

□ B Sodium Monoxides

B1 NaO

NEUTRAL $^2\Pi$ _____ UKS/SVP

$E_{abs} = -237.3058$ H
 $D_e = 209$ kJ/mol to Na+O

ANION $^3\Sigma^-$ _____ UKS/SVP

$E_{abs} = -237.3349$ H
 $E_a = 76.6$ kJ/mol = 0.79 eV

NEUTRAL $^2\Pi$ _____ UKS/SVP+

$E_{abs} = -237.3238$ H
 $D_e = 237$ kJ/mol to Na+O
 See table 3.3

ANION $^3\Sigma^-$ _____ UKS/SVP+

$E_{abs} = -237.3570$ H
 $E_a = 87.2$ kJ/mol = 0.90 eV

B2

Na₂O
 $D_{\infty h}$



NEUTRAL $^1\Sigma_g^+$ _____ RKS/SVP

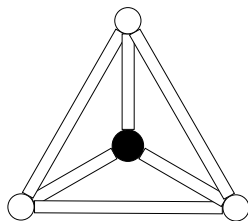
$E_{abs} = -399.6334$ H
 Global Minimum $E_i = 4.93$ eV
 $\Delta E_{Na}^i = 260$ kJ/mol rel [B1]
 $R(\text{Na-O}) = 199$ pm
 $R(\text{Na-Na}) = 399$ pm

CATION $^2\Sigma_g^+$ _____ UKS/SVP

$E_{abs} = -399.4522$ H
 Global Minimum
 $\Delta E_{Na}^i = 291$ kJ/mol rel [B1] + Na⁺
 $R(\text{Na-O}) = 212$ pm
 $R(\text{Na-Na}) = 425$ pm

B3

Na₃O
 D_{3h}

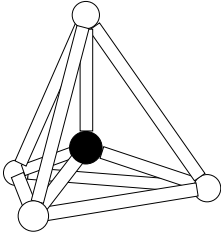
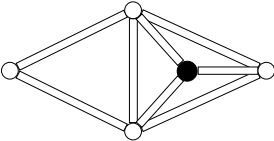
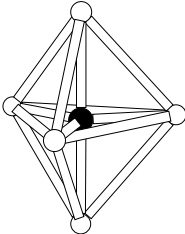


NEUTRAL $^2A'_1$ _____ UKS/SVP

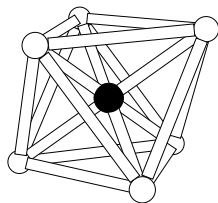
$E_{abs} = -561.9261$ H
 Global Minimum $E_i = 3.86$ eV
 $\Delta E_{Na}^i = 168$ kJ/mol rel [B2]
 $R(\text{Na-O}) = 207$ pm, $R(\text{Na-Na}) = 358$ pm

CATION $^1A'_1$ _____ UKS/SVP

$E_{abs} = -561.7844$ H
 Global Minimum
 $\Delta E_{Na}^i = 272$ kJ/mol rel [B2]
 $R(\text{Na-O}) = 207$ pm, $R(\text{Na-Na}) = 359$ pm

B4 Na₄O T_d		NEUTRAL ¹A₁ _____ RKS/SVP E_{abs}=-724.2116 H Global Minimum E_i=4.16 eV ΔE_{Na}ⁱ=149 kJ/mol rel B3 ΔE_{Na}^{io}=74.8 kJ/mol rel B5 ΔE_{Na₂}=250 kJ/mol rel B2+Na₂ R(Na-O)=213pm R(Na-Na)=347pm CATION ²A₁ _____ UKS/SVP E_{abs}=-724.0589 H Global Minimum ΔE_{Na}ⁱ=120 kJ/mol rel B3 ΔE_{Na}^{io}=83.0 kJ/mol rel B5 ΔE_{Na₂}=325 kJ/mol rel B2+Na₂ R(Na-O)=215pm R(Na-Na)=351pm
B5 Na₃O.Na C_{2v}		NEUTRAL ¹A₁ _____ RKS/SVP E_{abs}=-724.1831 H E=74.8 kJ/mol rel B4 ΔE_{Na}=74.3 kJ/mol rel B3 Triplet E_{abs}=-724.1574 H CATION ²A₁ _____ UKS/SVP E_{abs}=-724.0273 H E=83.0 kJ/mol rel B4 ΔE_{Na}=37.3 kJ/mol rel B3
B6 Na₅O D_{3h}		NEUTRAL ²A₁' _____ UKS/SVP E_{abs}=-886.4585 H Global Minimum ≈ B7, B8 E_i=3.78 eV ΔE_{Na}ⁱ=47.8 kJ/mol rel B4 ΔE_{Na}^{io}=6.3 kJ/mol rel B8 CATION ¹A₁' _____ RKS/SVP E_{abs}=-886.3170 H E=6.8 kJ/mol rel B8 ΔE_{Na}ⁱ=77.2 kJ/mol rel B4 ΔE_{Na}^{io}=6.8 kJ/mol rel B8

B7		NEUTRAL 2A_1 _____ UKS/SVP $E_{abs} = -886.4581$ H $E = 1.1$ kJ/mol rel B6 $\Delta E_{Na}^i = 46.7$ kJ/mol rel B4 $\Delta E_{Na}^{io} = 5.2$ kJ/mol rel B8
Na_5O C_{2v}		CATION 1A_1 _____ RKS/SVP $E_{abs} = -886.3155$ H $E = 10.8$ kJ/mol rel B8 $\Delta E_{Na}^i = 73.3$ kJ/mol rel B4 $\Delta E_{Na}^{io} = 10.8$ kJ/mol rel B8
B8		NEUTRAL 2A_1 _____ UKS/SVP $E_{abs} = -886.4609$ H $E = 6.3$ kJ/mol rel B6 $\Delta E_{Na}^i = 129$ kJ/mol rel B5 $\Delta E_{Na} = 54.1$ kJ/mol rel B4 CATION 1A_1 _____ RKS/SVP $E_{abs} = -886.3196$ H Global Minimum $\approx$ B6 , B7 $\Delta E_{Na}^i = 167$ kJ/mol rel B5 $\Delta E_{Na} = 84.0$ kJ/mol rel B4 $\Delta E_{Na_2} = 137$ kJ/mol rel B3 + Na_2
B9		NEUTRAL ${}^1A'$ _____ RKS/SVP $E_{abs} = -1048.7184$ H Global Minimum $E_i = 4.07$ eV $\Delta E_{Na}^i = 75.6$ kJ/mol rel B8 $\Delta E_{Na}^{io} = 26.3$ kJ/mol rel B12 $\Delta E_{Na} = 81.9$ kJ/mol rel B6 $\Delta E_{Na_2} = 62.2$ kJ/mol rel B4 + Na_2 $\Delta E_{frag} = 280$ kJ/mol rel B2 + A4 CATION ${}^2A'$ _____ UKS/SVP $E_{abs} = -1048.5688$ H Global Minimum $\approx$ B12 $\Delta E_{Na}^i = 53.8$ kJ/mol rel B8 $\Delta E_{Na}^{io} = 0.8$ kJ/mol rel B12 $\Delta E_{Na} = 60.6$ kJ/mol rel B6
$Na_5O.Na$ C_s		

B10Na₆O
D_{3d}NEUTRAL ³A_{1g} _____ UKS/SVPE_{abs}=-1048.7111 H

E=19.2 kJ/mol rel [B9]

ΔE_{Na}ⁱ=62.7 kJ/mol rel [B6]ΔE_{Na}^{io}=-19.2 kJ/mol rel [B9]

R(Na-O)=231pm

R(Na-Na)=314pm, 340pm

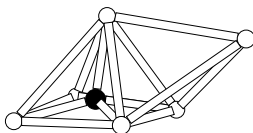
Singlet E_{abs}=-1048.7030CATION ²A_{1g} _____ UKS/SVPE_{abs}=-1048.5612 H

E=20.0 kJ/mol rel [B9]

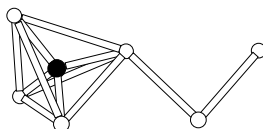
ΔE_{Na}ⁱ=40.7 kJ/mol rel [B6]ΔE_{Na}^{io}=-20.0 kJ/mol rel [B9]

R(Na-O)=235pm

R(Na-Na)=316pm, 346pm

Anion quartet E_{abs}=-1048.7540 O_h**B11**Na₅O.Na
C_sNEUTRAL ³A' _____ UKS/SVPE_{abs}=-1048.7095 H

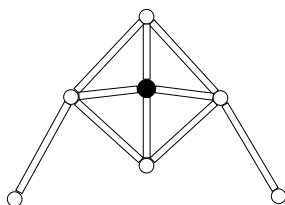
E=23.4 kJ/mol rel [B9]

ΔE_{Na}ⁱ=52.2 kJ/mol rel [B8]ΔE_{Na}^{io}=2.9 kJ/mol rel [B12]ΔE_{Na}=59.6 kJ/mol rel [B7]**B12**Na₄O.Na₂
C_sNEUTRAL ¹A' _____ RKS/SVPE_{abs}=-1048.7084 H

E=26.3 kJ/mol rel [B9]

ΔE_{Na}=49.4 kJ/mol rel [B8]ΔE_{Na2}=36.0 kJ/mol rel [B4]+Na₂CATION ²A' _____ UKS/SVPE_{abs}=-1048.5685 H

E=0.8 kJ/mol rel [B9]

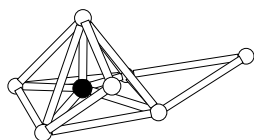
ΔE_{Na}=53.0 kJ/mol rel [B8]ΔE_{Na2}=69.6 kJ/mol rel [B4]+Na₂**B13**Na₄O.2Na
C_{2v}NEUTRAL ¹A₁ _____ RKS/SVPE_{abs}=-1048.6944 H

E=63.0 kJ/mol rel [B9]

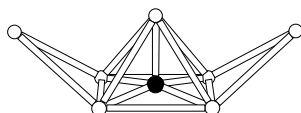
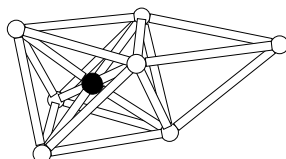
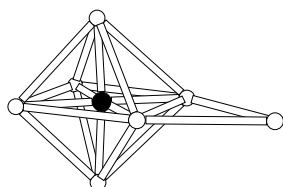
ΔE_{Na}=12.6 kJ/mol rel [B8]CATION ²A₁ _____ UKS/SVPE_{abs}=-1048.5440 H

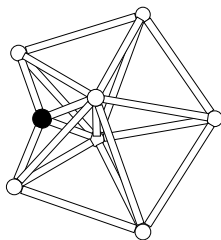
E=65.1 kJ/mol rel [B9]

ΔE_{Na}=11.3 kJ/mol rel [B8]

B14
 $\text{Na}_5\text{O} \cdot 2\text{Na}$
 C_1
 $\text{Na}_5\text{O} \cdot 2\text{Na}^+$
 C_{2v}
NEUTRAL ^2A _____ UKS/SVP $E_{\text{abs}} = -1210.9727 \text{ H}$ Global Minimum $\approx$ [B15] $E_i = 3.73 \text{ eV}$ $\Delta E_{\text{Na}}^i = 93.5 \text{ kJ/mol rel [B12]}$ $\Delta E_{\text{Na}}^{\text{io}} = 10.0 \text{ kJ/mol rel [B17]}$ $\Delta E_{\text{Na}} = 67.2 \text{ kJ/mol rel [B9]}$ CATION $^1\text{A}_1$ _____ UKS/SVP $E_{\text{abs}} = -1210.8358 \text{ H}$

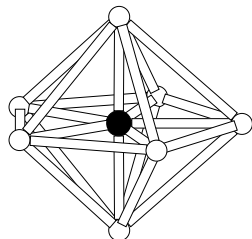
Global Minimum

 $\Delta E_{\text{Na}}^i = 102 \text{ kJ/mol rel [B12]}$ $\Delta E_{\text{Na}}^{\text{io}} = 26.6 \text{ kJ/mol rel [B17]}$ $\Delta E_{\text{Na}} = 101 \text{ kJ/mol rel [B9]}$ $\Delta E_{\text{Na}_2} = 93.7 \text{ kJ/mol rel [B4]} + \text{Na}_2$ $\Delta E_{\text{frag}} = 192 \text{ kJ/mol rel [B3]} + \text{[A4]}$ **B15**
 $\text{Na}_6\text{O} \cdot \text{Na}$
 C_{3v}
NEUTRAL $^2\text{A}_1$ _____ UKS/SVP $E_{\text{abs}} = -1210.9711 \text{ H}$ $E = 4.2 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}}^i = 63.0 \text{ kJ/mol rel [B9]}$ $\Delta E_{\text{Na}}^{\text{io}} = -4.2 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}} = 82.2 \text{ kJ/mol rel [B10]}$ CATION $^1\text{A}_1$ _____ RKS/SVP $E_{\text{abs}} = -1210.8274 \text{ H}$ $E = 22.1 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}}^i = 78.5 \text{ kJ/mol rel [B9]}$ $\Delta E_{\text{Na}}^{\text{io}} = -22.1 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}} = 98.5 \text{ kJ/mol rel [B10]}$ Triplet $E_{\text{abs}} = -1210.8149$ **B16**
 $\text{Na}_6\text{O} \cdot \text{Na}$
 C_{2v}
NEUTRAL $^2\text{A}_1$ _____ UKS/SVP $E_{\text{abs}} = -1210.9695 \text{ H}$ $E = 8.4 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}}^i = 58.8 \text{ kJ/mol rel [B9]}$ $\Delta E_{\text{Na}}^{\text{io}} = 8.4 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}} = 78.0 \text{ kJ/mol rel [B10]}$ CATION $^1\text{A}_1$ _____ RKS/SVP $E_{\text{abs}} = -1210.8241 \text{ H}$ $E = 30.8 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}}^i = 69.8 \text{ kJ/mol rel [B9]}$ $\Delta E_{\text{Na}}^{\text{io}} = -30.8 \text{ kJ/mol rel [B14]}$ $\Delta E_{\text{Na}} = 89.8 \text{ kJ/mol rel [B10]}$

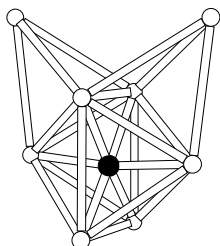
B17
 $\text{Na}_4\text{O}.\text{Na}_3$
 C_{2v}


NEUTRAL $^2\text{A}_1$ _____ UKS/SVP
 $E_{\text{abs}} = -1210.9689 \text{ H}$
 $E = 10.0 \text{ kJ/mol rel [B14]}$
 $\Delta E_{\text{Na}} = 83.5 \text{ kJ/mol rel [B12]}$
 $\Delta E_{\text{Na}_2} = 65.4 \text{ kJ/mol rel [B8]} + \text{Na}_2$

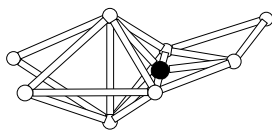
CATION $^1\text{A}_1$ _____ RKS/SVP
 $E_{\text{abs}} = -1210.8257 \text{ H}$
 $E = 26.6 \text{ kJ/mol rel [B14]}$
 $\Delta E_{\text{Na}} = 74.8 \text{ kJ/mol rel [B12]}$
 $\Delta E_{\text{Na}_2} = 60.4 \text{ kJ/mol rel [B8]} + \text{Na}_2$
 $^3\text{B}_1 \text{ } E = -1210.8197 \text{ H}$

B18
 Na_7O
 D_{5h}


NEUTRAL $^4\text{A}'_1$ _____ UKS/SVP
 $E_{\text{abs}} = -1210.9436 \text{ H}$
 $E = 76.4 \text{ kJ/mol rel [B14]}$
 $\Delta E_{\text{Na}}^i = 9.8 \text{ kJ/mol rel [B10]}$
 $\Delta E_{\text{Na}}^{\text{io}} = -72.2 \text{ kJ/mol rel [B15]}$

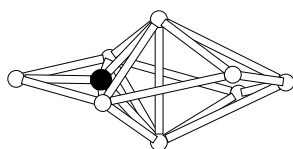
B19
 $\text{Na}_6\text{O}.\text{Na}_2$
 C_{2v}


NEUTRAL $^1\text{A}_1$ _____ RKS/SVP
 $E_{\text{abs}} = -1373.2333 \text{ H}$
Global Minimum $\approx$ [B20] $E_i = 4.02 \text{ eV}$
 $\Delta E_{\text{Na}}^i = 83.8 \text{ kJ/mol rel [B14]}$
 $\Delta E_{\text{Na}}^{\text{io}} = 2.9 \text{ kJ/mol rel [B20]}$
 $\Delta E_{\text{Na}} = 87.9 \text{ kJ/mol rel [B15]}$
 $\Delta E_{\text{Na}_2} = 83.5 \text{ kJ/mol rel [B9]} + \text{Na}_2$
 $\Delta E_{\text{frag}} = 286 \text{ kJ/mol rel [B2]} + \text{[A11]}$
 $\Delta E_{\text{frag}} = 114 \text{ kJ/mol rel [A4]} + \text{[A4]}$
CATION $^2\text{A}_1$ _____ UKS/SVP
 $E_{\text{abs}} = -1373.0834 \text{ H}$
 $E = 5.5 \text{ kJ/mol rel [B21]}$
 $\Delta E_{\text{Na}}^i = 49.6 \text{ kJ/mol rel [B14]}$
 $\Delta E_{\text{Na}}^{\text{io}} = -5.5 \text{ kJ/mol rel [B21]}$
 $\Delta E_{\text{Na}} = 71.7 \text{ kJ/mol rel [B15]}$

B20
 $\text{Na}_5\text{O}.\text{Na}_3$
 C_1


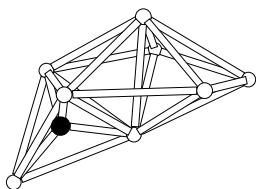
NEUTRAL ^1A _____ RKS/SVP
 $E_{\text{abs}} = -1373.2322 \text{ H}$
 $E = 2.9 \text{ kJ/mol rel [B19]}$
 $\Delta E_{\text{Na}}^{\text{i}} = 90.8 \text{ kJ/mol rel [B17]}$
 $\Delta E_{\text{Na}}^{\text{o}} = 18.1 \text{ kJ/mol rel [B22]}$
 $\Delta E_{\text{Na}} = 80.9 \text{ kJ/mol rel [B14]}$

CATION ^2A _____ UKS/SVP
 $E_{\text{abs}} = -1373.0850 \text{ H}$
 $E = 1.3 \text{ kJ/mol rel [B21]}$
 $\Delta E_{\text{Na}}^{\text{i}} = 80.3 \text{ kJ/mol rel [B17]}$
 $\Delta E_{\text{Na}}^{\text{o}} = 0.8 \text{ kJ/mol rel [B22]}$
 $\Delta E_{\text{Na}} = 16.3 \text{ kJ/mol rel [B14]}$

B21
 $\text{Na}_5\text{O}.\text{Na}_3$
 C_1, C_2


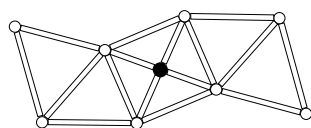
NEUTRAL ^1A _____ UKS/SVP
 $E_{\text{abs}} = -1373.2320 \text{ H}$
 $E = 3.4 \text{ kJ/mol rel [B19]}$
 $\Delta E_{\text{Na}}^{\text{i}} = 90.4 \text{ kJ/mol rel [B17]}$
 $\Delta E_{\text{Na}} = 80.3 \text{ kJ/mol rel [B14]}$
 Spin-contaminated singlet
 C_s triplet $E_{\text{abs}} = -1373.2221$

CATION ^2A _____ UKS/SVP
 $E_{\text{abs}} = -1373.0856 \text{ H}$
 Global Minimum $\approx$ [B20], [B22]
 $\Delta E_{\text{Na}}^{\text{i}} = 81.9 \text{ kJ/mol rel [B17]}$
 $\Delta E_{\text{Na}} = 55.4 \text{ kJ/mol rel [B14]}$
 C_s quartet $E_{\text{abs}} = -1373.073350$

B22
 $\text{Na}_4\text{O}.\text{Na}_4$
 C_s


NEUTRAL $^1\text{A}'$ _____ RKS/SVP
 $E_{\text{abs}} = -1373.2253 \text{ H}$
 $E = 21.0 \text{ kJ/mol rel [B19]}$
 $\Delta E_{\text{Na}} = 72.8 \text{ kJ/mol rel [B17]}$

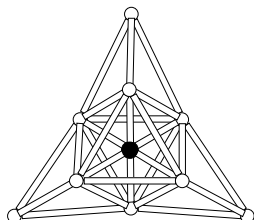
CATION $^2\text{A}'$ _____ UKS/SVP
 $E_{\text{abs}} = -1373.0847 \text{ H}$
 $E = 2.1 \text{ kJ/mol rel [B21]}$
 $\Delta E_{\text{Na}} = 79.6 \text{ kJ/mol rel [B17]}$

B23
 $\text{Na}_4\text{O}.\text{Na}_4$
 D_{2h}


NEUTRAL $^3\text{A}_g$ _____ UKS/SVP
 $E_{\text{abs}} = -1373.1977 \text{ H}$
 $E = 93.5 \text{ kJ/mol rel [B21]}$
 $\Delta E_{\text{Na}} = 0.3 \text{ kJ/mol rel [B17]}$

B24

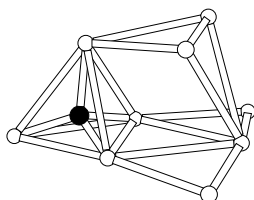
$\text{Na}_6\text{O} \cdot 3\text{Na}$
 $\text{C}_{3v}, \text{C}_1$

NEUTRAL ${}^2\text{A}_1$ _____ UKS/SVP $E_{\text{abs}} = -1535.4921 \text{ H}$ Global Minimum $E_i = 3.87 \text{ eV}$ $\Delta E_{\text{Na}}^i = 81.9 \text{ kJ/mol rel } \boxed{\text{B20}}$ $\Delta E_{\text{Na}}^{\text{io}} = 23.1 \text{ kJ/mol rel } \boxed{\text{B26}}$ $\Delta E_{\text{Na}} = 79.0 \text{ kJ/mol rel } \boxed{\text{B19}}$ Anion $E_{\text{abs}} = -1535.5342$ CATION ${}^1\text{A}$ _____ RKS/SVP $E_{\text{abs}} = -1535.3497 \text{ H}$ Global Minimum $\approx \boxed{\text{B25}}, \boxed{\text{B26}}$ $\Delta E_{\text{Na}}^i = 92.9 \text{ kJ/mol rel } \boxed{\text{B21}}$ $\Delta E_{\text{Na}}^{\text{io}} = 2.1 \text{ kJ/mol rel } \boxed{\text{B26}}$ $\Delta E_{\text{Na}} = 98.7 \text{ kJ/mol rel } \boxed{\text{B19}}$ $\Delta E_{\text{Na}_2} = 80.9 \text{ kJ/mol rel } \text{Na}_2 + \boxed{\text{B14}}^+$ $\Delta E_{\text{frag}} = 196 \text{ kJ/mol rel } \boxed{\text{A11}} + \boxed{\text{B3}}^+$ $\Delta E_{\text{frag}} = 136 \text{ kJ/mol rel } \boxed{\text{A4}} + \boxed{\text{B6}}^+$

Tetragonally distorted

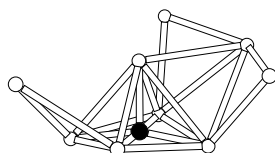
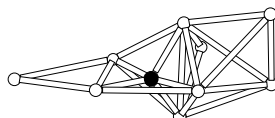
Triplet $E_{\text{abs}} = -1535.3412$ **B25**

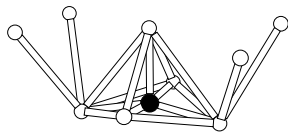
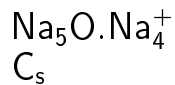
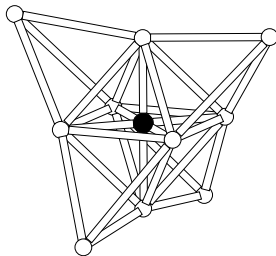
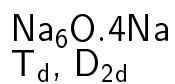
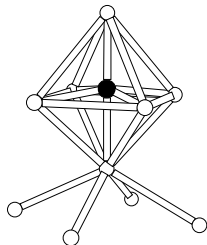
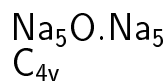
$\text{Na}_4\text{O} \cdot \text{Na}_5$
 C_s

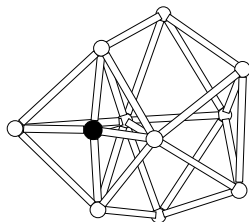
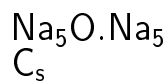
NEUTRAL ${}^2\text{A}'$ _____ UKS/SVP $E_{\text{abs}} = -1535.4849 \text{ H}$ $E = 18.9 \text{ kJ/mol rel } \boxed{\text{B24}}$ $\Delta E_{\text{Na}} = 81.1 \text{ kJ/mol rel } \boxed{\text{B22}}$ CATION ${}^1\text{A}'$ _____ RKS/SVP $E_{\text{abs}} = -1535.3487 \text{ H}$ $E = 2.6 \text{ kJ/mol rel } \boxed{\text{B24}}$ $\Delta E_{\text{Na}} = 92.7 \text{ kJ/mol rel } \boxed{\text{B22}}$ **B26**

$\text{Na}_5\text{O} \cdot \text{Na}_4$
 C_1

$\text{Na}_5\text{O} \cdot \text{Na}_4^+$
 C_s

NEUTRAL ${}^2\text{A}$ _____ UKS/SVP $E_{\text{abs}} = -1535.4833 \text{ H}$ $E = 23.1 \text{ kJ/mol rel } \boxed{\text{B24}}$ $\Delta E_{\text{Na}}^i = 79.9 \text{ kJ/mol rel } \boxed{\text{B22}}$ $\Delta E_{\text{Na}}^{\text{io}} = -4.2 \text{ kJ/mol rel } \boxed{\text{B25}}$ $\Delta E_{\text{Na}} = 58.8 \text{ kJ/mol rel } \boxed{\text{B20}}$ CATION ${}^1\text{A}'$ _____ RKS/SVP $E_{\text{abs}} = -1535.3489 \text{ H}$ $E = 2.1 \text{ kJ/mol rel } \boxed{\text{B24}}$ $\Delta E_{\text{Na}}^i = 93.2 \text{ kJ/mol rel } \boxed{\text{B22}}$ $\Delta E_{\text{Na}}^{\text{io}} = 0.5 \text{ kJ/mol rel } \boxed{\text{B25}}$ $\Delta E_{\text{Na}} = 92.4 \text{ kJ/mol rel } \boxed{\text{B20}}$

B27CATION $^3\text{A}'$ _____ UKS/SVP $E_{\text{abs}} = -1535.3334 \text{ H}$ $E = 41.7 \text{ kJ/mol rel [B24]}$ $\Delta E_{\text{Na}}^i = 52.5 \text{ kJ/mol rel [B22]}$ $\Delta E_{\text{Na}}^{\text{io}} = -40.2 \text{ kJ/mol rel [B25]}$ $\Delta E_{\text{Na}} = 51.7 \text{ kJ/mol rel [B20]}$ **B28**NEUTRAL $^1\text{A}_1$ _____ RKS/SVP $E_{\text{abs}} = -1697.7556 \text{ H}$ Global Minimum $E_i = 4.02 \text{ eV}$ $\Delta E_{\text{Na}}^i = 114 \text{ kJ/mol rel [B26]}$ $\Delta E_{\text{Na}}^{\text{io}} = 6.8 \text{ kJ/mol rel [B29]}$ $\Delta E_{\text{Na}} = 91.4 \text{ kJ/mol rel [B24]}$ $\Delta E_{\text{Na}_2} = 103 \text{ kJ/mol rel Na}_2 + \text{[B19]}$ $\Delta E_{\text{frag}} = 289 \text{ kJ/mol rel [A19] + [B2]}$ $\Delta E_{\text{frag}} = 155 \text{ kJ/mol rel [A4] + [B9]}$ CATION $^2\text{B}_2$ _____ UKS/SVP $E_{\text{abs}} = -1697.5980 \text{ H}$ $E = 25.5 \text{ kJ/mol rel [B31]}$ $\Delta E_{\text{Na}}^i = 53.6 \text{ kJ/mol rel [B26]}$ $\Delta E_{\text{Na}}^{\text{io}} = -23.1 \text{ kJ/mol rel [B29]}$ $\Delta E_{\text{Na}} = 51.5 \text{ kJ/mol rel [B24]}$ **B29**NEUTRAL $^1\text{A}_1$ _____ RKS/SVP $E_{\text{abs}} = -1697.7533 \text{ H}$ $E = 6.0 \text{ kJ/mol rel [B28]}$ $\Delta E_{\text{Na}}^i = 104 \text{ kJ/mol rel [B25]}$ $\Delta E_{\text{Na}}^{\text{io}} = 13.1 \text{ kJ/mol rel [B31]}$ $\Delta E_{\text{Na}} = 108 \text{ kJ/mol rel [B26]}$ CATION $^2\text{A}_1$ _____ UKS/SVP $E_{\text{abs}} = -1697.6068 \text{ H}$ $E = 2.4 \text{ kJ/mol rel [B31]}$ $\Delta E_{\text{Na}}^i = 77.2 \text{ kJ/mol rel [B25]}$ $\Delta E_{\text{Na}}^{\text{io}} = -2.4 \text{ kJ/mol rel [B31]}$ $\Delta E_{\text{Na}} = 76.7 \text{ kJ/mol rel [B26]}$

B30NEUTRAL $^1\text{A}'$ _____ RKS/SVP

$$E_{\text{abs}} = -1697.7530 \text{ H}$$

$$E = 6.8 \text{ kJ/mol rel } \boxed{\text{B28}}$$

$$\Delta E_{\text{Na}}^{\text{i}} = 103 \text{ kJ/mol rel } \boxed{\text{B25}}$$

$$\Delta E_{\text{Na}}^{\text{o}} = 12.3 \text{ kJ/mol rel } \boxed{\text{B31}}$$

$$\Delta E_{\text{Na}} = 108 \text{ kJ/mol rel } \boxed{\text{B26}}$$

CATION $^2\text{A}'$ _____ UKS/SVP

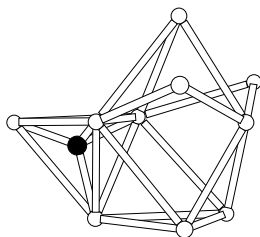
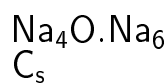
$$E_{\text{abs}} = -1697.6074 \text{ H}$$

$$E = 0.8 \text{ kJ/mol rel } \boxed{\text{B31}}$$

$$\Delta E_{\text{Na}}^{\text{i}} = 78.8 \text{ kJ/mol rel } \boxed{\text{B25}}$$

$$\Delta E_{\text{Na}}^{\text{o}} = -0.8 \text{ kJ/mol rel } \boxed{\text{B31}}$$

$$\Delta E_{\text{Na}} = 78.2 \text{ kJ/mol rel } \boxed{\text{B26}}$$

B31NEUTRAL $^1\text{A}'$ _____ RKS/SVP

$$E_{\text{abs}} = -1697.7483 \text{ H}$$

$$E = 19.2 \text{ kJ/mol rel } \boxed{\text{B28}}$$

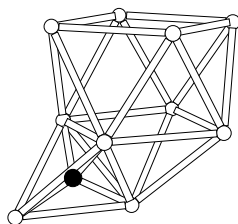
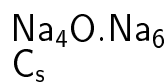
$$\Delta E_{\text{Na}} = 91.1 \text{ kJ/mol rel } \boxed{\text{B25}}$$

CATION $^2\text{A}'$ _____ UKS/SVP

$$E_{\text{abs}} = -1697.6077 \text{ H}$$

$$\text{Global Minimum} \approx \boxed{\text{B30}}, \boxed{\text{B29}}$$

$$\Delta E_{\text{Na}} = 79.6 \text{ kJ/mol rel } \boxed{\text{B25}}$$

B32NEUTRAL $^2\text{A}'$ _____ RKS/SVP

$$E_{\text{abs}} = -1697.7473 \text{ H}$$

$$E = 21.8 \text{ kJ/mol rel } \boxed{\text{B28}}$$

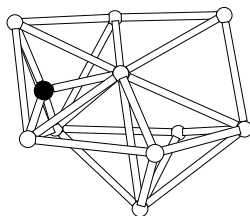
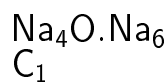
$$\Delta E_{\text{Na}} = 88.5 \text{ kJ/mol rel } \boxed{\text{B25}}$$

CATION $^2\text{A}'$ _____ UKS/SVP

$$E_{\text{abs}} = -1697.6054 \text{ H}$$

$$E = 6.0 \text{ kJ/mol rel } \boxed{\text{B31}}$$

$$\Delta E_{\text{Na}} = 73.5 \text{ kJ/mol rel } \boxed{\text{B25}}$$

B33NEUTRAL ^1A _____ RKS/SVP

$$E_{\text{abs}} = -1697.7472 \text{ H}$$

$$E = 22.1 \text{ kJ/mol rel } \boxed{\text{B28}}$$

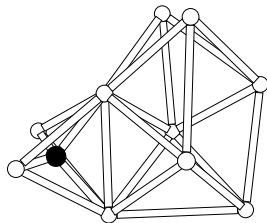
$$\Delta E_{\text{Na}} = 88.2 \text{ kJ/mol rel } \boxed{\text{B25}}$$

CATION ^2A _____ UKS/SVP

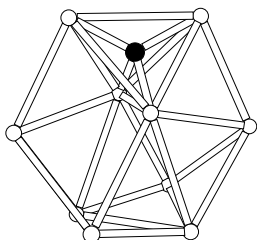
$$E_{\text{abs}} = -1697.6032 \text{ H}$$

$$E = 11.8 \text{ kJ/mol rel } \boxed{\text{B31}}$$

$$\Delta E_{\text{Na}} = 67.7 \text{ kJ/mol rel } \boxed{\text{B25}}$$

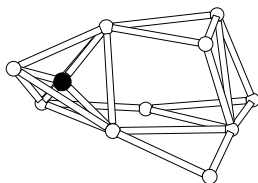
B34
 $\text{Na}_4\text{O}.\text{Na}_6$
 C_1


NEUTRAL ^1A _____ RKS/SVP
 $E_{\text{abs}} = -1697.7464 \text{ H}$
 $E = 24.2 \text{ kJ/mol rel [B28]}$
 $\Delta E_{\text{Na}} = 86.1 \text{ kJ/mol rel [B25]}$

B35
 $\text{Na}_4\text{O}.\text{Na}_6$
 C_2


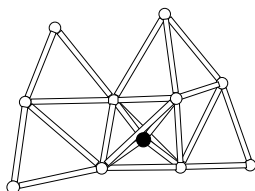
NEUTRAL ^1A _____ RKS/SVP
 $E_{\text{abs}} = -1697.7455 \text{ H}$
 $E = 26.5 \text{ kJ/mol rel [B28]}$
 $\Delta E_{\text{Na}} = 83.8 \text{ kJ/mol rel [B25]}$

CATION ^2A _____ UKS/SVP
 $E_{\text{abs}} = -1697.5977 \text{ H}$
 $E = 26.3 \text{ kJ/mol rel [B31]}$
 $\Delta E_{\text{Na}} = 53.3 \text{ kJ/mol rel [B25]}$

B36
 $\text{Na}_4\text{O}.\text{Na}_6$
 C_1


NEUTRAL ^1A _____ RKS/SVP
 $E_{\text{abs}} = -1697.7393 \text{ H}$
 $E = 42.8 \text{ kJ/mol rel [B28]}$
 $\Delta E_{\text{Na}} = 64.5 \text{ kJ/mol rel [B25]}$

CATION ^2A _____ UKS/SVP
 $E_{\text{abs}} = -1697.5991 \text{ H}$
 $E = 22.6 \text{ kJ/mol rel [B31]}$
 $\Delta E_{\text{Na}} = 57.0 \text{ kJ/mol rel [B25]}$

B37
 $\text{Na}_4\text{O}.\text{Na}_6$
 C_1


NEUTRAL ^1A _____ RKS/SVP
 $E_{\text{abs}} = -1697.7381 \text{ H}$
 $E = 45.9 \text{ kJ/mol rel [B28]}$
 $\Delta E_{\text{Na}} = 64.3 \text{ kJ/mol rel [B25]}$

CATION ^2A _____ UKS/SVP
 $E_{\text{abs}} = -1697.5976 \text{ H}$
 $E = 26.5 \text{ kJ/mol rel [B31]}$
 $\Delta E_{\text{Na}} = 53.0 \text{ kJ/mol rel [B25]}$