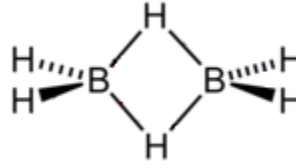# Diborane - D_{2h} Symmetry

Diborane has 18 vibrational degrees of freedom. Nine modes are Raman active and eight are IR active. The experimental results are provided in the table below. Do a symmetry analysis to confirm the assignments given below, and identify stretches and bends.

D_{2h}	A_g	A_g	A_g	A_g	B_{1g}	B_{1g}	B_{2g}	B_{2g}	B_{3g}
$\dfrac{Raman}{cm}$	2524	2104	1180	794	1768	1035	2591	920	1012
D_{2h}	A_u	B_{1u}	B_{1u}	B_{1u}	B_{2u}	B_{2u}	B_{3u}	B_{3u}	B_{3u}
$\dfrac{IR}{cm}$	0	2612	950	368	1915	973	2525	1606	1177

$E \ \ C_2{}^z \ \ C_2{}^y \ \ C_2{}^x \ \ i \ \ \sigma_{xy} \ \ \sigma_{xz} \ \ \sigma_{yz}$

$$C_{D2h} := \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix} \begin{matrix} A_g\text{: } x^2,\ y^2,\ z^2 \\ B_{1g}\text{: } R_z,\ xy \\ B_{2g}\text{: } R_y,\ xz \\ B_{3g}\text{: } R_x,\ yz \\ A_u \\ B_{1u}\text{: } z \\ B_{2u}\text{: } y \\ B_{3u}\text{: } x \end{matrix}$$

$$D2h := \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad \Gamma_{uma} := \begin{pmatrix} 8 \\ 0 \\ 2 \\ 2 \\ 0 \\ 4 \\ 6 \\ 2 \end{pmatrix} \qquad \Gamma_{bonds} := \begin{pmatrix} 8 \\ 0 \\ 0 \\ 0 \\ 0 \\ 4 \\ 4 \\ 0 \end{pmatrix}$$

$$A_g := \left(C_{D2h}{}^T\right)^{\langle 1 \rangle} \qquad B_{1g} := \left(C_{D2h}{}^T\right)^{\langle 2 \rangle} \qquad B_{2g} := \left(C_{D2h}{}^T\right)^{\langle 3 \rangle} \qquad B_{3g} := \left(C_{D2h}{}^T\right)^{\langle 4 \rangle}$$

$$A_u := \left(C_{D2h}{}^T\right)^{\langle 5 \rangle} \qquad B_{1u} := \left(C_{D2h}{}^T\right)^{\langle 6 \rangle} \qquad B_{2u} := \left(C_{D2h}{}^T\right)^{\langle 7 \rangle} \qquad B_{3u} := \left(C_{D2h}{}^T\right)^{\langle 8 \rangle} \qquad h := \sum D2h$$

$$\Gamma_{trans} := B_{1u} + B_{2u} + B_{3u} \qquad \Gamma_{rot} := B_{1g} + B_{2g} + B_{3g} \qquad \Gamma_{tot} := \overrightarrow{\left(\Gamma_{uma} \cdot \Gamma_{trans}\right)}$$

$$\Gamma_{vib} := \Gamma_{tot} - \Gamma_{trans} - \Gamma_{rot} \qquad \Gamma_{vib}{}^T = (18 \ \ 2 \ \ 0 \ \ 0 \ \ 0 \ \ 4 \ \ 6 \ \ 2) \qquad i := 1..8$$

$$\Gamma_{stretch} := \Gamma_{bonds} \qquad \Gamma_{bend} := \Gamma_{vib} - \Gamma_{stretch}$$

$$\text{Vib}_i := \frac{\sum \overrightarrow{\left[\text{D2h} \cdot \left(C_{\text{D2h}}{}^T \right)^{\langle i \rangle} \cdot \Gamma_{\text{vib}} \right]}}{h} \qquad \text{Stretch}_i := \frac{\sum \overrightarrow{\left[\text{D2h} \cdot \left(C_{\text{D2h}}{}^T \right)^{\langle i \rangle} \cdot \Gamma_{\text{stretch}} \right]}}{h} \qquad \text{Bend}_i := \frac{\sum \overrightarrow{\left[\text{D2h} \cdot \left(C_{\text{D2h}}{}^T \right)^{\langle i \rangle} \cdot \Gamma_{\text{bend}} \right]}}{h}$$

$$\text{Vib} = \begin{pmatrix} 4 \\ 2 \\ 2 \\ 1 \\ 1 \\ 3 \\ 2 \\ 3 \end{pmatrix} \quad \begin{matrix} A_g: \ x^2, y^2, z^2 \\ B_{1g}: \ R_z, xy \\ B_{2g}: \ R_y, xz \\ B_{3g}: \ R_x, yz \\ A_u \\ B_{1u}: \ z \\ B_{2u}: \ y \\ B_{3u}: \ x \end{matrix} \qquad \text{Stretch} = \begin{pmatrix} 2 \\ 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ 1 \\ 2 \end{pmatrix} \quad \begin{matrix} A_g: \ x^2, y^2, z^2 \\ B_{1g}: \ R_z, xy \\ B_{2g}: \ R_y, xz \\ B_{3g}: \ R_x, yz \\ A_u \\ B_{1u}: \ z \\ B_{2u}: \ y \\ B_{3u}: \ x \end{matrix} \qquad \text{Bend} = \begin{pmatrix} 2 \\ 1 \\ 1 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \end{pmatrix} \quad \begin{matrix} A_g: \ x^2, y^2, z^2 \\ B_{1g}: \ R_z, xy \\ B_{2g}: \ R_y, xz \\ B_{3g}: \ R_x, yz \\ A_u \\ B_{1u}: \ z \\ B_{2u}: \ y \\ B_{3u}: \ x \end{matrix}$$

This analysis is in agreement with the experimental data. There are 9 Raman active modes and 8 IR active modes. Furthermore there are 4 Raman stretches at 2524 (Ag), 2104 (Ag), 1768 (B1g), and 2591 (B2g). The five Raman bends occur at 1180 (Ag), 794 (Ag), 1035 (B1g), 920 (B2g), and 1012 (B3g).

The 4 IR stretches occur at 2612 (B1u), 1915 (B2u), 2525 (B3u), and 1606 (B3u). The bends appear at 950 (B1u), 368 (B1u), 973 (B2u), 1177 (B3u).