
H	-3.84227681	0.27357089	0.36401332	H	0.30939562	2.51198087	1.24074451
H	-2.95422219	0.33376700	-1.19273385	H	1.71244826	1.59260445	1.77535754
C	-1.96944668	1.35089567	0.46740258	C	-0.10831743	1.11869093	2.86435815
H	-2.38781430	2.31817135	0.16245572	H	-0.01813413	0.03353013	3.00957994
H	-1.97012841	1.26981320	1.55802825	H	0.34886869	1.61241779	3.72560101
C	-2.20047058	-1.14631736	0.19866331	C	0.46417248	0.55629984	0.38693229
O	-1.65920489	-1.75676879	-0.77533737	O	1.42964895	0.37127593	-0.38599056
O	-2.09946906	-1.48442283	1.41538339	O	-0.68670156	-0.00293164	0.24434318
C	-0.52109566	1.27341473	-0.03555442	C	-1.59784694	1.47308814	2.90322712
O	0.33318927	0.74639547	0.77558324	O	-2.33114096	1.05900447	1.87441504
O	-0.25122073	1.68633644	-1.18623189	O	-2.08608576	2.09107994	3.83807125
H	1.87754234	0.91851992	0.67258032	H	-1.74182867	0.57925529	1.18584710
O	2.05713218	0.45548024	-2.05219314	O	2.41666454	-1.61643358	-2.54520995
H	2.65549810	0.90545013	-1.43462032	H	1.71668655	-1.40428647	-3.24348404
H	1.18264760	0.87840993	-1.84569367	H	2.46087550	-0.84318216	-1.96375678
O	2.41851459	-1.67324156	-0.29671645	O	0.05431867	-3.50428703	-2.54374738
H	2.22385873	-1.13765105	-1.10320788	H	1.00232766	-3.50966785	-2.34346498
H	2.86516774	-1.00423918	0.25537878	H	0.00876544	-2.81584225	-3.28323072
Na	0.25903175	-1.56333092	0.53919956	Na	0.00484153	-1.16797851	-1.69775753

3I

C	-0.95202788	0.21996514	0.13606247
C	-2.45049360	0.21784541	0.55312846
C	1.08233652	-0.96487205	-0.66499789
C	-0.41290427	-1.09784273	-0.45546724
H	-0.63437271	-1.92204546	0.22493389
H	-0.83247388	1.03011710	-0.59418902
H	-0.37181410	0.49699365	1.02837855
H	-0.91248172	-1.28611925	-1.41104629
O	1.87056808	-1.55094586	0.14832171
O	-2.85172177	1.32116642	1.02691914
O	-3.10516765	-0.84426548	0.38470529
O	1.50068248	-0.17556065	-1.58331329
Na	3.18546392	0.69949867	-0.36462172
O	1.54617882	2.34781244	-0.68432238
H	1.20197205	1.56376906	-1.18126926
H	0.81605004	2.60764596	-0.10717496
O	4.40791003	-1.10790269	0.25791598
H	3.45523562	-1.46576492	0.19288801
H	4.80363184	-1.49660755	1.04455257
O	-5.47717143	0.37679813	1.46048261
H	-4.99013710	-0.37610218	1.07412838
H	-4.73145843	1.01362459	1.45640502

3J

O	1.29589828	-1.96116041	-0.44419672
H	1.77386485	-1.70161918	0.35643722
C	0.64980561	0.43395290	1.68749776
H	0.53992330	-0.65249345	1.79569827
H	1.48792881	0.61610307	0.99924669
C	-0.65544936	1.01904050	1.11235655
H	-1.47237110	0.75589050	1.79231364
H	-0.58467413	2.10754139	1.06405450
C	1.07064483	0.98057648	3.09755289
O	0.26024859	1.74901946	3.67473505
O	2.19079370	0.55173529	3.48483632
C	-0.92263571	0.45989219	-0.26541854
O	-1.17381339	-0.81449671	-0.36203017
O	-0.82061947	1.19338942	-1.29009142
H	0.36330626	-1.68208229	-0.26419259
Na	-0.59524102	-0.54218001	-2.75637885
O	-2.61769537	-1.66347198	-2.38323537
H	-2.25514398	-1.39958515	-1.48389733
H	-3.52604075	-1.34527428	-2.41933786
O	1.64848366	-0.18809990	-2.47597255
H	1.43187146	0.64206484	-2.02184698
H	1.70915005	-0.85004296	-1.74036413

3K

C	-0.27733303	0.53231058	0.24538908
C	-1.81723407	0.49794956	0.40202660
C	1.80776975	-0.42933319	-0.73331661
C	0.30437721	-0.58556658	-0.64079200
H	0.05227987	-1.55549936	-0.20462655
H	-0.00888064	1.51449986	-0.16479646
H	0.15951148	0.48092395	1.25076630
H	-0.13982532	-0.51933055	-1.63705637
O	2.53019652	-0.98884871	0.16927148
O	-2.28708069	1.41808209	1.14002033
O	-2.45504071	-0.40444368	-0.19927926
O	2.29785885	0.30275046	-1.65491589
Na	4.31944630	0.41121582	-0.87080869
O	5.07552743	-1.37541811	0.28785393
H	4.06440710	-1.42412145	0.34181343
H	5.44076315	-1.78421632	1.07841218
O	-4.90853740	1.85569793	1.29089960
H	-3.91916322	1.67458912	1.27718641
H	-5.13629804	1.92101219	0.35527439
O	-5.08433395	-0.98039448	0.59719069
H	-5.23523896	-0.15090179	1.08250209
H	-4.15983366	-0.85942363	0.27743930

Table S6. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_4$ using B3LYP exchange-correlation functional with dispersion correction.

4A

C	-0.02747766	-2.27353123	-0.88783388
H	0.96740052	-2.14491634	-1.32643780
H	-0.45202360	-3.22583474	-1.22489486
C	0.09391834	-2.30812561	0.65770428
H	-0.89712869	-2.46820930	1.09183330
H	0.76178363	-3.12940993	0.94332445
C	-0.96474477	-1.13210060	-1.32203368
O	-2.19404860	-1.29217091	-1.15377754
O	-0.40448489	-0.06381562	-1.76052478
C	0.67691158	-0.99408396	1.17975627
O	1.90886276	-0.76511405	0.96137982
O	-0.10984594	-0.15732113	1.72516962
Na	0.60248623	1.43778327	-0.04685214
O	1.94493362	1.82083001	1.94540358
H	1.13198511	1.54707358	2.40240883
H	2.26350177	0.93488009	1.65329511
O	2.25106972	0.44478067	-1.57215796
H	2.43155272	-0.11821486	-0.79619154
H	1.36499926	0.12833794	-1.87241566
O	-2.72028901	0.47454633	0.95977259
H	-1.88783462	0.17413471	1.38280030
H	-2.80665754	-0.14119774	0.20154291
O	-1.47371539	2.27439944	-0.75561603
H	-1.34798969	1.53747075	-1.39385803
H	-2.04551999	1.85007636	-0.07507415

4B

C	0.00304288	-2.07009808	-0.77717726
H	1.03451737	-2.14766306	-1.13383247
H	-0.56834111	-2.93755782	-1.12765765
C	-0.00294515	-2.07006999	0.77723004
H	-1.03440122	-2.14776896	1.13385902
H	0.56864017	-2.93737923	1.12775770
C	-0.63737351	-0.78866093	-1.33247361
O	-1.89460583	-0.69194097	-1.31963984
O	0.15243596	0.14175178	-1.70441395
C	0.63742106	-0.78855969	1.33234897
O	1.89461073	-0.69177200	1.31975035
O	-0.15249850	0.14181971	1.70429325
Na	-0.00002519	1.68458088	-0.00009177
O	2.26263871	1.98678590	0.50350159
H	2.18716872	1.22785758	1.12398752
H	2.66266098	1.54265999	-0.27340642
O	2.84852891	-0.10438446	-1.30329925
H	2.77353221	-0.55797305	-0.44215074
H	1.90537433	-0.06520193	-1.59725870
O	-2.84856196	-0.10446691	1.30335017
H	-1.90539327	-0.06523971	1.59727454
H	-2.77352672	-0.55813219	0.44222929
O	-2.26274320	1.98668592	-0.50353507
H	-2.18724961	1.22774823	-1.12399921
H	-2.66273034	1.54254649	0.27338650

4C

C	-0.89217609	-2.04493880	0.63715316
H	-1.93014354	-1.71639990	0.52328967
H	-0.87104177	-3.05348919	1.06690285
C	-0.21462316	-2.08890407	-0.75877695
H	0.82817083	-2.39833323	-0.63877303
H	-0.74554188	-2.81604219	-1.38463835
C	-0.12249157	-1.09470884	1.56969731
O	1.00177980	-1.47816292	1.98124262
O	-0.63548533	0.05627086	1.79219736
C	-0.29297585	-0.71499302	-1.44012004
O	-1.41046724	-0.34230745	-1.87756302
O	0.77202073	-0.00101463	-1.45037202
Na	0.55919306	1.46854997	0.46298320
O	0.32312978	2.71442596	-1.58812174
H	0.47396554	1.77538268	-1.85929659
H	-0.61049184	2.71620923	-1.32175286
O	-1.95045634	1.62394469	-0.01469439
H	-1.96700504	1.01420835	-0.78624132
H	-1.75963298	1.01063265	0.73303220
O	2.62645063	0.31556868	0.65305947
H	2.27971754	-0.01436596	-0.20073725
H	2.24635646	-0.32132910	1.30155710
O	1.16039705	1.53564471	1.63021054
H	0.35872186	1.03662938	1.80312841
H	1.83175382	0.94978416	1.27293266

4D

C	1.55743018	0.19766399	1.78591550
H	1.72504697	0.39488926	2.85199403
H	2.46532885	0.43599245	1.22449642
C	1.21434405	-1.30347818	1.60265086
H	2.06917232	-1.90233397	1.93660542
H	0.33832436	-1.54834737	2.21114151
C	0.39744860	1.07350463	1.30119803
O	0.57704588	1.76698472	0.24416723
O	-0.70412123	0.99208151	1.91238724
C	0.94648187	-1.60780909	0.11773183
O	-0.28355691	-1.71426296	-0.23809386
O	1.93028350	-1.65787931	-0.65348777
O	-1.58047442	2.54435669	-1.23717948
H	-1.30059184	2.09226218	-2.04662678
H	-0.78251622	2.50850630	-0.65131773
O	1.79841806	0.77231523	-2.03696399
H	1.53210926	1.23036151	-1.20926532
H	2.04557155	-0.12188628	-1.71913154
O	-2.37943511	-1.21086591	1.43424970
H	-1.64132068	-1.65302784	0.95129072
H	-1.90964327	-0.53082288	1.95466062
Na	-1.62641287	0.35017712	-0.29775465
O	-0.75203400	-0.19749539	-2.49680234
H	-0.56336898	-1.00074871	-1.96111633
H	0.14049675	0.22118294	-2.53903759

4E

C	0.40021899	-0.58879774	2.43968184
H	-0.39641479	-1.33878127	2.46124683
H	0.79851591	-0.44213204	3.45033309
C	1.54846065	-1.09986001	1.52890538
H	2.35121181	-0.35706661	1.50411006
H	1.93110019	-2.04276347	1.93741056
C	-0.14250513	0.75739317	1.92204390
O	0.55940923	1.77788584	2.11895768
O	-1.24279012	0.72179037	1.26763596
C	1.02125195	-1.35422016	0.11537172
O	0.21722001	-2.31506175	-0.04500161
O	1.33020420	-0.51321046	-0.79536658
O	-1.01135417	2.11574407	-1.09311073
H	-1.24308396	1.93935483	-0.15091530
H	-0.04875859	2.32451717	-1.01274936
O	-0.23873993	-0.02538527	-2.95506260
H	-0.53633283	0.85476570	-2.66405859
H	0.48084100	-0.25776209	-2.31446974
O	1.65786569	2.22403234	-0.40917874
H	1.39079400	2.29023807	0.53323012
H	1.74720533	1.25480353	-0.54093549
Na	-1.30296921	-0.34987498	-0.68698021
O	-1.69761158	-2.30403067	-2.04069343
H	-0.94972988	-2.54844236	-1.44637001
H	-1.28873475	-1.70617702	-2.69323759

4F

C	0.88728363	0.13024035	2.23978830
H	0.08914091	-0.41165461	2.75539383
H	1.49969493	0.61843112	3.01176176
C	1.75867105	-0.83188838	1.42579513
H	2.59639395	-0.29992982	0.96554169
H	2.18543346	-1.59589902	2.09186181
C	0.22745604	1.24699977	1.41352407
O	-0.84256324	1.74888561	1.84669068
O	0.79004295	1.58598627	0.31525455
C	1.01256799	-1.57551883	0.30567591
O	-0.25091478	-1.73171615	0.43463082
O	1.67783559	-1.96736357	-0.68858272
O	-1.34317862	2.60151061	-1.01289654
H	-1.90390449	2.58117720	-0.22326085
H	-0.45017377	2.52722915	-0.59608780
O	1.44092505	0.44291607	-2.09617763
H	1.49829827	0.96132970	-1.26809244
H	1.74283956	-0.44285777	-1.81272661
O	-2.49542810	-0.16267757	0.63450703
H	-2.17546142	0.55821669	1.21242125
H	-1.83889185	-0.87052472	0.79492856
Na	-0.83056753	0.21830805	-1.15095107
O	-0.95736671	-1.99710334	-2.16869028
H	-0.85445607	-2.18645639	-1.20423163
H	-0.03569197	-2.07151794	-2.45753545

4G

C	1.13927404	-2.02427885	-0.78780205
H	1.44836382	-2.50417484	-1.72821486
H	0.96962066	-2.80929920	-0.04719492
C	2.24038936	-1.06564015	-0.30259296
H	3.12412808	-1.65233592	-0.01495028
H	2.53869811	-0.37796004	-1.09911483
C	-0.20913488	-1.33319639	-1.03577606
O	-1.25751999	-2.00540369	-0.83476827
O	-0.19327265	-0.11538942	-1.41866965
C	1.78059403	-0.24898848	0.92280458
O	2.02202440	1.00338406	0.91921396
O	1.14145144	-0.86330499	1.81775061
O	-1.11956928	0.63351033	2.19159966
H	-1.80901552	0.07618403	1.78263222
H	-0.31481848	0.06341268	2.27202536
O	-3.04151623	-0.68663542	0.53921123
H	-3.70476631	-1.30967071	0.85437605
H	-2.41110782	-1.21370461	-0.05124782
Na	-0.21469396	1.62457373	0.29734445
O	-2.28462152	1.57589117	-0.98450002
H	-1.69307278	0.90953581	-1.40750128
H	-2.86003622	1.01851790	-0.43185762
O	1.47689597	2.15601235	-1.46954035
H	1.03313580	1.34607499	-1.78635905
H	1.96438295	1.82043837	-0.67960934

4H

C	1.29258546	-0.15449820	2.12851709
H	1.35326862	-0.61713449	3.12426914
H	1.92037130	0.74024936	2.14300362
C	1.79594088	-1.13909778	1.06206509
H	2.87189098	-1.31201901	1.20835648
H	1.29247393	-2.10620355	1.14802836
C	-0.15769330	0.31795769	1.91542115
O	-0.48146334	1.41936178	2.43556830
O	-0.93402048	-0.41428501	1.22104212
C	1.59314925	-0.59946133	-0.36362439
O	1.18112587	-1.43083516	-1.24713901
O	1.79502067	0.62443121	-0.56764165
O	-0.51720803	1.79847115	-1.44509626
H	-0.97198725	2.27629038	-0.71305127
H	0.38685619	1.56931566	-1.12458395
O	-0.27625019	-0.39329561	-3.32730982
H	0.45666827	-0.75674456	-2.77181397
H	-0.27235924	0.55755837	-3.13183258
O	-1.83834105	2.89981670	0.72239354
H	-1.48707260	3.76794398	0.95257514
H	-1.46013189	2.28623193	1.42394728
Na	-1.12083738	-0.44883039	-1.03424926
O	-1.00530610	-2.78435818	-0.19912950
H	-0.98131403	-2.18170776	0.57350268
H	-0.12866795	-2.62264949	-0.61044688

4I

C	1.58164879	0.31216803	1.95737727
H	2.04504642	0.27144872	2.94960501
H	2.03380353	1.12667808	1.38235083
C	1.84799307	-1.03492946	1.23442653
H	2.92784951	-1.14889046	1.08146791
H	1.46873899	-1.85301571	1.85283009
C	0.06727473	0.53961256	2.12633480
O	-0.48637492	1.34012989	1.26929716
O	-0.53824587	-0.09536658	3.00327541
C	1.14332753	-1.05819017	-0.12204479
O	0.05947998	-1.71350119	-0.20704722
O	1.62494289	-0.33885524	-1.05413586
Na	-0.73256414	0.63278142	-1.05609561
O	0.92554834	2.45404291	-0.74048207
H	1.50421218	1.69364189	-0.92725296
H	0.52980095	2.22716970	0.13702242
O	-2.54699420	-0.19276445	0.46335265
H	-2.06684209	-0.96843238	0.79683216
H	-2.08823038	0.52688462	0.96476512
O	-1.86374323	-1.51048590	-2.04668157
H	-1.11749896	-1.74453217	-1.43008615
H	-2.53716300	-1.14117690	-1.45467266
O	0.05239990	0.12373589	-3.32974481
H	0.75833765	-0.16497543	-2.70868334
H	-0.64764963	-0.54602239	-3.22888719

4J

C	1.28641508	0.20163342	2.23738272
H	1.40319858	0.05697840	3.32105692
H	1.89710989	1.06839055	1.96553981
C	1.76066483	-1.05254233	1.49395798
H	2.83498621	-1.20557492	1.67646576
H	1.23400648	-1.94023319	1.85390093
C	-0.18568298	0.58225201	1.97728900
O	-0.53346379	1.76403630	2.21582609
O	-0.93863895	-0.33324593	1.49563317
C	1.55674393	-0.99540030	-0.02552618
O	1.38188235	-2.07291402	-0.64391685
O	1.55920663	0.16546916	-0.57815229
O	-0.09943789	2.34300406	-0.51156809
H	-0.44961862	2.47899313	0.39196732
H	0.69012452	1.78272243	-0.35438337
O	0.48373237	0.77311374	-2.94597835
H	0.19774417	1.65958282	-2.68210638
H	1.06718935	0.48031476	-2.19323605
O	-3.14996808	0.03331333	0.11944220
H	-3.47819973	-0.86979783	0.03365995
H	-2.47339777	-0.00784398	0.85684909
Na	-0.93029135	0.04751939	-0.87863821
O	-0.68968297	-1.78460731	-2.40190422
H	0.11022519	-2.03190283	-1.87273751
H	-0.36872009	-1.09095283	-3.00166960

4K			
C	-2.43883735	0.74576842	-0.32368651
C	-2.27831684	-0.14683059	0.92168103
C	-0.27858146	-0.00180236	-1.48701760
C	-1.80133258	0.10390522	-1.57860046
H	-2.21922158	-0.89391687	-1.74283919
H	-3.50788487	0.89509631	-0.50771826
H	-1.96030199	1.71688110	-0.15169177
H	-2.03679834	0.73471633	-2.44647703
O	0.25264255	-1.14514685	-1.53006656
O	-3.21556902	-0.86808477	1.28456271
O	-1.11339357	-0.07282746	1.48944216
O	0.37244772	1.09166665	-1.33788111
Na	1.17553124	-0.41324408	0.76404866
O	0.53235464	-1.58525585	2.78474354
H	-0.30762007	-1.14461322	2.45610547
H	0.67854402	-1.23823435	3.67136804
O	2.91174475	1.29143581	-2.10530447
H	1.94721945	1.24399378	-1.83945790
H	2.91798508	1.13572200	-3.05677641
O	0.68791306	1.93796665	1.32837776
H	0.63490368	2.01337013	0.35753801
H	-0.11680032	1.40108932	1.52493347
O	2.88456229	-1.15042290	-0.72711363
H	2.03867646	-1.31543575	-1.20739415
H	3.20277825	-0.32878147	-1.15129550

4L			
C	-1.52771477	-1.72936405	-0.52217757
H	-2.55845648	-2.10194811	-0.43303474
H	-0.85760808	-2.59523921	-0.52815832
C	-1.41152600	-0.93387979	-1.83734373
H	-1.85742240	-1.50270089	-2.65965148
H	-1.97945841	-0.00108669	-1.72338538
C	-1.25318083	-0.91111544	0.73881406
O	-1.85275991	0.21599773	0.85503892
O	-0.45937088	-1.36220574	1.61169339
C	0.03318475	-0.56611278	-2.23894991
O	0.38782162	-0.71580655	-3.41594884
O	0.76537297	-0.09942486	-1.27897582
Na	0.68992079	0.98622724	0.71468426
O	-0.44623770	1.24937405	2.90996980
H	-1.14380719	0.89837074	2.29233891
H	-0.09710374	0.41972630	3.26667926
O	2.80617598	1.48720854	-0.44388850
H	3.19168447	0.75498341	0.06003234
H	2.23265470	1.02335706	-1.09895235
O	-0.98738349	2.76887701	0.36272039
H	-1.50429912	1.93640615	0.30911329
H	-0.98736574	2.98115874	1.30610073
O	2.15857140	-1.13311538	0.79390403
H	1.36217504	-1.46291562	1.25808811
H	1.80664230	-1.01665221	-0.11745480

4M

C	-0.88932594	-2.20712095	0.36993827
C	-0.11713721	-2.06655206	-0.96601883
C	-0.70246198	-0.95408152	-1.86079643
O	-1.51793187	-1.24947141	-2.74282336
C	-0.79100636	-0.95282754	1.23447235
O	-1.82796633	-0.26027554	1.42762466
O	0.36542484	-0.62000902	1.68032084
O	-0.28220649	0.23996773	-1.57957019
H	-1.94381111	-2.41697383	0.16784520
H	-0.45670500	-3.04484680	0.93285946
H	0.93528542	-1.85645435	-0.74605729
H	-0.18642402	-3.01722883	-1.50518431
Na	-0.20124744	1.50677629	0.39420505
O	-0.29170230	2.90024943	-1.61746691
H	0.67644430	2.91767634	-1.62114693
H	-0.49577078	1.98190022	-1.92521970
O	2.81982562	-1.01589953	0.85674445
H	3.34937417	-0.95229271	1.65948297
H	1.86579638	-0.99579175	1.16638886
O	2.02430012	1.23262389	-0.66575551
H	1.34181342	0.70000651	-1.14732908
H	2.52367804	0.56605238	-0.15406392
O	-0.69361876	1.83412429	2.75719727
H	0.05789256	1.23271965	2.89068388
H	-1.36335811	1.17193739	2.45348194

4N

C	-0.86395931	-1.16184159	-0.10040491
H	-1.38717160	-2.12705937	-0.07127799
H	0.20912412	-1.37947401	-0.05545456
C	-1.20482327	-0.43928723	-1.41777216
H	-2.28760744	-0.35279039	-1.51859435
H	-0.75976055	0.56183988	-1.39032843
C	-1.27318789	-0.35706633	1.14815177
O	-0.41785678	-0.35011149	2.10837533
O	-2.36689310	0.25456767	1.13854914
C	-0.63933308	-1.20380683	-2.61146779
O	-1.34367707	-1.90703037	-3.32810513
O	0.66833681	-1.08835358	-2.80505347
Na	1.32862204	0.60828573	0.99552740
O	-1.39111501	1.93785163	3.14198065
H	-0.94324728	1.05524297	3.14875640
H	-2.10183294	1.69406657	2.51234856
O	1.83335006	0.47912251	-1.24317348
H	1.14675431	-0.41178523	-2.14017760
H	2.25977271	1.17515557	-1.75541990
O	0.59382748	2.79110372	1.51343916
H	0.20899199	3.18049743	0.71971500
H	-0.17154124	2.60618112	2.12636041
O	3.32419891	-0.70493328	0.47131334
H	3.25194632	-1.66409909	0.40922232
H	2.88604229	-0.32457998	-0.36666807

4O

C	0.08494603	0.02913552	2.00151648
H	-0.60332211	0.41636607	1.23782539
H	-0.45333303	-0.68902842	2.62548791
C	1.28389185	-0.67915499	1.30280856
H	2.06269094	0.05626795	1.08204669
H	1.68783931	-1.44874172	1.96778229
C	0.55725812	1.23829962	2.85233537
O	0.95188348	2.25036106	2.16800841
O	0.53037868	1.13585659	4.09299570
C	0.80184573	-1.30102009	0.00594753
O	0.18562168	-2.40675318	0.04309675
O	0.95014669	-0.60774566	-1.06367345
Na	-1.14164060	-0.07548620	-1.83134071
O	-1.73575002	1.96805871	-1.21054998
H	-2.09892434	2.81371460	-1.48724971
H	-0.79986829	2.14765789	-0.81108278
O	0.64968577	2.13929267	-0.35815460
H	1.02261689	1.27365569	-0.61628046
H	0.77977976	2.20782535	0.67426986
O	-1.77798969	-2.34060521	-1.60156021
H	-0.98188011	-2.47975459	-0.97010094
H	-2.52900225	-2.78866526	-1.19866442
O	0.04833107	-1.35236996	-3.56375675
H	0.63335709	-1.25281730	-2.77698624
H	-0.55175669	-2.06927815	-3.30378413

4P

C	-1.97755178	0.05347441	1.64546738
C	-2.94256730	1.24122613	1.37106308
C	-0.09306814	-1.10021641	0.24611450
C	-1.54125321	-0.64334040	0.34232187
H	-2.18989828	-1.48907742	0.09355641
H	-1.08744514	0.44762128	2.15030071
H	-2.46158747	-0.65914087	2.32084837
H	-1.64120053	0.08093169	-0.47945734
O	0.18492374	-2.01225925	-0.61025338
O	-4.07905876	1.21273204	1.88039385
O	-2.46011262	2.16425993	0.61803261
O	0.81323999	-0.48765360	0.89875902
Na	1.90155036	-0.27107481	-1.23219127
O	2.63626890	-2.64340032	0.10460128
H	1.68600305	-2.57317870	-0.22896637
H	2.58222473	-2.08286365	0.89479307
O	0.79940143	1.50124323	-2.08509412
H	0.46627663	1.86401698	-1.18319822
H	0.02108282	1.46129940	-2.65126315
O	0.07972648	2.18749355	0.27821400
H	0.36186362	1.39737276	0.77715393
H	-0.94808242	2.21629833	0.40975681
O	3.92640339	-1.29637218	-1.74539223
H	4.23217391	-1.79773218	-2.50807433
H	3.60579627	-1.94999174	-1.06079700

4Q

C	0.43841295	0.21705523	0.93466897
H	0.48310371	1.31378959	0.98394774
H	-0.56001684	-0.04576936	0.56542501
C	1.52544099	-0.29417851	-0.04154953
H	2.44360564	0.28326298	0.09137867
H	1.73388973	-1.34527306	0.17208187
C	0.52973438	-0.30970545	2.39294259
O	-0.56450612	-0.25975253	3.02935246
O	1.65453000	-0.70249534	2.79646448
C	0.97272919	-0.14233276	-1.44413696
O	0.34674663	-1.12070502	-1.95934090
O	1.01353901	1.01515686	-1.99728295
O	-1.34857433	2.06755523	-1.06278172
H	-1.38833070	1.96520768	-0.10204210
H	-0.39547629	1.93832435	-1.28204583
O	-0.64507214	1.22763361	-4.07019684
H	-0.80016870	2.17780205	-4.12881921
H	0.13099523	1.12821744	-3.44058585
O	0.69119934	-0.98548838	5.48387480
H	1.37981643	-1.02971815	4.79269777
H	-0.04977456	-0.72065937	4.90240016
Na	-1.63155786	0.07074820	-2.29556545
O	-1.98182338	-1.73972215	-0.78531218
H	-1.02123767	-1.81808775	-1.00094247
H	-2.03061963	-1.67629336	0.17827684

4R

C	0.46262471	-0.08618849	2.07633553
H	0.13894768	0.91557957	1.75855032
H	-0.43921156	-0.69603415	2.20326498
C	1.36028351	-0.71685456	0.99781458
H	2.35014729	-0.25827599	1.02310177
H	1.48212685	-1.78334799	1.22287801
C	1.09890162	0.07432967	3.49948200
O	0.31583468	0.60901402	4.33106035
O	2.27720783	-0.33431925	3.65243909
C	0.75656542	-0.56923853	-0.38218644
O	-0.43716681	-1.00240609	-0.59065726
O	1.41647521	0.03689471	-1.28651942
O	-1.85078722	2.33008678	-0.82982122
H	-2.14991923	1.65020255	-0.15982636
H	-1.30952020	2.95925091	-0.33913751
O	0.84983991	0.15758028	-3.80111805
H	1.57419098	0.48792440	-4.34300277
H	1.20505132	0.03063818	-2.86202993
O	-2.42366717	0.25873740	0.73097908
H	-2.17900983	0.38809419	1.65860227
H	-1.72137046	-0.34905871	0.37909093
Na	-0.88070911	0.75234078	-2.16405835
O	-1.48307283	-1.36837030	-3.13931470
H	-1.12333295	-1.56265849	-2.24506210
H	-0.69474847	-1.24450692	-3.69288813

4S

C	0.11143417	0.12396599	0.47385583
H	0.18869215	1.17989958	0.18337096
H	-0.95142019	-0.08717839	0.65427969
C	0.64822617	-0.76033945	-0.66794517
H	1.68081192	-0.46734058	-0.87992882
H	0.63596461	-1.80927389	-0.36488252
C	0.84543560	-0.00615459	1.83209596
O	0.29047127	0.59349491	2.78995662
O	1.91997151	-0.67410266	1.84378383
C	-0.21876141	-0.55788431	-1.89467387
O	-1.04037796	-1.47633410	-2.22856687
O	-0.17590602	0.57518777	-2.48881033
O	-1.90664652	2.24001091	-1.30558843
H	-1.93540524	2.23222569	-0.34039231
H	-1.02488752	1.85625326	-1.53785204
O	3.30037949	-1.13414050	4.08806121
H	2.70188615	-1.72721613	4.55754718
H	2.80954674	-0.92485643	3.23911367
O	1.74566739	1.08784521	5.15077641
H	2.48822211	0.49202933	4.94750638
H	1.17216881	0.96972168	4.35966817
Na	-2.43318610	0.58257309	-2.86899550
O	-2.56662510	-1.20039280	-4.33000118
H	-1.89278258	-1.47151851	-3.62585697
H	-2.12763457	-1.29148871	-5.18238777

4T

C	0.12563757	-0.02432985	0.15058150
H	0.03581496	1.06574378	0.04435565
H	-0.89598403	-0.41641777	0.24693263
C	0.81055877	-0.60739850	-1.10211866
H	1.80282481	-0.16199952	-1.20554642
H	0.91263992	-1.68973350	-0.99340921
C	0.84390921	-0.27510872	1.50057774
O	0.17993487	0.05662229	2.51846201
O	2.00881711	-0.76395309	1.45139933
C	-0.06951348	-0.27188520	-2.28845164
O	-0.95889010	-1.11194226	-2.65672284
O	0.00165783	0.89920982	-2.79502388
O	-1.60910699	2.64824279	-1.61976256
H	-1.59092022	2.64551528	-0.65484504
H	-0.76840445	2.20451141	-1.90210302
O	3.36265720	-1.36341085	3.69119654
H	2.77945268	-2.01366885	4.10067604
H	2.88146525	-1.10937478	2.85051165
O	1.54438074	0.56929485	4.92688653
H	2.36836877	0.11129693	4.68659435
H	0.99416463	0.42852026	4.12292954
Na	-2.36896826	0.83128525	-2.90592077
O	-3.38206211	-0.88671622	-1.64474928
H	-3.46754031	-0.91876938	-0.68437621
H	-2.48301826	-1.25355070	-1.85569980

Table S7. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_5$ using B3LYP exchange-correlation functional with dispersion correction.

5A				5B			
C	-0.38000690	-2.40673256	0.25338866	C	-0.98740683	-2.28634247	0.08544123
H	0.59922633	-2.78579148	-0.05299270	H	-2.00225432	-2.09274666	-0.27400320
H	-1.07596190	-3.24501964	0.36771989	H	-0.95173983	-3.26021032	0.58654785
C	-0.24665866	-1.68702076	1.62373388	C	-0.02006170	-2.31158067	-1.12680143
H	-1.24206249	-1.43273881	1.99891772	H	1.00634142	-2.45580728	-0.77347177
H	0.24447080	-2.36675723	2.32942264	H	-0.29837089	-3.15189334	-1.77244661
C	-0.91763522	-1.44125168	-0.81275184	C	-0.57040428	-1.21199006	1.09236573
O	-2.15440509	-1.19499989	-0.82486962	O	0.44172022	-1.45858848	1.81306109
O	-0.06173928	-0.87950205	-1.57265628	O	-1.21399108	-0.11340778	1.09794799
C	0.59440344	-0.41237660	1.49611119	C	-0.14659996	-1.01457296	-1.94349368
O	1.84210861	-0.52755865	1.36068268	O	-1.18384449	-0.86195222	-2.62670693
O	-0.03582170	0.69927770	1.46345955	O	0.78934400	-0.14523617	-1.81486483
Na	0.06110808	1.33915455	-0.87015626	Na	0.45708459	1.36193972	0.13396427
O	2.50024561	1.22417603	-0.61871552	O	-0.13501595	2.48377923	-1.84748825
H	2.37432024	0.74578939	0.23913661	H	0.20592984	1.64464171	-2.22578710
H	2.76771890	0.48600600	-1.20007660	H	-1.07051541	2.25783241	-1.65303154
O	2.57804532	-1.51051947	-1.30155312	O	-2.45273512	1.09874948	-1.11145993
H	2.58092112	-1.49707679	-0.32870271	H	-2.21087150	0.44529629	-1.80206702
H	1.61812968	-1.37458486	-1.50307688	H	-2.20683735	0.64198298	-0.27994368
O	-2.80834733	0.64549102	1.25253472	O	2.42985774	-0.13322099	0.30085014
H	-1.85429196	0.71499051	1.48062053	H	2.04184706	-0.25966376	-0.60237104
H	-2.82916595	-0.14592188	0.68135482	H	1.95280330	-0.79788936	0.83303412
O	-2.21169945	1.53783622	-1.40246966	O	1.87433337	0.38657091	3.24602231
H	-2.26544852	0.56376471	-1.53106256	H	1.29096588	-0.31856115	2.86664819
H	-2.58750713	1.62978399	-0.50561502	H	2.55627087	0.50315911	2.56951428
O	0.85190990	3.18884862	0.60595092	O	-0.09647234	2.12829750	2.32990140
H	0.63168540	2.41632324	1.17226803	H	-0.70444479	1.37407951	2.18101470
H	1.70593137	2.94707077	0.21449276	H	0.63663480	1.71618197	2.83416230

5C

C	0.45464653	-1.03240122	2.36053496
H	0.09254954	-2.04657602	2.16591978
H	0.68041004	-0.92268235	3.42795036
C	1.76219442	-0.79344551	1.56054864
H	2.15503971	0.19785642	1.80577147
H	2.49394455	-1.55764063	1.84336945
C	-0.63018732	-0.01791679	1.96871871
O	-0.49302561	1.17558884	2.37475500
O	-1.56276643	-0.42090088	1.21290312
C	1.50966393	-0.89470460	0.05464899
O	1.54835177	-2.01426672	-0.49448230
O	1.22040688	0.21438274	-0.54365370
O	-1.31562984	2.71503051	0.21840577
H	-1.34179494	2.23303218	1.07967240
H	-0.38456002	3.01076717	0.20957397
O	-0.05762891	-2.26129471	-2.70308988
H	0.04964874	-1.39395290	-3.12889016
H	0.60030456	-2.24426039	-1.96400068
O	1.45253263	2.57548682	0.88468013
H	0.95829547	2.22964472	1.65485983
H	1.50809795	1.77265157	0.31881676
Na	-1.19944516	0.63303878	-0.83667288
O	-2.29498261	-1.42199122	-1.29703180
H	-2.10067446	-1.51654895	-0.34624170
H	-1.57247169	-1.88354643	-1.78204579
O	0.23942979	0.58062023	-2.88928260
H	0.80204092	0.39399279	-2.07085040
H	0.66928950	1.29368179	-3.37323018

5D

C	0.93664787	0.01018179	2.50340424
H	0.32635235	-0.72364999	3.03527585
H	1.53278430	0.56856661	3.23895408
C	1.89298489	-0.70897567	1.53052857
H	2.56460175	0.01285075	1.05914243
H	2.49442967	-1.43146004	2.09761707
C	-0.01096798	1.00418223	1.80890241
O	-1.21766505	1.00785916	2.14887752
O	0.49178943	1.75331814	0.89669789
C	1.12084015	-1.48306872	0.45333616
O	0.30367250	-2.35548745	0.81114782
O	1.35281716	-1.14450197	-0.77116819
O	-1.31680347	2.93402106	-0.81329719
H	-2.09492753	2.37731508	-0.65622543
H	-0.74120087	2.74462044	-0.03303395
O	2.19397641	1.41323747	-1.26594147
H	1.84913680	1.73292877	-0.40691374
H	2.18037361	0.44040811	-1.13481026
O	-2.32686531	0.25180104	-0.26505022
H	-2.12695820	0.44940145	0.67672253
H	-2.37694709	-0.72763898	-0.35243614
Na	-0.22233185	0.78091820	-1.24444128
O	-1.96363972	-2.44801545	-0.76738287
H	-1.16980893	-2.55581629	-0.18917064
H	-1.58735516	-2.25491769	-1.64318115
O	-0.28410953	-1.22696155	-2.73538720
H	0.40701054	-1.39391185	-2.01446461
H	0.14134804	-1.39964141	-3.58187434

5E

C	0.85388132	-0.00157615	2.27894644
H	-0.05765262	-0.36028537	2.76604225
H	1.47298893	0.46144200	3.06068576
C	1.61570621	-1.16369504	1.63838517
H	2.54264788	-0.81125592	1.17604906
H	1.90155964	-1.88772302	2.41465557
C	0.44780290	1.12172246	1.31198422
O	-0.51876501	1.85668838	1.67457225
O	1.07477231	1.23433607	0.21384040
C	0.83567265	-1.94508357	0.56724592
O	-0.44208112	-1.88290966	0.58658926
O	1.50105531	-2.58557591	-0.28740573
O	-2.27524980	3.16463821	0.02720555
H	-2.89312594	2.42264377	-0.02446389
H	-1.57602377	2.84976827	0.65425026
O	1.91887247	-0.35057011	-1.90704923
H	1.95047924	0.26654226	-1.15062940
H	2.02430009	-1.22655829	-1.48592624
O	-2.31061724	0.07815804	0.39003810
H	-1.91007132	0.72808671	0.99800900
H	-1.83657010	-0.74644610	0.62927679
Na	-0.47412689	-0.08133666	-1.32335896
O	-0.92449421	-2.35455103	-2.04430777
H	-0.95305796	-2.44273907	-1.06149816
H	-0.01078687	-2.62773070	-2.21589241
O	-0.42684358	2.24573543	-1.88083946
H	0.25122095	2.17982857	-1.17412448
H	-1.16197791	2.70595665	-1.42785221

5F

C	1.44980142	0.07183813	2.19517836
H	1.56756269	-0.13976790	3.26718778
H	2.18547761	0.83878447	1.93705094
C	1.69470938	-1.20089805	1.38130492
H	2.73677988	-1.52735323	1.50958790
H	1.05869090	-2.02146785	1.72746239
C	0.06176019	0.70790175	2.00377394
O	-0.06314209	1.90311861	2.38025695
O	-0.86904675	0.01130933	1.47317197
C	1.44840100	-1.01972540	-0.12133102
O	1.06689537	-2.03955659	-0.77547093
O	1.57620661	0.14398002	-0.61112369
O	-0.66828787	2.00380994	-1.01563113
H	-1.28596502	2.36020328	-0.33096514
H	0.15342814	1.80477477	-0.53476745
O	1.04123952	1.02569239	-3.15050686
H	0.39630746	1.68157291	-2.84283388
H	1.40710503	0.66909964	-2.30399569
O	-2.31534694	2.57160744	1.12821857
H	-2.62890810	1.65700474	1.19473079
H	-1.50831797	2.50522049	1.71561333
Na	-1.00316791	-0.34292351	-0.91099201
O	-0.45116820	-1.32896906	-2.98962966
H	0.20792506	-1.75236526	-2.39352294
H	0.02646004	-0.54345898	-3.33004640
O	-1.49537159	-2.40749623	0.37500510
H	-1.26884253	-1.71393585	1.03207982
H	-0.62593630	-2.65617684	0.00646897

5G				5H			
C	-1.35527911	-1.79824267	0.32317819	C	0.86941582	-0.61649251	2.51651793
H	-2.35068816	-1.39056746	0.12462122	H	0.07562373	-1.35756229	2.65067497
H	-1.44302460	-2.79329366	0.77270264	H	1.40557285	-0.46906803	3.46075431
C	-0.58182069	-1.94084053	-1.01460784	C	1.87390081	-1.13602398	1.45425661
H	0.40740972	-2.35902025	-0.81348748	H	2.68416617	-0.41016952	1.33822872
H	-1.13947506	-2.63044784	-1.65774676	H	2.28144567	-2.09629899	1.79056097
C	-0.59861294	-0.88869481	1.29194732	C	0.27440556	0.72551502	2.06383367
O	0.44758851	-1.34823891	1.83850750	O	0.97552967	1.75399072	2.17950281
O	-1.01102277	0.30580628	1.44803341	O	-0.88573215	0.67397862	1.51399834
C	-0.47295375	-0.58951498	-1.72850113	C	1.16633556	-1.34421954	0.11547700
O	-1.50781750	-0.11769336	-2.25960414	O	0.39167180	-2.32739828	-0.00669140
O	0.65905294	0.01474408	-1.67925957	O	1.32772852	-0.43945744	-0.77985774
Na	0.39347456	1.77155601	0.01790795	O	-1.12041462	2.14355830	-0.74338831
O	0.54593988	2.68240238	-2.22067322	H	-1.05419345	1.89641252	0.21113313
H	0.59817653	1.69863389	-2.32086134	H	-0.18870562	2.39241415	-0.93130273
H	-0.40517330	2.85558701	-2.17522302	O	0.64637727	-0.52186691	-3.35176658
O	-1.98621520	1.98175756	-0.55469208	H	0.53487945	0.41103789	-3.56990405
H	-1.98737719	1.33374069	-1.29507689	H	0.98501525	-0.53359821	-2.41400599
H	-1.98525610	1.40093127	0.23379695	O	1.64525678	2.30268908	-0.51789692
O	2.30132067	0.22273501	0.51168113	H	1.50309990	2.39254217	0.44701722
H	1.93399187	-0.03530107	-0.36364433	H	1.71581027	1.32889780	-0.62316277
H	1.83536039	-0.38268155	1.12726969	Na	-1.21396185	-0.31006981	-0.66593099
O	0.81914382	2.13426814	2.37061248	O	-1.32139575	-2.13932583	-2.17813450
H	0.14131538	1.41675319	2.34206263	H	-0.67052598	-2.45279625	-1.50854598
H	1.65344715	1.66629985	2.21758904	H	-0.76887045	-1.69258638	-2.84824875
O	1.27150004	-3.89022104	1.24951085	O	-3.34791559	0.50774499	0.32245690
H	2.08171061	-3.69951657	0.76205288	H	-2.70169389	0.55859146	1.05487648
H	0.93304569	-2.99877910	1.51335029	H	-3.20364882	1.33185167	-0.16542706

5I

C	1.46415330	0.67369658	2.00886157
H	1.65000325	0.79545056	3.08240262
H	2.14709179	1.31163468	1.43957764
C	1.71722760	-0.80938484	1.62884568
H	2.76340070	-1.05559401	1.84493315
H	1.05524273	-1.44847578	2.22033807
C	0.00773028	1.05396721	1.70766720
O	-0.89188989	0.58686257	2.44337165
O	-0.20874571	1.75983320	0.65747045
C	1.45975332	-1.02717662	0.13490904
O	0.35812914	-1.60708058	-0.18705197
O	2.28119446	-0.56733616	-0.69014308
O	1.19236261	3.14855348	-1.05034979
H	0.65425661	3.94484397	-1.12491166
H	0.76991660	2.62244205	-0.30480979
O	0.69319893	0.79608571	-2.46395860
H	0.90216560	1.71757637	-2.20326280
H	1.36507617	0.25670163	-1.97734097
O	-2.86668486	-0.11111842	0.61749834
H	-2.75526875	-1.08009463	0.69468212
H	-2.33613416	0.25711941	1.36395171
Na	-1.06611021	0.22992774	-0.84143711
O	-0.90077763	-1.57373419	-2.57855455
H	-0.27431905	-1.76221745	-1.83666870
H	-0.44992088	-0.86311506	-3.06273242
O	-1.96026475	-2.78713119	0.45023421
H	-1.04065986	-2.42377529	0.44416315
H	-2.12264429	-2.99681816	-0.47905623

5J

C	1.53866986	-0.11587019	2.20206931
H	1.61487022	-0.71283416	3.12362073
H	1.95570064	0.87206581	2.41341832
C	2.30860303	-0.80377982	1.06898678
H	3.38320971	-0.80885881	1.29946555
H	2.00281240	-1.84986193	0.96506801
C	0.05166003	0.09124436	1.91164623
O	-0.55131438	1.04056993	2.45964483
O	-0.51353677	-0.73777434	1.09562134
C	2.11826948	-0.13290528	-0.30846420
O	2.40190207	-0.82018852	-1.32413594
O	1.64435035	1.04882011	-0.30793145
O	0.08165549	2.78728772	-1.77677711
H	-0.49771620	2.95872510	-1.01522066
H	0.87250702	2.34839111	-1.39344281
O	-0.01943691	-1.09551517	-2.58130296
H	-0.31746709	-1.88378958	-2.08784388
H	0.93757978	-1.00557454	-2.35403403
O	-2.85872689	-0.46269749	0.13850887
H	-3.60315809	-0.60546640	0.73381110
H	-2.00872677	-0.55775620	0.69688022
Na	-0.56331491	0.52742400	-1.01067541
O	-1.84761701	2.19981408	0.34781191
H	-1.42523232	1.91800721	1.19726979
H	-2.53609799	1.52823496	0.20496983
O	-1.13782747	-2.81473250	-0.61277144
H	-0.63007860	-2.33244729	0.07060112
H	-1.98811866	-2.34724123	-0.60025318

5K

C	-2.05118505	-1.14352515	1.30022702
C	-2.00715438	0.38137254	1.11893134
C	-0.55822934	-1.67145402	-0.66229284
C	-1.94818588	-1.88314833	-0.05706842
H	-2.10949473	-2.95444397	0.10223274
H	-1.24729698	-1.47719516	1.96595297
H	-3.01466787	-1.39416623	1.76131940
H	-2.71388313	-1.47871846	-0.72663860
O	0.33122257	-2.53130599	-0.44490149
O	-0.98391993	1.00312415	1.62771842
O	-2.91495664	0.94055263	0.48664039
O	-0.38281354	-0.56698888	-1.28805029
Na	0.90137390	0.87486612	-0.06643737
O	-0.62083697	2.76480499	-0.40160690
H	-1.33647921	2.34541546	-0.90323347
H	-0.85086751	2.45733928	0.50548299
O	2.55565500	-1.16230915	0.27310172
H	1.85514729	-1.76077965	-0.09453184
H	2.23957984	-0.90947188	1.16007194
O	1.31508088	0.23828849	-3.13690561
H	0.71568008	-0.21946463	-2.47835764
H	0.75218092	0.90018126	-3.55521506
O	3.03582202	1.15036991	-1.14023862
H	3.13229741	0.27719114	-0.70185520
H	2.59352936	0.93153566	-1.98772250
O	1.26970875	0.12479244	2.39135013
H	1.62099458	0.72784422	3.05461762
H	0.30034612	0.38949042	2.22517532

5L

C	-1.45303825	-1.26664554	-0.65050753
H	-2.42201718	-0.78126909	-0.50194478
H	-1.59362403	-2.34837384	-0.75488654
C	-0.80538685	-0.71866523	-1.95045440
H	0.17302782	-1.18631897	-2.09547633
H	-1.45862394	-0.97080731	-2.79348492
C	-0.54322253	-1.00105028	0.55038444
O	0.49872990	-1.72755156	0.65104024
O	-0.81389476	-0.03816250	1.32329284
C	-0.66709104	0.80866665	-1.88223596
O	-1.71645879	1.49599135	-1.93772569
O	0.50894766	1.28503851	-1.69655101
Na	0.49299370	1.76902967	0.70295135
O	0.54942022	3.78709918	-0.60718435
H	0.52420265	3.04434984	-1.26202232
H	-0.38179333	3.92228900	-0.37982298
O	-1.90796310	2.40947295	0.64826059
H	-2.01655717	2.24677310	-0.31633265
H	-1.86929589	1.49852147	1.00763233
O	2.33832886	0.35225712	0.16368186
H	1.93926047	0.52403242	-0.71598710
H	1.90511800	-0.48137028	0.43987252
O	1.63629239	-2.81485858	2.90114886
H	2.56047605	-2.55919198	2.79627592
H	1.15942847	-2.29349903	2.21197338
O	0.84971532	-4.53222062	0.55858495
H	0.64928692	-3.61041379	0.30505121
H	1.15706971	-4.41468321	1.47155682

5M

C	-0.88007020	0.17976744	-0.58810801
C	-2.28118600	-0.05937441	0.02617758
C	1.21846991	-0.80143626	-1.46813354
C	-0.28443373	-0.98680773	-1.40553936
H	-0.53635742	-1.92731117	-0.91150393
H	-0.93150359	1.08907394	-1.19720431
H	-0.22856867	0.40854030	0.26869357
H	-0.71291436	-0.98262247	-2.41288070
O	1.95017548	-1.44750453	-0.65034926
O	-2.81746091	0.97619755	0.52271645
O	-2.73512452	-1.23363973	0.02922466
O	1.69174126	0.10457669	-2.24232096
Na	2.79321574	0.74814140	0.11038386
O	1.50449686	2.43375476	-0.85371010
H	1.39443049	1.76455595	-1.57084910
H	0.61426406	2.57233003	-0.50423204
O	1.79139806	-0.47713174	1.83679079
H	1.64098508	-1.11143188	1.09538837
H	0.95270125	-0.39289792	2.30796619
O	-2.90968301	0.54220006	3.30659191
H	-3.57881531	-0.15064582	3.17318956
H	-2.79489130	0.86552691	2.38806039
O	4.32454639	0.00545363	-1.54963551
H	4.22312704	-0.90891166	-1.24182352
H	3.47806757	0.10791315	-2.05811168
O	-4.93711868	-0.86674307	1.63825791
H	-4.20483592	-1.21575250	1.07177364
H	-4.88579447	0.07123522	1.39857592

Table S8. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_6$ using B3LYP exchange-correlation functional with dispersion correction.

6A

C	0.05767111	-2.47348781	-0.72102389
H	1.10815238	-2.54522298	-1.01588047
H	-0.48354349	-3.35374292	-1.08479040
C	-0.04312915	-2.43801640	0.82852640
H	-1.09284235	-2.50576993	1.12703145
H	0.50637539	-3.29526684	1.23249144
C	-0.56599516	-1.21565970	-1.33443686
O	-1.82261751	-1.13422143	-1.38183922
O	0.23377344	-0.28694771	-1.69523113
C	0.56876351	-1.14715716	1.38196124
O	1.82445974	-1.05164912	1.42517283
O	-0.24014902	-0.21010888	1.69840772
Na	-0.00659204	1.50065484	-0.04100884
O	2.35728817	1.48559552	0.60048175
H	2.24319171	0.64094211	1.10303755
H	2.80114733	1.17178715	-0.20848544
O	2.94070141	-0.62750569	-1.22996178
H	2.82545308	-1.03326789	-0.35268249
H	2.00980000	-0.52879978	-1.53611714
O	-2.94408273	-0.60466345	1.25117077
H	-2.01502533	-0.48046260	1.55315160
H	-2.82243556	-1.04701599	0.39254139
O	-2.37629487	1.43177610	-0.66842994
H	-2.25667523	0.56619387	-1.13273946
H	-2.81665960	1.15175439	0.15468115
O	0.24781426	2.47165126	2.23838943
H	0.12186093	1.50269577	2.33811309
H	1.16753838	2.54924232	1.93908763
O	-0.28797097	2.36641200	-2.35023020
H	-0.15061387	1.39636558	-2.41654759
H	-1.20512310	2.44244157	-2.04217675

6B

C	-1.36225810	-2.21529465	0.11960448
H	-2.30125857	-1.86185166	-0.31521245
H	-1.52535613	-3.17827451	0.61514410
C	-0.31727859	-2.41252094	-1.00907937
H	0.61082689	-2.80735920	-0.58429481
H	-0.71706669	-3.13984125	-1.72561416
C	-0.85350292	-1.20612522	1.15365611
O	-0.02118898	-1.61155781	2.01373081
O	-1.24206041	0.00064188	1.02653941
C	-0.02820655	-1.10653349	-1.76247735
O	-0.95556259	-0.59638486	-2.44542615
O	1.12864591	-0.58710938	-1.61415642
Na	0.71859664	1.22304939	0.08346710
O	-0.77584566	2.04032764	-1.72102001
H	-0.74860845	1.17680242	-2.19935359
H	-1.68304699	2.03236600	-1.36451939
O	-3.10461843	0.60539468	-0.91391821
H	-2.67533869	0.06864112	-1.60366507
H	-2.55356639	0.39570414	-0.12520403
O	2.31106270	-0.59682080	0.81533812
H	2.12774772	-0.76574111	-0.13611748
H	1.64606320	-1.14927256	1.26958174
O	1.48957976	0.12959018	3.59274738
H	0.85082042	-0.49535296	3.17301868
H	2.25731966	0.09141205	3.00426767
O	0.06881499	2.11554468	2.21621757
H	-0.61663352	1.44100973	2.02216914
H	0.63943800	1.64510745	2.85872605
O	2.03128973	2.02365383	-1.86597400
H	1.81512268	1.08459150	-2.05544166
H	1.19879624	2.48332401	-2.06112112

6C

C	0.71196388	-1.56131221	2.10632124
H	0.37449913	-2.57914656	1.89486711
H	0.85659415	-1.46764557	3.19198896
C	2.04887519	-1.29525462	1.38850922
H	2.43481188	-0.30197618	1.62921401
H	2.78083318	-2.03786493	1.73324023
C	-0.42215356	-0.60325213	1.71248564
O	-0.10903995	0.60297706	1.42062599
O	-1.59408483	-1.06194472	1.66362403
C	1.89889593	-1.44992635	-0.13214667
O	1.39379829	-2.51278906	-0.56701692
O	2.26111919	-0.46047504	-0.86495962
O	-1.71760254	2.76667394	0.72328913
H	-1.17980952	2.06917419	1.16153703
H	-1.20022286	2.98593044	-0.07266657
O	-3.13490362	0.51283757	-0.07915152
H	-2.94322320	1.42904327	0.20682634
H	-2.77579457	-0.04144036	0.64948770
O	2.06472656	1.92952579	0.38118353
H	1.39521232	1.53217960	0.97881911
H	2.37296682	1.12540681	-0.10352823
Na	-0.87340357	0.43012278	-0.91006142
O	-1.21758885	-1.91914088	-1.10469477
H	-1.59040599	-1.99908245	-0.21136233
H	-0.30923698	-2.29027588	-1.02960061
O	0.69566155	0.26595591	-2.78374515
H	1.37415049	-0.13162579	-2.14872225
H	0.60427805	-0.35383641	-3.51477905
O	0.15468613	2.63484082	-1.40161218
H	0.92522505	2.51833314	-0.78447541
H	0.38973594	2.11864601	-2.19124503

6D

C	1.19132753	-0.50186860	2.39819016
H	0.62177515	-1.38848847	2.69116882
H	1.75938854	-0.12720882	3.25769048
C	2.18652961	-0.88141361	1.27202604
H	2.81224759	-0.01548924	1.03596355
H	2.81906085	-1.70154319	1.62798148
C	0.22945227	0.59002661	1.93091176
O	0.66615059	1.76607285	1.80344188
O	-0.95910256	0.22936101	1.63146690
C	1.44039768	-1.34384995	0.01234555
O	1.03344222	-2.52540782	-0.04177936
O	1.24189735	-0.45237467	-0.89801203
O	-0.43495459	2.65565246	-0.53200792
H	-0.18381966	2.49754146	0.41282075
H	0.44783840	2.69800211	-0.94904026
O	-2.90241158	1.65308419	0.44656502
H	-2.46750833	2.33538367	-0.08772288
H	-2.19408953	1.34466683	1.06729289
O	2.30977340	2.04136811	-0.60694289
H	2.11061288	2.13655245	0.34021719
H	2.02928967	1.10840379	-0.78147044
Na	-0.96479205	0.31240656	-0.79659160
O	0.34122582	-2.41920585	-2.72311525
H	0.44210199	-2.79624009	-1.81974294
H	0.82524975	-1.58608769	-2.57178506
O	-2.93006599	-1.16665645	0.19449986
H	-2.23281884	-1.14592304	0.87547360
H	-3.27360959	-0.25358903	0.20425634
O	-2.01217114	-1.00120637	-2.46347589
H	-2.46626167	-1.36937988	-1.68317264
H	-1.27111513	-1.62134252	-2.66141579

6E

C	0.51495932	-1.29173977	2.40551994
H	0.12265399	-2.28400212	2.16964226
H	0.70537343	-1.21866464	3.48414459
C	1.84620890	-1.07539953	1.65371526
H	2.24307556	-0.08137873	1.87803252
H	2.56717356	-1.82787031	1.99772261
C	-0.53243038	-0.23554546	2.03531278
O	-0.24778201	0.98374552	2.29202611
O	-1.59830933	-0.61144397	1.47670305
C	1.68056729	-1.25141792	0.13627863
O	1.26428316	-2.35160149	-0.28782407
O	1.97327032	-0.23267378	-0.59265871
O	-1.96265455	2.70502915	1.14403620
H	-1.38902790	2.11900635	1.71382496
H	-1.34754278	3.29800783	0.69329894
O	-0.22842077	-2.25646970	-2.57727941
H	0.14141663	-1.45500610	-2.99068956
H	0.36787643	-2.40065941	-1.79961663
O	1.45766433	2.20182272	0.48236367
H	0.94527006	1.87995593	1.25491725
H	1.83343774	1.36183373	0.11919073
Na	-1.82708201	0.85741242	-0.32083339
O	-2.34277945	-1.26156034	-1.14832755
H	-2.10339423	-1.51652696	-0.23876367
H	-1.65191046	-1.67332226	-1.72531549
O	1.09248363	0.21774430	-2.96635856
H	1.49504162	-0.03688594	-2.06447856
H	1.83277599	0.39344377	-3.55763770
O	-0.38259321	2.16386830	-1.56828713
H	0.29647593	2.31646670	-0.86647189
H	0.07448005	1.59853236	-2.22360185

6F

C	0.61043101	-0.81437235	2.58828663
H	-0.04244618	-1.68756707	2.66193935
H	1.00014999	-0.56167549	3.58274539
C	1.80087958	-1.14177338	1.66074485
H	2.45520513	-0.26983661	1.57342491
H	2.37177144	-1.96718141	2.10473843
C	-0.20175978	0.38049599	2.07733378
O	0.40389379	1.50262605	1.99041484
O	-1.40334723	0.19606235	1.74341620
C	1.33388393	-1.59649636	0.26939857
O	0.60390680	-2.60887530	0.19386024
O	1.72375414	-0.88130851	-0.72631407
O	-1.02350016	3.31375775	0.61166482
H	-0.51982684	2.73836786	1.25410283
H	-0.36530712	3.60921338	-0.03058117
O	0.58216122	-0.76168562	-3.02729882
H	1.22939710	-0.93467523	-3.71985424
H	1.06164603	-0.90440854	-2.13842965
O	1.97640304	1.77979285	-0.27402256
H	1.55421531	1.79010426	0.61173936
H	2.07831978	0.81041487	-0.44373395
Na	-1.60070821	1.23015013	-0.33576289
O	-1.20458978	-2.62090829	-1.85906476
H	-0.53291973	-2.74573211	-1.14200583
H	-0.73219340	-2.06581309	-2.50622627
O	-2.74079578	-0.79784077	-0.51081929
H	-2.40792139	-0.89772987	0.39960830
H	-2.27868222	-1.49841775	-1.03561668
O	-0.13894378	1.77322062	-2.04211315
H	0.66357802	1.89524542	-1.47865881
H	0.05829084	0.97232808	-2.56904361

6G

C	-2.31616018	-1.42939278	1.30000018
C	-2.19259070	0.09096934	1.13343478
C	-0.68658979	-1.91293118	-0.56936506
C	-2.10624004	-2.15690825	-0.05365226
H	-2.24929855	-3.23260974	0.09833614
H	-1.57912989	-1.79373582	2.02289062
H	-3.32562697	-1.65493602	1.66292539
H	-2.83545901	-1.77780811	-0.77582006
O	0.24580476	-2.61244886	-0.10024457
O	-1.07624272	0.62264943	1.53414568
O	-3.11409754	0.72421717	0.59578720
O	-0.53917911	-0.93838034	-1.38931879
Na	0.66349479	0.54184184	-0.10179325
O	-0.67954080	2.70491822	0.03249734
H	-1.46187408	2.77890788	-0.52758073
H	-0.96303775	2.04615352	0.74076151
O	2.49003025	-1.18878725	0.33811151
H	1.76171535	-1.82532343	0.10895276
H	2.25719542	-0.81347829	1.21386485
O	1.19628037	-0.24457482	-3.22322353
H	0.58076087	-0.65086389	-2.54209911
H	0.61914238	0.26004788	-3.80773769
O	2.80875847	0.92216461	-1.33744619
H	2.91889839	0.09894430	-0.80283827
H	2.35124097	0.62299148	-2.15546524
O	1.49586927	0.41000924	2.38222248
H	1.73772358	1.28761822	2.02252450
H	0.51373887	0.37281329	2.33472704
O	1.99942468	2.63125855	0.68526869
H	2.41588316	2.23322719	-0.10912950
H	1.13644583	2.98116004	0.39085830

6H

C	0.12296657	-1.54078507	1.86186271
H	-0.32462120	-2.46605434	1.48774604
H	0.32233048	-1.63047433	2.93519136
C	1.48041109	-1.30232981	1.14772526
H	1.96564805	-0.43037659	1.59329199
H	2.11087045	-2.18356530	1.30273710
C	-0.84411656	-0.37919275	1.61467693
O	-0.64675763	0.70483095	2.26316036
O	-1.74184879	-0.52496573	0.74365179
C	1.28899134	-1.09468546	-0.35475644
O	1.22949723	-2.09032767	-1.10375190
O	1.15232190	0.13224854	-0.74353332
O	-1.25600573	2.64719608	0.29465556
H	-1.37076251	2.05089406	1.06848930
H	-0.31986717	2.90417701	0.37846340
O	-0.23749043	-1.78811847	-3.38528264
H	-0.01401906	-0.88004005	-3.65072624
H	0.37174946	-1.96690488	-2.62512442
O	1.47436583	2.15388244	1.10315636
H	0.80804654	1.74866214	1.69184390
H	1.53200742	1.47161972	0.39488231
Na	-1.20090597	0.78311969	-1.11302716
O	-2.46052232	-1.02390266	-1.94933482
H	-2.33452921	-1.32794809	-1.03327904
H	-1.75425574	-1.45216404	-2.48910434
O	0.37297876	0.98536328	-3.04296199
H	0.86436091	0.61249206	-2.24350658
H	0.89190388	1.72354657	-3.37967293
O	1.55102254	0.76533640	4.00794485
H	2.09623070	1.27435550	3.39231370
H	0.69534401	0.67859028	3.53208560

6I

C	1.65345217	-0.08986295	2.16254795
H	1.62851542	-0.56335232	3.15469772
H	2.42440711	0.68409575	2.17756975
C	1.96461622	-1.14697092	1.08947262
H	3.00188605	-1.48912500	1.21005264
H	1.31628505	-2.02156599	1.18678504
C	0.31103037	0.61450203	1.94566810
O	0.18396793	1.80342899	2.33328865
O	-0.61657693	-0.04884271	1.36107855
C	1.80961037	-0.57065080	-0.32618051
O	1.26711305	-1.32378903	-1.20776077
O	2.16984311	0.61811877	-0.52266100
O	0.06216527	1.97040149	-1.52729812
H	-0.33552694	2.51752010	-0.82041826
H	0.93091665	1.63919680	-1.18764766
O	-0.01028792	-0.22100192	-3.38686980
H	0.67104977	-0.64433080	-2.81292198
H	0.07189925	0.72484131	-3.18199572
O	-1.24871857	3.21533249	0.64432169
H	-1.05420768	4.14242568	0.82045331
H	-0.77158114	2.68970152	1.36305780
Na	-0.90074824	-0.19962787	-1.10295357
O	-2.78955600	0.83931118	0.13662581
H	-2.07392308	0.64180537	0.79665179
H	-2.74982714	1.80558119	0.06854911
O	0.26340073	-3.81693434	-0.44279895
H	-0.65717252	-3.54565587	-0.31447181
H	0.70362015	-2.99488180	-0.75464871
O	-2.00052790	-2.02674744	0.18283109
H	-1.40724098	-1.57269607	0.82180884
H	-2.82831187	-1.52816234	0.22947617

6J

C	1.97057337	-0.17668976	2.05850289
H	2.06228706	-0.64349844	3.04963913
H	2.60019354	0.71631483	2.05324203
C	2.42943520	-1.15962538	0.96993865
H	3.51051317	-1.32872366	1.07212782
H	1.93349552	-2.12877759	1.07458971
C	0.51957073	0.29578647	1.89928883
O	0.20281615	1.40480525	2.39485343
O	-0.28403807	-0.46598650	1.25648631
C	2.16738919	-0.61090619	-0.44264804
O	1.72300856	-1.43428800	-1.31693425
O	2.36398071	0.61392980	-0.64140553
O	0.04434191	1.78787120	-1.45740014
H	-0.41758002	2.23959912	-0.72038901
H	0.95309232	1.56491464	-1.14675161
O	0.34144308	-0.37633204	-3.42797899
H	1.05882979	-0.73236331	-2.84885641
H	0.34047366	0.57713849	-3.25020800
O	-1.38214793	2.71856153	0.77749739
H	-1.28456241	3.64522337	1.02379149
H	-0.87139694	2.19475094	1.47243882
Na	-0.59991157	-0.45571994	-1.18251720
O	-4.09616040	1.77503423	0.51716515
H	-3.90814075	0.84295740	0.32264690
H	-3.20869160	2.16602291	0.62531037
O	-0.40287837	-2.77936875	-0.19544266
H	-0.27806522	-2.15641415	0.55224100
H	0.43362588	-2.64482234	-0.69267018
O	-2.66417218	-0.74210985	0.10170709
H	-1.96655272	-0.50573433	0.76325049
H	-2.58463815	-1.70199977	0.00902078

6K

C	0.86993301	-0.49808850	2.60420247
H	0.03453631	-1.19820218	2.70726344
H	1.34165324	-0.33984137	3.57992473
C	1.92213928	-1.10122971	1.63514537
H	2.74201664	-0.38817178	1.50465067
H	2.30515548	-2.03576320	2.05966220
C	0.38627392	0.85546360	2.06667284
O	1.13063289	1.84723002	2.22498237
O	-0.72050084	0.86034680	1.41168586
C	1.26665746	-1.40754270	0.29094972
O	0.53762539	-2.43122521	0.20903383
O	1.40255841	-0.54632460	-0.64942110
O	-0.75876045	2.83427208	-0.45934853
H	-0.79569400	2.32277984	0.38993385
H	0.19621721	2.75106064	-0.68487818
O	1.13451766	-1.06490928	-3.25645189
H	1.17497823	-0.19445243	-3.66891577
H	1.29721378	-0.90161403	-2.28666449
O	1.94026686	2.19028927	-0.44868633
H	1.83751035	2.30868918	0.51822168
H	1.86515046	1.21571236	-0.54879229
Na	-1.17297530	-0.61746775	-0.50787200
O	-1.03030804	-2.43906198	-2.07307940
H	-0.41663718	-2.69376566	-1.34673806
H	-0.43711095	-2.05666065	-2.74686954
O	-3.19900160	-0.16746807	0.84517094
H	-2.45018658	0.23182478	1.33630899
H	-3.33455271	0.42900762	0.09078637
O	-2.33851989	1.13700892	-1.61327568
H	-1.73503981	1.88738994	-1.30558757
H	-2.49480992	1.23534759	-2.55739847

6L

C	1.56898942	-0.65512215	2.08117167
H	1.49817768	-1.57129517	2.68492151
H	2.09991385	0.10321257	2.66023889
C	2.31718303	-0.95817691	0.76404827
H	3.38081792	-1.11245313	0.98928753
H	1.93180248	-1.86767343	0.29699015
C	0.15236582	-0.13676065	1.83088004
O	-0.32213058	0.76608697	2.56108741
O	-0.47720092	-0.64317381	0.82747041
C	2.18184800	0.21961280	-0.21880403
O	1.81016584	-0.02716456	-1.40989008
O	2.37402046	1.37497876	0.25197826
O	0.50400773	3.04670051	-0.75669854
H	-0.09084587	3.05372972	0.01022541
H	1.32569216	2.58056606	-0.44775686
O	0.21730960	-1.99430115	-2.36619772
H	0.05441704	-2.59086336	-1.61066107
H	0.91506239	-1.36896785	-2.04336140
O	-3.01828891	-0.21985216	0.04112861
H	-3.06064913	0.73032267	0.23800798
H	-2.15895235	-0.46128258	0.46731159
Na	-0.37864519	0.88734336	-1.10017877
O	-1.75471212	2.20911946	0.90608864
H	-1.30299113	1.66569413	1.62820239
H	-2.13062311	2.98322557	1.33982981
O	-0.32824761	-3.21382620	0.13924994
H	-0.32379989	-2.26766418	0.44869360
H	-1.24861693	-3.49351997	0.21081531
O	-1.85578407	-0.19862356	-2.52823708
H	-1.21235432	-0.94788818	-2.57279983
H	-2.43568656	-0.36947905	-1.75860431

6M

C	-1.91002581	-1.32873199	0.15814056
H	-2.82717044	-0.73305585	0.17301938
H	-2.14057119	-2.37430774	0.39132011
C	-1.28495944	-1.26988391	-1.26199875
H	-0.36125242	-1.85430371	-1.28525017
H	-2.00081714	-1.70641418	-1.96668968
C	-0.92452314	-0.80128605	1.19967706
O	0.06482623	-1.53933165	1.50246304
O	-1.08246314	0.37197610	1.65818206
C	-1.02797427	0.18555294	-1.66827532
O	-2.01900560	0.91097658	-1.92047075
O	0.18888570	0.59569127	-1.64997723
Na	0.51006436	1.84813183	0.39648006
O	0.59159305	3.30006909	-1.53620970
H	0.41201158	2.39267300	-1.88435580
H	-0.28253331	3.61932489	-1.26941136
O	-1.83129252	2.63683788	0.21101346
H	-2.04869306	2.18922257	-0.63841759
H	-1.89094254	1.90351577	0.85556465
O	2.05221267	-0.17577597	0.15573158
H	1.50202424	-0.07424920	-0.65918740
H	1.49934650	-0.74971542	0.72840344
O	1.23214716	1.47703703	2.65381326
H	0.40113612	0.94943601	2.59178311
H	1.91838970	0.87317770	2.33542716
O	0.59481465	-3.81238512	0.20399888
H	0.33374428	-2.99156395	0.70451370
H	0.87285854	-4.44258284	0.87902905
O	3.18789248	-2.80351279	-0.62959139
H	2.31006015	-3.19979029	-0.47021789
H	3.05618349	-1.85848010	-0.43995214

6N

C	0.89069900	-1.34629410	2.14275751
H	0.64068438	-2.35226011	1.79498390
H	0.99517865	-1.38035612	3.23673421
C	2.21728223	-0.87843090	1.51464802
H	2.44298728	0.13875807	1.84270566
H	3.01759009	-1.55788618	1.83442700
C	-0.27889842	-0.40568717	1.83150996
O	-0.02440880	0.83615048	1.77212213
O	-1.42314276	-0.91552494	1.62307027
C	2.14287714	-0.92605794	-0.01722874
O	1.97357008	-2.04805539	-0.55520929
O	2.23474723	0.19096472	-0.63961716
O	-1.49270536	2.95438531	1.12687027
H	-0.93493741	2.23613973	1.52921214
H	-0.97368864	3.22157337	0.35276975
O	-3.53128488	0.89267430	1.23842849
H	-3.11222029	1.75133572	1.41820111
H	-2.90537959	0.22110944	1.59562822
O	0.42012264	-1.96622332	-2.77047093
H	1.06061317	-2.09586998	-2.02264538
H	0.70852559	-1.11808510	-3.15536334
Na	-1.60243829	0.78741769	-0.26497002
O	-1.73823762	-1.25523067	-1.27821013
H	-1.62449110	-1.66494364	-0.40483547
H	-0.99248546	-1.57853330	-1.84759373
O	1.57573382	0.60832485	-3.08086756
H	1.93695207	0.34603108	-2.15955913
H	2.34158733	0.78360559	-3.63867285
O	0.21555080	2.05215878	-1.05749520
H	0.88162019	1.56305892	-0.52426856
H	0.51024963	1.86350720	-1.96712357

6O

C	0.66502116	-1.59154965	2.14536347
H	0.33139130	-2.60718622	1.91904019
H	0.86891876	-1.53596442	3.22483324
C	1.94289869	-1.26224549	1.36314016
H	2.31947652	-0.27118493	1.63050559
H	2.72449581	-1.98746920	1.63043696
C	-0.50400178	-0.64250466	1.86227945
O	-0.23907821	0.56993872	1.56911014
O	-1.67531500	-1.11394334	1.91931447
C	1.76028618	-1.33921642	-0.16645870
O	0.94331237	-2.17186130	-0.62625821
O	2.47429938	-0.53766241	-0.86312943
O	-1.12424916	3.03780085	0.73616953
H	-0.96754644	2.30166310	1.36047481
H	-0.24201078	3.23314760	0.38790867
O	-3.54443030	0.29667683	0.55815404
H	-3.77005354	-0.40392911	-0.06798028
H	-2.94530605	-0.15039356	1.21421429
O	1.69711517	1.89292605	0.15733120
H	1.12035346	1.41217552	0.79353915
H	2.22203601	1.15309433	-0.22921307
Na	-1.48060126	0.89912234	-0.51438653
O	-1.65606654	-1.46147010	-0.96433240
H	-1.78344035	-1.70418525	-0.03071111
H	-0.73171163	-1.76084365	-1.12594815
O	1.62278009	-0.07823273	-3.34118833
H	1.95049568	-0.40080852	-2.44860507
H	2.38041150	0.36721830	-3.73808944
O	-0.01346490	1.75990806	-2.06785665
H	0.64267909	1.95706837	-1.36462494
H	0.45478715	1.11780719	-2.64798735

6P

C	-1.33100834	-1.54324781	1.43978130
C	-1.84667060	-0.25865487	0.78190630
C	0.52095648	-2.01316990	-0.23988879
C	-0.76214615	-2.54434884	0.40640602
H	-0.53950500	-3.49141342	0.90768651
H	-0.57122115	-1.30652330	2.19161535
H	-2.18278086	-2.01787822	1.94328005
H	-1.51955158	-2.70133266	-0.36929581
O	1.62433229	-2.49603101	0.10477764
O	-2.81626812	-0.35209103	-0.00479654
O	-1.24716681	0.83890290	1.08624264
O	0.35449785	-1.06336998	-1.08718408
Na	0.57349273	1.19021666	-0.56029341
O	-1.21159865	2.76266281	-0.84297136
H	-1.91607215	2.47203236	-1.45744893
H	-1.43856437	2.25555723	-0.02948983
O	3.65131993	-0.67264451	-0.20638799
H	2.99320456	-1.40636982	-0.09713754
H	3.47301900	-0.33638936	-1.10137337
O	-3.40202010	1.41144352	-1.92680124
H	-4.22284454	1.82145171	-1.63104273
H	-3.18778574	0.73342456	-1.22259436
O	2.08455154	0.28965930	-2.39273132
H	1.47723845	-0.41197771	-1.98258429
H	1.95407680	0.25384039	-3.34616965
O	2.29711643	1.42646323	0.95646115
H	2.87803193	0.67348537	0.69274447
H	1.86833480	1.19055774	1.80363616
O	0.51099711	0.96149977	3.06010359
H	-0.19902378	0.88495125	2.35791765
H	0.34238235	1.79918762	3.50649531

Table S9. The Cartesian atomic coordinates of the typical low-lying isomers of Na$^+$(DC$_2^{2-}$)(H$_2$O)$_7$ using B3LYP exchange-correlation functional with dispersion correction.

7A				7B			
C	-2.24694843	-0.21485323	1.56954001	C	-2.24203639	0.58074227	-1.43272732
H	-2.97771462	0.42284582	1.06562170	H	-2.99926670	0.06198604	-0.83916329
H	-2.59328052	-0.36795443	2.60115269	H	-2.67025855	0.76522446	-2.42778226
C	-2.12490144	-1.57600115	0.86338993	C	-1.86037685	1.92060914	-0.79026355
H	-1.58533592	-2.29485671	1.48598861	H	-1.28933246	2.53794853	-1.48982576
H	-3.12747365	-1.98938380	0.68691885	H	-2.76959896	2.48569950	-0.54417408
C	-0.91753680	0.54746292	1.62732676	C	-1.04834548	-0.36254756	-1.60392200
O	0.15008768	-0.14230308	1.77087675	O	0.08136755	0.14433225	-1.90205031
O	-0.93575513	1.79979549	1.48237679	O	-1.23407174	-1.59495288	-1.38270975
C	-1.41026284	-1.48253739	-0.49377107	C	-1.03403259	1.80114456	0.50189197
O	-1.46917676	-0.38732344	-1.12717306	O	-1.03899065	0.69854413	1.13417487
O	-0.74915966	-2.48679677	-0.89591287	O	-0.36876617	2.82060355	0.84478346
O	2.73242817	0.82425478	1.50468508	O	2.43748056	-1.23966906	-1.49807651
H	1.85968129	0.50885526	1.83243686	H	1.65377969	-0.75560402	-1.84957157
H	2.99978731	0.14485359	0.85460209	H	2.82364112	-0.63968495	-0.83532668
O	1.31503325	2.76475981	0.20831185	O	0.79352486	-3.25723592	-0.57657875
H	2.03601829	2.28845271	0.67535767	H	1.57633391	-2.78723588	-0.92975195
H	0.52138886	2.58835214	0.76692901	H	0.03921156	-2.80592790	-1.02146077
O	1.08852955	-2.70755026	1.15987075	O	1.46562308	2.48637097	-1.29505376
H	0.70373889	-1.90754641	1.57666347	H	0.90300363	1.77292104	-1.66651624
H	0.43450757	-2.92121291	0.45925829	H	0.88747650	2.92065216	-0.63780088
Na	0.81809550	0.39198047	-0.51994758	Na	0.66869649	-0.82465831	0.42621162
O	-2.20505169	2.19409731	-1.05631647	O	-2.38515108	-1.68827107	1.17993794
H	-1.91432628	2.36602431	-0.14122817	H	-2.22278080	-1.88208115	0.23566376
H	-2.18635722	1.21083680	-1.08711574	H	-2.09905493	-0.75016718	1.24316322
O	1.01373197	-1.10991262	-2.57596476	O	1.22683734	1.69444664	2.76330918
H	0.30739702	-1.67248885	-2.17406144	H	0.68380111	2.26901728	2.16423098
H	0.56812685	-0.29122473	-2.84767903	H	0.60349411	0.97289648	2.93430545
O	2.75717312	-1.20259268	-0.41016818	O	2.52091156	0.69941250	0.53911303
H	2.27874970	-1.87462402	0.13655977	H	2.27601432	1.41631771	-0.09316413
H	2.38391688	-1.27293198	-1.31202054	H	2.26039646	1.04329574	1.42583836
O	0.33771619	1.98322208	-2.29705397	O	0.15969190	-2.49515200	2.03982865
H	0.82788016	2.52279867	-1.64624302	H	0.41285074	-3.06024468	1.28224051
H	-0.60064487	2.13391204	-2.04289650	H	-0.80447819	-2.34502583	1.91912849

7C

C	-0.84049074	2.91660824	-0.05445439
H	-0.95217930	2.97477398	-1.14142917
H	-0.83740886	3.93011089	0.36346913
C	-2.03832794	2.13965223	0.55067706
H	-1.95330104	2.15124428	1.64074968
H	-2.96813572	2.62812967	0.23860518
C	0.48930202	2.23615366	0.29508629
O	0.87668601	2.25285766	1.48487184
O	1.09011121	1.62818790	-0.66605946
C	-2.04298689	0.68888315	0.06231130
O	-2.48860464	0.44327889	-1.09802737
O	-1.52888181	-0.18595702	0.82974132
Na	0.64339855	-0.68528096	-0.00029931
O	-0.07767369	0.01057218	-2.43024225
H	-1.02580693	0.05631564	-2.19161124
H	0.32000237	0.78928290	-1.96936544
O	-2.59080466	-2.35145983	-0.75396834
H	-2.58534388	-1.44516385	-1.13951276
H	-2.60712382	-2.11720996	0.18728017
O	3.15899505	-0.14410104	-0.53567146
H	3.09078822	-0.29695103	0.43035809
H	2.60911709	0.66789171	-0.64393739
O	2.12334440	-0.13866310	1.98967483
H	1.44295311	-0.73923248	2.36008881
H	1.73624464	0.77166691	1.94486900
O	-0.00663351	-1.87243670	2.35046073
H	0.04152137	-2.49938859	1.59894337
H	-0.70514333	-1.24262028	2.08555853
O	1.74423734	-2.00511310	-1.99285311
H	2.42679240	-1.43578681	-1.56878446
H	1.10409043	-1.37167389	-2.38473226
O	0.03411785	-3.10008253	-0.16523923
H	0.69172030	-2.94742977	-0.88112560
H	-0.85841355	-2.94493069	-0.54934533

7D

C	-0.27196402	-2.25360770	1.75403668
H	-1.26738487	-2.01219100	2.13744917
H	0.19042538	-3.00723653	2.40153730
C	-0.40130626	-2.84721396	0.32448326
H	0.57679540	-3.20139698	-0.01174946
H	-1.09351809	-3.69502303	0.36761624
C	0.60500416	-0.99590291	1.75906433
O	1.84643278	-1.12965848	1.60354623
O	0.00482126	0.13265170	1.84251917
C	-0.96180022	-1.80920994	-0.66342736
O	-2.18575705	-1.55963979	-0.63573783
O	-0.10800871	-1.20602690	-1.41491862
Na	0.09536458	0.87377940	-0.32855017
O	-2.76044701	0.15339742	1.45185592
H	-2.77277630	-0.56232386	0.78116289
H	-1.83462698	0.13440260	1.78254506
O	-0.68230236	1.30017414	-2.61926032
H	-0.65010191	0.32591655	-2.49304189
H	-1.41224780	1.60457136	-2.04175379
O	2.61207398	0.70515126	-0.26432347
H	2.46499775	0.28672171	0.61720276
H	2.77056353	-0.08575308	-0.82580208
O	0.10604975	2.96283545	1.27631119
H	0.69654414	3.08530199	0.50532132
H	0.33812315	2.11728523	1.70605226
O	1.34294449	2.89075954	-1.27251097
H	0.75997351	2.50555534	-1.95671204
H	2.00675511	2.19906996	-1.06275920
O	2.51294520	-1.91019700	-1.13342719
H	2.49174866	-2.01720987	-0.16573066
H	1.55993253	-1.75115629	-1.35145098
O	-2.06017617	2.13418635	-0.30707668
H	-1.49401468	2.65862184	0.29472294
H	-2.50670902	1.48057983	0.28497772

7E

C	-1.16492393	1.07026649	-2.16728300
H	-1.22761926	0.12866268	-2.71809369
H	-1.37955325	1.90399924	-2.84416958
C	-2.22403967	1.07648649	-1.02846543
H	-2.30737335	2.08562243	-0.61587062
H	-3.18972947	0.77590180	-1.44986203
C	0.24525856	1.23990987	-1.59291148
O	0.62981135	2.39861943	-1.28279904
O	0.92066191	0.17341488	-1.38877753
C	-1.84028658	0.10566294	0.09353545
O	-2.00440773	-1.13339035	-0.09855595
O	-1.31075259	0.60879905	1.13631403
Na	1.02242209	-0.17388914	1.06911945
O	0.66305561	-4.18661703	-0.74549405
H	0.32906317	-3.47089203	-1.35657718
H	0.05666691	-4.92816385	-0.85316600
O	-0.36925977	-2.13329680	-2.11081319
H	-1.12988593	-1.89810326	-1.53759716
H	0.22636665	-1.35841310	-1.96017593
O	-0.71472029	3.31762345	1.12774238
H	-1.03114637	2.39071874	1.22353487
H	-0.39170467	3.33031415	0.20954947
O	1.90588704	2.12110055	1.09501474
H	1.63460508	2.28099969	0.15668775
H	1.23590758	2.62829215	1.58622699
O	3.28895249	-0.12417736	0.05933332
H	2.65059066	0.03428142	-0.66929895
H	3.31405663	0.72561042	0.52736983
O	0.01732287	-0.51653454	3.33952316
H	0.04244354	-1.42545870	2.99026128
H	-0.67594274	-0.10109555	2.78807536
O	0.02244547	-2.37197778	1.28168404
H	-0.80786107	-2.03870217	0.86198419
H	0.33323612	-3.10746546	0.71411417

7F

C	1.36281590	2.40476100	0.67157946
H	2.40668455	2.20933762	0.40887425
H	1.31571165	3.23722888	1.38304003
C	0.57846488	2.80184245	-0.60934909
H	-0.42431301	3.13550000	-0.32724976
H	1.11125029	3.62344522	-1.09903385
C	0.76927831	1.15613117	1.32691369
O	-0.33823079	1.25073121	1.92882183
O	1.38958551	0.05502478	1.15613692
C	0.49127479	1.61128994	-1.57884035
O	1.45056444	1.39034237	-2.34492396
O	-0.56020400	0.87605302	-1.46245958
Na	-0.67854888	-0.86022132	0.18584976
O	2.04371393	-2.63677478	1.46284441
H	2.78527638	-2.40250889	0.88707142
H	1.65839146	-1.76544382	1.68799695
O	-1.76111876	-1.49408714	-2.08996966
H	-1.06153912	-2.14525501	-1.89772833
H	-1.28438646	-0.63681867	-2.17817404
O	-1.35290032	-1.32926905	2.46043074
H	-2.20451799	-1.28061990	1.98960211
H	-1.02472333	-0.40545473	2.51671240
O	-3.19843687	-0.95113151	0.28562901
H	-3.16834534	0.03499471	0.26161006
H	-2.95275050	-1.24015266	-0.61718176
O	-2.52025839	1.70114545	0.21998667
H	-1.88194244	1.52927170	-0.51644576
H	-1.92168955	1.75658513	0.99052084
O	2.52581641	-0.85954448	-1.14408107
H	2.26936717	-0.40723734	-0.30648245
H	2.29459996	-0.18983743	-1.82301203
O	0.51398161	-2.65638174	-0.89926860
H	1.26037334	-2.06014040	-1.16779287
H	0.83722609	-3.02482710	-0.05448518

7G				**7H**			
C	-2.26045208	1.12613818	-1.10299870	C	1.78821102	-0.98732707	-1.91951474
H	-1.90482391	1.53545001	-2.05168029	H	1.05665659	-1.23517115	-2.69321991
H	-3.25907041	1.54926610	-0.92679817	H	2.73767968	-1.45619837	-2.21382722
C	-2.36439917	-0.40272302	-1.17861558	C	1.98157754	0.52690618	-1.81814320
H	-2.96274992	-0.79475618	-0.35288505	H	2.84703486	0.76815675	-1.19327057
H	-2.86861305	-0.68469805	-2.11356666	H	2.18791724	0.94867715	-2.81143255
C	-1.34032681	1.64091904	0.01853192	C	1.33911016	-1.64944745	-0.60808231
O	-1.20702480	0.91349964	1.05531316	O	1.68403051	-1.09902755	0.48610995
O	-0.77620504	2.75034617	-0.17084165	O	0.65072551	-2.70237143	-0.69754720
C	-1.00529523	-1.10812607	-1.16017069	C	0.78703363	1.29406873	-1.23974896
O	-0.05005485	-0.59515257	-1.82173588	O	-0.34104172	0.69529819	-1.16377145
O	-0.91219156	-2.16766341	-0.47045065	O	1.00033777	2.46449317	-0.82837854
Na	0.35749832	-0.96668086	1.48794423	Na	-0.06940074	0.60967552	1.48743233
O	0.60963548	2.06332368	-2.58174673	O	-1.50245374	-1.66510982	-2.21841832
H	0.01481889	2.55393761	-1.98238658	H	-0.77180529	-2.27676755	-2.00364407
H	0.36245149	1.13020078	-2.41172765	H	-1.12774508	-0.80624624	-1.93043254
O	1.38636573	-3.01893105	0.67664545	O	-0.77064189	2.90993761	1.21378473
H	2.09222935	-2.73344087	0.07492469	H	-1.65859191	2.82300498	0.83461745
H	0.57926200	-2.94230547	0.11793802	H	-0.17737242	2.95063570	0.42777001
O	0.59788716	0.86017141	3.13084041	O	0.23143895	-1.48985590	2.72526332
H	1.45837394	0.94153677	2.69439709	H	-0.59042872	-1.93526044	2.48014243
H	-0.05281658	1.18475739	2.46820951	H	0.83875520	-1.61501889	1.95709055
O	-1.99347818	-1.59337666	2.02357830	O	2.28729802	1.34922041	1.54035031
H	-1.85822848	-2.03367093	1.16079825	H	2.13919077	1.99547391	0.82992613
H	-2.02365411	-0.64662096	1.77933821	H	2.34266410	0.48190678	1.08444110
O	1.96072257	2.65858030	-0.11287380	O	-1.81115520	-2.58268505	0.48749629
H	1.02222610	2.81948826	0.13772883	H	-0.85702656	-2.74374383	0.29649891
H	1.87259311	2.48238472	-1.06939322	H	-2.12874214	-2.33069033	-0.40097783
O	2.42281607	-1.42342881	-1.43771166	O	-2.68481975	1.71739274	-0.56448175
H	1.46753797	-1.17231018	-1.63420263	H	-1.78144729	1.40619995	-0.86998343
H	2.94397463	-1.14931476	-2.20027854	H	-3.27244404	1.66541776	-1.32612366
O	2.37158464	0.16463377	0.87401084	O	-2.33753381	-0.07091719	1.58153548
H	2.58589488	-0.38264546	0.09329675	H	-2.70349099	0.46220788	0.85154581
H	2.27605553	1.08627237	0.52363055	H	-2.23182623	-0.98298138	1.23510831

7I

C	-0.35206487	-1.42457762	-2.33883857
H	-1.44395981	-1.43874812	-2.38634918
H	0.01012472	-2.15110128	-3.07936933
C	0.18670301	-0.03031893	-2.67745208
H	1.26658810	-0.05828012	-2.84451643
H	-0.28274061	0.32299854	-3.60598158
C	0.06614682	-1.93433954	-0.95263266
O	1.13537568	-1.47821395	-0.43847383
O	-0.69731007	-2.77355610	-0.39672600
C	-0.10111393	1.01116915	-1.58895933
O	-1.22518485	0.97232728	-0.99411079
O	0.81727949	1.84611915	-1.33872305
Na	1.39830771	0.65664052	0.98948541
O	-3.09515579	-1.27613826	-0.30544678
H	-2.42191074	-1.96445419	-0.47167663
H	-2.65864063	-0.46233839	-0.61579568
O	1.19769120	3.06204978	1.07589177
H	0.27521864	3.26150536	1.32829363
H	1.09711949	2.87927160	0.11669482
O	1.62510524	-1.46308960	2.21527524
H	0.79312543	-1.65588322	2.66943561
H	1.46496603	-1.74480651	1.28223557
O	3.12509440	0.42395139	-0.77026808
H	2.53325321	1.07579683	-1.19729131
H	2.61951313	-0.40760102	-0.86296042
O	-1.44761799	-2.21126633	2.11759119
H	-1.03877019	-2.55509329	1.28108751
H	-2.36291441	-2.03726294	1.84539908
O	-1.65769697	3.08545443	1.07063485
H	-1.57727278	2.63427106	0.20736770
H	-1.68138941	2.33348212	1.68675956
O	-0.85540460	0.46382513	1.67872399
H	-1.11445149	0.52437998	0.73413890
H	-1.05759290	-0.45904016	1.94433123

7J

C	-1.18518839	-1.91548649	-1.61154803
H	-1.68645747	-2.57499990	-0.89704459
H	-1.06507378	-2.49089822	-2.53958704
C	-2.03701619	-0.66989703	-1.87494660
H	-1.63876215	-0.09012265	-2.71153343
H	-3.05516842	-0.98278013	-2.14463134
C	0.22505079	-1.64262342	-1.06494734
O	0.72839985	-0.48219056	-1.20755354
O	0.79001889	-2.61519741	-0.49140510
C	-2.13963130	0.24358419	-0.64931696
O	-2.28886326	-0.28732815	0.48985149
O	-2.04032987	1.49563260	-0.84791100
Na	0.37233169	1.70811006	-0.05770648
O	-0.72742964	-2.21852578	1.89704541
H	-0.23709067	-2.63845894	1.16610199
H	-1.42808731	-1.71979859	1.42957206
O	-1.23529121	3.26994756	1.03358245
H	-1.13713213	2.79842019	1.87179863
H	-1.78023839	2.67887084	0.46215880
O	2.20117622	2.16220263	1.36847081
H	1.61048410	1.82534806	2.05749256
H	2.66255073	1.36037223	1.00772818
O	3.10522482	-0.07531884	0.18319859
H	3.10201202	-0.82491133	0.81308437
H	2.35555631	-0.28605819	-0.42065711
O	0.14580229	1.92394830	-2.50887271
H	-0.78124365	1.94023194	-2.19423255
H	0.39744472	0.98868756	-2.37773596
O	2.46603212	-2.39851133	1.60959267
H	1.95345943	-2.54447111	0.77343607
H	1.78012420	-2.26618236	2.27764094
O	-0.35446876	0.66031252	2.09988383
H	-1.20684774	0.48124358	1.62886832
H	-0.07190344	-0.24711635	2.30916478

7K				7L			
C	-2.13095704	1.44293869	0.82641507	C	-2.55323376	-0.26564092	0.43713048
H	-2.75987241	1.31516244	-0.05779551	H	-2.86913408	-0.57845293	-0.56056294
H	-2.57762780	2.25384997	1.41853736	H	-3.45010081	0.06507746	0.97935146
C	-2.08808655	0.16306271	1.66902049	C	-1.90391827	-1.43990906	1.18916508
H	-1.68005621	0.36173568	2.66373190	H	-1.77415995	-1.19765425	2.24696013
H	-3.10768802	-0.22314106	1.80716473	H	-2.56086129	-2.31649852	1.11545148
C	-0.74568238	1.92891967	0.37185116	C	-1.63274675	0.95275340	0.29891501
O	0.25295103	1.67180346	1.11562117	O	-0.83339582	1.20722111	1.26218167
O	-0.68624055	2.56630120	-0.71904041	O	-1.70569621	1.64273503	-0.75598371
C	-1.25339894	-0.95585768	1.03856382	C	-0.53756760	-1.81134278	0.59873561
O	-1.21045936	-1.03159945	-0.23436512	O	-0.45900070	-1.92748383	-0.67022741
O	-0.62745740	-1.72697241	1.81921509	O	0.44406065	-1.93094032	1.38050008
Na	1.48781578	-0.39431518	0.63990615	Na	1.44710049	0.30204878	1.00908448
O	-1.94360687	0.80819712	-2.48464101	O	-1.46321095	-0.31159636	-2.80914142
H	-1.58424535	1.58897367	-2.00803480	H	-1.84340256	0.38608823	-2.24129563
H	-2.04760826	0.15482241	-1.77041140	H	-1.17956849	-0.99076927	-2.16279614
O	1.54311982	-2.75952085	0.52561526	O	2.28092264	2.32336127	0.07998715
H	1.19621220	-3.14164529	-0.30298440	H	2.19384395	2.12495040	-0.86426800
H	0.73122913	-2.64890443	1.06999735	H	1.57398803	2.98655340	0.25754659
O	2.62769513	0.48106037	-1.17374973	O	-0.01761798	3.72737972	0.65060864
H	1.98727647	0.14791781	-1.83479965	H	-0.55118484	3.77607247	-0.15565876
H	2.49372577	1.45517212	-1.13732259	H	-0.33332959	2.87009764	1.03390769
O	1.99396654	3.15785047	-0.70731794	O	0.62666613	-0.02341797	3.32181693
H	1.03481255	3.06459108	-0.92778827	H	0.51776054	-0.90056483	2.89089761
H	1.95256271	2.97309153	0.24406770	H	-0.09468409	0.49151161	2.91531338
O	1.20122809	0.00033183	3.06946305	O	0.61313559	1.54080754	-2.33304236
H	0.54782998	-0.72031124	2.98960293	H	-0.06538827	1.78642937	-1.66825979
H	0.75333678	0.75422471	2.63214420	H	0.10467915	0.90713685	-2.88084361
O	-0.24773830	-3.37903176	-1.60387408	O	1.56327238	-3.63868072	-1.91269486
H	-0.77196553	-2.76639330	-1.04867474	H	0.78592200	-3.27477176	-1.44963176
H	0.04573113	-2.80586425	-2.33032937	H	2.19893441	-2.91066627	-1.86942229
O	0.42770993	-0.66948903	-2.44971214	O	1.93493400	-0.62168348	-1.09226310
H	0.00240501	-0.81663618	-1.57997208	H	1.14981086	-1.21000859	-1.00910966
H	-0.22153337	-0.06429932	-2.86272007	H	1.61269622	0.11950365	-1.64312485

Table S10. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_8$ using B3LYP exchange-correlation functional with dispersion correction.

8A

C	-0.13933706	-2.51918072	-1.76123270
H	0.28781700	-1.94036968	-2.58474716
H	-0.55113117	-3.45637318	-2.14921412
C	0.97737896	-2.86031787	-0.73770407
H	0.58956678	-3.57063348	-0.00216476
H	1.81980118	-3.31415139	-1.27274293
C	-1.26030421	-1.72483520	-1.07349793
O	-2.13693651	-2.34349125	-0.44154140
O	-1.15425432	-0.44006473	-1.14273494
C	1.46893966	-1.60955187	-0.00801467
O	2.12508762	-0.74454498	-0.66356833
O	1.12346035	-1.46491587	1.20681071
O	0.77930857	2.64982481	-0.98696944
H	0.79559850	2.05605198	-1.77725901
H	-0.01730173	3.22224950	-1.06001715
O	0.78689471	0.57736250	-2.73451259
H	1.48438971	0.07394443	-2.26987406
H	-0.02777494	0.20174728	-2.31502255
O	-1.41624999	-1.90902640	2.22392468
H	-0.48091321	-1.98071085	1.93715242
H	-1.91372239	-2.08320286	1.39756308
O	-1.31976699	0.78620545	2.48689454
H	-1.44347873	-0.19862636	2.50487464
H	-0.41184667	0.95262275	2.81314120
O	1.44130581	0.81933687	2.70578223
H	1.48980592	-0.09320298	2.34255030
H	2.05518237	1.31370243	2.11697295
O	-2.43036341	1.55719729	0.12010930
H	-2.17480591	0.73801561	-0.37424581
H	-2.19265417	1.38671815	1.05713046
O	2.84504677	1.65350944	0.52694099
H	2.75826407	0.77065757	0.09689462
H	2.29478721	2.25057444	-0.01712790
O	-1.68292134	3.84359104	-0.97565354
H	-2.15223115	3.92767353	-1.81333087
H	-2.03909118	3.01477165	-0.54378159
Na	0.18686607	0.79445123	0.44096653

8B

C	1.01888564	3.33121263	0.41757527
H	2.07257626	3.18850008	0.66827854
H	0.74068336	4.37995051	0.58073824
C	0.77258478	2.96911479	-1.06955368
H	-0.26421647	3.19868837	-1.32952957
H	1.45420844	3.56249971	-1.68825469
C	0.19003041	2.45182004	1.33726604
O	-1.11029810	2.60136713	1.16653205
O	0.69689187	1.66129158	2.13065582
C	1.05098227	1.47807214	-1.29869131
O	2.24293174	1.10485985	-1.38895081
O	0.03251150	0.70071420	-1.31148025
O	2.33652485	-1.46859315	-0.52109747
H	2.38554817	-0.55517969	-0.90806032
H	2.12987254	-1.35018588	0.42897823
O	-2.68574727	0.54006570	-1.20380272
H	-2.62607901	-0.30524128	-1.67862378
H	-1.76076134	0.87584991	-1.24564179
O	1.12944408	-1.09609396	1.97813773
H	1.14609719	-0.13650787	2.14893820
H	0.17805099	-1.37001629	2.15397785
O	0.09600880	-3.79314040	0.87952768
H	-0.57156318	-3.14426613	1.29013328
H	0.92584363	-3.59579024	1.33431572
O	-1.34703888	-1.86376844	1.81468502
H	-2.06402180	-0.34201697	1.70795919
H	-1.91216798	-2.20993655	2.51357261
O	-2.52772992	0.52922218	1.53751241
H	-2.81061773	0.47125214	0.59559313
H	-1.64025001	1.77649999	1.49623755
O	0.72761422	-3.30825325	-1.74643868
H	0.43581010	-3.71233480	-0.89997637
H	1.46128373	-2.71573175	-1.46068791
O	-1.14665714	-1.49113748	-2.54313752
H	-0.57132160	-0.70325098	-2.49877724
H	-0.53335919	-2.25718173	-2.45571472
Na	-0.19923872	-1.34200053	-0.19544089

8C

C	-0.97348131	-2.62295949	0.51969128
H	-1.80480479	-2.63163554	-0.18934516
H	-1.16276307	-3.41625895	1.25612676
C	0.35638754	-2.90291629	-0.18817355
H	1.13229286	-3.16678974	0.53621150
H	0.24624360	-3.77058740	-0.85242795
C	-0.99197571	-1.28625661	1.26473428
O	0.06564790	-0.90398563	1.85318481
O	-2.06291278	-0.60801989	1.21345022
C	0.91533975	-1.75268031	-1.04240295
O	0.12248671	-0.79690478	-1.38115672
O	2.12991954	-1.80578558	-1.34411037
O	0.37823181	1.76263046	2.54841047
H	0.26451851	0.78471300	2.53770085
H	1.16343194	1.90995823	1.98675950
O	-2.17599622	2.07880277	1.51967406
H	-1.35032803	2.28725813	2.00212304
H	-2.25096585	1.09837939	1.60483577
O	2.80647851	-1.23754924	1.39144729
H	1.85732967	-1.29534545	1.63800239
H	2.84754493	-1.62944960	0.49909673
Na	-0.21625926	1.10803067	0.13109909
O	-2.64209709	-0.53785914	-1.50107586
H	-2.74510608	-0.65996870	-0.53424226
H	-1.69409607	-0.75887175	-1.63138216
O	1.97274374	0.94182921	-2.31442343
H	2.68465209	0.29119767	-2.40322904
H	1.20538131	0.34418701	-2.11091339
O	2.24123855	1.33381404	0.52348152
H	2.59836647	0.46073582	0.80443395
H	2.29047558	1.36089129	-0.45191547
O	-2.22858434	2.17536334	-1.25503813
H	-2.38395937	2.29821679	-0.29421600
H	-2.50555210	1.25348800	-1.46543015
O	0.34938145	3.01400923	-1.27650180
H	-0.57135689	2.84200999	-1.56774978
H	0.94717509	2.60265530	-1.91996569

8D

C	-0.27923415	-2.81168453	1.07109138
H	-1.29041367	-2.66874477	1.46249525
H	0.16777655	-3.69857886	1.53288290
C	-0.34945209	-3.03701097	-0.46408083
H	0.62917866	-3.36218725	-0.82814749
H	-1.09032178	-3.81752072	-0.66855502
C	0.57579414	-1.58334763	1.39888491
O	1.82715032	-1.67493751	1.34102593
O	-0.05833123	-0.49654362	1.63556718
C	-0.76316306	-1.75602508	-1.19529420
O	-1.96374450	-1.38944013	-1.17422712
O	0.18174436	-1.08197615	-1.74717136
Na	-0.02096891	0.94104191	-0.26423061
O	-2.78102510	-0.37645817	1.29019936
H	-2.75750919	-0.81831379	0.41794760
H	-1.85613703	-0.50288546	1.60573410
O	-1.15442177	1.00979193	-2.69559445
H	-0.54134203	0.23850999	-2.57607931
H	-1.98183084	0.62663212	-2.36319371
O	2.42083325	0.61933825	-0.05462260
H	2.30984310	-0.01798423	0.68936979
H	2.75322071	0.03338795	-0.76418068
O	0.18311473	2.14073248	2.43800320
H	0.83876072	2.59122020	1.85753054
H	0.33858364	1.17760710	2.34953862
O	1.75257314	3.21877188	0.43622719
H	1.09287979	3.37325155	-0.27126361
H	2.23120928	2.40411558	0.18129346
O	2.78863097	-1.81429311	-1.39870444
H	2.70072595	-2.07620711	-0.46477873
H	1.85203045	-1.64694140	-1.65898165
O	-1.94334657	2.18808965	0.75487883
H	-1.31262110	2.27201075	1.51145016
H	-2.45744834	1.36456617	0.92704763
O	-0.45363741	3.25243145	-1.28152247
H	-1.15666988	3.09605180	-0.61487658
H	-0.67248729	2.61360396	-1.99346601

8E				**8F**		
C	-0.19765410	3.18826943	-0.20706137	C	-1.69078603	-2.36679785	-0.47716203
H	0.67960201	3.35454795	0.42469291	H	-2.03425305	-2.05795068	-1.46904020
H	-0.71393134	4.13893126	-0.37420919	H	-2.41619803	-3.10563357	-0.10964293
C	0.25999261	2.62835465	-1.58168465	C	-0.29570112	-3.00100930	-0.55290078
H	-0.59437784	2.60091904	-2.26394154	H	-0.04811081	-3.51197039	0.38128656
H	1.03331356	3.28835424	-1.99163414	H	-0.28809799	-3.76071194	-1.34702156
C	-1.16170945	2.19945513	0.46593930	C	-1.78291694	-1.13600620	0.43539129
O	-2.37161963	2.24183598	0.16847480	O	-0.87270711	-0.97649674	1.31589808
O	-0.61000670	1.32591923	1.23647865	O	-2.72598985	-0.32669452	0.22737615
C	0.83304070	1.21803960	-1.44581046	C	0.82831994	-1.99997223	-0.86255434
O	1.95338847	1.07414641	-0.87412021	O	0.53290451	-0.99183467	-1.58555754
O	0.10899393	0.25026534	-1.85275057	O	1.96710847	-2.21445600	-0.37219043
O	1.97838016	1.65550131	1.90664929	O	-0.17070179	1.27442162	2.58692849
H	2.29218616	1.63130423	0.98382742	H	-0.48654849	0.38671971	2.27761590
H	0.99586974	1.67199075	1.77194920	H	0.78576433	1.27076137	2.45099628
O	0.88957188	-2.38059377	-1.81331817	O	-2.02047277	2.25082968	0.78869188
H	1.68213618	-2.24147384	-1.24623683	H	-1.47834832	2.17960516	1.59694929
H	0.59790630	-1.46543202	-2.02964233	H	-2.42149206	1.35500149	0.67452503
O	-2.60567478	-0.12570985	-1.25626531	O	1.31293556	-2.32152269	2.37521510
H	-2.77540496	0.66220352	-0.69509323	H	0.42795658	-2.00514018	2.09225033
H	-1.74090367	0.07709741	-1.66967489	H	1.69989572	-2.62803045	1.53137136
O	-1.03211982	-0.88642332	2.74301234	O	-1.44601024	0.72616148	-2.10395067
H	-1.48039533	-1.47304879	2.10044098	H	-2.21090129	0.51997737	-1.54153673
H	-1.12810909	0.01055876	2.34593713	H	-0.91090912	-0.09556775	-2.09473622
O	-1.77793539	-2.07937598	0.38723836	O	1.55408280	1.46896398	-2.18801212
H	-2.22852544	-1.43909727	-0.22501259	H	1.35328398	0.50710041	-2.13545465
H	-1.64836064	-2.92101807	-0.09803700	H	0.70115639	1.92575134	-2.30038874
O	-0.92217546	-4.22131903	-1.14003640	O	2.20964249	0.03504505	1.17965188
H	-0.21616143	-3.59642588	-1.45915991	H	1.99544268	-0.61924656	1.87967666
H	-0.46157976	-4.92921303	-0.67540308	H	2.37727474	-0.56478475	0.41788449
O	1.69113239	-1.02574345	2.40342147	O	2.16136352	2.61455306	0.23549259
H	0.76114897	-1.08234978	2.72643196	H	2.44988705	1.84774648	0.76227161
H	1.91606176	-0.06414442	2.41490221	H	2.16814017	2.27614859	-0.68852366
O	2.75761133	-1.42697357	-0.11964440	O	-0.26104593	3.44072261	-0.99909357
H	2.61761618	-0.49671696	-0.42617561	H	0.44006208	3.56985366	-0.34015400
H	2.55527782	-1.43382502	0.83839425	H	-1.05054628	3.15827309	-0.49290269
Na	0.23810474	-0.79063504	0.35898391	Na	0.09688386	1.01605492	-0.06556574

8G

C	0.32090568	-3.03655568	-0.69389215
H	1.23068713	-3.09657442	-1.29802195
H	-0.28307382	-3.93700543	-0.85566482
C	0.70862497	-2.96030915	0.80852212
H	-0.19053189	-3.07424475	1.42040127
H	1.40303734	-3.77826978	1.02599809
C	-0.48417259	-1.81359221	-1.13637728
O	-1.67662318	-1.68719313	-0.72799379
O	0.11963117	-0.94108888	-1.84003733
C	1.39664010	-1.61989982	1.11596655
O	2.61684391	-1.50443063	0.88789184
O	0.61692096	-0.67729042	1.51973066
O	1.13946039	2.23918966	-1.08957224
H	1.82604872	1.52796941	-1.21291242
H	0.52985387	2.17579241	-1.86173275
O	2.65934971	0.05618207	-1.40962596
H	2.87800816	-0.34921205	-0.54292167
H	1.88883227	-0.47349451	-1.70867850
O	-1.97171052	-1.32635964	2.03681202
H	-0.99670741	-1.15568288	2.02904098
H	-2.11084493	-1.66894106	1.13217421
O	-2.41442539	1.32530569	1.56519431
H	-2.41528807	0.38855480	1.88099077
H	-1.58182743	1.70868339	1.91695535
O	0.19656930	1.91412017	2.14376722
H	0.67432179	1.05732490	2.08436725
H	0.78449775	2.63556857	1.83714668
O	-2.79378022	0.81267804	-1.10781080
H	-2.54922470	-0.14292209	-1.06332597
H	-2.87170763	1.11051200	-0.17590860
O	1.59550267	3.97059790	0.87789415
H	1.02997279	4.74640822	0.79040360
H	1.47942050	3.45009799	0.04109222
O	-0.77512988	1.46180203	-2.85538168
H	-0.49143212	0.52955456	-2.72158953
H	-1.62956728	1.47816680	-2.37528269
Na	-0.46802058	0.74173363	-0.05530241

8H

C	0.04451459	3.04113093	0.97507364
H	0.95378820	2.81634126	1.54201296
H	-0.42140951	3.94708747	1.37732305
C	0.41381068	3.29347480	-0.50999646
H	-0.49656721	3.53062061	-1.06856151
H	1.11393022	4.13413507	-0.56462340
C	-0.95828057	1.88423557	1.07828156
O	-2.14548884	2.09905717	0.76455656
O	-0.47616902	0.73783159	1.41833189
C	1.08651047	2.05655807	-1.10287272
O	2.29256466	1.83134710	-0.83556266
O	0.34590174	1.26305531	-1.79454575
O	1.39892618	-2.60584769	0.78143113
H	1.86411186	-1.78601866	1.05553168
H	0.86208802	-2.91237379	1.55055218
O	2.10223599	0.00407886	1.25266728
H	2.42552653	0.63239337	0.57538867
H	1.23213267	0.38404489	1.53341522
O	-2.34349204	0.76706588	-1.68372247
H	-1.43512569	1.09644154	-1.86489849
H	-2.55376093	1.17836551	-0.81830656
O	-1.98220709	-1.79572557	-0.95756487
H	-2.19507435	-0.92116183	-1.37543364
H	-1.30544818	-2.26831819	-1.48385764
O	0.43193116	-2.89409205	-1.78759906
H	0.81387075	-3.03682603	-0.89520383
H	1.06174126	-2.26679699	-2.20210498
O	-2.00097192	-1.49362034	1.78268464
H	-1.58915334	-0.59512178	1.77573163
H	-2.13170544	-1.69942842	0.83200264
O	1.97156088	-0.72141137	-2.42243549
H	1.35403765	0.05913324	-2.38583297
H	2.74311090	-0.38614504	-1.94488602
O	-0.33056135	-3.26341643	2.78046048
H	-0.75595449	-4.12622227	2.71979517
H	-1.01330239	-2.59439685	2.46800984
Na	0.17465858	-0.72397947	-0.34819483

8I

C	-2.15924775	-2.07094433	0.04865084
H	-2.35715132	-2.17303883	-1.02236506
H	-3.06556014	-2.40627826	0.57264850
C	-0.97331206	-2.94039125	0.46571171
H	-0.84000856	-2.92299231	1.55111666
H	-1.17516724	-3.98556975	0.19188400
C	-2.00196978	-0.57470806	0.33912968
O	-1.18530967	-0.20427660	1.24735518
O	-2.67799016	0.21577523	-0.37765844
C	0.37440151	-2.57434774	-0.17561517
O	0.36126819	-1.93584914	-1.28968429
O	1.41888468	-2.92866603	0.41847026
O	-0.84370050	2.53300304	2.07545735
H	-0.97364469	1.56767745	1.97166046
H	0.05887520	2.74710774	1.77248621
O	-1.83769250	2.81909200	-0.51744607
H	-1.66727619	3.03733627	0.41968597
H	-2.33903789	1.97444868	-0.45579101
O	0.99496577	-1.26351371	2.62985557
H	0.11551800	-1.00341817	2.27805486
H	1.23522034	-2.04652316	2.09248151
O	-0.73575121	0.23091596	-2.43241351
H	-1.62940773	0.35270326	-2.06596028
H	-0.45072898	-0.65422218	-2.09935122
O	2.67243020	-0.77552225	-1.56653135
H	3.38572288	-1.41629041	-1.46543708
H	1.81646392	-1.31777025	-1.52348876
O	2.10210807	0.46904027	0.83343855
H	1.82780230	-0.14009738	1.56216187
H	2.42616838	-0.07269801	0.08282345
O	1.59853638	3.07549428	0.64297947
H	2.02513814	2.19774717	0.78217645
H	1.60778250	3.18847320	-0.32072261
O	1.56305159	1.78692758	-2.09761110
H	2.16107565	1.01788220	-2.03605420
H	0.76165551	1.42591127	-2.52652523
Na	0.01268571	1.27189614	-0.25128220

8J

C	-1.34935412	1.35867077	2.25979970
H	-1.89986053	2.18214654	1.79766952
H	-1.31610708	1.56154132	3.33928681
C	-2.06164453	0.02655116	2.01191250
H	-1.63444749	-0.76749736	2.62974593
H	-3.11927925	0.12260223	2.29495998
C	0.09550205	1.41197511	1.74570525
O	0.74751681	0.32082859	1.64473393
O	0.55809787	2.54614562	1.45058528
C	-2.02471804	-0.43491192	0.55078361
O	-2.05868390	0.44759151	-0.36174523
O	-1.96442350	-1.68432986	0.34718952
Na	1.33682058	-1.14893823	-0.36917885
O	-1.30229471	3.19241250	-0.61751604
H	-0.79357897	3.29409231	0.20866474
H	-1.63374520	2.27310887	-0.54979816
O	-0.37538929	-2.46902463	-1.63792105
H	-0.59110522	-1.92605068	-2.41217764
H	-1.09362496	-2.25433216	-0.98790773
O	3.14080550	0.34220864	0.35108608
H	3.12032871	1.03765824	-0.31996750
H	2.40500594	0.55909939	0.96942864
O	0.33488565	-2.36857343	1.73368931
H	-0.57144144	-2.36251125	1.35870109
H	0.48471975	-1.42262313	1.95536201
O	1.53912357	2.74404936	-1.07539064
H	1.41898350	2.65634907	-0.09975854
H	0.65261319	3.05327636	-1.34034442
O	-1.42615071	-0.13331370	-2.84611369
H	-1.75214888	0.05314297	-1.91188769
H	-1.94073166	0.42199128	-3.44153306
O	1.27071699	0.24026582	-2.22738570
H	0.35648693	0.22071573	-2.57224981
H	1.40993628	1.14727202	-1.87574549
O	1.85414894	-3.57384014	-0.30560272
H	1.11701234	-3.51649641	-0.94064702
H	1.42616128	-3.39513062	0.55498235

8K

C	-0.96585696	2.36077979	1.35221831
H	-1.12120710	3.08795713	0.55101415
H	-0.92962753	2.92520990	2.29410166
C	-2.12064071	1.35450490	1.39790512
H	-2.10410288	0.77976465	2.32676416
H	-3.07400449	1.89949480	1.36376742
C	0.41711559	1.72907818	1.14490832
O	0.60039380	0.52094396	1.50764486
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C	-2.10787000	0.37547599	0.22000918
O	-1.83158288	0.83198873	-0.93223871
O	-2.36954668	-0.83797817	0.47283785
Na	0.11509220	-1.70721290	0.44247550
O	-0.01649071	2.81658991	-1.91724368
H	0.43401198	3.05183687	-1.08536406
H	-0.69463487	2.17635304	-1.61941125
O	-1.46759154	-2.90420636	-1.01313802
H	-1.33932224	-2.55881284	-1.91005745
H	-2.03437729	-2.22085650	-0.58852511
O	2.25018529	-2.86834537	0.37490495
H	2.10548523	-2.64298087	-0.56012742
H	2.72061766	-2.07613903	0.71888792
O	3.18001670	-0.35885171	1.10335321
H	3.45795856	0.07640441	0.28609525
H	2.30418032	0.04757722	1.31725727
O	-0.87498120	-1.53095030	2.71360017
H	-1.65195630	-1.38825030	2.13642246
H	-0.37002568	-0.70175822	2.59999218
O	2.47639790	1.28564408	-1.49356753
H	2.20257819	1.67822802	-0.62570353
H	1.86721214	1.73565835	-2.10483320
O	-1.19484757	-0.76918045	-2.91767481
H	-1.52730270	-0.17413190	-2.17666808
H	-1.27463726	-0.26568856	-3.73529103
O	1.23085965	-1.17280500	-1.63430333
H	0.47421029	-1.02631830	-2.23739706
H	1.72153584	-0.32016594	-1.58253483

8L

C	-1.69078603	-2.36679785	-0.47716203
H	-2.03425305	-2.05795068	-1.46904020
H	-2.41619803	-3.10563357	-0.10964293
C	-0.29570112	-3.00100930	-0.55290078
H	-0.04811081	-3.51197039	0.38128656
H	-0.28809799	-3.76071194	-1.34702156
C	-1.78291694	-1.13600620	0.43539129
O	-0.87270711	-0.97649674	1.31589808
O	-2.72598985	-0.32669452	0.22737615
C	0.82831994	-1.99997223	-0.86255434
O	0.53290451	-0.99183467	-1.58555754
O	1.96710847	-2.21445600	-0.37219043
O	-0.17070179	1.27442162	2.58692849
H	-0.48654849	0.38671971	2.27761590
H	0.78576433	1.27076137	2.45099628
O	-2.02047277	2.25082968	0.78869188
H	-1.47834832	2.17960516	1.59694929
H	-2.42149206	1.35500149	0.67452503
O	1.31293556	-2.32152269	2.37521510
H	0.42795658	-2.00514018	2.09225033
H	1.69989572	-2.62803045	1.53137136
O	-1.44601024	0.72616148	-2.10395067
H	-2.21090129	0.51997737	-1.54153673
H	-0.91090912	-0.09556775	-2.09473622
O	1.55408280	1.46896398	-2.18801212
H	1.35328398	0.50710041	-2.13545465
H	0.70115639	1.92575134	-2.30038874
O	2.20964249	0.03504505	1.17965188
H	1.99544268	-0.61924656	1.87967666
H	2.37727474	-0.56478475	0.41788449
O	2.16136352	2.61455306	0.23549259
H	2.44988705	1.84774648	0.76227161
H	2.16814017	2.27614859	-0.68852366
O	-0.26104593	3.44072261	-0.99909357
H	0.44006208	3.56985366	-0.34015400
H	-1.05054628	3.15827309	-0.49290269
Na	0.09688386	1.01605492	-0.06556574

8M				8N			
C	-2.48667381	1.17959654	0.74529591	C	-2.72953019	1.38822689	-0.09025278
H	-2.97422208	1.05515030	-0.22380619	H	-2.86984523	0.98279506	-1.09657577
H	-3.09654866	1.88031947	1.33300623	H	-3.50024598	2.13858078	0.11355579
C	-2.41144465	-0.15824616	1.48746285	C	-2.86903630	0.24308538	0.94521590
H	-1.99255586	-0.01873351	2.48770127	H	-2.82146498	0.65597099	1.95627796
H	-3.42643439	-0.56131038	1.61123040	H	-3.83844240	-0.24699557	0.79334183
C	-1.12519401	1.85570176	0.53878906	C	-1.35053506	2.04835105	0.02136368
O	-0.25884757	1.75216110	1.46047508	O	-1.18226047	2.94199292	0.87892105
O	-0.94898407	2.51059907	-0.53318887	O	-0.43611041	1.58390007	-0.75526230
C	-1.58927651	-1.23972444	0.77294324	C	-1.76215714	-0.79961750	0.78599138
O	-1.56561124	-1.24321427	-0.50216033	O	-1.73868211	-1.48476928	-0.29276421
O	-0.98403334	-2.07015620	1.50842941	O	-0.89252602	-0.88834907	1.69524829
Na	1.93863792	-0.92101563	0.52130354	Na	0.76762268	-0.38677529	-0.14772284
O	-1.92488442	0.88896227	-2.59483747	O	-1.06960276	-0.23063747	-2.67013753
H	-1.78350738	1.59824023	-1.93346161	H	-1.49087928	-0.83426241	-2.02578723
H	-1.94298336	0.08536786	-2.04386706	H	-0.92311858	0.57063863	-2.11155624
O	1.33058179	-3.19717518	0.61693077	O	-0.50568478	-3.84338771	0.01659125
H	1.06401235	-3.51194109	-0.26799901	H	-1.01355231	-2.99481122	-0.11327989
H	0.45900386	-2.94124516	1.00357756	H	-0.44818254	-3.94052753	0.97571616
O	3.11842500	0.95217644	-0.32318717	O	1.36880665	3.23550248	1.65401964
H	2.79661761	1.02124409	-1.23369371	H	0.41142184	3.16009610	1.37946211
H	2.79385178	1.78949906	0.09473990	H	1.80033721	3.67845384	0.91259851
O	1.89879092	3.15325765	0.71996043	O	2.19706073	1.64230835	-1.42276126
H	1.52150613	3.65329567	-0.01598938	H	2.58066951	1.36778079	-0.56617493
H	1.10577435	2.66848803	1.08329404	H	1.27179276	1.88634250	-1.18873138
O	0.98581220	-0.41000916	2.58520978	O	2.46460271	0.79143982	1.17624287
H	0.29185061	-1.09608190	2.53270772	H	2.32275918	0.01156663	1.75785914
H	0.50808756	0.41197433	2.33744579	H	2.04156281	1.59414155	1.56396345
O	0.88560580	1.77854140	-2.39496910	O	1.71588647	-1.65522486	2.11880655
H	0.39217623	2.14626010	-1.62111254	H	1.94484929	-2.10940345	1.28160535
H	0.15873093	1.55805725	-3.00355342	H	0.74251251	-1.53041711	2.08347178
O	-0.15977809	-3.48581291	-1.81414487	O	1.59489051	-0.82282526	-2.51075347
H	-0.82550743	-2.96723463	-1.31896416	H	1.94386493	0.07813626	-2.32198612
H	0.36705695	-2.78692925	-2.23537111	H	0.64768696	-0.69353332	-2.76050761
O	0.90563743	-0.86133686	-1.56476168	O	1.89397842	-2.62807225	-0.47438703
H	-0.01149188	-0.95407018	-1.21724438	H	1.91367159	-2.14979294	-1.33267604
H	0.95924089	0.05922952	-1.89936513	H	1.08909751	-3.19564296	-0.46240690

Table S11. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_9$ using B3LYP exchange-correlation functional with dispersion correction.

9A

C	-1.74047704	2.38119149	-0.80064075
H	-2.65329438	1.81238909	-0.99922425
H	-1.81886096	3.36628281	-1.27219635
C	-1.58203852	2.58351628	0.73607752
H	-0.84942640	3.37241821	0.91953054
H	-2.55382198	2.87547768	1.14779360
C	-0.54315476	1.63515140	-1.39769413
O	0.51624234	2.26082278	-1.63547128
O	-0.68760446	0.36718972	-1.56291268
C	-1.10991309	1.29383684	1.41082206
O	-1.97753899	0.41196254	1.69663121
O	0.14038448	1.14498194	1.57392222
Na	0.72294943	-0.70618353	0.12770535
O	-2.00451800	-3.20196224	-0.30751732
H	-2.44006408	-2.30737921	-0.48910464
H	-2.65120398	-3.89097436	-0.49264086
O	-2.90966630	-0.78291275	-0.63264431
H	-2.84725959	-0.36521898	0.25383994
H	-2.15255440	-0.34802950	-1.11212205
O	1.58438804	3.49069097	0.72497097
H	1.19702226	2.71268070	1.16967249
H	1.31066367	3.34663298	-0.19774504
O	2.53461141	0.42836322	-1.12414567
H	1.95928015	1.20001814	-1.32945621
H	2.84672516	0.51755222	-0.20022291
O	1.92734091	-2.57127093	1.58422577
H	1.01521364	-2.43999876	1.92537549
H	1.76635556	-2.90813834	0.68065031
O	1.15063431	-1.17945839	-2.90845546
H	0.43545721	-0.56289485	-2.62487263
H	1.93473616	-0.75872576	-2.50649726
O	2.76351796	0.06100986	1.62172295
H	2.62479508	-0.90602567	1.72701700
H	1.95709406	0.48816540	1.95885319
O	0.73206818	-2.94431146	-0.91470490
H	0.87227589	-2.46239937	-1.76882628
H	-0.21739885	-3.16353794	-0.84343907
O	-0.69357804	-1.93360329	1.84696983
H	-1.18952983	-1.07735230	1.95596588
H	-1.24634607	-2.52102584	1.30217087

9B

C	-0.84795936	-2.92249915	1.27442958
H	-1.77093678	-2.55033819	1.72777842
H	-0.59243227	-3.89056105	1.71832728
C	-1.06715069	-3.12323651	-0.25066211
H	-0.23152400	-3.69462571	-0.66473140
H	-1.99689370	-3.68355760	-0.39803403
C	0.29117879	-1.93117367	1.53084130
O	1.47924319	-2.32908377	1.42717855
O	-0.04854519	-0.71858784	1.75573731
C	-1.17394609	-1.78405034	-0.98771823
O	-2.23271667	-1.11392939	-0.91316667
O	-0.12086293	-1.39075770	-1.61036929
Na	0.30801972	0.69194282	-0.22684285
O	-2.71814086	-0.07164359	1.61208419
H	-2.82413367	-0.50115078	0.73797085
H	-1.80616485	-0.35480521	1.85900433
O	-0.87280978	0.94618793	-2.59271876
H	-0.51832031	0.02626765	-2.46329055
H	-1.71843340	0.87552323	-2.12230028
O	2.57101059	-0.30789350	-0.05088635
H	2.32306868	-0.89542611	0.70268401
H	2.71516764	-0.95892987	-0.76591142
O	0.77875683	1.85339990	2.18209572
H	1.57857065	2.10111365	1.65856048
H	0.74857016	0.87539716	2.24266689
O	2.76050510	2.37505202	0.36806909
H	2.20361617	2.64879634	-0.38980120
H	2.98368407	1.44064116	0.17865099
O	2.22065298	-2.77581107	-1.34936739
H	2.11251360	-2.97435382	-0.40188652
H	1.35279015	-2.36726891	-1.57815710
O	-1.44953535	2.16658515	0.71584960
H	-0.71327160	2.20711800	1.37796819
H	-2.09196309	1.50197011	1.06539211
O	-1.32632178	4.42719516	-0.67714701
H	-1.55019914	3.64789519	-0.10488806
H	-1.99756932	4.45422077	-1.36871561
O	0.80779793	2.83841739	-1.56523552
H	0.18356351	3.53549939	-1.27131909
H	0.25451375	2.23576424	-2.11091362

9C

C	2.22805359	2.32150048	0.00541109
H	2.49801898	2.59440628	-1.01741369
H	3.08275207	2.54796070	0.65799502
C	1.00665462	3.15036195	0.46481841
H	0.83763972	3.02452689	1.53596384
H	1.21733545	4.20721277	0.26201972
C	2.00687167	0.80409005	0.04782371
O	1.38176008	0.31289606	1.03819071
O	2.43745950	0.13059018	-0.93710570
C	-0.24079056	2.73901775	-0.33296829
O	-0.21038260	2.90505675	-1.57805993
O	-1.19032531	2.16892699	0.30791402
Na	-0.73281792	-0.31149726	0.04574206
O	2.04480967	-2.39966800	-1.43953118
H	2.53435602	-2.52551902	-2.26006401
H	2.24322789	-1.45756548	-1.13820282
O	-3.16788746	0.29673827	-0.05089248
H	-3.12703444	-0.13019178	-0.93672808
H	-2.67486457	1.14417399	-0.11175388
O	0.91250631	-4.21034417	0.61812086
H	1.56196939	-3.85015563	-0.00890350
H	0.87817353	-3.52950085	1.33380716
O	0.64045724	-2.07440718	2.28129541
H	-0.30859890	-1.84105847	2.30021129
H	1.07663934	-1.31189108	1.84807523
O	-1.91503298	-0.88823852	2.16293109
H	-1.57351295	-0.06107849	2.58204831
H	-2.59569807	-0.59867109	1.52100443
O	-0.58534197	1.39650428	2.81774448
H	-0.90232025	1.84494824	1.99321785
H	0.28264339	1.06302151	2.52376981
O	-0.65725419	-2.51500680	-0.90849718
H	-0.45239002	-3.24976417	-0.29086995
H	0.19954445	-2.41711839	-1.37486246
O	-0.13959997	0.33245687	-2.27488703
H	0.82045128	0.19834824	-2.19773742
H	-0.26354410	1.31485164	-2.20489819
O	-2.53421227	-1.09271859	-2.36235020
H	-1.75802225	-0.56321535	-2.62988211
H	-2.10911643	-1.84984521	-1.91365494

9D

C	-1.68950930	2.55966886	-1.09481852
H	-1.71543423	2.06607319	-2.07084752
H	-2.04006578	3.59172607	-1.19684167
C	-2.63274820	1.81088150	-0.12272229
H	-2.66836741	2.33499458	0.83604510
H	-3.63881030	1.79192055	-0.56092455
C	-0.25522995	2.57680124	-0.55446680
O	0.08036722	3.48383283	0.23540248
O	0.50009216	1.60216543	-0.92798475
C	-2.19284049	0.36673364	0.12289380
O	-2.12124482	-0.41967119	-0.88363138
O	-1.88596776	0.02217151	1.29720542
Na	0.33578486	-0.61108505	0.14064735
O	-0.27754896	-0.03451904	-2.91678552
H	-1.09205352	-0.29440845	-2.44030899
H	0.02588426	0.71890717	-2.35110074
O	-2.56274457	-2.80012053	0.34415523
H	-2.43531738	-2.01659388	-0.25151917
H	-2.76002427	-2.36445555	1.18631068
O	2.30093523	2.82875803	1.62399836
H	1.50060672	3.13558535	1.11639868
H	2.96768636	2.65857061	0.94390417
O	3.01599138	0.70673319	-0.61151697
H	2.94649174	0.33417291	0.28639425
H	2.17407063	1.22171990	-0.70388770
O	1.84614963	0.14255397	1.85275847
H	1.26189664	-0.26806246	2.52835812
H	1.87879863	1.11826491	1.98990620
O	-0.14768346	-1.26056211	3.09567435
H	0.02178319	-2.03375775	2.52103338
H	-0.85904292	-0.78055327	2.62797252
O	1.72337772	-1.43664220	-1.75322971
H	2.36364307	-0.72501051	-1.51931254
H	1.03828475	-1.03418299	-2.34463148
O	1.82140274	-3.99621575	-0.99622020
H	1.87287448	-3.07949243	-1.37229584
H	1.44909664	-4.54901972	-1.69254807
O	0.10621968	-2.90210358	0.87863775
H	0.68548363	-3.45921165	0.31658077
H	-0.83200110	-3.07461750	0.63131789

9E				9F			
C	-2.05272979	-2.23644365	0.73835701	C	-1.07689501	2.06716846	1.74666576
H	-2.92327214	-1.88404367	0.17918031	H	-0.92193559	3.04859210	1.29476160
H	-2.41728281	-2.88512759	1.54702654	H	-1.19609617	2.23078988	2.82680686
C	-1.09591664	-3.02928758	-0.16694152	C	-2.35350368	1.41376735	1.19655520
H	-0.37225620	-3.59624624	0.42507428	H	-2.72864630	0.64963001	1.87952423
H	-1.66517745	-3.75764925	-0.76053855	H	-3.13231155	2.18377617	1.10986374
C	-1.38022863	-1.01886899	1.37940059	C	0.20978574	1.25016292	1.56575578
O	-0.15105396	-1.12797126	1.70455122	O	0.13421147	-0.02625519	1.60749305
O	-2.05759968	0.03876402	1.51698087	O	1.28172418	1.89740333	1.41791042
C	-0.32043884	-2.13103176	-1.14356786	C	-2.17856704	0.78153498	-0.18789554
O	-0.83135194	-1.01376440	-1.45445445	O	-1.46781573	1.40020154	-1.04296665
O	0.80797686	-2.52820858	-1.55815026	O	-2.75179350	-0.32740639	-0.39358098
O	1.49432069	0.88536898	2.49560145	Na	0.58128730	-1.67761219	-0.12640275
H	0.88649048	0.11102485	2.43908429	O	0.38746206	3.51159328	-0.86883771
H	2.16919778	0.69268503	1.81903670	H	0.72246171	3.35695916	0.03160457
O	-0.65250053	2.34164971	1.63082341	H	-0.31753262	2.83227979	-0.95654021
H	0.20231014	2.09810074	2.04642923	O	-1.23152924	-2.06448145	-1.73802669
H	-1.23631087	1.54942117	1.74028891	H	-0.99698186	-1.62451610	-2.57064292
O	2.08214956	-2.62702357	0.92898685	H	-1.89893154	-1.45014891	-1.33526610
H	1.26299055	-2.26580093	1.33108130	O	2.92719765	-2.32116178	-0.12584325
H	1.79395606	-2.84941127	0.01797148	H	2.88511626	-1.77350622	-0.92755247
Na	0.39185991	0.68688387	0.00139230	H	3.11194606	-1.70410019	0.61434234
O	-2.89528034	0.63584198	-1.16914205	O	2.83279041	-0.56821836	2.03151551
H	-2.88925116	0.64015354	-0.19411092	H	3.06155073	0.36187262	1.89131920
H	-2.33521020	-0.15308612	-1.35688972	H	1.85032196	-0.51901550	2.02003636
O	1.73731961	0.02410892	-2.26172153	O	-2.04254981	-1.75600540	1.90301667
H	1.43272655	-0.91540615	-2.24979912	H	-2.54380681	-1.37933785	1.14942096
H	0.91908460	0.53986330	-2.39081850	H	-1.30085385	-1.11943938	1.99466936
O	2.87902606	-0.10820437	0.23057443	O	2.68549886	1.83861609	-0.95729224
H	2.78188052	-1.04798911	0.52598850	H	2.36236551	1.73527426	-0.03589512
H	2.60940829	-0.10140374	-0.71601024	H	2.05903393	2.50398066	-1.30284522
O	-0.44854609	1.92949126	-1.92140565	O	-0.62800414	0.22272080	-3.23880670
H	-0.54243872	2.81965071	-1.51317998	H	-1.02450746	0.68082659	-2.43237422
H	-1.33985701	1.53088915	-1.82765128	H	-0.69872500	0.83610415	-3.97799634
O	2.04752680	2.54542907	-0.35909839	O	1.71387312	-0.49981021	-1.91744179
H	1.91849399	2.41715181	-1.30901608	H	0.98508182	-0.26001337	-2.52461328
H	2.76238991	1.93899294	-0.11331836	H	2.11564610	0.35806634	-1.63268994
O	-0.94284129	4.13708298	-0.35249104	O	-0.62805206	-3.67563745	0.53146443
H	-1.89704191	4.27788415	-0.37415171	H	-1.00020272	-3.55712109	-0.35775095
H	-0.78748693	3.55677360	0.43684926	H	-1.21594973	-3.14684428	1.11867778

9G

C	-1.25833590	-2.36892229	-1.46661831
H	-1.93966204	-2.69430037	-0.67786100
H	-1.21437446	-3.17062350	-2.21717336
C	-1.77571626	-1.09102805	-2.13467260
H	-1.12955177	-0.80666054	-2.96929694
H	-2.77872128	-1.27673053	-2.54382859
C	0.15551456	-2.23375985	-0.88890446
O	1.00429730	-1.55342979	-1.54732061
O	0.41386293	-2.83354472	0.19704246
C	-1.89655912	0.11449729	-1.19377028
O	-2.19054871	-0.09467261	0.02942030
O	-1.69432530	1.25369391	-1.70343102
Na	0.86880155	2.01814814	0.30176579
O	-1.76404998	-2.40210705	1.89414223
H	-1.09508175	-2.79910004	1.29782054
H	-2.09420623	-1.64970211	1.36970269
O	-1.05673248	3.30845057	-0.04900893
H	-1.69168945	3.19682222	0.68392814
H	-1.39590055	2.66124059	-0.71428256
O	2.73203582	0.62409855	1.23205951
H	2.33208131	0.29018629	2.04749368
H	2.98523012	-0.20117970	0.73694981
O	3.24959235	-1.64367177	-0.12156687
H	3.04069568	-2.39586974	0.44877368
H	2.46767195	-1.62494961	-0.74456350
O	3.01537418	2.78165117	-0.63190254
H	2.59443940	2.26963677	-1.34761309
H	3.30703839	2.11288735	0.01086784
O	1.07378383	1.14428775	-1.94324200
H	0.13952267	1.34431775	-2.15414163
H	1.09350384	0.16117672	-1.88455827
O	0.94396633	-1.52648958	2.54200354
H	0.97593801	-1.94603689	1.64967459
H	0.09405947	-1.86205406	2.88063478
O	-2.92791383	2.12119068	1.76858324
H	-2.94196651	1.42164889	1.08372180
H	-2.21001973	1.82313803	2.34979597
O	-0.36342266	0.81652385	1.84536486
H	-1.01031051	0.46647317	1.18980339
H	0.13185837	0.02641165	2.14968374

9H

C	-2.72259789	-0.13890297	-0.21840436
H	-3.09345419	0.43875709	0.62972479
H	-3.53997335	-0.76994241	-0.58982257
C	-2.27852737	0.80008244	-1.36093949
H	-2.05945378	0.22022364	-2.25990016
H	-3.10674574	1.48305741	-1.58730008
C	-1.59951088	-1.06925604	0.24410131
O	-1.07126382	-1.82706070	-0.63683211
O	-1.24205334	-1.04522290	1.45629395
C	-1.05993035	1.65972609	-0.99451188
O	-1.16033785	2.42019877	0.01135232
O	-0.02770118	1.56400592	-1.73148293
O	2.39594188	0.62130259	-0.81841781
O	-1.84953611	1.45876824	2.58149470
H	-1.67630267	0.51764877	2.36114674
H	-1.91061367	1.87397752	1.69757116
O	0.44256971	4.44565453	-1.56771557
H	-0.16263517	4.31778538	-0.82251890
H	0.56052247	3.52786150	-1.86887727
O	2.30595899	-3.51600249	-0.10514242
H	2.30061119	-2.95850791	0.69614649
H	1.45811124	-4.00108943	-0.01618459
Na	1.35201760	-1.43741724	-0.87972399
O	-0.33993333	-4.21001181	0.45522032
H	-0.36844893	-4.00966978	1.39979839
H	-0.66480148	-3.37619055	0.03168344
O	0.19864522	-0.93746351	-2.94237785
H	0.14249443	0.01680488	-2.71105955
H	-0.51742582	-1.33394715	-2.41164840
O	1.45786476	-1.48299677	1.60935449
H	0.47997050	-1.36711273	1.67727033
H	1.87190630	-0.63864625	1.87702962
O	0.58900986	2.68500145	2.12424683
H	0.19834034	2.75350071	1.22328400
H	-0.15145888	2.26246249	2.61413206
O	2.58632116	1.04579294	1.95072249
H	1.83287223	1.71071441	2.07015083
H	3.35080087	1.37907758	2.43221296
H	2.58458491	0.87130117	0.10627983
H	1.63610382	1.17047604	-1.10535518

9I

C	1.75286768	-2.25256478	-1.10931267
H	1.57771888	-3.03960363	-0.37286339
H	2.63308986	-2.54081291	-1.70119226
C	0.54972843	-2.12240132	-2.05091722
H	0.73761308	-1.35486861	-2.80622845
H	0.40662222	-3.07324192	-2.58330613
C	2.12734781	-0.95314905	-0.38122177
O	2.08230906	0.12670354	-1.06157458
O	2.48723787	-1.02670296	0.82306160
C	-0.78526041	-1.80731184	-1.35987640
O	-0.99341546	-2.28579376	-0.20153381
O	-1.60872825	-1.09776212	-2.00828322
Na	-1.11575422	1.92641929	0.13329760
O	0.65848305	-2.78746950	2.05856811
H	1.49154605	-2.41851213	1.70148527
H	0.04698691	-2.69538670	1.29798814
O	-3.07335444	0.81058307	-0.73106587
H	-3.49561582	0.36168588	0.01564554
H	-2.66628147	0.06269717	-1.23139369
O	0.54237458	2.62227146	1.74952267
H	0.62700398	1.90645944	2.39766463
H	1.36682700	2.60739267	1.21810114
O	2.52496251	2.52151223	-0.12259993
H	3.45310190	2.64300114	0.10463516
H	2.42890467	1.56672554	-0.43951592
O	-0.03233204	3.78032505	-1.15411400
H	-0.08001308	3.03746033	-1.78832629
H	0.85706675	3.69402050	-0.77404996
O	-0.15359845	1.22723065	-2.09223457
H	-0.76159781	0.49344331	-2.31896447
H	0.69179351	0.78640551	-1.84307958
O	0.88793552	-0.07890000	2.85671468
H	1.53771615	-0.15795606	2.12277712
H	0.62253351	-1.01479395	2.96375525
O	-3.13391060	-1.47775510	1.10127141
H	-2.37325486	-1.82921775	0.54247121
H	-3.38380905	-2.18725024	1.70319894
O	-1.72551796	0.70498177	2.06832730
H	-2.23139005	-0.10331342	1.84655886
H	-0.84901530	0.40602671	2.38000824

9J

C	-2.18773751	0.79889848	-1.38784644
H	-2.69802989	1.55479168	-0.78675138
H	-2.85990793	0.51860148	-2.21103377
C	-0.88607336	1.37143520	-1.97005494
H	-0.44342630	0.68642564	-2.69610002
H	-1.12070151	2.30534789	-2.49761808
C	-1.99505370	-0.44772430	-0.52158704
O	-1.11096531	-1.30475442	-0.89068871
O	-2.70521172	-0.58743792	0.50359721
C	0.14696149	1.71430063	-0.88908595
O	-0.26257846	2.33354574	0.13652895
O	1.35056260	1.35631583	-1.07397842
O	1.69225015	0.03952168	1.41567974
O	-2.37512785	1.91298595	1.91855124
H	-2.82694700	1.17860932	1.46506004
H	-1.67268517	2.16897946	1.28273347
O	3.09123214	3.71914319	-0.95795557
H	2.68535702	4.00183289	-0.11723429
H	2.65611088	2.86474171	-1.12295116
O	0.31916145	-2.91254886	2.18201623
H	-0.08212318	-2.15838765	2.64863791
H	-0.39231435	-3.35053868	1.67930763
Na	1.13317428	-1.82058103	0.25948227
O	-1.21400586	-3.76460644	-0.01325482
H	-2.08971601	-4.16448391	-0.05666296
H	-1.31513903	-2.81259782	-0.32085135
O	1.26598349	-1.17982200	-2.15385775
H	1.53579507	-0.25587319	-1.94556090
H	0.30465144	-1.16450068	-1.95186453
O	-0.89728167	-0.39086585	2.59864568
H	-1.52099576	-0.67150418	1.89404734
H	-1.24133210	0.50080332	2.80612894
O	1.41413668	4.11315605	1.35361789
H	0.85189036	3.38886600	0.98195672
H	0.85751825	4.89892269	1.30216669
O	1.44710669	-3.80546533	-1.08142515
H	1.47128408	-3.11814840	-1.77129451
H	0.51171989	-4.03854658	-0.94125772
H	0.83761624	0.13103963	1.87882257
H	1.71844432	0.74339196	0.73885285

9K

C	-2.27473147	1.16988263	-1.24454490
H	-2.67361808	1.83326380	-0.47328868
H	-3.06053323	1.05060152	-2.00364790
C	-1.03033390	1.78632963	-1.89129911
H	-0.69555786	1.19827269	-2.74895577
H	-1.28096557	2.78839022	-2.26590942
C	-2.05796761	-0.21304675	-0.62041037
O	-1.14671393	-0.96394008	-1.11375100
O	-2.81264230	-0.55151990	0.33120184
C	0.14095441	1.96133258	-0.92008749
O	-0.12928124	2.25879466	0.28119168
O	1.31596331	1.81109437	-1.37728915
O	2.52356921	0.19444256	0.52079285
O	-2.05869328	1.62430900	2.15973226
H	-2.66765398	1.04961924	1.66469278
H	-1.42569006	1.92481753	1.47183126
O	3.03335065	3.83700208	-0.10661798
H	2.81210149	3.56238885	0.79762787
H	2.51837704	3.22117109	-0.65871269
O	0.23642539	-2.93418014	1.46278520
H	-0.13481176	-2.26339289	2.08228724
H	-0.55305236	-3.26078472	0.97204165
Na	1.16372364	-1.43954260	-0.28881924
O	-1.90761125	-3.40177698	-0.18930033
H	-2.68849222	-3.07758863	0.28221639
H	-1.61533194	-2.58050687	-0.66184053
O	1.15309317	-0.71582656	-2.60345951
H	1.39236738	0.21464054	-2.41493289
H	0.20096378	-0.74663451	-2.38137168
O	-1.37429626	-1.11000898	2.64269358
H	-1.93619051	-1.10794972	1.83702836
H	-1.29589205	-0.15471674	2.82287987
O	1.76373187	2.36174517	2.12541466
H	1.03521137	2.36595660	1.43838762
H	1.33162689	2.50570038	2.97505782
O	2.26191343	-3.63524867	-0.17465175
H	1.66367020	-3.62395729	0.60302316
H	1.91955610	-4.31344362	-0.76830935
H	2.42203972	0.71221318	1.33970970
H	2.31484255	0.85303970	-0.17645387

Table S12. The Cartesian atomic coordinates of the typical low-lying isomers of $Na^+(DC_2^{2-})(H_2O)_{10}$ using B3LYP exchange-correlation functional with dispersion correction.

10A

C	-0.40550000	-2.71412072	1.68662829
H	-1.11791342	-2.25763383	2.37948348
H	-0.09296454	-3.68966784	2.07308777
C	-1.09429670	-2.93263140	0.31114760
H	-0.43856115	-3.53154987	-0.32733763
H	-2.03397046	-3.47016975	0.47315481
C	0.82274601	-1.81256646	1.53902250
O	1.90302313	-2.31977897	1.14323907
O	0.64426756	-0.56572185	1.75859184
C	-1.39649037	-1.60790905	-0.39055053
O	-2.47774168	-1.01552776	-0.10864984
O	-0.51276028	-1.15907747	-1.19253040
Na	0.68785427	0.78727527	-0.27565201
O	-1.85393300	0.23412053	2.49249238
H	-2.33254146	-0.08212543	1.70735954
H	-0.92937098	-0.07319703	2.32358771
O	-0.95856533	0.59183042	-3.26695193
H	-0.81032239	-0.12764872	-2.61247596
H	-1.81111932	0.95928804	-2.97496115
O	2.82365238	-0.48488530	-0.62846667
H	2.69032439	-1.03684672	0.18055986
H	2.65803457	-1.12886323	-1.34354134
O	1.58458493	2.01262329	1.88766528
H	2.18375895	2.20557725	1.13253794
H	1.54785529	1.04171016	1.99748970
O	2.96631709	2.21862756	-0.49696613
H	2.36884131	2.41996479	-1.24738323
H	3.19334440	1.27326626	-0.61815763
O	1.67054796	-2.80711464	-1.70628597
H	1.85019946	-3.01877676	-0.77260662
H	0.84572695	-2.27532102	-1.64489728
O	-1.04006021	2.89758660	2.33197897
H	-0.07401082	2.72780959	2.33752091
H	-1.44258145	2.02138580	2.52743636
O	-1.03731663	2.52245966	-0.32855217
H	-1.14641715	2.78789093	0.62113849
H	-1.88961529	2.17363806	-0.65881153
O	0.84069622	2.42090914	-2.25781496
H	0.16661996	2.77296948	-1.63832049
H	0.32256208	1.79063701	-2.81076082
O	-3.11528656	1.12684494	-1.47164895
H	-4.06533244	1.26214276	-1.38810250

10B

C	-1.33597381	2.57563867	-1.26399281
H	-2.13857127	2.05755185	-1.79648114
H	-1.20851018	3.57741092	-1.68636916
C	-1.73063421	2.72044608	0.23227922
H	-1.03173558	3.40046651	0.72715267
H	-2.73980275	3.14321913	0.28222873
C	-0.02727068	1.79449767	-1.43479496
O	1.06340804	2.40696945	-1.35282602
O	-0.14165269	0.52590143	-1.60056211
C	-1.71943236	1.36792393	0.95133543
O	-2.68874243	0.57727365	0.76023909
O	-0.69491866	1.09312011	1.65507858
Na	0.46571190	-0.65487379	0.44422518
O	-1.89343430	-2.96401848	-1.40641237
H	-2.23200938	-2.05597210	-1.68533754
H	-2.39330580	-3.63362861	-1.88477398
O	-2.59011062	-0.48746549	-1.84402790
H	-2.92151439	-0.13356704	-0.99332263
H	-1.67714306	-0.08858349	-1.87915970
O	1.45842000	2.82125837	1.42960414
H	0.63771337	2.31487257	1.63069844
H	1.41047730	2.95449590	0.46366785
O	2.60429643	0.31909115	1.21393528
H	2.37149585	1.26782739	1.34645684
H	2.26555429	-0.12750770	2.01988995
O	0.44003326	-3.34956271	2.10989379
H	-0.46396938	-3.01925141	1.93124448
H	0.84488728	-3.34345041	1.22133045
O	3.42073581	0.81532426	-1.42437222
H	2.65004135	1.42364765	-1.47785027
H	3.40820828	0.51956691	-0.49551835
O	0.95348138	-0.80621116	3.06163796
H	0.78662709	-1.75896551	2.88284851
H	0.13966253	-0.31088154	2.85559363
O	0.85079104	-2.75979006	-0.64029636
H	1.35681405	-2.31545277	-1.37160539
H	-0.02972664	-2.96205061	-1.01025800
O	-1.64096319	-1.86895098	1.15462142
H	-2.13730215	-1.00941901	1.16350120
H	-1.93011687	-2.35899235	0.36415089
O	1.86010876	-1.14810415	-2.53240269
H	1.11624235	-0.52141050	-2.39438669

H	-2.88947827	0.28045283	-0.96845543	H	2.62475216	-0.59865648	-2.24131105

10C **10D**

C	2.50386979	-0.74688441	-1.75837815	C	-1.01818062	-3.12366818	0.87214115
H	1.88004116	-1.04539456	-2.60706289	H	-2.00890477	-2.79578295	1.19960391
H	3.50501738	-1.15583620	-1.94782810	H	-0.80946906	-4.11860806	1.27919613
C	2.56633126	0.77794926	-1.64849633	C	-0.99522713	-3.20942167	-0.67905037
H	3.32214411	1.09449357	-0.92443612	H	-0.07301517	-3.70311840	-1.00014511
H	2.85534304	1.20213482	-2.62038521	H	-1.85671257	-3.79935878	-1.00916427
C	1.93684728	-1.46851015	-0.52706892	C	0.03844982	-2.13710643	1.37736259
O	1.75215133	-0.79556505	0.54213130	O	1.23481628	-2.51346166	1.46558240
O	1.67257399	-2.69024549	-0.66486936	O	-0.36411217	-0.94560668	1.61069559
C	1.23365547	1.41949805	-1.25395549	C	-1.06820149	-1.81652876	-1.30953167
O	0.15635542	0.82304386	-1.58864465	O	-2.18395527	-1.24644756	-1.40977434
O	1.26657927	2.49055985	-0.58845693	O	0.04914114	-1.28582908	-1.63991577
Na	-0.36044242	0.40224452	0.82039959	Na	0.49200018	0.66293954	-0.07560277
O	-0.74762861	-3.61660731	-0.58568237	O	-2.98692009	-0.30054405	1.21539068
H	-0.71739128	-4.51306017	-0.93833206	H	-3.04725428	-0.61702123	0.29613253
H	0.20927454	-3.31697053	-0.50179873	H	-2.07168111	-0.57510335	1.46892295
O	-0.90519702	2.76496228	1.06996963	O	-1.44522361	1.38457163	-1.32507060
H	-1.80212396	2.71313703	0.65688419	H	-1.80861677	0.49147769	-1.53303848
H	-0.23753848	2.87142006	0.35452285	H	-1.84415173	1.65221512	-0.47095863
O	-2.06869260	-2.74677725	1.76597548	O	2.61607276	-0.34040923	0.57976974
H	-1.65703423	-3.21849645	1.01541223	H	2.19689370	-1.02142571	1.16165306
H	-1.31164107	-2.34038959	2.24375725	H	2.87007083	-0.88232452	-0.19353413
O	0.14291268	-1.36219245	2.66629618	O	0.22193822	1.60504038	2.29063146
H	0.19254832	-0.46116007	3.04841178	H	1.15734529	1.90029246	2.18433570
H	0.85360068	-1.39478966	1.98565990	H	0.20745610	0.62652739	2.33572046
O	0.39645246	1.37881488	3.06335903	O	2.75693999	2.27504660	1.48874246
H	1.30811920	1.53821504	2.72187765	H	2.39980404	2.67670432	0.66907079
H	-0.16292434	2.03437744	2.59611850	H	2.99131204	1.36488047	1.21920261
O	2.73844298	1.56961057	1.62736608	O	2.44170985	-2.48594837	-1.20878152
H	2.41331979	2.15849758	0.91701782	H	2.26399727	-2.89617186	-0.34468278
H	2.59638271	0.67781128	1.24262675	H	1.55187641	-2.12773908	-1.45201181
O	-2.50633590	-0.45387625	0.37169104	O	-2.16913231	2.35411230	1.18949166
H	-2.54314971	-1.27648815	0.92028827	H	-1.32033309	2.20400862	1.66707082
H	-2.30725608	-0.75790790	-0.54268269	H	-2.68552465	1.52930776	1.33816924
O	-1.48197884	-1.31205894	-2.05203038	O	-1.22025026	4.13279433	-0.92090749
H	-1.22110676	-2.19500134	-1.72024417	H	-1.64641349	3.81582484	-0.10279543
H	-0.68876830	-0.73717445	-2.00260773	H	-1.45101516	3.43251649	-1.55619000
O	-3.31765728	2.17878475	-0.07007043	O	1.31974141	2.92896052	-0.78956558
H	-3.09249916	2.09626792	-1.02295708	H	0.49488765	3.46144312	-0.81058943
H	-3.28982818	1.25090180	0.23807602	H	1.32958661	2.37184222	-1.59337342
O	-2.27915656	1.57036868	-2.58436095	O	1.36892773	0.81938364	-2.59062921
H	-1.35877291	1.49244671	-2.24214749	H	0.68342219	0.12525915	-2.42767492
H	-2.52048605	0.65033724	-2.76510672	H	2.19714832	0.33177186	-2.67768625

10E

C	1.61715515	2.80193727	0.73576912
H	2.31055996	2.73331483	-0.10549594
H	2.16805934	3.23814429	1.58153509
C	0.42164173	3.69810252	0.38440108
H	-0.17887171	3.91152249	1.27269314
H	0.79110879	4.65673951	-0.00546506
C	1.21992006	1.38340062	1.15215133
O	0.15729853	1.22296182	1.82353171
O	1.98982987	0.43010525	0.80241246
C	-0.51148887	3.07804841	-0.67024333
O	0.02592892	2.30489753	-1.54259428
O	-1.73789324	3.32228380	-0.59055286
O	-1.40899245	-3.03341635	-0.32151237
H	-1.52300439	-2.87880847	-1.27758858
H	-0.54234913	-3.49008070	-0.21411198
O	2.29457279	0.80787145	-1.91892106
H	2.49652297	0.68491353	-0.96765611
H	1.54171509	1.44506339	-1.88514282
O	-2.49498327	1.18841295	0.97709384
H	-2.56498654	2.03131162	0.47601396
H	-1.61469534	1.27314045	1.40433788
O	2.15975959	-2.13660898	1.85908135
H	2.32367256	-1.21091660	1.57698002
H	1.31751992	-2.06076903	2.35594170
O	1.25112142	-3.68729847	-0.20535978
H	1.71556582	-3.27231734	0.55875501
H	1.49511517	-3.13761359	-0.97811558
O	-0.32677932	-1.32812761	2.57683469
H	-0.17152377	-0.35808862	2.47195861
H	-1.28826205	-1.48195568	2.43378429
O	-1.42751606	-1.87090197	-2.87801815
H	-2.00736587	-1.77811153	-3.64115235
H	-1.50698379	-1.03881732	-2.31738833
O	-2.87584585	-1.59144003	1.59991710
H	-2.98769732	-0.66980956	1.30305035
H	-2.52000686	-2.10596208	0.84715806
O	1.29437408	-1.68583521	-2.09125838
H	1.67899546	-0.77370311	-2.18671733
H	0.48943944	-1.73586605	-2.63579710
O	-1.24227629	0.05913695	-1.20082769
H	-0.79981413	0.91332314	-1.49423722
H	-1.88091792	0.35395147	-0.51572237
Na	0.29486549	-1.22272133	0.15887619

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C	-1.09674956	-3.03934568	-0.72690960
H	-1.22943259	-2.84937007	-1.79489817
H	-1.70592409	-3.91615875	-0.46643404
C	0.37058303	-3.33588686	-0.39472619
H	0.46084499	-3.66335772	0.64608285
H	0.74351408	-4.15949459	-1.01732302
C	-1.64647963	-1.84735792	0.06121860
O	-1.31467852	-1.73851377	1.27759235
O	-2.37671610	-1.01016222	-0.56191199
C	1.33629337	-2.15141407	-0.56709987
O	0.89291223	-1.07199567	-1.08066748
O	2.51390218	-2.32657865	-0.15628149
O	-1.82461613	0.55930240	2.72959278
H	-1.70323061	-0.34419927	2.35411891
H	-0.92874473	0.93176411	2.77812569
O	-2.95621632	1.42837190	0.47333885
H	-2.65239669	1.26321286	1.40136629
H	-2.90122743	0.53785020	0.04644640
O	3.51137899	-0.42143577	1.31052292
H	4.19261689	-0.83973738	1.84781627
H	3.23070063	-1.10419620	0.62279428
Na	-0.38239693	0.57934872	0.24872354
O	-1.13991974	-0.53237579	-2.96134629
H	-1.80982901	-0.74917611	-2.27559268
H	-0.32113462	-0.84671252	-2.52296788
O	2.30096025	1.21431669	-1.85571418
H	2.04073260	0.30243789	-1.59819824
H	1.43430494	1.62625043	-2.04533307
O	2.70781290	2.24805972	0.63690127
H	3.08237153	1.45490901	1.05957033
H	2.64589335	1.97305394	-0.31211528
O	-0.37849790	1.83193471	-1.86934465
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H	-0.81228952	1.15051853	-2.43357039
O	0.08973304	2.60259024	1.35681946
H	-0.31520725	3.28282905	0.79783541
H	1.05886959	2.57664144	1.15579370
O	-1.94846184	3.61378807	-0.51918501
H	-2.62972309	4.27766727	-0.66760732
H	-2.40106241	2.80322389	-0.13047528
O	0.86806816	-0.29483264	2.17532714
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C	0.19684310	-3.36528464	0.98268718
H	-0.57082811	-3.21703703	1.74883326
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C	-0.50400172	-3.62227341	-0.37651768
H	0.24014125	-3.65530271	-1.17898796
H	-1.01366201	-4.59115649	-0.32005597
C	1.10759432	-2.14438057	0.88985724
O	2.29216094	-2.33234790	0.50593743
O	0.60568757	-0.99704381	1.15522037
C	-1.56318283	-2.54641546	-0.65568172
O	-2.56994511	-2.52457495	0.09496131
O	-1.33281957	-1.71619642	-1.60100411
Na	0.11719378	1.04770808	-0.13433170
O	-1.95837821	-0.61976333	1.94551495
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H	-1.01800970	-0.85640923	1.74250016
O	-2.25775668	0.60924739	-0.71526354
H	-2.41728596	0.34456968	0.20691214
H	-2.07715851	-0.25374689	-1.18335951
O	3.30449544	-0.51631714	-0.98000180
H	2.97817208	-1.20607608	-0.30535902
H	4.13780671	-0.83382626	-1.34297149
O	1.61173720	1.27341027	2.30366679
H	2.03383079	1.71484433	1.53833711
H	1.47766277	0.34766543	1.99817501
O	2.42527962	1.97351034	-0.24202663
H	2.10330810	2.36497723	-1.09052100
H	2.89274396	1.14976480	-0.49937622
O	1.18053266	2.56461066	-2.59909532
H	0.33049197	2.90731014	-2.24699363
H	1.00206769	1.61274619	-2.73797607
O	-0.95940829	1.95353757	1.96893135
H	-0.04120245	1.78326588	2.30045763
H	-1.49052413	1.14959920	2.13831701
O	-1.84084325	4.33185883	1.11991849
H	-1.54802516	3.50131272	1.57350377
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O	-1.14851164	3.01681108	-1.24335972
H	-1.39306607	3.62293288	-0.51390607
H	-1.73053853	2.22891695	-1.15789333
O	0.76735592	-0.15145124	-2.13291417
H	0.09749345	-0.87482910	-2.02589496
H	1.64875819	-0.48824705	-1.88667667

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C	-1.17769476	2.56223054	1.38268970
H	-0.58610684	3.42969800	1.08441241
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C	-2.29836216	2.28672905	0.36592454
H	-3.09221112	1.68580775	0.81437525
H	-2.74331187	3.24245770	0.05684668
C	-0.24057615	1.36869117	1.60267570
O	-0.71251233	0.20314983	1.47578708
O	0.96768789	1.61284193	1.91823815
C	-1.81552812	1.56519492	-0.89831219
O	-0.68455192	1.90581902	-1.38134381
O	-2.55992923	0.66907013	-1.38230096
Na	0.32745827	-1.44131536	0.10904587
O	1.42049920	3.49429963	-0.51654574
H	1.37047689	3.37068285	0.44354234
H	0.64199777	2.98640381	-0.84751842
O	-1.10775598	-1.55282658	-1.84819737
H	-0.49375841	-1.36464736	-2.57312147
H	-1.69216297	-0.75556759	-1.80846584
O	1.52863552	-3.42327346	-1.01910314
H	2.05892471	-2.61525147	-1.13816675
H	1.52388029	-3.62235467	-0.06093862
O	2.00551917	-0.97921813	1.95696806
H	2.86214992	-0.81288549	1.54374103
H	1.60376367	-0.09034537	2.11298967
O	-3.13611895	-0.88114800	0.93029729
H	-3.24930108	-0.46272323	0.05409249
H	-2.34738795	-0.40002081	1.27458053
O	3.14422528	1.38973633	0.21861916
H	2.43640109	1.43605816	0.89774737
H	2.89989809	2.14475017	-0.35103764
O	0.53673938	0.39044795	-3.14395661
H	0.00334091	0.98942250	-2.53155423
H	0.80114641	0.92451138	-3.90058934
O	2.19338820	-0.70714127	-1.24991129
H	1.72632227	-0.30376351	-2.01387216
H	2.62571223	0.03278683	-0.76356217
O	-1.55365213	-3.07509345	0.50327641
H	-1.43033346	-3.01642130	-0.46045196
H	-2.23641864	-2.38688584	0.70100639
O	0.90347967	-3.55486024	1.70493656
H	-0.04880291	-3.45645261	1.49063654
H	1.21421806	-2.70770020	2.07314827

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C	2.67515595	1.04362508	0.91207427
H	3.24672423	0.82557832	0.00502245
H	3.36909651	0.99392918	1.76299374
C	2.06165695	2.44615047	0.85247063
H	1.54737800	2.66085502	1.79766254
H	2.84238457	3.20662998	0.74374213
C	1.63980233	-0.06137124	1.10685132
O	0.68710513	0.12572606	1.91636999
O	1.77034624	-1.11536797	0.39646960
C	1.02206367	2.67743126	-0.25549159
O	0.52378933	1.64010692	-0.83298099
O	0.68375139	3.85630069	-0.48498604
Na	-0.62518917	-0.42769587	-0.24260341
O	1.59723441	-3.75773631	0.26344818
H	2.51852226	-4.03091090	0.33413791
H	1.59368957	-2.77564120	0.42072652
O	-1.99413316	3.77366891	-0.11882124
H	-2.37337542	3.17937304	-0.78179727
H	-1.07257108	3.94949958	-0.42684864
O	-1.10536309	-4.43851568	0.94645196
H	-0.13356731	-4.48001347	0.97144523
H	-1.29423519	-3.54667272	1.30953804
O	-1.31735015	-1.79627703	1.72397145
H	-2.06603489	-1.20201666	1.51587136
H	-0.57826427	-1.21895748	2.02229075
O	-2.87267076	0.23856353	0.68400640
H	-2.49288630	0.94229048	1.27140339
H	-2.81873288	0.61295586	-0.21845895
O	-1.45019262	2.07781672	2.03701986
H	-1.51166061	2.77163573	1.34092383
H	-0.57373033	1.65270149	1.98825511
O	-0.47462420	-3.89118592	-1.71491850
H	-0.99717227	-4.12113835	-0.91492395
H	0.43009476	-3.89807120	-1.35266872
O	1.87274080	-0.30121988	-2.25926199
H	2.08041824	-0.74494400	-1.41088632
H	1.52584663	0.55868354	-1.94015726
O	-0.70769699	-1.26375714	-2.42967896
H	0.23381434	-1.02309487	-2.59143320
H	-0.72079459	-2.24130312	-2.28553979
O	-1.93769689	1.22694761	-1.78340043
H	-1.77699930	0.44733668	-2.34525701
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C	1.85379036	-2.49335807	-1.04247239
H	1.59078575	-3.29890638	-0.35356009
H	2.77739440	-2.78811414	-1.56045721
C	0.74729557	-2.29105755	-2.08353485
H	1.02327721	-1.49830845	-2.78378432
H	0.62836678	-3.21457353	-2.66741522
C	2.19301687	-1.23211914	-0.23802545
O	2.20102637	-0.12416780	-0.87662811
O	2.47371035	-1.35378087	0.98236595
C	-0.63583079	-1.96330915	-1.50348816
O	-0.94947659	-2.46358382	-0.37748204
O	-1.38576489	-1.22329601	-2.20342758
Na	-1.37272715	1.66927939	0.11452099
O	0.47232732	-3.06633472	2.00889647
H	1.35280810	-2.73618165	1.74014935
H	-0.05895733	-2.93232539	1.19589200
O	-3.12507463	0.45221920	-0.96339536
H	-3.56362901	-0.08707468	-0.28780363
H	-2.60634132	-0.21723837	-1.47295647
O	0.44124651	2.29428352	1.75525204
H	0.44627303	1.56291042	2.39315492
H	1.31138441	2.26837055	1.29724904
O	-1.10232639	4.08128439	0.23612502
H	-0.64071291	3.80304682	1.04596320
H	-0.37976214	4.12663237	-0.43010251
O	2.69535340	2.16059481	0.22041309
H	3.56940660	2.19428609	0.62426405
H	2.58062344	1.22389266	-0.15663338
O	1.01494898	3.69622185	-1.54667954
H	0.61888985	2.87898830	-1.91135691
H	1.73874529	3.36257967	-0.98432689
O	-0.00499281	1.13495789	-1.79897209
H	-0.55861775	0.45148947	-2.22876262
H	0.81029651	0.64627506	-1.53352952
O	0.70834512	-0.38272561	2.87123793
H	1.42528712	-0.46734934	2.20375734
H	0.41407160	-1.31458384	2.93479891
O	-3.17348629	-1.78182611	0.83332386
H	-2.36793187	-2.08154676	0.30565113
H	-3.46895091	-2.54062058	1.34806718
O	-1.90744647	0.38568365	2.00845593
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C	-1.97893858	0.02070409	-2.03283675
H	-2.93976209	0.12543668	-1.52295097
H	-2.18326550	-0.49901166	-2.97942009
C	-1.36129211	1.39347846	-2.31298520
H	-0.55247547	1.32348073	-3.04392278
H	-2.13300963	2.04728239	-2.74126672
C	-1.10865601	-0.91831496	-1.19691908
O	0.14161879	-0.72515154	-1.13378302
O	-1.7136806	-1.86497217	-0.5964551
C	-0.81928876	2.08422207	-1.05434375
O	-1.48122947	1.95049653	0.02911263
O	0.24857209	2.74272469	-1.17770966
Na	1.70168637	0.32226864	0.77491395
O	-3.33495282	-0.13169214	1.06807786
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H	-2.86483833	0.65972578	0.74097879
O	1.95837798	2.66776201	0.92657501
H	1.40228294	3.02519842	1.64303460
H	1.40047799	2.84697768	0.13442810
O	1.74926934	-1.74849552	2.00291879
H	0.83184247	-1.91221725	2.27200821
H	1.87490320	-2.27591544	1.18381187
O	-0.55352322	-4.33913770	0.02336957
H	-0.66071407	-4.22688383	0.97868312
H	-1.01998806	-3.55852534	-0.34742065
O	3.45937849	-0.44646812	-0.61453866
H	3.13323137	0.04908894	-1.39783717
H	3.26021839	-1.38121285	-0.77792519
O	1.91871433	0.87820341	-2.50237271
H	1.57225577	1.74100541	-2.19945050
H	1.21072596	0.26746297	-2.20747763
O	-1.22747766	-2.05591035	2.06607270
H	-1.31812757	-1.99220393	1.08317817
H	-2.07637957	-1.71224801	2.38582268
O	-0.40506844	3.46307001	2.38147421
H	-0.81926205	3.27692150	1.51687209
H	-0.42108860	2.58925317	2.80576551
O	-0.24609565	0.66174713	2.06916983
H	-0.75205229	1.07472683	1.33166810
H	-0.62038375	-0.22743921	2.18994520
O	1.76451429	-2.84188521	-0.54093134
H	1.17474000	-3.61385159	-0.42860350
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C	-1.64792786	-1.30694242	-2.10408967
H	-2.43216234	-1.90900714	-1.63822085
H	-1.54789937	-1.65710621	-3.14119376
C	-2.01916113	0.17453731	-2.09402605
H	-1.29833931	0.76014579	-2.67257753
H	-3.00020500	0.31687216	-2.56745837
C	-0.32430644	-1.62252130	-1.40487882
O	0.56548360	-0.71356475	-1.33561780
O	-0.17170774	-2.79304147	-0.94711858
C	-2.09366163	0.78741098	-0.69186780
O	-2.26786488	0.02543701	0.30881062
O	-1.97169052	2.04622575	-0.61646257
Na	1.20838755	0.86180510	0.60974613
O	-2.37579380	-2.86744718	0.84820167
H	-1.78179922	-3.09878561	0.10965918
H	-2.50726807	-1.90787109	0.72314296
O	-0.14052050	2.78106918	1.19048042
H	-0.50710934	2.67768139	2.08617170
H	-0.91943153	2.55821113	0.62341739
O	2.80827883	-0.98543763	1.28994379
H	2.25123004	-1.49313332	1.89697097
H	2.92262699	-1.56923238	0.50163485
O	2.77567236	-2.30794769	-1.08579146
H	2.24715384	-3.11555950	-1.00895561
H	2.07636781	-1.64527459	-1.30596718
O	3.55652799	1.70034968	0.64668019
H	3.27253239	1.69465142	-0.28740160
H	3.65433664	0.76904506	0.90695087
O	1.91711286	1.62701006	-1.67595576
H	1.30210579	2.39191580	-1.76910764
H	1.39228332	0.82943038	-1.87928388
O	0.44502148	-2.92630177	1.71359974
H	0.42850189	-2.88557697	0.72685583
H	-0.46660782	-3.20190887	1.91509441
O	-1.99171483	1.65476336	3.07698082
H	-2.45318483	1.43869515	2.24894190
H	-1.36273705	0.91476386	3.16065663
O	-0.23711149	-0.27123837	2.07226736
H	-0.99011475	-0.21002152	1.43787898
H	0.02622102	-1.21595301	2.06053487
O	0.03256042	3.63395941	-1.60812080
H	0.22789301	3.93587242	-0.70686910
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C	-0.49225205	3.28356314	-0.52641308
H	-0.45113667	3.66082738	0.49876557
H	-0.96683738	4.06198682	-1.14006523
C	0.92592297	3.01818909	-1.05219871
H	0.89786906	2.70636283	-2.09807244
H	1.49851398	3.95361440	-0.99391093
C	-1.43255079	2.07150276	-0.55295420
O	-1.28314745	1.21280446	-1.48182396
O	-2.31651088	2.01176704	0.34668821
C	1.68437278	1.97839738	-0.21594819
O	1.65901191	2.12133233	1.04202555
O	2.29544425	1.04833507	-0.82879847
Na	0.05373913	-2.02539872	0.10075023
O	2.24194900	0.25841222	2.91942604
H	2.18788365	0.99363190	2.25666544
H	1.37203971	0.26834243	3.34235014
O	-0.57857179	1.55321961	2.54544080
H	0.19163289	1.86917837	2.02305272
H	-1.34597056	1.85777472	2.02185950
O	0.83141672	0.31950415	-3.00646523
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H	0.02467412	0.70954360	-2.60216739
O	-1.79819619	-1.34210157	-1.45152079
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H	-1.46213318	-1.62627295	-2.31018979
O	1.73480528	-3.91484925	0.31631356
H	1.57030824	-3.99839031	-0.63297012
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O	-3.63061006	-0.31616405	0.58936842
H	-3.26249395	0.59538929	0.43184019
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O	1.24338172	-2.15709846	-2.03815604
H	1.00955683	-1.31539968	-2.51519856
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H	2.33051732	-0.91705414	1.55037030

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C	-0.92084801	-3.89297634	-0.15077246
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C	-1.79824704	-2.88557240	-0.90540203
H	-1.46671703	-2.80811256	-1.94441262
H	-2.84343879	-3.22932837	-0.91942950
C	0.58135817	-3.55749681	-0.25063424
O	1.00527023	-3.16940283	-1.37832952
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C	-1.83511520	-1.47140407	-0.31956558
O	-1.54775980	-1.30542418	0.90817505
O	-2.18524475	-0.53582830	-1.10240656
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O	1.32175526	3.04384369	-2.63623591
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H	1.95622481	-1.79653722	-1.16937400
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H	0.88168850	-0.04793296	-1.70241132
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H	-2.49831964	2.27468475	-1.75886043
H	-2.30715073	1.08501868	-0.77315078
O	2.35239847	0.93633537	2.37595548
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H	2.93491218	0.83699575	3.13637542
O	-2.08068964	0.78773928	2.39398336
H	-1.95005109	0.02679986	1.75132903
H	-2.15167660	0.37638165	3.26291862
O	0.02216583	2.36118234	1.87386184
H	-0.73701275	1.78508327	2.14840992
H	0.83762998	1.96371585	2.23374343
Na	0.14338204	2.42516679	-0.52700570