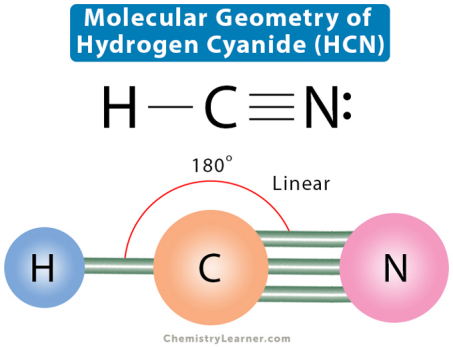
Feature construction

Coulomb matrix for molecules



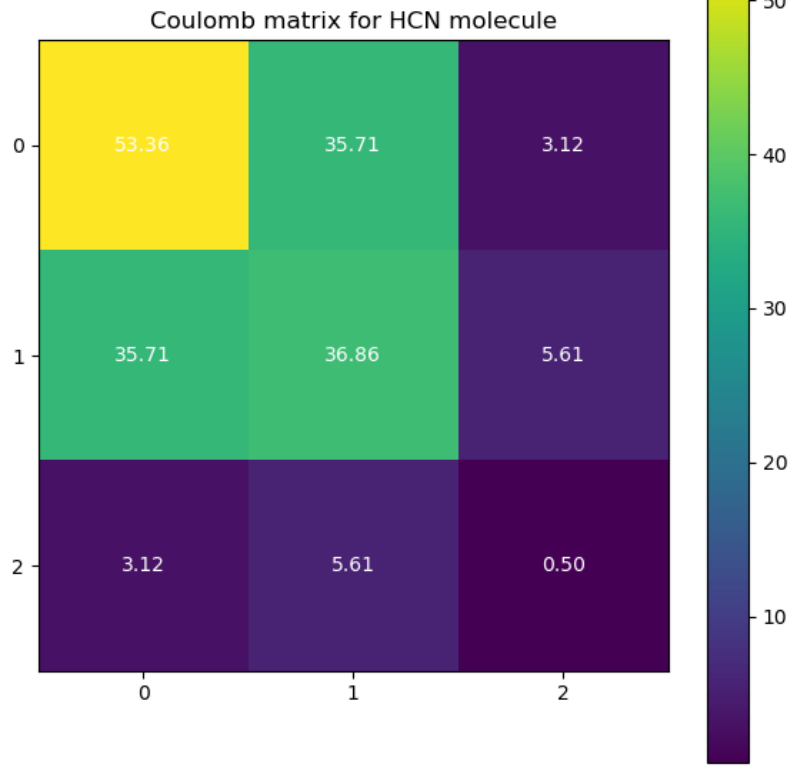
- DScribe library GitHub page

- Examples and comparison with features created by hand
  - Coulomb matrix of HCN
  - $d_{\mathrm{HC}} = 1.07\ \text{Å}, \quad d_{\mathrm{CN}} = 1.17\ \text{Å}; \quad$ so $d_{\mathrm{HN}} = 2.24\ \text{Å}.$
  - $Z_{\mathrm{H}} = 1, Z_{\mathrm{C}} = 6, Z_{\mathrm{N}} = 7.$
  - Diagonal elements
    - $\mathrm{M}_{\mathrm{HH}} = (0.5)1^{2.4} = 0.5, \quad \mathrm{M}_{\mathrm{CC}} = (0.5)6^{2.4} = 36.86, \quad \mathrm{M}_{\mathrm{NN}} = (0.5)7^{2.4} = 53.36.$
  - Off-diagonal elements
    - $\mathrm{M}_{\mathrm{CH}} = \mathrm{M}_{\mathrm{HC}} = \dfrac{1 \times 6}{1.07} = 5.61, \quad \mathrm{M}_{\mathrm{CN}} = \mathrm{M}_{\mathrm{NC}} = \dfrac{6 \times 7}{1.17} = 35.89,$

      $\mathrm{M}_{\mathrm{HN}} = \mathrm{M}_{\mathrm{NH}} = \dfrac{1 \times 7}{2.24} = 3.12.$
  - Coulomb matrix using DScribe

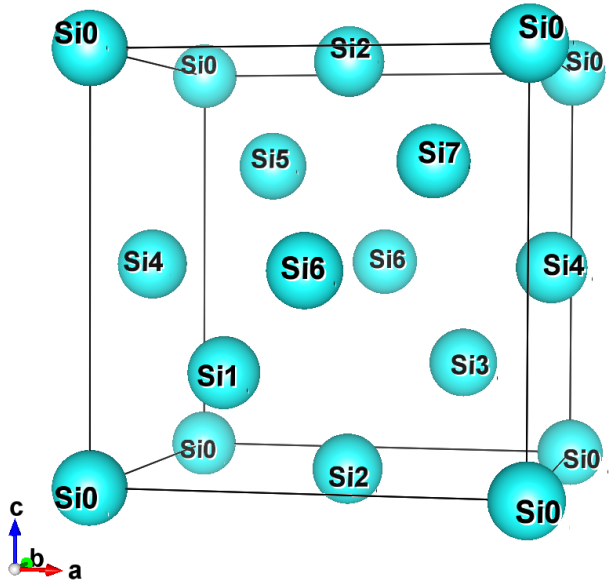
$$H - C \equiv N$$

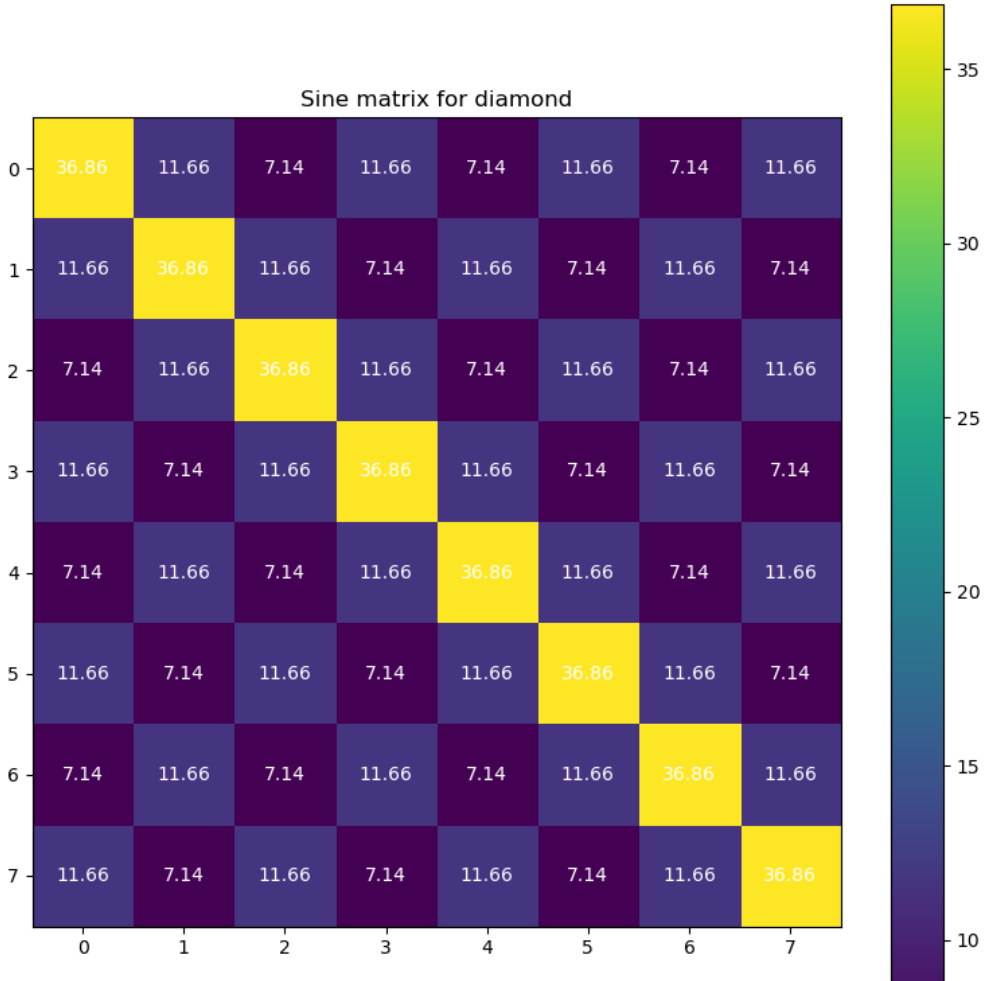
$$d_{HC} = 1.07 \text{ Å}; d_{CN} = 1.176 \text{ Å}$$



Sine matrix for crystalline solids

- Diamond as an example
  - FCC lattice with two atoms in the unit cell
    - At $(0,0,0)$, $a(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
  - Conventional cubic unit cell, 8 atoms in the cell





Sine matrix of a diamond conventional cell
Using DScribe libraries

- Calculating sine matrix by hand for diamond
- $\vec{a}_1 = a(1,0,0),\ \vec{a}_2 = a(0,1,0),\ \vec{a}_3 = a(0,0,1)$
- Matrix $\mathbf{B} = a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.
- 8 C atoms in the unit cell
- $\vec{R}_0 = a(0,0,0),\quad \vec{R}_1 = a\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right),\quad \vec{R}_2 = a\left(\frac{1}{2},0,\frac{1}{2}\right),\ \vec{R}_3 = a\left(\frac{3}{4},\frac{1}{4},\frac{3}{4}\right).$
- $\vec{R}_4 = a\left(0,\frac{1}{2},\frac{1}{2}\right),\ \vec{R}_5 = a\left(\frac{1}{4},\frac{3}{4},\frac{3}{4}\right),\ \vec{R}_6 = a\left(\frac{1}{2},\frac{1}{2},0\right),\ \vec{R}_7 = a\left(\frac{3}{4},\frac{3}{4},\frac{1}{4}\right).$
- $\mathbf{B}^{-1} = \frac{1}{a}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.
- Work out $\mathbf{M}_{10}^{\text{sine}} = \mathbf{M}_{01}^{\text{sine}}$:
  - $\vec{R}_{10} = \vec{R}_1 - \vec{R}_0 = (a/4,a/4,a/4).$
  - $\mathbf{B}^{-1}\,.\,\vec{R}_{10} = \frac{1}{a}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.\begin{pmatrix} a/4 \\ a/4 \\ a/4 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$

REPEAT

3. **Sine matrix**

- Ewald matrix is computationally expensive to calculate.
- Can we construct a quantity akin to EM, yet easy to calculate? Sine matrix.
- $$M_{ij}^{\text{sine}} = \begin{cases} 0.5 Z_i^{2.4} & \forall i = j, \\ \phi_{ij} & \forall i \neq j, \end{cases}$$

$$\phi_{ij} = Z_i Z_j \, || \, \mathbf{B} \, . \sum_{k=1}^{3} \hat{e}_k \sin^2(\pi \hat{e}_k \, . \, \mathbf{B}^{-1} \, . \, (\vec{R}_i - \vec{R}_j)) \, ||_2^{-1} .$$

- $\mathbf{B}$ is a 3×3 matrix whose columns are the lattice vectors written column-wise: $B_{11} = a_{11}, B_{21} = a_{12}$ and $B_{31} = a_{13}$.
- a_{ij} is component of $\vec{a}_i$ along Cartesian direction j.
- $\hat{e}_k$: Cartesian unit vector along direction k.
- Captures the infinite, periodic arrangement of the atoms.

  No physical meaning.

$$\vec{a}_i = \begin{pmatrix} a_{i1} \\ a_{i2} \\ a_{i3} \end{pmatrix} \quad i = 1, 2, 3.$$

$$\mathbf{B} = \begin{pmatrix} (\vec{a}_1) & (\vec{a}_2) & (\vec{a}_3) \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}$$

Arxiv:1904.08875

- For $k = 1$: $\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$
  - $\pi \hat{e}_1 \mathbf{B}^{-1} \,.\, \overrightarrow{R}_{10} = \pi(1\ 0\ 0)\frac{1}{4}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \pi/4.$
  - $\sin^2(\pi/4) = \frac{1}{2}.$
- Same contributions for $k = 2,\ 3.$
- Vector in the denominator: $\frac{1}{2}\mathbf{B} \,.\, (\hat{e}_1 + \hat{e}_2 + \hat{e}_3) = \frac{1}{2}a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{a}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$
- $|\,|\mathbf{B} \,.\, \sum_{k=1}^{3} \hat{e}_k \sin^2(\pi \hat{e}_k \mathbf{B}^{-1} \,.\, (\overrightarrow{R}_1 - \overrightarrow{R}_0)\,|\,|_2 = \frac{\sqrt{3}}{2}a.$
- $a = 3.567$ Å for diamond.
- Therefore, $M_{10}^{\text{sine}} = 6 \times 6 \times \frac{2}{\sqrt{3} \times 3.567} = 11.65.$