CrysMMNet - Supplementary Materials

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A QUALITATIVE ANALYSIS OF THE ATTENTION LAYERS

uai2023-supplimentary In this section, we aim to visualize and understand attention in different tokens in the material description and we perform a qualitative analysis of the attention layer in MatSciBert. We utilized the standard BertViz tool [1] to analyze and visualize the attention scores in the MatSciBert Model. We present a case study of the textual data of $FeH_8(ClO_2)_2$ in figure 3 and 4, where we have examined the attention score of the [CLS] token at the 5th layer of MatSciBert. From figure 3 and 4, it is clearly observed, MatSciBert allocates higher attention scores to tokens that define global features of the crystal, such as 'Formula', 'Mineral', 'Crystal System', 'Space Group Number', and 'Dimensionality'. Further, we observe for local information corresponding to Fe, H, and O atoms. MatScibert provides more attention score to tokens related to bond types (octahedral geometry, equivalent bond, distorted water-like geometry etc) and bond lengths (2.08 Å, 2.10 Å and 2.53 Å bond length). It is evident from these observations that MatSciBert is attending the important tokens related to global and local material information, to generate more expressive multimodal representation.

[1]https://github.com/jessevig/bertviz

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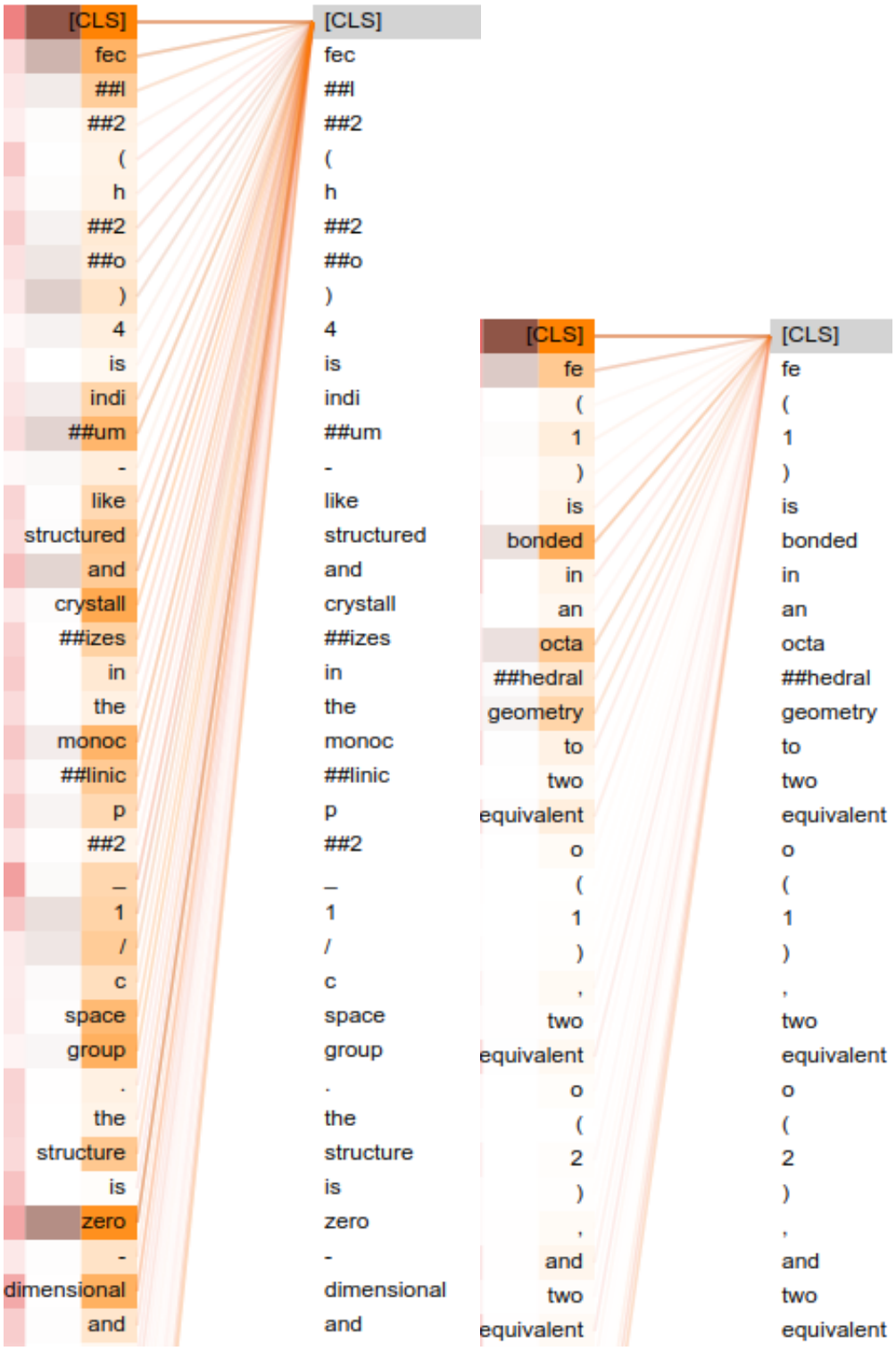

Figure 3: Attention weights of 5th Layer at MatSciBert between [CLS] token and other tokens in material's description for $\mathbf{FeH_8(ClO_2)_2}$.

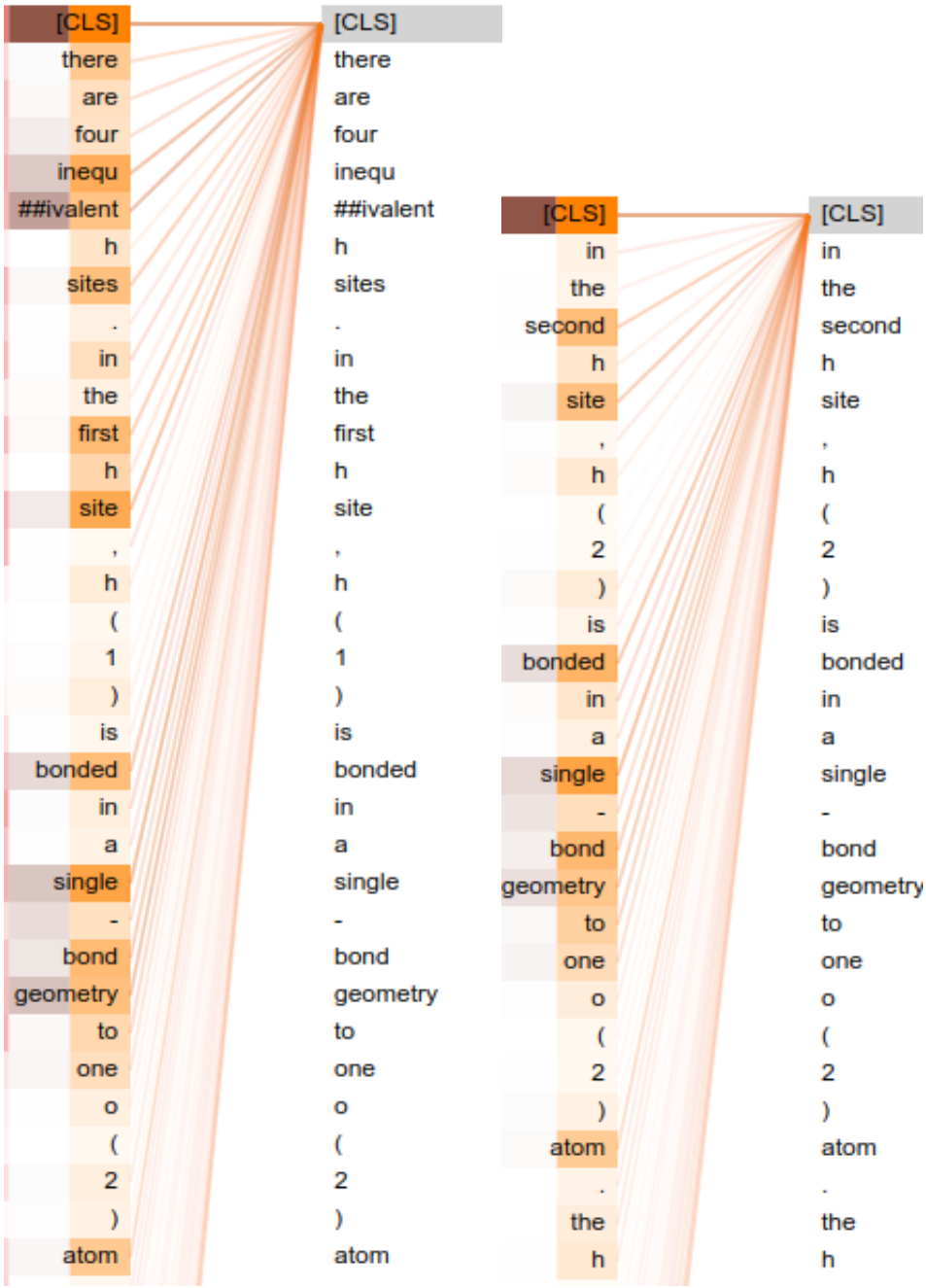

Figure 4: Attention weights of 5th Layer at MatSciBert between [CLS] token and other tokens in material's description for $\mathbf{FeH_8(ClO_2)_2}$.