C Oxygen, Sodium Superoxides and Peroxides

C1 O

NEUTRAL ^3P ——— UKS/SVP+
E_{abs}=-75.0049 H

NEUTRAL ^3P ——— UKS/SVP
E_{abs}=-74.9974 H

ANION ^2P ——— UKS/SVP+
E_{abs}=-75.0735 H

ANION ^2P ——— UKS/SVP
E_{abs}=-74.9892 H

C2 O_2

NEUTRAL $^3\Sigma_g^-$ ——— UKS/SVP+
E_{abs}=-150.2313 H
E_a=44.7 kJ/mol =0.463 eV
R=122 pm

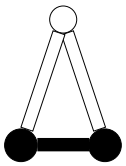
NEUTRAL $^3\Sigma_g^-$ ——— UKS/SVP
E_{abs}=-150.2258 H
E_a=-66.4 kJ/mol =-0.688 eV

ANION $^2\Pi_g$ ——— UKS/SVP+
E_{abs}=-150.2483 H
R=136 pm

ANION $^2\Pi_g$ ——— UKS/SVP
E_{abs}=-150.2005 H

C3

Superoxide
$Na(O_2)$
C_{2v}



NEUTRAL $^2B_1$ ——— UKS/SVP+
E_{abs}=-312.5086 H
Global Minimum E_i=6.34 eV rel C4
R_{O-O}=136 pm
$D_e=\Delta E^i_{Na}$=128 kJ/mol rel O_2+Na
$D_e=\Delta E^i_{Na}$=590 kJ/mol rel $(O_2)^-+Na^+$
See table 3.3

NEUTRAL $^2B_1$ ——— UKS/SVP
E_{abs}=-312.4934 H

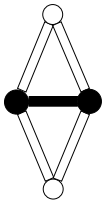
C4

$(O_2).Na^+$
$C_{\infty v}$

CATION $^3\Sigma$ ——— UKS/SVP+
E_{abs}=-312.2757 H
Global Minimum
ΔE^i_{Na}=23.4 kJ/mol rel O_2+Na^+
R_{O-O}=121pm

C5

Peroxide
$Na_2(O_2)$
D_{2h}

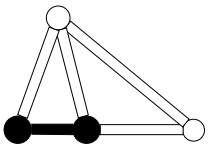


NEUTRAL ^1A_g _____ RKS/SVP+
E_{abs}=-474.7959 H
Global Minimum E_i=4.58 eV
R_{O-O}=160 pm
ΔE^i_{Na}=154 kJ/mol rel C3

NEUTRAL ^1A_g _____ RKS/SVP
E_{abs}=-474.7674 H
ΔE_{ox}=154 kJ/mol rel Na_2+O_2

C6

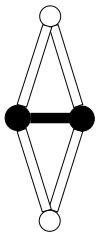
Superoxide
$Na_2(O_2)$
C_s



NEUTRAL $^3A''$ _____ UKS/SVP+
E_{abs}=-474.7633 H
E=85.6 kJ/mol rel C5
ΔE^i_{Na}=68.3 kJ/mol rel C3
R_{O-O}=134pm

C7

Superoxide
$Na_2(O_2)$
D_{2h}



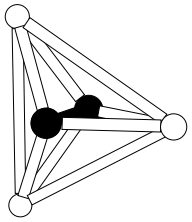
NEUTRAL $^3B_{1g}$ _____ UKS/SVP+
E_{abs}=-474.7713 H
E=64.6 kJ/mol rel C5
R_{O-O}=137 pm
ΔE^i_{Na}=129 kJ/mol rel C3
Molecule in yz plane (see fig 3.5)

CATION $^2B_{2u}$ _____ UKS/SVP+
E_{abs}=-474.6277 H
Global Minimum
ΔE^i_{Na}=324 kJ/mol rel C4
R_{O-O}=137 pm

CATION $^2B_{2u}$ _____ UKS/SVP
E_{abs}=-474.5919 H

C8

Peroxide
$Na_3(O_2)$
D_{3h}



NEUTRAL $^2A'_1$ ——— UKS/SVP+
E_{abs}=-637.0736 H
E=46.7 kJ/mol rel D1
R_{O-O}=160 pm
ΔE^i_{Na}=129 kJ/mol rel C5

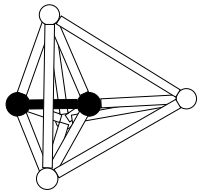
NEUTRAL $^2A'_1$ ——— UKS/SVP
E_{abs}=-637.0581 H
E=29.9 kJ/mol rel D1
ΔE^i_{Na}=163 kJ/mol rel C5
ΔE_{ox}=285 kJ/mol rel A3+O_2

CATION $^1A'_1$ ——— UKS/SVP+
E_{abs}=-636.9400 H
Global Minimum
ΔE^i_{Na}=220 kJ/mol rel C7

CATION $^1A'_1$ ——— UKS/SVP
E_{abs}=-636.9241 H
ΔE^i_{Na}=272 kJ/mol rel C7

C9

Peroxide
$Na_4(O_2)$
C_{3v}

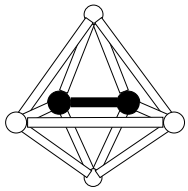


NEUTRAL $^1A_1$ ——— RKS/SVP+
E_{abs}=-799.3386 H
E=121 kJ/mol rel D3
R_{O-O}=159 pm
ΔE^i_{Na}=48.8 kJ/mol rel D1
Cation & Triplet → D3

NEUTRAL $^1A_1$ ——— RKS/SVP
E_{abs}=-799.3214 H
E=104 kJ/mol rel D3
ΔE_{ox}=353 kJ/mol rel A4+O_2

C10

Peroxide
$Na_4(O_2)$
C_{2v}



NEUTRAL $^1A_1$ ——— RKS/SVP+
E_{abs}=-799.3336 H
E=134 kJ/mol rel D3
R_{O-O}=157 pm
ΔE^i_{Na}=35.7 kJ/mol rel D1

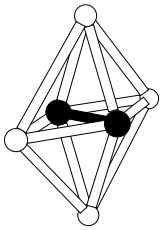
NEUTRAL $^1A_1$ ——— RKS/SVP
E_{abs}=-799.3173 H

CATION $^2A_1$ ——— UKS/SVP+
E_{abs}=-799.1920 H
E=102 kJ/mol rel D3
ΔE^i_{Na}=61.2 kJ/mol rel C8

CATION $^2A_1$ ——— UKS/SVP
E_{abs}=-799.1744 H

C11

Peroxide
$Na_4(O_2)$
D_{4h}



NEUTRAL $^1A_{1g}$ ——— RKS/SVP+
E_{abs}=-799.3246 H
E=157 kJ/mol rel D3
R_{O-O}=158 pm
ΔE^i_{Na}=12.1 kJ/mol rel D1

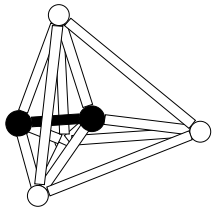
NEUTRAL $^1A_{1g}$ ——— RKS/SVP
E_{abs}=-799.3123 H

CATION $^2A_{1g}$ ——— UKS/SVP+
E_{abs}=-799.1685 H
E=164 kJ/mol rel D3
ΔE^i_{Na}=-0.5 kJ/mol rel C8

CATION $^2A_{1g}$ ——— UKS/SVP
E_{abs}=(-799.1554) H
Not a minimum → D6

C12

Peroxide
$Na_4(O_2).Na$
C_1



NEUTRAL ^2A ——— UKS/SVP+
E_{abs}=-961.5951 H
E=233 kJ/mol rel D7
R_{O-O}=156 pm
ΔE_{Na}=-47.5 kJ/mol rel D3
ΔE_{Na}=73.0 kJ/mol rel C9

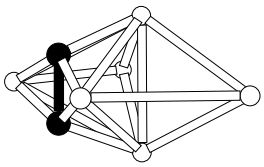
NEUTRAL ^2A ——— UKS/SVP
E_{abs}=-961.5792 H
E=215 kJ/mol rel D7
ΔE_{ox}=362 kJ/mol rel A6+O_2

CATION ^1A ——— RKS/SVP+
E_{abs}=-961.4623 H
E=262 kJ/mol rel D7
ΔE_{Na}=7.1 kJ/mol rel D3
ΔE_{Na}=109 kJ/mol rel C10
Almost C_s

CATION ^1A ——— RKS/SVP
E_{abs}=-961.4466 H
E=231 kJ/mol rel D7

C13

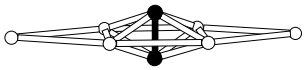
Peroxide
$Na_4(O_2).Na_2$
C_{2v}



NEUTRAL $^1A_1$ ——— RKS/SVP
E_{abs}=-1123.8405 H
E=252 kJ/mol rel D14
R_{O-O}=154 pm
ΔE_{Na}=85.6 kJ/mol rel C12
ΔE_{ox}=325 kJ/mol rel A11+O_2

CATION $^2A_1$ ——— UKS/SVP
E_{abs}=-1123.6861 H
E=300 kJ/mol rel D14
ΔE_{Na}=28.4 kJ/mol rel C12
Distorted to C_s

C14

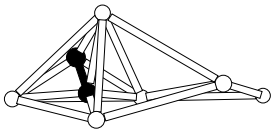


Peroxide
$Na_4(O_2).Na_2$
D_{2h}

NEUTRAL ^1A_g — RKS/SVP
E_{abs}=-1123.8372 H
E=261 kJ/mol rel D14
R_{O-O}=157 pm
ΔE_{Na}=76.9 kJ/mol rel C12

CATION ^2A_g — UKS/SVP
E_{abs}=-1123.6757 H
E=327 kJ/mol rel D14
ΔE_{Na}=1.1 kJ/mol rel C12

C15

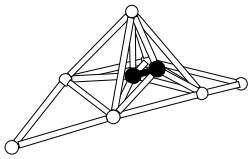


Peroxide
$Na_4(O_2).Na_2$
C_1

NEUTRAL ^1A — RKS/SVP
E_{abs}=-1123.8304 H
E=279 kJ/mol rel D14
R_{O-O}=158 pm
ΔE_{Na}=59.1 kJ/mol rel C12

CATION ^2A — UKS/SVP
E_{abs}=-1123.6931 H
E=282 kJ/mol rel D14
ΔE_{Na}=46.7 kJ/mol rel C12

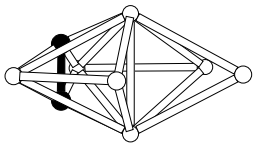
C16



Peroxide
$Na_5(O_2).Na_2$
C_s

NEUTRAL $^2A''$ — UKS/SVP
E_{abs}=-1286.0950 H
ΔE^{i}_{Na}=67.7 kJ/mol rel C13
ΔE^{io}_{Na}=8.1 kJ/mol rel C17
ΔE_{ox}=310 kJ/mol rel A16+O_2
E=278 kJ/mol rel D23
R_{O-O}=157 pm
ΔE^{i}_{Na}=67.7 kJ/mol rel C13

C17



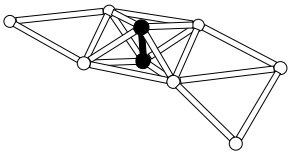
Peroxide
$Na_4(O_2).Na_3$
C_{2v}

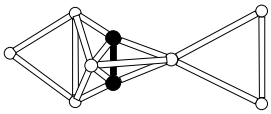
NEUTRAL $^2A_1$ — UKS/SVP
E_{abs}=-1286.0919 H
E=286 kJ/mol rel D23
R_{O-O}=154 pm
ΔE^{i}_{Na}=59.6 kJ/mol rel C13

CATION $^1A_1$ — RKS/SVP
E_{abs}=-1285.9538 H
E=288 kJ/mol rel D23
ΔE_{Na}=84.0 kJ/mol rel C15

C18

Peroxide
$Na_4(O_2).Na_3$
C_s

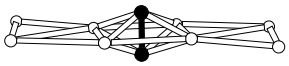




NEUTRAL $^2A'$ _____ UKS/SVP
E_{abs}=-1286.0851 H
E=304 kJ/mol rel D23
R_{O-O}=157 pm
ΔE_{Na}=41.7 kJ/mol rel C13
Cation → C18
CATION $^1A'$ _____ RKS/SVP
E_{abs}=-1285.9554 H
E=284 kJ/mol rel D23
ΔE_{Na}=88.2 kJ/mol rel C15

C19

Peroxide
$Na_4(O_2).Na_4$
C_s

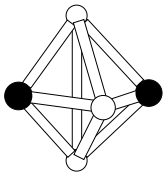


NEUTRAL $^3A'$ _____ RKS/SVP
E_{abs}=-1448.3323 H
E=344 kJ/mol rel D33
R_{O-O}=157 pm
ΔE_{Na}=22.6 kJ/mol rel C16
Singlet E_{abs}=-1448.3235 H
CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1448.1874 H
E=352 kJ/mol rel D33
ΔE_{Na}=8.7 kJ/mol rel C18

D Sodium-Bridged Bis-Monoxides

D1

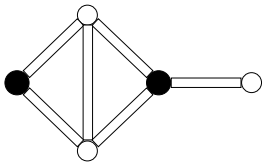
μ-η^3-Na_3O_2
D_{3h}



NEUTRAL $^2A_2''$ _____ UKS/SVP
E_{abs}=-637.0695 H
Global Minimum E_i=3.96 eV rel C8
R_{O-O}=261 pm
ΔE^i_{Na}=193 kJ/mol rel C5
ΔE_{ox}=315 kJ/mol rel A3+O_2
Cation → C8
Anion E_{abs}=-637.0972 H
NEUTRAL $^2A_2''$ _____ UKS/SVP+
E_{abs}=-637.0913 H

D2

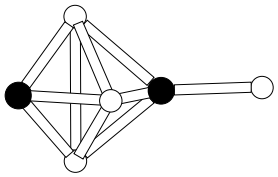
μ-η^2-Na_3O_2
C_{2v}



NEUTRAL $^2A_1$ _____ UKS/SVP
E_{abs}=-637.0473 H
E=58.3 kJ/mol rel D1
R_{O-O}=308 pm
ΔE^i_{Na}=134 kJ/mol rel C5

D3

μ-η^3-Na_4O_2
C_{3v}

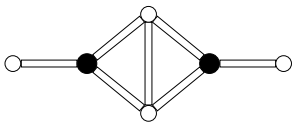


NEUTRAL A_1 _____ UKS/SVP+
E_{abs}=-799.3611 H
Global Minimum ≈ D5 E_i=4.16 eV
R_{O-O}=291 pm
ΔE^i_{Na}=165 kJ/mol rel D1
Spin-contaminated singlet
NEUTRAL $^2A_2''$ _____ UKS/SVP+
E_{abs}=-799.3845 H
ΔE_{frag}=248 kJ/mol rel B30+B30
ΔE_{ox}=412 kJ/mol rel A4+O_2
CATION $^2A_1$ _____ UKS/SVP
E_{abs}=-799.2084 H
Global Minimum
ΔE_{frag}=322 kJ/mol rel B30+B30$^+$

CATION $^2A_1$ _____ UKS/SVP+
E_{abs}=-799.2309 H

D4

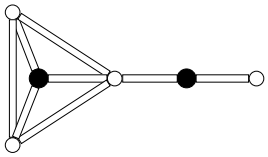
μ-η^2-Na_4O_2
D_{2h}



NEUTRAL ^1A_g _____ RKS/SVP
E_{abs}=-799.3603 H
E=2.1 kJ/mol rel D3
R_{O-O}=334 pm
ΔE^i_{Na}=163 kJ/mol rel D1
CATION ^2A_g _____ UKS/SVP
E_{abs}=-799.1869 H
E=56.4 kJ/mol rel D3

D5

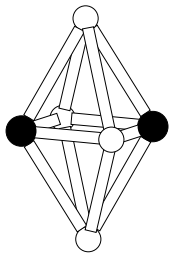
μ-η^1-Na_4O_2
C_{2v}



NEUTRAL $^1A_1$ ——— RKS/SVP
E_{abs}=-799.3185 H
E=112 kJ/mol rel D3
R_{O-O}=422 pm
ΔE^i_{Na}=53.3 kJ/mol rel D1
CATION $^2A_1$ ——— UKS/SVP
E_{abs}=-799.1738 H
E=90.8 kJ/mol rel D3

D6

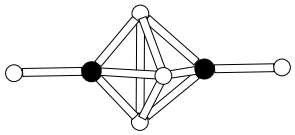
μ-η^4-Na_4O_2
D_{4h}



NEUTRAL A_{1g} ——— UKS/SVP
E_{abs}=-799.3157 H
E=119 kJ/mol rel D3
R_{O-O}=237 pm
ΔE^i_{Na}=45.9 kJ/mol rel D1
Singlet/Triplet mixture
CATION $^2A_{1g}$ ——— UKS/SVP
E_{abs}=-799.1628 H
E=120 kJ/mol rel D3

D7

μ-η^3-Na_5O_2
D_{3h}

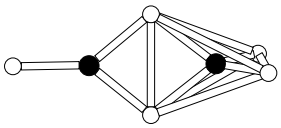


NEUTRAL $^2A'_1$ ——— UKS/SVP
E_{abs}=-961.6610 H
Global Minimum E_i=3.44 eV
R_{O-O}=300 pm
ΔE^i_{Na}=187 kJ/mol rel D3
ΔE_{frag}=266 kJ/mol rel B30+B31
ΔE_{ox}=534 kJ/mol rel A6+O_2
NEUTRAL $^1A'_1$ ——— UKS/SVP
E_{abs}=-961.6837 H

CATION $^1A'_1$ ——— RKS/SVP
E_{abs}=-961.5347 H
Global Minimum
ΔE^i_{Na}=256 kJ/mol rel D3
ΔE_{frag}=307 kJ/mol rel B30+B31$^+$
CATION $^1A'_1$ ——— RKS/SVP
E_{abs}=-961.5621 H

D8

μ-η^2-Na_5O_2
C_{2v}

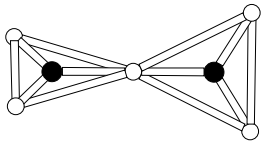


NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-961.6479 H
E=34.4 kJ/mol rel D7
R_{O-O}=272 pm
ΔE^i_{Na}=153 kJ/mol rel D3
ΔE^i_{Na}=155 kJ/mol rel D4

CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-961.5130 H
E=57.0 kJ/mol rel D7
ΔE^i_{Na}=199 kJ/mol rel D3
ΔE^i_{Na}=256 kJ/mol rel D4

D9

μ-η^1-Na_5O_2
D_{2d}

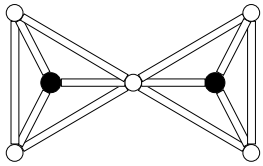


NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-961.6224 H
E=101 kJ/mol rel D7
R_{O-O}=362 pm
ΔE^i_{Na}=85.6 kJ/mol rel D3
ΔE^i_{Na}=197 kJ/mol rel D5

CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-961.5001 H
E=90.8 kJ/mol rel D7
ΔE^i_{Na}=165 kJ/mol rel D3
ΔE^i_{Na}=256 kJ/mol rel D5

D10

μ-η^1-Na_5O_2
D_{2h}

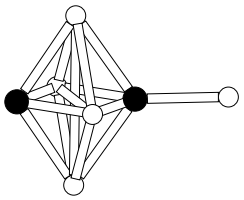


NEUTRAL ^2A_g ——— UKS/SVP
E_{abs}=-961.6213 H
E=104 kJ/mol rel D7
R_{O-O}=428 pm
ΔE^i_{Na}=82.7 kJ/mol rel D3
ΔE^i_{Na}=195 kJ/mol rel D5

CATION ^1A_g ——— RKS/SVP
E_{abs}=-961.4967 H
E=99.8 kJ/mol rel D7
ΔE^i_{Na}=156 kJ/mol rel D3
ΔE^i_{Na}=247 kJ/mol rel D5

D11

μ-η^4-Na_5O_2
C_{4v}

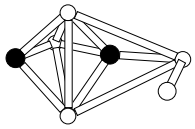


NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-961.6080 H
E=139 kJ/mol rel D7
R_{O-O}=264 pm
ΔE^{i}_{Na}=47.8 kJ/mol rel D3
ΔE^{i}_{Na}=167 kJ/mol rel D6

CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-961.4520 H
E=217 kJ/mol rel D7
ΔE^{i}_{Na}=39.1 kJ/mol rel D3
ΔE^{i}_{Na}=159 kJ/mol rel D6

D12

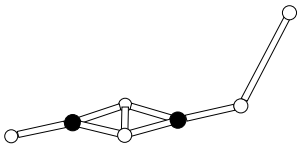
$Na_4O_2.Na$
C_s



NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-961.6109 H
E=132 kJ/mol rel D7
R_{O-O}=268 pm
ΔE_{Na}=55.4 kJ/mol rel D3
Cation → D7

D13

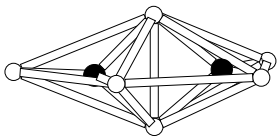
$Na_4O_2.Na$
C_s



NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-961.6001 H
E=160 kJ/mol rel D7
R_{O-O}=334 pm
ΔE_{Na}=27.0 kJ/mol rel D3
ΔE_{Na}=29.1 kJ/mol rel D4
Cation → D7

D14

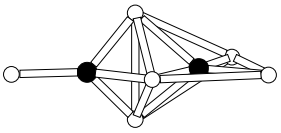
μ-η^2-Na_6O_2
C_{2v}



NEUTRAL $^1A_1$ ——— RKS/SVP
E_{abs}=-1123.9366 H
Global Minimum E_i=3.71 eV
R_{O-O}=335 pm
ΔE^{i}_{Na}=123 kJ/mol rel D7
ΔE^{i}_{Na}=158 kJ/mol rel D8
ΔE^{io}_{Na}=54.9 kJ/mol rel D16
ΔE_{frag}=240 kJ/mol rel B30+B32
ΔE_{Na_2}=243 kJ/mol rel D3+Na_2
ΔE_{ox}=578 kJ/mol rel A11+O_2

CATION $^2A_1$ ——— UKS/SVP
E_{abs}=-1123.8004 H
Global Minimum
ΔE^{i}_{Na}=97.1 kJ/mol rel D7
ΔE^{i}_{Na}=154 kJ/mol rel D8
ΔE^{io}_{Na}=65.4 kJ/mol rel D19
ΔE_{frag}=236 kJ/mol rel B31+$B31^+$

D15

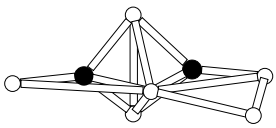


μ-η^3-Na_6O_2
C_s

NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1123.9343 H
E=6.0 kJ/mol rel D14
R_{O-O}=308 pm
ΔE^{i}_{Na}=117 kJ/mol rel D7
ΔE^{io}_{Na}=48.8 kJ/mol rel D16

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1123.7939 H
E=17.1 kJ/mol rel D14
ΔE^{i}_{Na}=80.1 kJ/mol rel D7
ΔE^{io}_{Na}=48.3 kJ/mol rel D19

D16

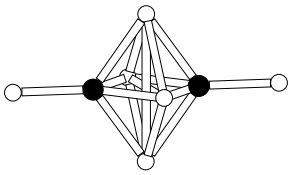


μ-η^3-Na_5O_2.Na
C_s

NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1123.9157 H
E=54.9 kJ/mol rel D14
R_{O-O}=300 pm
ΔE_{Na}=68.3 kJ/mol rel D7
ΔE_{Na_2}=188 kJ/mol rel D3+Na_2

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1123.7741 H
E=69.1 kJ/mol rel D14
ΔE_{Na}=28.1 kJ/mol rel D7
ΔE_{Na_2}=217 kJ/mol rel D3+Na_2

D17



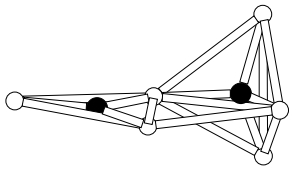
μ-η^4-Na_6O_2
D_{4h}

NEUTRAL $^1A_{1g}$ _____ RKS/SVP
E_{abs}=-1123.9125 H
E=63.3 kJ/mol rel D14
R_{O-O}=274 pm
ΔE^{i}_{Na}=59.9 kJ/mol rel D7
ΔE^{i}_{Na}=199 kJ/mol rel D11
ΔE^{io}_{Na}=-8.4 kJ/mol rel D16

CATION $^2A_{1g}$ _____ UKS/SVP
E_{abs}=-1123.7712 H
E=76.7 kJ/mol rel D14
ΔE^{i}_{Na}=20.5 kJ/mol rel D7
ΔE^{i}_{Na}=238 kJ/mol rel D11
ΔE^{io}_{Na}=-11.3 kJ/mol rel D19

D18

μ-η^1-Na_6O_2
C_s

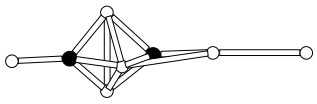


NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1123.9109 H
E=67.5 kJ/mol rel D14
R_{O-O}=411 pm
ΔE^{i}_{Na}=55.7 kJ/mol rel D7
ΔE^{i}_{Na}=157 kJ/mol rel D9
ΔE^{io}_{Na}=-12.6 kJ/mol rel D16

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1123.7752 H
E=66.2 kJ/mol rel D14
ΔE^{i}_{Na}=31.0 kJ/mol rel D7
ΔE^{i}_{Na}=122 kJ/mol rel D9
ΔE^{io}_{Na}=-0.8 kJ/mol rel D19

D19

μ-η^3-Na_5O_2.Na
C_s

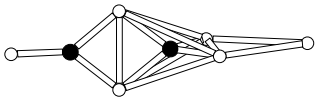


NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1123.9088 H
E=73.0 kJ/mol rel D14
R_{O-O}=299 pm
ΔE_{Na}=50.1 kJ/mol rel D7
Triplet D_{3h} E_{abs}=-1123.8952

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1123.7755 H
E=65.4 kJ/mol rel D14
ΔE_{Na}=31.8 kJ/mol rel D7

D20

μ-η^2-Na_5O_2.Na
C_{2v}

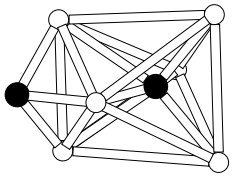


NEUTRAL $^1A_1$ _____ RKS/SVP
E_{abs}=-1123.9083 H
E=74.3 kJ/mol rel D14
R_{O-O}=340 pm
ΔE_{Na}=48.8 kJ/mol rel D7
ΔE_{Na}=83.2 kJ/mol rel D8

CATION $^2A_1$ _____ UKS/SVP
E_{abs}=-1123.7562 H
E=116 kJ/mol rel D14
ΔE_{Na}=-18.9 kJ/mol rel D7
ΔE_{Na}=38.1 kJ/mol rel D8

D21

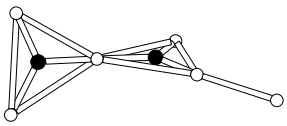
μ-η^3-Na_6O_2
C_{3v}



NEUTRAL $^1A_1$ _____ RKS/SVP
E_{abs}=-1123.8963 H
E=106 kJ/mol rel D14
R_{O-O}=322 pm
ΔE^{i}_{Na}=17.3 kJ/mol rel D7
ΔE^{io}_{Na}=-50.9 kJ/mol rel D16

D22

μ-η^1-Na_5O_2.Na
C_s

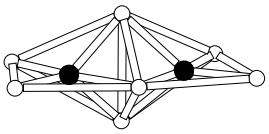


NEUTRAL A' — UKS/SVP
E_{abs}=-1123.8703 H
E=174 kJ/mol rel D14
R_{O-O}=426 pm
ΔE_{Na}=-50.9 kJ/mol rel D7
ΔE_{Na}=50.4 kJ/mol rel D9
Spin-contaminated singlet

CATION $^2A'$ — UKS/SVP
E_{abs}=-1123.7404 H
E=158 kJ/mol rel D14
ΔE_{Na}=-60.4 kJ/mol rel D7
ΔE_{Na}=30.5 kJ/mol rel D9

D23

μ-η^3-Na_7O_2
C_{2v}

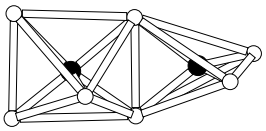


NEUTRAL $^2A_1$ — UKS/SVP
E_{abs}=-1286.2008 H
Global Minimum ≈ D24 E_i=3.73 eV
R_{O-O}=315 pm
ΔE^i_{Na}=93.2 kJ/mol rel D14
ΔE^i_{Na}=99.2 kJ/mol rel D15
ΔE^{io}_{Na}=19.7 kJ/mol rel D27
ΔE_{frag}=166 kJ/mol rel B32+B31
ΔE_{ox}=588 kJ/mol rel A16+O_2

CATION $^1A_1$ — RKS/SVP
E_{abs}=-1286.0636 H
E=6.8 kJ/mol rel D27
ΔE^i_{Na}=90.6 kJ/mol rel D14
ΔE^i_{Na}=108 kJ/mol rel D15
ΔE^{io}_{Na}=-6.8 kJ/mol rel D27

D24

μ-η^2-Na_7O_2
C_1

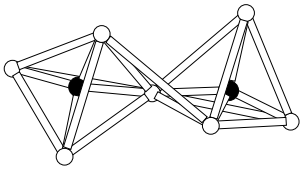


NEUTRAL ^2A — UKS/SVP
E_{abs}=-1286.1992 H
E=4.2 kJ/mol rel D23
R_{O-O}=350 pm
ΔE^i_{Na}=89.0 kJ/mol rel D14
ΔE^{io}_{Na}=15.5 kJ/mol rel D27

CATION ^1A — RKS/SVP
E_{abs}=-1286.0653 H
E=2.4 kJ/mol rel D27
ΔE^i_{Na}=95.0 kJ/mol rel D14
ΔE^{io}_{Na}=-2.4 kJ/mol rel D27

D25

μ-η^1-Na_7O_2
C_2

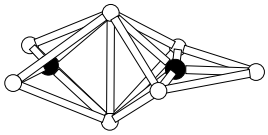


NEUTRAL ^2A ——— UKS/SVP
E_{abs}=-1286.1949 H
E=15.5 kJ/mol rel D23
R_{O-O}=391 pm
ΔE^i_{Na}=77.7 kJ/mol rel D14
ΔE^i_{Na}=83.8 kJ/mol rel D15
$\Delta E^{i_o}_{Na}$=152 kJ/mol rel D27

CATION ^1A ——— RKS/SVP
E_{abs}=-1286.0655 H
E=1.8 kJ/mol rel D27
ΔE^i_{Na}=95.6 kJ/mol rel D14
ΔE^i_{Na}=113 kJ/mol rel D15
$\Delta E^{i_o}_{Na}$=-1.8 kJ/mol rel D27

D26

μ-η^2-Na_7O_2
C_{2v}

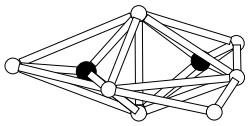


NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-1286.1933 H
E=19.7 kJ/mol rel D23
R_{O-O}=335 pm
ΔE^i_{Na}=73.5 kJ/mol rel D14
$\Delta E^{i_o}_{Na}$=0.0 kJ/mol rel D27

CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-1286.0587 H
E=19.7 kJ/mol rel D27
ΔE^i_{Na}=77.7 kJ/mol rel D14
$\Delta E^{i_o}_{Na}$=-19.7 kJ/mol rel D27

D27

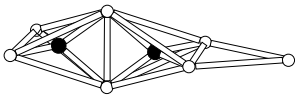
μ-η^2-Na_6O_2.Na
C_{2v}



NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-1286.1933 H
E=19.7 kJ/mol rel D23
R_{O-O}=335 pm
ΔE^i_{Na}=128 kJ/mol rel D16
ΔE^i_{Na}=148 kJ/mol rel D20
ΔE_{Na}=73.5 kJ/mol rel D14
ΔE_{Na_2}=129 kJ/mol rel D7+Na_2

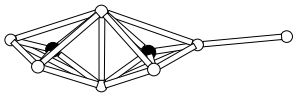
CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-1286.0662 H
Global Minimum ≈ D25
ΔE^i_{Na}=163 kJ/mol rel D19
ΔE^i_{Na}=213 kJ/mol rel D20
ΔE_{Na}=97.4 kJ/mol rel D14
ΔE_{Na_2}=127 kJ/mol rel D7+Na_2
ΔE_{frag}=184 kJ/mol rel B32+B31$^+$

D28



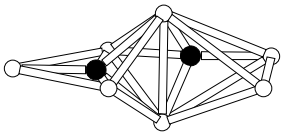
μ-η^2-Na_6O_2.Na
C_{2v}

NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-1286.1913 H
E=24.9 kJ/mol rel D23
R_{O-O}=343 pm
ΔE^i_{Na}=123 kJ/mol rel D16
ΔE^i_{Na}=143 kJ/mol rel D20
ΔE_{Na}=68.3 kJ/mol rel D14



CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-1286.0519 H
E=37.5 kJ/mol rel D27
ΔE^i_{Na}=125 kJ/mol rel D19
ΔE^i_{Na}=176 kJ/mol rel D20
ΔE_{Na}=59.9 kJ/mol rel D14
Triplet E_{abs}=-1286.0420

D29

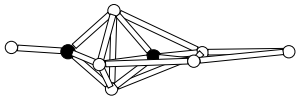


μ-η^3-Na_6O_2.Na
C_s

NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1286.1878 H
E=34.1 kJ/mol rel D23
R_{O-O}=309 pm
ΔE^i_{Na}=114 kJ/mol rel D16
ΔE_{Na}=59.1 kJ/mol rel D14
ΔE_{Na}=65.1 kJ/mol rel D15

CATION $^1A'$ ——— RKS/SVP
E_{abs}=-1286.0554 H
E=29.4 kJ/mol rel D27
ΔE^i_{Na}=134 kJ/mol rel D19
ΔE_{Na}=69.1 kJ/mol rel D14
ΔE_{Na}=86.1 kJ/mol rel D15

D30

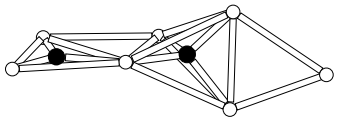


μ-η^3-Na_6O_2.Na
C_s

NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1286.1857 H
E=39.6 kJ/mol rel D23
R_{O-O}=309 pm
ΔE^i_{Na}=108 kJ/mol rel D16
ΔE_{Na}=53.6 kJ/mol rel D14
ΔE_{Na}=59.6 kJ/mol rel D15

CATION $^1A'$ ——— RKS/SVP
E_{abs}=-1286.0552 H
E=28.9 kJ/mol rel D27
ΔE^i_{Na}=134 kJ/mol rel D19
ΔE_{Na}=68.5 kJ/mol rel D14
ΔE_{Na}=85.6 kJ/mol rel D15

D31

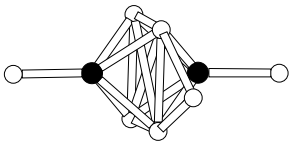


μ-η^1-Na_6O_2.Na
C_s

NEUTRAL $^2A'$ _____ UKS/SVP
E_{abs}=-1286.1674 H
E=87.7 kJ/mol rel D23
R_{O-O}=411 pm
ΔE^i_{Na}=60.4 kJ/mol rel D16
ΔE^i_{Na}=180 kJ/mol rel D22
ΔE_{Na}=5.5 kJ/mol rel D14

CATION $^1A'$ _____ RKS/SVP
E_{abs}=-1286.0383 H
E=73.3 kJ/mol rel D27
ΔE^i_{Na}=89.5 kJ/mol rel D19
ΔE^i_{Na}=182 kJ/mol rel D22
ΔE_{Na}=24.2 kJ/mol rel D14

D32



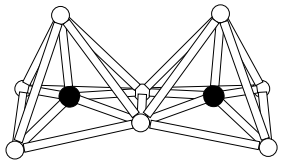
μ-η^4-Na_6O_2.Na
C_{2v}

NEUTRAL $^2A_1$ _____ UKS/SVP
E_{abs}=-1286.1589 H
E=110 kJ/mol rel D23
R_{O-O}=274 pm
ΔE^i_{Na}=38.1 kJ/mol rel D16
ΔE_{Na}=-16.8 kJ/mol rel D14
ΔE_{Na}=46.5 kJ/mol rel D17

CATION $^1A_1$ _____ RKS/SVP
E_{abs}=-1286.0305 H
E=93.7 kJ/mol rel D27
ΔE^i_{Na}=69.1 kJ/mol rel D19
ΔE_{Na}=3.7 kJ/mol rel D14
ΔE_{Na}=80.3 kJ/mol rel D17

D33

μ-η^2-Na_8O_2
C_1



NEUTRAL ^1A ——— RKS/SVP

E_{abs}=-1448.4632 H

Global Minimum ≈ D34 E_i=3.85 eV

R_{O-O}=367 pm

ΔE^i_{Na}=88.5 kJ/mol rel D23

ΔE^i_{Na}=92.7 kJ/mol rel D24

ΔE^{io}_{Na}=8.9 kJ/mol rel D35

Two C_1 minima

ΔE_{Na_2}=114 kJ/mol rel D14+Na_2

ΔE_{frag}=105 kJ/mol rel B32+B32

ΔE_{frag}=325 kJ/mol rel D3+A4

ΔE_{ox}=591 kJ/mol rel A19+O_2

Triplet C_s E_{abs}=-1448.4551

CATION ^2A ——— UKS/SVP

E_{abs}=-1448.3216 H

E=1.3 kJ/mol rel D38

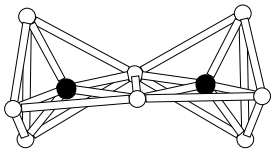
ΔE^i_{Na}=71.9 kJ/mol rel D25

ΔE^i_{Na}=72.5 kJ/mol rel D24

ΔE^{io}_{Na}=-1.3 kJ/mol rel D38

D34

μ-η^2-Na_8O_2
C_{2v}



NEUTRAL $^1A_1$ ——— RKS/SVP

E_{abs}=-1448.4631 H

E=0.3 kJ/mol rel D33

R_{O-O}=368 pm

ΔE^i_{Na}=88.2 kJ/mol rel D23

ΔE^i_{Na}=92.4 kJ/mol rel D24

ΔE^{io}_{Na}=8.7 kJ/mol rel D35

CATION $^2A_1$ ——— UKS/SVP

E_{abs}=-1448.3210 H

E=2.9 kJ/mol rel D38

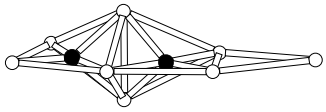
ΔE^i_{Na}=70.9 kJ/mol rel D24

ΔE^i_{Na}=72.5 kJ/mol rel D24

ΔE^{io}_{Na}=-2.9 kJ/mol rel D38

D35

μ-η^3-Na_7O_2.Na
C_s

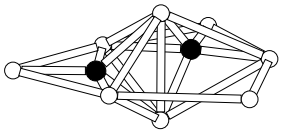


NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1448.4598 H
E=8.9 kJ/mol rel D33
R_{O-O}=316 pm
ΔE^i_{Na}=99.2 kJ/mol rel D27
ΔE^i_{Na}=114 kJ/mol rel D29
ΔE^o_{Na}=7.9 kJ/mol rel D39
ΔE_{Na}=79.6 kJ/mol rel D23

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1448.3157 H
E=16.8 kJ/mol rel D38
ΔE^i_{Na}=54.6 kJ/mol rel D27
ΔE^i_{Na}=81.1 kJ/mol rel D29
ΔE^o_{Na}=20.7 kJ/mol rel D39
ΔE_{Na}=56.4 kJ/mol rel D25
ΔE_{Na}=61.4 kJ/mol rel D23

D36

μ-η^3-Na_7O_2.Na
C_{2v}

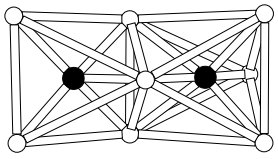


NEUTRAL $^3A_1$ _____ UKS/SVP
E_{abs}=-1448.4591 H
E=10.8 kJ/mol rel D33
R_{O-O}=317 pm
ΔE^i_{Na}=97.4 kJ/mol rel D27
ΔE^i_{Na}=112 kJ/mol rel D29
ΔE^o_{Na}=6.0 kJ/mol rel D39
ΔE_{Na}=77.7 kJ/mol rel D23

CATION $^2A_1$ _____ UKS/SVP
E_{abs}=-1448.3210 H
E=2.9 kJ/mol rel D38
ΔE^i_{Na}=68.5 kJ/mol rel D27
ΔE^i_{Na}=96.9 kJ/mol rel D29
ΔE^o_{Na}=34.7 kJ/mol rel D39
ΔE_{Na}=70.4 kJ/mol rel D25
ΔE_{Na}=75.4 kJ/mol rel D23

D37

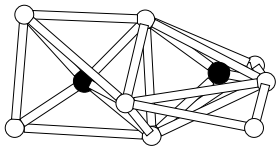
μ-η^3-Na_8O_2
C_s



NEUTRAL $^1A'$ _____ RKS/SVP
E_{abs}=-1448.4589 H
E=11.3 kJ/mol rel D33
R_{O-O}=327 pm
ΔE^i_{Na}=77.2 kJ/mol rel D23
ΔE^o_{Na}=-2.4 kJ/mol rel D35

CATION $^2A'$ _____ UKS/SVP
E_{abs}=-1448.3203 H
E=4.7 kJ/mol rel D38
ΔE^i_{Na}=68.5 kJ/mol rel D25
ΔE^o_{Na}=-4.7 kJ/mol rel D38

D38

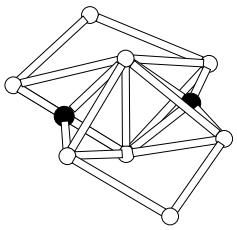


μ-η^2-Na_7O_2.Na
C_1

NEUTRAL A — UKS/SVP
E_{abs}=-1448.4573 H
E=15.5 kJ/mol rel D33
R_{O-O}=347 pm
ΔE^{i}_{Na}=92.7 kJ/mol rel D27
ΔE^{io}_{Na}=1.3 kJ/mol rel D39
ΔE_{Na}=73.0 kJ/mol rel D23
ΔE_{Na}=77.2 kJ/mol rel D24
Spin-contaminated singlet

CATION ^{2}A — UKS/SVP
E_{abs}=-1448.3221 H
Global Minimum ≈ D33, D34, D37, D36
ΔE^{i}_{Na}=71.4 kJ/mol rel D27
ΔE^{io}_{Na}=37.5 kJ/mol rel D39
ΔE_{Na}=73.3 kJ/mol rel D25
ΔE_{Na}=73.8 kJ/mol rel D24
ΔE_{frag}=135 kJ/mol rel B32 + B32$^+$

D39

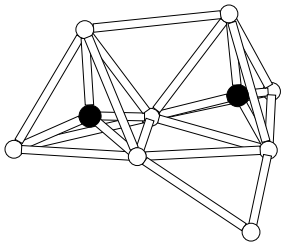


μ-η^2-
Na_6O_2.2Na
C_{2v}

NEUTRAL $^1A_1$ — RKS/SVP
E_{abs}=-1448.4568 H
E=16.8 kJ/mol rel D33
R_{O-O}=340 pm
ΔE_{Na}=91.4 kJ/mol rel D27
ΔE_{Na_2}=97.4 kJ/mol rel D14+Na_2

CATION $^2A_1$ — UKS/SVP
E_{abs}=-1448.3078 H
E=37.5 kJ/mol rel D38
ΔE_{Na}=33.7 kJ/mol rel D27
ΔE_{Na_2}=63.8 kJ/mol rel D14+Na_2

D40



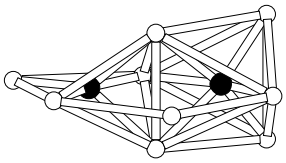
μ-η^1-Na_7O_2.Na
C_1

NEUTRAL A — UKS/SVP
E_{abs}=-1448.4533 H
E=26.0 kJ/mol rel D33
R_{O-O}=397 pm
ΔE^{i}_{Na}=82.2 kJ/mol rel D27
ΔE^{io}_{Na}=150 kJ/mol rel D31
ΔE_{Na}=62.5 kJ/mol rel D23
ΔE_{Na}=78.0 kJ/mol rel D25
Spin-contaminated singlet

CATION ^{2}A — UKS/SVP
E_{abs}=-1448.3201 H
E=5.3 kJ/mol rel D38
ΔE^{i}_{Na}=66.2 kJ/mol rel D27
ΔE^{io}_{Na}=139 kJ/mol rel D31
ΔE_{Na}=68.0 kJ/mol rel D25

D41

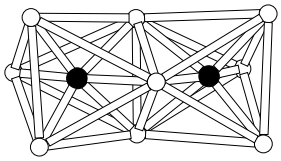
μ-η^3-Na_8O_2.Na
C_s



NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1610.7242 H
Global Minimum ≈ D42 E_i=3.75 eV
R_{O-O}=327 pm
ΔE^i_{Na}=93.7 kJ/mol rel D35
ΔE^{io}_{Na}=10.5 kJ/mol rel D43
ΔE_{Na}=84.8 kJ/mol rel D33
ΔE_{Na}=96.1 kJ/mol rel D37
ΔE_{frag}=136 kJ/mol rel B32 + B36
ΔE_{ox}=630 kJ/mol rel A23 + O_2
CATION $^1A'$ ——— RKS/SVP
E_{abs}=-1610.5820 H
E=11.6 kJ/mol rel D43
ΔE^i_{Na}=81.9 kJ/mol rel D38
ΔE^i_{Na}=84.8 kJ/mol rel D36
ΔE^{io}_{Na}=-11.6 kJ/mol rel D43
ΔE_{Na}=83.2 kJ/mol rel D33
ΔE_{Na}=86.6 kJ/mol rel D37

D42

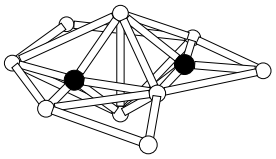
μ-η^3-Na_9O_2
C_{3v}



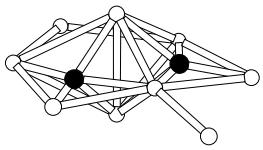
NEUTRAL $^2A_1$ ——— UKS/SVP
E_{abs}=-1610.7229 H
E=3.4 kJ/mol rel D41
R_{O-O}=334 pm
ΔE^i_{Na}=81.4 kJ/mol rel D33
ΔE^i_{Na}=92.7 kJ/mol rel D37
ΔE^{io}_{Na}=-3.4 kJ/mol rel D41
Quartet D_{3h} E_{abs}=-1610.7169 H
CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-1610.5830 H
E=8.9 kJ/mol rel D43
ΔE^i_{Na}=85.9 kJ/mol rel D33
ΔE^i_{Na}=89.3 kJ/mol rel D37
ΔE^{io}_{Na}=-4.5 kJ/mol rel D47
ΔE^{io}_{Na}=-1.1 kJ/mol rel D46
Triplet E_{abs}=-1610.5741
Anion E_{abs}=-1610.7599

D43

μ-η^3-
$Na_7O_2.2Na$
C_s



C_{2v}

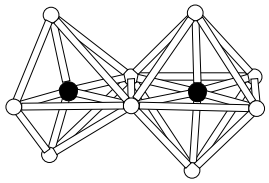


NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1610.7202 H
E=10.5 kJ/mol rel D41
R_{O-O}=319 pm
ΔE^{i}_{Na}=91.1 kJ/mol rel D39
ΔE_{Na}=83.2 kJ/mol rel D35
ΔE_{Na_2}=95.3 kJ/mol rel D23+Na_2

CATION $^1A_1$ ——— RKS/SVP
E_{abs}=-1610.5864 H
Global Minimum ≈ D47
ΔE^{i}_{Na}=131 kJ/mol rel D39
ΔE_{Na}=93.5 kJ/mol rel D38
ΔE_{Na}=110 kJ/mol rel D35
ΔE_{Na_2}=104 kJ/mol rel D23+Na_2
ΔE_{frag}=133 kJ/mol rel B32+B36$^+$
ΔE_{frag}=193 kJ/mol rel A4+D7$^+$

D44

μ-η^2-Na_9O_2
C_s

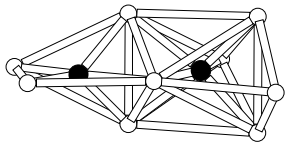


NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1610.7191 H
E=13.4 kJ/mol rel D41
R_{O-O}=364 pm
ΔE^{i}_{Na}=71.4 kJ/mol rel D33
ΔE^{io}_{Na}=-13.4 kJ/mol rel D41
ΔE^{io}_{Na}=3.4 kJ/mol rel D47

CATION $^1A'$ ——— RKS/SVP
E_{abs}=-1610.5745 H
E=31.2 kJ/mol rel D43
ΔE^{i}_{Na}=63.5 kJ/mol rel D33
ΔE^{io}_{Na}=-26.8 kJ/mol rel D47

D45

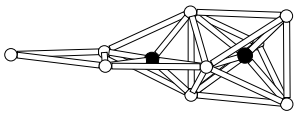
μ-η^3-Na_8O_2.Na
C_s



NEUTRAL $^2A'$ ——— UKS/SVP
E_{abs}=-1610.7185 H
E=15.0 kJ/mol rel D41
R_{O-O}=324 pm
ΔE^{i}_{Na}=78.8 kJ/mol rel D35
ΔE^{io}_{Na}=-4.5 kJ/mol rel D43
ΔE_{Na}=69.8 kJ/mol rel D33
ΔE_{Na}=81.1 kJ/mol rel D37

CATION $^1A'$ ——— RKS/SVP
E_{abs}=-1610.5810 H
E=14.2 kJ/mol rel D43
ΔE^{i}_{Na}=79.3 kJ/mol rel D38
ΔE^{i}_{Na}=96.1 kJ/mol rel D36
ΔE^{io}_{Na}=-14.2 kJ/mol rel D43
ΔE_{Na}=80.6 kJ/mol rel D33
ΔE_{Na}=84.0 kJ/mol rel D37

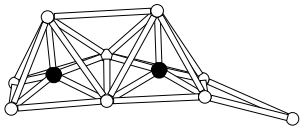
D46



μ-η^3-Na_8O_2.Na
C_s

NEUTRAL $^2A'$ _____ UKS/SVP
E_{abs}=-1610.7180 H
E=16.3 kJ/mol rel D41
R_{O-O}=325 pm
ΔE^{i}_{Na}=77.4 kJ/mol rel D35
ΔE^{io}_{Na}=-5.8 kJ/mol rel D43
ΔE_{Na}=68.5 kJ/mol rel D33
ΔE_{Na}=79.8 kJ/mol rel D37
CATION $^1A'$ _____ RKS/SVP
E_{abs}=-1610.5834 H
E=7.9 kJ/mol rel D43
ΔE^{i}_{Na}=85.6 kJ/mol rel D38
ΔE^{i}_{Na}=102 kJ/mol rel D36
ΔE^{io}_{Na}=-7.9 kJ/mol rel D43
ΔE_{Na}=86.9 kJ/mol rel D33
ΔE_{Na}=90.3 kJ/mol rel D37

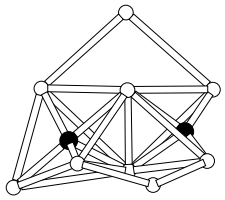
D47



μ-η^2-Na_8O_2.Na
C_1

NEUTRAL ^2A _____ UKS/SVP
E_{abs}=-1610.7178 H
E=16.8 kJ/mol rel D41
R_{O-O}=362 pm
ΔE^{i}_{Na}=76.9 kJ/mol rel D35
ΔE^{i}_{Na}=83.5 kJ/mol rel D38
ΔE^{io}_{Na}=0.3 kJ/mol rel D48
ΔE^{io}_{Na}=-6.3 kJ/mol rel D43
ΔE_{Na}=68.0 kJ/mol rel D33
CATION ^1A _____ RKS/SVP
E_{abs}=-1610.5847 H
E=4.5 kJ/mol rel D43
ΔE^{i}_{Na}=89.0 kJ/mol rel D38
ΔE^{io}_{Na}=-4.5 kJ/mol rel D43
ΔE_{Na}=90.3 kJ/mol rel D33

D48

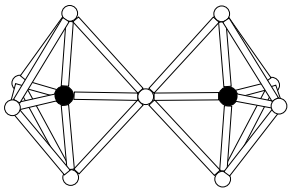


μ-η^2-
Na_7O_2.2Na
C_1

NEUTRAL ^2A _____ UKS/SVP
E_{abs}=-1610.7177 H
ΔE^{i}_{Na}=84.5 kJ/mol rel D39
= kJ/mol
= kJ/mol
E=17.1 kJ/mol rel D41
R_{O-O}=348 pm
ΔE^{i}_{Na}=84.5 kJ/mol rel D39
ΔE_{Na}=76.7 kJ/mol rel D35
ΔE_{Na}=83.2 kJ/mol rel D38
ΔE_{Na_2}=88.7 kJ/mol rel D23+Na_2
Cation → D43

D49

μ-η^1-Na_9O_2
D_{2h}



NEUTRAL ^2A_g ——— UKS/SVP
E_{abs}=-1610.7096 H
E=38.3 kJ/mol rel D41
R_{O-O}=448 pm
ΔE^{i}_{Na}=46.5 kJ/mol rel D33
ΔE^{io}_{Na}=-38.3 kJ/mol rel D41

CATION ^1A_g ——— RKS/SVP
E_{abs}=-1610.5638 H
E=59.3 kJ/mol rel D43
ΔE^{i}_{Na}=35.4 kJ/mol rel D33
ΔE^{io}_{Na}=-54.9 kJ/mol rel D47