Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary materials for:

Microscopic solvation of $NaBO_2$ in water: Anion photoelectron spectroscopy and *ab initio* calculations

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Contents

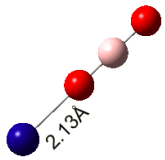
Figure S1: Structures of the low-lying isomers of $NaBO_2^-(H_2O)_n^-$ (n=0-4) clusters.

Table S1: Cartesian coordinates of the low-lying isomers of $NaBO_2^-(H_2O)_n$ (n=0-4) clusters.

Figure S2: Structures of the low-lying isomers of neutral $NaBO_2(H_2O)_n$ (n=0-4) clusters.

Table S2: Cartesian coordinates of the low-lying isomers of neutral $NaBO_2(H_2O)_n$(n=0-4) clusters.

0



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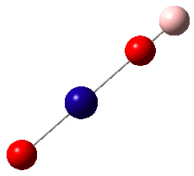

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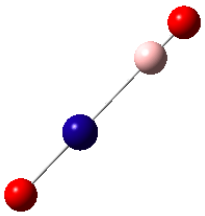

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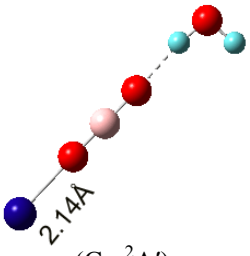

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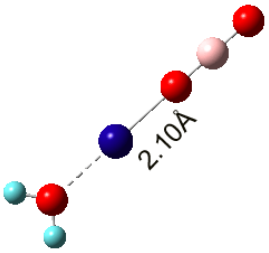
1A 0.00eV



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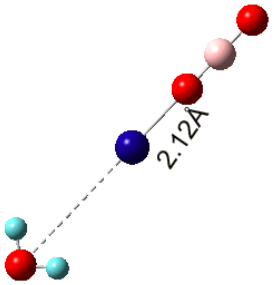

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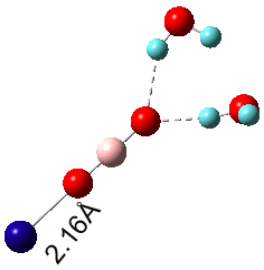
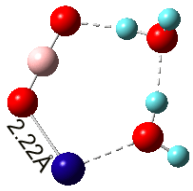


(C_1 ^2A)
2A 0.00eV



(C_1 ^2A)
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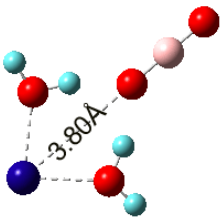

(C_2 ^2A)
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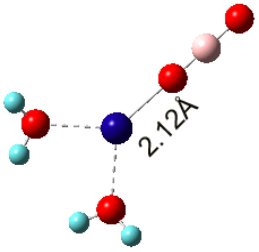

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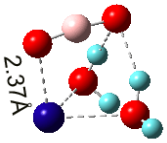
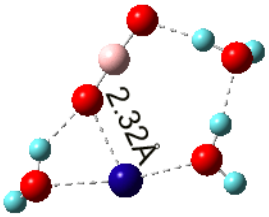
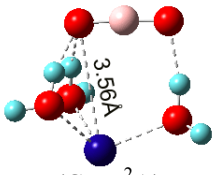


(C_1 ^2A)
2E 0.22eV

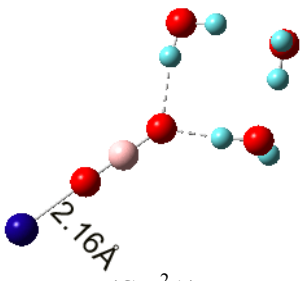
3



(C_1 ^2A)
3A 0.00eV



(C_1 ^2A)
3B 0.00eV



(C_1 ^2A)
3C 0.03eV

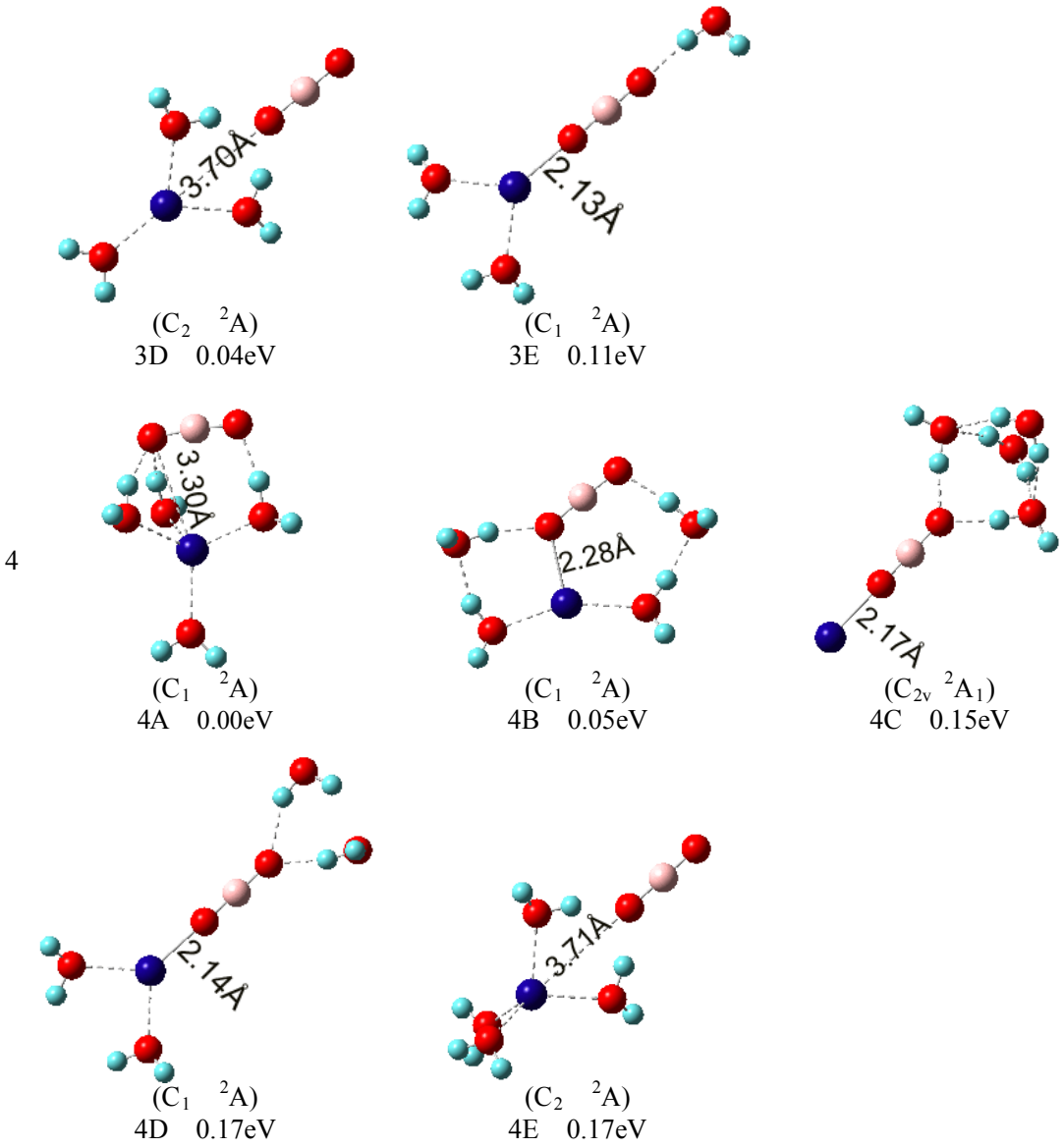


Fig. S1 Optimized geometries of the typical low-lying isomers of $NaBO_2^-(H_2O)_n$ (n=0-4).

Table S1 Cartesian coordinates of the low-lying isomers of $NaBO_2^-(H_2O)_n$ (n=0-4) clusters.

$NaBO_2^-$			
0A			
Na	0.00000000	0.00000000	2.22470200
O	0.00000000	0.00000000	0.09829900
B	0.00000000	0.00000000	-1.17444100
O	0.00000000	0.00000000	-2.42323900
0B			
Na	0.00000000	0.00000000	0.52888600
O	0.00000000	0.00000000	2.69061300
O	0.00000000	0.00000000	-1.62497300
B	0.00000000	0.00000000	-2.86857400
0C			
Na	0.00000000	0.00000000	0.81246800
O	0.00000000	0.00000000	2.98425100
B	0.00000000	0.00000000	-1.76938400
O	0.00000000	0.00000000	-2.99553100

$NaBO_2^-(H_2O)$			
1A			
Na	-2.73272500	2.08988600	0.00000000
O	-1.00968500	0.81845300	0.00000000
B	0.00000000	0.05551400	0.00000000
O	0.99547400	-0.70373200	0.00000000
H	2.44228100	-1.71095600	0.00000000
O	3.13820500	-2.40672200	0.00000000
H	2.62574800	-3.21936100	0.00000000
1B			
Na	-1.12100500	-0.00119600	-0.03038400
O	0.97908300	-0.00020300	-0.00797200
B	2.25320700	0.00016500	0.00415500
O	3.49972200	0.00061200	0.01619100
O	-3.35852900	0.00104300	0.03510900
H	-3.94776300	-0.77778700	-0.01608500
H	-3.94942300	0.77850700	-0.01708200
1C			
Na	0.00000000	0.00000000	0.69581800
O	0.00000000	0.00000000	-1.42430200
B	0.00000000	0.00000000	-2.69742700
O	0.00000000	0.00000000	-3.94558800
H	0.00000000	0.75147700	4.38996000
O	0.00000000	0.00000000	5.00154200
H	0.00000000	-0.75147700	4.38996000

$NaBO_2^-(H_2O)_2$

2A			
Na	4.06180600	-0.00586700	0.01773600
O	1.90644700	-0.04316000	-0.01322700
B	0.64712500	-0.05330400	-0.02005300
O	-0.61150500	-0.06314100	-0.02100300
O	-3.14095900	-1.49851800	0.02917600
H	-2.18498800	-1.32085500	0.03418800
H	-3.49349700	-0.60308300	-0.06674800
H	-1.97333100	1.03970900	-0.13668300
O	-2.83307500	1.51933500	-0.08532900
H	-2.83093100	1.89916100	0.79748100

2B			
Na	2.16409900	0.12660700	0.02031800
O	0.84768600	-1.66108200	0.04746600
B	-0.40638900	-1.55291700	-0.01364800
O	-1.65474400	-1.38535900	-0.07174300
O	0.64270400	1.83974600	-0.01694200
H	-0.33637100	1.71938900	-0.04246800
H	0.83052100	2.73747500	-0.31268700
O	-2.05857500	1.24139600	-0.02429400
H	-1.99492100	0.24494100	-0.09832500
H	-2.48894800	1.39248600	0.82232700

2C			
Na	0.00000000	0.00000000	2.72716700
O	0.00000000	0.00000000	-1.07222500
B	0.00000000	0.00000000	-2.35114100
O	0.00000000	0.00000000	-3.59435500
O	0.00000000	1.56372800	1.05598400
O	0.00000000	-1.56372800	1.05598400
H	-0.38127100	-2.43565600	0.92757100
H	-0.00149200	-1.10841700	0.16931600
H	0.38127100	2.43565600	0.92757100
H	0.00149200	1.10841700	0.16931600

2D			
Na	0.69775100	-0.01050100	-0.01660000
O	-1.41899600	-0.00820400	0.01344300
B	-2.69177300	-0.00811500	0.00392600
O	-3.93967700	-0.00763200	-0.00531200
O	2.30790900	1.62869800	-0.01647800
O	2.36034700	-1.62541100	-0.05207500
H	3.23175600	1.31720300	0.04576400
H	2.33432700	2.56698400	0.22446500
H	3.25904500	-1.26978600	-0.19599900
H	2.48180800	-2.35791200	0.57212000

2E			
Na	0.72980700	1.41398100	-0.15757800
O	-1.19601300	-1.40812000	0.11126600
B	-1.49583200	-0.18078900	0.03689900
O	-1.60946400	1.06736800	-0.04546500
O	1.14638000	-0.34154000	1.57340200
O	1.11743000	-0.69408600	-1.33325800
H	1.20521400	-0.78869500	-2.28898900
H	0.31514400	-1.19225100	-1.06020000
H	1.88507900	-0.75795400	1.11078200
H	0.37918300	-0.89992200	1.33970400
H	-2.83093100	1.89916100	0.79748100

$NaBO_2^-(H_2O)_3$

3A			
Na	-1.28384600	1.06595200	0.25591800
O	-0.79861000	-1.20181100	0.16778800
B	0.39683300	-1.59272300	0.03596700
O	1.60315700	-1.91621500	-0.09069400
O	0.72786800	2.03971100	-0.19055200
O	-3.23252800	-0.18909300	-0.29013700
H	-3.91314400	-0.31316700	0.38108900
H	-2.56923200	-0.89843400	-0.15466500
H	1.57155100	1.52887000	-0.16555000
H	0.93802500	2.93997300	0.08644900
O	2.96907600	0.40184700	-0.07065200
H	3.40761800	0.40516300	0.78589400
H	2.55161900	-0.49977500	-0.13418500

3B			
Na	-1.49956500	1.03544100	-0.01533500
O	0.74253400	-1.72533400	0.01289200
B	1.64982000	-0.83843200	-0.02779200
O	2.47213600	0.10641300	-0.05606700
O	-1.29218700	-0.73504800	-1.55637900
O	-1.21788800	-0.64067800	1.60482900
O	0.56583500	2.08676200	-0.00851800
H	-0.97784200	-0.52395000	2.52945900
H	-0.49905300	-1.17582100	1.19178000
H	-2.02085700	-1.34513300	-1.71137100
H	-0.57216300	-1.26163800	-1.13633300
H	0.79339200	2.87724600	-0.50821200
H	1.35919400	1.49470000	-0.03174100

3C			
Na	-4.69618600	-0.01922100	0.16533500
O	-2.54034200	0.03012600	0.03171600
B	-1.28658800	0.02917500	-0.05758700
O	-0.02900800	0.02345200	-0.15251200
O	1.89822500	-1.79576600	-0.21099400
H	1.13341500	-1.15894100	-0.16375700
H	1.86588200	-2.15137000	-1.10330900
H	1.30769700	1.49022800	-0.23225100
O	2.08946300	2.06865400	-0.25228200
H	2.82956500	1.46049500	-0.10588000
O	4.02769500	-0.15262200	0.40179400
H	4.06359000	-0.16724100	1.36230700
H	3.32256400	-0.79837100	0.17036900

3D			
Na	0.00000000	0.00000000	1.85171900
O	0.00000000	0.00000000	-1.84665300
B	0.00000000	0.00000000	-3.1270530
O	0.00000000	0.00000000	-4.36865400
O	0.00000000	1.58077600	0.24444200
O	0.00000000	-1.58077600	0.24444200
O	0.00000000	0.00000000	4.09857300
H	-0.23642700	-2.49888200	0.09774400
H	0.00041400	-1.12402600	-0.64395700
H	0.23642700	2.49888200	0.09774400
H	-0.00041400	1.12402600	-0.64395700
H	-0.09796500	0.77022200	4.69079000
H	0.09796500	-0.77022200	4.69079000

3E			
Na	-1.77070400	0.00295100	-0.01235000
O	0.35754300	-0.0320590	0.01651000
B	1.62330100	-0.0410400	0.00896700
O	2.87407200	-0.0446430	0.00321400
O	-3.40311500	-1.6071930	-0.02252700
O	-3.37721800	1.66563400	-0.05521900
H	-4.28109400	1.32645800	-0.21062800
H	-3.49143200	2.38724700	0.58341200
H	-4.31747700	-1.26396800	0.01973000
H	-3.46280000	-2.53660200	0.24609700
O	5.61723000	-0.04397500	-0.00813400
H	5.72591000	0.91054800	-0.01509600
H	4.64004400	-0.15304900	-0.00325200

$NaBO_2^-(H_2O)_4$

4A

Na	-1.26408200	-0.07423400	0.07002400
O	2.17753300	-1.07338900	-0.03550400
B	2.41306800	0.17169300	-0.11470700
O	2.54872300	1.41484700	-0.17869100
O	0.04502300	-1.16352400	1.70551500
O	-0.14469700	1.96357600	0.03097500
H	0.27088800	-0.76612600	2.55116700
H	0.89665400	-1.25880000	1.21766000
H	-0.44560500	2.77289300	-0.39397300
H	0.83916600	1.93788300	-0.05774900
O	-0.14504600	-1.47882500	-1.42844300
H	0.77796800	-1.46566200	-1.08140900
H	-0.08309700	-1.41367600	-2.38552900
O	-3.51896000	0.25435300	-0.04133200
H	-4.17002500	-0.31161300	-0.49178400
H	-3.94699300	1.12691000	0.02473200

4B

Na	0.64879100	1.18557000	0.06267600
O	0.40379700	-1.07441500	-0.07016600
B	-0.76381900	-1.56389500	-0.13914800
O	-1.94270700	-1.98250800	-0.20058500
O	-3.52809400	0.18598200	0.07218200
O	2.90121500	1.28560400	-0.27288500
O	-1.45793000	2.02292900	-0.01171200
H	3.21727400	0.36985400	-0.10461800
H	3.52507200	1.88855500	0.15082700
H	-3.03507200	-0.66361200	-0.07808500
H	-3.94031600	0.08019300	0.93531600
H	-2.25687100	1.44464000	0.01553700
H	-1.72584400	2.89006500	0.31581300
O	3.07208200	-1.44220900	0.18470500
H	3.21855300	-1.72007600	1.09516800
H	2.09269900	-1.47447600	0.06403700

4C

Na	0.00000000	0.00000000	5.09854500
O	0.00000000	0.00000000	2.92779000
B	0.00000000	0.00000000	1.67379100
O	0.00000000	0.00000000	0.41050600
O	0.00000000	1.74596200	-1.65590200
O	0.00000000	-1.74596200	-1.65590200
H	0.00000000	2.65858100	-1.35563300
H	0.00000000	1.19377200	-0.83610100
H	0.00000000	-1.19377200	-0.83610100
H	0.00000000	-2.65858100	-1.35563300
O	-1.97344500	0.00000000	-3.08134100
O	1.97344500	0.00000000	-3.08134100
H	-1.46697800	-0.75445000	-2.74499100
H	-1.46697800	0.754450000	-2.74499100
H	1.46697800	-0.75445000	-2.74499100
H	1.46697800	0.75445000	-2.74499100

4D

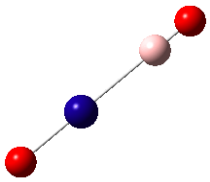
Na	2.45661200	-0.01628600	-0.02862800
O	0.31691900	-0.02661300	-0.01411500
B	-0.94285100	-0.03340000	-0.02171700
O	-2.20002500	-0.04212700	-0.02312400
O	4.06197900	-1.62718400	0.30132000
O	4.04479900	1.61573400	-0.36700800
O	-4.72112900	-1.45856300	-0.40214300
O	-4.44842500	1.47094600	0.34432500
H	4.97487500	-1.28263300	0.23291700
H	4.11541500	-2.36561400	0.92798200
H	-3.58197400	1.03711200	0.16863600
H	-4.46208000	1.57964800	1.29912800
H	-5.08414700	-0.57563500	-0.24743300
H	-3.76768900	-1.28107500	-0.33883400
H	4.10443700	2.50663100	0.01279800
H	4.95974400	1.27016400	-0.34574200

4E

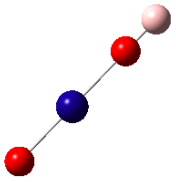
Na	0.00000000	0.00000000	1.44678900
O	0.00000000	0.00000000	-2.26503000
B	0.00000000	0.00000000	-3.54481400
O	0.00000000	0.00000000	-4.78708000
O	0.00000000	1.61682000	-0.18397300
O	1.66216500	-0.01438800	3.08573300
O	-1.66216500	0.01438800	3.08573300
H	2.17605500	-0.80135300	3.32537600
H	1.34940600	0.34255800	3.93748600
H	-0.00913500	1.13229800	-1.05557600
H	0.55445800	2.39048100	-0.30823300
H	-2.17605500	0.80135300	3.32537600
H	-1.34940600	-0.34255800	3.93748600
O	0.00000000	-1.61682000	-0.18397300
H	-0.55445800	-2.39048100	-0.30823300
H	0.00913500	-1.13229800	-1.05557600

0

($C_{\infty v}$ $^1\Sigma$)
0A′ 0.00eV

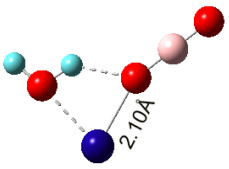


($C_{\infty v}$ $^1\Sigma$)
0B′ 9.69eV

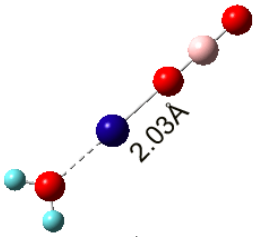


($C_{\infty v}$ $^1\Sigma$)
0C′ 9.66eV

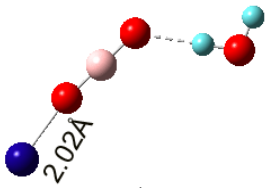
1



(C_s $^1A'$)
1A′ 0.00eV

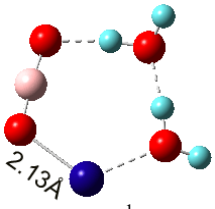


(C_{2v} $^1A_1$)
1B′ 0.19eV

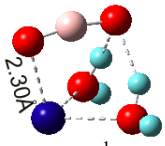


(C_s $^1A'$)
1C′ 0.32eV

2

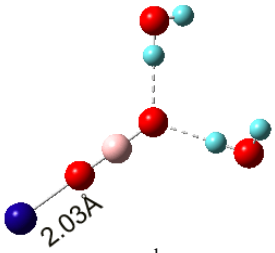


(C_1 ^1A)
2A′ 0.00eV



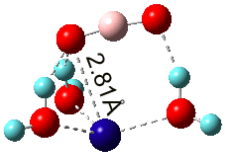
(C_1 ^1A)
2B′ 0.04eV

(C_{2v} $^1A_1$)
2C′ 0.13eV

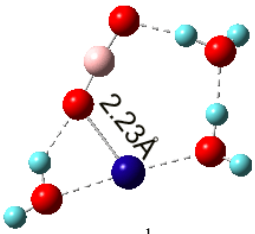


(C_2 ^1A)
2D′ 0.76eV

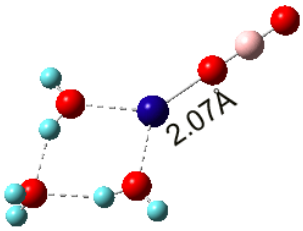
3



(C_1 ^1A)
3A′ 0.00eV



(C_1 ^1A)
3B′ 0.01eV



(C_{2v} $^1A_1$)
3C′ 0.85eV

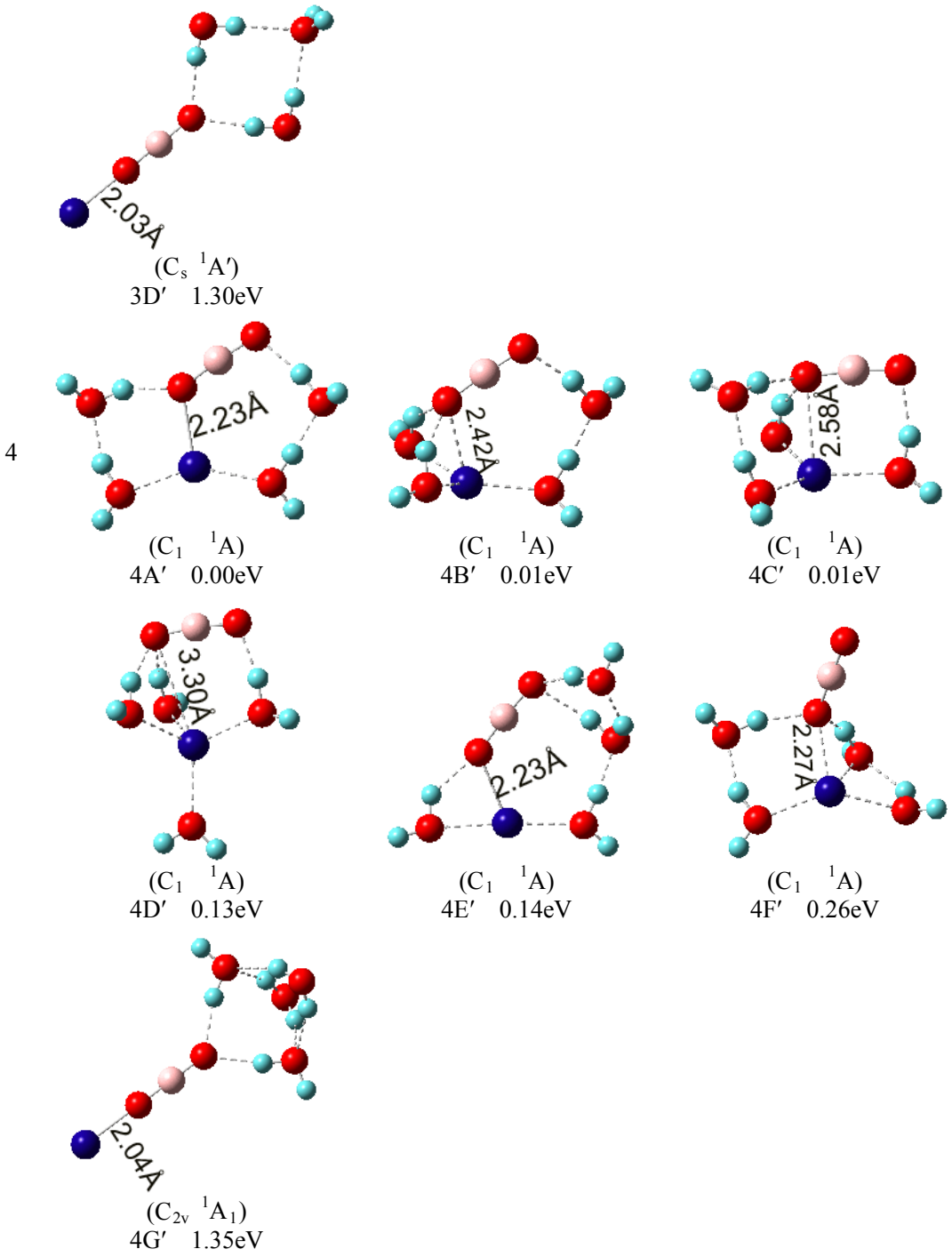


Fig. S2 Optimized geometries of the typical low-lying isomers of $NaBO_2(H_2O)_n$ (n=0-4) neutrals.

Table S2 Cartesian coordinates of the low-lying isomers of neutral $NaBO_2(H_2O)_n$ (n=0-4) clusters.

$NaBO_2$			
0A'			
Na	0.00000000	0.00000000	2.15149700
O	0.00000000	0.00000000	0.13816000
B	0.00000000	0.00000000	-1.14466300
O	0.00000000	0.00000000	-2.38105400
0B'			
Na	0.00000000	0.00000000	0.81272600
O	0.00000000	0.00000000	2.89085000
B	0.00000000	0.00000000	-1.72327900
O	0.00000000	0.00000000	-2.93129800
0C'			
Na	0.00000000	0.00000000	0.53316900
O	0.00000000	0.00000000	2.64496300
O	0.00000000	0.00000000	-1.60736100
B	0.00000000	0.00000000	-2.83313500

$NaBO_2(H_2O)$			
1A'			
Na	-1.43743400	-1.12060200	0.00124700
O	0.39785700	-0.09342900	-0.00215100
B	1.67700200	0.04847700	-0.00062000
O	2.90467500	0.17882200	0.00137300
H	-2.32282300	1.93432100	0.01874100
O	-1.96179200	1.04613300	-0.00264100
H	-0.97633000	1.09771400	-0.00200200
1B'			
Na	0.00000000	0.00000000	1.07600500
O	0.00000000	0.00000000	-0.95884400
B	0.00000000	0.00000000	-2.23976000
O	0.00000000	0.00000000	-3.47845400
O	0.00000000	0.00000000	3.36983600
H	0.00000000	0.76840000	3.95122000
H	0.00000000	-0.76840000	3.95122000
1C'			
Na	-3.07439000	-0.54381300	0.00000000
O	-1.23447800	0.29673100	0.00000000
B	0.00000000	0.61722100	0.00000000
O	1.20363900	0.92155200	0.00000000
H	2.63535500	-0.20363100	0.00000000
O	3.40799300	-0.80416900	0.00000000
H	4.16569700	-0.21344100	0.00000000

$NaBO_2(H_2O)_2$

2A'				**2C'**			
Na	1.30114300	-1.40251700	0.04101000	Na	0.79257600	-1.45776200	0.00000000
O	-0.79892700	-1.76007700	0.03485200	O	-0.13615900	0.56603100	0.00000000
B	-1.51838800	-0.71996400	-0.02211700	B	-0.16724100	1.85597700	0.00000000
O	-2.13101100	0.37241300	-0.07605500	O	-0.19881200	3.08871400	0.00000000
O	1.98480700	0.70531600	-0.04029600	O	-0.19881200	-1.20547600	1.99204400
H	1.20354800	1.32968000	0.00161600	O	-0.19881200	-1.20547600	-1.99204400
H	2.73022500	1.22462700	-0.35130700	H	-0.56726800	-1.25813600	2.87610500
O	-0.20827900	2.18772300	0.00540400	H	-0.44342100	-0.33928800	1.59701800
H	-1.00928000	1.58853700	-0.06011200	H	-0.44342100	-0.33928800	-1.59701800
H	2.84166100	-0.41785300	0.67803600	H	-0.56726800	-1.25813600	-2.87610500
2B'				**2D'**			
Na	0.64664600	0.14698200	1.26700100	Na	0.00000000	0.00000000	3.71975200
O	-0.95719800	-0.22146700	-1.41729000	O	0.00000000	0.00000000	1.68928900
B	-1.42756200	-0.12363600	-0.24668200	B	0.00000000	0.00000000	0.42033100
O	-1.63392600	-0.00162800	0.98570200	O	0.00000000	0.00000000	-0.82642600
O	1.16692600	-1.54657700	-0.21172400	O	0.00000000	2.29549600	-2.48473500
O	0.97914300	1.60821800	-0.52246700	H	0.03235100	1.50593300	-1.91248300
H	0.88578600	2.54353400	-0.72236300	H	-0.63276500	2.06566100	-3.17054900
H	0.35761700	1.13352800	-1.11921600	H	0.63276500	-2.06566100	-3.17054900
H	1.85224600	-2.05947700	-0.64621800	O	0.00000000	-2.29549600	-2.48473500
H	0.48949900	-1.32457000	-0.88956200	H	-0.03235100	-1.50593300	-1.91248300

$NaBO_2(H_2O)_3$

3A'			
Na	-0.63026400	1.20163000	0.02238100
O	-0.23597500	-1.58435700	-0.04262600
B	1.01553600	-1.36074300	-0.05349300
O	2.20674800	-0.98405700	-0.05060700
O	-1.59851200	0.03905700	-1.67230800
O	-1.48965800	-0.02310900	1.74761400
O	1.58806500	1.62459100	-0.00560000
H	-1.48584200	-0.16967700	2.69636200
H	-1.13156000	-0.83549500	1.31906700
H	-2.33707200	-0.18416700	-2.24256400
H	-1.23510200	-0.79737800	-1.29837200
H	2.25909400	2.26797800	-0.24408200
H	2.02037300	0.72751500	-0.02091600

3B'			

3C'			
Na	0.00000000	0.00000000	0.13889300
O	0.00000000	0.00000000	2.20581400
B	0.00000000	0.00000000	3.48369600
O	0.00000000	0.00000000	4.72555500
O	0.00000000	1.56016800	-1.56163700
O	0.00000000	-1.56016800	-1.56163700
O	0.00000000	0.00000000	-4.01855300
H	0.00000000	-1.28671200	-2.49089500
H	0.00000000	-2.52140000	-1.54053100
H	0.00000000	1.28671200	-2.49089500
H	0.00000000	2.52140000	-1.54053100
H	0.76989700	0.00000000	-4.59989100
H	-0.76989700	0.00000000	-4.59989100

3D'			
Na	0.45903400	4.67000500	0.00000000
O	0.16455600	2.66561800	0.00000000
B	0.00993000	1.40314700	0.00000000
O	-0.13993700	0.16828100	0.00000000
O	-0.13993700	-1.90063600	2.00869900
H	-0.15172400	-1.14234000	1.39944500
H	-0.08530800	-2.66490900	1.42203400
H	-0.15172400	-1.14234000	-1.39944500
O	-0.13993700	-1.90063600	-2.00869900
H	-0.08530800	-2.66490900	-1.42203400
O	-0.23031100	-4.19082500	0.00000000
H	-1.11686800	-4.56738900	0.00000000
H	0.37643800	-4.93832300	0.00000000

$NaBO_2(H_2O)_4$

4A'

Na	0.57613800	1.10652800	0.03722900
O	0.42289500	-1.11436000	0.02161900
B	-0.74323200	-1.61705000	-0.03248300
O	-1.92485600	-2.01591900	-0.07796400
O	-3.40828400	0.20604600	0.01237800
O	2.81622400	1.34670000	0.03923000
O	-1.46650800	2.04658200	-0.03597900
H	3.13496500	0.41036600	0.02122700
H	3.54880500	1.90690400	-0.22638700
H	-2.96910600	-0.68440300	-0.05778900
H	-4.06574000	0.12409200	0.70892400
H	-2.23369700	1.41443700	0.00817000
H	-1.82458000	2.87746100	-0.35844000
O	3.08708600	-1.31349400	-0.06722700
H	3.46575200	-1.92387700	0.57130200
H	2.10978700	-1.45598400	-0.05056900

4B'

Na	-1.04719500	1.00629800	0.07420400
O	-0.65072800	-1.37347100	-0.06978200
B	0.58325700	-1.68080200	-0.13557800
O	1.81022400	-1.89795900	-0.18351100
O	0.90860800	2.13402200	-0.05309300
O	-1.96120800	-0.08722300	1.88459300
O	3.01911700	0.48080100	0.03308500
H	-2.02235300	-0.26128800	2.82647400
H	-1.57749100	-0.88015400	1.45443700
H	1.16072200	2.89664500	-0.58042500
H	1.72704500	1.57617100	0.01897300
H	3.68200600	0.44675000	0.72820200
H	2.68655900	-0.44901300	-0.08061400
O	-2.16480200	0.10060200	-1.72298100
H	-1.77989600	-0.74027200	-1.39934300
H	-2.96341100	-0.10827900	-2.21255200

4C'

Na	0.04511900	-1.21889200	0.22105300
O	-0.08005600	1.35079800	0.42853500
B	-1.22302600	1.42954700	-0.12981000
O	-2.33980000	1.33882200	-0.67529000
O	2.37915000	1.34426000	-0.68737500
O	0.26010100	-0.4555360	2.38092000
O	-2.02696100	-1.35825600	-0.73761200
H	-0.06447700	-0.44301000	3.28416200
H	0.12392800	0.43780000	1.99819800
H	3.03214300	1.82110100	-0.16772900
H	1.50051000	1.52912200	-0.27806000
H	-2.65752700	-1.9323350	-1.17799600
H	-2.36081200	-0.42954300	-0.82437100
O	1.98796700	-1.30359700	-0.94831200
H	2.31761200	-0.37320300	-0.92387400
H	2.28424800	-1.68179100	-1.77979700

4D'

Na	-1.04631100	0.14484300	0.00172900
O	1.95352400	-1.23157100	-0.01123900
B	2.30745400	-0.01245800	-0.00319800
O	2.52593200	1.21970400	0.00802500
O	-0.20123000	-1.27308600	1.61602800
O	0.03273200	2.15544100	-0.00102000
H	-0.05631300	-1.29112800	2.56503300
H	0.67527700	-1.44026700	1.19092100
H	-0.05494700	3.07383500	-0.26512600
H	1.01061700	1.95486400	0.01255300
O	-0.22775200	-1.30710500	-1.59654500
H	0.65762400	-1.45680700	-1.18195500
H	-0.10183100	-1.36471300	-2.54657500
O	-3.36752400	0.25473600	-0.00093300
H	-3.91382000	-0.5352160	-0.06969100
H	-3.96990400	0.98350600	0.17728600

4E'

Na	1.81168100	0.78986900	0.20071000
O	1.03658800	-1.24587000	-0.27521400
B	-0.18894900	-1.46253400	-0.50153300
O	-1.41777600	-1.57753900	-0.71867900
O	3.53664800	-0.67753900	0.36417900
O	0.28333300	2.39359100	-0.00905700
O	-3.20560100	-0.59950600	1.12645900
O	-2.05344700	1.26888900	-0.59934600
H	4.34908000	-1.14442900	0.56898700
H	2.85023100	-1.33294000	0.12473400
H	-2.61330700	0.97334300	0.14353000
H	-1.87268800	0.41992600	-1.04099600
H	-2.65087500	-1.15951300	0.54047200
H	-4.07531800	-1.00797000	1.14543200
H	-0.62598200	2.03077100	-0.20756000
H	0.21716700	3.34871900	-0.08147300

4F'				**4G'**			
Na	1.00150900	0.44677800	-0.53996600	Na	0.00000000	0.00000000	5.00161800
O	-0.90905400	-0.55912000	0.17371400	O	0.00000000	0.00000000	2.96339500
B	-1.67535400	-1.49460400	-0.28581200	B	0.00000000	0.00000000	1.69622100
O	-2.40468000	-2.38106300	-0.73166200	O	0.00000000	0.00000000	0.44874400
O	-1.84385500	1.94467700	0.64066200	O	0.00000000	1.75157100	-1.71707700
O	2.76623300	-1.01823500	-0.59512100	O	0.00000000	-1.75157100	-1.71707700
O	0.40850000	2.61583900	-0.63916700	H	0.00000000	2.67931500	-1.46649300
H	2.54516500	-1.33016400	0.30083300	H	0.00000000	1.24013300	-0.88231900
H	3.12910100	-1.76281500	-1.08170000	H	0.00000000	-1.24013300	-0.88231900
H	-1.66646900	0.97765600	0.54090200	H	0.00000000	-2.67931500	-1.46649300
H	-2.77208800	2.07704800	0.42775200	O	-2.08063000	0.00000000	-2.98167300
H	-0.47688100	2.61666600	-0.20268500	O	2.08063000	0.00000000	-2.98167300
H	0.74394400	3.51490200	-0.62384600	H	-1.53076300	-0.75552900	-2.72959700
O	1.26595700	-0.83654600	1.65602800	H	-1.53076300	0.75552900	-2.72959700
H	1.26720900	-0.75341400	2.61314200	H	1.53076300	-0.75552900	-2.72959700
H	0.32538000	-0.90583800	1.35865600	H	1.53076300	0.75552900	-2.72959700