# Jahn-Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations

*Jules Tshishimbi Muya[1], Arnout Ceulemans[2], Gopinadhanpillai Gopakumar[3,4] and Carol A. Parish[1*]*

*[1]Department of Chemistry, University of Richmond, Richmond, Virginia 23173, USA*

*[2]Department of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001, Belgium*

*[3]Fuel Chemistry Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamilnadu 603102, India.*

*[4]Max-Planck Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, Mülheim an der Ruhr, 45470, Germany*

**ELECTRONIC SUPPLEMENTARY INFORMATION**

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Corresponding author: Carol Parish

E-mail: cparish@richmond.edu

**Table S1.** Sample command file: Fractional occupation calculation performed for the $Si_8O_{12}(C(CH_3)_3)_8$ cation with the TURBOMOLE program

```
$uhfmo_alpha   file=alpha
$uhfmo_beta   file=beta
$uhf
$alpha shells
Sym….MOs                    Number of electron
 a1g    1-12                 ( 1 )
 a2g    1-2                  ( 1 )
 eg     1-10                 ( 1 )
 t1g    1-9                  ( 1 )
 t2g    1-19                 ( 1 )
 a1u    1                    ( 1 )
 a2u    1-10                 ( 1 )
 eu     1-7                  ( 1 )
 t1u    1-20                 ( 1 )
 t2u    1-11                 ( 1 )
$beta shells
 a1g    1-12                 ( 1 )
 a2g    1-2                  ( 1 )
 eg     1-10                 ( 1 )
 t1g    1-9                  ( 1 )
 t2g    1-18                 ( 1 )
 t2g    19                   (2/3)
 a1u    1                    ( 1 )
 a2u    1-10                 ( 1 )
 eu     1-7                  ( 1 )
 t1u    1-20                 ( 1 )
 t2u    1-11                 ( 1 )
```

**Table S2.** The total contributions (in %) of $a_{1g}$, $a_{2u}$, $e_g$ and $t_{2g}$ active modes

| Modes | V($O_h \downarrow C_{3v}$) | V($Si_8O_{12}$) | V(*tert*-but) |
|---|---|---|---|
| $A_{1g}$ | 1.55 | 6.75 | 1.30 |
| $A_{2u}$ | 17.28 | 0.77 | 18.16 |
| $E_g$ | 30.04 | 40.32 | 28.31 |
| $T_{2g}$ | 51.12 | 52.15 | 52.22 |

**Table S3.** The coefficients ($C_i^j$) of $a_{2u}$ and $a_{1g}$ active normal modes ($\vec{Q}_{\Gamma_i^j}$) in the expansion of the distortion vector $\vec{\Delta} = \sum_{i,j} C_i^j \times \vec{Q}_{\Gamma_i^j}$ for octatertbutylsilsesquioxane monocation.

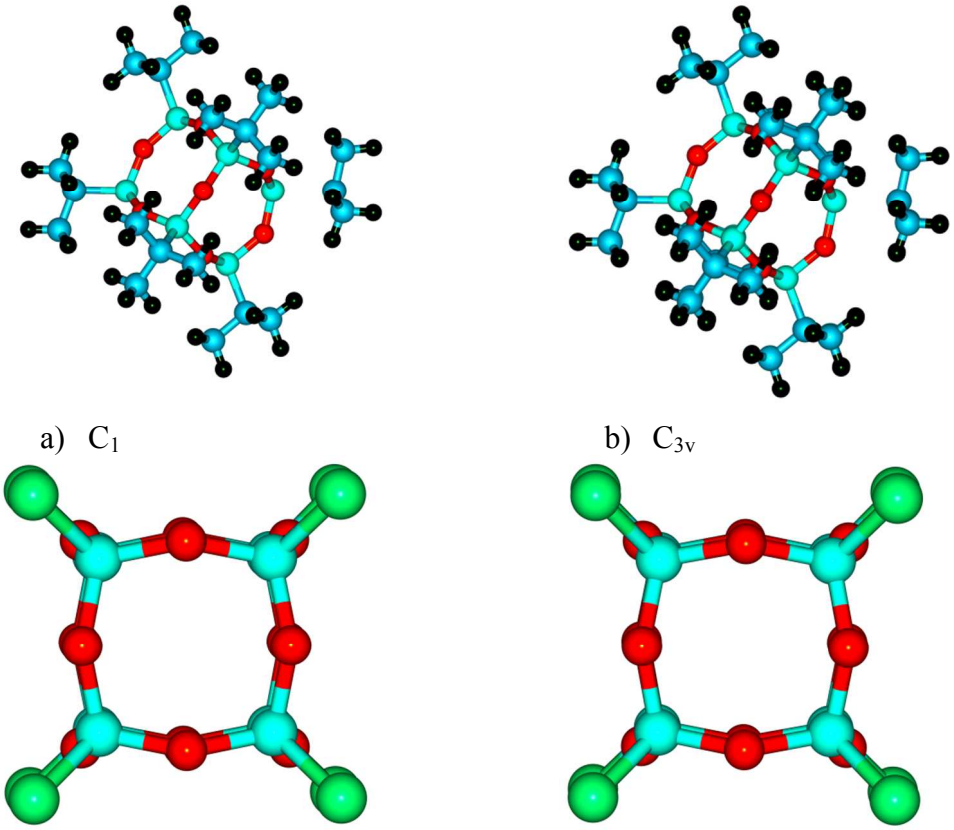
| **Modes** | V($O_h \downarrow C_{3v}$) | **V($Si_8O_{12}$)** | **V(*tert*-but)** |
|---|---|---|---|
| **$1a_{1g}$** | 0.000 | -0.006 | 0.006 |
| **$2a_{1g}$** | 0.020 | 0.020 | 0.000 |

| | | | |
|---|---|---|---|
| **$3a_{1g}$** | 0.004 | 0.005 | -0.001 |
| **$4a_{1g}$** | 0.007 | 0.014 | -0.007 |
| **$5a_{1g}$** | -0.015 | -0.004 | -0.011 |
| **$6a_{1g}$** | 0.003 | -0.002 | 0.006 |
| **$7a_{1g}$** | 0.022 | 0.000 | 0.022 |
| **$8a_{1g}$** | -0.011 | 0.000 | -0.011 |
| **$9a_{1g}$** | -0.022 | 0.000 | -0.022 |
| **$10a_{1g}$** | -0.024 | 0.000 | -0.024 |
| **$1a_{2u}$** | 0.061 | -0.003 | 0.064 |
| **$2a_{2u}$** | 0.003 | 0.005 | -0.002 |
| **$3a_{2u}$** | 0.077 | 0.004 | 0.072 |
| **$4a_{2u}$** | 0.066 | -0.001 | 0.067 |
| **$5a_{2u}$** | -0.017 | -0.005 | -0.012 |
| **$6a_{2u}$** | 0.017 | 0.001 | 0.016 |
| **$7a_{2u}$** | 0.081 | 0.000 | 0.081 |
| **$8a_{2u}$** | -0.037 | 0.000 | -0.037 |
| **$9a_{2u}$** | 0.058 | 0.000 | 0.058 |
| **$10_{2u}$** | 0.024 | 0.000 | 0.024 |

**Table S4.** Contributions of JT active vibrational normal modes (in %) to the distortion vectors, V($O_h \downarrow C_{3v}$) and that of its components V(**$Si_8O_{12}$**) and V(tert-but) in $Si_8O_{12}(C(CH_3)_3)^+$.

| **Modes** | **V($O_h \downarrow C_{3v}$)** | **V($Si_8O_{12}$)** | **V(*tert*-but)** |
|---|---|---|---|
| **$1a_{1g}$** | 0.000 | 0.345 | 0.028 |
| **$2a_{1g}$** | 0.273 | 3.915 | 0.000 |
| **$3a_{1g}$** | 0.011 | 0.233 | 0.000 |
| **$4a_{1g}$** | 0.032 | 2.000 | 0.038 |
| **$5a_{1g}$** | 0.154 | 0.206 | 0.079 |
| **$6a_{1g}$** | 0.007 | 0.051 | 0.023 |
| **$7a_{1g}$** | 0.321 | 0.000 | 0.341 |
| **$8a_{1g}$** | 0.083 | 0.000 | 0.088 |
| **$9a_{1g}$** | 0.303 | 0.000 | 0.322 |
| **$10a_{1g}$** | 0.368 | 0.000 | 0.391 |
| **$1a_{2u}$** | 2.441 | 0.096 | 2.869 |
| **$2a_{2u}$** | 0.008 | 0.268 | 0.002 |
| **$3a_{2u}$** | 3.842 | 0.171 | 3.640 |
| **$4a_{2u}$** | 2.860 | 0.010 | 3.135 |
| **$5a_{2u}$** | 0.192 | 0.217 | 0.106 |
| **$6a_{2u}$** | 0.188 | 0.012 | 0.1734 |
| **$7a_{2u}$** | 4.265 | 0.000 | 4.528 |
| **$8a_{2u}$** | 0.897 | 0.000 | 0.953 |
| **$9a_{2u}$** | 2.213 | 0.000 | 2.349 |
| **$10_{2u}$** | 0.375 | 0.000 | 0.399 |
| **$1e_g$** | 5.673 | 0.190 | 6.534 |
| **$2e_g$** | 4.299 | 1.573 | 3.456 |

| | | | |
|---|---|---|---|
| **$3e_g$** | 1.928 | 0.000 | 2.047 |
| **$4e_g$** | 0.241 | 0.000 | 0.256 |
| **$5e_g$** | 1.252 | 0.073 | 1.346 |
| **$6e_g$** | 2.778 | 37.92 | 0.068 |
| **$7e_g$** | 0.128 | 0.566 | 0.0725 |
| **$8e_g$** | 1.691 | 0.000 | 1.796 |
| **$9e_g$** | 0.084 | 0.000 | 0.0316 |
| **$10e_g$** | 1.346 | 0.000 | 1.429 |
| **$11e_g$** | 2.804 | 0.000 | 2.977 |
| **$12e_g$** | 0.213 | 0.000 | 0.296 |
| **$13e_g$** | 4.922 | 0.000 | 5.227 |
| **$14e_g$** | 1.694 | 0.000 | 1.799 |
| **$15e_g$** | 0.279 | 0.000 | 0.296 |
| **$16e_g$** | 0.707 | 0.000 | 0.751 |
| **$1t_{2g}$** | 0.382 | 0.000 | 0.405 |
| **$2t_{2g}$** | 3.952 | 8.303 | 2.012 |
| **$3t_{2g}$** | 1.807 | 0.094 | 1.828 |
| **$4t_{2g}$** | 1.390 | 2.219 | 1.902 |
| **$5t_{2g}$** | 1.511 | 0.591 | 1.503 |
| **$6t_{2g}$** | 1.029 | 0.355 | 0.905 |
| **$7t_{2g}$** | 1.274 | 7.043 | 1.903 |
| **$8t_{2g}$** | 5.563 | 2.747 | 5.205 |
| **$9t_{2g}$** | 6.814 | 5.700 | 7.123 |
| **$10t_{2g}$** | 0.344 | 0.315 | 0.417 |
| **$11t_{2g}$** | 1.404 | 0.000 | 1.491 |
| **$12t_{2g}$** | 0.148 | 0.000 | 0.157 |
| **$13t_{2g}$** | 1.472 | 24.6613 | 1.979 |
| **$14t_{2g}$** | 1.977 | 0.000 | 2.099 |
| **$15t_{2g}$** | 1.478 | 0.130 | 1.442 |
| **$16t_{2g}$** | 4.303 | 0.000 | 4.569 |
| **$17t_{2g}$** | 10.826 | 0.000 | 11.495 |
| **$18t_{2g}$** | 0.310 | 0.000 | 0.329 |
| **$19t_{2g}$** | 0.262 | 0.000 | 0.279 |
| **$20t_{2g}$** | 1.547 | 0.000 | 1.643 |
| **$21t_{2g}$** | 1.582 | 0.000 | 1.680 |
| **$22t_{2g}$** | 1.522 | 0.000 | 1.616 |
| **$23t_{2g}$** | 0.037 | 0.000 | 0.039 |
| **$24t_{2g}$** | 0.188 | 0.000 | 0.200 |
| **Sum** | **100** | **100** | **100** |
| **Norm** | **0.647** | **0.233** | **0.603** |



a) $C_1$ b) $C_{3v}$

c) $C_1$ d) $D_{4h}$

**Figure S1.** Optimized geometries of $[Si_8O_{12}(tert\text{-but})_8]^+$ in $C_1$ (a) and $C_{3v}$ (b) symmetry as well as $[Si_8O_{12}Cl_8]^+$ in $C_1$ (c) and $D_{4h}$ (d) symmetry. As shown in (a) and (b), upon symmetry lowering from $O_h$ symmetry, one of Si-C bonds elongates detaching one of the tert-butyl groups.

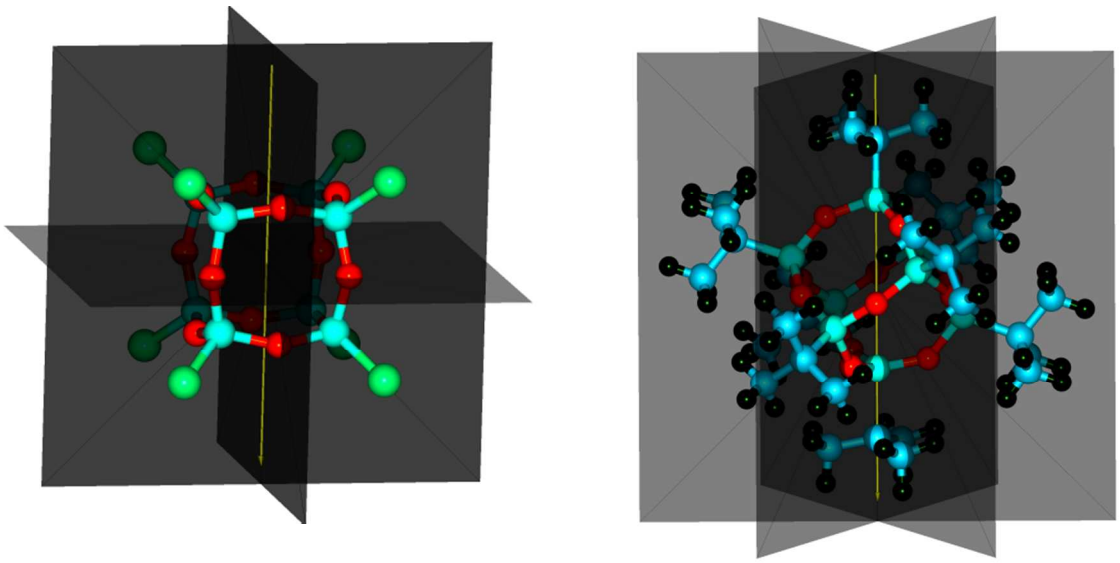
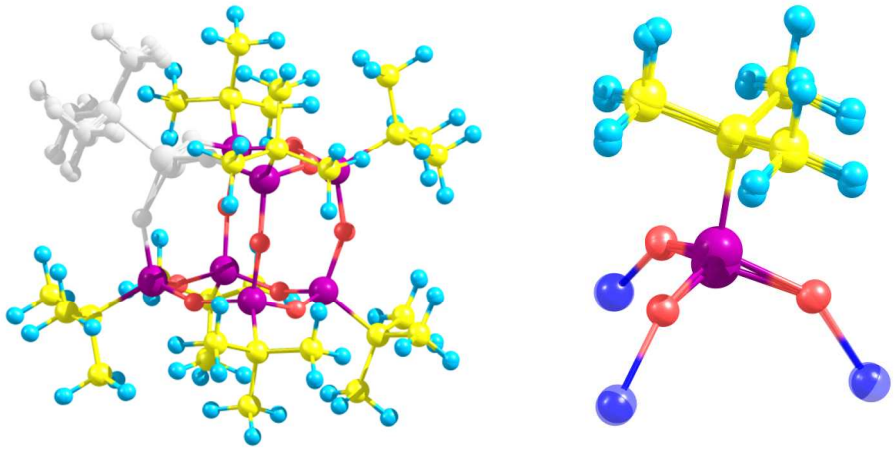
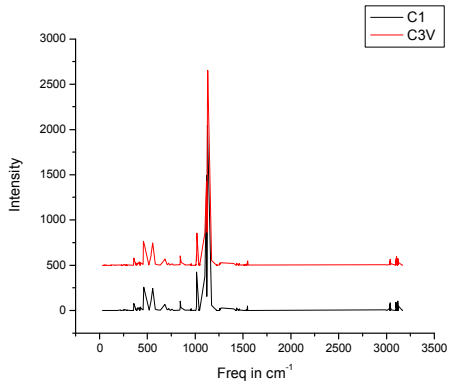


**Figure S2.** Tetragonal and trigonal axes (depicted in yellow) for $Si_8O_{12}Cl_8^+$ (left) and $Si_8O_{12}(tert\text{-}but)_8^+$ (right).

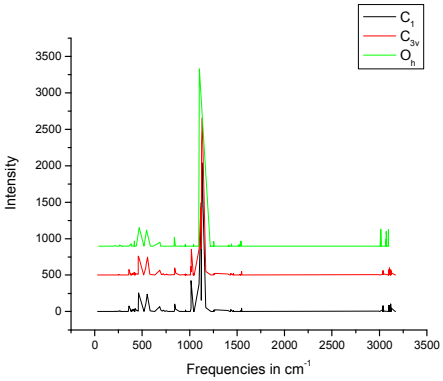


**a.** **b.**

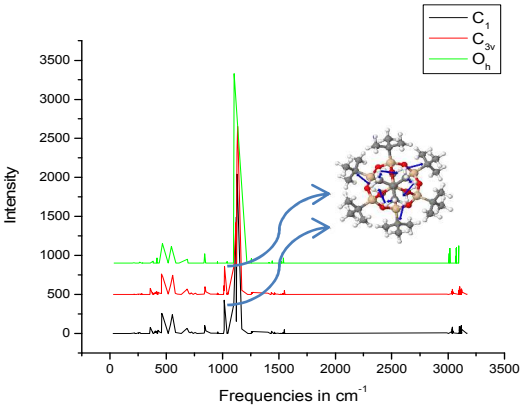
**Figure S3.** Superposition of $D_{3d}$ and $C_{3v}$ symmetric structures of $Si_8O_{12}(tert\text{-}but)_8$ (a) and the selected fragment section (b).



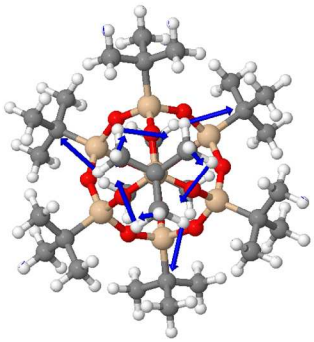

**a.**




**b.**

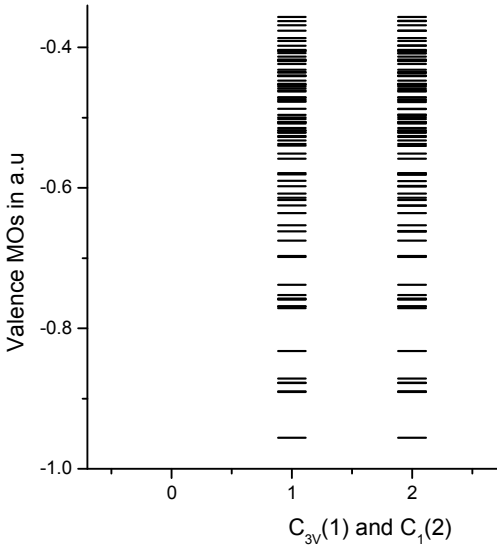



**d.**

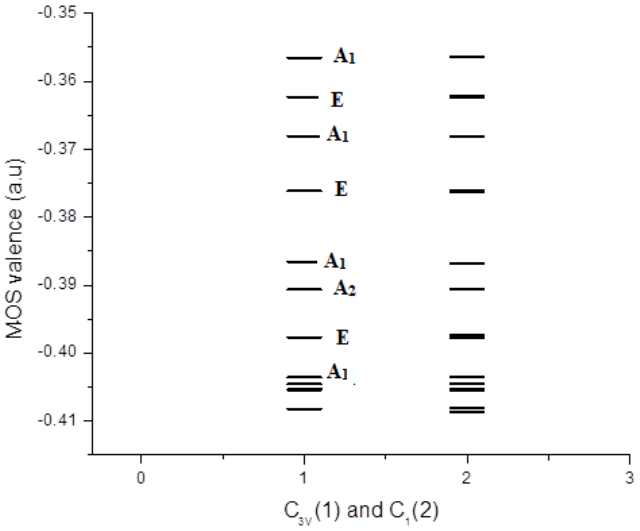


**e.** $A_1$ mode, characteristic of $Si_8O_{12}$(*tert*-but)$_8^+$ involved only the detached tert-butyl group

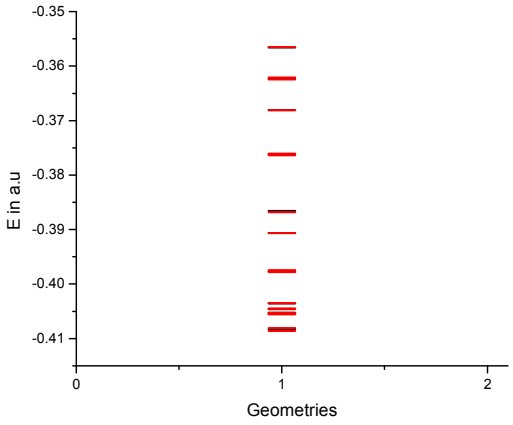
**Figure S4.** Superposition of infrared (IR) spectra for $O_h$, $C_1$ and $C_{3v}$ symmetric neutral and cationic $Si_8O_{12}$(tert-but)$_8$.




a. All valence MOs

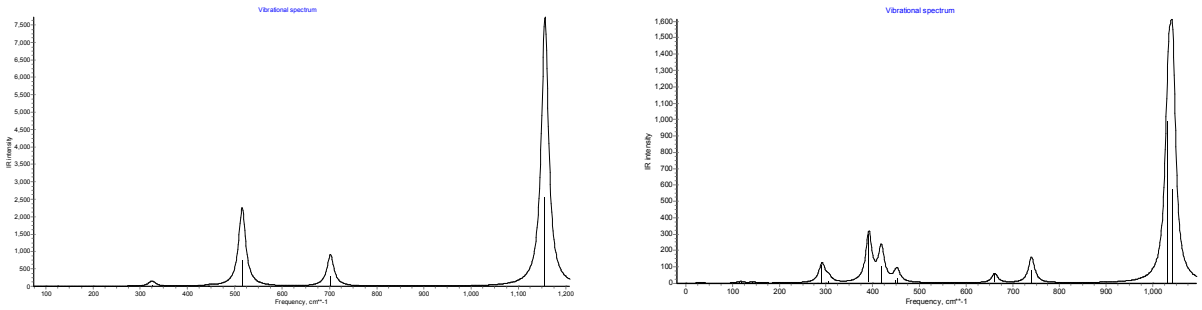



b. High-lying valence MOs




c. Superposition of high-lying MOs (red $C_1$ and black $C_{3v}$)

**Figure S5** Comparison between valence shell molecular orbitals under $C_1$ and $C_{3v}$ symmetries at ROB3LYP/6-31G(d) level.




a. neutral b. cation

**Figure S6** IR spectra for $O_h$ (a), and $D_{4h}$ (b) symmetric neutral and cationic $Si_8O_{12}(Cl)_8$.

**Steps followed in the JT vibrational analysis**

Let $\vec{R}_{HS}$ and $\vec{R}_{LS}$ be the cartesian coordinates of the high and low symmetric POSS cation (e.g $\vec{R}_{HS}$ belongs to $O_h$ symmetry for both cations studied here, whereas the $\vec{R}_{LS}$ corresponds to $C_{3v}$ and $D_{4h}$ symmetry for $Si_8O_{12}(C(CH_3)_3)_8)^+$ and $Si_8O_{12}Cl_8^+$, respectively).

The distortion vector is defined by:

$$\vec{\Delta} = \vec{R}_{HS} - \vec{R}_{LS}$$

This distortion vector is then decomposed to its components (*ie*. inorganic core and substituents):

$$\vec{\Delta} = \vec{\Delta}_{But} + \vec{\Delta}_{Si_8O_{12}}$$

The normal vectors are given by :

$$N\vec{\Delta} = \frac{\vec{\Delta}}{\sqrt{\vec{\Delta}\cdot\vec{\Delta}}},$$

$$N\vec{\Delta}_{But} = \frac{\vec{\Delta}_{But}}{\sqrt{\vec{\Delta}_{But}\cdot\vec{\Delta}_{But}}},$$

and $N\vec{\Delta}_{Si_8O_{12}} = \frac{\vec{\Delta}_{Si_8O_{12}}}{\sqrt{\vec{\Delta}\cdot\vec{\Delta}}}$

The normal distortion vector can be also expressed by:

$$\frac{\vec{\Delta}}{\sqrt{\vec{\Delta}\cdot\vec{\Delta}}} = \frac{\vec{\Delta}_{But}}{\sqrt{\vec{\Delta}\cdot\vec{\Delta}}} + \frac{\vec{\Delta}_{Si_8O_{12}}}{\sqrt{\vec{\Delta}\cdot\vec{\Delta}}},$$

The contribution of each component (butyl groups and inorganic core) for the distortion vector can be estimated as follows:

$$\%\vec{\Delta}_{But} = \frac{\vec{\Delta}_{But} \cdot \vec{\Delta}}{\vec{\Delta} \cdot \vec{\Delta}} \times 100$$

$$\%\vec{\Delta}_{But} = \frac{\vec{\Delta}_{Si_8O_{12}} \cdot \vec{\Delta}}{\vec{\Delta} \cdot \vec{\Delta}} \times 100$$

As $\vec{R}_{HS}$ is not in equilibrium with some of its nuclear displacements (normal vibrational modes, $\vec{Q}$), of representation $\Gamma \in \{A_{1g}, A_{2u}, E_g, T_{2g}\}$ for $[Si_8O_{12}(tert\text{-}But)_8]^+$and $\Gamma \in \{A_{1g}, E_g\}$ for $[Si_8O_{12}(Cl)_8]^+$, the distortion vector can be expanded in active vibrational modes. The corresponding Jahn-Teller active modes are predicted using the application of group theory to molecular systems (*ie.* the symmetrical products of the electronically degenerate orbitals expressed by $\Gamma \subset \Gamma_{\deg,el} \times \Gamma_{\deg,el}$ should contain the active modes).

Where, $\Gamma_{\deg,el} = \{^2t_{2g}, ^2e_g\}$ for $[Si_8O_{12}(tert\text{-}But)_8]^+$ and $[Si_8O_{12}(Cl)_8]^+$, respectively.

We can now express the distortion vector $\vec{\Delta}$ and its main components $\vec{\Delta}_{But}$ and $\vec{\Delta}_{Si_8O_{12}}$ as a function of high symmetry $\vec{Q}_{\Gamma_i^j}$ vibrational modes as:

$$\vec{\Delta} = \sum_{i,j} C_i^j \times \vec{Q}_{\Gamma_i^j}$$

Here, the expression $\vec{Q}_{\Gamma_k} \times \vec{Q}_{\Gamma_l} \cong \delta_{kl}$

The $C_i^j$ coefficients of different vibrational modes are evaluated by:

$C_k^j = \vec{\Delta} \times \vec{Q}_{\Gamma_k^j}$, and $C_k^\Gamma = \sqrt{\sum_\gamma \left| C_k^{\Gamma_k^\gamma} \right|^2}$

**Cartesian Coordinates for the optimized geometries of Octatert-butyl and Octachloro silsesquioxane monocations ($Si_8O_{12}Cl_8^+$ and $Si_8O_{12}(C(CH_3)_3)_8^+$) at UB3LYP/6-31G(d)**

1. **$Si_8O_{12}Cl_8^+$**

**Symmetry $D_{4h}$**

| | | | |
|---|---|---|---|
| O | -1.328273000 | -1.328273000 | 1.896817000 |
| Si | 0.000000000 | -2.229138000 | 1.577955000 |
| O | 1.328273000 | -1.328273000 | 1.896817000 |
| Si | 2.229138000 | 0.000000000 | 1.577955000 |
| O | 1.328273000 | 1.328273000 | 1.896817000 |
| Si | 0.000000000 | 2.229138000 | 1.577955000 |
| O | 0.000000000 | 2.647170000 | 0.000000000 |
| Si | 0.000000000 | 2.229138000 | -1.577955000 |
| O | -1.328273000 | 1.328273000 | -1.896817000 |
| Si | -2.229138000 | 0.000000000 | -1.577955000 |
| O | -2.647170000 | 0.000000000 | 0.000000000 |
| Si | -2.229138000 | 0.000000000 | 1.577955000 |
| O | -1.328273000 | 1.328273000 | 1.896817000 |
| O | 1.328273000 | 1.328273000 | -1.896817000 |
| Si | 2.229138000 | 0.000000000 | -1.577955000 |
| O | 1.328273000 | -1.328273000 | -1.896817000 |
| Si | 0.000000000 | -2.229138000 | -1.577955000 |
| O | -1.328273000 | -1.328273000 | -1.896817000 |
| O | 2.647170000 | 0.000000000 | 0.000000000 |
| O | 0.000000000 | -2.647170000 | 0.000000000 |
| Cl | -3.879123000 | 0.000000000 | 2.747558000 |
| Cl | 0.000000000 | -3.879123000 | -2.747558000 |
| Cl | 0.000000000 | -3.879123000 | 2.747558000 |
| Cl | 3.879123000 | 0.000000000 | 2.747558000 |
| Cl | 0.000000000 | 3.879123000 | 2.747558000 |
| Cl | 0.000000000 | 3.879123000 | -2.747558000 |
| Cl | -3.879123000 | 0.000000000 | -2.747558000 |
| Cl | 3.879123000 | 0.000000000 | -2.747558000 |

**Symmetry $O_h$ ($Si_8O_{12}Cl_8$ neutral)**

| | | | |
|---|---|---|---|
| O | -1.879684000 | 0.000000000 | 1.879684000 |
| Si | -1.575960000 | -1.575960000 | 1.575960000 |
| O | 0.000000000 | -1.879684000 | 1.879684000 |
| Si | 1.575960000 | -1.575960000 | 1.575960000 |
| O | 1.879684000 | 0.000000000 | 1.879684000 |
| Si | 1.575960000 | 1.575960000 | 1.575960000 |
| O | 1.879684000 | 1.879684000 | 0.000000000 |
| Si | 1.575960000 | 1.575960000 | -1.575960000 |
| O | 0.000000000 | 1.879684000 | -1.879684000 |

| | | | |
|---|---|---|---|
| Si | -1.575960000 | 1.575960000 | -1.575960000 |
| O | -1.879684000 | 1.879684000 | 0.000000000 |
| Si | -1.575960000 | 1.575960000 | 1.575960000 |
| O | 0.000000000 | 1.879684000 | 1.879684000 |
| O | 1.879684000 | 0.000000000 | -1.879684000 |
| Si | 1.575960000 | -1.575960000 | -1.575960000 |
| O | 0.000000000 | -1.879684000 | -1.879684000 |
| Si | -1.575960000 | -1.575960000 | -1.575960000 |
| O | -1.879684000 | 0.000000000 | -1.879684000 |
| O | 1.879684000 | -1.879684000 | 0.000000000 |
| O | -1.879684000 | -1.879684000 | 0.000000000 |
| Cl | -2.744744000 | 2.744744000 | 2.744744000 |
| Cl | -2.744744000 | -2.744744000 | -2.744744000 |
| Cl | -2.744744000 | -2.744744000 | 2.744744000 |
| Cl | 2.744744000 | -2.744744000 | 2.744744000 |
| Cl | 2.744744000 | 2.744744000 | 2.744744000 |
| Cl | 2.744744000 | 2.744744000 | -2.744744000 |
| Cl | -2.744744000 | 2.744744000 | -2.744744000 |
| Cl | 2.744744000 | -2.744744000 | -2.744744000 |

2. **$Si_8O_{12}(C(CH_3)_3)_8^+$**

**Symmetry $D_{3d}$**

| | | | |
|---|---|---|---|
| O | -2.321927000 | 1.340565000 | 0.000000000 |
| Si | -1.312151000 | 2.272174000 | 0.908498000 |
| O | 0.000000000 | 2.679127000 | 0.000000000 |
| Si | 1.312151000 | 2.272174000 | -0.908498000 |
| O | 0.781161000 | 1.351497000 | -2.193567000 |
| Si | 0.000000000 | 0.000000000 | -2.674853000 |
| O | 0.779850000 | -1.352254000 | -2.193567000 |
| Si | 1.311685000 | -2.272443000 | -0.908498000 |
| O | 0.000000000 | -2.681130000 | 0.000000000 |
| Si | -1.311685000 | -2.272443000 | 0.908498000 |
| O | -2.320192000 | -1.339564000 | 0.000000000 |
| Si | -2.623836000 | 0.000269000 | -0.908498000 |
| O | -1.561011000 | 0.000757000 | -2.193567000 |
| O | 2.320192000 | -1.339564000 | 0.000000000 |
| Si | 2.623836000 | 0.000269000 | 0.908498000 |
| O | 1.561011000 | 0.000757000 | 2.193567000 |
| Si | 0.000000000 | 0.000000000 | 2.674853000 |
| O | -0.779850000 | -1.352254000 | 2.193567000 |
| O | 2.321927000 | 1.340565000 | 0.000000000 |
| O | -0.781161000 | 1.351497000 | 2.193567000 |
| C | -4.391456000 | -0.000017000 | -1.548500000 |
| C | -5.364628000 | 0.004954000 | -0.347975000 |
| C | -4.627128000 | 1.259882000 | -2.410251000 |

| | | | |
|---|---|---|---|
| C | -4.630932000 | -1.264440000 | -2.402492000 |
| H | -5.236158000 | -0.880330000 | 0.284979000 |
| H | -5.233988000 | 0.893879000 | 0.279352000 |
| H | -6.401141000 | 0.005003000 | -0.710225000 |
| H | -3.957550000 | 1.294454000 | -3.277734000 |
| H | -5.657398000 | 1.264073000 | -2.790244000 |
| H | -4.483429000 | 2.181596000 | -1.835247000 |
| H | -5.661235000 | -1.267688000 | -2.782418000 |
| H | -3.961674000 | -1.306683000 | -3.269892000 |
| H | -4.490220000 | -2.183000000 | -1.821745000 |
| C | -2.195743000 | -3.803104000 | 1.548500000 |
| C | -3.410503000 | -3.378284000 | 2.402492000 |
| C | -2.678024000 | -4.648382000 | 0.347975000 |
| C | -1.222474000 | -4.637152000 | 2.410251000 |
| H | -3.112457000 | -2.777569000 | 3.269892000 |
| H | -4.135644000 | -2.797144000 | 1.821745000 |
| H | -3.928467000 | -4.268929000 | 2.782418000 |
| H | -1.842872000 | -4.979706000 | -0.279352000 |
| H | -3.196238000 | -5.546052000 | 0.710225000 |
| H | -3.380467000 | -4.094481000 | -0.284979000 |
| H | -1.733980000 | -5.531487000 | 2.790244000 |
| H | -0.352397000 | -4.973561000 | 1.835247000 |
| H | -0.857744000 | -4.074566000 | 3.277734000 |
| C | 0.000000000 | 0.000000000 | 4.646740000 |
| C | -1.470377000 | -0.010624000 | 5.076231000 |
| C | 0.744390000 | -1.268072000 | 5.076231000 |
| C | 0.725988000 | 1.278696000 | 5.076231000 |
| H | -2.011164000 | 0.874213000 | 4.727228000 |
| H | -1.997031000 | -0.905267000 | 4.730746000 |
| H | -1.511673000 | -0.008528000 | 6.177243000 |
| H | 1.782500000 | -1.276846000 | 4.730746000 |
| H | 0.763222000 | -1.304884000 | 6.177243000 |
| H | 0.248491000 | -2.178825000 | 4.727228000 |
| H | 0.748451000 | 1.313412000 | 6.177243000 |
| H | 1.762672000 | 1.304613000 | 4.727228000 |
| H | 0.214531000 | 2.182113000 | 4.730746000 |
| C | -2.195714000 | 3.803121000 | 1.548500000 |
| C | -2.686605000 | 4.643427000 | 0.347975000 |
| C | -3.404654000 | 3.377269000 | 2.410251000 |
| C | -1.220428000 | 4.642725000 | 2.402492000 |
| H | -1.855691000 | 4.974811000 | -0.284979000 |
| H | -3.391116000 | 4.085827000 | -0.279352000 |
| H | -3.204903000 | 5.541049000 | 0.710225000 |
| H | -3.099805000 | 2.780111000 | 3.277734000 |
| H | -3.923418000 | 4.267414000 | 2.790244000 |
| H | -4.131032000 | 2.791965000 | 1.835247000 |

| | | | |
|---|---|---|---|
| H | -1.732767000 | 5.536617000 | 2.782418000 |
| H | -0.849216000 | 4.084252000 | 3.269892000 |
| H | -0.354576000 | 4.980145000 | 1.821745000 |
| C | 2.195714000 | 3.803121000 | -1.548500000 |
| C | 1.220428000 | 4.642725000 | -2.402492000 |
| C | 2.686605000 | 4.643427000 | -0.347975000 |
| C | 3.404654000 | 3.377269000 | -2.410251000 |
| H | 0.849216000 | 4.084252000 | -3.269892000 |
| H | 0.354576000 | 4.980145000 | -1.821745000 |
| H | 1.732767000 | 5.536617000 | -2.782418000 |
| H | 3.391116000 | 4.085827000 | 0.279352000 |
| H | 3.204903000 | 5.541049000 | -0.710225000 |
| H | 1.855691000 | 4.974811000 | 0.284979000 |
| H | 3.923418000 | 4.267414000 | -2.790244000 |
| H | 4.131032000 | 2.791965000 | -1.835247000 |
| H | 3.099805000 | 2.780111000 | -3.277734000 |
| C | 0.000000000 | 0.000000000 | -4.646740000 |
| C | -0.744390000 | -1.268072000 | -5.076231000 |
| C | -0.725988000 | 1.278696000 | -5.076231000 |
| C | 1.470377000 | -0.010624000 | -5.076231000 |
| H | -0.248491000 | -2.178825000 | -4.727228000 |
| H | -1.782500000 | -1.276846000 | -4.730746000 |
| H | -0.763222000 | -1.304884000 | -6.177243000 |
| H | -0.214531000 | 2.182113000 | -4.730746000 |
| H | -0.748451000 | 1.313412000 | -6.177243000 |
| H | -1.762672000 | 1.304613000 | -4.727228000 |
| H | 1.511673000 | -0.008528000 | -6.177243000 |
| H | 2.011164000 | 0.874213000 | -4.727228000 |
| H | 1.997031000 | -0.905267000 | -4.730746000 |
| C | 2.195743000 | -3.803104000 | -1.548500000 |
| C | 2.678024000 | -4.648382000 | -0.347975000 |
| C | 1.222474000 | -4.637152000 | -2.410251000 |
| C | 3.410503000 | -3.378284000 | -2.402492000 |
| H | 3.380467000 | -4.094481000 | 0.284979000 |
| H | 1.842872000 | -4.979706000 | 0.279352000 |
| H | 3.196238000 | -5.546052000 | -0.710225000 |
| H | 0.857744000 | -4.074566000 | -3.277734000 |
| H | 1.733980000 | -5.531487000 | -2.790244000 |
| H | 0.352397000 | -4.973561000 | -1.835247000 |
| H | 3.928467000 | -4.268929000 | -2.782418000 |
| H | 3.112457000 | -2.777569000 | -3.269892000 |
| H | 4.135644000 | -2.797144000 | -1.821745000 |
| C | 4.391456000 | -0.000017000 | 1.548500000 |
| C | 4.630932000 | -1.264440000 | 2.402492000 |
| C | 5.364628000 | 0.004954000 | 0.347975000 |
| C | 4.627128000 | 1.259882000 | 2.410251000 |

| | | | |
|---|---|---|---|
| H | 3.961674000 | -1.306683000 | 3.269892000 |
| H | 4.490220000 | -2.183000000 | 1.821745000 |
| H | 5.661235000 | -1.267688000 | 2.782418000 |
| H | 5.233988000 | 0.893879000 | -0.279352000 |
| H | 6.401141000 | 0.005003000 | 0.710225000 |
| H | 5.236158000 | -0.880330000 | -0.284979000 |
| H | 5.657398000 | 1.264073000 | 2.790244000 |
| H | 4.483429000 | 2.181596000 | 1.835247000 |
| H | 3.957550000 | 1.294454000 | 3.277734000 |

**Symmetry $D_{4h}$**

| | | | |
|---|---|---|---|
| O | -1.903571000 | 0.000000000 | 1.903571000 |
| Si | -1.587761000 | -1.587761000 | 1.587761000 |
| O | 0.000000000 | -1.903571000 | 1.903571000 |
| Si | 1.587761000 | -1.587761000 | 1.587761000 |
| O | 1.903571000 | 0.000000000 | 1.903571000 |
| Si | 1.587761000 | 1.587761000 | 1.587761000 |
| O | 1.903571000 | 1.903571000 | 0.000000000 |
| Si | 1.587761000 | 1.587761000 | -1.587761000 |
| O | 0.000000000 | 1.903571000 | -1.903571000 |
| Si | -1.587761000 | 1.587761000 | -1.587761000 |
| O | -1.903571000 | 1.903571000 | 0.000000000 |
| Si | -1.587761000 | 1.587761000 | 1.587761000 |
| O | 0.000000000 | 1.903571000 | 1.903571000 |
| O | 1.903571000 | 0.000000000 | -1.903571000 |
| Si | 1.587761000 | -1.587761000 | -1.587761000 |
| O | 0.000000000 | -1.903571000 | -1.903571000 |
| Si | -1.587761000 | -1.587761000 | -1.587761000 |
| O | -1.903571000 | 0.000000000 | -1.903571000 |
| O | 1.903571000 | -1.903571000 | 0.000000000 |
| O | -1.903571000 | -1.903571000 | 0.000000000 |
| C | -2.684784000 | 2.684784000 | 2.684784000 |
| C | -4.160930000 | 2.371331000 | 2.371331000 |
| C | -2.371331000 | 2.371331000 | 4.160930000 |
| C | -2.371331000 | 4.160930000 | 2.371331000 |
| H | -4.412703000 | 2.581364000 | 1.326046000 |
| H | -4.412703000 | 1.326046000 | 2.581364000 |
| H | -4.809532000 | 2.998930000 | 2.998930000 |
| H | -1.326046000 | 2.581364000 | 4.412703000 |
| H | -2.998930000 | 2.998930000 | 4.809532000 |
| H | -2.581364000 | 1.326046000 | 4.412703000 |
| H | -2.998930000 | 4.809532000 | 2.998930000 |
| H | -1.326046000 | 4.412703000 | 2.581364000 |
| H | -2.581364000 | 4.412703000 | 1.326046000 |
| C | -2.684784000 | 2.684784000 | -2.684784000 |
| C | -4.160930000 | 2.371331000 | -2.371331000 |

| | | | |
|---|---|---|---|
| C | -2.371331000 | 4.160930000 | -2.371331000 |
| C | -2.371331000 | 2.371331000 | -4.160930000 |
| H | -4.412703000 | 1.326046000 | -2.581364000 |
| H | -4.412703000 | 2.581364000 | -1.326046000 |
| H | -4.809532000 | 2.998930000 | -2.998930000 |
| H | -1.326046000 | 4.412703000 | -2.581364000 |
| H | -2.998930000 | 4.809532000 | -2.998930000 |
| H | -2.581364000 | 4.412703000 | -1.326046000 |
| H | -2.998930000 | 2.998930000 | -4.809532000 |
| H | -1.326046000 | 2.581364000 | -4.412703000 |
| H | -2.581364000 | 1.326046000 | -4.412703000 |
| C | -2.684784000 | -2.684784000 | -2.684784000 |
| C | -4.160930000 | -2.371331000 | -2.371331000 |
| C | -2.371331000 | -2.371331000 | -4.160930000 |
| C | -2.371331000 | -4.160930000 | -2.371331000 |
| H | -4.412703000 | -2.581364000 | -1.326046000 |
| H | -4.412703000 | -1.326046000 | -2.581364000 |
| H | -4.809532000 | -2.998930000 | -2.998930000 |
| H | -1.326046000 | -2.581364000 | -4.412703000 |
| H | -2.998930000 | -2.998930000 | -4.809532000 |
| H | -2.581364000 | -1.326046000 | -4.412703000 |
| H | -2.998930000 | -4.809532000 | -2.998930000 |
| H | -1.326046000 | -4.412703000 | -2.581364000 |
| H | -2.581364000 | -4.412703000 | -1.326046000 |
| C | -2.684784000 | -2.684784000 | 2.684784000 |
| C | -2.371331000 | -2.371331000 | 4.160930000 |
| C | -4.160930000 | -2.371331000 | 2.371331000 |
| C | -2.371331000 | -4.160930000 | 2.371331000 |
| H | -1.326046000 | -2.581364000 | 4.412703000 |
| H | -2.581364000 | -1.326046000 | 4.412703000 |
| H | -2.998930000 | -2.998930000 | 4.809532000 |
| H | -4.412703000 | -2.581364000 | 1.326046000 |
| H | -4.809532000 | -2.998930000 | 2.998930000 |
| H | -4.412703000 | -1.326046000 | 2.581364000 |
| H | -2.998930000 | -4.809532000 | 2.998930000 |
| H | -2.581364000 | -4.412703000 | 1.326046000 |
| H | -1.326046000 | -4.412703000 | 2.581364000 |
| C | 2.684784000 | -2.684784000 | 2.684784000 |
| C | 2.371331000 | -2.371331000 | 4.160930000 |
| C | 2.371331000 | -4.160930000 | 2.371331000 |
| C | 4.160930000 | -2.371331000 | 2.371331000 |
| H | 2.581364000 | -1.326046000 | 4.412703000 |
| H | 1.326046000 | -2.581364000 | 4.412703000 |
| H | 2.998930000 | -2.998930000 | 4.809532000 |
| H | 2.581364000 | -4.412703000 | 1.326046000 |
| H | 2.998930000 | -4.809532000 | 2.998930000 |

| | | | |
|---|---|---|---|
| H | 1.326046000 | -4.412703000 | 2.581364000 |
| H | 4.809532000 | -2.998930000 | 2.998930000 |
| H | 4.412703000 | -2.581364000 | 1.326046000 |
| H | 4.412703000 | -1.326046000 | 2.581364000 |
| C | 2.684784000 | 2.684784000 | 2.684784000 |
| C | 2.371331000 | 4.160930000 | 2.371331000 |
| C | 2.371331000 | 2.371331000 | 4.160930000 |
| C | 4.160930000 | 2.371331000 | 2.371331000 |
| H | 2.581364000 | 4.412703000 | 1.326046000 |
| H | 1.326046000 | 4.412703000 | 2.581364000 |
| H | 2.998930000 | 4.809532000 | 2.998930000 |
| H | 2.581364000 | 1.326046000 | 4.412703000 |
| H | 2.998930000 | 2.998930000 | 4.809532000 |
| H | 1.326046000 | 2.581364000 | 4.412703000 |
| H | 4.809532000 | 2.998930000 | 2.998930000 |
| H | 4.412703000 | 1.326046000 | 2.581364000 |
| H | 4.412703000 | 2.581364000 | 1.326046000 |
| C | 2.684784000 | 2.684784000 | -2.684784000 |
| C | 2.371331000 | 2.371331000 | -4.160930000 |
| C | 2.371331000 | 4.160930000 | -2.371331000 |
| C | 4.160930000 | 2.371331000 | -2.371331000 |
| H | 2.581364000 | 1.326046000 | -4.412703000 |
| H | 1.326046000 | 2.581364000 | -4.412703000 |
| H | 2.998930000 | 2.998930000 | -4.809532000 |
| H | 2.581364000 | 4.412703000 | -1.326046000 |
| H | 2.998930000 | 4.809532000 | -2.998930000 |
| H | 1.326046000 | 4.412703000 | -2.581364000 |
| H | 4.809532000 | 2.998930000 | -2.998930000 |
| H | 4.412703000 | 2.581364000 | -1.326046000 |
| H | 4.412703000 | 1.326046000 | -2.581364000 |
| C | 2.684784000 | -2.684784000 | -2.684784000 |
| C | 2.371331000 | -2.371331000 | -4.160930000 |
| C | 4.160930000 | -2.371331000 | -2.371331000 |
| C | 2.371331000 | -4.160930000 | -2.371331000 |
| H | 1.326046000 | -2.581364000 | -4.412703000 |
| H | 2.581364000 | -1.326046000 | -4.412703000 |
| H | 2.998930000 | -2.998930000 | -4.809532000 |
| H | 4.412703000 | -2.581364000 | -1.326046000 |
| H | 4.809532000 | -2.998930000 | -2.998930000 |
| H | 4.412703000 | -1.326046000 | -2.581364000 |
| H | 2.998930000 | -4.809532000 | -2.998930000 |
| H | 2.581364000 | -4.412703000 | -1.326046000 |
| H | 1.326046000 | -4.412703000 | -2.581364000 |

**Symmetry $D_{2h}$**

| | | | |
|---|---|---|---|
| O | 0.000000000 | 2.686923000 | 0.000000000 |

| | | | |
|---|---|---|---|
| Si | 0.000000000 | 2.244311000 | 1.588722000 |
| O | 1.346168000 | 1.346168000 | 1.907671000 |
| Si | 2.244311000 | 0.000000000 | 1.588722000 |
| O | 2.686923000 | 0.000000000 | 0.000000000 |
| Si | 2.244311000 | 0.000000000 | -1.588722000 |
| O | 1.346168000 | -1.346168000 | -1.907671000 |
| Si | 0.000000000 | -2.244311000 | -1.588722000 |
| O | -1.346168000 | -1.346168000 | -1.907671000 |
| Si | -2.244311000 | 0.000000000 | -1.588722000 |
| O | -1.346168000 | 1.346168000 | -1.907671000 |
| Si | 0.000000000 | 2.244311000 | -1.588722000 |
| O | 1.346168000 | 1.346168000 | -1.907671000 |
| O | 0.000000000 | -2.686923000 | 0.000000000 |
| Si | 0.000000000 | -2.244311000 | 1.588722000 |
| O | -1.346168000 | -1.346168000 | 1.907671000 |
| Si | -2.244311000 | 0.000000000 | 1.588722000 |
| O | -2.686923000 | 0.000000000 | 0.000000000 |
| O | 1.346168000 | -1.346168000 | 1.907671000 |
| O | -1.346168000 | 1.346168000 | 1.907671000 |
| C | 0.000000000 | 3.796775000 | -2.683963000 |
| C | -1.265573000 | 4.617727000 | -2.369223000 |
| C | 1.265573000 | 4.617727000 | -2.369223000 |
| C | 0.000000000 | 3.352293000 | -4.159608000 |
| H | -2.182145000 | 4.056035000 | -2.579788000 |
| H | -1.294936000 | 4.942497000 | -1.323324000 |
| H | -1.282084000 | 5.521297000 | -2.995171000 |
| H | 2.182145000 | 4.056035000 | -2.579788000 |
| H | 1.282084000 | 5.521297000 | -2.995171000 |
| H | 1.294936000 | 4.942497000 | -1.323324000 |
| H | 0.000000000 | 4.238457000 | -4.810067000 |
| H | 0.887508000 | 2.760921000 | -4.409709000 |
| H | -0.887508000 | 2.760921000 | -4.409709000 |
| C | -3.796775000 | 0.000000000 | -2.683963000 |
| C | -4.617727000 | 1.265573000 | -2.369223000 |
| C | -3.352293000 | 0.000000000 | -4.159608000 |
| C | -4.617727000 | -1.265573000 | -2.369223000 |
| H | -4.942497000 | 1.294936000 | -1.323324000 |
| H | -4.056035000 | 2.182145000 | -2.579788000 |
| H | -5.521297000 | 1.282084000 | -2.995171000 |
| H | -2.760921000 | -0.887508000 | -4.409709000 |
| H | -4.238457000 | 0.000000000 | -4.810067000 |
| H | -2.760921000 | 0.887508000 | -4.409709000 |
| H | -5.521297000 | -1.282084000 | -2.995171000 |
| H | -4.056035000 | -2.182145000 | -2.579788000 |
| H | -4.942497000 | -1.294936000 | -1.323324000 |
| C | -3.796775000 | 0.000000000 | 2.683963000 |

| | | | |
|---|---|---|---|
| C | -4.617727000 | 1.265573000 | 2.369223000 |
| C | -4.617727000 | -1.265573000 | 2.369223000 |
| C | -3.352293000 | 0.000000000 | 4.159608000 |
| H | -4.056035000 | 2.182145000 | 2.579788000 |
| H | -4.942497000 | 1.294936000 | 1.323324000 |
| H | -5.521297000 | 1.282084000 | 2.995171000 |
| H | -4.056035000 | -2.182145000 | 2.579788000 |
| H | -5.521297000 | -1.282084000 | 2.995171000 |
| H | -4.942497000 | -1.294936000 | 1.323324000 |
| H | -4.238457000 | 0.000000000 | 4.810067000 |
| H | -2.760921000 | -0.887508000 | 4.409709000 |
| H | -2.760921000 | 0.887508000 | 4.409709000 |
| C | 0.000000000 | 3.796775000 | 2.683963000 |
| C | 1.265573000 | 4.617727000 | 2.369223000 |
| C | -1.265573000 | 4.617727000 | 2.369223000 |
| C | 0.000000000 | 3.352293000 | 4.159608000 |
| H | 2.182145000 | 4.056035000 | 2.579788000 |
| H | 1.294936000 | 4.942497000 | 1.323324000 |
| H | 1.282084000 | 5.521297000 | 2.995171000 |
| H | -2.182145000 | 4.056035000 | 2.579788000 |
| H | -1.282084000 | 5.521297000 | 2.995171000 |
| H | -1.294936000 | 4.942497000 | 1.323324000 |
| H | 0.000000000 | 4.238457000 | 4.810067000 |
| H | -0.887508000 | 2.760921000 | 4.409709000 |
| H | 0.887508000 | 2.760921000 | 4.409709000 |
| C | 3.796775000 | 0.000000000 | 2.683963000 |
| C | 4.617727000 | 1.265573000 | 2.369223000 |
| C | 3.352293000 | 0.000000000 | 4.159608000 |
| C | 4.617727000 | -1.265573000 | 2.369223000 |
| H | 4.942497000 | 1.294936000 | 1.323324000 |
| H | 4.056035000 | 2.182145000 | 2.579788000 |
| H | 5.521297000 | 1.282084000 | 2.995171000 |
| H | 2.760921000 | -0.887508000 | 4.409709000 |
| H | 4.238457000 | 0.000000000 | 4.810067000 |
| H | 2.760921000 | 0.887508000 | 4.409709000 |
| H | 5.521297000 | -1.282084000 | 2.995171000 |
| H | 4.056035000 | -2.182145000 | 2.579788000 |
| H | 4.942497000 | -1.294936000 | 1.323324000 |
| C | 3.796775000 | 0.000000000 | -2.683963000 |
| C | 3.352293000 | 0.000000000 | -4.159608000 |
| C | 4.617727000 | 1.265573000 | -2.369223000 |
| C | 4.617727000 | -1.265573000 | -2.369223000 |
| H | 2.760921000 | -0.887508000 | -4.409709000 |
| H | 2.760921000 | 0.887508000 | -4.409709000 |
| H | 4.238457000 | 0.000000000 | -4.810067000 |
| H | 4.942497000 | 1.294936000 | -1.323324000 |

| | | | |
|---|---|---|---|
| H | 5.521297000 | 1.282084000 | -2.995171000 |
| H | 4.056035000 | 2.182145000 | -2.579788000 |
| H | 5.521297000 | -1.282084000 | -2.995171000 |
| H | 4.942497000 | -1.294936000 | -1.323324000 |
| H | 4.056035000 | -2.182145000 | -2.579788000 |
| C | 0.000000000 | -3.796775000 | -2.683963000 |
| C | -1.265573000 | -4.617727000 | -2.369223000 |
| C | 0.000000000 | -3.352293000 | -4.159608000 |
| C | 1.265573000 | -4.617727000 | -2.369223000 |
| H | -1.294936000 | -4.942497000 | -1.323324000 |
| H | -2.182145000 | -4.056035000 | -2.579788000 |
| H | -1.282084000 | -5.521297000 | -2.995171000 |
| H | 0.887508000 | -2.760921000 | -4.409709000 |
| H | 0.000000000 | -4.238457000 | -4.810067000 |
| H | -0.887508000 | -2.760921000 | -4.409709000 |
| H | 1.282084000 | -5.521297000 | -2.995171000 |
| H | 2.182145000 | -4.056035000 | -2.579788000 |
| H | 1.294936000 | -4.942497000 | -1.323324000 |
| C | 0.000000000 | -3.796775000 | 2.683963000 |
| C | -1.265573000 | -4.617727000 | 2.369223000 |
| C | 1.265573000 | -4.617727000 | 2.369223000 |
| C | 0.000000000 | -3.352293000 | 4.159608000 |
| H | -2.182145000 | -4.056035000 | 2.579788000 |
| H | -1.294936000 | -4.942497000 | 1.323324000 |
| H | -1.282084000 | -5.521297000 | 2.995171000 |
| H | 2.182145000 | -4.056035000 | 2.579788000 |
| H | 1.282084000 | -5.521297000 | 2.995171000 |
| H | 1.294936000 | -4.942497000 | 1.323324000 |
| H | 0.000000000 | -4.238457000 | 4.810067000 |
| H | 0.887508000 | -2.760921000 | 4.409709000 |
| H | -0.887508000 | -2.760921000 | 4.409709000 |

**Symmetry $C_{3v}$**

| | | | |
|---|---|---|---|
| O | 2.252084000 | 1.479340000 | -0.038591000 |
| Si | 1.190029000 | 2.326194000 | 0.916524000 |
| O | 0.717499000 | 1.368918000 | 2.162895000 |
| Si | 0.000000000 | 0.000000000 | 2.749028000 |
| O | 0.826768000 | -1.305831000 | 2.162895000 |
| Si | 1.419529000 | -2.193692000 | 0.916524000 |
| O | 0.155104000 | -2.690032000 | -0.038591000 |
| Si | -1.200903000 | -2.364896000 | -0.894428000 |
| O | -0.712101000 | -1.406319000 | -2.219876000 |
| Si | 0.000000000 | 0.000000000 | -2.533047000 |
| O | 1.573958000 | 0.086462000 | -2.219876000 |
| Si | 2.648511000 | 0.142436000 | -0.894428000 |

| | | | |
|---|---|---|---|
| O | 2.371806000 | -1.215711000 | -0.027744000 |
| O | -2.238740000 | -1.446189000 | -0.027744000 |
| Si | -2.609558000 | -0.132502000 | 0.916524000 |
| O | -2.407188000 | 1.210692000 | -0.038591000 |
| Si | -1.447609000 | 2.222460000 | -0.894428000 |
| O | -0.861858000 | 1.319857000 | -2.219876000 |
| O | -1.544267000 | -0.063087000 | 2.162895000 |
| O | -0.133066000 | 2.661900000 | -0.027744000 |
| C | 4.400235000 | 0.228021000 | -1.561333000 |
| C | 4.561047000 | 1.487302000 | -2.441251000 |
| C | 5.379883000 | 0.307313000 | -0.366628000 |
| C | 4.710305000 | -1.033561000 | -2.396359000 |
| H | 3.900235000 | 1.462555000 | -3.316440000 |
| H | 4.349004000 | 2.406360000 | -1.883887000 |
| H | 5.592316000 | 1.554206000 | -2.811508000 |
| H | 5.305839000 | -0.573241000 | 0.281494000 |
| H | 6.412100000 | 0.359372000 | -0.736588000 |
| H | 5.203819000 | 1.197635000 | 0.247419000 |
| H | 5.737667000 | -0.983380000 | -2.779783000 |
| H | 4.623703000 | -1.949391000 | -1.801440000 |
| H | 4.042526000 | -1.127928000 | -3.261484000 |
| C | 0.000000000 | 0.000000000 | -4.750089000 |
| C | 0.660107000 | 1.325852000 | -5.053072000 |
| C | 0.818168000 | -1.234595000 | -5.053072000 |
| C | -1.478275000 | -0.091257000 | -5.053072000 |
| H | 0.078812000 | 2.178718000 | -4.694536000 |
| H | 1.681455000 | 1.386686000 | -4.669352000 |
| H | 0.719939000 | 1.408992000 | -6.152508000 |
| H | 0.360178000 | -2.149526000 | -4.669352000 |
| H | 0.860253000 | -1.327982000 | -6.152508000 |
| H | 1.847419000 | -1.157612000 | -4.694536000 |
| H | -1.580192000 | -0.081010000 | -6.152508000 |
| H | -1.926231000 | -1.021106000 | -4.694536000 |
| H | -2.041633000 | 0.762840000 | -4.669352000 |
| C | -2.397590000 | 3.696705000 | -1.561333000 |
| C | -1.460062000 | 4.596024000 | -2.396359000 |
| C | -3.568565000 | 3.206332000 | -2.441251000 |
| C | -2.956082000 | 4.505459000 | -0.366628000 |
| H | -0.623629000 | 4.978940000 | -1.801440000 |
| H | -1.044449000 | 4.064894000 | -3.261484000 |
| H | -2.017201000 | 5.460655000 | -2.779783000 |
| H | -4.258471000 | 2.563168000 | -1.883887000 |
| H | -4.142140000 | 4.065985000 | -2.811508000 |
| H | -3.216727000 | 2.646425000 | -3.316440000 |
| H | -3.517275000 | 5.373356000 | -0.736588000 |
| H | -3.639092000 | 3.907822000 | 0.247419000 |

| | | | |
|---|---|---|---|
| H | -2.156478000 | 4.881612000 | 0.281494000 |
| C | 1.981565000 | 3.912154000 | 1.532688000 |
| C | 3.220469000 | 3.567413000 | 2.390520000 |
| C | 2.414147000 | 4.783399000 | 0.332480000 |
| C | 0.962730000 | 4.692186000 | 2.394513000 |
| H | 2.957308000 | 2.959507000 | 3.263519000 |
| H | 3.977812000 | 3.022755000 | 1.814686000 |
| H | 3.687260000 | 4.490365000 | 2.759074000 |
| H | 1.561649000 | 5.063662000 | -0.297122000 |
| H | 2.877401000 | 5.711464000 | 0.692377000 |
| H | 3.149511000 | 4.272012000 | -0.299519000 |
| H | 1.420448000 | 5.618052000 | 2.767054000 |
| H | 0.071709000 | 4.973062000 | 1.820897000 |
| H | 0.635692000 | 4.112514000 | 3.265185000 |
| C | 0.000000000 | 0.000000000 | 4.625819000 |
| C | 1.451339000 | 0.120165000 | 5.143173000 |
| C | -0.829735000 | 1.196814000 | 5.143173000 |
| C | -0.621604000 | -1.316979000 | 5.143173000 |
| H | 2.076281000 | -0.715554000 | 4.807428000 |
| H | 1.926127000 | 1.051330000 | 4.813277000 |
| H | 1.457845000 | 0.116502000 | 6.241190000 |
| H | -1.873542000 | 1.142410000 | 4.813277000 |
| H | -0.829816000 | 1.204280000 | 6.241190000 |
| H | -0.418453000 | 2.155889000 | 4.807428000 |
| H | -0.628029000 | -1.320782000 | 6.241190000 |
| H | -1.657828000 | -1.440335000 | 4.807428000 |
| H | -0.052585000 | -2.193740000 | 4.813277000 |
| C | 2.397242000 | -3.672163000 | 1.532688000 |
| C | 2.935472000 | -4.482412000 | 0.332480000 |
| C | 3.582187000 | -3.179842000 | 2.394513000 |
| C | 1.479236000 | -4.572715000 | 2.390520000 |
| H | 2.124915000 | -4.863563000 | -0.299519000 |
| H | 3.604435000 | -3.884259000 | -0.297122000 |
| H | 3.507572000 | -5.347634000 | 0.692377000 |
| H | 3.243696000 | -2.606782000 | 3.265185000 |
| H | 4.155152000 | -4.039170000 | 2.767054000 |
| H | 4.270943000 | -2.548633000 | 1.820897000 |
| H | 2.045140000 | -5.438443000 | 2.759074000 |
| H | 1.084354000 | -4.040857000 | 3.263519000 |
| H | 0.628877000 | -4.956264000 | 1.814686000 |
| C | -2.002646000 | -3.924726000 | -1.561333000 |
| C | -3.250243000 | -3.562463000 | -2.396359000 |
| C | -0.992482000 | -4.693634000 | -2.441251000 |
| C | -2.423801000 | -4.812772000 | -0.366628000 |
| H | -4.000074000 | -3.029549000 | -1.801440000 |
| H | -2.998077000 | -2.936966000 | -3.261484000 |

| | | | |
|---|---|---|---|
| H | -3.720466000 | -4.477275000 | -2.779783000 |
| H | -0.090533000 | -4.969528000 | -1.883887000 |
| H | -1.450176000 | -5.620191000 | -2.811508000 |
| H | -0.683508000 | -4.108980000 | -3.316440000 |
| H | -2.894825000 | -5.732728000 | -0.736588000 |
| H | -1.564727000 | -5.105457000 | 0.247419000 |
| H | -3.149361000 | -4.308371000 | 0.281494000 |
| C | -4.378807000 | -0.239991000 | 1.532688000 |
| C | -5.349619000 | -0.300987000 | 0.332480000 |
| C | -4.544917000 | -1.512344000 | 2.394513000 |
| C | -4.699705000 | 1.005302000 | 2.390520000 |
| H | -5.274426000 | 0.591551000 | -0.299519000 |
| H | -5.166084000 | -1.179403000 | -0.297122000 |
| H | -6.384973000 | -0.363830000 | 0.692377000 |
| H | -3.879388000 | -1.505732000 | 3.265185000 |
| H | -5.575600000 | -1.578882000 | 2.767054000 |
| H | -4.342653000 | -2.424429000 | 1.820897000 |
| H | -5.732400000 | 0.948078000 | 2.759074000 |
| H | -4.041662000 | 1.081350000 | 3.263519000 |
| H | -4.606689000 | 1.933509000 | 1.814686000 |

**Symmetry $C_1$**

| | | | |
|---|---|---|---|
| O | 2.330911000 | 1.349350000 | 0.025110000 |
| Si | 1.312472000 | 2.257818000 | -0.920530000 |
| O | 0.007548000 | 2.646080000 | 0.027542000 |
| Si | -1.331379000 | 2.292699000 | 0.895707000 |
| O | -0.799285000 | 1.365164000 | 2.226250000 |
| Si | -0.007484000 | 0.000012000 | 2.530031000 |
| O | -0.799271000 | -1.365135000 | 2.226201000 |
| Si | -1.331381000 | -2.292714000 | 0.895693000 |
| O | 0.007548000 | -2.646137000 | 0.027542000 |
| Si | 1.312467000 | -2.257830000 | -0.920527000 |
| O | 2.330879000 | -1.349370000 | 0.025154000 |
| Si | 2.656310000 | 0.000001000 | 0.890814000 |
| O | 1.565381000 | 0.000039000 | 2.203221000 |
| O | -2.348364000 | -1.332304000 | 0.047309000 |
| Si | -2.615047000 | 0.000001000 | -0.908068000 |
| O | -1.522990000 | 0.000027000 | -2.132185000 |
| Si | 0.010630000 | 0.000009000 | -2.748395000 |
| O | 0.794777000 | -1.339891000 | -2.179304000 |
| O | -2.348369000 | 1.332272000 | 0.047353000 |
| O | 0.794795000 | 1.339908000 | -2.179335000 |
| C | 4.405493000 | -0.000005000 | 1.569777000 |
| C | 5.392342000 | -0.000015000 | 0.378404000 |
| C | 4.638548000 | 1.262775000 | 2.428219000 |

| | | | |
|---|---|---|---|
| C | 4.638536000 | -1.262781000 | 2.428230000 |
| H | 5.269349000 | -0.887035000 | -0.252964000 |
| H | 5.269357000 | 0.887000000 | -0.252971000 |
| H | 6.424525000 | -0.000019000 | 0.752021000 |
| H | 3.968849000 | 1.299668000 | 3.296380000 |
| H | 5.667883000 | 1.269017000 | 2.809844000 |
| H | 4.494168000 | 2.182697000 | 1.851069000 |
| H | 5.667872000 | -1.269031000 | 2.809854000 |
| H | 3.968838000 | -1.299659000 | 3.296394000 |
| H | 4.494144000 | -2.182708000 | 1.851087000 |
| C | 2.182735000 | -3.808025000 | -1.520016000 |
| C | 3.401943000 | -3.409262000 | -2.382405000 |
| C | 2.660527000 | -4.643335000 | -0.311190000 |
| C | 1.205236000 | -4.648886000 | -2.372348000 |
| H | 3.107251000 | -2.817750000 | -3.256388000 |
| H | 4.133723000 | -2.827047000 | -1.810410000 |
| H | 3.910903000 | -4.310691000 | -2.748221000 |
| H | 1.825205000 | -4.956945000 | 0.325970000 |
| H | 3.165962000 | -5.552538000 | -0.662345000 |
| H | 3.373138000 | -4.090111000 | 0.311597000 |
| H | 1.707243000 | -5.558740000 | -2.726810000 |
| H | 0.325254000 | -4.961400000 | -1.797933000 |
| H | 0.856062000 | -4.099707000 | -3.254020000 |
| C | -0.023167000 | -0.000005000 | -4.624861000 |
| C | 1.424450000 | -0.000031000 | -5.166218000 |
| C | -0.759950000 | -1.261440000 | -5.128773000 |
| C | -0.759910000 | 1.261445000 | -5.128789000 |
| H | 1.981561000 | 0.886561000 | -4.842227000 |
| H | 1.981531000 | -0.886642000 | -4.842226000 |
| H | 1.412494000 | -0.000031000 | -6.264168000 |
| H | -1.799046000 | -1.293946000 | -4.781057000 |
| H | -0.779440000 | -1.269945000 | -6.226589000 |
| H | -0.264332000 | -2.182316000 | -4.800472000 |
| H | -0.779403000 | 1.269935000 | -6.226604000 |
| H | -1.799004000 | 1.293991000 | -4.781071000 |
| H | -0.264262000 | 2.182309000 | -4.800503000 |
| C | 2.182715000 | 3.808037000 | -1.519977000 |
| C | 2.660509000 | 4.643309000 | -0.311127000 |
| C | 3.401917000 | 3.409310000 | -2.382388000 |
| C | 1.205202000 | 4.648913000 | -2.372272000 |
| H | 1.825194000 | 4.956874000 | 0.326058000 |
| H | 3.373143000 | 4.090078000 | 0.311624000 |
| H | 3.165915000 | 5.552535000 | -0.662255000 |
| H | 3.107222000 | 2.817827000 | -3.256387000 |
| H | 3.910868000 | 4.310752000 | -2.748176000 |
| H | 4.133704000 | 2.827080000 | -1.810419000 |

| | | | |
|---|---|---|---|
| H | 1.707191000 | 5.558787000 | -2.726701000 |
| H | 0.856033000 | 4.099764000 | -3.253963000 |
| H | 0.325220000 | 4.961391000 | -1.797844000 |
| C | -2.187612000 | 3.827648000 | 1.551399000 |
| C | -1.202154000 | 4.656590000 | 2.404144000 |
| C | -2.668013000 | 4.676299000 | 0.350162000 |
| C | -3.405323000 | 3.422067000 | 2.410878000 |
| H | -0.854861000 | 4.101843000 | 3.284410000 |
| H | -0.321473000 | 4.965058000 | 1.829997000 |
| H | -1.697274000 | 5.567171000 | 2.765754000 |
| H | -3.381628000 | 4.129830000 | -0.276659000 |
| H | -3.172664000 | 5.580624000 | 0.714327000 |
| H | -1.834115000 | 4.997203000 | -0.284355000 |
| H | -3.913821000 | 4.320778000 | 2.783444000 |
| H | -4.136041000 | 2.841952000 | 1.836798000 |
| H | -3.110952000 | 2.826717000 | 3.283770000 |
| C | 0.007608000 | -0.000016000 | 4.747876000 |
| C | 0.749446000 | -1.282635000 | 5.047397000 |
| C | 0.749404000 | 1.282622000 | 5.047424000 |
| C | -1.472104000 | -0.000042000 | 5.057965000 |
| H | 0.225074000 | -2.168873000 | 4.682150000 |
| H | 1.773993000 | -1.276522000 | 4.667696000 |
| H | 0.809443000 | -1.368206000 | 6.146642000 |
| H | 0.224995000 | 2.168849000 | 4.682210000 |
| H | 0.809416000 | 1.368162000 | 6.146670000 |
| H | 1.773945000 | 1.276557000 | 4.667707000 |
| H | -1.567542000 | -0.000036000 | 6.157978000 |
| H | -1.980934000 | 0.893702000 | 4.688892000 |
| H | -1.980900000 | -0.893811000 | 4.688902000 |
| C | -2.187626000 | -3.827642000 | 1.551435000 |
| C | -2.668021000 | -4.676337000 | 0.350224000 |
| C | -1.202175000 | -4.656560000 | 2.404215000 |
| C | -3.405345000 | -3.422034000 | 2.410893000 |
| H | -3.381619000 | -4.129880000 | -0.276631000 |
| H | -1.834115000 | -4.997280000 | -0.284270000 |
| H | -3.172693000 | -5.580642000 | 0.714418000 |
| H | -0.854879000 | -4.101780000 | 3.284461000 |
| H | -1.697304000 | -5.567125000 | 2.765861000 |
| H | -0.321493000 | -4.965058000 | 1.830080000 |
| H | -3.913843000 | -4.320735000 | 2.783491000 |
| H | -3.110981000 | -2.826649000 | 3.283766000 |
| H | -4.136062000 | -2.841941000 | 1.836787000 |
| C | -4.377986000 | 0.000008000 | -1.551340000 |
| C | -4.611576000 | -1.261368000 | -2.413539000 |
| C | -5.365525000 | 0.000002000 | -0.363207000 |
| C | -4.611571000 | 1.261394000 | -2.413524000 |

| | | | |
|---|---|---|---|
| H | -3.936389000 | -1.299052000 | -3.276003000 |
| H | -4.474033000 | -2.182749000 | -1.835653000 |
| H | -5.639658000 | -1.264539000 | -2.799092000 |
| H | -5.243172000 | 0.887160000 | 0.268843000 |
| H | -6.398199000 | 0.000006000 | -0.735959000 |
| H | -5.243176000 | -0.887166000 | 0.268833000 |
| H | -5.639652000 | 1.264573000 | -2.799077000 |
| H | -4.474026000 | 2.182766000 | -1.835628000 |
| H | -3.936383000 | 1.299087000 | -3.275986000 |

**Coordinates of the neutral $Si_8O_{12}(C(CH_3)_3)_8$ in $O_h$ symmetry**

| | | | |
|---|---|---|---|
| O | -1.895501000 | 0.000000000 | 1.895501000 |
| Si | -1.592593000 | -1.592593000 | 1.592593000 |
| O | 0.000000000 | -1.895501000 | 1.895501000 |
| Si | 1.592593000 | -1.592593000 | 1.592593000 |
| O | 1.895501000 | 0.000000000 | 1.895501000 |
| Si | 1.592593000 | 1.592593000 | 1.592593000 |
| O | 1.895501000 | 1.895501000 | 0.000000000 |
| Si | 1.592593000 | 1.592593000 | -1.592593000 |
| O | 0.000000000 | 1.895501000 | -1.895501000 |
| Si | -1.592593000 | 1.592593000 | -1.592593000 |
| O | -1.895501000 | 1.895501000 | 0.000000000 |
| Si | -1.592593000 | 1.592593000 | 1.592593000 |
| O | 0.000000000 | 1.895501000 | 1.895501000 |
| O | 1.895501000 | 0.000000000 | -1.895501000 |
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