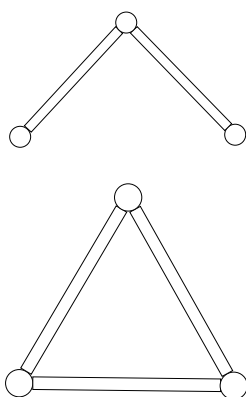
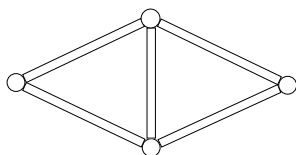
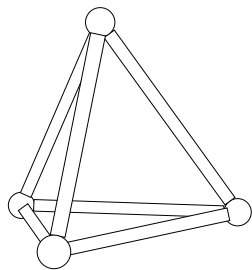
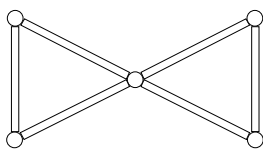
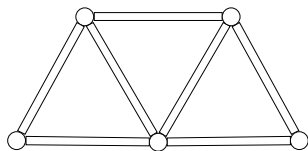
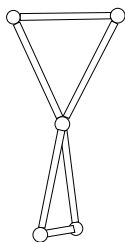
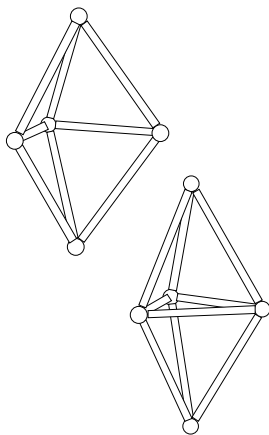
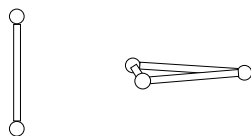
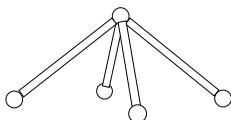
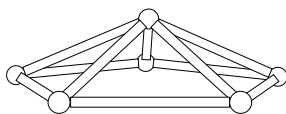


**A** Pure Sodium

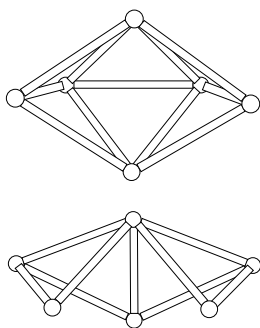
**A1** NaNEUTRAL  $^2S$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -162.2287 \text{ H}$  $E_i = 5.26 \text{ eV}$  (Expt: 5.14 eV)CATION  $^1S$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -162.0355 \text{ H}$ **A2** Na<sub>2</sub>NEUTRAL  $^1\Sigma_g^+$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -324.4831 \text{ H}$  $D_e = 67.5 \text{ kJ/mol}$  (Expt: 72.0 kJ/mol) $R = 317.2 \text{ pm}$ , HOMO  $\varepsilon = -0.116 \text{ H} = 3.16 \text{ eV}$  $E_i = 5.03 \text{ eV}$  (Expt: 4.91 eV)Triplet  $E_{\text{abs}} = -324.4581$ ,  $R = 475 \text{ pm}$ CATION  $^2\Sigma_g^+$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -324.2984 \text{ H}$  $\Delta E_{\text{Na}} = 89.8 \text{ kJ/mol}$  $R = 377.6 \text{ pm}$ **A3**Na<sub>3</sub>  
C<sub>2v</sub>Na<sub>3</sub><sup>+</sup>  
D<sub>3h</sub>NEUTRAL  $^2B_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -486.7238 \text{ H}$  $E_i = 4.08 \text{ eV}$  $\Delta E_{\text{coh}} = 33.0 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 31.5 \text{ kJ/mol}$  rel **A2** $R = 332, 457 \text{ pm}$ ;  $\angle = 87.2^\circ$ CATION  $^1A'_1$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -486.5737 \text{ H}$  $\Delta E_{\text{coh}} = 70.7 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 122 \text{ kJ/mol}$  rel **A2** $\Delta E_{\text{Na}_2} = 145 \text{ kJ/mol}$  rel Na<sub>2</sub> + Na<sup>+</sup> $R = 352.1 \text{ pm}$ Linear triplet  $E_{\text{abs}} = -486.5463$ **A4**Na<sub>4</sub>  
D<sub>2h</sub>NEUTRAL  $^1A_g$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -648.9782 \text{ H}$  $E_i = 4.24 \text{ eV}$  $\Delta E_{\text{coh}} = 41.6 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 67.5 \text{ kJ/mol}$  rel **A3** $\Delta E_{\text{Na}_2} = 31.5 \text{ kJ/mol}$  rel **A2** $R = 316, 361 \text{ pm}$ Triplet  $E_{\text{abs}} = -648.9702 \text{ H}$  expandedCATION  $^2B_{3u}$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -648.8225 \text{ H}$  $\Delta E_{\text{coh}} = 60.6 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 52.8 \text{ kJ/mol}$  rel **A3** $\Delta E_{\text{Na}_2} = 107 \text{ kJ/mol}$  rel **A2** $R = 332, 374 \text{ pm}$

**A5**
 $\text{Na}_4^-$   
 $T_d$ 
ANION  $^4T$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -649.0029 \text{ H}$  $E_a = 64.8 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = \text{kJ/mol}$  $R = 371.0 \text{ pm}$ Neutral and cationic  $\rightarrow 2\text{Na}_2$ **A6**
 $\text{Na}_5$   
 $C_{2v}$ 
 $\text{Na}_5^+$   
 $D_{2h}$ 
NEUTRAL  $^2B_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -811.2316 \text{ H}$ Global Minimum  $E_i = 3.98 \text{ eV}$  $\Delta E_{\text{coh}} = 46.3 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 70.1 \text{ kJ/mol}$  rel **A4** $\Delta E_{\text{Na}_2} = 64.8 \text{ kJ/mol}$  rel  $\text{Na}_2 + \text{A3}$ CATION  $^1A_g$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -811.0849 \text{ H}$  $E = 1.3 \text{ kJ/mol}$  rel **A7** $\Delta E_{\text{coh}} = 70.7 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 88.5 \text{ kJ/mol}$  rel **A4** $\Delta E_{\text{Na}_2} = 73.8 \text{ kJ/mol}$  rel  $\text{Na}_2 + \text{A3}^+$ Triplet  $E_{\text{abs}} = -811.0677 \text{ H}$  pentagonal segment**A7**
 $\text{Na}_5^+$   
 $D_{2d}$ 
CATION  $^1A_1$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -811.0854 \text{ H}$ Global minimum  $\approx \text{A6}$  $\Delta E_{\text{coh}} = 70.9 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 89.8 \text{ kJ/mol}$  rel **A4** $\Delta E_{\text{Na}_2} = 75.1 \text{ kJ/mol}$  rel  $\text{Na}_2 + \text{A3}^+$

**A8**Na<sub>5</sub>  
C<sub>2v</sub>Na<sub>5</sub><sup>+</sup>  
D<sub>3h</sub>NEUTRAL <sup>2</sup>A<sub>1</sub> \_\_\_\_\_ UKS/SVPE<sub>abs</sub>=-811.2251 HE=17.1 kJ/mol rel **A6**ΔE<sub>coh</sub>=42.8 kJ/molΔE<sub>Na</sub>=47.8 kJ/mol rel **A4**Quartet E<sub>abs</sub>=-811.2194 shorter and broaderCATION <sup>1</sup>A<sub>1</sub>' \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-811.0744 HE=28.9 kJ/mol rel **A7**ΔE<sub>coh</sub>=65.2 kJ/molΔE<sub>Na</sub>=60.9 kJ/mol rel **A4**Triplet → **A10****A9**Na<sub>5</sub><sup>+</sup>  
C<sub>2v</sub>CATION <sup>1</sup>A<sub>1</sub> \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-811.0818 HE=9.45 kJ/mol rel **A7**ΔE<sub>coh</sub>=69.1 kJ/molΔE<sub>Na</sub>=80.3 kJ/mol**A10**Na<sub>5</sub><sup>+</sup>  
C<sub>2v</sub>CATION <sup>3</sup>B<sub>1</sub> \_\_\_\_\_ UKS/SVPE<sub>abs</sub>=-811.0704 HE=39.4 kJ/mol rel **A7**ΔE<sub>coh</sub>=63.1 kJ/molΔE<sub>Na</sub>=50.4 kJ/mol rel **A4**Singlet and doublet → **A8****A11**Na<sub>6</sub>  
C<sub>5v</sub>NEUTRAL <sup>1</sup>A<sub>1</sub> \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-973.4908 HGlobal minimum E<sub>i</sub>=4.21 eVΔE<sub>coh</sub>=51.9 kJ/molΔE<sub>Na</sub>=80.0 kJ/mol rel **A6**ΔE<sub>Na<sub>2</sub></sub>=77.5 kJ/mol rel Na<sub>2</sub>+ **A4**

**A12**

Na<sub>6</sub>  
C<sub>2v</sub>  
Na<sub>6</sub><sup>+</sup>  
C<sub>s</sub>

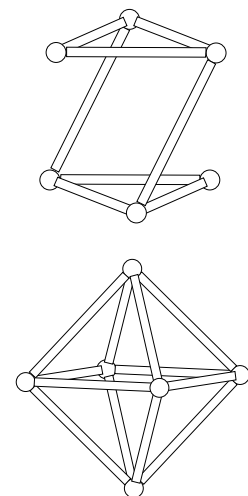


NEUTRAL <sup>3</sup>B<sub>2</sub> \_\_\_\_\_ UKS/SVP  
E<sub>abs</sub>=-973.4840 H  
E=17.9 kJ/mol rel **A11**  
ΔE<sub>coh</sub>=48.9 kJ/mol  
ΔE<sub>Na</sub>=62.2 kJ/mol rel **A6**

CATION <sup>2</sup>A'' \_\_\_\_\_ UKS/SVP  
E<sub>abs</sub>=-973.3360 H  
Global minimum ≈ **A14**  
ΔE<sub>coh</sub>=68.7 kJ/mol  
ΔE<sub>Na</sub>=57.5 kJ/mol rel **A7**  
ΔE<sub>Na<sub>2</sub></sub>=79.8 kJ/mol rel Na<sub>2</sub>+**A4**<sup>+</sup>

**A13**

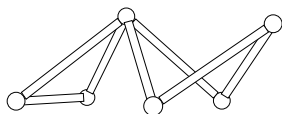
Na<sub>6</sub>  
D<sub>3d</sub>  
Na<sub>6</sub><sup>+</sup>  
O<sub>h</sub>



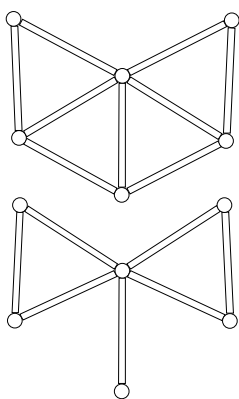
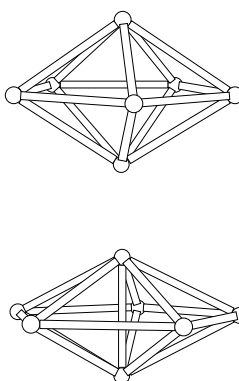
NEUTRAL <sup>3</sup>A<sub>1g</sub> \_\_\_\_\_ UKS/SVP  
E<sub>abs</sub>=-973.4820 H  
E=23.1 kJ/mol rel **A11**  
ΔE<sub>coh</sub>=48.1 kJ/mol  
ΔE<sub>Na</sub>=57.0 kJ/mol rel **A6**  
ΔE<sub>Na<sub>2</sub></sub>=54.3 kJ/mol rel Na<sub>2</sub>+**A4**  
CATION <sup>4</sup>A<sub>1g</sub> \_\_\_\_\_ UKS/SVP  
E<sub>abs</sub>=-973.3267 H  
E=24.3 kJ/mol rel **A11**  
ΔE<sub>coh</sub>=64.7 kJ/mol  
ΔE<sub>Na</sub>=33.2 kJ/mol rel **A7**

**A14**

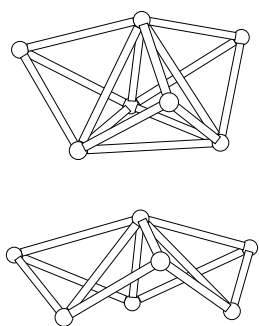
Na<sub>6</sub><sup>+</sup>  
C<sub>s</sub>

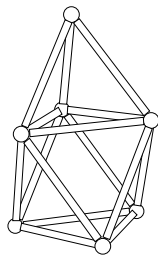
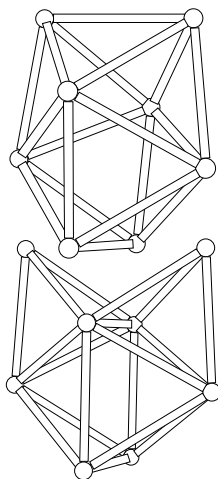
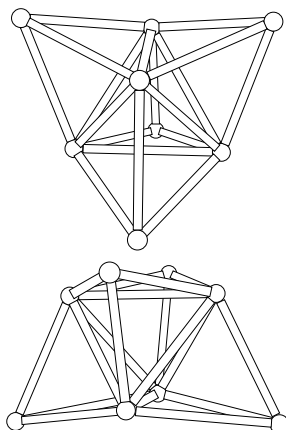


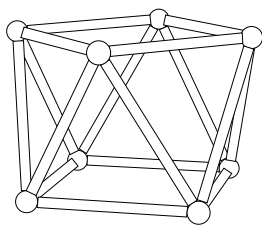
CATION <sup>2</sup>A<sub>1</sub> \_\_\_\_\_ UKS/SVP  
E<sub>abs</sub>=-973.3352 H  
E=2.1 kJ/mol rel **A12**  
ΔE<sub>coh</sub>=68.4 kJ/mol  
ΔE<sub>Na</sub>=55.4 kJ/mol rel **A7**

**A15**Na<sub>6</sub>  
C<sub>2v</sub>Na<sub>6</sub><sup>+</sup>  
C<sub>2v</sub>NEUTRAL <sup>3</sup>B<sub>2</sub> \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-973.4681 HE=59.6 kJ/mol rel **A11**ΔE<sub>coh</sub>=42.0 kJ/molΔE<sub>Na</sub>=20.5 kJ/mol rel **A6**Singlet → **A11**CATION <sup>2</sup>A<sub>1</sub> \_\_\_\_\_ UKS/SVPE<sub>abs</sub>=-973.3328 HE=8.4 kJ/mol rel **A12**ΔE<sub>coh</sub>=67.3 kJ/molΔE<sub>Na</sub>=49.1 kJ/mol rel **A7****A16**Na<sub>7</sub>  
D<sub>5h</sub>Na<sub>7</sub><sup>+</sup>  
D<sub>5h</sub>NEUTRAL <sup>2</sup>A<sub>1</sub> \_\_\_\_\_ UKS/SVPE<sub>abs</sub>=-1135.7510 HGlobal minimum E<sub>i</sub>=3.99 eVΔE<sub>coh</sub>=56.3 kJ/molΔE<sub>Na</sub>=82.7 kJ/mol rel **A11**ΔE<sub>Na<sub>2</sub></sub>=95.3 kJ/mol rel Na<sub>2</sub>+ **A6**CATION <sup>1</sup>A<sub>1</sub> \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-1135.6045 H

Global minimum

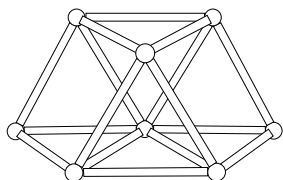
ΔE<sub>coh</sub>=73.8 kJ/molΔE<sub>Na</sub>=104 kJ/mol rel **A12**ΔE<sub>Na<sub>2</sub></sub>=95.8 kJ/mol rel Na<sub>2</sub>+ **A6**<sup>+</sup>ΔE<sub>frag</sub>=401 kJ/mol rel **A4**+**A3**<sup>+</sup>Triplet E<sub>abs</sub>=-1135.5871 expanded**A17**Na<sub>7</sub>  
C<sub>3v</sub>Na<sub>7</sub><sup>+</sup>  
C<sub>3v</sub>NEUTRAL <sup>2</sup>A<sub>1</sub> \_\_\_\_\_ UKS/SVPE<sub>abs</sub>=-1135.7469 HE=10.8 kJ/mol rel **A16**ΔE<sub>coh</sub>=54.8 kJ/molΔE<sub>Na</sub>=71.9 kJ/mol rel **A11**CATION <sup>1</sup>A<sub>1</sub> \_\_\_\_\_ RKS/SVPE<sub>abs</sub>=-1135.6021 HE=6.3 kJ/mol rel **A16**ΔE<sub>coh</sub>=72.9 kJ/molΔE<sub>Na</sub>=98.2 kJ/mol rel **A12**

**A18**
 $\text{Na}_7^+$   
 $\text{C}_{3v}$ 
CATION  $^3\text{A}_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1135.5927 \text{ H}$  $E = 31.0 \text{ kJ/mol rel } \boxed{\text{A16}}$  $\Delta E_{\text{coh}} = 69.4 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 73.5 \text{ kJ/mol rel } \boxed{\text{A12}}$ **A19**
 $\text{Na}_8$   
 $\text{D}_{2d}$   
 $\text{Na}_8^+$   
 $\text{C}_{2v}$ 
NEUTRAL  $^1\text{A}_1$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1298.0123 \text{ H}$ Global minimum  $E_i = 4.17 \text{ eV}$  $\Delta E_{\text{coh}} = 60.0 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 85.6 \text{ kJ/mol rel } \boxed{\text{A16}}$  $\Delta E_{\text{Na}_2} = 101 \text{ kJ/mol rel } \text{Na}_2 + \boxed{\text{A11}}$  $\Delta E_{\text{frag}} = 147 \text{ kJ/mol rel } \boxed{\text{A4}} + \boxed{\text{A4}}$ Triplet  $E_{\text{abs}} = -1297.9890$ CATION  $^2\text{A}_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1297.8589 \text{ H}$ Global minimum  $\approx \boxed{\text{A22}}$  $\Delta E_{\text{coh}} = 73.0 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 67.5 \text{ kJ/mol rel } \boxed{\text{A16}}$  $\Delta E_{\text{Na}_2} = 104 \text{ kJ/mol rel } \text{Na}_2 + \boxed{\text{A12}}^+$ **A20**
 $\text{Na}_8$   
 $\text{T}_d$   
 $\text{Na}_8^+$   
 $\text{D}_{2d}$ 
NEUTRAL  $^1\text{A}_1$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1298.0098 \text{ H}$  $E = 6.6 \text{ kJ/mol rel } \boxed{\text{A19}}$  $\Delta E_{\text{coh}} = 59.1 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 79.0 \text{ kJ/mol rel } \boxed{\text{A16}}$ CATION  $^2\text{A}_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1297.8514 \text{ H}$  $E = 19.7 \text{ kJ/mol rel } \boxed{\text{A19}}$  $\Delta E_{\text{coh}} = 70.6 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 47.8 \text{ kJ/mol rel } \boxed{\text{A16}}$

**A21** $\text{Na}_8$   
 $D_{4d}$ 

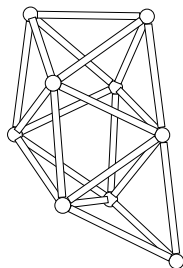
NEUTRAL  $^1A_1$  \_\_\_\_\_ RKS/SVP  
 $E_{\text{abs}} = -1298.0091 \text{ H}$   
 $E = 8.4 \text{ kJ/mol rel [A19]}$   
 $\Delta E_{\text{coh}} = 59.0 \text{ kJ/mol}$   
 $\Delta E_{\text{Na}} = 77.2 \text{ kJ/mol rel [A16]}$

CATION  $^2B_2$  \_\_\_\_\_ UKS/SVP  
 $E_{\text{abs}} = -1297.8525 \text{ H}$   
 $E = 16.8 \text{ kJ/mol rel [A19]}$   
 $\Delta E_{\text{coh}} = 70.9 \text{ kJ/mol}$   
 $\Delta E_{\text{Na}} = 50.7 \text{ kJ/mol rel [A16]}$

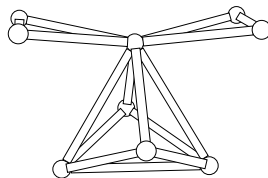
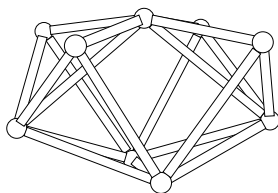
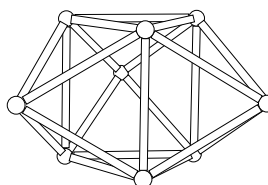
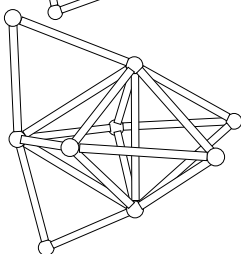
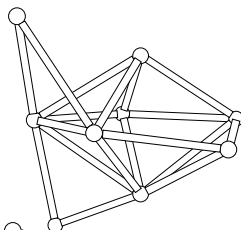
**A22** $\text{Na}_8$   
 $C_{2v}$ 

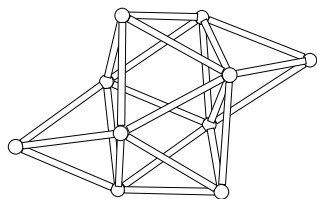
NEUTRAL  $^1A_1$  \_\_\_\_\_ RKS/SVP  
 $E_{\text{abs}} = -1298.0077 \text{ H}$   
 $E = 12.1 \text{ kJ/mol rel [A19]}$   
 $\Delta E_{\text{coh}} = 58.5 \text{ kJ/mol}$   
 $\Delta E_{\text{Na}} = 73.5 \text{ kJ/mol rel [A16]}$   
Triplet  $E_{\text{abs}} = -1297.9912$

CATION  $^2B_1$  \_\_\_\_\_ UKS/SVP  
 $E_{\text{abs}} = -1297.8576 \text{ H}$   
 $E = 3.4 \text{ kJ/mol rel [A19]}$   
 $\Delta E_{\text{coh}} = 72.6 \text{ kJ/mol}$   
 $\Delta E_{\text{Na}} = 64.1 \text{ kJ/mol rel [A16]}$

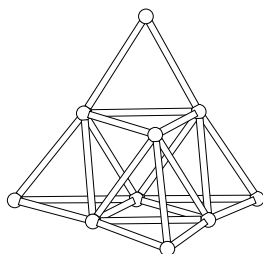
**A23** $\text{Na}_9$   
 $C_s$ 

NEUTRAL  $^2A'$  \_\_\_\_\_ UKS/SVP  
 $E_{\text{abs}} = -1460.2584 \text{ H}$   
Global minimum  $\approx$  [A24]  $E_i = 3.62 \text{ eV}$   
 $\Delta E_{\text{coh}} = 58.4 \text{ kJ/mol}$   
 $\Delta E_{\text{Na}} = 45.7 \text{ kJ/mol rel [A19]}$   
 $\Delta E_{\text{Na}_2} = 63.8 \text{ kJ/mol rel Na}_2 + \text{[A16]}$   
Occupy other face:  $E_{\text{abs}} = -1460.2574$

**A24** $\text{Na}_9$  $\text{C}_{2v}$  $\text{Na}_9^+$  $\text{C}_{2v}$ NEUTRAL  $^2A_2$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1460.2577 \text{ H}$  $E = 1.8 \text{ kJ/mol rel [A23]}$  $\Delta E_{\text{coh}} = 58.2 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 43.8 \text{ kJ/mol rel [A19]}$ CATION  $^1A_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1460.1240 \text{ H}$  $E = 3.9 \text{ kJ/mol rel [A25]}$  $\Delta E_{\text{coh}} = 75.5 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 95.6 \text{ kJ/mol rel [A19]}$ Triplet  $E_{\text{abs}} = -1460.1070$  contracted**A25** $\text{Na}_9, \text{Na}_9^+$  $\text{C}_{2v}, \text{D}_{3h}$ NEUTRAL  $^2B_1$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1460.2558 \text{ H}$  $E = 6.8 \text{ kJ/mol rel [A23]}$  $\Delta E_{\text{coh}} = 57.6 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 38.9 \text{ kJ/mol rel [A19]}$ CATION  $^1A'_1$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1460.1255 \text{ H}$ Global minimum  $\approx$  [A24] $\Delta E_{\text{coh}} = 76.0 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 99.5 \text{ kJ/mol rel [A19]}$  $\Delta E_{\text{Na}_2} = 99.5 \text{ kJ/mol rel Na}_2 + [\text{A16}]^+$  $\Delta E_{\text{frag}} = 164 \text{ kJ/mol rel [A4]} + [\text{A7}]^+$ **A26** $\text{Na}_9$  $\text{C}_1$  $\text{Na}_9^+$  $\text{C}_2$ NEUTRAL  $^2A$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1460.2534 \text{ H}$  $E = 13.1 \text{ kJ/mol rel [A23]}$  $\Delta E_{\text{coh}} = 56.9 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 32.6 \text{ kJ/mol rel [A19]}$ CATION  $^1A$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1460.1225 \text{ H}$  $E = 7.9 \text{ kJ/mol rel [A25]}$  $\Delta E_{\text{coh}} = 75.1 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 91.6 \text{ kJ/mol rel [A19]}$

**A27** $\text{Na}_{10}$   
 $\text{C}_2$ NEUTRAL  $^1\text{A}$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1622.5160 \text{ H}$ Global Minimum:  $E_i = 3.87$  $\Delta E_{\text{coh}} = 60.1 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 75.9 \text{ kJ/mol rel } \boxed{\text{A23}}$  $\Delta E_{\text{Na}_2} = 54.1 \text{ kJ/mol rel Na}_2 + \boxed{\text{A19}}$  $\Delta E_{\text{frag}} = 123 \text{ kJ/mol rel } \boxed{\text{A4}} + \boxed{\text{A11}}$ Triplet  $E_{\text{abs}} = -1622.5043 \text{ H flattened}$ CATION  $^2\text{A}$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1622.3736 \text{ H}$ 

Global Minimum

 $\Delta E_{\text{coh}} = 73.6 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 50.9 \text{ kJ/mol rel } \boxed{\text{A25}}$  $\Delta E_{\text{Na}_2} = 30.5 \text{ kJ/mol rel Na}_2 + \boxed{\text{A19}}^+$ **A28** $\text{Na}_{10}$   
 $\text{C}_s$ NEUTRAL  $^3\text{A}'$  \_\_\_\_\_ RKS/SVP $E_{\text{abs}} = -1622.4984 \text{ H}$  $E = 69.8 \text{ kJ/mol rel } \boxed{\text{A28}}$  $\Delta E_{\text{coh}} = 55.5 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 29.8 \text{ kJ/mol rel } \boxed{\text{A23}}$ Singlet  $E_{\text{abs}} = -1622.4939$ CATION  $^2\text{A}'$  \_\_\_\_\_ UKS/SVP $E_{\text{abs}} = -1622.3679 \text{ H}$  $E = 14.9 \text{ kJ/mol rel } \boxed{\text{A27}}$  $\Delta E_{\text{coh}} = 72.0 \text{ kJ/mol}$  $\Delta E_{\text{Na}} = 26.0 \text{ kJ/mol rel } \boxed{\text{A25}}$