# Fine-Grained Chemical Entity Typing with Multimodal Knowledge Representation

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## Abstract

How to extract knowledge about chemical reactions from the core chemistry literature is a new emerging challenge that has not been well studied. In this paper, we introduce a new benchmark data set (CHEMET) to facilitate the study of knowledge extraction in this new domain. Fine-grained chemical entity typing poses interesting new challenges especially because of the complex name mentions frequently occurring in chemistry literature and graphic representation of entities. At the same time, there are also interesting new opportunities to leverage external chemistry knowledge resources. We propose a novel multi-modal representation learning framework to solve the problem of fine-grained chemical entity typing by leveraging external resources with chemical structures and using cross-modal attention to learn effective representation of text in the chemistry domain. Experiment results show that the proposed framework outperforms multiple state-of-the-art methods.[1]

## 1 Introduction

*Heng* **[story: In Chemistry literature, many entities are not explained or defined in local context, so if we only use the local sentence context it's difficult to decide the type of the entities. Recent work [cite Tuan's ACL21 paper] tries to explore additional knowledge from the external KB. But for chemistry literature, only the natural language description is still not enough, we need to use the graph structures of these entities for disambiguation, give an example here. Correct KB to Multimedia definition.]**

As the amount of research literature is growing exponentially, accurate and efficient information extraction (IE) methods are crucial for many downstream applications including question answering and knowledge reasoning. One domain largely overlooked by previous IE research is Chemistry (an example sentence is shown in Figure 2), where the papers often mention chemicals and reactions they are involved. What benefit can it bring if we develop well-performing IE methods for chemistry domain? If a comprehensive chemistry knowledge base can be efficiently constructed, chemicals can be discovered at a faster pace since models can learn from existing reactions to infer never-imagined ones, thus benefiting downstream applications such as those in biomedical research and chemical engineering industry.

One fundamental building-block of information extraction is fine-grained entity typing (FET), which is the task of classifying entity mentions into subset of pre-defined hierarchical classes *Heng* **[change this to the type examples in Chemistry]** (e.g., Organic Chemistry/Organic Compounds/Organonitrogen Compounds/Amides), and doing well in such task typically requires the system to understand the mention and its context well. The task is particularly challenging for chemistry articles, where domain-specific knowledge is heavily required to understand the text; for instance, one needs to understand the reaction mechanism in the literature described by both equation image and text (about experiment conditions), and since a reaction is based upon chemical compounds, it additionally assumes one to have knowledge about the chemical entity mentions as well. Many mentions, however, are not explained or defined in local context, and it would thus be difficult to decide the type of the mentions if we only use the sentence itself. Recent work (Lai et al., 2021) explores additional knowledge from the external Knowledge Base (KB), but for chemistry literature, only using the natural language description is less optimal a solution (as shown in our experiment in section 4) than also using graph structures of these chemical entities for further disambiguation.

In scientific domains, information extraction models have been widely developed for biomedical

[1]The programs, data and resources will be made publicly available for research purpose.

context (Liu et al., 2016; Poon and Vanderwende, 2010; Li et al., 2019a, 2017; Cho and Lee, 2019; Beltagy et al., 2019; Lee et al., 2020; Liu et al., 2018; Tian et al., 2020; Lai et al., 2021; Zhang and Ji, 2021; Zhang et al., 2021). However, while chemistry research shapes the foundation of many biomedical studies, there has been little work done in extracting knowledge from core chemistry research literature. Previous work in Chemistry IE (ChemIE) mainly focuses on name tagging (e.g., recognizing chemical name spans), and there is only one work we were able to find (Nguyen et al., 2020) on tasks other than name tagging (e.g., reaction event extraction). Different from in biomedical literature where chemical compounds are often expressed in natural language (e.g., water, aspirin), in chemistry they are often complex formula-like names (e.g., 5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid, $H_2O$), which is hard to be understood by existing language models because such complex names do not follow morphological structure like other commonly used words. Furthermore, many chemicals simply have never been coined with any nomenclature in natural language. The chemical mentions are essentially rare terms that are not to be learned well by only language model.

Although there has been a line of methods in FET applied to news domain (Choi et al., 2018; Xiong et al., 2019; Dai et al., 2019a; Lin and Ji, 2019; Jin et al., 2019; López et al., 2019), none has been developed for core chemistry literature and they do not consider any types of domain-specific knowledge. While language model may have a hard time understanding the chemical mention purely based on its surface form and contextual representation, we can understand the identity through its multimedia representation such as natural language description about its properties and its structure (or graph). To show an example, in Figure 2, where the description text and chemical structure are from external database about the chemical "Ethyl Acetate", some substructures are correlated with phrases in the description; what this implies that because external textual knowledge correlates with labels (indicated by the success of knowledge-enhanced NLP methods), the chemical structure will also likely contribute to disambiguating types.

Utilizing multimodal defnition of entities *Heng* **[do you want to call it as entity linking instead?]**, we introduce the first deep learning based method that uses cross-modal attention to embed the structure and description text of chemicals into a common space as core features for classification. Since the proposed task has not been studied in the previous work, there is no dataset available for training or evaluating the task. To facilitate the study of this new task, we construct CHEMET[2], the first dataset for fine-grained typing in the chemistry literature domain, for which we utilize external database for taxonomy construction, distant supervision for training data labeling, and human annotation for evaluation data labeling, *Heng* **[I don't understand 'Wikipedia category for ontology construction'. you should write clearly the procedure of distant supervision, and motivate it at the beginning, no training data etc.]**. The corpus consists of 100 open access papers from PubChem [3] on Suzuki-Coupling[4] theme. *Heng* **[give details about what database, what theme?]** We will discuss the data construction details in Section 2. Experimental results on this new benchmark show that our method outperforms the state-of-the-art FET methods.

Overall, our contributions can be summarized as the following:

- We are the first to study the task of fine-grained chemical entity typing in chemistry literature, a largely under-explored yet promising field for NLP that has a great need for information extraction methods.
- We construct the first human-annotated dataset in fine-grained chemical entity typing and will release it to the public.
- We introduce a novel method that utilizes multimodal knowledge to enrich entity mention representation. The multimodal component of our model is based on chemical structure and text alignment, which has never been explored before and can be applied to a variety of ChemIE tasks such as relation extraction and event extraction.
- Experiments on the dataset show that our model outperforms the state-of-the-arts entity typing models.

[2]Both the dataset and the code will be released to public
[3]https://pubchem.1ncbi.nlm.nih.gov/
[4]https://en.wikipedia.org/wiki/Suzuki_reaction

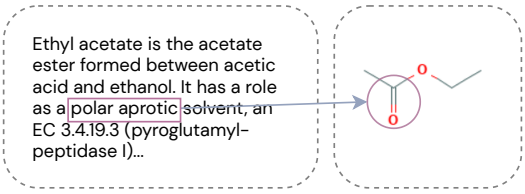


Figure 1: The example shows multimedia definition (description text and chemical structure) from chemical database about "Ethyl Acetate". The circled substructure often indicates the "polar aprotic" property of chemicals

Table 1: Dataset Statistics for CHEMET

| Setting | Anno. | #Inst. | #Mention | #Types |
|---|---|---|---|---|
| Train | Distant | 8000 | NA | 43 |
| Dev | Human | 1000 | NA | NA |
| Test | Human | 1000 | NA | NA |

## 2 Dataset

*Cheng* **["limited dataset" is a bit vague. Is there any such data set available? If so, we should try to use it. My sense is that there isn't(?), so the novelty and significance of the data set could be more clearly articulated.]** Since there is no dataset available for fined-grained chemical entity typing, we have collected and annotated a dataset, CHEMET, based on a corpus of 100 papers from PubChem) with Suzuki-Coupling (a popular reaction mechanism) theme; the theme was chosen to align with chemistry annotators' domain knowledge. We will discuss the steps taken to construct the dataset below.

**Taxonomy Construction**. *Cheng* **[how was the number xx determined? try to give a justification or explanation of the process that reached the number xx. ]**In taxonomy construction, we focus on collecting the types that belong to chemicals commonly occurring in Suzuki-Coupling literature. We carefully select sub-categories from wikipedia chemistry category page [5] as fine-grained ontology; for example, Organic chemistry→Organic compounds→Esters is a fined-grained type where right of the arrow is the sub-category of the left. The ontology is shown in Appendix A

**Distant Supervision**

*Cheng* **[Provide a reference to this string matching algorithm or elaborate.]**

*Jinfeng* **[I'm re-writing this section as below. Free free to use any part of it.]**

We employed distant supervision from Wikipedia and PubChem to create noisy entity labels for the corpus. This process involves the following steps. 1) We first populated entities into the nodes (i.e., entity types) of the taxonomy. That generated an *entity dictionary*. More details are given in the next paragraph. 2) We then tokenized the corpus using (Jessop et al., 2011), a texting mining framework for chemistry that recognizes complex chemical name well. 3) Finally, we distantly labeled the corpus with the entity dictionary by following the procedure of training data generation in AutoNER (Shang et al., 2018).

Now we give more detailed description of our process of automatically assigning entities to types. Each type (except those starting with "Other") is a node in our taxonomy that corresponds to a category in Wikipedia. Each category can have sub-categories and associated pages. Starting from each type, we traced its sub-categories recursively by performing a depth-first search (DFS) with a maximum depth of three. In the DFS we skipped those sub-categories that are probably irrelevant to Chemistry. We used a spell-checker dictionary (Azman, 2012) with over 104,000 technical chemistry terms, and dropped a category from the search if less than 20% of the 1-grams in its name and the names of all its direct children were covered by the dictionary. The maximum depth of three and threshold of 20% were selected empirically by manually checking the quality of the results for some types. After the DFS, we populated the Wikipedia page titles associated with any sub-category of a type as entities of that type. For each type starting with "Other", we took the difference between the entities assigned to its direct parent category and those assigned to all its siblings as its entity list. Finally, we expanded each entity with its synonyms from the PubChem database[6].

**Human Annotation**. Note: talk about agreement metric

We hired five undergraduate chemistry students as annotators. The annotators were instructed to identify and type spans in the assigned samples using Brat (Stenetorp et al., 2012) interface. To ensure the diversity of the testing data, we ran-

[5] https://en.wikipedia.org/wiki/Category:Chemistry

[6] https://ftp.ncbi.nlm.nih.gov/pubchem/Compound/Extras/CID-Synonym-filtered.gz

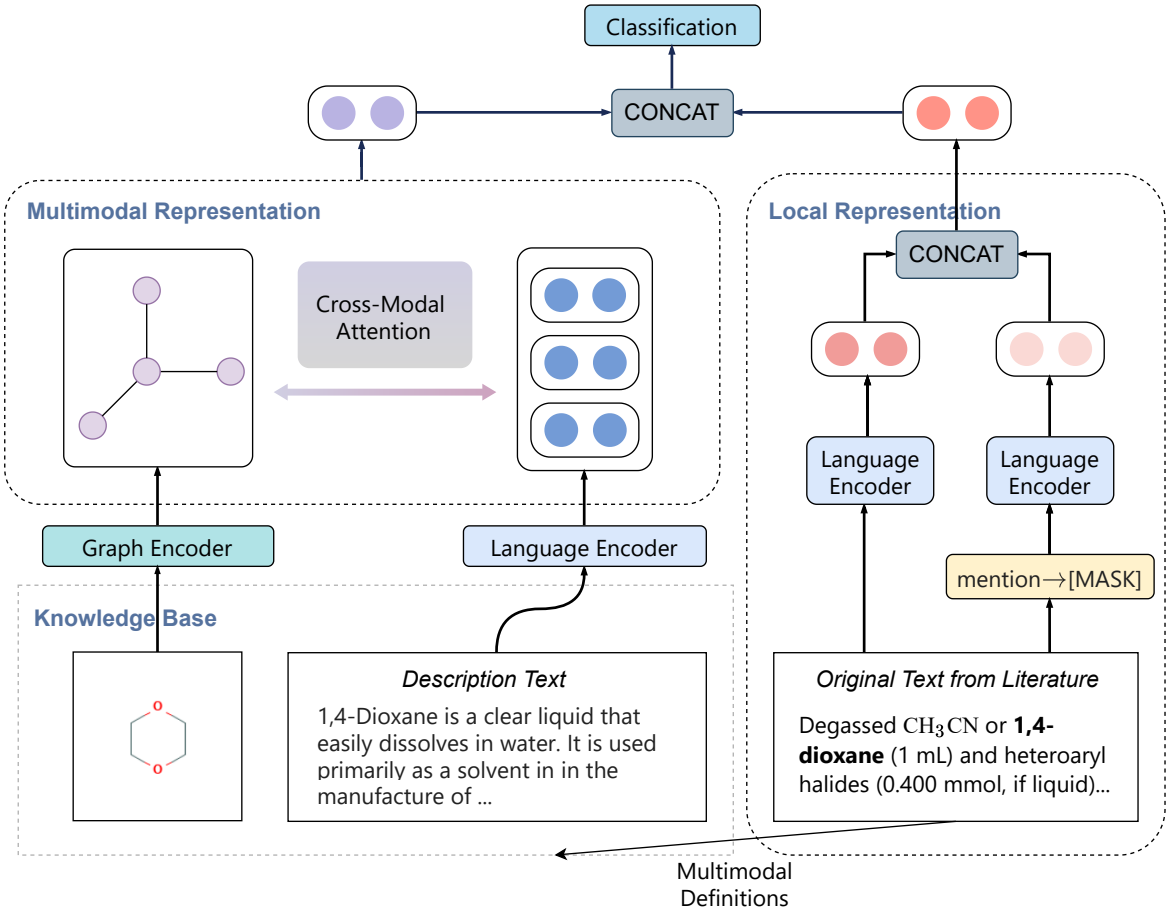


Figure 2: Our fine-grained chemical entity typing model architecture. Please refer to Section 3 for details. *Heng* **[1. label "KB" and "Literature"; 2. make font bigger. ]**

domly select the test samples from the corpus for annotation. In order to mitigate annotator bias, we distributed each sentence to three annotators, and take majority vote from the results. The dataset statistics is shown in Table 1.

## 3 Method

Chemistry literature is unique in that the mentions are often expressed in complex, unnatural forms, as shown in the snippet in Figure 2. At the same time, external databases contains multimedia definition about chemical entity, such as chemical structure and natural language description. It is thus a natural idea to incorporate these different forms of representation of an entity to enhance the system's understanding on a chemicals. In our methodology, we develop an effective deep learning based model to implement such idea.

The overall model architecture is presented in Figure 2. Given a sentence $S$ marked with mentions, we first extract external information (chemical structure and natural language description) by linking to PubChem, one of the mostly used chemical database; we use its search API to fetch entity information given a mention name. We also used a modified version of $S$ that mask the entire mention name, to combat the issue of complex chemical name (3.1). We then proceed to extract features from local context and from external multimodal definition. The multimodal features are passed through cross-attention stage (3.2) to learn a unified representation. Finally we use all features learned to classify the mention.

### 3.1 Original Text Embedding

Given the original sentence $S$, we first insert a marker symbol "*" at the start and end of the mention $m$ during preprocessing, following (Zhou et al., 2020); similar approach is also used in (Zhang et al., 2017; Shi and Lin, 2019). The model first encodes the original sentence with SciBERT (Beltagy et al., 2019), a Transformer (Vaswani et al., 2017) based language model pre-trained on biomedical text. Let $T = [t_1, t_2, ..., t_z]$ be the tokens in $S$ after

tokenization (we implicitly assume the presence of [CLS] and [SEP] tokens and omit them from for cleanness), where $z$ is the number of tokens. Then we pass the tokens into SciBERT to to obtain contextual representations:

$$[\mathbf{t}_1, \mathbf{t}_2, ..., \mathbf{t}_z] = \text{SciBERT}([t_1, t_2, ..., t_z]) \quad (1)$$

Where $\mathbf{T} = [\mathbf{t}_1, \mathbf{t}_2, ..., \mathbf{t}_z] \in \mathbb{R}^d$ and $d$ is the number of hidden dimensions. We then use the embedding of "*" before $m$ as the mention embedding. Let us denote the mention embedding as $\mathbf{m}$.

#### 3.1.1 Context-only Embedding

Since chemical entities often involve complex names that are difficult to be understood, we also produce a representation that rely less on the word structure of the mention, since the mention often not follows morphology (e.g., [3H]MK-801, NSC-406186, 8-azido-[alpha-32P]ATP). We first replace the entire span of mention by [MASK], then the modified sentence is embedded by SciBERT and the embedding for the [MASK] token is used as the corresponding context-only embedding for the mention, denoted $\mathbf{m}_{\text{MASK}}$. The context-focused embedding is then concatenated with mention embedding to represent local information, denoted by $\mathbf{m}_{\text{L}} = [\mathbf{m}; \mathbf{m}_{\text{MASK}}]$.

### 3.2 Multimodal Encoder

As one of our core contributions, we propose to incorporate multimodal definition to expand chemical representation, and to combat the difficulty of understanding complex chemical mention name (e.g., (E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid) purely based on context and morphological structure.

Specifically, we use API provided by PubChem as the entity linker to retrieve chemical structure and natural language description for each chemical mention. Chemical structure refers to a graph where bonds are edges and atoms are nodes, and description text discusses chemical properties (e.g., Aspirin is an orally administered non-steroidal antiinflammatory agent).

To learn concepts from multiple modalities that better correlate with target label and to build more accurate representation of a molecule, we made use of the recently successful attention mechanism to co-embed concepts (or molecule property) in text and substructure in chemical graph in order to capture interaction between different modalities.

Formally, let $G = (V, E)$ denote the chemical graph with $a$ nodes, and $D = [d_1, d_2, ..., d_b]$ denote the sequence of $b$ tokens after tokenizing description sentences. Similar to the embedding the sentence from literature, we embed the tokens with SciBERT for which output is $\mathbf{D} = [\mathbf{d}_1, \mathbf{d}_2, ..., \mathbf{d}_b]$. We also embed the nodes in chemical structure using Graph Isomorphism Network (with edge features) (Xu et al., 2018), a powerful graph neural network that can well capture different graph patterns. We randomly initialize embedding for each atom and bond type and use them to initialize node and edge embedding, and update node embeddings as below

$$\mathbf{n}_i^{l+1} = \text{FFNN}^{l+1}\left((1+\epsilon)\mathbf{n}_i^l + \sum_{j \in \mathcal{N}(i)} \mathbf{n}_j^l + \mathbf{e}_{j,i}^l\right) \quad (2)$$

where $\mathbf{n}_i^l \in \mathbb{R}^d$ is node representation for node $i$ at $l$-th layer, $\epsilon$ is a tuning hyperparameter, $\mathcal{N}(i)$ is the set of neighbours of node $i$, and FFNN is a feed forward neural network with two hidden layers (the first one maps from $\mathbb{R}^d$ to $\mathbb{R}^{2d}$ with Tanh activation, and the second one maps $\mathbb{R}^{2d}$ back to $\mathbb{R}^d$ without activation). We denote node representation $\mathbf{N} = [\mathbf{n}_1, \mathbf{n}_2, ..., \mathbf{n}_a]$.

We leverage self-attention mechanism of (Vaswani et al., 2017) to learn dependency between different modalities. To achieve this, we first stack node and token embeddings as

$$\mathbf{X} = \begin{pmatrix} \mathbf{N} \\ \mathbf{D} \end{pmatrix}, \ \mathbf{X} \in \mathbb{R}^d \quad (3)$$

where $\mathbf{X} \in \mathbb{R}^d$. Then the stacked embedding is passed through a Transformer layer to learn cross-modal association

$$[\tilde{\mathbf{n}}_1, \tilde{\mathbf{n}}_2, ..., \tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2...] = \text{Transformer}(\mathbf{X}) \quad (4)$$

and the cross-modal feature is then obtained by maxpooling the output from transformer layer

$$\mathbf{f}_{\text{cm}} = \text{MaxPool}([\tilde{\mathbf{n}}_1, \tilde{\mathbf{n}}_2, ..., \tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2...]) \quad (5)$$

In addition, we preserve the unimodal graph representation by mean pooling over the node representation $\mathbf{N}$, to get $\mathbf{f}_g$. We also use the [CLS] token embedding $\mathbf{d}_{[CLS]}$ to represent unimodal text features. We then obtain a the multimodal definition vector

$$\mathbf{f} = [\mathbf{f}_{\text{cm}}; \mathbf{f}_g; \mathbf{f}_{[CLS]}] \quad (6)$$

### 3.3 Final Prediction

Let E denote the set of entity types. Lastly, we predict the final entity type by using features from both local context and multimodal information

$$\mathbf{p} = \text{Sigmoid}(\text{FFNN}([\mathbf{m}_\text{L}; \mathbf{f}])) \tag{7}$$

where FFNN is a feed forward neural network mapping from $\mathbb{R}^d$ to $\mathbb{R}^{|\text{E}|}$. $\mathbf{p}$ is the final probability distribution of classes.

### 3.4 Training

We use multi-label soft margin loss for training, that is,

$$\mathcal{L} = \frac{1}{C}\sum_{i=1}^{C}\left(y_i \log\left(\frac{1}{1+e^{-x_i}}\right) + (1-y_i)\log\left(\frac{e^{-x_i}}{1+e^{-x_i}}\right)\right) \tag{8}$$

In the equation, $C$ is number of classes, $y_i$ indicates true (binary) label for class $i$ and $x_i$ is the predicted probability for class $i$.

## 4 Experiments

Since there is no other fine-grained chemical entity typing datasets, we evaluate fine-grained chemical entity typing on CHEMET. The experiments can be reproduced using implementations provided in Appendix B.

### 4.1 Baseline Methods

In the experiment, we compared our method with the following state-of-the-art baselines,

**SciBERT**. SciBert (Beltagy et al., 2019) is a Transformer based language model pretrained on sample of 1.14M papers from Semantic Scholar, in which 82% are from the broad biomedical domain. A linear layer is applied on the embedding of the marker "*" embedding for classification.

**SciBERT-D** and **SciBERT-G**. Based on Scibert, we also create variants that additionally use either description sentences (D) or chemical structure graph (G) as features.

**Latent Type Representation**. Lin and Ji (2019) used a hybrid classification method beyond binary relevance to exploit type inter-dependency with latent type representation

**Fine-Grained Entity Typing in Hyperbolic Space** Utilized hyperbolic embeddings. @Nik

### 4.2 Implementation Detail

Our model is implemented using PyTorch (Paszke et al., 2019) and Huggingface Transformers (Wolf et al., 2019) with SciBERT as text encoder. We left model parameters and reproducibility details in the appendix.

### 4.3 Result

Table 2 shows the overall result for developement and test set on CHEMET. We can see that our model achieves a higher performance on F1 than every other baseline. We can see a performance of SciBERT, which only uses the local context, is not as good as other baselines, and this shows the importance of incorporating non-local features, which adds information that assists disambiguating mention types. We can also see a clear increase of performance from SciBERT-D and SciBERT-G from our model, which shows the importance of incorporating multimodal definition for chemical entities in chemistry literature.

### 4.4 Ablation Study

To show the improvement made by each of the submodules in our method, we perform an ablation study on CHEMET developement set and show results in Table 3. For model [w/o graph] and [w/o description], we discard $\mathbf{f}_c m$ and correspondingly $\mathbf{f}_g$ or $\mathbf{d}_{\text{[CLS]}}$. For model [w/o cross-modal attention], we left out $\mathbf{f}_c m$, and For model [w/o context-only repr.], we keep every thing other than $\mathbf{m}_{\text{MASK}}$

### 4.5 Cross-Modal Attention Analysis

We show a heatmap visualization of transformer attention scores (between $[\mathbf{n}_1, \mathbf{n}_2, ...]$ and $[\mathbf{d}_1, \mathbf{d}_2, ...]$) in Figure 4 where lighter color corresponds to higher values. We take an example from the chemical . We show that the text concepts and graph substructure indeed have reasonable correlation with each other.

While we apply multimodal entity representation technique to fine-grained chemical entity typing, the idea can be well generalized to other ChemIE tasks such as relation extraction and reaction event extraction, in which chemical entities play a major role. We will release new datasets on other ChemIE task in the near future.

### 4.6 Qualitative Analysis

Here we analyzed the remaining errors and categorize the into different cases (shown in Figure 3). We discuss the most common ones below,

Table 2: FET performance on CHEMET

| Model | Dev | | | Test | | |
|---|---|---|---|---|---|---|
| | Accuracy | Macro F1 | Micro F1 | Accuracy | Macro F1 | Micro F1 |
| BioBERT | 1 | 2 | 3 | 1 | 2 | 3 |
| SciBERT | 1 | 2 | 3 | 1 | 2 | 3 |
| FETBSL1 | 1 | 2 | 3 | 1 | 2 | 3 |
| FETBSL2 | 1 | 2 | 3 | 1 | 2 | 3 |
| Our Model | 1 | 2 | 3 | 1 | 2 | 3 |

Table 3: Ablation Study

| Model | Macro-F1 | Micro-F1 |
|---|---|---|
| Full Model | 1 | 2 |
| w/o description | 1 | |
| w/o graph | 1 | 2 |
| w/o cross-modal attention | 1 | 2 |
| w/o context-only repr. | 1 | 2 |

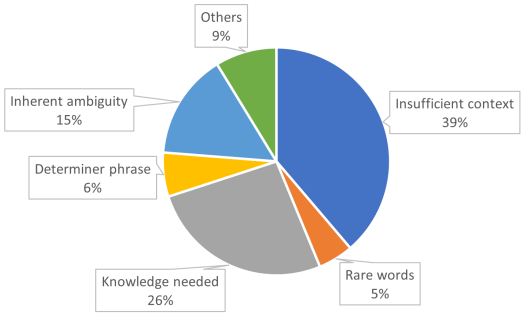


Figure 3: Distribution of remaining errors on the test set.

## 5 Related Work

### 5.1 Fine-Grained Entity Typing

There has been a wave of Fine-Grained Entity Typing (FET) methods in recent years (Choi et al., 2018; Xiong et al., 2019; Dai et al., 2019a; Lin and Ji, 2019; Jin et al., 2019; López et al., 2019). Xiong et al. (2019) propose to capture label correlation by employing graph convolution network on label co-occurrence matrix. Dai et al. (2019a) makes use of an existing entity linker to obtain noisy external data in order to enrich and disambiguate mention representation. The authors also use entity linking scores as additional features. Lin and Ji (2019) exploit type inter-dependency with latent type representation. Previous FET methods, however, only focused on news domain where text comes from news or wikipedia article and speech.

### 5.2 Multimodal Representation

Multi-modal knowledge representation methods have been widely applied to tasks such as visual question answering and cross-modal retrieval between image and text. One line of deep-learning based alignment methods (Diao et al., 2021; Wei et al., 2020; Ye et al., 2019; Nam et al., 2017; Li et al., 2020; Radford et al., 2021) involves cross-modal alignment between separately learned word and image region representation. A recent popular line of research, including VisualBERT (Li et al., 2019c) and VL-BERT(Su et al., 2019), integrates the reasoning process into pretraining, inspired from (Devlin et al., 2018). These models are fed with image-caption pairs and proceed to align regions and phrases by attention mechanism.

Different from alignment among image, text, and audio, our method involves cross-modal alignment between chemical structure and description text, which is a phenomenon specific to chemistry and has never been explored in previous work.

### 5.3 Knowledge-Enhanced Language Representation

Recently, there has been a lot of work (Peters et al., 2019; Zhang et al., 2019; Qin et al., 2020; He et al., 2020; Liu et al., 2020; Yang and Mitchell, 2019; Wang et al., 2020, 2021; Xu et al., 2021) on incorporating external knowledge into language understanding. In (Liu et al., 2020), triples are injected into the sentences as domain knowledge and attach to the tokens in the sentence. (Liu et al., 2020), on the other hand, embed words with KB concepts in an LSTM framework.

As a unique contribution, our work is the first to draw a line between local context and external (chemical) entity structure information.

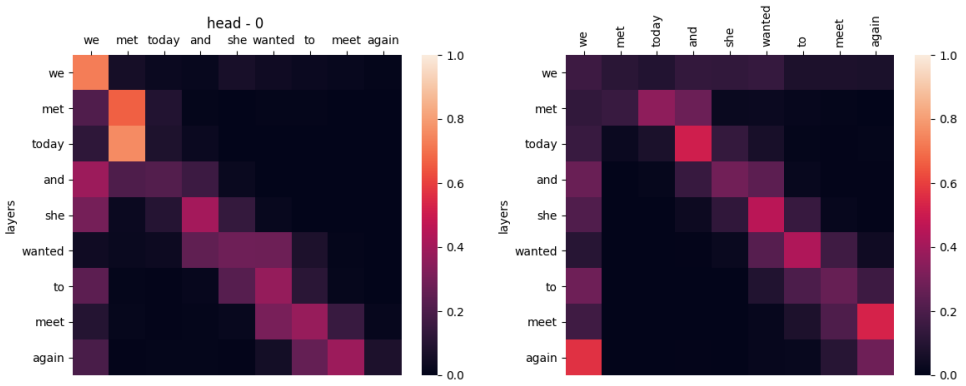


Figure 4: Attention visualization heatmap for chemical

### 5.4 Improve Information Extraction with External Knowledge

There have been recent studies on improve information extraction with external data (Dai et al., 2019b; Li et al., 2019d; Lai et al., 2021; Zhang and Ji, 2021; Zhang et al., 2021; Li et al., 2019b; Huang et al., 2020), to help enrich or disambiguate local information. In (Lai et al., 2021), the authors develop a model that aligns nodes in span graph and knowledge graph to learn a more distinctive concept embedding for joint biomedical entity and relation extraction. In (Zhang et al., 2021), the authors employ Abstract Meaning Representation (AMR) to uncover a clear semantic structure of sentences and used sentence-level knowledge graph to enrich the AMR graph. There, however, has not been work that takes in physical structures of entity to enrich representation.

## 6 Conclusions and Future Work

In this work, we take the first step to explore the task of fine-grained entity typing in chemistry domain and introduced a dataset, CHEMET, to facilitate the study of the task. Meanwhile, we also developed a deep-learning based model that effectively incorporates multimodal definition of chemical mentions to improve the model's understanding on chemistry text, and showed through experiments that our model achieved state-of-the-art on the dataset. We would like to point out that the multimodal entity representation can be applied to other ChemIE tasks.

One big challenge from our findings is that many chemicals cannot be linked to external database, either due to its varying mention form or the database simply does not contain that particular entity (which is relatively more obvious for newer chemistry articles). In the future, we will develop entity linking algorithm to not only match mention to database better but also do cross-document linking (i.e., retrieve context for a mention from other documents).

## 7 Introduction

These instructions are for authors submitting papers to EMNLP 2021 using LaTeX. They are not self-contained. All authors must follow the general instructions for *ACL proceedings,[7] as well as guidelines set forth in the EMNLP 2021 call for papers. This document contains additional instructions for the LaTeX style files.

The templates include the LaTeX source of this document (`emnlp2021.tex`), the LaTeX style file used to format it (`emnlp2021.sty`), an ACL bibliography style (`acl_natbib.bst`), an example bibliography (`custom.bib`), and the bibliography for the ACL Anthology (`anthology.bib`).

## 8 Engines

To produce a PDF file, pdfLaTeX is strongly recommended (over original LaTeX plus dvips+ps2pdf or dvipdf). XeLaTeX also produces PDF files, and is especially suitable for text in non-Latin scripts.

## 9 Preamble

The first line of the file must be

```
\documentclass[11pt]{article}
```

[7] http://acl-org.github.io/ACLPUB/formatting.html

To load the style file in the review version:

```
\usepackage[review]{emnlp2021}
```

For the final version, omit the `review` option:

```
\usepackage{emnlp2021}
```

To use Times Roman, put the following in the preamble:

```
\usepackage{times}
```

(Alternatives like txfonts or newtx are also acceptable.)

Please see the LaTeX source of this document for comments on other packages that may be useful.

Set the title and author using `\title` and `\author`. Within the author list, format multiple authors using `\and` and `\And` and `\AND`; please see the LaTeX source for examples.

By default, the box containing the title and author names is set to the minimum of 5 cm. If you need more space, include the following in the preamble:

```
\setlength\titlebox{<dim>}
```

where `<dim>` is replaced with a length. Do not set this length smaller than 5 cm.

# 10 Document Body

## 10.1 Footnotes

Footnotes are inserted with the `\footnote` command.[8]

## 10.2 Tables and figures

See Table 4 for an example of a table and its caption.
**Do not override the default caption sizes.**

## 10.3 Hyperlinks

Users of older versions of LaTeX may encounter the following error during compilation:

```
\pdfendlink ended up in
different nesting level
than \pdfstartlink.
```

This happens when pdfLaTeX is used and a citation splits across a page boundary. The best way to fix this is to upgrade LaTeX to 2018-12-01 or later.

| Command | Output | Command | Output |
|---|---|---|---|
| `{\"a}` | ä | `{\c c}` | ç |
| `{\^e}` | ê | `{\u g}` | ğ |
| `{\`i}` | ì | `{\l}` | ł |
| `{\.I}` | İ | `{\~n}` | ñ |
| `{\o}` | ø | `{\H o}` | ő |
| `{\'u}` | ú | `{\v r}` | ř |
| `{\aa}` | å | `{\ss}` | ß |

Table 4: Example commands for accented characters, to be used in, *e.g.*, BibTeX entries.

## 10.4 Citations

Table 5 shows the syntax supported by the style files. We encourage you to use the natbib styles. You can use the command `\citet` (cite in text) to get "author (year)" citations, like this citation to a paper by Gusfield (1997). You can use the command `\citep` (cite in parentheses) to get "(author, year)" citations (Gusfield, 1997). You can use the command `\citealp` (alternative cite without parentheses) to get "author, year" citations, which is useful for using citations within parentheses (e.g. Gusfield, 1997).

## 10.5 References

The LaTeX and BibTeX style files provided roughly follow the American Psychological Association format. If your own bib file is named `custom.bib`, then placing the following before any appendices in your LaTeX file will generate the references section for you:

```
\bibliographystyle{acl_natbib}
\bibliography{custom}
```

You can obtain the complete ACL Anthology as a BibTeX file from https://aclweb.org/anthology/anthology.bib.gz. To include both the Anthology and your own .bib file, use the following instead of the above.

```
\bibliographystyle{acl_natbib}
\bibliography{anthology,custom}
```

Please see Section 11 for information on preparing BibTeX files.

[8] This is a footnote.

| Output | natbib command | Old ACL-style command |
|---|---|---|
| (Gusfield, 1997) | \citep | \cite |
| Gusfield, 1997 | \citealp | no equivalent |
| Gusfield (1997) | \citet | \newcite |
| (1997) | \citeyearpar | \shortcite |

Table 5: Citation commands supported by the style file. The style is based on the natbib package and supports all natbib citation commands. It also supports commands defined in previous ACL style files for compatibility.

### 10.6 Appendices

Use \appendix before any appendix section to switch the section numbering over to letters. See Appendix **??** for an example.

## 11 BibTeX Files

Unicode cannot be used in BibTeX entries, and some ways of typing special characters can disrupt BibTeX's alphabetization. The recommended way of typing special characters is shown in Table 4.

Please ensure that BibTeX records contain DOIs or URLs when possible, and for all the ACL materials that you reference. Use the doi field for DOIs and the url field for URLs. If a BibTeX entry has a URL or DOI field, the paper title in the references section will appear as a hyperlink to the paper, using the hyperref LaTeX package.

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# A Dataset Ontology

# B Hyperparameters

| | | | | |
|---|---|---|---|---|
| Chemistry | Organic_Chemistry | Organic_Compounds | Aromatic_Compounds | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Aromatic_Compounds | Aryl_Groups |
| Chemistry | Organic_Chemistry | Organic_Compounds | Carbenes | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Esters | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Ethers | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Hydrocarbons | Alkanes |
| Chemistry | Organic_Chemistry | Organic_Compounds | Hydrocarbons | Alkenes |
| Chemistry | Organic_Chemistry | Organic_Compounds | Hydrocarbons | Alkynes |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Acids | Carboxylic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Acids | Phosphonic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Acids | Phosphinic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Acids | Sulphinic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Acids | Sulphonic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organohalides | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organometallic_Compounds | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organonitrogen_Compounds | Amides |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organonitrogen_Compounds | Amines |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organonitrogen_Compounds | Nitriles |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organonitrogen_Compounds | Nitro_Compounds |
| Chemistry | Organic_Chemistry | Organic_Compounds | Heterocyclic_Compounds | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organophosphorus_Compounds | Phosphinic_Acids_And_Derivatives |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organophosphorus_Compounds | Phosphonic_Acids_And_Derivatives |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organosulfur_Compounds | Sulfonic_Acids |
| Chemistry | Organic_Chemistry | Organic_Compounds | Polycyclic_Organic_Compounds | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Organic_Polymers | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Reactive_Intermediates | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Thiols | |
| Chemistry | Organic_Chemistry | Organic_Compounds | Other_Compounds | |
| Chemistry | Organic_Chemistry | Functional_Groups | Carbonyl_Group | Ketones |
| Chemistry | Organic_Chemistry | Functional_Groups | Carbonyl_Group | |
| Chemistry | Organic_Chemistry | Functional_Groups | Hydroxyl_Group | |
| Chemistry | Organic_Chemistry | Functional_Groups | Acyl_Groups | |
| Chemistry | Organic_Chemistry | Functional_Groups | Amides | |
| Chemistry | Organic_Chemistry | Functional_Groups | Amines | |
| Chemistry | Organic_Chemistry | Functional_Groups | Esters | |
| Chemistry | Organic_Chemistry | Functional_Groups | Ethers | |
| Chemistry | Organic_Chemistry | Functional_Groups | Nitriles | |
| Chemistry | Inorganic_Chemistry | Inorganic_Compounds | | |
| Chemistry | Chemical_Reactions | Catalysis | Catalysts | |

Figure 5: Ontology Screenshot