

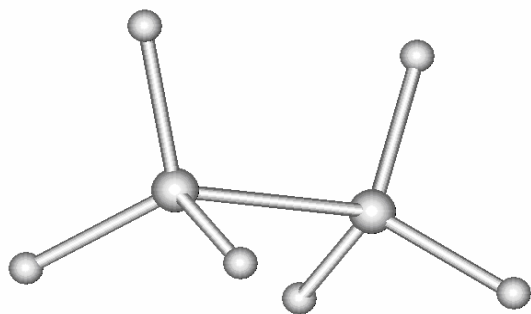
Anna Kaleta
Piotr Chojnacki
IV rok informatyki chemicznej

21 kwietnia 2006 r.

Przedmiot specjalizacyjny II

Konstruowanie macierzy Z

Grupa punktowa D_{3h}

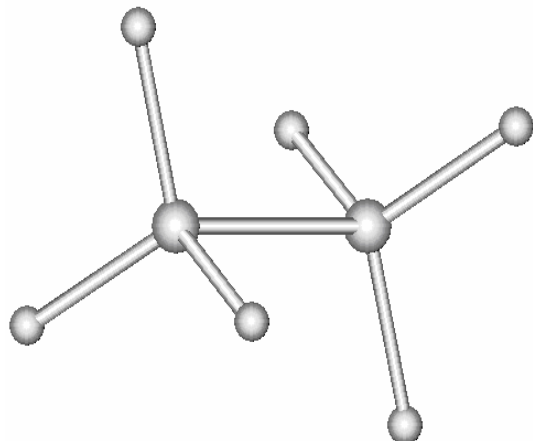


Name:
macierz Z dla czasteczki SiH₆

| | | | | | | | | | |
|----|------|---|--------|---|--------|---|---|---|---|
| Si | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| Si | 2.33 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| H | 1.48 | 0 | 107.80 | 0 | 000.00 | 0 | 1 | 2 | 0 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 1 | 2 | 3 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 2 | 1 | 3 |
| H | 1.48 | 0 | 107.80 | 0 | 000.00 | 0 | 2 | 1 | 4 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 2 | 1 | 4 |
| H | 1.48 | 0 | 107.80 | 0 | 000.00 | 0 | 1 | 2 | 5 |
| 0 | | | | | | | | | |

$$r_{(\text{Si1-Si2})} = 2.33 \text{ \AA}, r_{(\text{Si1-H3})} = 1.48 \text{ \AA}, \angle_{\text{H3Si2Si1}} = 107.80^\circ, \angle_{\text{H4H3Si2Si1}} = 120^\circ, \angle_{\text{H6H4Si2Si1}} = 0.00^\circ$$

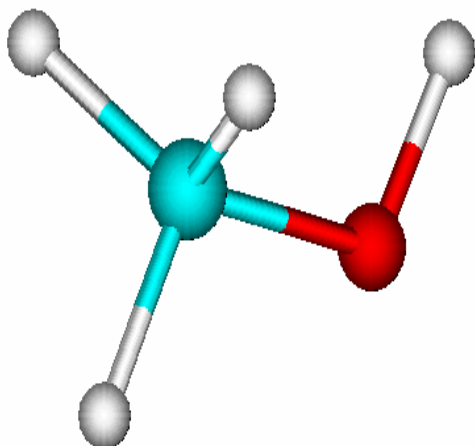
Grupa punktowa D_{3d}



Name:
macierz Z dla czasteczki SiH₆

| | | | | | | | | | |
|----|------|---|--------|---|--------|---|---|---|---|
| Si | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| Si | 2.33 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| H | 1.48 | 0 | 107.80 | 0 | 000.00 | 0 | 1 | 2 | 0 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 1 | 2 | 3 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 1 | 2 | 4 |
| H | 1.48 | 0 | 107.80 | 0 | 180.00 | 0 | 2 | 1 | 4 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 2 | 1 | 6 |
| H | 1.48 | 0 | 107.80 | 0 | 120.00 | 0 | 2 | 1 | 7 |
| 0 | | | | | | | | | |

$$r_{(\text{Si1-Si2})} = 2.33 \text{ \AA}, r_{(\text{Si1-H3})} = 1.48 \text{ \AA}, \angle_{\text{H3Si2Si1}} = 107.80^\circ, \angle_{\text{H4H3Si2Si1}} = 120.00^\circ, \angle_{\text{H6H4Si2Si1}} = 180.00^\circ$$



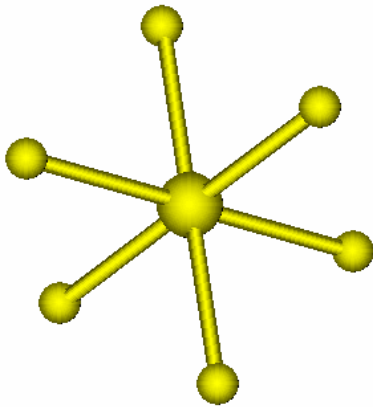
Name:
macierz Z dla czasteczki CH₃OH

| | | | | | | | | | |
|----|------|---|--------|---|--------|---|---|---|---|
| C | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| O | 1.44 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| H | 0.96 | 0 | 110.00 | 0 | 000.00 | 0 | 2 | 1 | 0 |
| H | 1.09 | 0 | 107.00 | 0 | 180.00 | 0 | 1 | 2 | 3 |
| XX | 1.00 | 0 | 125.00 | 0 | 000.00 | 0 | 1 | 2 | 3 |
| H | 1.09 | 0 | 054.50 | 0 | 100.00 | 0 | 1 | 5 | 2 |
| H | 1.09 | 0 | 054.50 | 0 | 260.00 | 0 | 1 | 5 | 2 |
| 0 | | | | | | | | | |

$$r_{(\text{C1-O2})} = 1.44 \text{ \AA}, r_{(\text{C1-H4})} = 1.09 \text{ \AA}, r_{(\text{C1-H6})} = r_{(\text{C1-H7})} = 1.09 \text{ \AA}, r_{(\text{O2-H3})} = 0.96 \text{ \AA},$$

$$\angle_{\text{H4C1O2}} = 107.00^\circ, \angle_{\text{XX5C1O2}} = 125.00^\circ, \angle_{\text{XXH3O2C1}} = 0.00^\circ, \angle_{\text{H4H3O2C1}} = 180.00^\circ,$$

$$\angle_{\text{H7O2XX5C1}} = 260.00^\circ$$

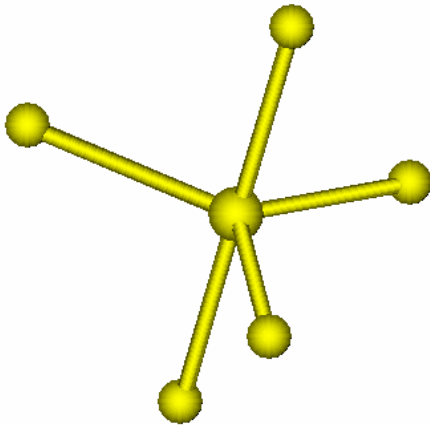


Name:

macierz Z dla czasteczki SF6

| | | | | | | | | | |
|---|------|---|--------|---|--------|---|---|---|---|
| S | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| F | 1.56 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| F | 1.56 | 0 | 180.00 | 0 | 000.00 | 0 | 1 | 2 | 0 |
| F | 1.56 | 0 | 090.00 | 0 | 180.00 | 0 | 1 | 2 | 3 |
| F | 1.56 | 0 | 090.00 | 0 | 090.00 | 0 | 1 | 4 | 3 |
| F | 1.56 | 0 | 090.00 | 0 | 090.00 | 0 | 1 | 5 | 3 |
| F | 1.56 | 0 | 090.00 | 0 | 270.00 | 0 | 1 | 6 | 2 |
| 0 | | | | | | | | | |

$r_{(S-F)} = 1.56 \text{ \AA}$, $\angle_{F_3F_2S_1} = 180.00^\circ$, $\angle_{F_4F_2S_1} = 90.00^\circ$, $\angle_{F_4F_3F_2S_1} = 180.00^\circ$, $\angle_{F_5F_4F_3S_1} = 90.00^\circ$,
 $\angle_{F_7F_6F_2S_1} = 270.00^\circ$

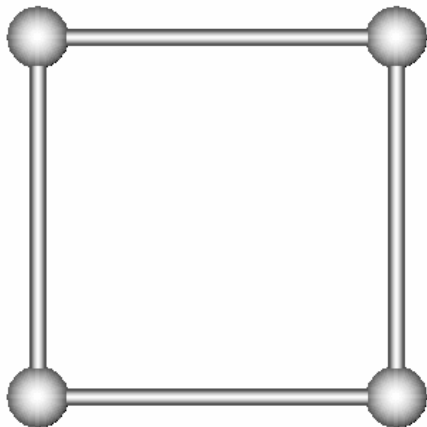


Name:

macierz Z dla czasteczki PF5

| | | | | | | | | | |
|---|------|---|--------|---|--------|---|---|---|---|
| P | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| F | 1.53 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| F | 1.53 | 0 | 180.00 | 0 | 000.00 | 0 | 1 | 2 | 0 |
| F | 1.58 | 0 | 090.00 | 0 | 090.00 | 0 | 1 | 3 | 2 |
| F | 1.58 | 0 | 120.00 | 0 | 090.00 | 0 | 1 | 4 | 3 |
| F | 1.58 | 0 | 120.00 | 0 | 090.00 | 0 | 1 | 5 | 3 |
| 0 | | | | | | | | | |

$r_{(P-F_{ax})} = 1.58 \text{ \AA}$, $r_{(P-F_{eq})} = 1.53 \text{ \AA}$, $\angle_{F_{eq}PF_{eq}} = 120.00^\circ$, $\angle_{F_{ax}PF_{eq}} = 90.00^\circ$, $\angle_{F_{ax}F_{ax}PF_{eq}} = 90.00^\circ$
gdzie *ax*- oznacza pozycję aksjalną, a *eq*- oznacza pozycję ekwatorialną.



Name:

macierz Z dla czasteczki Pd4

| | | | | | | | | | |
|----|------|---|--------|---|--------|---|---|---|---|
| Pd | 0.00 | 0 | 000.00 | 0 | 000.00 | 0 | 0 | 0 | 0 |
| Pd | 2.60 | 0 | 000.00 | 0 | 000.00 | 0 | 1 | 0 | 0 |
| Pd | 2.60 | 0 | 090.00 | 0 | 000.00 | 0 | 2 | 1 | 0 |
| Pd | 2.60 | 0 | 090.00 | 0 | 000.00 | 0 | 3 | 2 | 1 |
| 0 | | | | | | | | | |

$r_{(Pd-Pd)} = 2.60 \text{ \AA}$, $\angle_{PdPdPd} = 90.00^\circ$