Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## 5-steps algorithm to accelerate the prediction of $[Au_{25}(SR)_{19}]^z$ clusters (z=1-, 0, 1+)

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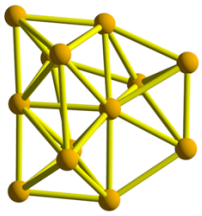
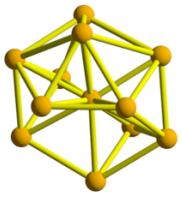
**Fig. S1.** Inner cores of all calculated isomers of $Au_{25}(SR)_{19}$ [z] cluster (z= 0, 1-, 1+). Colour code: Gold adatoms are shown in yellow; core gold atoms are shown in orange colour; chlorine atoms in green; sulphur atoms in red colour. First row stands for core size; second row shows relative energy values; third row indicates the number of octahedra and tetrahedra; four row provides with number of compact tetrahedra and last row indicates the symmetry displayed by each inner core.

**CHLORIDE-PROTECTED CLUSTERS**

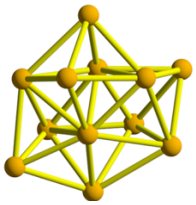
**NEUTRAL/ PBE**



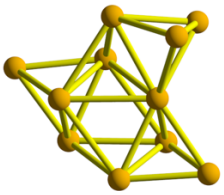
**1.$Au_{13}$**
**0.0 eV**
**2 O + 8 T**
**3 compact T**
**C1**



**2.$Au_{12}$**
**0.014 eV**
**15 T**
**9 compact T**
**Cs**

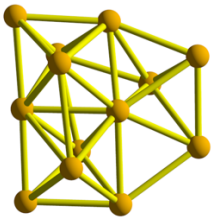


**3.$Au_{12}$**
**0.38 eV**
**1 O + 6 T**
**6 compact T**
**C5v**

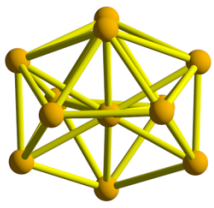


**4.$Au_{11}$**
**0.53 eV**
**1 O + 5 T**
**4 compact T**
**C1**

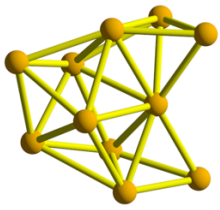
**NEUTRAL/ TPSS**



**1a. $Au_{13}$**
**0.0 eV**
**2 O + 10 T**
**5 Compact T**
**Cs**

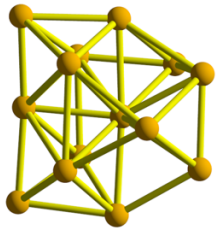


**2a.$Au_{12}$**
**0.039 eV**
**25 T**
**22 Compact T**
**Cs**

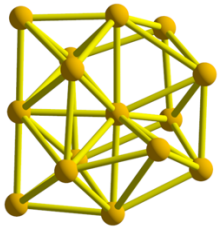


**3a.$Au_{11}$**
**0.91 eV**
**10 T**
**7 Compact T**
**C1**

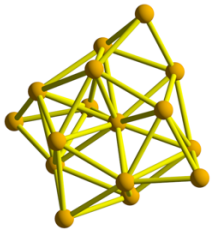
**ANIONIC/ PBE**



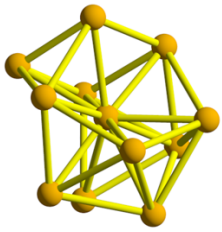
**1j. $Au_{14}$**
**0.0 eV**
**2 O + 10 T**
**7 Compact T**
**C1**



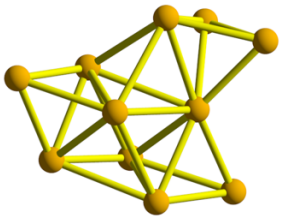
**2j.$Au_{15}$**
**0.2 eV**
**4 O + 9 T**
**3 Compact T**
**C1**



**3j.$Au_{16}$ ($Au_{18}$ changed to $Au_{16}$)**
**0.34 eV**
**1 O + 14 T**
**7 compact T**
**C1**

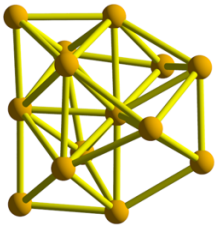


**4j.$Au_{12}$**
**0.40 eV**
**17 T**
**11 Compact T**
**Cs**

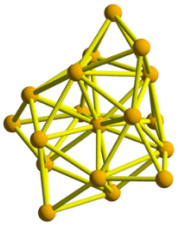


**5j.$Au_{11}$**
**1.45 eV**
**1 O + 5 T**
**3 Compact T**

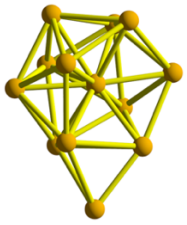
**ANIONIC/ TPSS**



**1k.$Au_{14}$**
**0.0 eV**
**2 O + 15 T**
**9 Compact T**
**C1**



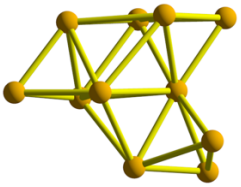
**2k.Au$_{18}$ (obtained from opt. of $Au_{11}$)**
**0.17 eV**
**2 O + 23 T**
**19 Compact T**
**C1**



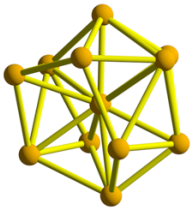
**3k.$Au_{13}$**
**0.48 eV**
**25 T**
**21 Compact T**
**C1**

**-H PROTECTED CLUSTERS**

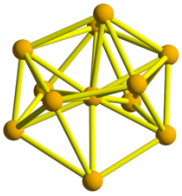
**NEUTRAL/ PBE**



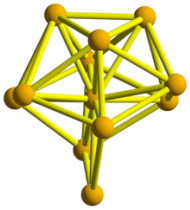
**1b.$Au_{11}$**
**0.0 eV**
**1 O + 5 T**
**3 Compact T**
**Cs**



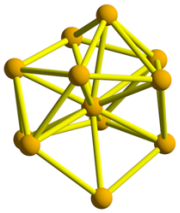
**2b.$Au_{12}$**
**0.12 eV**
**11 T**
**6 Compact T**
**C1**



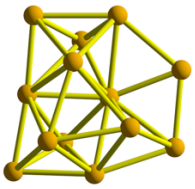
**3b.$Au_{11}$**
**0.19 eV**
**18 T**
**8 Compact T**
**Cs**



**4b.$Au_{12}$**
**0.22 eV**
**19 T**
**10 Compact T**
**C2v**

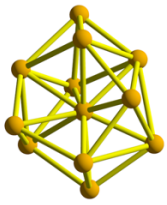


**5b.$Au_{12}$**
**0.26 eV**
**13 T**
**8 Compact T**
**C2v**

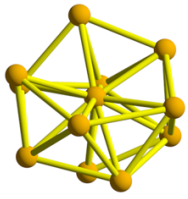


**6b.$Au_{13}$**
**0.60 eV**
**2 O + 5 T**
**1 Compact T**
**C1**

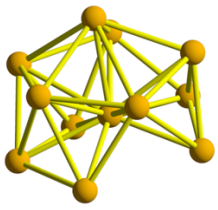
**NEUTRAL/ TPSS**



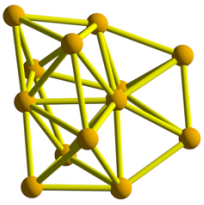
**1c.$Au_{12}$**
**0.0 eV**
**1 O + 10 T**
**6 Compact T**
**C2**



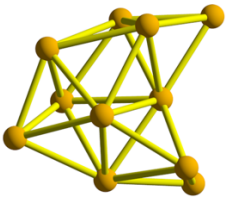
**2c.$Au_{12}$**
**0.026 eV**
**24 T**
**15 compact T**
**C5v**



**3c.$Au_{12}$**
**0.13 eV**
**25 T**
**12 Compact T**
**C5v**

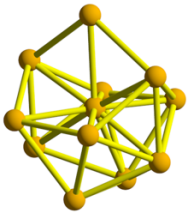


**4c.$Au_{13}$**
**0.16 eV**
**2 O + 9 T**
**4 Compact T**
**C1**

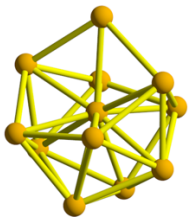


**5c.$Au_{11}$**
**0. 17 eV**
**8 T**
**7 Compact T**
**C1**

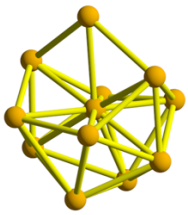
**ANIONIC/ PBE**



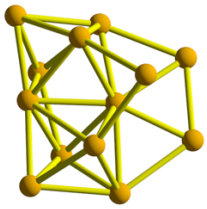
**1f.$Au_{12}$**
**0.0 eV**
**18 T**
**12 Compact T**
**C2v**



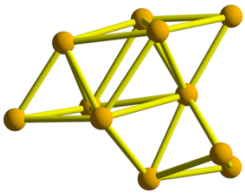
**2f.$Au_{12}$**
**0.023 eV**
**16 T**
**10 Compact T**
**C2v**



**3f.$Au_{12}$**
**0.059 eV**
**18 T**
**10 compact T**
**C2v**

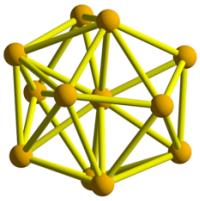


**4f.$Au_{13}$**
**0.35 eV**
**1 O + 4T**
**1 compact T**
**C1**

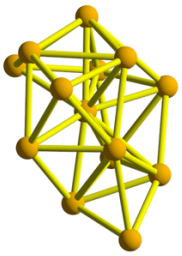


**5f.$Au_{11}$**
**0.44 eV**
**1 O + 5T**
**1 compact T**
**Cs**

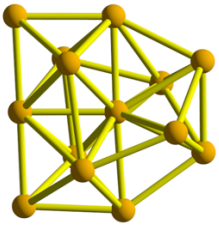
**ANIONIC/ TPSS**



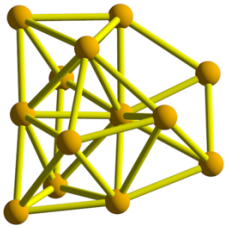
**1g.$Au_{12}$**
**0.0 eV**
**23 T**
**16 compact T**
**C5v**



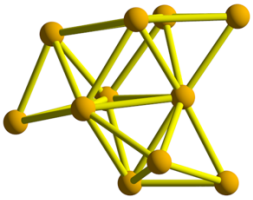
**2g.$Au_{14}$**
**0.19 eV**
**1 O + 16 T**
**11 compact T**
**C1**



**3g.$Au_{14}$**
**0.25 eV**
**3 O + 13 T**
**5 compact T**
**C2**



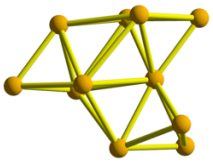
**4g.$Au_{13}$**
**0.34 eV**
**1 O + 8 T**
**5 compact T**
**C1**



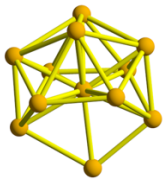
**5g.$Au_{11}$**
**0.96 eV**
**1 O + 10 T**
**5 Compact T**
**C1**

**-$CH_3$ PROTECTED CLUSTERS**

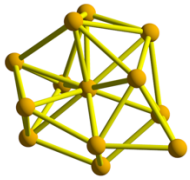
**NEUTRAL/ PBE**



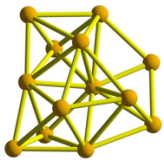
**1d.$Au_{11}$**
**0.0 eV**
**1 O + 5T**
**4 compact T**
**Cs**



**2d.$Au_{11}$**
**0.14 eV**
**19 T**
**12 compact T**
**C2v**

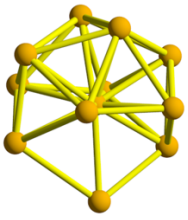


**3d.$Au_{13}$**
**1.05 eV**
**8 T**
**7 compact T**
**C1**

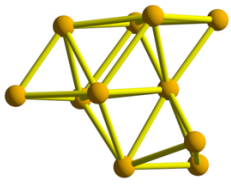


**4d.$Au_{13}$**
**1.24 eV**
**1 O + 2T**
**1 compact T**
**C1**

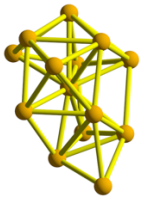
**NEUTRAL/ TPSS**



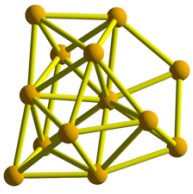
**1e.$Au_{11}$**
**0.0 eV**
**20 T**
**12 compact T**
**C2v**



**2e.$Au_{11}$**
**0.2 eV**
**1 O + 6 T**
**4 compact T**
**Cs**

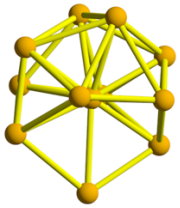


**3e.$Au_{14}$**
**0.53 eV**
**2 O + 9T**
**5 compact T**
**C1**

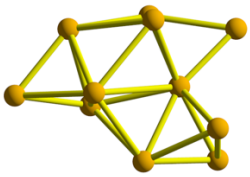


**4e.$Au_{13}$**
**0.6 eV**
**1 O + 10T**
**1 compact T**
**C1**

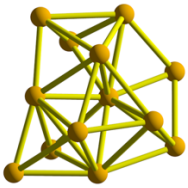
**ANIONIC/ PBE**



**1h.$Au_{11}$**
**0.0 eV**
**18 T**
**12 compact T**
**C2v**

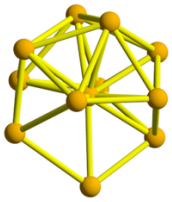


**2h.$Au_{11}$**
**0.42 eV**
**1 O + 4 T**
**2 compact T**
**C1**

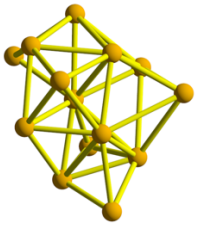


**3h.$Au_{13}$**
**1.07 eV**
**1 O + 6 T**
**1 compact T**
**C1**

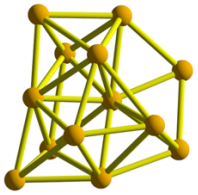
**ANIONIC/ TPSS**



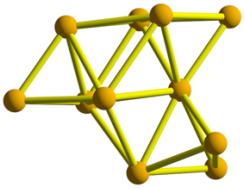
**1i.$Au_{11}$**
**0.0 eV**
**20 T**
**18 compact T**
**C2v**



**2i.$Au_{14}$**
**0.43 eV**
**2 O + 14 T**
**9 compact T**
**C1**



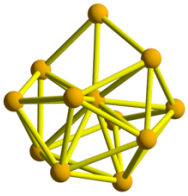
**3i.$Au_{13}$**
**0.62 eV**
**2 O + 9 T**
**1 compact T**
**C1**



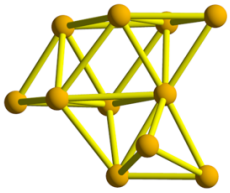
**4i.$Au_{11}$**
**0.69 eV**
**2 O + 7 T**
**6 compact T**
**Cs**

**-H PROTECTED CLUSTERS**

**CATION/ PBE**

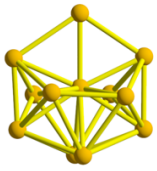


**6a.Au12**
**0.0 eV**
**18 T**
**12 compact T**
**$C_{2v}$**

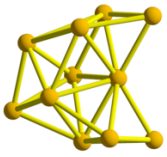


**6b.Au11**
**0.31 eV**
**1 O + 5 T**
**3 compact T**
**$C_1$**

**CATION/ TPSS**



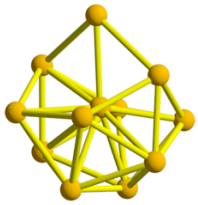
**7a.Au12**
**0.0 eV**
**22 T**
**12 compact T**
**$C_{2v}$**



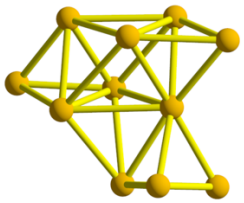
**7b.Au11**
**0.17 eV**
**11 T**
**3 compact T**
**$C_1$**

## -$CH_3$ PROTECTED CLUSTERS

**CATION/ PBE**



**8a.Au12**
**0.0 eV**
**21 T**
**10 compact T**
**$C_{2v}$**

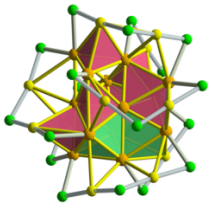


**8b.Au11**
**0.53 eV**
**4 T**
**4 compact T**
**$C_1$**

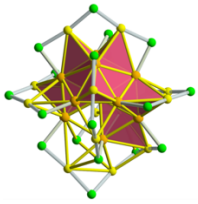
**Fig. S2.** All calculated isomers of $Au_{25}(SR)_{19}^{[z]}$ cluster (z=0,1-, 1+) displaying comprising tetrahedra (red planes) and octahedra (green planes). Colour code: Gold adatoms are shown in yellow; core gold atoms are shown in orange color; chlorine atoms in green; sulphur atoms in red colour. Under each figure is indicated the number of constituting octahedra and tetrahedra. Same order is giving as in Fig. S1.

**CHLORIDE-PROTECTED**

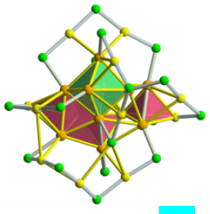
**NEUTRAL/ PBE**



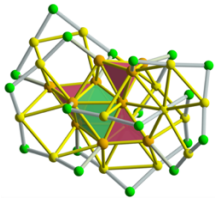
**2 O + 8 T**



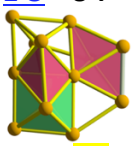
**15 T**



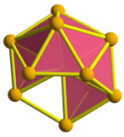
**1 O + 6 T**



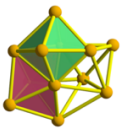
**1 O + 5 T ← < 3.4 Å.**



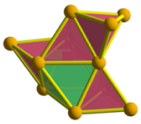
**1 O + 3 T**



**9 T**



**1 O + 3 T**



**1 O + 4 T**

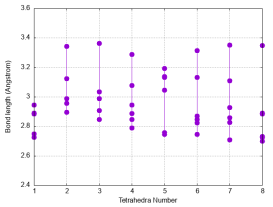
**NOTES:**

**Counting of polyhedra (tetrahedra or octahedra) edges considers bond lengths as larger as 3.4 Å.**
**Compact tetrahedra have edges with bond lengths included in the range from 2.6 to 3.2 Å.**

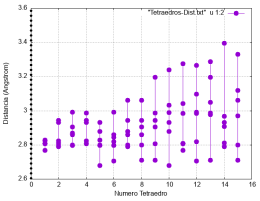
**ALGORITHM**

1. **Sort isomers according to number of tetrahedra with bond lengths included in the range from 2.6 to 3.4 Å.**
2. **Form sets with isomers displaying same type of polyhedra (i.e all containing tetrahedra or combination of tetrahedra and octahedra).**
3. **Calculate T factor= (#O + #T)/#cT, where O stands for octahedra, T for tetrahedra and cT for compact tetrahedra found in the inner core. Sometimes is necessary to consider long bond distances to avoid division by zero.**
4. **Use factor values to sort between sets. Make a general consideration that more tetrahedra is better.**

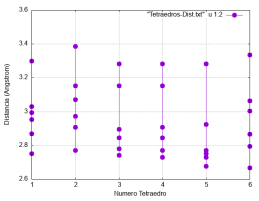
**NUMBER OF COMPACT TETRAHEDRA**



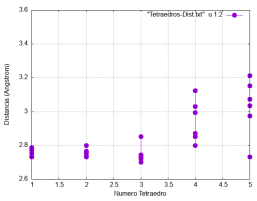
**2** cT< 3.2



**9** cT< 3.2

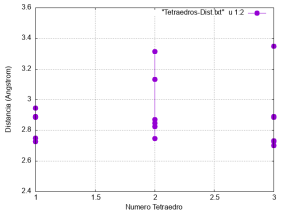


6 cT< **3.4**

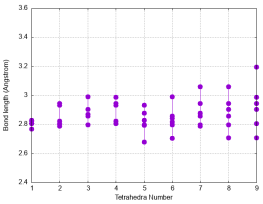


4 cT< 3.2

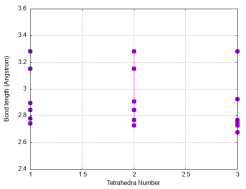
**TOTAL STRUCTURE**



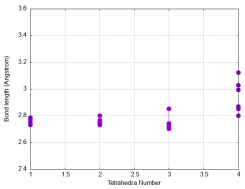
1 cT< 3.2



9 cT< 3.2



3 cT< 3.4



4 cT< 3.2

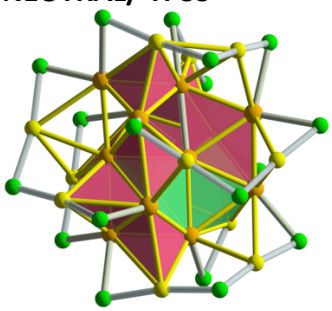
**INNER CORE**

**STEPS:**

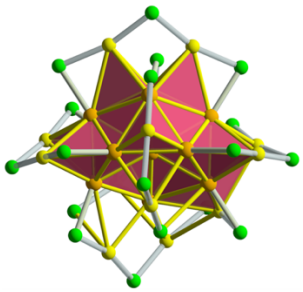
| | | | | | |
|---|---|---|---|---|---|
| 1. | **15 T** | **2 O + 8 T** | **1 O + 6 T** | **1 O + 5 T** | **2 subgroups** |
| 2. | **9** | **1** | **3** | **4** | **compact T in inner core** |
| 3. | **1.66** | **10** | **2.33** | **1.5** | **T-Factor** |
| 4. | **2 O + 8 T(10)** | **1 O + 6 T (2.33)** | **15 T (1.66)** | **1 O + 5 T (1.5)** | **ISOMERS ENERGY ORDER** |

**Trend in energy is large T-factor value corresponds with energy minimum.**

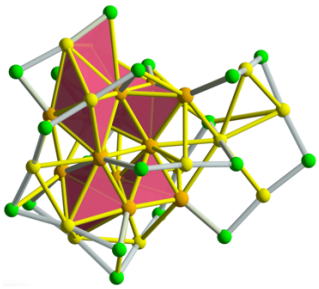
**NEUTRAL/ TPSS**



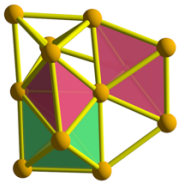
2 O + 10 T



25 T

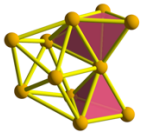


10 T

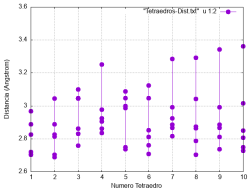


1 O + 3 T

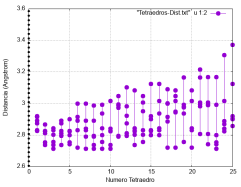
15 T



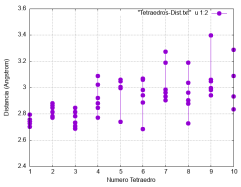
3 T



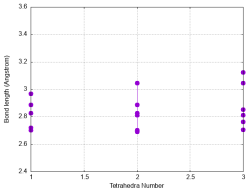
5 cT < 3.2



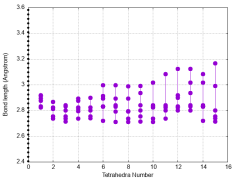
22 cT < 3.2



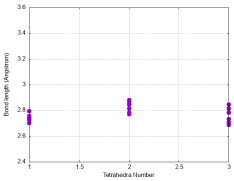
7 cT < 3.2



3 cT < 3.2



15 cT < 3.2



3 cT < 3

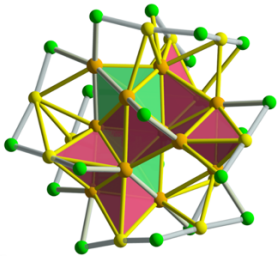
**STEPS:**

| | | | | |
|---|---|---|---|---|
| **1.** | **25 T** | **10 T** | **2 O + 10 T** | **2 subgroups** |
| **2.** | **15** | **3** | **3** | **# of compact T in core** |
| **3.** | **1.67** | **3.333** | **4** | **T-factor values** |
| **4.** | **2 O + 10 T (4)** | **25 T (1.67)** | **10 T(3.33)** | **ISOMERS ENERGY ORDER** |

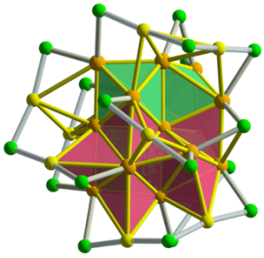
In each subgroup more stable isomer has large number of tetrahedra, for example, isomer including 25 T is more stable than isomer including 10 T.
2O + 10 T was moved toward left side given its large T-factor value. It seems that T-factor value has more weight in deciding the energy order than the number of tetrahedra in the full structure.

**Minimum has the large T-factor value.**

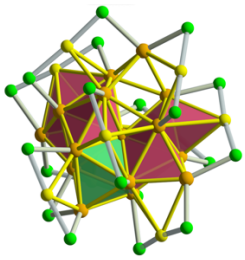
**ANIONIC/ PBE**



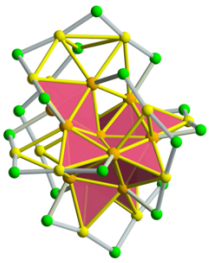
2 O + 10 T



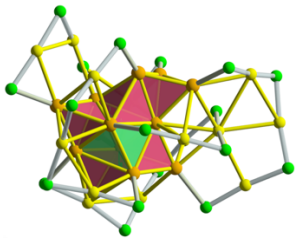
4 O + 9T



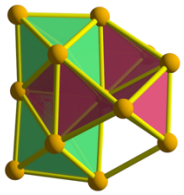
1 O + 14 T



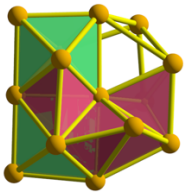
17 T



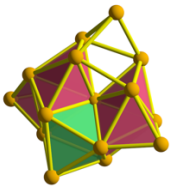
1 O + 5T



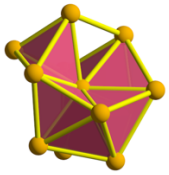
2 O + 6 T



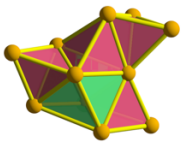
2 O + 5 T



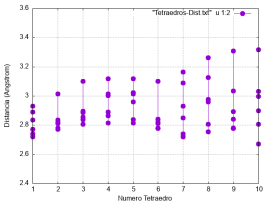
1 O +10 T



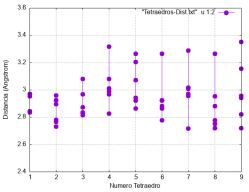
10 T



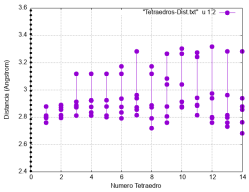
1 O + 4T



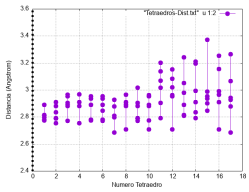
7 cT < 3.2



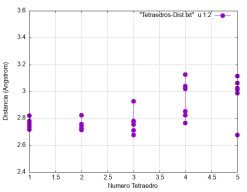
3 cT < 3.2



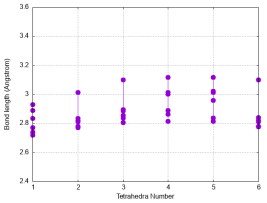
7 cT < 3.2



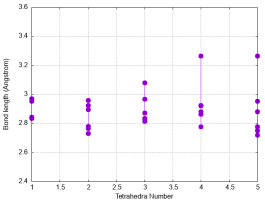
11 cT < 3.2



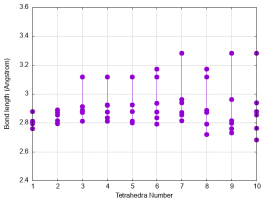
3 cT < 3.2



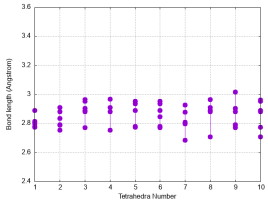
6 cT < 3.2



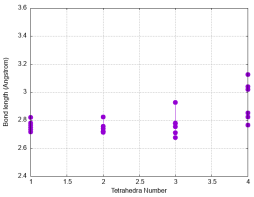
3 cT < 3.2



7 cT < 3.2



10 cT < 3.2



4 cT < 3.2

**ISOMERS ENERGY ORDER**

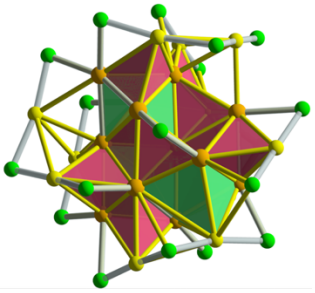
**STEPS:**

| | | | | |
|---|---|---|---|---|
| **1.** | **17 T** | **1 O + 14 T** | **2 O + 10 T** | **4 O + 9 T** | **1 O + 5 T** |
| **2.** | **10** | **7** | **6** | **3** | **4** |
| **3.** | **1.7** | **2.14** | **2** | **4.33** | **1.5** |
| **4.** | **2 O + 10 T (2)** | **4 O + 9 T (4.33)** | **1 O + 14 T (2.14)** | **17 T (1.7)** | **1 O + 5 T (1.5)** |

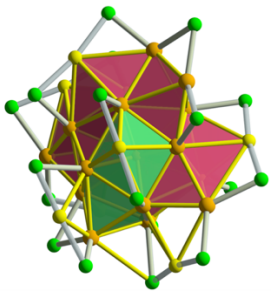
**Isomers constituted by 1 octahedron form one subgroup (highlighted in cyan color)**
**Isomers comprised by 2 or more Octahedra form second subgroup (red color)**
**Third set is formed by isomer containing only tetrahedra.**

**More stable isomer is contained in the group holding a large T-factor value.**
**Conclusion: Energy order is given as decrement of T-factor value.**

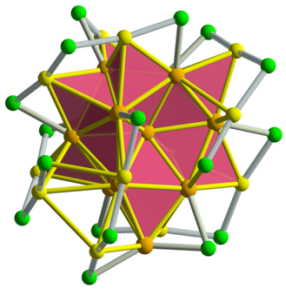
**ANIONIC/ TPSS**



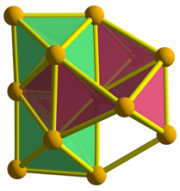
2 O + 15 T



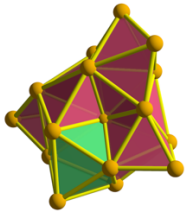
2 O + 23 T



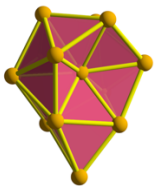
25 T



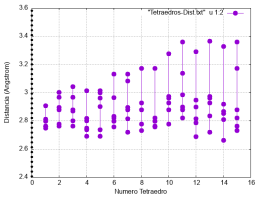
2 O + 6 T



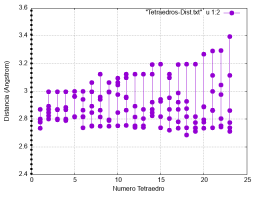
1 O + 16 T



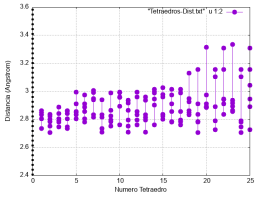
16 T



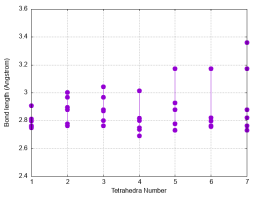
9 cT < 3.2



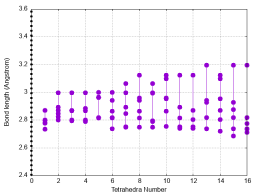
19 cT < 3.2



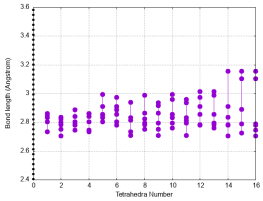
21 cT < 3.2



6 cT < 3.2



16 cT < 3.2



16 cT < 3.2

**ISOMERS ENERGY ORDER**

STEPS

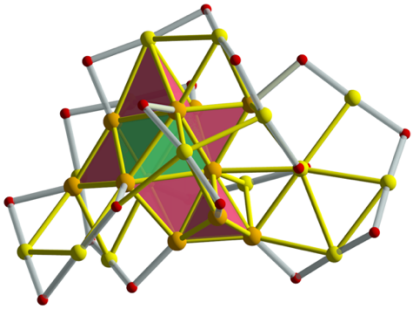
| | | | |
|---|---|---|---|
| **1.** | **25 T** | **2 O + 23 T** | **2 O + 15 T** |
| **2.** | **16** | **16** | **6** |
| **3.** | **1.56** | **1.56** | **2.83** |
| **4.** | **2 O + 15 T (2.83)** | **2 O + 23 T (1.56)** | **25 T (1.56)** |

**More stable isomer has large T-factor value.**

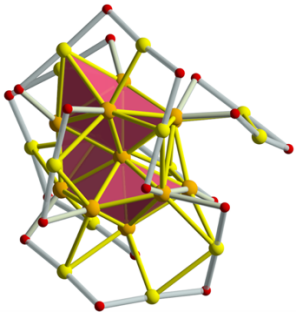
GENERAL CONCLUSION. For chloride-protected the energy order is consistent with **decrement** of T-factor values, independently of charge-state [z= 0, 1-] and XC functional.

## H-PROTECTED

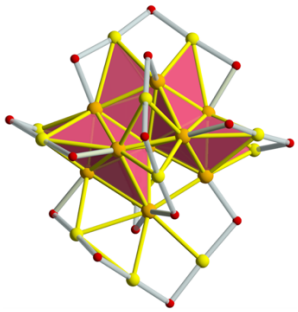
**NEUTRAL/ PBE**



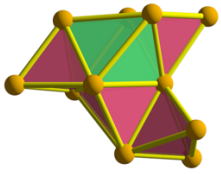
**1 O + 5 T**



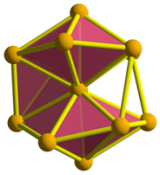
**11 T**



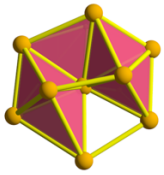
**18 T**



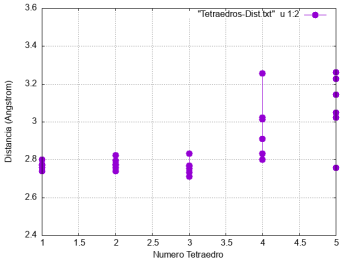
**1 O + 4 T**



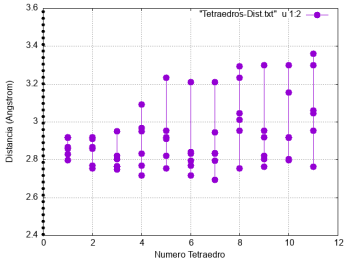
**9 T**



**11 T**




3 cT < 3.2

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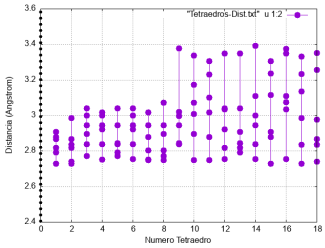
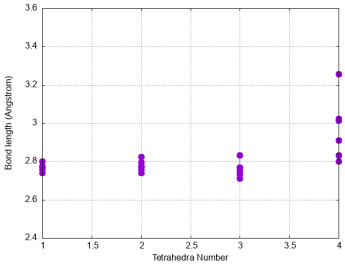



8 cT< 3.2

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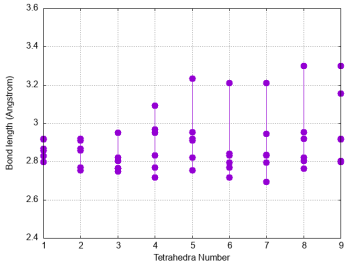


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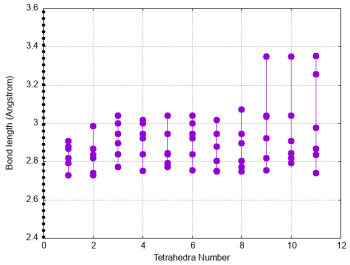


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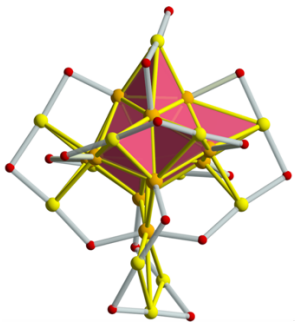
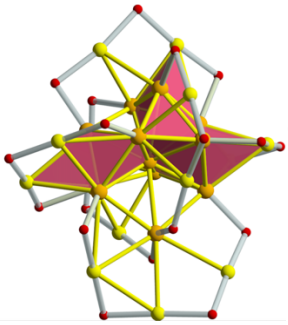
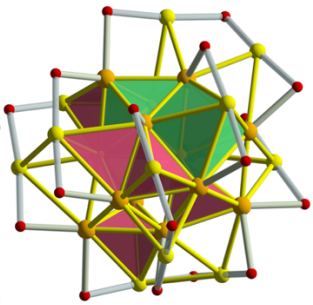


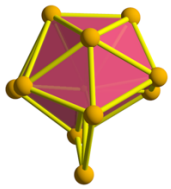
**19 T**



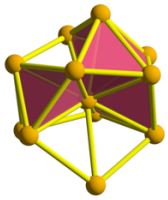
**13 T**



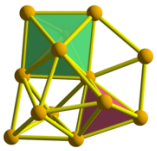
**2 O + 5 T**



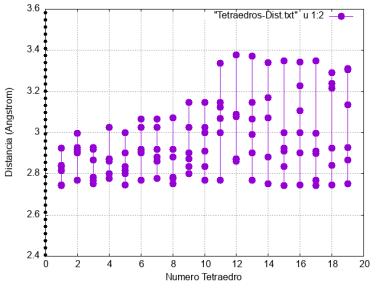
**12 T**



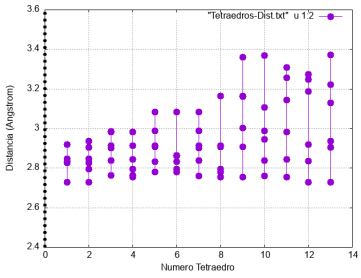
**8 T**



**1 O + 1 T**




10 cT < 3.2

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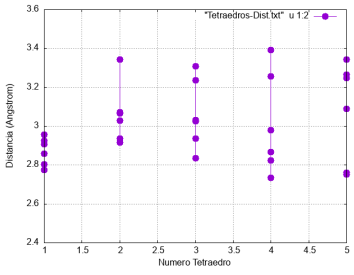


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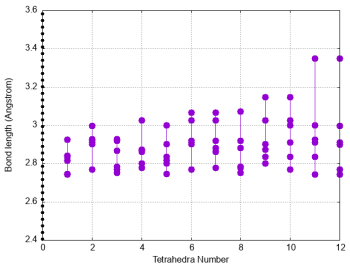


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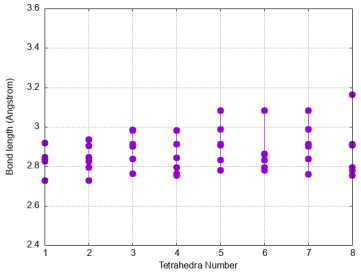


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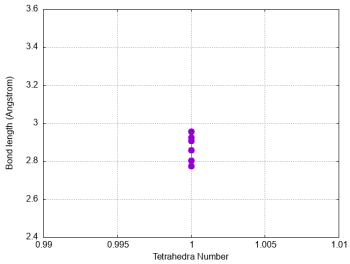


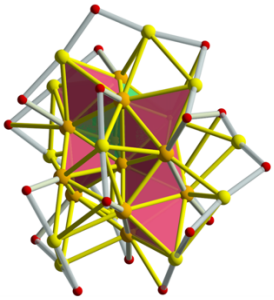

1 cT< 3.2

**STEPS**

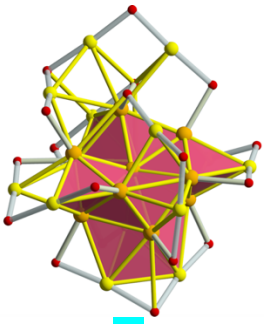
| | | | **ISOMERS ENERGY ORDER** | | | |
|---|---|---|---|---|---|---|
| **1.** | **19 T** | **18 T** | **13 T** | **11 T** | **1 O + 5 T** | **2 O + 5 T** |
| **2.** | **10** | **8** | **8** | **6** | **3** | **1** |
| **3.** | **1.9** | **2.25** | **1.62** | **1.83** | **2** | **7** |
| 4. | **1 O + 5 T (2)** | **13 T (1.62)** | **11 T (1.83)** | **19 T (1.9)** | **18 T (2.25)** | **2 O + 5 T (7)** |

Minimum corresponds with an isomer with small T-factor value being part of a subgroup.
Energy order is given in terms of **increment of T-factor values**.

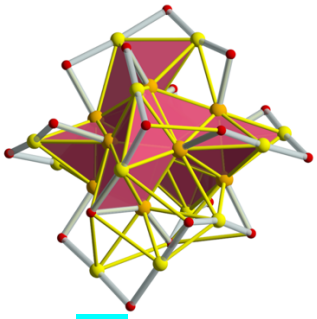
**NEUTRAL/ TPSS**



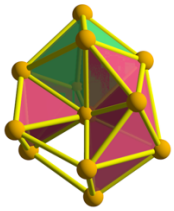
1 O + 10 T



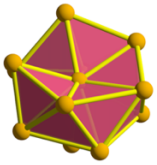
24 T



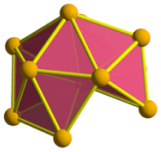
25 T



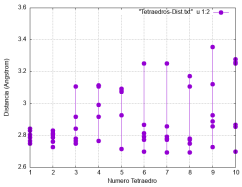
1 O + 6 T



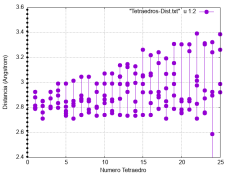
12 T



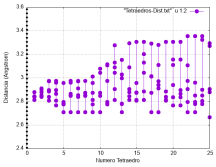
12 T



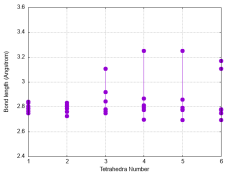
6 cT < 3.2



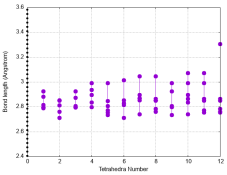
**15** cT < 3.2



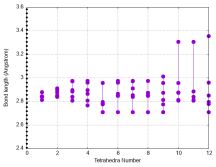
12 cT< 3.2



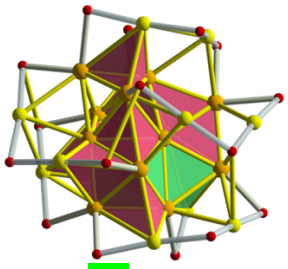
4 cT < 3.2



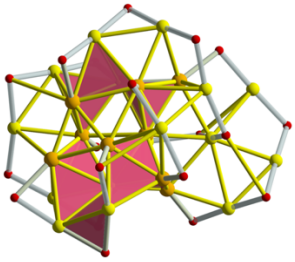
11 cT < 3.2



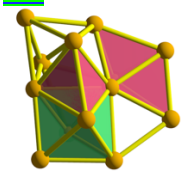
9 cT< 3.2



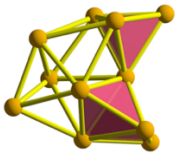
2 O + 9 T



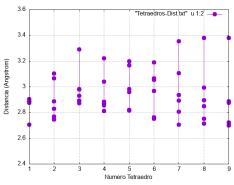
8 T



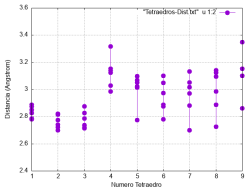
1 O + 3 T



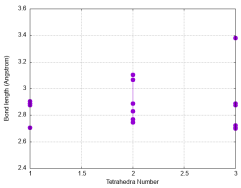
3T



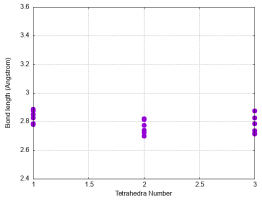
4 cT < 3.2



7 cT < 3.2



2 cT < 3.2



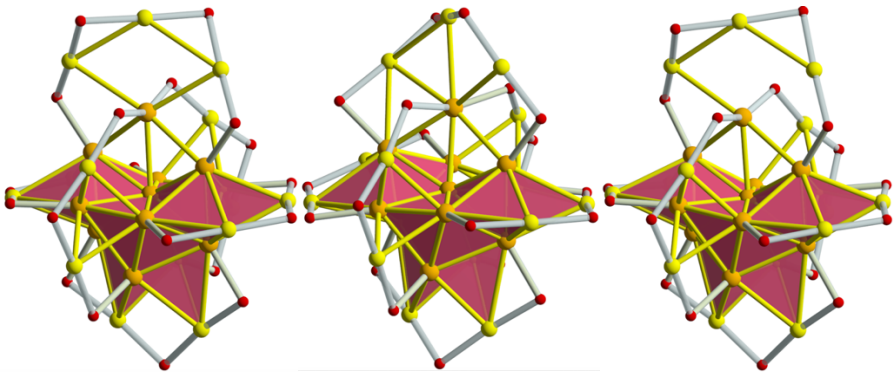
3 cT < 3.2

**STEPS**

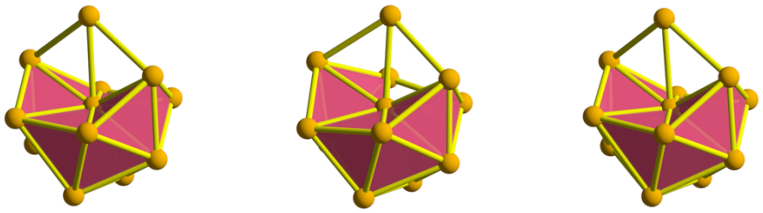
| | | | ISOMERS ENERGY ORDER | | |
|---|---|---|---|---|---|
| **1.** | **25 T** | **24 T** | **1 O + 10T** | **2 O + 9 T** | **8 T** |
| **2.** | **9** | **11** | **4** | **2** | **3** |
| **3.** | **2.78** | **2.18** | **2.75** | **5.55** | **2.67** |
| 4. | **1 O + 10 T (2.75)** | **25 T (2.78)** | **24 T (2.18)** | **2 O + 9 T (5.55)** | **8 T (2.67)** |

Isomer constituted by 8 T occupies the last place because there are isomers with more Tetrahedra.
Minimum **has small** T-factor value.
Inside its subgroup (cyan color), structure constituted by 1 O + 10 T has a smaller factor value.

**ANIONIC/ PBE**

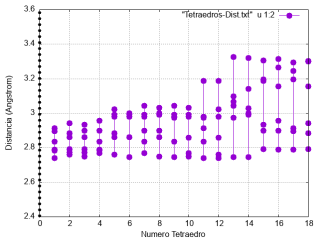


18 T 16 T 18 T

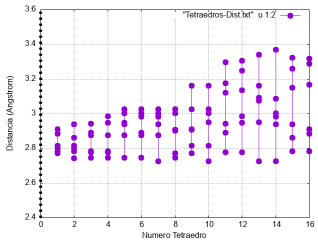


12 T 10 T 12T

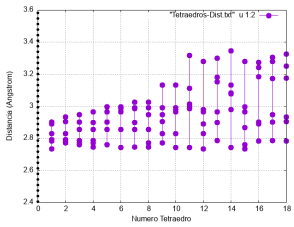
**Isomers with same number of tetrahedra, have different number of compact tetrahedra in their inner cores. More stable has 4 T more than others and less stable displays longer edges.**



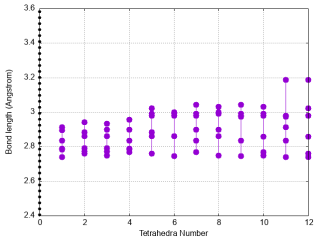

12 cT < 3.2



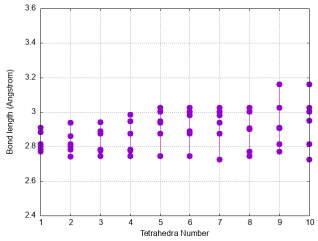

**10** cT < 3.2



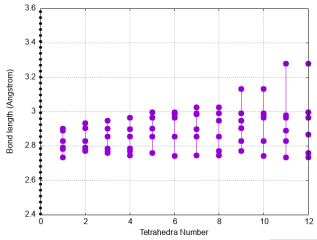

10 cT< 3.2



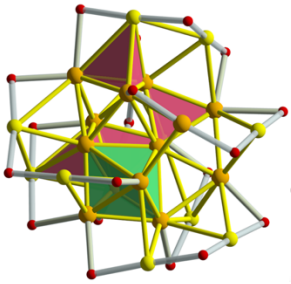

12 cT < 3.2

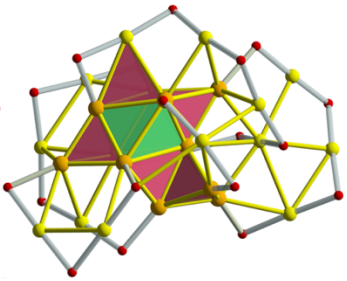



**10** cT < 3.2

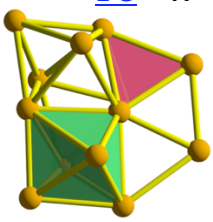


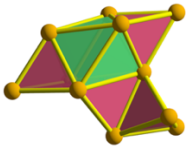

10 cT< 3.2; 2 T >3.2



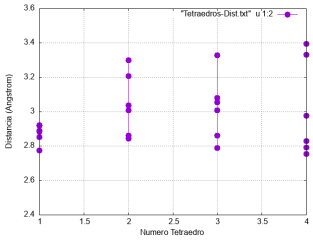


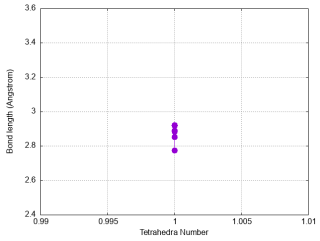
**1 O + 4T** **1 O + 5T**



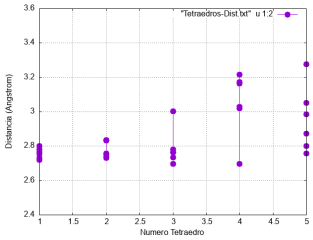


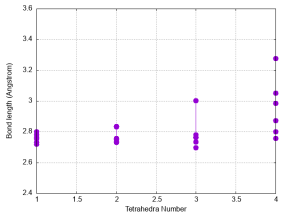
1 O+ 1 T 1 O+ 3 T




1 cT < 3.2 1 cT < 3.2



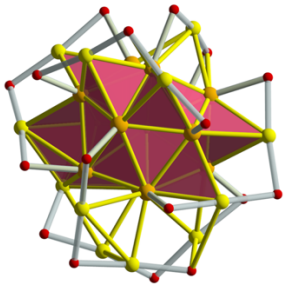

3 cT < 3.2 3 cT < 3.2

**STEPS**

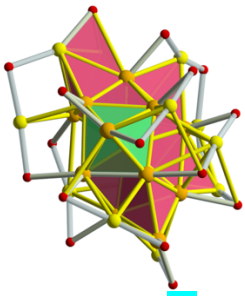
| | | | | **ISOMERS ENERGY ORDER** | |
|---|---|---|---|---|---|
| **1.** | **18 T** | **18 T** | **16 T** | **1 O + 4 T** | **1 O + 5 T** |
| **2.** | **12** | **10** | **10** | **3** | **3** |
| **3.** | **1.5** | **1.8** | **1.6** | **1.67** | **2** |
| 4. | **18 T (1.5)** | **16 T (1.6)** | **18 T (1.8)** | **1 O + 4 T (1.67)** | **1 O + 5 T (2)** |

**Minimum corresponds with smaller T-factor value.**

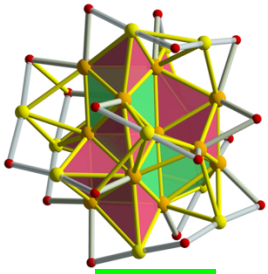
**ANIONIC/ TPSS**



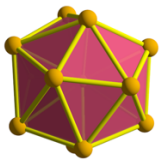
**23 T**



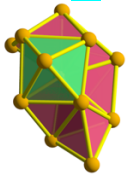
**1 O + 16 T**



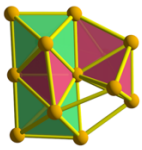
**3 O + 13 T**



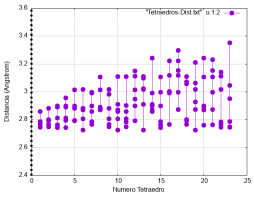
**14 T**



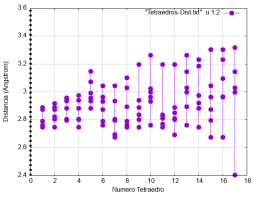
**1 O + 10 T**



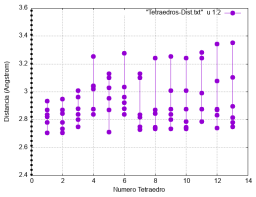
**2 O + 6 T**



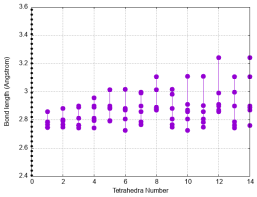

16 cT < 3.2



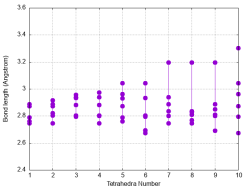

**11** cT < 3.2



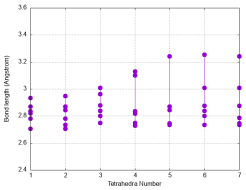

5 cT< 3.2



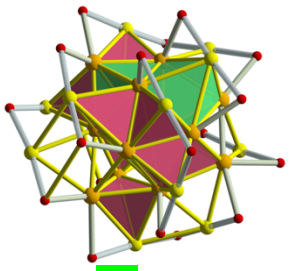

12 cT < 3.2



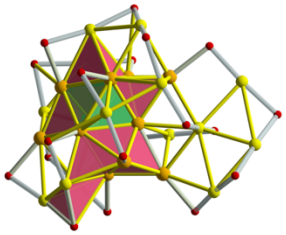

**9** cT < 3.2



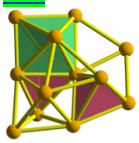

4 cT< 3.2



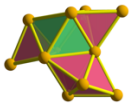
**1 O + 8 T**



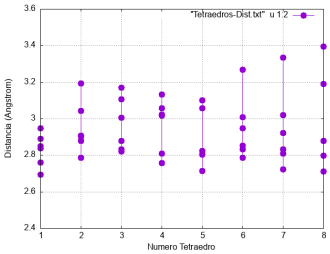
**1 O + 10 T**



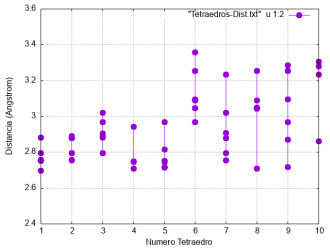
1 O + 2 T



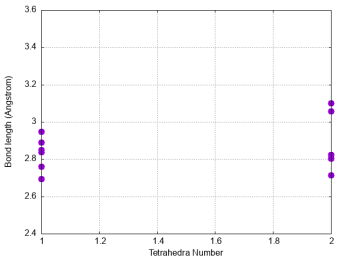
1 O + 5 T



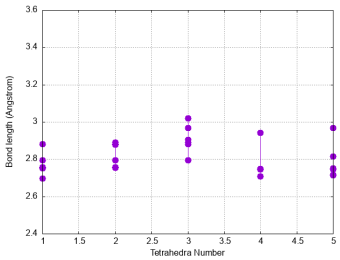

5 cT < 3.2




**5** cT < 3.2




2 cT < 3.2




**5** cT < 3.2

| **STEPS** | | **ISOMERS ENERGY ORDER** | | | |
|---|---|---|---|---|---|
| **1.** | **23 T** | **1 O + 16 T** | **3 O + 13 T** | **1 O + 10 T** | **1 O + 8 T** |
| **2.** | **12** | **9** | **4** | **5** | **2** |
| **3.** | **1.92** | **1.89** | **4** | **2.2** | **4.5** |
| **4.** | **23 T (1.92)** | **1 O + 16 T (1.89)** | **3 O + 13 T (4)** | **1 O + 8 T (4.5)** | **1 O + 10 T(2.2)** |

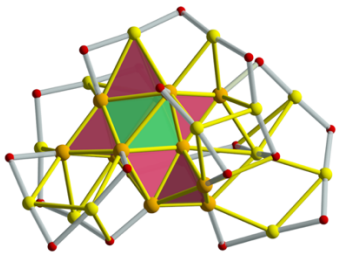
**In subgroup formed by isomers including 1 octahedron, reordering of isomers with similar number of tetrahedra (8 and 10).**

In general, energy order goes from **small to large T-factor** values.

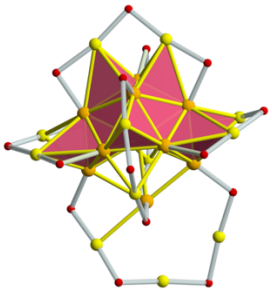
GENERAL CONCLUSION. For SH-protected the energy order is consistent with **increment** of T-factor values, independently of charge-state [z= 0, 1-] and XC functional.

**-$CH_3$-PROTECTED**

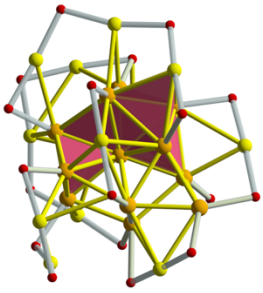
**NEUTRAL/ PBE**



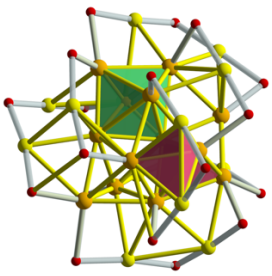
**1 O + 5 T**



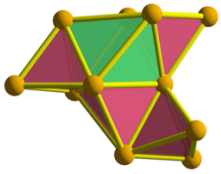
**19 T**



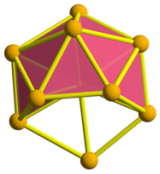
**8 T**



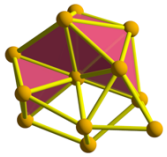
**1 O + 2T**



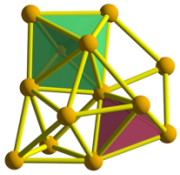
**1 O + 4 T**



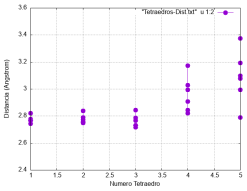
**12 T**



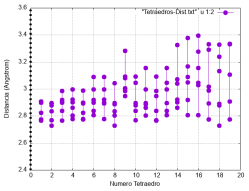
**7 T**



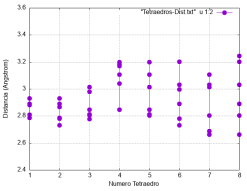
**1 O +T**



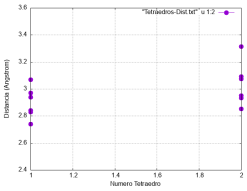
4 cT < 3.2



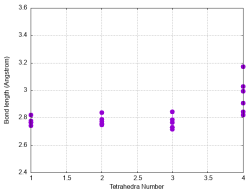
**12** cT < 3.2



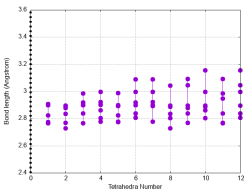
7 cT< 3.2



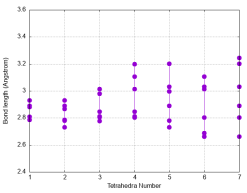
1 cT< 3.2



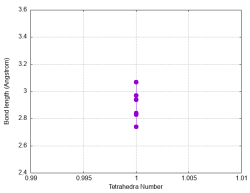
4 cT < 3.2



**12** cT < 3.2



6 cT< 3.2



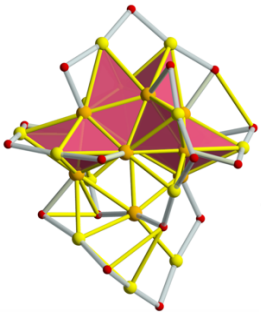
1 cT< 3.2

Minimum has compact tetrahedra constituting its inner core (around 2.88 Å)

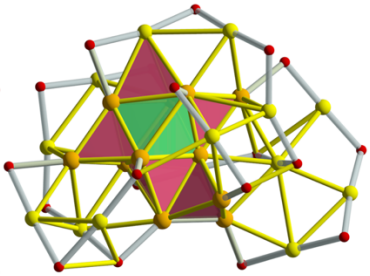
| | **STEPS** | | **ISOMERS ENERGY ORDER** | |
|---|---|---|---|---|
| **1.** | **19 T** | **8 T** | **1 O + 5 T** | **1 O + 2 T** |
| **2.** | **12** | **6** | **4** | **1** |
| **3.** | **1.58** | **1.33** | **1.5** | **3** |
| **4.** | **1 O + 5 T (1.5)** | **19 T (1.58)** | **8 T (1.33)** | **1 O + 2 T (3)** |

**Small to large values** of T-factor in each subgroup gave the correct energy order.

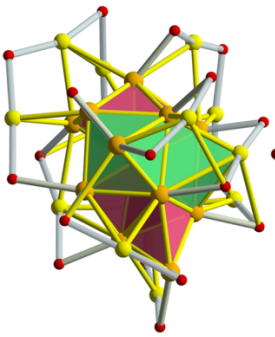
**NEUTRAL/ TPSS**



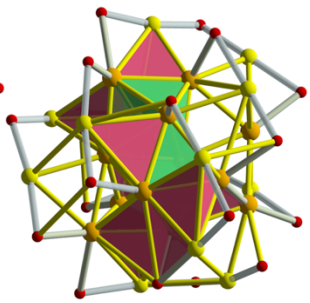
**20 T**



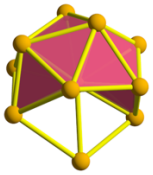
**1 O + 6 T**



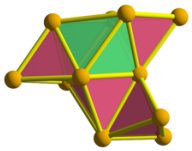
**2 O + 9 T**



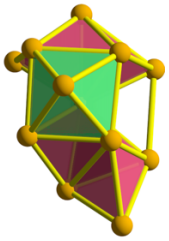
**1 O + 10 T**



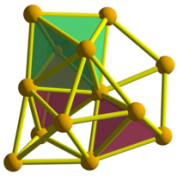
**12 T**



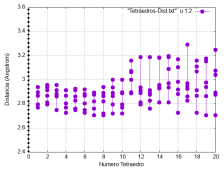
**1 O + 4 T**



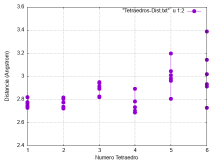
**1 O + 5 T**



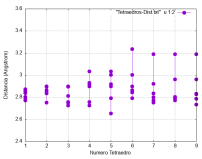
**1 O + 1 T**



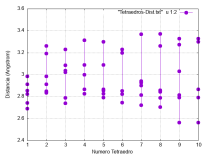
20 T < 3.4



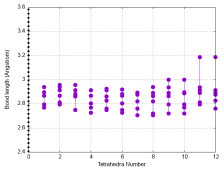
**6** T < 3.4



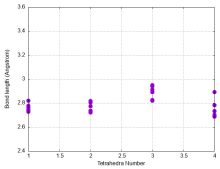
9 T< 3.4



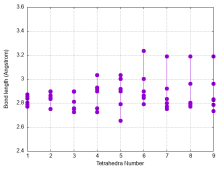
10 T< 3.4



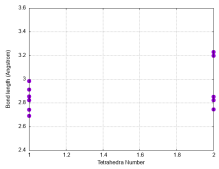
12 cT < 3.2



**4** cT < 3.2



5 cT< 3.2



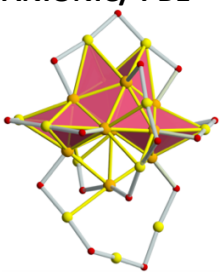
1 cT< 3.2

**STEPS**

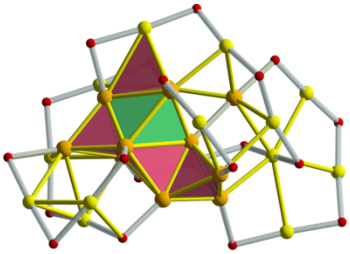
| | | ISOMERS ENERGY ORDER | | |
|---|---|---|---|---|
| 1. | **20 T** | **1 O + 10 T** | **2 O + 9 T** | **1 O + 6 T** |
| 2. | **12** | **1** | **5** | **4** |
| 3. | **1.67** | **11** | **2.2** | **1.75** |
| 4. | **20 T (1.67)** | **1 O + 6 T (1.75)** | **2 O + 9 T (2.2)** | **1 O + 10 T (11)** |

Isomer constituted by 1 O + 10 T has a T-factor value of 11 then it is changed to last place.
In this case, it is evident the energy order. Increment in T-factor value corresponds with less stability. Minimum has smaller factor value. It means that for this ligand XC functional and charge-state the energy **order is given as increment in the T-factor value.**

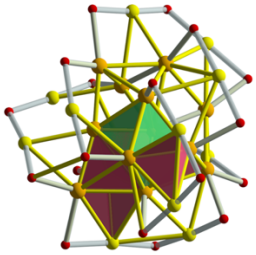
**ANIONIC/ PBE**



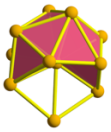
**18 T**



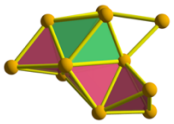
**1 O + 4 T**



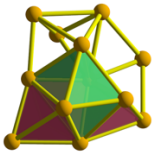
**1 O + 6 T**



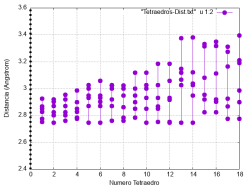
**12 T**



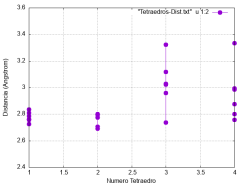
**1 O+ 3T**



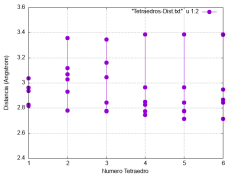
**1 O+ 4 T**



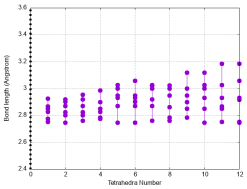
12 cT < 3.2



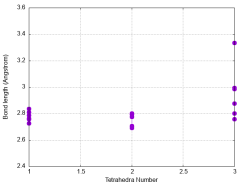
**2** cT < 3.2



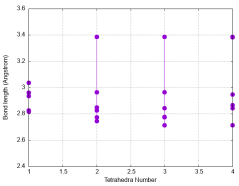
1 cT< 3.2



12 cT < 3.2



**2** cT < 3.2



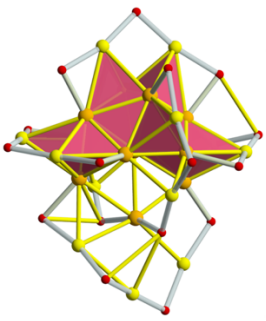
1 cT< 3.2

**STEPS**

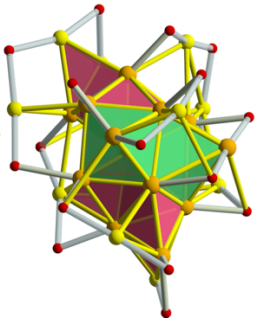
| | | | **ISOMERS ENERGY ORDER** |
|---|---|---|---|
| 1. | **18 T** | **1 O + 6 T** | **1 O + 4 T** |
| 2. | **12** | **1** | **2** |
| 3. | **1.5** | **7** | **7** |
| 4. | **18 T (1.5)** | **1 O + 4 T (7)** | **10 O + 6 T (7)** |

**Minimum has smaller T-factor value.**

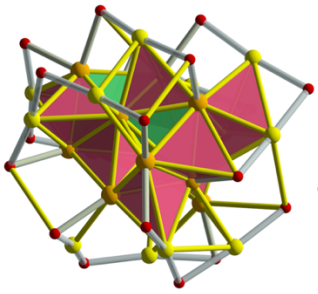
**ANIONIC/ TPSS**



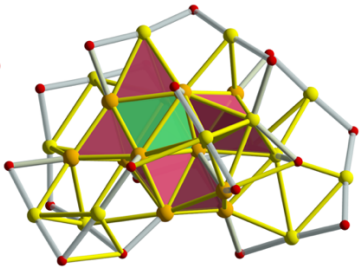
**20 T**



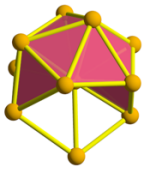
**2 O+ 14 T**



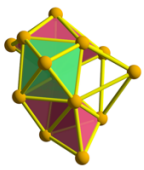
**2 O + 9 T**



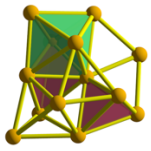
**2 O + 7 T**



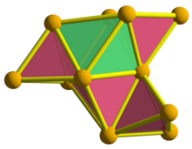
**12 T**



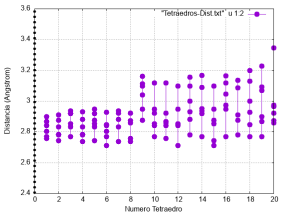
**1 O + 9 T**



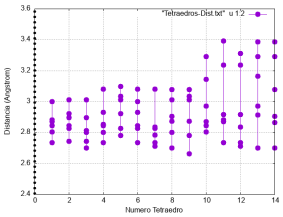
**1 O + 2T**



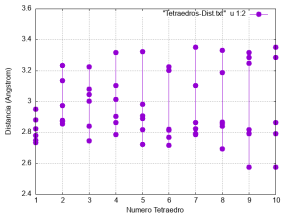
**1 O + 4 T**



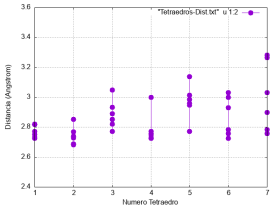

18 cT < 3.2



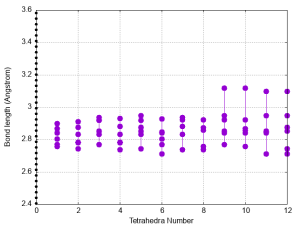

**9** cT < 3.2



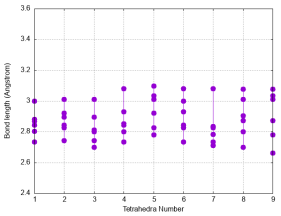

1 cT< 3.2



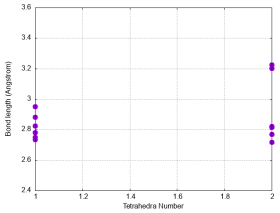

6 cT< 3.2



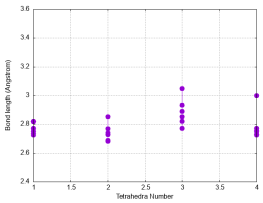

12 cT < 3.2




**9** cT < 3.2




1 cT< 3.2




4 cT< 3.2

**STEPS**

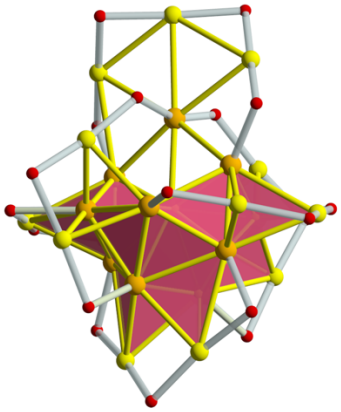
| | | ISOMERS ENERGY ORDER | | |
|---|---|---|---|---|
| 1. | **20 T** | **2 O + 14 T** | **2 O + 9 T** | **2 O + 7 T** |
| 2. | **12** | **9** | **1** | **4** |
| 3. | **1.67** | **1.78** | **11** | **2.25** |
| 4. | **20 T (1.67)** | **2 O + 14 T (1.78)** | **2 O + 7 T (2.25)** | **2 O + 9 T (11)** |

**Energy order is given by increment in T-factor value. In this case, smaller T-factor value corresponds with minimum.**

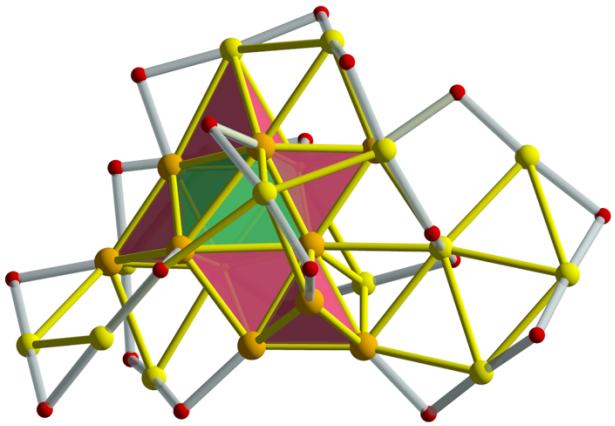
GENERAL CONCLUSION. For $SCH_3$-protected the energy order is consistent with **increment** of T-factor values, independently of charge-state [z= 0, 1-] and XC functional.

## CATIONIC H-PROTECTED

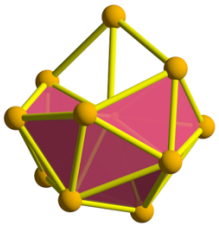
**PBE**



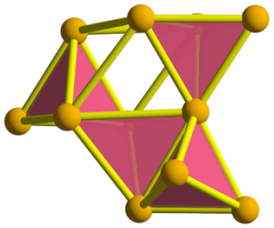
**18 T**



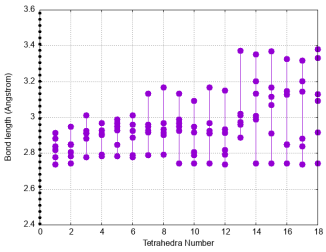
**1 O + 5 T**



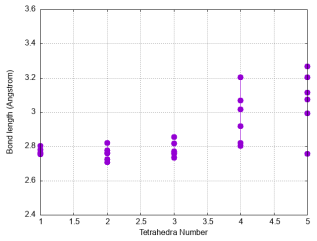
**12 T**



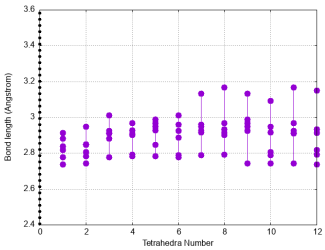
**4 T**



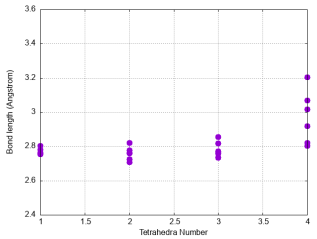

18 cT < 3.2




3 cT < 3.2




12 cT < 3.2




4 cT < 3.2

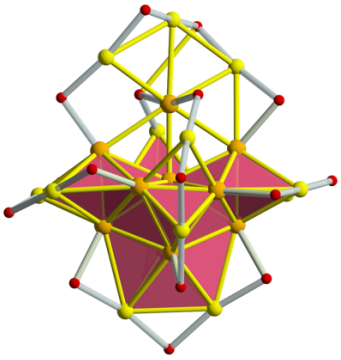
**STEPS**

**ISOMERS ENERGY ORDER**

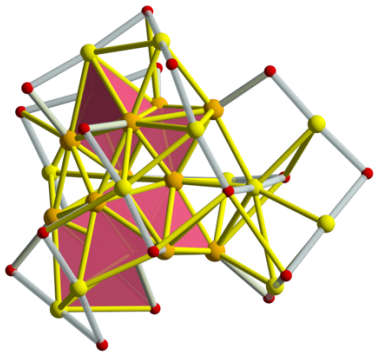
| | | |
|---|---|---|
| **1.** | **18 T** | **1 O + 5 T** |
| **2.** | **12** | **3** |
| **3.** | **1.5** | **2.0** |

**Minimum has smaller T-factor value and many compact tetrahedra in the inner core.**

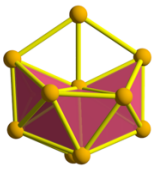
**TPSS**



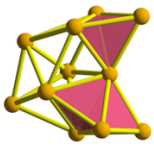
**21 T**



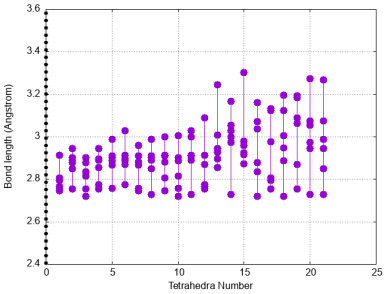
**10 T**



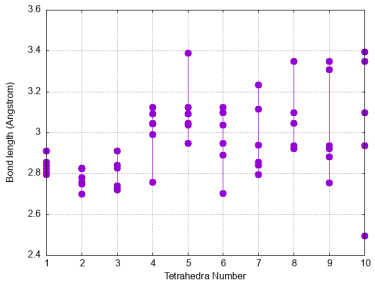
**12 T**



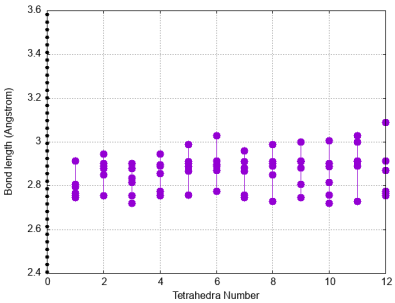
**3 T**



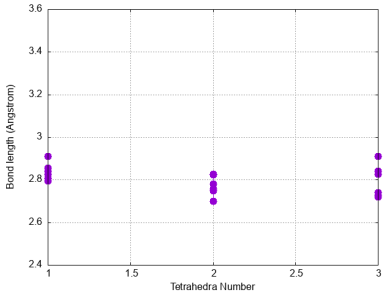

17 cT < 3.2




5 cT < 3.2




12 cT < 3.2




3 cT < 3.2

**STEPS**

**ISOMERS ENERGY ORDER**

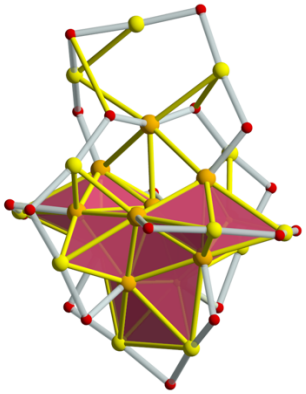
| | | |
|---|---|---|
| **1.** | **21 T** | **10 T** |
| **2.** | **12** | **3** |
| **3.** | **1.75** | **3.33** |

**Minimum has smaller T-factor value.**

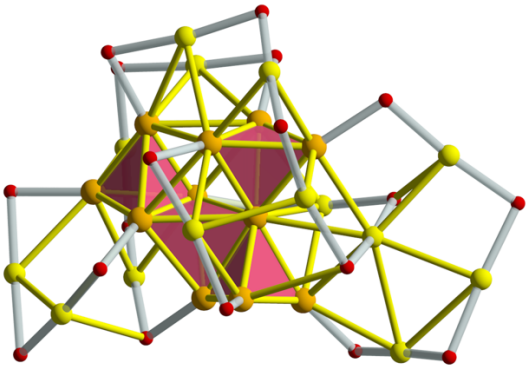
GENERAL CONCLUSION. For cationic SH-protected, the energy order is consistent with **increment** of T-factor values, independently of XC functional.

## CATIONIC $CH_3$-PROTECTED

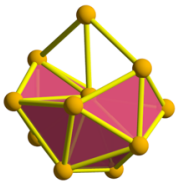
**PBE**



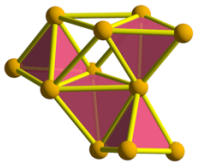
**21 T**



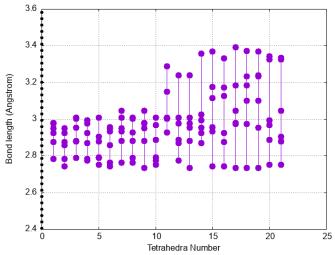
**4 T**



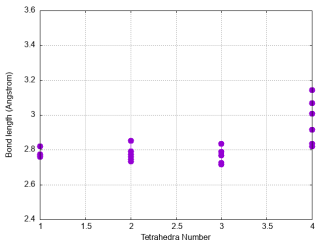
**12 T**



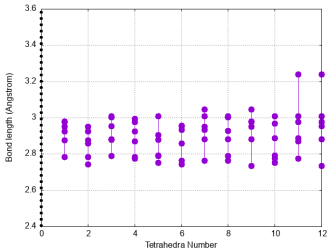
**4 T**



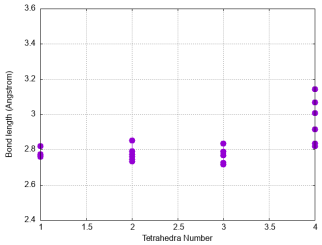

21 cT < 3.2




4 T< 3.2




10 cT < 3.2




4 T< 3.2

**STEPS**

**ISOMERS ENERGY ORDER**

| | | |
|---|---|---|
| **1.** | **21 T** | **4 T** |
| **2.** | **10** | **4** |
| **3.** | **2.1** | **1** |

**Minimum has larger T-factor value.**

GENERAL CONCLUSION. For cationic $SCH_3$-protected isomers, the energy order is consistent with **decrement** of T-factor values, with PBE XC functional.

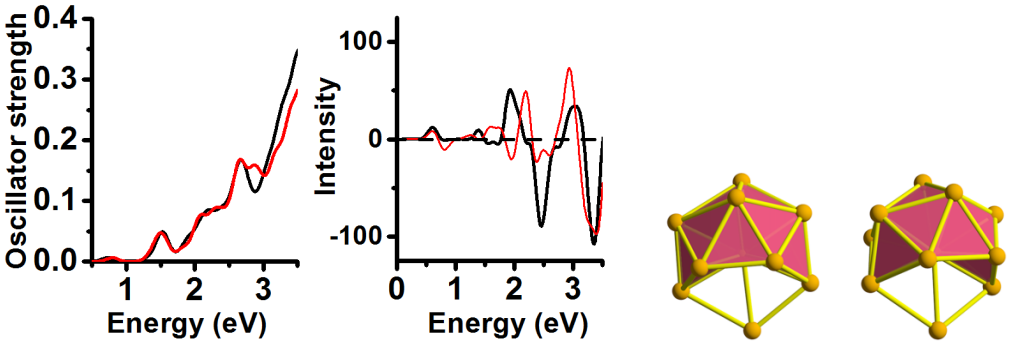



**Fig. S3.** Comparison of UV and CD spectra of **second in energy isomer** (PBE) and the **energy minimum** (TPSS optimization) of $Au_{25}(\mathbf{SCH_3})_{19}^{[0]}$ cluster. Black lines correspond with PBE calculations and red lines are lineshapes of optimized isomer with TPSS functional. UV spectra show major coincidence in position and intensity of their peaks. However, CD spectra show differences in the range from 1.0 to 2.0 eV. Three peaks included in mentioned energy range correspond with featured by enantiomers (1.55, 1.71, and 1.92 eV). Peaks located at 0.60, and 3.36 eV are common to both isomers. First inner core corresponds with $Au_{11}$ core and $C_{2v}$ symmetry, calculated with PBE functional. This comparison allows us to know about XC-**functionals effect on optical and chiroptical properties**. (2d, 1e)

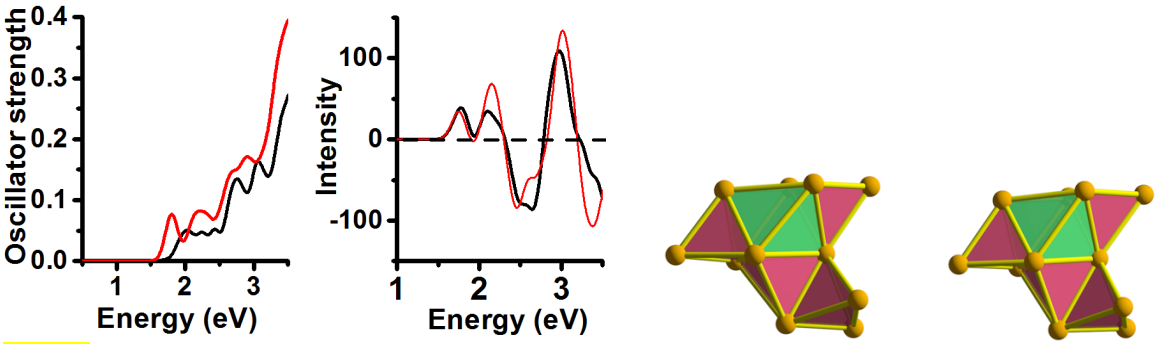



**Fig. S4.** Comparison of UV and CD spectra of a pair of $Au_{25}(SCH_3)_{19}^{[0]}$ clusters optimized with PBE and TPSS XC functionals. Black lines correspond with **PBE** calculations and red lines are lineshapes of optimized isomer with **TPSS** functional. Absorption spectra display a peak width of 0.1 eV. The isomer constituted by one $Au_{11}$ inner core and sustaining $C_s$ symmetry is found as second in energy during TPSS calculations, but it corresponds with the energy minimum during PBE calculations. Their UV spectra show differences in intensity. However, their CD spectra feature major coincidence along lineshapes. This comparison is done to get insight into **XC functionals effect on optical and chiroptical properties**. (1d, 2e)

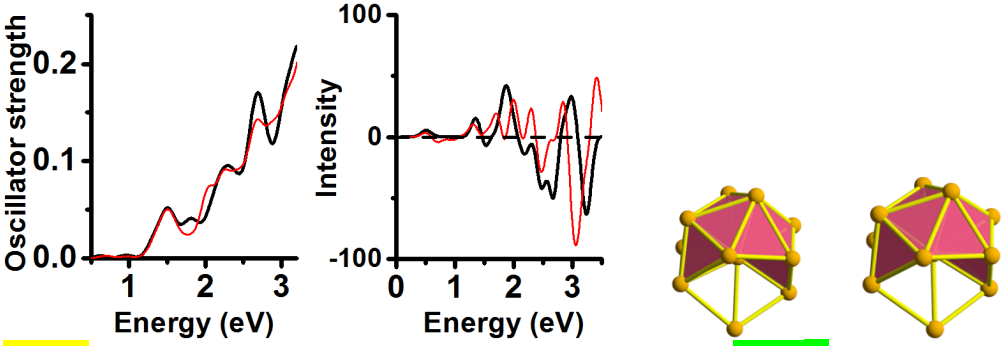



**Fig. S5.** Comparison of calculated UV and CD spectra of **anionic** isomers comprised by one $Au_{11}$ inner core ($C_{2v}$ symmetry) and protected by -$CH_3$ ligands. Anionic/**PBE** (Black line; $C_{2v}$ point group), anionic/**TPSS** (Red line; $C_{2v}$) clusters. Absorption spectra display a peak width of 0.1 eV. This comparison let us get insight into the **XC functional effect on optical and chiroptical properties**. Both isomers are constituted by 12 tetrahedra. For anionic clusters, is obtained large coincidences in their UV spectra and slightly different CD spectra. (1h, 1i)

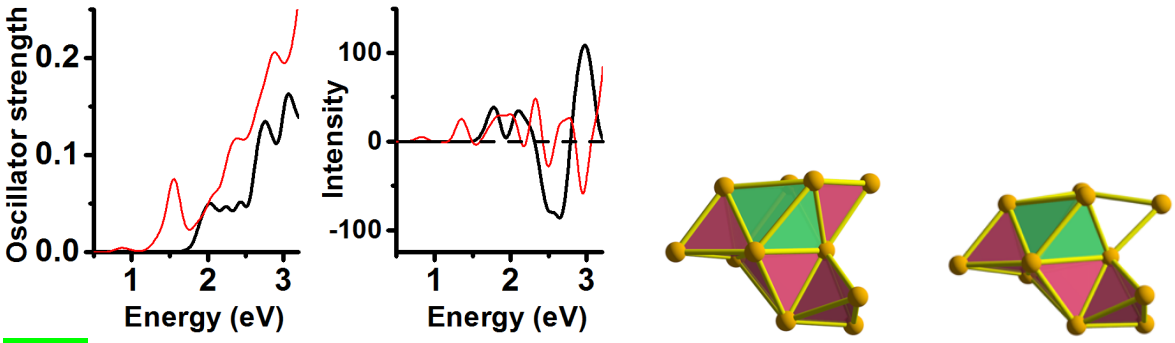



**Fig. S6.** Comparison of calculated UV and CD spectra of isomers comprised by one $Au_{11}$ inner core with 0 and 1- charge-states and protected by -$CH_3$ ligands. **Neutral/PBE** (Black line; $C_s$ point group) and **anionic/PBE** (Red line; $C_1$) clusters. Absorption spectra display a peak width of 0.1 eV. The anionic cluster displays peaks under 2.0 eV, while neutral cluster features peaks in agreement with experimental values. First inner core corresponds with neutral/PBE case. It is evident that for this kind of isomers, anionic structure shows less tetrahedra. This comparison let us get insight into **the charge-state effect on optical and chiroptical properties**. (1d, 2h)

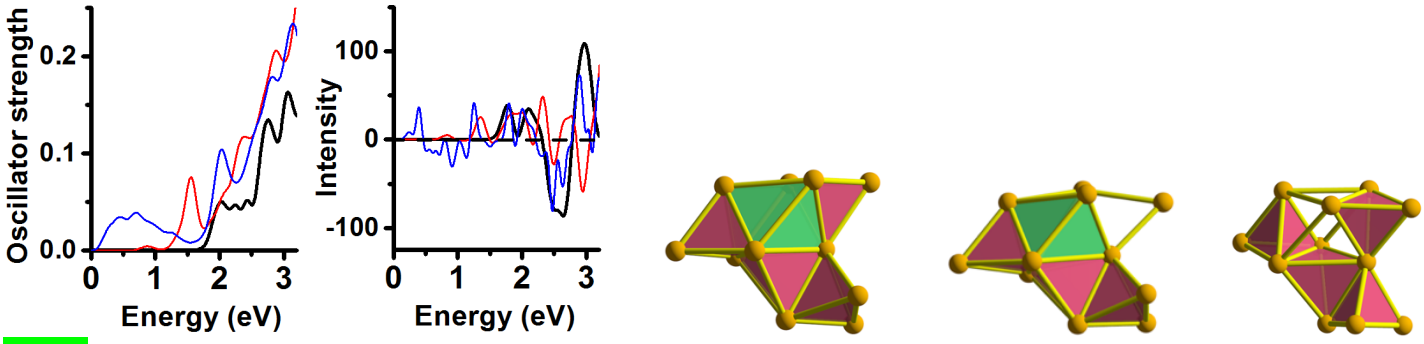



**Fig. S7.** Comparison of calculated UV and CD spectra of isomers comprised by one $Au_{11}$ inner core with 0, 1- and 1+ charge-states and protected by -$CH_3$ ligands. Neutral/PBE (Black line; $C_s$ point group), anionic/PBE (Red line; $C_1$) and cationic/PBE (Blue line; $C_1$) clusters. Absorption spectra display a peak width of 0.1 eV. The anionic cluster displays peaks under 2.0 eV, while neutral cluster features peaks in agreement with experimental values. First inner core corresponds with neutral/PBE case. This comparison let us get insight into the **charge-state effect on optical and chiroptical properties**. Inner cores displaying tetrahedra (red color) and octahedra (green color) constituting $Au_{11}$ inner cores. It is evident that cationic cluster holding one $Au_{11}$ core is more distorted and only tetrahedra are found. (1d, 2h, 8b)

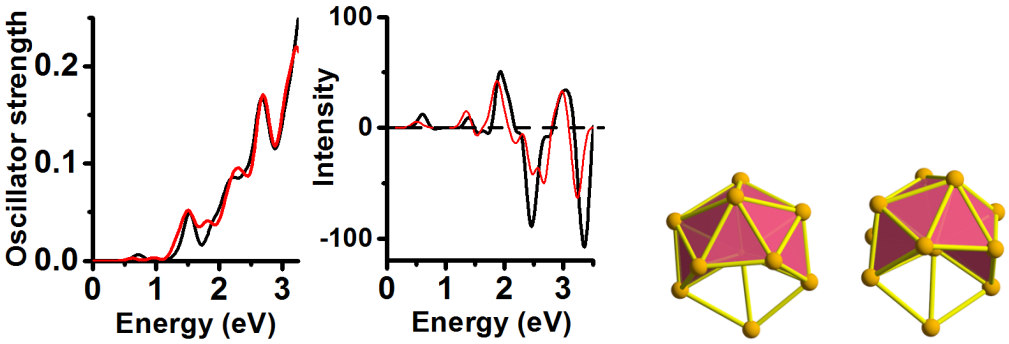



**Fig. S8.** Comparison of calculated UV and CD spectra of isomers comprised by one $Au_{11}$ inner core ($C_{2v}$ symmetry) and protected by $-CH_3$ ligands. Neutral/**PBE** (Black line; $C_{2v}$ point group), anionic/**PBE** (Red line; $C_{2v}$) clusters. Absorption spectra display a peak width of 0.1 eV. This comparison let us get insight into the **charge-state** effect **on optical and chiroptical properties**. It is evident that despite change in their charge-state, this pair of isomers show similar UV and CD spectra. Both isomers are constituted by 12 tetrahedra. (2d, 1h)

Minimum
120

| | | | |
|---|---|---|---|
| Au | -2.232520 | -0.072528 | 1.387264 |
| Au | -4.814965 | 0.304602 | -3.193674 |
| Au | 6.852988 | -2.182759 | -0.874854 |
| Au | -1.013753 | -2.538769 | 0.446681 |
| S | 6.318054 | -4.043826 | 0.413575 |
| S | 3.491736 | -0.576171 | -2.670087 |
| Au | -4.067746 | -2.722591 | -1.341525 |
| Au | -1.974519 | -0.344869 | -1.408526 |
| Au | -2.420373 | 2.821503 | -3.262582 |
| Au | 1.032987 | -1.898850 | 2.194198 |
| Au | 1.559283 | -2.786828 | -0.394403 |
| Au | 0.639331 | -0.257092 | 0.048444 |
| Au | 3.913143 | -0.926171 | -0.369221 |
| S | -0.650458 | 2.473782 | 3.512322 |
| Au | 0.202129 | 1.975890 | -1.506202 |
| Au | 0.130358 | 2.157986 | 1.277358 |
| Au | 2.563109 | 1.730315 | -0.120082 |
| S | 4.269265 | -1.057280 | 1.957029 |
| Au | -4.455841 | 0.110029 | -0.268629 |
| Au | -2.535306 | 2.100649 | -0.300644 |
| Au | 1.192461 | -0.884782 | -2.847642 |
| S | -3.121601 | 4.352781 | 0.203051 |
| Au | -0.850013 | 4.792491 | 0.026898 |
| Au | 3.526691 | 1.077313 | 2.556368 |
| S | 1.343245 | 5.475962 | -0.315876 |
| S | 3.366142 | 3.299207 | 3.266236 |
| Au | 2.278845 | 4.304516 | 1.461749 |
| S | 4.547568 | 2.913492 | -0.797397 |
| Au | 6.015154 | 1.224643 | -1.380680 |
| Au | 0.641564 | 0.600770 | 4.008964 |
| S | 1.651842 | -1.464959 | 4.433425 |
| S | 7.541934 | -0.356842 | -2.123036 |
| S | -0.143206 | 3.176504 | -3.518672 |
| S | -4.734616 | 2.626682 | -3.173168 |
| S | -5.101328 | -1.999662 | -3.301851 |
| S | -2.986517 | -3.828892 | 0.398293 |
| S | -1.034717 | -1.249295 | -3.422045 |
| S | -2.490521 | -0.756734 | 3.658769 |
| S | -6.813715 | 0.177507 | 0.020615 |
| Au | -4.127997 | -2.293341 | 3.100195 |
| Au | -6.411508 | -1.802594 | 1.164961 |
| S | -5.864584 | -3.704543 | 2.406387 |
| S | 2.231962 | -4.693334 | -1.662690 |
| Au | 4.254237 | -4.318263 | -0.597722 |
| C | -2.481762 | -5.418522 | -0.366735 |
| H | -1.809899 | -5.926556 | 0.335054 |

| | | | |
|---|---|---|---|
| H | -3.383295 | -6.021760 | -0.523589 |
| H | -1.972112 | -5.254973 | -1.321024 |
| C | -6.892854 | -2.229311 | -2.985581 |
| H | -7.439700 | -1.836455 | -3.850026 |
| H | -7.080335 | -3.303357 | -2.878720 |
| H | -7.203489 | -1.705644 | -2.076939 |
| C | 0.366286 | 2.060764 | -4.882925 |
| H | 0.111468 | 2.551044 | -5.830017 |
| H | 1.450668 | 1.919055 | -4.812244 |
| H | -0.133448 | 1.090882 | -4.816111 |
| C | -5.272228 | 3.135307 | -4.855287 |
| H | -6.343833 | 2.921833 | -4.942865 |
| H | -5.097857 | 4.213233 | -4.950777 |
| H | -4.720311 | 2.597061 | -5.629803 |
| C | -1.164462 | -3.071578 | -3.331373 |
| H | -2.223009 | -3.338867 | -3.440720 |
| H | -0.576482 | -3.497765 | -4.152200 |
| H | -0.782943 | -3.431446 | -2.370170 |
| C | 4.188193 | -1.994967 | -3.588583 |
| H | 3.939577 | -1.861380 | -4.647758 |
| H | 5.276525 | -1.980595 | -3.451498 |
| H | 3.785861 | -2.944003 | -3.222761 |
| C | 6.067543 | -0.763730 | 2.201807 |
| H | 6.219549 | -0.537055 | 3.263040 |
| H | 6.600495 | -1.683736 | 1.936156 |
| H | 6.419289 | 0.064959 | 1.578624 |
| C | 7.358175 | -5.401178 | -0.255174 |
| H | 8.394880 | -5.211126 | 0.044968 |
| H | 7.009754 | -6.339310 | 0.190687 |
| H | 7.286474 | -5.456274 | -1.344462 |
| C | 9.150478 | 0.123146 | -1.380436 |
| H | 9.881213 | -0.657334 | -1.620602 |
| H | 9.455498 | 1.071551 | -1.836136 |
| H | 9.068592 | 0.239861 | -0.296663 |
| C | 4.009410 | 3.591316 | -2.413822 |
| H | 3.186782 | 4.288379 | -2.213984 |
| H | 4.854479 | 4.118485 | -2.871282 |
| H | 3.665092 | 2.786128 | -3.070309 |
| C | 1.358478 | 7.240024 | 0.190782 |
| H | 2.399736 | 7.581412 | 0.185605 |
| H | 0.776594 | 7.806521 | -0.544924 |
| H | 0.929293 | 7.371626 | 1.187725 |
| C | 5.097713 | 3.860706 | 3.031061 |
| H | 5.136444 | 4.932961 | 3.255528 |
| H | 5.733665 | 3.309324 | 3.732049 |
| H | 5.422976 | 3.683160 | 2.001056 |
| C | -3.498614 | 4.271128 | 1.993463 |
| H | -3.506039 | 5.290065 | 2.397017 |
| H | -4.494411 | 3.823984 | 2.098318 |

| | | | |
|---|---|---|---|
| H | -2.762204 | 3.656262 | 2.522881 |
| C | -0.007028 | 4.007943 | 4.269157 |
| H | -0.350106 | 4.849912 | 3.655553 |
| H | -0.431808 | 4.080098 | 5.277428 |
| H | 1.084157 | 4.008989 | 4.320114 |
| C | -7.015975 | 1.448052 | 1.329777 |
| H | -6.836747 | 2.425777 | 0.867025 |
| H | -8.042901 | 1.397911 | 1.709622 |
| H | -6.305716 | 1.288630 | 2.145816 |
| C | -7.088114 | -3.734567 | 3.776053 |
| H | -8.036537 | -4.109897 | 3.376072 |
| H | -6.714085 | -4.419590 | 4.545731 |
| H | -7.233647 | -2.739872 | 4.204430 |
| C | -3.504699 | 0.574596 | 4.412684 |
| H | -3.882762 | 0.210744 | 5.374045 |
| H | -2.848828 | 1.440102 | 4.559960 |
| H | -4.338496 | 0.843242 | 3.757452 |
| C | 0.434581 | -2.354086 | 5.479687 |
| H | 0.692882 | -3.419273 | 5.461563 |
| H | 0.522436 | -1.968293 | 6.502078 |
| H | -0.584135 | -2.203308 | 5.110126 |
| C | 1.461454 | -6.093685 | -0.758878 |
| H | 0.422609 | -6.171589 | -1.097572 |
| H | 2.004283 | -7.011402 | -1.011304 |
| H | 1.484233 | -5.924253 | 0.320725 |

Iso2

120

| | | | |
|---|---|---|---|
| Au | -2.345625 | 0.659563 | 1.059104 |
| Au | -2.287880 | 3.414070 | 2.934211 |
| Au | 1.186010 | 4.172966 | 2.636258 |
| Au | 2.225025 | 1.707010 | 0.650556 |
| Au | 0.557972 | -1.820568 | 2.333995 |
| Au | -3.425355 | -1.950888 | 1.677331 |
| Au | -4.533595 | 0.025519 | -1.013193 |
| Au | -1.628487 | 1.366618 | -1.750599 |
| Au | 0.068963 | 1.077204 | 2.621767 |
| Au | 1.112225 | -0.565072 | 5.976839 |
| Au | 0.861338 | -4.960408 | 2.117860 |
| Au | 0.668659 | -2.691363 | -0.704261 |
| S | -3.836279 | 1.691513 | 2.680036 |
| S | -0.822248 | 5.205757 | 3.221170 |
| S | 3.290380 | 3.342069 | 2.092118 |
| S | -5.444563 | -1.301604 | 0.693083 |
| S | -3.829242 | 1.546104 | -2.646944 |
| S | -1.605965 | -2.519162 | 3.008825 |
| S | 0.515038 | 1.410724 | 4.944499 |

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|---|---|---|---|
| S | 1.566409 | -2.480174 | 7.202352 |
| S | 1.843361 | -4.615050 | 0.050693 |
| C | -5.265432 | 2.414947 | 1.791825 |
| H | -4.950822 | 2.882092 | 0.855319 |
| H | -5.961878 | 1.596672 | 1.575940 |
| C | -0.681172 | 5.468322 | 5.029352 |
| H | -1.667791 | 5.750796 | 5.413106 |
| H | -0.323815 | 4.567562 | 5.536852 |
| C | 3.779786 | 2.326913 | 3.535034 |
| H | 2.920599 | 1.788286 | 3.943545 |
| H | 4.534598 | 1.604456 | 3.195957 |
| C | -2.024914 | -1.500017 | 4.463099 |
| H | -2.973026 | -1.868619 | 4.870321 |
| H | -1.222242 | -1.617142 | 5.204594 |
| C | -6.135225 | -2.788412 | -0.111610 |
| H | -5.349759 | -3.343657 | -0.636785 |
| C | -3.706494 | 0.596016 | -4.205940 |
| H | -3.248446 | 1.253404 | -4.955727 |
| H | -3.071273 | -0.283270 | -4.068186 |
| C | -1.062217 | 1.794799 | 5.791602 |
| H | -1.728546 | 0.928519 | 5.821756 |
| H | -0.827372 | 2.122638 | 6.810542 |
| C | 3.389840 | -2.626125 | 7.307624 |
| H | 3.864047 | -2.537162 | 6.326944 |
| H | 3.748943 | -1.829909 | 7.969061 |
| C | 1.242991 | -6.027721 | -0.947485 |
| H | 1.664326 | -5.932788 | -1.954793 |
| H | 1.612088 | -6.948009 | -0.480270 |
| Au | 2.560876 | -0.390153 | -1.328439 |
| Au | 2.340601 | -3.086546 | -3.389360 |
| Au | -1.083611 | -3.953444 | -2.975299 |
| Au | -1.990207 | -1.565404 | -0.840172 |
| Au | 1.098394 | 1.964931 | -2.032119 |
| Au | 4.373107 | 2.087161 | -1.466622 |
| Au | 4.245535 | -0.333634 | 1.051235 |
| Au | 0.129952 | 0.000297 | 0.011874 |
| Au | 0.095564 | -0.946774 | -2.723984 |
| Au | -0.292325 | 1.774839 | -4.715481 |
| Au | -0.776145 | 4.327809 | -2.487207 |
| Au | -0.451231 | 2.796017 | 0.506614 |
| S | 4.074934 | -1.706963 | -2.672853 |
| S | 0.780449 | -4.611559 | -4.199429 |
| S | -3.078554 | -3.496494 | -1.864196 |
| S | 2.946689 | 3.344739 | -2.812047 |
| S | 5.867772 | 0.882952 | -0.131662 |
| S | 2.910123 | -1.941773 | 2.063643 |
| S | -0.051511 | -0.501957 | -5.058314 |
| S | -0.490889 | 4.085043 | -4.779830 |
| S | -1.195876 | 4.922816 | -0.296010 |

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|---|---|---|---|
| C | 4.980530 | -2.777096 | -1.492857 |
| H | 4.297002 | -3.214405 | -0.757534 |
| H | 5.727446 | -2.154140 | -0.986886 |
| C | 0.387866 | -4.081036 | -5.906196 |
| H | 1.295429 | -4.180839 | -6.512550 |
| H | 0.026613 | -3.047227 | -5.923548 |
| C | -4.153160 | -2.901532 | -3.224355 |
| H | -3.581128 | -2.326988 | -3.956831 |
| H | -4.932164 | -2.258128 | -2.792542 |
| C | 3.343746 | 2.810865 | -4.518177 |
| H | 4.264256 | 3.318472 | -4.828458 |
| H | 2.513097 | 3.112198 | -5.167737 |
| C | 6.558251 | 2.128043 | 1.015269 |
| H | 7.078469 | 1.603329 | 1.824197 |
| H | 5.766526 | 2.770154 | 1.418177 |
| C | 3.525217 | -2.016765 | 3.776055 |
| H | 3.053287 | -2.888048 | 4.250242 |
| H | 3.257688 | -1.111484 | 4.336962 |
| C | 1.675843 | -0.582750 | -5.670218 |
| H | 1.962811 | -1.638935 | -5.743076 |
| H | 2.351215 | -0.081792 | -4.971845 |
| C | -2.183654 | 4.361494 | -5.433904 |
| H | -2.925364 | 3.821610 | -4.837134 |
| H | -2.210307 | 4.018607 | -6.474306 |
| C | -3.023428 | 4.809036 | -0.228634 |
| H | -3.318440 | 4.892560 | 0.825757 |
| H | -3.368850 | 3.854225 | -0.637171 |
| H | -5.745144 | 3.156412 | 2.440986 |
| H | 0.030004 | 6.286493 | 5.189717 |
| H | 4.200994 | 2.987902 | 4.301393 |
| H | -2.114894 | -0.447788 | 4.171555 |
| H | -6.564395 | -3.416388 | 0.677634 |
| H | -6.920676 | -2.475235 | -0.808440 |
| H | -4.711052 | 0.298384 | -4.525691 |
| H | -1.554543 | 2.603287 | 5.231077 |
| H | 3.622442 | -3.602964 | 7.746201 |
| H | 0.150803 | -6.043040 | -1.003475 |
| H | 5.478651 | -3.570039 | -2.062166 |
| H | -0.390182 | -4.749918 | -6.290931 |
| H | -4.607486 | -3.771277 | -3.712813 |
| H | 3.485870 | 1.728034 | -4.571620 |
| H | 7.271353 | 2.737533 | 0.448276 |
| H | 4.613351 | -2.140890 | 3.740757 |
| H | 1.718906 | -0.104886 | -6.655315 |
| H | -2.387616 | 5.437281 | -5.390750 |
| H | -3.444236 | 5.640117 | -0.805589 |
| H | 1.739296 | -7.029196 | 4.602760 |
| H | 0.306698 | -7.345417 | 5.636375 |
| C | 0.648219 | -7.093604 | 4.626161 |

| | | | |
|---|---|---|---|
| H | 0.304964 | -7.857263 | 3.919464 |
| Au | 0.823383 | -3.969724 | 5.588884 |
| S | -0.133548 | -5.502541 | 4.142316 |

Iso3

120

| | | | |
|---|---|---|---|
| Au | -1.615736 | -0.190111 | 2.086721 |
| Au | -4.508687 | 1.745377 | -2.484075 |
| Au | 3.280492 | -2.840754 | 0.797634 |
| Au | -0.357314 | -2.775306 | -0.769107 |
| Au | -3.441343 | -1.846805 | -2.990722 |
| Au | -1.753620 | 0.509004 | -2.434729 |
| Au | -2.131361 | 4.100478 | -3.049846 |
| Au | 0.574630 | -2.110284 | 1.670412 |
| Au | 2.088596 | -1.410881 | -1.357237 |
| Au | -0.026128 | 0.050878 | -0.304837 |
| Au | 2.424156 | -0.049496 | 1.073484 |
| Au | 0.033113 | 2.776317 | -1.630303 |
| Au | 0.483748 | 2.492313 | 0.979171 |
| Au | 2.401084 | 1.552521 | -1.278954 |
| Au | -2.684857 | -1.184372 | -0.315391 |
| Au | -2.464199 | 1.579061 | -0.023862 |
| Au | 0.657386 | -0.705860 | -4.056888 |
| Au | -2.295653 | 4.601400 | 0.834135 |
| Au | 3.640902 | 2.877001 | 1.159958 |
| Au | 1.122468 | 5.321545 | 0.093800 |
| Au | 4.915513 | -0.694531 | -1.515747 |
| Au | 0.800444 | 0.645633 | 3.608754 |
| Au | -2.214656 | -2.060396 | 4.612917 |
| Au | -2.987269 | -3.721805 | 2.392051 |
| Au | 1.203236 | -4.946229 | 1.283517 |
| S | 3.163069 | -4.627578 | 2.506574 |
| S | 2.161809 | -2.410853 | -3.553123 |
| S | 0.781656 | 2.953818 | 3.309177 |
| S | 4.072971 | 1.007139 | 2.484821 |
| S | -3.639884 | 2.875047 | 1.585064 |
| S | -0.903709 | 6.400243 | 0.436807 |
| S | 3.375002 | 4.777120 | -0.161833 |
| S | 4.445820 | 1.366290 | -2.490028 |
| S | 0.893542 | -1.647475 | 4.047461 |
| S | 5.179253 | -2.864785 | -0.748443 |
| S | 0.052899 | 3.920439 | -3.793422 |
| S | -4.296673 | 4.067816 | -2.245323 |
| S | -5.251010 | -0.379039 | -3.077210 |
| S | -1.785876 | -3.461684 | -2.889518 |
| S | -0.957186 | 0.844708 | -4.666624 |
| S | -2.553782 | 0.210920 | 4.269141 |
| S | -4.145972 | -2.844152 | 0.601394 |
| S | -2.246231 | -4.402789 | 4.515941 |

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|---|---|---|---|
| S | -0.678308 | -5.159436 | -0.040423 |
| C | 4.342048 | -5.869379 | 1.850522 |
| C | 3.705281 | -2.000828 | -4.452978 |
| C | -0.827885 | 3.503948 | 3.979312 |
| C | 5.695735 | 0.407138 | 1.894553 |
| C | -5.364272 | 3.158056 | 1.048655 |
| C | -1.412885 | 7.104031 | -1.172689 |
| C | 4.216186 | 6.112295 | 0.777274 |
| C | 5.671703 | 2.526173 | -1.786978 |
| C | 2.646411 | -1.892270 | 4.514071 |
| C | 6.639900 | -2.908887 | 0.352804 |
| C | 0.934441 | 5.496865 | -3.497402 |
| C | -5.373146 | 4.718081 | -3.583744 |
| C | -6.353380 | -0.905447 | -1.713679 |
| C | -1.068147 | -3.605649 | -4.561133 |
| C | -2.121814 | -0.027559 | -5.776452 |
| C | -4.362105 | 0.259102 | 3.964283 |
| C | -4.351980 | -4.227388 | -0.572839 |
| C | -0.515302 | -4.984006 | 4.424185 |
| C | -0.012595 | -6.027936 | -1.512892 |
| H | 4.027453 | -6.867222 | 2.175924 |
| H | 5.329421 | -5.642921 | 2.271703 |
| H | 4.390384 | -5.831805 | 0.758031 |
| H | 3.553567 | -2.259269 | -5.507689 |
| H | 4.514419 | -2.605981 | -4.029479 |
| H | 3.951048 | -0.939681 | -4.359624 |
| H | -1.041585 | 4.497306 | 3.567503 |
| H | -0.737950 | 3.556296 | 5.070573 |
| H | -1.624785 | 2.805459 | 3.708338 |
| H | 6.463144 | 1.147259 | 2.147918 |
| H | 5.676566 | 0.229559 | 0.808976 |
| H | 5.899899 | -0.533558 | 2.419227 |
| H | -5.883818 | 2.193692 | 1.092875 |
| H | -5.402030 | 3.557373 | 0.031826 |
| H | -5.821305 | 3.863853 | 1.751981 |
| H | -0.668040 | 7.851498 | -1.468118 |
| H | -2.387752 | 7.583522 | -1.028635 |
| H | -1.500796 | 6.321221 | -1.939117 |
| H | 4.035809 | 7.059307 | 0.255557 |
| H | 5.290063 | 5.890595 | 0.787347 |
| H | 3.839664 | 6.170935 | 1.801789 |
| H | 5.370177 | 3.540418 | -2.070825 |
| H | 6.650755 | 2.283595 | -2.215482 |
| H | 5.699778 | 2.457634 | -0.693453 |
| H | 2.817646 | -2.965567 | 4.646142 |
| H | 2.815703 | -1.357814 | 5.455367 |
| H | 3.309609 | -1.501557 | 3.735170 |
| H | 7.542626 | -2.817974 | -0.262101 |
| H | 6.639161 | -3.876087 | 0.868606 |

| | | | |
|---|---|---|---|
| H | 6.611621 | -2.102681 | 1.089692 |
| H | 0.542628 | 6.261192 | -4.177516 |
| H | 1.993228 | 5.310453 | -3.713931 |
| H | 0.842825 | 5.826275 | -2.455243 |
| H | -5.196984 | 5.797522 | -3.658003 |
| H | -6.416370 | 4.529807 | -3.304120 |
| H | -5.149477 | 4.238028 | -4.539935 |
| H | -6.746182 | -1.896320 | -1.967269 |
| H | -7.176239 | -0.185338 | -1.649449 |
| H | -5.812278 | -0.955160 | -0.763791 |
| H | -1.836832 | -3.995765 | -5.238496 |
| H | -0.226910 | -4.305794 | -4.495271 |
| H | -0.684417 | -2.643707 | -4.924664 |
| H | -1.626571 | -0.203565 | -6.738050 |
| H | -2.988610 | 0.629029 | -5.916595 |
| H | -2.454913 | -0.977440 | -5.340144 |
| H | -4.590872 | 1.233873 | 3.518394 |
| H | -4.872910 | 0.154934 | 4.927958 |
| H | -4.667904 | -0.545836 | 3.289243 |
| H | -4.820405 | -3.842238 | -1.486866 |
| H | -5.000992 | -4.968198 | -0.091668 |
| H | -3.385168 | -4.676263 | -0.819916 |
| H | -0.518281 | -5.990795 | 3.993409 |
| H | -0.118650 | -5.011473 | 5.445440 |
| H | 0.095301 | -4.319465 | 3.806456 |
| H | -0.750656 | -5.911626 | -2.315895 |
| H | 0.115084 | -7.088035 | -1.267532 |
| H | 0.943641 | -5.595904 | -1.824482 |

Iso4
120

| | | | |
|---|---|---|---|
| Au | -0.428863 | -1.201169 | -3.065733 |
| Au | -1.109837 | -1.666750 | 1.987455 |
| Au | 1.430014 | -2.555692 | -1.574430 |
| Au | -1.808320 | 2.931004 | 0.171102 |
| Au | 0.858599 | 2.079365 | -0.639293 |
| Au | 4.292463 | 2.215598 | -0.502535 |
| Au | -1.167196 | 2.166721 | 4.456055 |
| Au | 2.097500 | -4.536199 | 0.418947 |
| Au | -1.355832 | 1.428340 | -2.315706 |
| Au | 2.705827 | -0.215778 | -0.931379 |
| Au | 0.604111 | -3.817092 | 3.261518 |
| Au | -3.967148 | 1.547200 | 2.261766 |
| Au | -0.475235 | 1.150187 | 1.774874 |
| Au | 4.932723 | -0.582270 | 1.155269 |
| Au | 0.962878 | 3.706030 | 2.412475 |
| Au | -1.524900 | -3.944371 | -2.348343 |
| Au | -4.028897 | 2.612626 | -2.508560 |

| | | | |
|---|---|---|---|
| Au | -3.361731 | -3.015468 | 0.493881 |
| Au | 0.611724 | -0.434312 | 3.742072 |
| Au | -2.821726 | -0.021504 | -4.682718 |
| Au | 1.468128 | 1.533756 | -3.642568 |
| Au | 1.635232 | -1.700816 | 1.366519 |
| Au | -2.855200 | 0.402792 | -0.341460 |
| Au | -0.210631 | -0.539184 | -0.456281 |
| Au | 2.470222 | 0.961991 | 1.658465 |
| S | -3.209173 | 3.080632 | 3.815311 |
| S | -0.315066 | 3.036279 | -3.852236 |
| S | 3.417562 | 0.318435 | -3.274777 |
| S | 0.304208 | -5.419080 | 1.586996 |
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| S | 0.669138 | -2.523601 | 5.177700 |
| S | -1.090030 | -1.411846 | -5.353572 |
| S | -4.778183 | 1.063387 | -4.064981 |
| S | -3.598620 | 4.280294 | -0.967545 |
| S | 3.796564 | -1.904933 | 2.671036 |
| S | 3.751433 | -3.555102 | -0.920709 |
| S | 2.552388 | 3.755119 | -0.654145 |
| S | 0.722091 | 1.281680 | 5.486944 |
| S | 0.647027 | -4.604656 | -2.811427 |
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| S | 6.192486 | 0.903118 | -0.117274 |
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| H | 3.394641 | -0.993657 | -5.298321 |
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| H | 2.418603 | -1.858769 | 6.677762 |
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| H | 4.331867 | 4.510048 | 3.490069 |
| H | 4.180065 | 3.995393 | 1.776895 |
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