Final Project

This notebook is adapted from here:
https://aiqm.github.io/torchani/examples/nnp_training.html

Checkpoint 1: Data preparation

1. Create a working directory: `/global/scratch/users/[USER_NAME]/[DIR_NAME]`. Replace the [USER_NAME] with yours and specify a [DIR_NAME] you like.
2. Copy this Jupyter Notebook to the working directory
3. Download the ANI dataset `ani_dataset_gdb_s01_to_s04.h5` from bCourses and upload it to the working directory
4. Complete this notebook (can be worked on with your laptop, but **must be run on the cluster** for the final outputs)

Hint: You can use ? to learn more about any python function, e.g. ?torch.nn.Linear

In [1]:
```
!pwd
```

```
/global/home/users/cah051/chem277b_final
```

In [2]:
```
import warnings
warnings.filterwarnings("ignore", category=UserWarning)
import numpy as np
from tqdm import tqdm
import torch
from torch.utils.data import DataLoader
import torch.nn as nn
import torchani
import torchani.data
```

Use GPU

In [3]:
```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)
```

```
cpu
```

Set up AEV computer

AEV: Atomic Environment Vector (atomic features)

Ref: Chem. Sci., 2017, 8, 3192

In [4]:
```
def init_aev_computer():
    Rcr = 5.2
    Rca = 3.5
    EtaR = torch.tensor([16], dtype=torch.float, device=device)
```

```
    ShfR = torch.tensor([
        0.900000, 1.168750, 1.437500, 1.706250,
        1.975000, 2.243750, 2.512500, 2.781250,
        3.050000, 3.318750, 3.587500, 3.856250,
        4.125000, 4.393750, 4.662500, 4.931250
    ], dtype=torch.float, device=device)


    EtaA = torch.tensor([8], dtype=torch.float, device=device)
    Zeta = torch.tensor([32], dtype=torch.float, device=device)
    ShfA = torch.tensor([0.90, 1.55, 2.20, 2.85], dtype=torch.float, device=dev
    ShfZ = torch.tensor([
        0.19634954, 0.58904862, 0.9817477, 1.37444680,
        1.76714590, 2.15984490, 2.5525440, 2.94524300
    ], dtype=torch.float, device=device)

    num_species = 4
    aev_computer = torchani.AEVComputer(
        Rcr, Rca, EtaR, ShfR, EtaA, Zeta, ShfA, ShfZ, num_species
    )
    return aev_computer

aev_computer = init_aev_computer()
aev_dim = aev_computer.aev_length
print(aev_dim)
```

```
384
```

Prepare dataset & split

In [5]:
```
def load_ani_dataset(dspath):
    self_energies = torch.tensor([
        0.500607632585, -37.8302333826,
        -54.5680045287, -75.0362229210
    ], dtype=torch.float, device=device)
    energy_shifter = torchani.utils.EnergyShifter(None)
    species_order = ['H', 'C', 'N', 'O']

    dataset = torchani.data.load(dspath)
    dataset = dataset.subtract_self_energies(energy_shifter, species_order)
    dataset = dataset.species_to_indices(species_order)
    dataset = dataset.shuffle()
    return dataset

dataset = load_ani_dataset("ani_gdb_s01_to_s04.h5")
```

In [6]:
```
# Use dataset.split method to do split
train_data, val_data, test_data = dataset.split(0.8, 0.1, None)

# Show amount of training data vs total data
print("Training data size:", len(train_data))
print("Validation data size:", len(val_data))
print("Test data size:", len(test_data))
print("Total data size:", len(dataset))
# assert(len(dataset) == len(val_data) + len(test_data) + len(train_data))
print(691918 + 86489 * 2)
```

```
Training data size: 691918
Validation data size: 86489
Test data size: 86491
Total data size: 864898
864896
```

Batching

In [7]:
```python
batch_size = 8192
# use dataset.collate(...).cache() method to do batching

train_data_loader = train_data.collate(batch_size).cache()
val_data_loader = val_data.collate(batch_size).cache()
test_data_loader = test_data.collate(batch_size).cache()
```

In [8]:
```python
# Show that batching is working correctly
train_data_loader_list = list(train_data_loader)
train_data_loader_list
```

Out[8]:
```
[defaultdict(list,
             {'species': tensor([[ 1,  3,  1,  ..., -1, -1, -1],
                     [ 1,  1,  1,  ...,  0, -1, -1],
                     [ 2,  1,  1,  ..., -1, -1, -1],
                     ...,
                     [ 3,  1,  1,  ..., -1, -1, -1],
                     [ 1,  1,  1,  ..., -1, -1, -1],
                     [ 3,  2,  1,  ..., -1, -1, -1]]),
              'coordinates': tensor([[[-1.1798, -0.1810,  0.0135],
                      [ 0.0076,  0.5872, -0.0313],
                      [ 1.1543, -0.1982,  0.0168],
                      ...,
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]],

                     [[ 1.2710, -0.6315,  0.0998],
                      [-0.0238,  0.0491, -0.3697],
                      [-1.2936, -0.6566,  0.0970],
                      ...,
                      [ 0.0663,  1.3313,  0.9864],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]],

                     [[ 1.5292, -0.5563, -0.1509],
                      [ 0.5789,  0.6241,  0.0566],
                      [-0.7831,  0.0703,  0.1310],
                      ...,
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]],

                     ...,

                     [[ 1.4368, -0.1143, -0.1775],
                      [ 0.2461,  0.0067,  0.4819],
                      [-0.8549,  0.7809, -0.1303],
                      ...,
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]],

                     [[ 1.4478, -0.4993,  0.0032],
                      [ 0.5233,  0.7326, -0.0351],
                      [-0.8278,  0.1537, -0.0830],
                      ...,
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]],

                     [[ 1.3134, -0.5351, -0.1324],
                      [ 0.5821,  0.6378,  0.1231],
                      [-0.8073,  0.4931,  0.0164],
                      ...,
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000],
                      [ 0.0000,  0.0000,  0.0000]]]),
              'energies': tensor([-0.0033, -0.0391,  0.0485,  ..., -0.0076, -
0.0183,  0.0017],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  3,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.8008, -0.3833,  0.3399],
                     [ 0.6719,  0.3059,  0.0262],
                     [-0.6707, -0.2899, -0.1753],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.0576, -0.1666, -0.1057],
                     [ 0.1651,  0.4555,  0.0050],
                     [ 1.1662, -0.2826,  0.0239],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1460, -0.1943, -0.0071],
                     [-0.0094,  0.6126, -0.0107],
                     [ 1.1622, -0.2101,  0.0078],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 0.0025, -1.0662,  0.0492],
                     [ 1.0353,  0.0678, -0.0693],
                     [ 0.0046,  1.0633,  0.0975],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0268, -0.2205,  1.1926],
                     [-0.0487,  0.5991, -0.0106],
                     [-0.0166, -0.2346, -1.1774],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.3764, -0.3919, -0.0289],
                     [-0.4762,  0.6964,  0.0058],
                     [ 0.8167,  0.4475, -0.0421],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0012,  0.0248, -0.0053,  ..., -0.0143, -
0.0054, -0.0597],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.7032, -0.1645, -0.0698],
                     [ 0.3850,  0.4308,  0.1409],
                     [-0.5960, -0.4519,  0.0278],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0059, -1.1064, -0.1472],
                     [ 1.0073,  0.0580,  0.1897],
                     [-0.0195,  1.1012, -0.2816],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0782, -0.0669,  1.9077],
                     [-0.0761,  0.1167,  0.7104],
                     [-0.0053,  0.0366, -0.7237],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.4090, -0.5840,  0.0269],
                     [-0.6744,  0.6413, -0.2759],
                     [ 0.7311,  0.5958,  0.3022],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2946, -0.6335,  0.0342],
                     [-0.6555,  0.6250, -0.2918],
                     [ 0.7538,  0.6517,  0.2771],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4398,  0.0236, -0.2300],
                     [-0.2056,  0.0193,  0.4664],
                     [ 0.8954,  0.7545, -0.1394],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0053,  0.0593,  0.0826,  ..., -0.0184, -
0.0063, -0.0130],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ...,  0, -1, -1],
                    ...,
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.3064, -0.5229,  0.0130],
                     [-0.5584,  0.7489,  0.0065],
                     [ 0.9224,  0.4429, -0.0182],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4950, -0.4203, -0.0946],
                     [ 0.5040,  0.6299,  0.2247],
                     [-0.8184,  0.4606, -0.0603],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5038,  0.5335, -0.0661],
                     [ 0.6003, -0.6396,  0.2226],
                     [-0.6656, -0.5744, -0.3775],
                     ...,
                     [-1.5630,  0.4724,  1.2232],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-0.1320,  1.3746,  0.0613],
                     [-0.0299,  0.0118, -0.3349],
                     [ 1.2283, -0.5399,  0.0661],
                     ...,
                     [-0.9843, -1.9383, -0.2508],
                     [-1.2876, -0.8438,  1.0918],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.8171, -0.3542,  0.3619],
                     [ 0.6310,  0.2695,  0.0479],
                     [-0.6261, -0.3093, -0.2312],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7426,  0.0894, -0.1001],
                     [-0.4575, -0.4675,  0.1359],
                     [ 0.6242,  0.3445,  0.0823],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0238,  0.0485, -0.0292,  ...,  0.0147,
0.0161,  0.0005],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 3,  2,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.9246e+00, -1.3995e-01,  5.4679e-02],
                     [ 5.6925e-01,  5.3969e-01, -1.0445e-01],
                     [-6.0007e-01, -4.7984e-01, -3.8140e-03],
                     ...,
                     [-2.0951e+00,  7.6528e-01,  7.7311e-01],
                     [-2.6547e+00, -5.4726e-01, -1.4724e-02],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4040e+00, -3.2828e-01, -7.3313e-03],
                     [ 5.9704e-02,  1.3558e-01, -2.0728e-02],
                     [ 1.0723e+00, -8.2607e-01,  6.4582e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.0470e+00,  2.5486e-01, -6.4050e-04],
                     [-1.4710e-01, -5.2528e-01,  1.1445e-03],
                     [ 1.0660e+00,  7.4774e-02, -1.0986e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.2066e+00, -2.5255e-01, -3.1946e-02],
                     [ 1.6065e-02,  5.6917e-01,  9.9403e-02],
                     [ 1.1861e+00, -3.1393e-01, -1.6713e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-5.7255e-02, -8.8096e-01,  9.0359e-03],
                     [ 7.7016e-01,  4.0047e-01, -1.1036e-02],
                     [-7.0460e-01,  4.7847e-01,  6.7406e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1066e+00,  1.5009e-01, -1.0087e-01],
                     [ 8.4826e-02, -5.3012e-01,  5.1952e-03],
                     [ 1.1408e+00,  1.6887e-01,  1.0450e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0321,  0.0234,  0.0274,  ...,  0.0030,
0.0021,  0.0042],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  3,  ...,  0, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.6268e+00,  4.3150e-01, -1.8552e-01],
                     [ 5.5600e-01, -5.4014e-01,  2.7657e-01],
                     [-6.2042e-01, -4.3063e-01, -4.2220e-01],
                     ...,
                     [-2.2182e+00, -2.3486e-01,  1.2171e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 7.5300e-01, -3.1079e-04, -2.4437e-03],
                     [-7.5285e-01, -1.1358e-03,  8.8117e-04],
                     [ 1.2059e+00,  9.8742e-01, -3.0409e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2095e-02, -2.4442e-01,  1.1678e+00],
                     [-8.8686e-02,  6.5039e-01,  2.8876e-02],
                     [ 1.9109e-02, -2.3800e-01, -1.1846e+00],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.4764e+00, -4.8973e-01,  2.6764e-04],
                     [-5.2848e-01,  7.1094e-01,  6.7220e-02],
                     [ 7.5968e-01,  7.0911e-01,  5.1630e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5033e+00, -1.0071e-01, -1.5412e-01],
                     [ 2.4459e-01, -9.1419e-03,  4.4157e-01],
                     [-8.8628e-01,  7.6379e-01, -1.3493e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4398e+00,  3.9284e-02, -1.9625e-01],
                     [-2.4225e-01, -4.2259e-02,  4.4899e-01],
                     [ 8.9169e-01,  7.4004e-01, -1.4018e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0769, -0.0074,  0.0190,  ...,  0.1629, -
0.0082, -0.0006],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0,  0,  0],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.7425e+00, -1.3101e-01, -2.1500e-02],
                     [ 3.7100e-01,  3.6193e-01,  2.1828e-01],
                     [-5.9974e-01, -4.4541e-01, -2.1067e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-2.1484e-02,  2.9849e-02,  1.9226e+00],
                     [ 7.1196e-03, -8.9264e-02,  6.7918e-01],
                     [ 4.4627e-02,  2.3557e-02, -7.0334e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1516e+00, -2.1902e-01, -9.3056e-04],
                     [-5.1803e-03,  6.2843e-01, -9.0859e-03],
                     [ 1.1395e+00, -1.9776e-01,  2.6631e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.9852e+00, -1.5727e-01, -1.2112e-01],
                     [ 5.3911e-01,  5.4924e-01,  9.1642e-02],
                     [-5.5421e-01, -5.0291e-01,  8.6527e-02],
                     ...,
                     [-2.1930e+00,  4.4954e-01, -1.2170e+00],
                     [-2.7091e+00, -6.5803e-01,  1.6996e-01],
                     [-2.0865e+00,  1.0760e+00,  6.1367e-01]],

                    [[-1.2066e+00,  1.2828e-02,  1.7840e-02],
                     [ 2.9277e-01, -8.5396e-02,  6.3240e-02],
                     [ 1.4598e+00,  4.6787e-02, -4.1602e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4803e+00, -4.8815e-01,  3.8089e-04],
                     [ 5.4693e-01,  7.1475e-01,  2.3110e-02],
                     [-7.5389e-01,  6.9154e-01,  3.1079e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.3469,  0.0823,  0.0063,  ..., -0.0057, -
0.0332, -0.0105],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.1957e+00, -5.0025e-01,  9.8049e-03],
                     [ 2.3189e-02,  4.2416e-01,  3.0793e-02],
                     [ 1.3261e+00,  1.8953e-01, -2.9508e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3787e-01, -1.2410e-02,  1.9063e+00],
                     [ 1.4696e-01,  2.2576e-02,  6.9826e-01],
                     [ 1.6118e-01, -5.5986e-02, -6.9206e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 3.5645e-02, -1.4813e-03,  1.8817e+00],
                     [-1.5684e-02, -1.6597e-02,  6.9361e-01],
                     [-7.4997e-02,  2.3913e-02, -7.0225e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 9.4485e-03, -1.0670e+00, -8.3338e-02],
                     [ 1.0352e+00,  5.4104e-02,  1.1432e-01],
                     [-8.2307e-03,  1.0802e+00, -1.4901e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5899e+00, -4.8727e-01,  8.3233e-02],
                     [-6.8640e-01,  5.7813e-01, -3.5095e-01],
                     [ 7.3151e-01,  5.1974e-01,  2.9322e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7368e+00,  1.3302e-01, -7.9583e-02],
                     [-3.8099e-01, -3.9229e-01,  1.7346e-01],
                     [ 7.4327e-01,  3.8541e-01,  2.5499e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0275,  0.0828,  0.0722,  ..., -0.0072, -
0.0167, -0.0358],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-1.2213, -0.1195, -0.0268],
                     [ 0.2290,  0.3428,  0.1349],
                     [ 1.2620, -0.2553, -0.1044],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.1455,  1.3284,  0.0983],
                     [ 0.0151,  0.0041, -0.4042],
                     [ 1.2327, -0.5408,  0.0380],
                     ...,
                     [-0.7686, -2.0390,  0.2021],
                     [-1.5496, -0.4577,  1.1848],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7256,  0.1453, -0.0205],
                     [-0.3800, -0.4367,  0.0945],
                     [ 0.7095,  0.3495,  0.0135],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.5368, -0.5073,  0.1220],
                     [-0.6226,  0.6442, -0.3006],
                     [ 0.7705,  0.5438,  0.3038],
                     ...,
                     [ 1.5114, -0.6445, -1.0283],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2493, -0.2795, -0.0338],
                     [ 0.1059,  0.6028,  0.0031],
                     [ 1.2647, -0.2590, -0.0806],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2746, -0.6821,  0.0881],
                     [ 0.0031,  0.0144, -0.3794],
                     [-1.2202, -0.6102,  0.1218],
                     ...,
                     [-0.2505,  1.4627,  1.0023],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
              'energies': tensor([ 0.0227,  0.0300, -0.0585,  ..., -0.0397, -
0.0020, -0.0266],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ...,  0,  0, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.5334e+00,  4.8379e-01, -1.5398e-01],
                     [-6.4428e-01, -5.6377e-01,  3.2937e-01],
                     [ 6.5153e-01, -6.3059e-01, -3.1096e-01],
                     ...,
                     [ 1.8190e+00,  2.7943e-01,  1.2782e+00],
                     [ 2.5394e+00,  1.9881e-01, -3.0917e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6618e+00,  2.0986e-01, -1.0242e-01],
                     [ 4.4140e-01, -4.7717e-01,  8.1571e-02],
                     [-6.4765e-01,  3.4796e-01, -1.0296e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4212e+00, -1.3029e-02, -2.4863e-01],
                     [-2.0503e-01,  3.2252e-02,  5.1105e-01],
                     [ 9.1980e-01,  7.8322e-01, -1.4090e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.1378e+00, -5.0590e-01, -3.9313e-03],
                     [ 1.4078e-03,  4.7138e-01,  1.1766e-02],
                     [ 1.2813e+00,  1.5918e-01, -8.5551e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7333e+00, -4.3718e-02,  8.7210e-02],
                     [-4.4647e-01,  4.5828e-01, -1.3955e-01],
                     [ 6.4811e-01, -3.7365e-01, -5.7841e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4219e+00, -1.5329e-01, -6.3330e-03],
                     [ 8.2913e-02,  1.1380e-01,  3.8165e-02],
                     [ 8.7754e-01, -9.9609e-01, -3.1717e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0002, -0.0048, -0.0056,  ..., -0.0049, -
0.0209, -0.0580],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  2,  ...,  0,  0, -1],
                    ...,
                    [ 2,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.0654, -0.1615, -0.0305],
                     [ 0.1621,  0.4109, -0.0048],
                     [ 1.1755, -0.2560,  0.0055],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5905,  0.4904, -0.1418],
                     [ 0.5802, -0.5706,  0.3079],
                     [-0.6234, -0.4817, -0.4030],
                     ...,
                     [-1.8437,  0.0261,  1.1668],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.6279,  0.4944, -0.1915],
                     [-0.6176, -0.5841,  0.3530],
                     [ 0.6479, -0.5353, -0.3042],
                     ...,
                     [ 2.1650,  0.1071,  1.2567],
                     [ 2.4674,  0.3187, -0.6610],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.9293, -0.0594, -0.0629],
                     [ 0.6144,  0.5417,  0.0458],
                     [-0.5409, -0.4642,  0.0701],
                     ...,
                     [-2.0282,  1.0401,  0.4777],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.6095, -0.4162, -0.0036],
                     [ 0.4721,  0.5817, -0.0252],
                     [-0.8877,  0.1225,  0.0571],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4498, -0.0162, -0.3000],
                     [-0.1608,  0.0154,  0.5629],
                     [ 0.9382,  0.7193, -0.1569],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0589, -0.0119,  0.0063,  ..., -0.0055, -
0.0410,  0.0055],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  1,  1,  ..., -1, -1, -1],
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                    [ 1,  1,  3,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.5678, -0.4592, -0.1183],
                     [ 0.5679,  0.5183,  0.0267],
                     [-0.7834,  0.0182,  0.0137],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.9129, -0.1578, -0.1219],
                     [ 0.5649,  0.5496,  0.1491],
                     [-0.5186, -0.4904,  0.1285],
                     ...,
                     [-1.9779,  0.5674, -1.1323],
                     [-2.7087, -0.7681, -0.0215],
                     [-2.4117,  0.9028,  0.5780]],

                    [[ 1.5845,  0.4692, -0.1747],
                     [ 0.5807, -0.5816,  0.3461],
                     [-0.6203, -0.4766, -0.4405],
                     ...,
                     [-2.1048, -0.1137,  1.1721],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-0.6310,  0.0320, -0.0517],
                     [ 0.6373, -0.0492,  0.0632],
                     [-1.3383, -0.7306,  0.1072],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.3003, -0.5502, -0.1232],
                     [ 0.6022,  0.6645,  0.1249],
                     [-0.8097,  0.4845,  0.0415],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4324, -0.5006,  0.0041],
                     [-0.5466,  0.7199, -0.0065],
                     [ 0.9265,  0.4304,  0.0030],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0317, -0.0213,  0.0119,  ...,  0.0287,
0.0068, -0.0533],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4838e+00,  1.1278e-01, -1.2887e-01],
                     [ 1.5624e-01, -7.9936e-02,  4.9795e-01],
                     [-1.0131e+00,  6.4917e-01, -1.4332e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 6.4973e-02,  3.6832e-02, -1.8330e+00],
                     [-6.7050e-02, -3.4823e-02, -6.3584e-01],
                     [-6.6996e-02, -1.3661e-01,  7.3490e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-7.2785e-01, -3.6274e-01, -1.1012e-02],
                     [ 7.3444e-01, -3.5916e-01, -6.7046e-03],
                     [-1.1651e-02,  8.5049e-01,  8.8495e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.1607e+00, -8.4733e-01,  8.7353e-02],
                     [ 2.2719e-02, -2.3060e-02, -4.0672e-01],
                     [ 1.4328e+00, -4.8169e-01,  7.3768e-02],
                     ...,
                     [-1.7191e-01,  1.1880e+00,  1.0994e+00],
                     [-1.2810e+00,  1.6098e+00,  1.7643e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4507e+00, -1.4748e-02, -2.3911e-01],
                     [-2.0423e-01,  3.2975e-02,  4.8537e-01],
                     [ 9.2355e-01,  7.4230e-01, -1.3396e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4537e+00, -1.1196e-01, -1.0427e-02],
                     [ 4.6400e-02,  1.5177e-01, -3.1336e-02],
                     [ 8.0803e-01, -1.0351e+00,  9.8268e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0394,  0.0163,  0.0137,  ...,  0.0060, -
0.0212,  0.0800],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  2,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  2,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[ 1.9556,  0.0192,  0.0433],
                     [ 0.5854,  0.4407, -0.1099],
                     [-0.6246, -0.5609, -0.0034],
                     ...,
                     [-2.0569,  0.4314,  1.0918],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4033,  0.6108, -0.0669],
                     [-0.6365, -0.6541,  0.2582],
                     [ 0.7193, -0.7781, -0.2178],
                     ...,
                     [ 1.5910,  0.7349,  1.1053],
                     [ 2.4001,  0.5221, -0.3755],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4069, -0.5001,  0.0154],
                     [ 0.6968,  0.6341, -0.0341],
                     [-0.8334,  0.4799,  0.0571],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.1683, -0.5785,  0.0288],
                     [ 0.0090,  0.1161,  0.0206],
                     [-1.1635, -0.5842,  0.0051],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5959,  0.2107,  0.1623],
                     [-0.5926, -0.3321, -0.4340],
                     [ 0.6046, -0.3385,  0.4320],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4759, -0.4924,  0.1893],
                     [-0.6199,  0.7208, -0.3395],
                     [ 0.7325,  0.5176,  0.3397],
                     ...,
                     [ 1.9603, -0.3958, -1.0299],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0058, -0.0077, -0.0243,  ..., -0.0907,
0.0103,  0.0088],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-7.8199e-01,  7.9845e-01,  2.9530e-03],
                     [-7.6292e-01, -7.8368e-01,  1.1244e-04],
                     [ 7.8522e-01, -7.8383e-01,  1.2097e-02],
                     ...,
                     [ 1.2298e+00,  1.2007e+00, -8.9938e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5889e+00, -3.9240e-01, -5.5786e-03],
                     [-6.7608e-01,  4.2032e-01,  1.6899e-03],
                     [ 7.4061e-01, -3.7788e-03,  3.5983e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4292e+00, -5.7181e-01,  4.7596e-02],
                     [-6.8604e-01,  7.1934e-01, -2.7990e-01],
                     [ 8.2354e-01,  6.1971e-01,  2.6927e-01],
                     ...,
                     [ 8.7405e-01, -1.2290e+00, -1.0201e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.4033e+00, -2.0779e-02,  1.1687e-01],
                     [ 1.3021e-01,  1.8836e-03, -5.7795e-01],
                     [-8.5357e-01, -7.2289e-01,  1.5632e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.0036e-03,  1.0769e+00, -7.6517e-02],
                     [-1.0441e+00, -4.2539e-02,  9.3287e-02],
                     [ 1.8202e-03, -1.0264e+00, -2.3644e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.9020e-02, -2.1728e-01,  1.2181e+00],
                     [-5.1861e-02,  5.7890e-01, -5.1027e-03],
                     [-9.7243e-03, -2.1931e-01, -1.2065e+00],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0241, -0.0431,  0.0327,  ...,  0.0133, -
0.0192, -0.0141],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 2,  2,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.8120e+00, -3.2470e-01,  4.1032e-01],
                     [ 6.5678e-01,  2.5036e-01,  5.8617e-03],
                     [-6.8670e-01, -3.5752e-01, -3.0313e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 7.0755e-01,  1.0130e-01,  1.1331e-01],
                     [-6.9412e-01,  4.4874e-02, -1.1736e-01],
                     [ 9.4415e-01, -7.1088e-01,  3.8922e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4484e+00, -4.9139e-01,  1.3011e-01],
                     [-6.2014e-01,  6.5152e-01, -3.3897e-01],
                     [ 7.1370e-01,  5.4166e-01,  3.1723e-01],
                     ...,
                     [ 1.3563e+00, -6.5366e-01, -1.0173e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.6117e+00, -4.8943e-01, -9.1470e-03],
                     [ 5.6497e-01,  6.3785e-01, -2.7072e-02],
                     [-8.5845e-01,  1.5804e-01,  7.4187e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3591e+00, -4.9203e-01,  1.2049e-02],
                     [ 4.9069e-01,  6.7369e-01,  1.4853e-02],
                     [-8.5494e-01,  5.4559e-01, -2.6072e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 8.8192e-04,  1.0794e+00, -1.2887e-01],
                     [-1.0257e+00, -7.6161e-02,  1.5847e-01],
                     [-3.8928e-02, -9.8207e-01, -3.2180e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0079,  0.0548, -0.0065,  ...,  0.0166, -
0.0234,  0.0040],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ...,  0,  0, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[ 1.6067e+00, -4.5981e-01,  1.2906e-02],
                     [ 4.5298e-01,  6.3904e-01,  3.2610e-03],
                     [-8.8032e-01,  6.0685e-02, -9.5687e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7000e+00,  8.5468e-02, -1.2678e-01],
                     [-4.2792e-01, -5.1905e-01,  3.8546e-02],
                     [ 5.8911e-01,  3.8627e-01,  2.8161e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5009e+00,  5.7827e-01, -6.8945e-02],
                     [-6.1596e-01, -6.2618e-01,  2.5127e-01],
                     [ 7.1285e-01, -6.7036e-01, -2.7138e-01],
                     ...,
                     [ 1.2175e+00,  8.5417e-01,  1.2271e+00],
                     [ 2.6471e+00,  2.0198e-01,  1.3446e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 5.6624e-02, -3.9714e-01,  7.4937e-01],
                     [ 3.0201e-02, -3.9574e-01, -7.5571e-01],
                     [ 3.3662e-02,  8.6262e-01,  1.5084e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1375e+00, -5.2387e-01,  5.3097e-03],
                     [ 1.8685e-03,  5.0932e-01, -6.0030e-03],
                     [ 1.2984e+00,  1.5567e-01,  2.8882e-04],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3890e+00,  6.3799e-01, -6.7761e-02],
                     [-6.2111e-01, -6.6591e-01,  2.8780e-01],
                     [ 7.2700e-01, -7.5194e-01, -2.4897e-01],
                     ...,
                     [ 1.0873e+00,  9.2558e-01,  1.2159e+00],
                     [ 2.4688e+00,  4.2299e-01, -2.7775e-02],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0454,  0.1122, -0.0054,  ...,  0.0089, -
0.0021,  0.0136],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  1,  3,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ...,  0, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.2873, -0.1852,  0.0034],
                     [ 0.0639, -0.1388, -0.0183],
                     [ 0.4584,  1.1461,  0.0106],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.9121, -0.0845, -0.0228],
                     [ 0.5806,  0.5605, -0.0252],
                     [-0.5298, -0.4474,  0.0786],
                     ...,
                     [-2.1727,  0.6610,  0.7152],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.6211,  0.1636,  0.1784],
                     [-0.5610, -0.2885, -0.4316],
                     [ 0.5817, -0.3224,  0.4588],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 0.6923,  0.0036,  0.0036],
                     [-0.7389, -0.0209, -0.1066],
                     [ 0.9930, -0.8247, -0.2215],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.0737, -0.9508,  0.1405],
                     [-0.0547,  0.0411, -0.4035],
                     [ 1.3432, -0.5041,  0.1178],
                     ...,
                     [-0.2722,  1.5128,  1.0307],
                     [-0.9875,  1.8442, -0.2921],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5776, -0.3613, -0.2967],
                     [ 0.5885,  0.5727,  0.3507],
                     [-0.6950, -0.2474,  0.4371],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.1038, -0.0314,  0.0441,  ...,  0.3045, -
0.0203, -0.0068],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.2283e+00, -5.9859e-01, -3.2737e-02],
                     [ 6.2009e-01,  6.5329e-01,  3.2811e-02],
                     [-8.0847e-01,  5.1438e-01, -2.3394e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3002e+00, -5.9976e-01, -1.2135e-02],
                     [ 6.8054e-01,  6.5467e-01,  1.0581e-02],
                     [-8.3773e-01,  5.1382e-01, -2.1732e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5985e+00, -3.9716e-01, -1.1351e-02],
                     [-7.1176e-01,  4.1207e-01, -1.8039e-03],
                     [ 7.6423e-01,  3.3275e-02,  8.4772e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.5495e+00, -4.8857e-01,  9.8378e-02],
                     [-6.8531e-01,  5.6975e-01, -3.4580e-01],
                     [ 7.0076e-01,  4.8699e-01,  3.1767e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5787e+00,  4.4900e-01, -1.3073e-01],
                     [ 6.0348e-01, -6.0804e-01,  2.5399e-01],
                     [-6.2879e-01, -4.5654e-01, -3.9940e-01],
                     ...,
                     [-1.8260e+00,  1.9220e-01,  1.1795e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5672e+00, -5.0610e-01, -7.8853e-03],
                     [ 5.3284e-01,  6.3940e-01,  3.9640e-02],
                     [-8.3289e-01,  2.2146e-01, -4.2395e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0258, -0.0418, -0.0425,  ..., -0.0213, -
0.0095,  0.0167],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 0.0416, -0.3976,  0.7544],
                     [ 0.0220, -0.3678, -0.7234],
                     [ 0.0507,  0.8576, -0.0220],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5982, -0.2747, -0.3334],
                     [ 0.5578,  0.5845,  0.3225],
                     [-0.6981, -0.2848,  0.3700],
                     ...,
                     [-2.5777, -0.6960, -0.2537],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5311, -0.4472, -0.0676],
                     [ 0.7388,  0.5750,  0.0756],
                     [-0.8439,  0.4148, -0.0869],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.3981,  0.3571,  0.0686],
                     [-0.5883, -0.4719, -0.3180],
                     [ 0.6228, -0.5639,  0.3665],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5277, -0.4438, -0.0736],
                     [-0.5606,  0.6980,  0.1135],
                     [ 0.9001,  0.3677, -0.1576],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4855, -0.4531, -0.0953],
                     [-0.5894,  0.6341,  0.0378],
                     [ 0.8197,  0.1269, -0.0294],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0150,  0.0020, -0.0128,  ...,  0.0167, -
0.0255, -0.0018],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-2.8247e-03,  1.0814e+00, -6.9813e-02],
                     [-1.0515e+00, -4.1050e-02,  8.2254e-02],
                     [-4.3009e-05, -1.0291e+00, -2.2572e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1676e+00, -2.0199e-01,  7.2158e-02],
                     [ 2.2816e-02,  5.7972e-01, -8.4834e-02],
                     [ 1.1504e+00, -1.9225e-01,  1.7170e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.9360e+00, -3.8149e-02, -4.0879e-02],
                     [ 5.9996e-01,  4.9950e-01,  5.2559e-03],
                     [-5.6631e-01, -4.7092e-01,  1.1589e-01],
                     ...,
                     [-2.2381e+00,  5.3818e-01,  7.6867e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.5524e+00, -4.8819e-01, -5.6326e-02],
                     [-5.0285e-01,  6.5182e-01,  5.6907e-02],
                     [ 9.5488e-01,  4.1742e-01, -4.8536e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2241e+00, -6.1477e-01,  3.9102e-02],
                     [ 6.4597e-01,  6.8318e-01, -6.7285e-02],
                     [-8.1647e-01,  5.1957e-01,  6.9274e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5326e+00, -4.9488e-01,  1.2378e-01],
                     [-6.0695e-01,  6.2010e-01, -2.8982e-01],
                     [ 7.5534e-01,  5.2557e-01,  2.9769e-01],
                     ...,
                     [ 1.7688e+00, -4.9500e-01, -9.8310e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0191,  0.0246, -0.0292,  ..., -0.0152, -
0.0245, -0.0344],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  3,  2,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.4104, -0.4626,  0.0247],
                     [-0.5429,  0.7188, -0.0761],
                     [ 0.7131,  0.6613,  0.0427],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1233, -0.1576,  0.0362],
                     [ 0.1270,  0.3921, -0.0111],
                     [ 1.2715, -0.1147, -0.0199],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4560, -0.4802,  0.0144],
                     [-0.5422,  0.6752, -0.0088],
                     [ 0.9804,  0.4450,  0.0549],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.7053,  0.1116, -0.0446],
                     [ 0.3693, -0.5015,  0.0361],
                     [-0.6179,  0.5204,  0.0475],
                     ...,
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                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2078, -0.2689, -0.0248],
                     [ 0.0699,  0.6066,  0.0499],
                     [ 1.1476, -0.3346, -0.1226],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.6645, -0.4228,  0.0171],
                     [ 0.4409,  0.5832, -0.0234],
                     [-0.9218,  0.1044,  0.0394],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0335, -0.0084, -0.0134,  ...,  0.0260, -
0.0042, -0.0453],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-4.2312e-02,  5.3926e-02, -1.8285e+00],
                     [ 5.7232e-02, -9.7017e-02, -6.1857e-01],
                     [ 1.1053e-01, -1.0619e-01,  7.2833e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2741e+00, -6.5313e-01,  1.1914e-01],
                     [ 1.8885e-02,  4.5488e-02, -3.9495e-01],
                     [-1.2799e+00, -6.5575e-01,  1.0310e-01],
                     ...,
                     [ 1.2365e-01,  1.4080e+00,  9.5150e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5532e+00,  1.2139e-01, -1.2256e-01],
                     [ 1.9487e-01, -2.9969e-02,  4.5334e-01],
                     [-1.0576e+00,  5.5344e-01, -7.6791e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.5059e+00, -4.4694e-01,  1.4474e-01],
                     [-6.0531e-01,  5.7395e-01, -3.2752e-01],
                     [ 7.0811e-01,  5.0816e-01,  3.0988e-01],
                     ...,
                     [ 1.7602e+00, -4.6936e-01, -1.0211e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4539e+00, -3.1181e-02,  1.0566e-01],
                     [ 1.2363e-01,  8.5017e-04, -5.7945e-01],
                     [-8.7475e-01, -7.4483e-01,  1.5610e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5049e+00,  9.9991e-02, -1.4593e-01],
                     [ 1.5155e-01, -4.0998e-02,  4.8841e-01],
                     [-1.0479e+00,  6.0645e-01, -5.9071e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0230, -0.0344,  0.0200,  ..., -0.0140,
0.0045, -0.0210],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 2,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 2,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.7115, -0.3177, -0.1641],
                     [ 0.5610,  0.4678,  0.2364],
                     [-0.6931, -0.3203,  0.2916],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.1157, -0.0626,  1.9158],
                     [ 0.1192,  0.0603,  0.6894],
                     [ 0.0949,  0.0261, -0.7093],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4093, -0.0217, -0.2798],
                     [-0.1857, -0.0047,  0.5355],
                     [ 0.8569,  0.7412, -0.1083],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.5410, -0.4721,  0.1485],
                     [-0.6565,  0.6383, -0.3606],
                     [ 0.7649,  0.5006,  0.3327],
                     ...,
                     [ 1.6062, -0.6790, -1.0186],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.9035, -0.0708,  0.0027],
                     [ 0.5805,  0.5541, -0.0601],
                     [-0.5403, -0.4827,  0.0153],
                     ...,
                     [-2.1899,  0.5879,  0.8212],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.7299, -0.4487,  0.2208],
                     [ 0.6780,  0.4213,  0.1567],
                     [-0.5857, -0.2498, -0.0074],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0109,  0.0823,  0.0002,  ..., -0.0272, -
0.0244,  0.0107],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
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                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4752e+00, -4.3509e-01,  2.4742e-02],
                     [ 5.1367e-01,  6.3999e-01, -5.6177e-02],
                     [-8.4337e-01,  4.7276e-01,  5.2910e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 5.3743e-02, -5.8688e-01,  0.0000e+00],
                     [ 7.6782e-02,  5.5422e-01,  0.0000e+00],
                     [-9.6571e-01,  7.2377e-01,  0.0000e+00],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6938e+00, -2.4320e-01, -3.1209e-01],
                     [ 5.4335e-01,  5.0960e-01,  3.3624e-01],
                     [-7.2700e-01, -2.8179e-01,  3.7450e-01],
                     ...,
                     [-2.7368e+00, -6.1976e-01, -2.7121e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.5187e+00, -4.5814e-01, -3.3301e-03],
                     [ 4.8442e-01,  6.8383e-01, -3.7039e-04],
                     [-8.6168e-01,  1.0688e-01,  1.7299e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.9056e+00, -1.3720e-01, -1.1085e-03],
                     [ 5.4164e-01,  5.3221e-01, -3.4438e-02],
                     [-5.9011e-01, -4.8845e-01,  5.4159e-02],
                     ...,
                     [-2.0472e+00,  7.7582e-01,  6.7681e-01],
                     [-2.6424e+00, -5.0030e-01, -1.0834e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5775e+00, -3.8638e-01,  2.9226e-03],
                     [-6.7150e-01,  3.9054e-01, -1.6334e-03],
                     [ 7.3477e-01,  4.6107e-02, -1.7208e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0400,  0.0753, -0.0245,  ..., -0.0597, -
0.0426, -0.0438],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ...,  0, -1, -1],
                    [ 1,  2,  1,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[ 1.5216,  0.1057, -0.1331],
                     [ 0.1524, -0.0560,  0.4726],
                     [-1.0521,  0.6078, -0.0620],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.1416,  1.3198,  0.0902],
                     [ 0.0278, -0.0541, -0.3764],
                     [ 1.2318, -0.4698,  0.0620],
                     ...,
                     [-1.0741, -1.7992, -0.3177],
                     [-1.1316, -0.8633,  1.1234],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2673, -0.2638, -0.0450],
                     [ 0.0823,  0.5062,  0.1043],
                     [ 1.1993, -0.2731, -0.1522],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.7442, -0.3231, -0.1614],
                     [ 0.6109,  0.4655,  0.2111],
                     [-0.7288, -0.2871,  0.2932],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4279,  0.6317, -0.0496],
                     [ 0.6259, -0.7091,  0.2140],
                     [-0.7348, -0.6523, -0.3333],
                     ...,
                     [-1.5828,  0.6822,  1.1874],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.2044,  1.3059,  0.0701],
                     [ 0.0556,  0.0295, -0.4060],
                     [ 1.2696, -0.5482,  0.0635],
                     ...,
                     [-1.0407, -1.8031, -0.1581],
                     [-1.1760, -0.7571,  1.2225],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0178,  0.0100,  0.0179,  ..., -0.0051, -
0.0100,  0.0021],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  2,  0,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.3067, -0.5855, -0.0186],
                     [ 0.0027,  0.1427, -0.0537],
                     [ 1.2872, -0.6109,  0.0109],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4976,  0.0244,  0.0887],
                     [ 0.1525, -0.0251, -0.5244],
                     [-0.9541, -0.7529,  0.1018],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.6904, -0.0060,  0.0237],
                     [-0.7508,  0.0401, -0.1255],
                     [ 1.1221, -1.0260, -0.6395],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.7253, -0.1701, -0.0448],
                     [ 0.4110,  0.4454,  0.1088],
                     [-0.6131, -0.4387,  0.0344],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0531, -0.4075,  0.7290],
                     [ 0.0126, -0.3755, -0.7286],
                     [ 0.0202,  0.8880, -0.0107],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7663,  0.0930, -0.0849],
                     [-0.4023, -0.4002,  0.1443],
                     [ 0.7328,  0.3686,  0.0294],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0373,  0.0028,  0.2637,  ...,  0.0074,
0.0365, -0.0592],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  1,  2,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[ 1.6759, -0.2084, -0.2868],
                     [ 0.5438,  0.4687,  0.2854],
                     [-0.7344, -0.3369,  0.3178],
                     ...,
                     [-2.8148, -0.3194, -0.2381],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.7655, -0.3850,  0.2451],
                     [ 0.6335,  0.3304,  0.1782],
                     [-0.6414, -0.3093, -0.0914],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0289,  1.2686, -0.2961],
                     [-0.0331, -0.0314,  0.6313],
                     [-0.0175, -1.2532, -0.2652],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-0.1113,  1.4018,  0.0342],
                     [-0.0303,  0.0064, -0.3287],
                     [ 1.2445, -0.5130,  0.0883],
                     ...,
                     [-1.1146, -1.9468, -0.4855],
                     [-1.1558, -1.2374,  1.1173],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.3940,  0.5631, -0.1137],
                     [-0.7010, -0.6731,  0.3568],
                     [ 0.6999, -0.6615, -0.1956],
                     ...,
                     [ 1.5732,  0.7107,  1.0588],
                     [ 2.4134,  0.3031, -0.4643],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.3012, -0.6757,  0.0169],
                     [ 0.0165,  0.0952, -0.1227],
                     [-1.3009, -0.6595,  0.0496],
                     ...,
                     [-0.8452,  2.0786,  0.0599],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
              'energies': tensor([ 0.0067, -0.0057,  0.0088,  ..., -0.0116,
0.1276, -0.0067],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 3.0037e-03, -1.9712e-01,  1.1800e+00],
                     [-6.9298e-02,  5.7886e-01,  1.3021e-02],
                     [-4.8039e-02, -2.4144e-01, -1.2104e+00],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3245e+00, -6.8272e-01,  8.5046e-02],
                     [ 7.2248e-01,  6.2284e-01, -1.3042e-01],
                     [-7.5874e-01,  5.4031e-01,  1.2199e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5404e+00, -4.1637e-01, -3.4419e-03],
                     [-6.9513e-01,  4.2987e-01,  2.4826e-03],
                     [ 7.3555e-01,  1.0153e-01,  1.9027e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.6678e+00, -3.0541e-01, -2.7854e-01],
                     [ 5.9495e-01,  4.4634e-01,  2.7689e-01],
                     [-7.3596e-01, -2.8142e-01,  4.5704e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7350e+00, -1.3502e-01,  4.9980e-02],
                     [ 3.9607e-01,  4.2012e-01, -1.1408e-01],
                     [-6.1777e-01, -4.3274e-01, -1.5739e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5778e+00, -5.1601e-01, -8.2900e-02],
                     [-6.5767e-01,  6.5382e-01,  1.1892e-03],
                     [ 7.8266e-01,  1.7158e-01, -2.4783e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0139,  0.0146, -0.0450,  ...,  0.0073,
0.0265,  0.0514],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  3,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.7298e+00,  4.7158e-02,  2.5058e-02],
                     [-4.3364e-01, -4.3145e-01, -1.1578e-01],
                     [ 6.3550e-01,  4.1564e-01,  1.5013e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3375e+00, -5.9017e-01,  1.3346e-02],
                     [-7.3215e-01,  6.2288e-01, -2.5147e-01],
                     [ 7.5833e-01,  6.1391e-01,  2.2594e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-6.6853e-01,  7.6112e-02, -3.9958e-02],
                     [ 6.7177e-01, -7.8900e-02,  4.3379e-02],
                     [-1.3414e+00, -7.9614e-01,  1.2489e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-7.8095e-01,  7.9742e-01, -1.9571e-02],
                     [-7.5624e-01, -7.7641e-01,  6.0230e-03],
                     [ 7.7147e-01, -7.8224e-01,  9.1583e-05],
                     ...,
                     [ 1.2714e+00,  1.2623e+00, -8.4924e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3850e+00, -5.5567e-01, -3.3113e-02],
                     [-7.7454e-01,  4.7455e-01,  3.8353e-02],
                     [ 7.8131e-01,  5.2340e-01, -8.4178e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3805e+00, -1.2421e-01, -1.6842e-02],
                     [ 1.0518e-01,  1.0712e-01, -2.2394e-02],
                     [ 9.0543e-01, -1.0626e+00,  9.3975e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0769, -0.0141,  0.0184,  ..., -0.0227, -
0.0307, -0.0270],
                       dtype=torch.float64)}),
```

```
            defaultdict(list,
                        {'species': tensor([[ 1,  1,  1,  ...,  0,  0,  0],
                                [ 1,  1,  2,  ..., -1, -1, -1],
                                [ 2,  1,  1,  ..., -1, -1, -1],
                                ...,
                                [ 1,  1,  1,  ..., -1, -1, -1],
                                [ 2,  1,  2,  ..., -1, -1, -1],
                                [ 1,  1,  2,  ..., -1, -1, -1]]),
                         'coordinates': tensor([[[ 1.8992e+00, -1.1024e-01, -1.6532e-02],
                                 [ 5.5562e-01,  5.1276e-01,  5.9842e-03],
                                 [-5.3721e-01, -5.2943e-01,  5.0583e-02],
                                 ...,
                                 [-2.0883e+00,  7.7562e-01, -9.6057e-01],
                                 [-2.7272e+00, -6.5468e-01,  1.5843e-02],
                                 [-1.9895e+00,  7.7319e-01,  8.4087e-01]],

                                [[ 1.4103e+00, -4.8139e-01,  9.6691e-03],
                                 [ 5.5622e-01,  7.3610e-01, -1.3395e-03],
                                 [-7.1959e-01,  6.7927e-01,  2.9335e-02],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[ 1.4976e+00, -5.1897e-01, -1.1978e-01],
                                 [ 6.0456e-01,  6.1942e-01,  5.1117e-02],
                                 [-8.0656e-01,  1.9946e-01, -1.2660e-01],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                ...,

                                [[ 1.8237e+00, -3.5726e-01,  2.1134e-01],
                                 [ 6.1876e-01,  2.8378e-01,  1.9525e-01],
                                 [-6.7711e-01, -3.3304e-01, -6.2511e-02],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[ 9.5695e-01, -8.9312e-01,  3.3664e-02],
                                 [-7.7779e-03,  1.2072e-01,  1.1598e-02],
                                 [-1.2314e+00, -3.5458e-01,  4.5153e-03],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[ 3.1747e-02, -3.5059e-01,  7.4970e-01],
                                 [ 3.2119e-02, -4.5563e-01, -7.7252e-01],
                                 [ 4.2408e-02,  8.9406e-01,  3.1634e-02],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
                         'energies': tensor([-0.0352,  0.0233,  0.0553,  ...,  0.0019, -
            0.0468,  0.0289],
                                dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  2,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 7.1909e-01,  2.9418e-02,  1.2281e-01],
                     [-7.1318e-01,  1.1446e-01, -1.2070e-01],
                     [ 6.6105e-01, -6.9086e-01,  1.7048e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2713e+00, -6.1305e-01,  1.1387e-01],
                     [ 3.6766e-02,  9.0809e-03, -4.2011e-01],
                     [-1.2613e+00, -6.1311e-01,  1.1299e-01],
                     ...,
                     [ 3.0010e-01,  1.3598e+00,  1.0115e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.1883e+00, -6.6804e-01, -1.5110e-01],
                     [ 7.6807e-01,  6.6525e-01,  1.2900e-01],
                     [-7.6729e-01,  5.5680e-01, -1.8812e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 2.2928e-02,  1.2298e+00, -2.7480e-01],
                     [-9.1573e-03, -4.4703e-04,  6.5762e-01],
                     [ 4.4388e-03, -1.2316e+00, -2.8877e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-6.4099e-01,  6.4738e-02, -2.9375e-02],
                     [ 6.4748e-01, -5.4481e-02,  3.1693e-02],
                     [-1.2329e+00, -8.3783e-01,  5.0533e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-4.3091e-02, -8.3778e-01, -1.6777e-03],
                     [ 7.7021e-01,  4.0448e-01, -1.4721e-02],
                     [-7.0862e-01,  4.4810e-01,  2.2418e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.2359, -0.0168,  0.0615,  ...,  0.0077,
0.0287,  0.0167],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.4073, -0.4924,  0.0411],
                     [-0.5542,  0.7416, -0.0661],
                     [ 0.9118,  0.3977,  0.0642],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2057, -0.2154, -0.0409],
                     [ 0.0378,  0.5712,  0.0413],
                     [ 1.1814, -0.3273, -0.1073],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.3874, -0.0909,  0.0165],
                     [ 0.1162,  0.1033,  0.0250],
                     [ 0.7855, -1.0689,  0.0528],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.5857, -0.3652, -0.2826],
                     [ 0.5684,  0.5500,  0.3103],
                     [-0.6627, -0.2372,  0.4392],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.7683,  0.7417, -0.0621],
                     [-0.7925, -0.7937,  0.0590],
                     [ 0.7543, -0.7357, -0.0817],
                     ...,
                     [ 1.2639,  1.4323, -0.6753],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7192,  0.1011, -0.0206],
                     [-0.4395, -0.5070, -0.0056],
                     [ 0.6225,  0.3961,  0.0465],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-4.5517e-02, -5.6957e-05, -1.3724e-02,  ...,
-6.5666e-03,
                    -7.8996e-03, -2.2090e-03], dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 3,  3,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  0,  0,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.5534e+00, -4.7500e-01, -1.1722e-01],
                     [ 5.7647e-01,  5.3282e-01,  3.4352e-02],
                     [-8.1173e-01,  1.3076e-01, -4.4540e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3088e+00, -2.3995e-01, -3.0407e-02],
                     [ 5.2020e-02,  5.3405e-01,  7.6654e-02],
                     [ 1.2250e+00, -3.3973e-01, -1.3466e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.9136e-02,  1.1238e+00, -2.2447e-01],
                     [-2.7530e-02,  2.5762e-02,  5.8978e-01],
                     [ 1.0812e-02, -1.1577e+00, -2.1651e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.4421e+00, -5.2892e-01, -2.5544e-02],
                     [-5.3565e-01,  7.6562e-01,  2.0528e-02],
                     [ 9.5752e-01,  4.5756e-01, -1.3003e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3057e+00, -5.9350e-01, -1.7617e-02],
                     [ 6.7697e-01,  6.4948e-01,  1.7577e-02],
                     [-8.2965e-01,  4.9843e-01, -2.5814e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.9577e-02, -1.3264e-02,  9.2066e-05],
                     [-8.5416e-01,  7.8033e-01, -2.3269e-01],
                     [-2.8105e-01, -9.0570e-01,  1.8305e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0365,  0.0153,  0.1519,  ..., -0.0071, -
0.0448,  0.0494],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.3767e+00, -1.2404e-01, -2.3048e-03],
                     [ 1.0273e-01,  1.3719e-01,  1.5875e-02],
                     [ 7.4442e-01, -1.0423e+00,  8.1239e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5306e+00,  8.7348e-02, -1.7597e-01],
                     [ 1.4501e-01, -2.1669e-02,  4.9111e-01],
                     [-1.0553e+00,  5.9030e-01, -3.4169e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4031e+00, -1.2692e-01,  1.0878e-02],
                     [ 4.4264e-02,  8.3361e-02, -5.9998e-02],
                     [ 8.7892e-01, -9.9602e-01,  4.9149e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-2.3789e-02,  1.3066e+00, -2.7571e-01],
                     [-7.6780e-03, -2.4069e-04,  5.7070e-01],
                     [ 1.1022e-02, -1.3174e+00, -2.3155e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6965e+00, -4.2528e-01,  4.0335e-01],
                     [ 6.7302e-01,  3.9826e-01, -9.3706e-03],
                     [-5.5168e-01, -2.6615e-01, -2.4546e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2406e+00, -2.5087e-01, -8.4068e-04],
                     [ 8.3097e-02,  5.3962e-01,  3.5004e-02],
                     [ 1.2602e+00, -2.8502e-01, -9.5638e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0938, -0.0046, -0.0404,  ..., -0.0072,
0.0183,  0.0321],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  3,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[-7.8290e-01,  7.7860e-01, -9.2577e-03],
                     [-7.7493e-01, -7.7738e-01,  1.5296e-02],
                     [ 7.8117e-01, -7.7039e-01, -9.9547e-03],
                     ...,
                     [ 1.2582e+00,  1.2348e+00, -8.6443e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2594e+00, -6.7509e-01,  8.8413e-02],
                     [ 3.4255e-03,  5.1844e-02, -3.7476e-01],
                     [-1.2572e+00, -6.6492e-01,  1.0086e-01],
                     ...,
                     [-2.3402e-02,  1.4157e+00,  9.9708e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-7.6879e-03,  1.1188e+00, -2.2646e-01],
                     [ 8.3475e-03,  9.6833e-03,  5.8771e-01],
                     [-2.1546e-03, -1.1136e+00, -2.4434e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.7776e+00,  3.8527e-02, -6.1151e-02],
                     [-4.6757e-01, -4.1278e-01, -2.0225e-03],
                     [ 6.5839e-01,  3.9430e-01,  1.1015e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5222e+00, -4.5599e-01,  5.4098e-04],
                     [ 4.8573e-01,  6.6978e-01,  4.7541e-03],
                     [-8.6610e-01,  1.1679e-01,  4.4634e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-2.2743e-01,  1.3107e+00,  1.0020e-01],
                     [ 5.5777e-02,  2.1471e-02, -3.8956e-01],
                     [ 1.3094e+00, -5.7890e-01,  4.5964e-02],
                     ...,
                     [-9.7772e-01, -1.8925e+00, -5.5540e-02],
                     [-1.3776e+00, -4.5667e-01,  1.1568e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0253, -0.0443,  0.1401,  ...,  0.0622, -
0.0616,  0.0051],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0,  0,  0],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  3,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[ 1.9512e+00, -5.7852e-02, -8.4843e-02],
                     [ 5.3514e-01,  4.9414e-01,  2.3068e-02],
                     [-5.8855e-01, -5.8811e-01,  1.6495e-01],
                     ...,
                     [-1.9021e+00,  7.0822e-01, -1.1215e+00],
                     [-2.8094e+00, -4.0788e-01, -3.9069e-02],
                     [-1.9966e+00,  8.2124e-01,  7.5735e-01]],

                    [[-1.1487e+00, -5.0766e-01, -1.4276e-04],
                     [ 3.8551e-03,  4.7871e-01,  7.2917e-03],
                     [ 1.2907e+00,  1.5306e-01, -2.4600e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6860e+00,  1.8297e-01, -1.4161e-01],
                     [ 4.3387e-01, -4.3302e-01,  1.3071e-01],
                     [-6.8590e-01,  3.8485e-01, -2.3482e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.3509e+00, -5.1303e-01,  1.6662e-02],
                     [ 5.4972e-01,  7.4276e-01,  4.9099e-03],
                     [-7.3490e-01,  6.7416e-01,  9.0344e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-5.2037e-01, -4.4776e-03, -3.9476e-03],
                     [ 6.6632e-01,  3.6896e-03,  9.2862e-04],
                     [-1.0492e+00,  9.5662e-01,  1.6253e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-7.8250e-01,  7.8007e-01,  1.9098e-03],
                     [-7.6826e-01, -7.7583e-01, -7.3854e-03],
                     [ 7.7690e-01, -7.7408e-01,  8.1407e-03],
                     ...,
                     [ 1.2364e+00,  1.2245e+00, -8.9262e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0228, -0.0057, -0.0127,  ...,  0.0085,
        0.0008, -0.0254],
                           dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  1,  3,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  0,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-0.0162,  0.0042,  1.1516],
                     [ 0.0433, -0.0111, -0.0251],
                     [-0.0162,  0.0042, -1.1327],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5169, -0.4517, -0.1168],
                     [-0.5552,  0.5758,  0.0295],
                     [ 0.8086,  0.0893,  0.0372],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.6050, -0.3739, -0.2403],
                     [ 0.5755,  0.5284,  0.3257],
                     [-0.6677, -0.2391,  0.3912],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.1952, -0.2375, -0.0303],
                     [ 0.0760,  0.6120,  0.0305],
                     [ 1.2339, -0.3130, -0.1078],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0748, -0.9013,  0.0363],
                     [ 0.8015,  0.4332, -0.0039],
                     [-0.7462,  0.4606, -0.0193],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.5350,  0.0031,  0.0119],
                     [ 0.6755, -0.0022, -0.0028],
                     [-1.0957,  0.9519, -0.0489],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0990, -0.0425, -0.0115,  ...,  0.0077,
0.0186,  0.0008],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4324, -0.0750, -0.2102],
                     [ 0.2508, -0.0315,  0.5341],
                     [-0.8396,  0.7279, -0.1621],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5667, -0.5053, -0.1204],
                     [-0.6179,  0.5465,  0.0497],
                     [ 0.8037,  0.2020, -0.0582],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2897, -0.5914,  0.0033],
                     [-0.0116,  0.1806, -0.0068],
                     [ 1.2659, -0.6335,  0.0026],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.1295, -0.8971,  0.1175],
                     [ 0.0676,  0.0327, -0.3313],
                     [ 1.4178, -0.4632,  0.0716],
                     ...,
                     [-0.1258,  1.5920,  1.0390],
                     [-1.1491,  1.6792, -0.1281],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4913, -0.0672, -0.1621],
                     [-0.1405, -0.0263,  0.5172],
                     [ 0.9985, -0.6603, -0.1471],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5966, -0.4990, -0.0173],
                     [ 0.5566,  0.6930,  0.0208],
                     [-0.8237,  0.0401,  0.0533],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0101,  0.0441, -0.0621,  ..., -0.0145, -
0.0192,  0.0358],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    ...,
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-1.5156e+00, -4.8745e-02, -1.4460e-01],
                     [-1.6010e-01, -5.1288e-02,  4.9724e-01],
                     [ 1.0282e+00, -6.4659e-01, -1.4024e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.8059e+00, -2.4298e-01, -3.0903e-01],
                     [ 6.0337e-01,  4.8145e-01,  3.0505e-01],
                     [-7.8441e-01, -2.6408e-01,  3.0193e-01],
                     ...,
                     [-2.7834e+00, -6.7177e-01, -3.2376e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1393e+00, -2.0068e-01,  1.7631e-02],
                     [-5.3466e-03,  6.0701e-01, -1.7271e-02],
                     [ 1.1420e+00, -1.9697e-01, -8.1946e-04],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.2737e+00, -6.7951e-01,  1.9149e-02],
                     [ 7.2000e-01,  6.4239e-01, -2.1347e-02],
                     [-7.8152e-01,  5.6078e-01,  4.3124e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.0915e+00, -8.8767e-01,  1.2910e-01],
                     [-1.4105e-02,  5.6859e-02, -4.0851e-01],
                     [ 1.3659e+00, -5.0100e-01,  7.2506e-02],
                     ...,
                     [-3.0586e-01,  1.3053e+00,  1.0914e+00],
                     [-1.1435e+00,  1.6791e+00, -2.8655e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2808e+00, -6.4870e-01,  1.0399e-01],
                     [ 1.9658e-02, -3.3213e-04, -3.8650e-01],
                     [-1.2731e+00, -6.0799e-01,  9.8640e-02],
                     ...,
                     [-3.9479e-01,  1.3598e+00,  1.0238e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0193,  0.0044, -0.0061,  ..., -0.0116, -
0.0295, -0.0085],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 2.8336e-02, -3.9650e-01,  7.5690e-01],
                     [ 4.6402e-02, -3.7820e-01, -7.5958e-01],
                     [ 3.1449e-02,  8.5148e-01,  1.8453e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.8785e+00, -1.4769e-01, -4.4318e-03],
                     [ 5.2498e-01,  5.5606e-01, -2.5529e-03],
                     [-6.1017e-01, -5.1004e-01,  4.6532e-02],
                     ...,
                     [-1.7263e+00,  1.1298e+00,  4.4060e-01],
                     [-2.7148e+00, -4.1419e-01,  3.8855e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3007e+00, -6.9188e-01, -1.4956e-02],
                     [ 7.3938e-01,  6.3377e-01,  3.1220e-02],
                     [-8.1383e-01,  5.6972e-01, -6.8697e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.7318e+00, -4.7186e-01, -7.4611e-03],
                     [ 5.5528e-01,  5.8997e-01, -2.3243e-02],
                     [-8.7355e-01,  1.0379e-01,  6.5550e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4937e+00, -4.5169e-01,  2.0918e-02],
                     [ 7.0028e-01,  5.9740e-01, -5.4613e-02],
                     [-8.3066e-01,  4.6905e-01,  7.5245e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7824e+00, -1.3060e-01, -3.7661e-02],
                     [ 4.0302e-01,  3.9805e-01,  1.3827e-01],
                     [-6.6451e-01, -4.4535e-01, -7.6806e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0087,  0.0005, -0.0038,  ...,  0.0368, -
0.0205,  0.0131],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  0,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-6.9368e-03, -3.4272e-02,  3.2867e-04],
                     [-8.2511e-01,  7.7568e-01, -2.1158e-01],
                     [-4.3405e-01, -9.0110e-01,  2.1692e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 2.9045e-02,  1.3134e+00, -2.5400e-01],
                     [-4.0149e-02,  2.0023e-02,  5.8280e-01],
                     [ 1.4361e-02, -1.3285e+00, -2.6623e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4281e+00, -4.5033e-01, -1.0885e-03],
                     [ 5.0864e-01,  6.4513e-01, -3.0998e-02],
                     [-8.6088e-01,  4.9382e-01,  7.8952e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.5778e-01,  1.3579e+00,  9.3252e-02],
                     [ 7.9212e-03, -6.8814e-02, -4.2009e-01],
                     [ 1.2881e+00, -5.2088e-01,  5.5446e-02],
                     ...,
                     [-1.0138e+00, -1.9115e+00, -1.3761e-01],
                     [-1.2959e+00, -7.1063e-01,  1.1673e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7837e-01,  1.3760e+00,  6.6327e-02],
                     [ 8.5042e-03, -6.1607e-03, -4.0025e-01],
                     [ 1.2521e+00, -5.4906e-01,  6.2948e-02],
                     ...,
                     [-1.0391e+00, -1.8364e+00, -3.3831e-01],
                     [-1.0915e+00, -9.1678e-01,  1.1826e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1536e+00, -1.9809e-01,  3.9712e-03],
                     [ 1.3429e-03,  5.8842e-01, -5.2909e-04],
                     [ 1.1592e+00, -1.8606e-01,  8.1722e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0439, -0.0169, -0.0468,  ..., -0.0157, -
0.0296, -0.0043],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4574e+00, -7.6867e-02, -2.0990e-01],
                     [ 2.5283e-01, -6.6132e-02,  5.2001e-01],
                     [-8.4086e-01,  7.5308e-01, -1.4484e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4621e+00, -4.8108e-01,  5.8319e-04],
                     [ 5.1212e-01,  7.2383e-01,  2.6714e-02],
                     [-8.8123e-01,  1.9677e-01, -4.5596e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3228e+00,  1.0233e+00, -2.2002e-03],
                     [-1.1898e-02,  7.6490e-01, -2.2628e-02],
                     [-5.0958e-01, -5.6651e-01, -1.6225e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.7059e+00,  8.9652e-02,  1.4836e-01],
                     [-4.3407e-01, -4.7514e-01, -1.9984e-01],
                     [ 6.1437e-01,  3.6015e-01, -1.1590e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-8.0306e-01,  8.0950e-01,  5.7456e-02],
                     [-8.0708e-01, -7.6043e-01, -4.2847e-02],
                     [ 7.9364e-01, -7.8465e-01,  3.8927e-02],
                     ...,
                     [ 1.1763e+00,  1.2285e+00, -9.6187e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.6294e+00,  1.5287e-01,  2.0262e-01],
                     [-5.1508e-01, -2.4273e-01, -4.6642e-01],
                     [ 5.4992e-01, -2.5551e-01,  4.5957e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0088, -0.0523, -0.0275,  ...,  0.0005, -
0.0039,  0.0343],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ...,  0,  0, -1],
                    [ 1,  3,  2,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  2,  ...,  0,  0, -1],
                    [ 2,  2,  0,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.5082e+00,  5.8113e-01, -1.1453e-01],
                     [-6.1909e-01, -6.1026e-01,  3.1276e-01],
                     [ 7.1714e-01, -6.7783e-01, -2.5213e-01],
                     ...,
                     [ 1.5804e+00,  5.6204e-01,  1.1240e+00],
                     [ 2.5364e+00,  3.8941e-01, -2.4248e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6913e+00,  1.5934e-01, -3.2096e-02],
                     [ 3.9104e-01, -5.2631e-01,  4.2965e-02],
                     [-5.8540e-01,  4.0860e-01,  1.9412e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2319e+00, -7.1748e-01, -4.1152e-02],
                     [ 6.9284e-01,  6.4263e-01, -1.1342e-02],
                     [-7.7727e-01,  6.3275e-01,  6.1012e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.6725e+00,  5.0581e-01, -1.7117e-01],
                     [-6.0465e-01, -5.5361e-01,  3.0409e-01],
                     [ 6.9197e-01, -5.9081e-01, -3.1272e-01],
                     ...,
                     [ 1.8969e+00,  2.1715e-01,  1.2181e+00],
                     [ 2.5809e+00,  3.2563e-01, -3.8044e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 6.3791e-01, -1.2294e-01, -1.2728e-03],
                     [-6.2987e-01, -1.1719e-01,  1.2728e-03],
                     [ 9.4371e-01,  8.1419e-01,  1.1142e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4848e-02,  1.0910e+00, -8.0115e-02],
                     [-1.0577e+00, -5.6076e-02,  8.0353e-02],
                     [-1.0084e-02, -1.0494e+00, -2.2170e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0160,  0.0255,  0.0141,  ..., -0.0016,
0.0403, -0.0106],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
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                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.2311e+00, -6.5656e-01,  1.1499e-01],
                     [-1.0422e-02,  6.4273e-02, -3.5764e-01],
                     [-1.2510e+00, -7.1453e-01,  9.5563e-02],
                     ...,
                     [ 4.2413e-02,  1.5032e+00,  9.5857e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2837e+00, -2.0932e-01, -1.7344e-03],
                     [ 6.0250e-02, -1.3434e-01,  2.9801e-02],
                     [ 4.8172e-01,  1.1743e+00,  6.8710e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3025e+00, -6.0248e-01,  3.6813e-02],
                     [ 2.9613e-02,  7.3048e-02, -2.2869e-02],
                     [-1.3320e+00, -6.8522e-01, -1.6877e-02],
                     ...,
                     [-8.1692e-01,  2.2007e+00, -6.4338e-02],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.1727e-02,  1.2698e+00, -2.5662e-01],
                     [ 7.4625e-02,  8.0024e-03,  6.0853e-01],
                     [-3.8921e-02, -1.2924e+00, -2.6899e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2026e+00,  1.7164e-02,  5.1895e-03],
                     [ 2.8335e-01, -7.3177e-02,  2.8743e-02],
                     [ 1.4539e+00,  4.0510e-02, -2.1972e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.1821e+00, -6.8653e-01, -3.7652e-02],
                     [ 7.5125e-01,  6.6533e-01,  4.3017e-02],
                     [-7.8390e-01,  6.1615e-01, -5.0662e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0374, -0.1035,  0.0122,  ..., -0.0043, -
0.0325, -0.0038],
                         dtype=torch.float64)}),
```

```
            defaultdict(list,
                        {'species': tensor([[ 1,  1,  1,  ...,  0,  0,  0],
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                                [ 2,  1,  3,  ..., -1, -1, -1],
                                ...,
                                [ 2,  1,  2,  ..., -1, -1, -1],
                                [ 1,  1,  3,  ..., -1, -1, -1],
                                [ 2,  1,  1,  ..., -1, -1, -1]]),
                         'coordinates': tensor([[[ 1.9514e+00, -1.1278e-01,  9.7491e-04],
                                 [ 5.5208e-01,  5.1049e-01, -2.0742e-03],
                                 [-5.6637e-01, -5.2691e-01,  9.5483e-04],
                                 ...,
                                 [-2.0827e+00,  7.6689e-01, -8.7521e-01],
                                 [-2.7342e+00, -6.1035e-01,  1.0049e-03],
                                 [-2.0446e+00,  7.8717e-01,  8.7843e-01]],

                                [[-1.4620e+00, -4.7191e-01, -1.1722e-01],
                                 [-5.8395e-01,  5.9972e-01,  3.8880e-02],
                                 [ 8.3616e-01,  1.7144e-01,  5.9120e-02],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[-1.0837e+00, -1.5829e-01,  4.2505e-02],
                                 [ 1.7139e-01,  3.8530e-01,  8.5873e-03],
                                 [ 1.1966e+00, -2.4026e-01, -4.7286e-03],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                ...,

                                [[ 9.7989e-01, -8.6491e-01, -9.3684e-03],
                                 [ 1.8864e-02,  1.2236e-01,  1.3438e-02],
                                 [-1.2877e+00, -3.4958e-01, -4.1928e-04],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[ 9.3405e-03, -1.0936e+00, -9.3646e-02],
                                 [ 1.0290e+00,  3.6755e-02,  1.1838e-01],
                                 [-1.0163e-02,  1.0938e+00, -1.6273e-01],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                                [[-1.3629e-01,  7.0307e-02,  1.8384e+00],
                                 [ 1.8608e-01, -1.0709e-01,  6.5920e-01],
                                 [ 9.9473e-02, -2.6854e-02, -6.7041e-01],
                                 ...,
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                                 [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
                         'energies': tensor([-0.0478, -0.0411, -0.0524,  ..., -0.0689,
            0.0087, -0.0253],
                                dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 2,  1,  2,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.2827, -0.6110,  0.0040],
                     [-0.0223,  0.1811, -0.0386],
                     [ 1.2385, -0.6438,  0.0061],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0058,  1.1061, -0.0662],
                     [-1.0285, -0.0629,  0.0933],
                     [ 0.0061, -1.0432, -0.2302],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.9130,  1.3170, -0.0552],
                     [ 0.4006,  0.3835,  0.1240],
                     [ 0.3887, -0.9419,  0.7389],
                     ...,
                     [-0.5905, -1.1607, -1.3145],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.1877, -0.5932, -0.0454],
                     [ 0.0295,  0.1177,  0.0089],
                     [-1.1804, -0.5894,  0.0159],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4614, -0.4337,  0.0034],
                     [-0.6869,  0.4450, -0.0367],
                     [ 0.7062,  0.1824,  0.0564],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5023, -0.5744, -0.1184],
                     [ 0.5784,  0.5893,  0.0888],
                     [-0.8481,  0.2485, -0.0805],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0553,  0.0025,  0.0068,  ..., -0.0928, -
0.0337,  0.0461],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ...,  0,  0, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0,  0,  0],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.6065e+00,  5.3337e-01, -1.7386e-01],
                     [-5.8243e-01, -5.7106e-01,  2.8752e-01],
                     [ 6.7336e-01, -6.0946e-01, -3.0644e-01],
                     ...,
                     [ 1.8824e+00,  2.7806e-01,  1.2325e+00],
                     [ 2.5441e+00,  4.2158e-01, -4.1690e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2033e+00, -6.0995e-03,  5.4958e-04],
                     [ 2.8412e-01, -5.1696e-02, -2.9793e-03],
                     [ 1.4518e+00,  3.5299e-02,  1.9515e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4200e+00,  5.5513e-01, -4.8467e-02],
                     [ 5.7504e-01, -6.2885e-01,  2.3057e-01],
                     [-6.5237e-01, -6.3836e-01, -3.8254e-01],
                     ...,
                     [-1.2723e+00,  4.6885e-01,  1.2120e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.9518e+00, -1.2017e-01,  6.2471e-03],
                     [ 5.6231e-01,  5.1722e-01, -5.5011e-03],
                     [-5.6502e-01, -5.1834e-01, -7.9174e-03],
                     ...,
                     [-2.1046e+00,  7.5031e-01, -8.7405e-01],
                     [-2.7500e+00, -6.3091e-01,  2.4604e-02],
                     [-2.0745e+00,  7.5491e-01,  8.8856e-01]],

                    [[-1.4278e+00, -5.3202e-01,  1.9471e-02],
                     [-8.0209e-01,  4.7055e-01, -2.4061e-02],
                     [ 7.8823e-01,  4.6393e-01,  4.9474e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3959e+00, -1.0461e-01,  2.1340e-02],
                     [ 5.7556e-02,  1.1552e-01,  5.9560e-02],
                     [ 7.7823e-01, -1.0138e+00, -2.5167e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0036, -0.0369, -0.0106,  ..., -0.0487, -
0.0345, -0.0766],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  3,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.5529e+00, -4.6436e-01,  5.1909e-02],
                     [ 4.9022e-01,  6.1737e-01, -9.4113e-02],
                     [-8.9140e-01,  4.8601e-01,  4.1873e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3089e+00, -3.9606e-01,  1.2351e-02],
                     [-4.8739e-01,  7.3935e-01, -1.2662e-02],
                     [ 7.9225e-01,  4.0693e-01,  2.5666e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6684e+00, -4.2485e-01, -2.4222e-02],
                     [ 6.6839e-01,  5.4037e-01, -2.8507e-02],
                     [-7.7305e-01,  1.7694e-01,  9.7352e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.6672e+00,  1.3064e-01, -9.4695e-02],
                     [ 3.7797e-01, -4.6217e-01,  1.8818e-01],
                     [-5.6445e-01,  4.4992e-01,  2.3925e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.0235e-04,  1.2503e+00, -2.5787e-01],
                     [-1.6014e-02, -1.5167e-02,  5.9460e-01],
                     [ 1.6829e-02, -1.2315e+00, -2.5048e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 9.7674e-03,  1.0895e+00, -5.3550e-02],
                     [-1.0400e+00, -5.7881e-02,  4.9893e-02],
                     [-5.4748e-03, -1.0367e+00, -2.0243e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.1007, -0.0548,  0.0478,  ...,  0.0335, -
0.0158, -0.0121],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 2,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-0.0193, -0.2182,  1.3022],
                     [ 0.0145,  0.5247, -0.0278],
                     [-0.0528, -0.1701, -1.2614],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7517, -0.0349,  0.1822],
                     [-0.4646,  0.4567, -0.2499],
                     [ 0.6719, -0.3840, -0.1469],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.8547,  1.2378, -0.0408],
                     [ 0.3488,  0.4531,  0.0741],
                     [ 0.4084, -0.9167,  0.7252],
                     ...,
                     [-0.6080, -1.2395, -1.1873],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.1316,  0.0804,  0.0132],
                     [-0.0705, -0.5583,  0.0027],
                     [-1.0572,  0.2114,  0.0310],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.9422, -0.1433,  0.0970],
                     [ 0.5634,  0.5302, -0.1755],
                     [-0.5930, -0.4864, -0.0449],
                     ...,
                     [-2.1646,  0.5022,  1.0229],
                     [-2.6584, -0.5028, -0.2487],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1627, -0.1922,  0.0328],
                     [ 0.1510,  0.3703,  0.0525],
                     [ 1.3048, -0.0867, -0.0435],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0108, -0.0124,  0.0020,  ...,  0.0617, -
0.0216,  0.0138],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  3,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.4105, -0.4204, -0.0198],
                     [-0.4831,  0.7540,  0.0274],
                     [ 0.8206,  0.4329, -0.0425],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.7610, -0.2724, -0.2382],
                     [ 0.5220,  0.5238,  0.2524],
                     [-0.6954, -0.3116,  0.2746],
                     ...,
                     [-2.8078, -0.5432, -0.1645],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.8577,  1.2576, -0.0110],
                     [ 0.3381,  0.3851, -0.0035],
                     [ 0.3212, -0.8975,  0.7524],
                     ...,
                     [-0.5373, -1.1753, -1.2204],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.6729, -0.3834,  0.0136],
                     [ 0.7212,  0.3533,  0.0119],
                     [-0.7192,  0.0610, -0.1262],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1186, -0.8847,  0.1000],
                     [-0.0261,  0.0332, -0.4131],
                     [ 1.3832, -0.4759,  0.0975],
                     ...,
                     [ 0.0056,  1.3570,  1.0797],
                     [-1.2548,  1.4954, -0.0519],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7536,  0.0557, -0.0884],
                     [-0.4233, -0.4152,  0.1160],
                     [ 0.5969,  0.3802,  0.0211],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0519, -0.0169, -0.0042,  ...,  0.0319, -
0.0267,  0.0139],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  0,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[ 7.9305e-01, -1.2747e-02,  1.3141e-02],
                     [-7.7103e-01,  8.1168e-03, -5.3868e-03],
                     [ 1.2544e+00,  9.9517e-01, -4.7153e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.3829e+00, -5.1575e-01,  1.8143e-02],
                     [ 5.5394e-01,  7.6334e-01,  7.6633e-03],
                     [-7.6330e-01,  6.9883e-01, -2.6059e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6322e+00,  1.5900e-01, -2.1654e-01],
                     [ 4.4291e-01, -4.2270e-01,  1.9900e-01],
                     [-6.6411e-01,  3.6558e-01,  9.3605e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-6.6123e-01,  3.7405e-02, -5.4041e-02],
                     [ 6.5321e-01, -4.3786e-02,  6.2795e-02],
                     [-1.2710e+00, -8.0567e-01,  2.2123e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5663e-01,  1.3609e+00,  7.5190e-02],
                     [-1.0466e-02, -1.6463e-03, -4.1681e-01],
                     [ 1.2764e+00, -5.2833e-01,  7.4115e-02],
                     ...,
                     [-9.9006e-01, -1.8914e+00, -2.7803e-01],
                     [-1.1993e+00, -8.5855e-01,  1.1578e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6398e+00, -2.7445e-01, -3.2872e-01],
                     [ 5.9542e-01,  5.7467e-01,  4.0866e-01],
                     [-6.9203e-01, -2.5785e-01,  3.3939e-01],
                     ...,
                     [-2.8282e+00, -5.7743e-01, -3.0021e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.1113,  0.0142, -0.0164,  ...,  0.0365, -
0.0281, -0.0035],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    [ 2,  2, -1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-0.0146,  0.0249,  1.8521],
                     [ 0.0227, -0.0313,  0.6912],
                     [ 0.0047, -0.0241, -0.6938],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1202, -0.2511, -0.0068],
                     [-0.0054,  0.6509,  0.0476],
                     [ 1.1553, -0.2176, -0.0120],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0000,  0.0000,  0.5580],
                     [ 0.0000,  0.0000, -0.5580],
                     [ 0.0000,  0.0000,  0.0000],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.5635, -0.3690, -0.3560],
                     [ 0.6329,  0.5108,  0.4140],
                     [-0.7016, -0.1177,  0.5329],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1206, -0.1224, -0.0253],
                     [ 0.2056,  0.4180,  0.0364],
                     [ 1.2080, -0.2932, -0.0258],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.3428, -0.4014, -0.0128],
                     [-0.4701,  0.7280,  0.0081],
                     [ 0.8150,  0.4481, -0.0283],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0466,  0.0205, -0.0835,  ...,  0.0247, -
0.0192, -0.0690],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.2701e+00, -5.2009e-01, -7.0309e-03],
                     [ 5.6653e-03,  1.6133e-01, -1.2214e-02],
                     [ 1.2846e+00, -6.2192e-01, -7.6472e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7336e+00, -3.8029e-01,  3.8342e-01],
                     [ 6.9158e-01,  3.6775e-01, -1.6699e-02],
                     [-5.8362e-01, -3.2492e-01, -2.4262e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4674e+00, -5.6821e-01,  4.1808e-02],
                     [-6.6447e-01,  6.4649e-01, -2.8775e-01],
                     [ 7.0652e-01,  6.2381e-01,  2.7373e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.4663e+00, -1.9495e-02,  9.6007e-02],
                     [ 1.2277e-01,  2.9666e-02, -5.4597e-01],
                     [-8.8074e-01, -7.6862e-01,  1.2400e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6425e+00, -4.1852e-01, -1.1940e-03],
                     [ 7.4379e-01,  4.1132e-01,  1.7611e-02],
                     [-7.0199e-01,  8.0787e-02, -3.0684e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4751e+00, -4.7872e-01,  5.0865e-02],
                     [-5.4453e-01,  7.3622e-01, -2.6652e-02],
                     [ 8.8472e-01,  4.0309e-01,  3.7642e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0876,  0.0176,  0.0086,  ...,  0.0036,
        0.0203, -0.0166],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  3,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-0.8917,  1.2832,  0.0087],
                     [ 0.3354,  0.3915, -0.0444],
                     [ 0.3568, -0.9243,  0.7558],
                     ...,
                     [-0.4859, -1.2519, -1.3061],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.7057, -0.0305,  0.0021],
                     [-0.7738,  0.1291,  0.0048],
                     [ 1.0677,  1.0464, -0.0406],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4662, -0.0563, -0.1613],
                     [-0.1671, -0.0151,  0.5252],
                     [ 1.0043, -0.6517, -0.1452],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.4604, -0.4837, -0.0172],
                     [-0.5707,  0.6805,  0.0104],
                     [ 0.9388,  0.4507, -0.0805],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7097, -0.0579,  0.1504],
                     [-0.4756,  0.4820, -0.2431],
                     [ 0.6496, -0.3649, -0.0657],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5002, -0.5414,  0.1106],
                     [-0.6724,  0.6864, -0.3553],
                     [ 0.8005,  0.5836,  0.2541],
                     ...,
                     [ 1.8415, -0.5393, -0.8608],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0137,  0.0366, -0.0093,  ..., -0.0141,
0.0112,  0.0113],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  3,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[-1.2103e+00, -1.3899e-01, -3.5827e-03],
                     [ 2.6739e-01,  4.1137e-01,  7.7480e-02],
                     [ 1.2438e+00, -2.7866e-01, -5.0460e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6334e+00,  1.3890e-01,  7.0993e-02],
                     [ 4.1349e-01, -5.1143e-01, -3.3151e-03],
                     [-5.7517e-01,  4.1407e-01, -1.8326e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4976e+00, -1.0470e-01, -1.7783e-01],
                     [-1.6310e-01,  7.2266e-02,  5.0946e-01],
                     [ 9.6222e-01, -6.6780e-01, -1.6808e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-4.0956e-04, -1.0880e+00,  7.3740e-02],
                     [ 1.0371e+00,  7.6814e-02, -7.2282e-02],
                     [ 9.7889e-03,  1.0367e+00,  1.4912e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4079e+00, -4.1170e-02, -2.6871e-01],
                     [-2.0434e-01,  6.6865e-02,  5.3802e-01],
                     [ 9.4365e-01,  7.3313e-01, -1.4587e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1322e+00, -8.7106e-01,  1.1876e-01],
                     [ 1.3637e-02,  3.4499e-02, -3.7911e-01],
                     [ 1.4064e+00, -4.6838e-01,  6.1589e-02],
                     ...,
                     [-6.0107e-01,  1.3340e+00,  1.1372e+00],
                     [-1.0209e+00,  1.7907e+00, -4.6435e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0220,  0.0722,  0.0124,  ...,  0.0326, -
0.0048, -0.0248],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    ...,
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.3866, -0.4486,  0.0470],
                     [ 0.5312,  0.6541, -0.0973],
                     [-0.8351,  0.4674,  0.0862],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4396, -0.5490,  0.0301],
                     [-0.8014,  0.4995, -0.0397],
                     [ 0.7687,  0.4521,  0.0569],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1756, -0.2691, -0.0365],
                     [ 0.0845,  0.6065,  0.1159],
                     [ 1.2086, -0.2784, -0.1641],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.7316, -0.0676,  0.0404],
                     [-0.4459,  0.4779, -0.0726],
                     [ 0.6245, -0.3790, -0.0288],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5039, -0.0526, -0.1574],
                     [-0.1584, -0.0413,  0.5125],
                     [ 1.0152, -0.6404, -0.1436],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.3134,  0.9749, -0.0237],
                     [-0.0104,  0.7818,  0.0258],
                     [-0.5100, -0.5762,  0.0065],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0479, -0.0296,  0.0200,  ..., -0.0107, -
0.0200, -0.0307],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  3,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.2284e+00, -1.3948e-03,  1.3750e-02],
                     [-2.0208e-01, -3.2415e-02, -5.9537e-02],
                     [-1.4175e+00,  1.9271e-04,  2.8115e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 6.5565e-01, -2.0108e-02, -9.7147e-03],
                     [-7.5003e-01,  1.1843e-01,  2.4634e-02],
                     [ 1.1056e+00,  9.7304e-01, -5.3808e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6718e+00, -3.7810e-01, -3.6625e-03],
                     [ 6.5454e-01,  5.0955e-01, -2.6228e-03],
                     [-7.3483e-01,  5.7263e-02, -6.6619e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-3.2845e-02, -2.2582e-02, -1.8490e+00],
                     [ 1.0050e-02,  4.7422e-02, -6.5369e-01],
                     [ 4.3165e-02,  4.9284e-02,  7.4138e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5360e+00, -1.4630e-02, -2.3615e-01],
                     [-2.3082e-01,  2.7308e-02,  4.4767e-01],
                     [ 9.4942e-01,  7.3692e-01, -1.1232e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3266e+00,  4.9547e-01,  7.3347e-02],
                     [-6.4780e-01, -6.6600e-01, -2.6725e-01],
                     [ 6.1772e-01, -6.0427e-01,  2.1195e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0382,  0.0190,  0.0326,  ...,  0.0100, -
0.0118,  0.0438],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  3,  2,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.8800e+00, -8.9526e-02,  9.8332e-02],
                     [ 5.3746e-01,  4.6542e-01, -4.4988e-02],
                     [-5.7060e-01, -5.3858e-01, -1.3825e-01],
                     ...,
                     [-1.8055e+00,  9.7645e-01,  7.0560e-01],
                     [-2.8401e+00, -2.7242e-01,  1.0727e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4508e+00,  3.5107e-01,  1.0554e-01],
                     [-6.0501e-01, -5.0103e-01, -3.1972e-01],
                     [ 5.9274e-01, -4.7331e-01,  3.0863e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6737e+00,  1.2708e-01, -5.0109e-03],
                     [ 3.9506e-01, -4.9553e-01, -7.8783e-03],
                     [-5.9927e-01,  4.7144e-01,  2.7106e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.4439e+00, -4.4223e-02, -1.8219e-01],
                     [-1.2562e-01, -7.5544e-02,  5.7966e-01],
                     [ 1.0067e+00, -6.6173e-01, -1.3056e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 3.5057e-03,  1.2414e+00, -2.7725e-01],
                     [ 2.2822e-02,  1.3372e-03,  6.2515e-01],
                     [-4.2227e-02, -1.2607e+00, -2.8380e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3809e+00, -1.0170e-01,  2.1869e-02],
                     [ 8.5996e-02,  8.3674e-02,  2.8969e-02],
                     [ 8.8260e-01, -1.0176e+00, -1.9368e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0235, -0.0025,  0.0127,  ...,  0.0139, -
0.0021, -0.0470],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 2,  2,  0,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  3,  ...,  0, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.9672e+00, -1.0528e-01, -1.9851e-02],
                     [ 5.1103e-01,  4.5772e-01,  5.6349e-03],
                     [-6.3297e-01, -5.1664e-01,  9.4057e-02],
                     ...,
                     [-2.1554e+00,  9.0044e-01,  6.0874e-01],
                     [-2.7121e+00, -4.0221e-01, -2.9283e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3610e+00, -3.4055e-01, -2.8218e-03],
                     [ 7.7831e-02,  1.3826e-01,  4.2484e-04],
                     [ 1.0394e+00, -8.2641e-01,  4.1080e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 7.1180e-01,  7.7186e-02,  1.1423e-01],
                     [-7.1144e-01,  8.1526e-02, -9.0616e-02],
                     [ 1.0673e+00, -8.3555e-01,  3.8945e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.4253e+00,  5.2933e-01, -8.6600e-02],
                     [ 6.7190e-01, -6.9158e-01,  2.4906e-01],
                     [-6.5992e-01, -5.6100e-01, -3.4730e-01],
                     ...,
                     [-1.7615e+00,  3.3021e-01,  1.0958e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-7.1899e-01, -3.5068e-01, -2.9370e-03],
                     [ 7.1820e-01, -3.7935e-01,  1.2092e-02],
                     [-6.9988e-03,  8.4399e-01,  2.1073e-04],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4351e+00,  1.5718e-01, -1.5632e-01],
                     [ 1.4430e-01, -1.0762e-01,  4.9668e-01],
                     [-9.5034e-01,  6.4427e-01, -1.9318e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0252, -0.0821,  0.0881,  ..., -0.0073,
0.0096,  0.0442],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.7035e+00, -1.7672e-01, -1.2512e-02],
                     [ 4.0565e-01,  4.6070e-01, -1.8055e-02],
                     [-5.8191e-01, -4.1193e-01,  7.2655e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4108e+00, -1.0454e-01, -7.2751e-03],
                     [ 8.2407e-02,  1.1850e-01, -1.7662e-02],
                     [ 7.9533e-01, -1.0440e+00, -2.3765e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3818e+00, -1.0557e-01, -7.5774e-03],
                     [ 1.1299e-01,  1.2742e-01,  1.8232e-02],
                     [ 7.5005e-01, -1.0374e+00, -7.1122e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.2669e+00, -5.7529e-01,  7.7698e-02],
                     [-7.6105e-03, -7.2759e-04, -4.0973e-01],
                     [-1.3001e+00, -5.9126e-01,  9.0956e-02],
                     ...,
                     [-3.3910e-01,  1.3399e+00,  1.0685e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.1271e+00,  8.3671e-02, -6.2775e-03],
                     [-6.4643e-02, -5.5953e-01,  3.1765e-03],
                     [-1.0754e+00,  1.9683e-01, -4.9168e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5213e+00, -4.4971e-01, -9.3552e-02],
                     [-5.6478e-01,  6.2581e-01, -1.0115e-02],
                     [ 8.0873e-01,  1.2027e-02,  3.8536e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0180, -0.0849, -0.0125,  ...,  0.0005,
0.0297, -0.0327],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -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]]),
             'coordinates': tensor([[[-1.7251e+00, -2.1259e-02, -3.8393e-02],
                     [-4.6978e-01,  4.3388e-01,  2.5254e-02],
                     [ 6.6850e-01, -4.0021e-01,  6.9523e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.6320e+00,  1.8199e-01,  1.8342e-01],
                     [-5.1260e-01, -2.7044e-01, -4.4436e-01],
                     [ 5.4881e-01, -3.0452e-01,  4.6472e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3247e+00, -5.9721e-01,  8.7410e-03],
                     [ 1.6506e-03,  1.6668e-01,  1.1467e-02],
                     [ 1.2964e+00, -6.2158e-01, -8.3808e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 9.6819e-03,  1.2878e+00, -2.6320e-01],
                     [-6.4208e-03, -1.8734e-03,  5.7161e-01],
                     [ 2.9483e-03, -1.2831e+00, -2.5198e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3897e+00, -5.5403e-01,  7.5884e-03],
                     [-5.5299e-01,  7.6930e-01,  6.1260e-03],
                     [ 9.5105e-01,  4.2969e-01, -5.0458e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6518e+00, -3.8152e-01,  4.0596e-03],
                     [ 6.4274e-01,  4.9263e-01,  1.7439e-03],
                     [-7.2627e-01,  1.1231e-01, -4.7871e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0058,  0.0292, -0.0623,  ..., -0.0252, -
0.0200,  0.0305],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0,  0],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.3290e+00,  9.2957e-01, -6.0184e-03],
                     [-9.7892e-03,  7.6250e-01,  6.1565e-03],
                     [-6.7271e-01, -4.7276e-01,  6.7274e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.9611e+00, -1.3574e-01, -3.1131e-02],
                     [ 6.2030e-01,  5.5040e-01,  1.8925e-02],
                     [-5.5762e-01, -4.9052e-01,  7.1323e-02],
                     ...,
                     [-2.1880e+00,  4.9911e-01, -1.0802e+00],
                     [-2.7845e+00, -6.4312e-01,  6.2544e-02],
                     [-2.1486e+00,  9.4729e-01,  7.5183e-01]],

                    [[ 1.3435e+00, -6.4749e-01, -2.2316e-02],
                     [-2.8605e-02,  8.9930e-02,  2.2562e-03],
                     [-1.3349e+00, -6.5193e-01, -1.3121e-02],
                     ...,
                     [-8.9135e-01,  2.0909e+00, -6.3362e-03],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.5182e+00, -1.1903e-01, -1.6704e-01],
                     [ 2.1794e-01, -4.7177e-02,  4.5028e-01],
                     [-8.9178e-01,  8.0592e-01, -1.5472e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5285e+00, -4.4298e-01, -1.0878e-01],
                     [-5.7319e-01,  5.7457e-01,  3.0304e-02],
                     [ 8.2470e-01,  8.1316e-02, -2.9049e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2912e+00, -6.4330e-01,  2.0853e-02],
                     [-1.9737e-02,  2.1345e-01, -6.2078e-02],
                     [ 1.2509e+00, -6.1064e-01,  1.1115e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0241,  0.0069, -0.0173,  ...,  0.0159, -
0.0442, -0.0388],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  3,  3,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  3,  0,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.7761e+00, -1.7356e-04, -1.4287e-02],
                     [-4.4941e-01,  3.8809e-01,  1.2850e-02],
                     [ 6.9465e-01, -3.7355e-01,  1.9828e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7307e+00, -3.7856e-01,  3.0156e-01],
                     [ 6.3726e-01,  3.2514e-01,  7.2658e-02],
                     [-6.0315e-01, -2.8280e-01, -1.1699e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4153e-02,  1.1083e+00, -2.1367e-01],
                     [-1.6962e-02,  2.6611e-02,  5.6955e-01],
                     [ 8.0077e-03, -1.1443e+00, -2.1676e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.7827e+00, -3.7749e-01,  1.6993e-01],
                     [ 6.4943e-01,  3.4923e-01,  2.4255e-01],
                     [-6.3211e-01, -3.0525e-01,  5.3003e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-8.8390e-01,  1.2367e+00, -2.4760e-02],
                     [ 3.8785e-01,  4.7343e-01,  7.3573e-02],
                     [ 3.4314e-01, -9.1700e-01,  7.3437e-01],
                     ...,
                     [-6.6511e-01, -1.0192e+00, -1.2854e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 6.4709e-01, -1.9839e-02, -1.6873e-02],
                     [-7.3408e-01,  1.1550e-01,  5.0110e-02],
                     [ 1.0471e+00,  1.0293e+00, -1.7315e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0137,  0.0163,  0.1420,  ...,  0.0143, -
0.0019,  0.0756],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.3667, -0.5384, -0.0883],
                     [-0.6763,  0.6476,  0.0609],
                     [ 0.7486,  0.3412, -0.1370],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2308, -0.7163,  0.0725],
                     [ 0.7069,  0.6160, -0.0182],
                     [-0.8289,  0.6441, -0.0164],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2597,  0.8769,  0.0306],
                     [-0.0700,  0.8822,  0.0222],
                     [-0.5447, -0.5157, -0.0478],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.2511, -0.6785,  0.0386],
                     [ 0.6997,  0.6492, -0.0919],
                     [-0.7607,  0.5465,  0.1036],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2386, -0.6758,  0.0706],
                     [ 0.7254,  0.6222, -0.0064],
                     [-0.7849,  0.5754, -0.0123],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4422,  0.0455, -0.2848],
                     [-0.1906,  0.0097,  0.4931],
                     [ 0.9006,  0.7712, -0.1591],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0415,  0.0398, -0.0203,  ...,  0.0051,
0.0173,  0.0107],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  3,  1,  ..., -1, -1, -1],
                    [ 2,  0,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 2,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-1.3669, -0.4017, -0.0275],
                     [-0.4835,  0.7478,  0.0245],
                     [ 0.8115,  0.4125, -0.0275],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.0074,  0.0027, -0.0797],
                     [ 0.3959, -0.7836,  0.0938],
                     [ 0.4592,  0.9368,  0.0797],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4740,  0.0864, -0.1567],
                     [ 0.1368, -0.0281,  0.4881],
                     [-1.0452,  0.5942, -0.0826],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.7201, -0.3202, -0.1312],
                     [ 0.5744,  0.4937,  0.2008],
                     [-0.7034, -0.3568,  0.2503],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2279, -0.6925,  0.1098],
                     [-0.0139,  0.0546, -0.4025],
                     [-1.2078, -0.6813,  0.0944],
                     ...,
                     [ 0.3770,  1.4203,  0.9878],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.8864, -0.0653,  0.0406],
                     [ 0.6088,  0.5028, -0.0798],
                     [-0.5792, -0.4323,  0.0166],
                     ...,
                     [-2.0602,  0.5993,  0.7838],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0666,  0.0327, -0.0023,  ..., -0.0150, -
0.0337, -0.0191],
                        dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.3644e+00, -5.4517e-01, -1.0598e-02],
                     [-5.2815e-01,  7.5733e-01, -3.5957e-02],
                     [ 9.4920e-01,  4.4817e-01, -3.5058e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4091e+00, -5.0932e-01, -1.2653e-02],
                     [-5.4662e-01,  7.3027e-01,  5.9848e-04],
                     [ 9.3229e-01,  4.4174e-01, -2.9320e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4639e+00, -5.3762e-01,  1.2818e-01],
                     [-6.5918e-01,  7.1813e-01, -3.2886e-01],
                     [ 7.8543e-01,  5.5972e-01,  2.2303e-01],
                     ...,
                     [ 1.9203e+00, -5.6993e-01, -9.1114e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.3423e+00, -3.7074e-01, -6.7072e-03],
                     [ 4.9985e-02,  1.5273e-01, -3.0669e-02],
                     [ 1.0116e+00, -8.1734e-01,  2.8767e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7358e+00, -2.7681e-01, -3.1801e-01],
                     [ 5.3545e-01,  5.4009e-01,  3.5495e-01],
                     [-7.3588e-01, -2.3043e-01,  3.5492e-01],
                     ...,
                     [-2.6434e+00, -7.3918e-01, -6.6059e-02],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1554e+00,  5.1851e-03, -4.7066e-04],
                     [ 2.8458e-01, -4.7473e-02, -2.4911e-03],
                     [ 1.4187e+00,  2.9343e-02,  1.0486e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0408, -0.0513,  0.0037,  ...,  0.2982, -
0.0157, -0.0399],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[ 1.1668e-02,  1.0768e+00, -8.9529e-02],
                     [-1.0463e+00, -4.4580e-02,  1.1241e-01],
                     [-2.8424e-03, -1.0347e+00, -2.6253e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6344e+00, -3.8602e-01, -1.2106e-02],
                     [ 6.4997e-01,  5.1235e-01,  4.0390e-03],
                     [-7.3382e-01,  1.3710e-01,  2.9156e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.6579e+00, -4.3900e-01,  2.3149e-02],
                     [ 5.5656e-01,  5.6712e-01, -5.2468e-02],
                     [-8.5495e-01,  1.4324e-01,  4.4799e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.7881e+00, -2.7809e-01, -1.7183e-01],
                     [ 5.0467e-01,  5.6459e-01,  1.8636e-01],
                     [-7.0199e-01, -3.4356e-01,  2.1760e-01],
                     ...,
                     [-2.7048e+00, -6.3107e-01, -1.0434e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-8.0890e-03,  1.2971e+00, -2.5564e-01],
                     [-2.6484e-03, -3.2471e-03,  5.4525e-01],
                     [ 1.0503e-02, -1.3073e+00, -2.4966e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-9.0425e-01,  1.2963e+00,  3.1334e-02],
                     [ 3.5448e-01,  3.8031e-01, -7.4981e-02],
                     [ 3.5469e-01, -8.8344e-01,  7.8365e-01],
                     ...,
                     [-6.1429e-01, -1.1777e+00, -1.1686e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0177,  0.0325,  0.0512,  ...,  0.0042, -
0.0223, -0.0001],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0,  0],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[ 1.3167, -0.6683, -0.0074],
                     [ 0.0352,  0.1124,  0.0832],
                     [-1.2984, -0.6906,  0.0127],
                     ...,
                     [-0.9232,  2.0684, -0.2219],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.9366, -0.1698,  0.1093],
                     [ 0.6271,  0.5670, -0.1101],
                     [-0.5484, -0.4653, -0.1376],
                     ...,
                     [-2.4335,  0.5254, -0.8419],
                     [-2.5585, -0.8985,  0.3920],
                     [-2.0179,  0.7901,  0.9934]],

                    [[-1.4945, -0.4432,  0.0109],
                     [-0.7688,  0.4711, -0.0075],
                     [ 0.7687,  0.1708, -0.0610],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.6840, -0.2754, -0.3193],
                     [ 0.5649,  0.5585,  0.3269],
                     [-0.7074, -0.2449,  0.3496],
                     ...,
                     [-2.6678, -0.7852, -0.1206],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2765, -0.5169, -0.1808],
                     [ 0.5519,  0.6391,  0.1778],
                     [-0.7461,  0.5135, -0.0592],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1495, -0.9406,  0.0771],
                     [-0.0205,  0.0426, -0.3334],
                     [ 1.3548, -0.4002,  0.1004],
                     ...,
                     [ 0.2324,  1.5606,  1.0688],
                     [-1.2241,  1.6516,  0.0584],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0033, -0.0132, -0.0349,  ..., -0.0162,
0.0191, -0.0050],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-0.0170, -1.0845,  0.1912],
                     [ 1.0663,  0.1038, -0.2853],
                     [ 0.0030,  1.0728,  0.3817],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0575, -0.2055,  1.2807],
                     [-0.0156,  0.5319, -0.0070],
                     [ 0.0219, -0.1959, -1.2506],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.9135,  1.3375,  0.0211],
                     [ 0.3171,  0.3977, -0.0584],
                     [ 0.3952, -0.8954,  0.7321],
                     ...,
                     [-0.4587, -1.4925, -1.2296],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.7418, -0.0237,  0.0075],
                     [-0.4423,  0.4348, -0.0448],
                     [ 0.6468, -0.4053,  0.0389],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2819, -0.6208,  0.0274],
                     [-0.7342,  0.6469, -0.2582],
                     [ 0.7230,  0.5979,  0.2529],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0218,  0.0260,  0.6156],
                     [ 0.0186,  0.0059, -0.6206],
                     [ 0.1057, -0.2295,  1.7098],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.1576,  0.0152,  0.0093,  ..., -0.0147,
0.0064,  0.0662],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 2,  2, -1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 0.0000e+00,  0.0000e+00,  5.3191e-01],
                     [ 0.0000e+00,  0.0000e+00, -5.3191e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4209e+00, -4.3598e-01, -1.1138e-01],
                     [ 5.2577e-01,  6.4988e-01,  2.0708e-01],
                     [-8.2928e-01,  4.6522e-01, -2.4133e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.3289e+00, -4.3182e-01, -3.1414e-03],
                     [-4.5653e-01,  7.5201e-01, -1.9313e-02],
                     [ 8.2915e-01,  4.4179e-01, -9.1340e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.5937e+00, -4.0409e-01, -2.1000e-02],
                     [ 6.9617e-01,  5.2260e-01, -9.3404e-03],
                     [-7.6766e-01,  2.3463e-01,  9.8173e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5653e+00, -4.4107e-01, -2.0014e-03],
                     [ 7.4860e-01,  4.2877e-01,  9.9966e-04],
                     [-6.8064e-01,  1.4791e-01,  1.0092e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2491e+00, -6.7786e-01,  1.5418e-02],
                     [ 7.2366e-01,  6.3073e-01, -1.0364e-02],
                     [-7.7694e-01,  5.7684e-01,  9.7421e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0793,  0.1365, -0.0530,  ...,  0.0407,
0.0167, -0.0152],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0,  0]]),
             'coordinates': tensor([[[-1.5440e+00, -7.8355e-02, -1.3929e-01],
                     [-1.5780e-01, -2.4283e-03,  5.0010e-01],
                     [ 9.9607e-01, -6.4820e-01, -1.4295e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-8.7020e-01,  1.2629e+00, -1.1101e-02],
                     [ 3.0692e-01,  3.8237e-01, -9.9233e-03],
                     [ 3.7642e-01, -9.2170e-01,  7.8647e-01],
                     ...,
                     [-5.9658e-01, -1.1418e+00, -1.2596e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-7.6825e-01,  7.8615e-01,  3.8829e-02],
                     [-7.4752e-01, -7.7762e-01, -1.3330e-02],
                     [ 7.5537e-01, -7.8422e-01,  1.7582e-02],
                     ...,
                     [ 1.1937e+00,  1.2037e+00, -9.3334e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-8.6671e-01,  1.2841e+00,  2.3891e-04],
                     [ 3.6385e-01,  4.1012e-01, -5.5618e-03],
                     [ 3.2510e-01, -8.9182e-01,  7.2427e-01],
                     ...,
                     [-5.2184e-01, -1.1143e+00, -1.3541e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2520e-02, -3.9413e-01,  7.6699e-01],
                     [ 4.8219e-02, -4.4236e-01, -7.4856e-01],
                     [ 5.4070e-02,  8.9475e-01,  8.1317e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.9536e+00, -1.3045e-01, -1.0272e-02],
                     [ 5.6613e-01,  5.2569e-01,  2.3560e-02],
                     [-5.6865e-01, -5.1394e-01,  4.4892e-03],
                     ...,
                     [-2.1197e+00,  7.3735e-01, -9.1565e-01],
                     [-2.7197e+00, -6.5614e-01,  3.9129e-02],
                     [-2.1241e+00,  7.3982e-01,  8.6567e-01]]]),
             'energies': tensor([-0.0124,  0.0015, -0.0185,  ..., -0.0083,
0.0290, -0.0456],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0,  0, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.1283e+00, -9.0875e-01,  1.1315e-01],
                     [-8.5177e-03,  2.3753e-02, -3.7342e-01],
                     [ 1.3849e+00, -4.6140e-01,  8.7132e-02],
                     ...,
                     [-2.0782e-01,  1.4703e+00,  1.0674e+00],
                     [-1.0683e+00,  1.7924e+00, -2.7462e-01],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.7955e+00, -3.6349e-01,  2.8092e-01],
                     [ 6.4738e-01,  3.0513e-01,  1.0907e-01],
                     [-6.6217e-01, -3.2601e-01, -1.2834e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2196e+00,  2.7514e-03,  4.7226e-03],
                     [-1.9830e-01, -4.9461e-02, -7.2887e-02],
                     [-1.4225e+00,  2.3922e-02,  5.0048e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.4673e+00, -5.5928e-01,  6.6739e-02],
                     [-6.9996e-01,  6.7691e-01, -3.1590e-01],
                     [ 7.0660e-01,  6.1549e-01,  2.6761e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 4.2725e-05, -1.0695e+00,  2.0834e-02],
                     [ 1.0372e+00,  5.9676e-02, -2.9859e-02],
                     [-1.4073e-03,  1.0646e+00,  4.6883e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5679e+00, -4.1195e-01, -9.7096e-02],
                     [-5.6941e-01,  5.7752e-01,  1.3920e-02],
                     [ 8.4135e-01, -1.1169e-02, -2.5496e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0460, -0.0108,  0.0369,  ...,  0.0029, -
0.0165, -0.0278],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4690,  0.1149, -0.1444],
                     [ 0.1660, -0.0380,  0.5057],
                     [-1.0824,  0.5878, -0.0377],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.3559, -0.5435,  0.0586],
                     [-0.8336,  0.5242, -0.0816],
                     [ 0.7620,  0.4764,  0.1100],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.4019, -0.5208, -0.1306],
                     [ 0.5536,  0.6525,  0.0668],
                     [-0.7772,  0.4889,  0.0253],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 0.0044,  1.2322, -0.2690],
                     [-0.0193,  0.0093,  0.6084],
                     [ 0.0211, -1.2431, -0.2679],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.7292, -0.2987, -0.1008],
                     [ 0.5459,  0.4645,  0.1130],
                     [-0.6801, -0.3940,  0.2598],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5233, -0.5202, -0.1259],
                     [ 0.5888,  0.5961,  0.0339],
                     [-0.8045,  0.1358,  0.0091],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([ 0.0085, -0.0213,  0.0228,  ..., -0.0261, -
0.0039,  0.0192],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 3,  2,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 3,  2,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-7.2439e-01,  1.7426e-02, -9.0454e-02],
                     [ 7.0157e-01, -1.5120e-02, -1.3198e-01],
                     [-1.0860e+00, -2.0331e-01,  7.6938e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5629e+00, -5.0643e-01,  1.2243e-01],
                     [-5.9745e-01,  6.1087e-01, -3.1327e-01],
                     [ 7.5903e-01,  5.4653e-01,  3.1483e-01],
                     ...,
                     [ 1.3865e+00, -6.3993e-01, -1.0132e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2851e+00, -5.9798e-01,  3.6875e-02],
                     [ 2.2376e-02,  1.9363e-01, -5.3111e-03],
                     [ 1.2905e+00, -6.5051e-01,  4.2843e-04],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.6358e+00,  1.8891e-01, -1.5816e-01],
                     [ 4.4594e-01, -4.8091e-01,  1.5171e-01],
                     [-6.5943e-01,  3.9585e-01, -7.8955e-04],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5774e+00, -4.9506e-01, -1.0500e-01],
                     [ 5.7976e-01,  5.4256e-01,  4.4605e-02],
                     [-8.1704e-01,  1.0251e-01, -4.1654e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7212e+00, -5.4633e-02,  1.3421e-01],
                     [-4.5478e-01,  4.6805e-01, -1.8649e-01],
                     [ 6.5036e-01, -3.4588e-01, -1.2659e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0596, -0.0316, -0.0435,  ..., -0.0116,
0.0244, -0.0150],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.4370e+00,  1.6331e-03,  9.7060e-02],
                     [ 1.3165e-01, -3.2054e-04, -5.7300e-01],
                     [-8.8363e-01, -7.2990e-01,  1.1235e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2019e+00, -2.3890e-01, -5.1961e-02],
                     [ 6.1347e-02,  5.7735e-01,  5.8422e-02],
                     [ 1.1552e+00, -3.3721e-01, -9.7837e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4733e+00, -3.4217e-01,  2.5433e-03],
                     [-4.5676e-01,  6.2797e-01,  5.8383e-02],
                     [ 8.3435e-01,  4.2002e-01, -2.6423e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 7.1283e-03,  1.3231e+00, -2.4689e-01],
                     [ 3.2221e-02, -1.6049e-02,  5.5092e-01],
                     [-4.2442e-02, -1.3323e+00, -2.3381e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2835e+00, -2.2316e-01, -2.8155e-02],
                     [ 7.0543e-02,  5.2771e-01,  5.3144e-02],
                     [ 1.2306e+00, -3.0634e-01, -1.2107e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.5234e+00, -5.1288e-01, -1.2664e-01],
                     [ 6.0291e-01,  5.8922e-01,  4.9978e-02],
                     [-7.9934e-01,  1.0838e-01,  2.4311e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0042, -0.0087, -0.0369,  ...,  0.0099, -
0.0203,  0.0215],
                         dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    ...,
                    [ 3,  1,  1,  ..., -1, -1, -1],
                    [ 2,  1,  2,  ..., -1, -1, -1],
                    [ 1,  3,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.6044, -0.5101,  0.1730],
                     [-0.6150,  0.6291, -0.3356],
                     [ 0.7990,  0.5405,  0.3920],
                     ...,
                     [ 1.7687, -0.2705, -1.0689],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4591, -0.4877, -0.0535],
                     [-0.5051,  0.6615,  0.0031],
                     [ 0.9063,  0.4460, -0.0521],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1592, -0.1445,  0.0332],
                     [ 0.2762,  0.4767, -0.0777],
                     [ 1.1906, -0.3190,  0.0531],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 1.2540, -0.5595,  0.0488],
                     [ 0.6739,  0.6497, -0.0636],
                     [-0.7703,  0.4599,  0.0777],
                     ...,
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                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.0065, -0.8808,  0.0045],
                     [ 0.0208,  0.0905,  0.0287],
                     [-1.2918, -0.3350,  0.0094],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.7333,  0.1275, -0.0378],
                     [-0.4630, -0.4920,  0.0743],
                     [ 0.6052,  0.3072,  0.0230],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0011,  0.0326, -0.0134,  ..., -0.0292, -
0.0585, -0.0026],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.6745, -0.4573,  0.1490],
                     [-0.5491,  0.5327, -0.2647],
                     [ 0.7724,  0.5201,  0.3326],
                     ...,
                     [ 1.5537, -0.4409, -1.1042],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.7057, -0.3247, -0.1260],
                     [ 0.5363,  0.5028,  0.1738],
                     [-0.6565, -0.3249,  0.2182],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1551,  0.0115,  0.0085],
                     [ 0.2668,  0.0789,  0.0031],
                     [ 1.4270, -0.0495, -0.0045],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[ 0.0489,  0.0140, -1.8251],
                     [-0.0783, -0.0119, -0.6441],
                     [ 0.0205, -0.0872,  0.7404],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.1353,  0.1218, -0.1093],
                     [ 0.0709, -0.4546,  0.0126],
                     [ 1.1684,  0.1511, -0.0067],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5632, -0.4987, -0.0130],
                     [ 0.5887,  0.6753,  0.0389],
                     [-0.8570,  0.1881, -0.0424],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0155, -0.0114, -0.0329,  ...,  0.0103,
0.0127,  0.0202],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 1,  1,  3,  ...,  0, -1, -1],
                    ...,
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0,  0, -1]]),
             'coordinates': tensor([[[-0.0134,  1.2387, -0.2265],
                     [-0.0118,  0.0390,  0.5147],
                     [ 0.0095, -1.2870, -0.2326],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4442, -0.4999,  0.0104],
                     [-0.5132,  0.7011, -0.0813],
                     [ 0.7913,  0.6984,  0.0033],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.5721,  0.4997, -0.1394],
                     [ 0.5773, -0.6063,  0.3095],
                     [-0.6149, -0.4997, -0.4215],
                     ...,
                     [-1.9535,  0.0329,  1.1457],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-0.0165, -0.2450,  1.1886],
                     [-0.0339,  0.5979, -0.0229],
                     [-0.0274, -0.2129, -1.1836],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.4210, -0.4593, -0.0167],
                     [-0.5356,  0.7158, -0.0529],
                     [ 0.7466,  0.6562, -0.0601],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.2254, -0.9169,  0.1242],
                     [ 0.0384,  0.0285, -0.4170],
                     [ 1.4253, -0.4110,  0.0659],
                     ...,
                     [-0.4487,  1.1745,  1.1694],
                     [-0.9411,  1.9093, -0.3276],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0103,  0.0732, -0.0210,  ...,  0.0002,
0.1616, -0.0091],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
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                    [ 2,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  2,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.1743e+00, -1.5689e-01,  3.0913e-02],
                     [ 9.5681e-02,  3.8215e-01, -1.8921e-02],
                     [ 1.3496e+00, -1.1296e-01, -1.2926e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.0656e+00, -4.8959e-01,  2.8333e-02],
                     [-3.1583e-02,  5.1550e-01, -3.7103e-03],
                     [ 1.2607e+00,  1.1115e-01,  1.9001e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4855e+00, -5.0672e-01,  7.9966e-02],
                     [-6.7260e-01,  5.8039e-01, -3.3744e-01],
                     [ 6.9276e-01,  5.4694e-01,  3.2340e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-1.3913e+00, -1.4480e-01,  4.3932e-03],
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                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7402e+00,  1.4806e-01, -4.0233e-02],
                     [-4.0963e-01, -4.1054e-01,  1.2340e-01],
                     [ 7.5224e-01,  3.6756e-01,  3.9240e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.4301e+00, -6.3715e-02, -1.8046e-01],
                     [-1.3637e-01, -1.6071e-02,  5.7316e-01],
                     [ 9.7892e-01, -6.9297e-01, -1.7303e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([-0.0188,  0.0144, -0.0296,  ..., -0.0543, -
0.0405,  0.0090],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 1,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.2877e+00, -7.0022e-01, -4.4075e-02],
                     [-4.7269e-02,  1.4566e-01,  1.3499e-02],
                     [-1.2875e+00, -7.3009e-01, -1.1720e-02],
                     ...,
                     [-8.3462e-01,  2.1543e+00,  6.3132e-02],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5733e+00,  2.2494e-01,  1.7337e-01],
                     [-5.8906e-01, -3.8675e-01, -3.6446e-01],
                     [ 5.4507e-01, -3.0624e-01,  3.2827e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.4291e+00, -4.3901e-01, -2.0744e-02],
                     [ 5.1420e-01,  6.3832e-01,  5.1435e-02],
                     [-8.4399e-01,  4.8635e-01, -2.9818e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-8.9657e-01,  1.2447e+00,  2.5228e-03],
                     [ 3.9361e-01,  4.3307e-01, -3.0102e-02],
                     [ 3.2881e-01, -8.6244e-01,  7.8818e-01],
                     ...,
                     [-6.0655e-01, -1.0846e+00, -1.2212e+00],
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                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2755e+00,  4.1672e-02, -1.0793e-03],
                     [-2.4073e-01, -1.3800e-01,  1.0518e-02],
                     [-1.4444e+00,  5.0245e-02, -1.1159e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-6.7162e-01,  5.7030e-02, -8.6715e-02],
                     [ 6.6726e-01, -6.9556e-02,  5.4375e-02],
                     [-1.4059e+00, -7.7516e-01,  2.7122e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0187,  0.0196, -0.0456,  ..., -0.0067,
0.0390,  0.0286],
                    dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  3,  ...,  0, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.5844,  0.4841, -0.1190],
                     [ 0.5394, -0.6075,  0.3220],
                     [-0.6102, -0.4454, -0.5152],
                     ...,
                     [-1.6060,  0.2021,  1.3042],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.8068, -0.3094, -0.0999],
                     [ 0.5872,  0.4486,  0.0951],
                     [-0.7369, -0.3451,  0.2036],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.2334, -0.6697,  0.0833],
                     [-0.0389,  0.0431, -0.3789],
                     [-1.2093, -0.6395,  0.0607],
                     ...,
                     [ 0.3881,  1.3759,  0.9854],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-1.7318, -0.4600,  0.1167],
                     [-0.6426,  0.6134, -0.2564],
                     [ 0.7651,  0.4693,  0.2775],
                     ...,
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                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-0.0230,  1.2948, -0.2500],
                     [-0.0358, -0.0181,  0.5627],
                     [ 0.0180, -1.2695, -0.2709],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[-1.5351, -0.4819, -0.0398],
                     [-0.5839,  0.7150,  0.0606],
                     [ 0.9301,  0.4052, -0.1010],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0012,  0.0014, -0.0221,  ..., -0.0008, -
0.0090, -0.0335],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ..., -1, -1, -1],
                    [ 1,  2,  2,  ..., -1, -1, -1],
                    [ 2,  2,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    [ 3,  3,  0,  ..., -1, -1, -1],
                    [ 3,  1,  3,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[ 1.6345e+00, -4.4956e-01, -1.6311e-03],
                     [ 5.8876e-01,  6.1534e-01, -1.3606e-02],
                     [-8.3609e-01,  6.6246e-02, -9.3606e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.5196e+00,  3.1294e-01,  1.2005e-01],
                     [-5.7943e-01, -4.3626e-01, -3.4098e-01],
                     [ 5.9263e-01, -4.4843e-01,  3.3704e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.7755e+00, -1.2262e-02, -2.2623e-02],
                     [-4.1877e-01,  4.1419e-01,  4.3938e-02],
                     [ 6.7074e-01, -4.1954e-01,  2.7289e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[ 1.7859e+00, -3.5571e-01,  3.1879e-01],
                     [ 6.4409e-01,  2.8909e-01,  5.9289e-02],
                     [-6.4842e-01, -3.4409e-01, -1.7130e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 7.3693e-01,  1.2028e-01, -1.0367e-02],
                     [-7.3483e-01, -1.2148e-01, -7.8853e-03],
                     [ 5.4813e-01, -6.9625e-01, -2.3398e-01],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.2779e+00, -1.9899e-01,  2.1425e-02],
                     [ 5.3152e-02, -1.4458e-01, -2.1999e-02],
                     [ 4.7340e-01,  1.1669e+00,  7.9882e-03],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0322, -0.0026, -0.0066,  ..., -0.0027,
0.1722, -0.0996],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  2,  1,  ..., -1, -1, -1],
                    [ 2,  1,  1,  ..., -1, -1, -1],
                    [ 2,  2,  0,  ..., -1, -1, -1],
                    ...,
                    [ 1,  2,  1,  ...,  0,  0, -1],
                    [ 3,  3,  0,  ..., -1, -1, -1],
                    [ 1,  1,  2,  ..., -1, -1, -1]]),
             'coordinates': tensor([[[-1.7149,  0.1573,  0.0421],
                     [-0.3872, -0.4912, -0.0521],
                     [ 0.6755,  0.3000, -0.1157],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.6523, -0.3155, -0.2395],
                     [ 0.5558,  0.4614,  0.2471],
                     [-0.6893, -0.3008,  0.3992],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.7180,  0.0622,  0.1161],
                     [-0.6917,  0.0902, -0.1204],
                     [ 0.9937, -0.9542,  0.4133],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    ...,

                    [[-0.1820,  1.3704,  0.0691],
                     [ 0.0186, -0.0038, -0.3994],
                     [ 1.2824, -0.5538,  0.0628],
                     ...,
                     [-0.9553, -1.8730, -0.1924],
                     [-1.2492, -0.7742,  1.1604],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 0.7180,  0.0887, -0.0340],
                     [-0.7247, -0.0841, -0.0425],
                     [ 0.9062, -0.6204,  0.1522],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]],

                    [[ 1.3707, -0.4959, -0.0249],
                     [ 0.5190,  0.7011,  0.0337],
                     [-0.7190,  0.7468, -0.0511],
                     ...,
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000],
                     [ 0.0000,  0.0000,  0.0000]]]),
             'energies': tensor([-0.0238, -0.0034,  0.0576,  ..., -0.0291,
0.3408,  0.0054],
                       dtype=torch.float64)}),
```

```
defaultdict(list,
            {'species': tensor([[ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  3,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ..., -1, -1, -1],
                    ...,
                    [ 1,  1,  1,  ...,  0, -1, -1],
                    [ 1,  1,  0,  ..., -1, -1, -1],
                    [ 1,  1,  1,  ...,  0, -1, -1]]),
             'coordinates': tensor([[[-1.5063e+00, -4.9278e-01,  1.3669e-01],
                     [-5.7493e-01,  5.7448e-01, -2.8932e-01],
                     [ 7.8171e-01,  5.1465e-01,  3.5760e-01],
                     ...,
                     [ 9.9330e-01, -5.6048e-01, -1.1081e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-1.1522e+00, -1.5090e-01, -3.4036e-02],
                     [ 2.4909e-01,  4.6849e-01,  6.6280e-02],
                     [ 1.1914e+00, -3.0789e-01, -4.8421e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[-5.4175e-02, -8.3738e-01,  4.2916e-03],
                     [ 7.8326e-01,  4.0171e-01, -1.6388e-02],
                     [-7.1745e-01,  4.5220e-01,  2.0213e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    ...,

                    [[-8.8924e-01,  1.2760e+00,  1.3547e-02],
                     [ 3.7969e-01,  3.9874e-01, -6.7113e-02],
                     [ 3.6007e-01, -8.6513e-01,  7.9582e-01],
                     ...,
                     [-6.3560e-01, -1.0521e+00, -1.3025e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 8.2305e-01,  1.9252e-02,  7.2332e-03],
                     [-8.2930e-01,  4.1186e-02, -1.0918e-02],
                     [ 1.0718e+00,  8.4149e-01,  2.3441e-02],
                     ...,
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]],

                    [[ 1.2938e+00, -7.3709e-01, -6.8136e-02],
                     [-1.9746e-03,  1.4076e-01,  6.7277e-02],
                     [-1.2232e+00, -6.5337e-01, -9.0104e-03],
                     ...,
                     [-9.1820e-01,  2.0970e+00, -2.3996e-04],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00],
                     [ 0.0000e+00,  0.0000e+00,  0.0000e+00]]]),
             'energies': tensor([ 0.0058, -0.0220,  0.0114,  ...,  0.0018,
0.3611,  0.0026],
                       dtype=torch.float64)})]
```

In [9]:
```
print(len(train_data_loader_list))
assert(len(train_data_loader_list) == len(train_data) // batch_size + 1)
```

```
85
```

The appropriate number of batches were created. For a dataset of size 691918, a total of 85 batches should be created and that is what is observed

In [10]:
```
display(len(train_data_loader_list[0]['species']))
display(len(train_data_loader_list[0]['coordinates']))
display(len(train_data_loader_list[0]['energies']))
```

```
8192
8192
8192
```

Batching is appropriately creating batches of size 8192. Each batch of the ANI dataset is of a dictionary with species, coordinates, and energies all stored in corresponding tensors.

In [11]:
```
# Training Data Batches
for i, batch in enumerate(train_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 8192
Batch # 11 is of size: 8192
Batch # 12 is of size: 8192
Batch # 13 is of size: 8192
Batch # 14 is of size: 8192
Batch # 15 is of size: 8192
Batch # 16 is of size: 8192
Batch # 17 is of size: 8192
Batch # 18 is of size: 8192
Batch # 19 is of size: 8192
Batch # 20 is of size: 8192
Batch # 21 is of size: 8192
Batch # 22 is of size: 8192
Batch # 23 is of size: 8192
Batch # 24 is of size: 8192
Batch # 25 is of size: 8192
Batch # 26 is of size: 8192
Batch # 27 is of size: 8192
Batch # 28 is of size: 8192
Batch # 29 is of size: 8192
Batch # 30 is of size: 8192
Batch # 31 is of size: 8192
Batch # 32 is of size: 8192
Batch # 33 is of size: 8192
Batch # 34 is of size: 8192
Batch # 35 is of size: 8192
Batch # 36 is of size: 8192
Batch # 37 is of size: 8192
Batch # 38 is of size: 8192
Batch # 39 is of size: 8192
Batch # 40 is of size: 8192
Batch # 41 is of size: 8192
Batch # 42 is of size: 8192
Batch # 43 is of size: 8192
Batch # 44 is of size: 8192
Batch # 45 is of size: 8192
Batch # 46 is of size: 8192
Batch # 47 is of size: 8192
Batch # 48 is of size: 8192
Batch # 49 is of size: 8192
Batch # 50 is of size: 8192
Batch # 51 is of size: 8192
Batch # 52 is of size: 8192
Batch # 53 is of size: 8192
Batch # 54 is of size: 8192
Batch # 55 is of size: 8192
Batch # 56 is of size: 8192
Batch # 57 is of size: 8192
Batch # 58 is of size: 8192
Batch # 59 is of size: 8192
```

```
Batch # 60 is of size: 8192
Batch # 61 is of size: 8192
Batch # 62 is of size: 8192
Batch # 63 is of size: 8192
Batch # 64 is of size: 8192
Batch # 65 is of size: 8192
Batch # 66 is of size: 8192
Batch # 67 is of size: 8192
Batch # 68 is of size: 8192
Batch # 69 is of size: 8192
Batch # 70 is of size: 8192
Batch # 71 is of size: 8192
Batch # 72 is of size: 8192
Batch # 73 is of size: 8192
Batch # 74 is of size: 8192
Batch # 75 is of size: 8192
Batch # 76 is of size: 8192
Batch # 77 is of size: 8192
Batch # 78 is of size: 8192
Batch # 79 is of size: 8192
Batch # 80 is of size: 8192
Batch # 81 is of size: 8192
Batch # 82 is of size: 8192
Batch # 83 is of size: 8192
Batch # 84 is of size: 3790
```

In [12]:
```
# Test Data Batches
for i, batch in enumerate(test_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 4571
```

In [13]:
```
# Val Data Batches
for i, batch in enumerate(val_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 4569
```

All the batching works well! Appropriate number of batches all of size 8192 except for the last batch were created

Torchani API

In [14]:
```
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.ReLU(),
            nn.Linear(128, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torchani.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [15]:
```
train_data_batch = next(iter(train_data_loader))

loss_func = nn.MSELoss()
species = train_data_batch['species'].to(device)
coords = train_data_batch['coordinates'].to(device)
true_energies = train_data_batch['energies'].to(device).float()
_, pred_energies = model((species, coords))
loss = loss_func(true_energies, pred_energies)
print(loss)
```

```
tensor(0.3071, grad_fn=<MseLossBackward0>)
```

In [ ]:
```

```