crystals

MDPI

Supplementary Materials: PRINCEPS: A Computer-Based Approach to the Structural Description and Recognition of Trends within Structural Databases, and its Application to the Ce-Ni-Si System

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S1. PRINCEPS Modules

The current PRINCEPS package is composed of the following modules (Table S1).

Table S1. List of PRINCEPS modules.

Module name	Function
Importcif	converts .cif files into .pos format for subsequent analysis
Cluster	performs clustering analysis on a group of phases
Coordmatch	project sites in a target phase into a collection of reference phases, and provide assessment of decomposition quality; also generates site projection maps
Terndist	generates ternary phase diagram connecting similar phases; also generates inter-phasic distance matrices
Figuretool_coord	auxiliary function for site projection map generation
Ternplot	auxiliary function for ternary phase diagram generation

All crystal structures used in this work were obtained in CIF format from the Inorganic Crystal Structure Database (ICSD). These CIF files are converted to .pos files using the *importcif* module in the PRINCEPS package, which is the format used for all subsequent analyses.

All CE match analyses are performed using the *coordmatch* module. The result of the analysis is printed in the MATLAB command window, and also saved as text files along with additional information about atomic CE of the phases involved in the analysis. When only one target phase is specified, *coordmatch* also generates the site projection map if the colors of reference phases are provided: this functionality utilizes the *figuretool_coord* module in the package, in which the user can control the appearance (such as camera settings and lighting parameters) of the figure, as well as customized structural features (bonds, polyhedra, unit cells, *etc.*).

The clustering analyses of binary phases and of ternary phases are performed using the *cluster* module. It also outputs a .csv table containing distances between the phases to be analyzed.

The ternary phase diagram with connected phases is generated using the *terndist* module. It also outputs a .csv table containing distances between all target phases and all (both target and reference) phases. The distance table is presented in Section S4.

S2. Algorithm Description for Match Quality Assessment and Projection Decomposition Weight Determination

S2.1. Assessment of CE Match Quality

The CE match quality of a site in the target phase is determined by its best match in the reference phases. If the distance between the CEs of target and best match reference site is d, the quality of the site is given by

$$quality = \frac{1}{1 + \frac{d}{cr^2}}$$

In this expression, $c = 0.5$ is an arbitrarily chosen factor, and r is the radius of the atom in the target phase: the reasoning behind dividing d by r^2 is that larger atoms in general have more atoms in their CEs, and hence have larger magnitude of the descriptors. Since the surface area of the coordination sphere is approximately proportional to r^2, including this factor in the formula helps correct this systematic effect due to the size of the central atom to provide a more consistent match quality.

From the definition of match quality, it can be seen that a distance of zero results in a match quality of 100%, while a distance of infinity results in a match quality of 0%. Changing the value of c will change the criterion for quality assessment: a smaller c value corresponds to a stricter criterion, which scores a lower match quality for the same distance. However, this will not affect the relative order of decomposition qualities between sites, but only their absolute magnitudes. In other words, the choice of c only sets the standard for what we would like to call a "good quality decomposition" for intuitive interpretation of the analysis result.

The overall decomposition quality of the target phase is then calculated as the average of CE match quality of each site, weighted by their multiplicities.

S2.2. Calculation of Decomposition Weight

The decomposition weights of a target phase onto reference phases are calculated in a site-wise fashion. In the following discussion, the target phase to be decomposed, and the collection of reference phases are denoted as P and $\mathcal{R}$, respectively.

For each site p in the target phase P and each site q in a reference phase $Q \in \mathcal{R}$, the weighting factor between these two sites is calculated as

$$w(p,q) = e^{-\frac{d(p,q)}{kr^2}}$$

where $d(p,q)$ is the distance between these two sites. $k = 0.05$ is an arbitrarily chosen factor, and r is the radius of the atom in the target phase: similar to the calculation of match quality, a factor of r^2 is used to correct the size effect of the central atom. From this expression, it is clear that a shorter distance corresponds to a higher weight: when $d(p,q) = 0$ we have $w(p,q) = 1$. The k factor controls the differentiation between difference sites: a smaller k value will result in larger difference in weighting factor for the reference sites, so a heavier weight will be assigned to the best matching phase, but the relative order of weights between phases is still preserved, i.e. it will not change which reference phase gets the highest weight. Similar to the choice of the c factor, these factors do not change the results of the core algorithm, but only in how the results are represented. As long as they are kept at a constant value throughout the analysis, any arbitrarily set value should lead to the same conclusions.

The weighting factor of a reference phase on the target site p is then defined as the maximal weighting factor among all sites in this reference phase, and normalized so that the weights on all reference phases add up to 1:

$$w(p,Q) = \frac{\max_{q \in Q} w(p,q)}{\sum_{Q \in \mathcal{R}} \max_{q \in Q} w(p,q)}$$

These site-wise decomposition weights are then averaged to give the overall decomposition weights, where the average is weighted by three factors: multiplicities, match qualities, and the user-defined weights of the elements.

S3. PRINCEPS Output for All Ce-Ni-Si Ternary Phases

The following result is directly copied from the output of PRINCEPS analysis.

```
--- Analysis of phase Ce14Ni6Si11 ---
site Ce1 (10.00,2.00,5.00): quality = 87.38%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.3764
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6093
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3912
site Ce2 (10.00,2.00,5.00): quality = 82.26%
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 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.7162
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.4652
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.5722
site Ce3 (9.00,2.00,6.00): quality = 75.71%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.1009
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.7717
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.2449
site Ce4 (10.00,2.00,5.00): quality = 89.16%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2437
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6821
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.2992
site Ce5 (10.00,2.00,5.00): quality = 87.84%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.3434
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6477
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3119
site Ce6 (11.00,1.00,5.00): quality = 82.61%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.6946
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.0807
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 6.5469
site Ce7 (9.00,2.00,6.00): quality = 62.72%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.8088
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.5916
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.6954
site Ce8 (8.00,6.00,6.00): quality = 93.58%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.8547
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.7543
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.6059
site Ce9 (10.00,2.00,5.00): quality = 87.52%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.3667
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6100
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3939
site Ce10 (10.00,2.00,5.00): quality = 88.87%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2659
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6749
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.2964
site Ce11 (11.00,1.00,5.00): quality = 80.83%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.8040
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.2775
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3386
site Ce12 (10.00,2.00,5.00): quality = 81.87%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.7407
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.3968
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3898
site Ce13 (8.00,6.00,6.00): quality = 89.40%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 2.2254
 2: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 3.6050
 3: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 5.5336
site Ce14 (8.00,4.00,8.00): quality = 96.27%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.5322
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.5797
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.4294
site Ce15 (8.00,4.00,8.00): quality = 96.19%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.5447
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.5746
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.4386
site Ni1 (6.00,0.00,3.00): quality = 95.07%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.7839
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.8749
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8443
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site Ni2 (6.00,0.00,3.00): quality = 82.67%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.2491
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.3059
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7250
site Ni3 (6.00,0.00,3.00): quality = 84.50%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.1947
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.2391
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7682
site Ni4 (6.00,0.00,3.00): quality = 83.24%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.2325
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.4488
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.6823
site Ni5 (6.00,0.00,3.00): quality = 95.91%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.7346
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.8609
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8307
site Ni6 (6.00,0.00,3.00): quality = 87.06%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.1137
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.2631
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7652
site Si1 (7.00,1.00,1.00): quality = 85.46%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.1839
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6832
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7863
site Si2 (7.00,2.00,0.00): quality = 78.72%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.3816
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6299
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7334
site Si3 (6.00,2.00,1.00): quality = 92.82%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.9102
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.0032
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7979
site Si4 (8.00,1.00,0.00): quality = 36.07%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.5860
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.3632
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4448
site Si5 (8.00,1.00,0.00): quality = 37.47%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.5343
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.4003
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4798
site Si6 (7.00,2.00,0.00): quality = 78.79%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.3796
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6779
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7795
site Si7 (7.00,2.00,0.00): quality = 71.66%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.5685
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.9631
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0496
site Si8 (7.00,2.00,0.00): quality = 79.40%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.3628
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6233
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7245
site Si9 (7.00,1.00,1.00): quality = 85.93%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.1690
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6755
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7780
site Si10 (6.00,2.00,1.00): quality = 92.55%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.9227
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.0028
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 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7922
site Si11 (7.00,2.00,0.00): quality = 68.08%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.6600
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.9916
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0787
Decomposition of Ce14Ni6Si11:
CeSi: 65.34%
CeNiSi#: 18.70%
CeSi2: 15.93%
Overall decomposition quality: 81.33%

--- Analysis of phase Ce15Ni4Si13 ---
site Ce1 (10.00,2.00,3.00): quality = 71.50%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.3336
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 5.7603
 3: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 5.7981
site Ce2 (10.00,1.00,6.00): quality = 88.67%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2815
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.8649
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3832
site Ce3 (10.00,1.50,5.50): quality = 88.15%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.3204
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6502
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3222
site Ce4 (10.00,2.00,5.00): quality = 86.66%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.4274
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.8533
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.4733
site Ce5 (8.00,2.00,10.00): quality = 96.88%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.4409
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.3836
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.4009
site Ni1 (6.00,2.00,0.00): quality = 23.15%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.1369
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.2033
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 3.5022
site Mx1 (7.00,0.50,1.50): quality = 78.89%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.3660
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.7846
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.8628
site Mx2 (6.00,0.50,2.50): quality = 81.55%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.2915
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.4781
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8027
site Si1 (8.00,0.50,0.50): quality = 43.73%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.3240
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.4525
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4955
site Si2 (7.00,0.50,1.50): quality = 89.51%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.0455
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.9218
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0113
site Si3 (6.00,0.50,2.50): quality = 89.00%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.0645
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.1369
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7311
site Si4 (6.00,0.00,3.00): quality = 96.05%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.7374
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.0398
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 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.9382
Decomposition of Ce15Ni4Si13:
CeSi: 68.43%
CeNiSi#: 24.59%
CeSi2: 6.90%
Overall decomposition quality: 80.09%

--- Analysis of phase Ce2Ni15Si2# ---
site Ce1 (1.00,17.11,1.89): quality = 64.25%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 3.7256
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.0059
 3: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 6.6823
site Ni1 (1.00,11.11,1.89): quality = 15.04%
 1: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 3.7450
 2: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 3.7527
 3: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 4.8923
site Mx1 (2.00,10.00,0.00): quality = 23.20%
 1: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 3.1655
 2: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 3.1660
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.1914
site Ni3 (2.00,8.74,1.26): quality = 16.51%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.6094
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 4.0633
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 4.4107
site Ni4 (3.00,7.74,1.26): quality = 25.58%
 1: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.0017
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.6090
 3: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 4.0767
Decomposition of Ce2Ni15Si2#:
CeNi5: 84.20%
Ni3Si: 11.07%
CeNi2Si2: 4.17%
Overall decomposition quality: 25.30%

--- Analysis of phase Ce2Ni17Si5# ---
site Ce1 (0.00,17.20,4.80): quality = 43.54%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 4.9398
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.7862
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 7.5103
site Mx1 (2.00,8.00,4.00): quality = 21.65%
 1: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 3.2492
 2: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 3.2625
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.4546
site Ni2 (2.00,7.60,2.40): quality = 14.84%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.7647
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 4.1476
 3: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 4.4011
site Si2 (2.00,9.20,0.80): quality = 27.31%
 1: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 2.9612
 2: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 2.9659
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.4118
Decomposition of Ce2Ni17Si5#:
CeNi5: 63.59%
Ni3Si: 24.48%
CeNi2Si2: 9.43%
Overall decomposition quality: 19.88%
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--- Analysis of phase Ce2Ni3Si5 ---
site Ce1 (4.00,7.00,10.00): quality = 76.39%
 1: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 3.0627
 2: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 3.6569
 3: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.3249
site Ni1 (4.00,2.00,6.00): quality = 44.94%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 2.2499
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.4567
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.5679
site Ni2 (5.00,0.00,5.00): quality = 72.01%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 1.5344
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.1804
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.1999
site Si1 (4.00,4.00,4.00): quality = 69.17%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.6321
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.5067
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.7712
site Si2 (4.00,3.00,5.00): quality = 72.35%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.5506
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.1857
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.8041
site Si3 (4.00,3.00,2.00): quality = 37.81%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.5223
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6101
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 2.7629
Decomposition of Ce2Ni3Si5:
CeNi2Si2: 80.69%
CeNi5: 10.79%
CeNiSi#: 4.97%
Overall decomposition quality: 63.12%

--- Analysis of phase Ce3Ni2Si8 ---
site Ce1 (4.00,2.00,16.00): quality = 89.08%
 1: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 2.2498
 2: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 3.5919
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.2332
site Ce2 (6.00,4.00,11.00): quality = 52.47%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 4.3831
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.3511
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.3578
site Ni1 (5.00,0.00,5.00): quality = 71.22%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 1.5545
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.2750
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.2868
site Si1 (4.00,2.00,6.00): quality = 82.56%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.2725
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.3576
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.8705
site Si2 (6.00,1.00,2.00): quality = 92.74%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.9142
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.0820
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7275
site Si3 (4.00,2.00,6.00): quality = 81.92%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.2912
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.4112
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.9065
site Si4 (5.00,0.00,5.00): quality = 72.29%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 1.5522
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.0736
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 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0831
Decomposition of Ce3Ni2Si8:
CeNi2Si2: 67.46%
CeSi2: 24.66%
CeNiSi#: 6.54%
Overall decomposition quality: 76.58%

--- Analysis of phase Ce3Ni4Si4 ---
site Ce1 (8.00,4.00,8.00): quality = 95.50%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.6363
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.0938
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.4767
site Ce2 (6.00,8.00,7.00): quality = 50.37%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 4.5077
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.2844
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.3993
site Ni1 (6.00,0.00,3.00): quality = 99.12%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.4357
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.9693
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8491
site Ni2 (4.00,4.00,4.00): quality = 78.95%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.3532
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.4116
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.8567
site Si1 (5.00,5.00,0.00): quality = 81.83%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 1.2937
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.0769
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0831
site Si2 (6.00,2.00,1.00): quality = 93.05%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.8998
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.0881
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7824
Decomposition of Ce3Ni4Si4:
CeSi2: 42.73%
CeNi2Si2: 31.58%
CeNiSi#: 24.87%
Overall decomposition quality: 82.01%

--- Analysis of phase Ce3Ni6Si2 ---
site Ce1 (5.00,8.00,4.00): quality = 33.16%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 5.7219
 2: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.9420
 3: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 6.2837
site Ni1 (4.00,6.00,2.00): quality = 57.52%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 1.9006
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 2.2000
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.6263
site Si1 (6.00,6.00,0.00): quality = 43.74%
 1: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 2.3238
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 4.0207
 3: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 4.0410
Decomposition of Ce3Ni6Si2:
CeNi5: 60.12%
CeSi: 14.97%
CeNi2Si2: 11.02%
Overall decomposition quality: 48.37%
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--- Analysis of phase Ce3NiSi3# ---
site Ce1 (10.00,0.88,6.12): quality = 88.58%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2879
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.5932
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.4222
site Ce2 (8.00,3.52,8.48): quality = 96.72%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.4668
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.6129
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.3801
site Mx1 (6.00,0.44,2.56): quality = 94.50%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 0.8225
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.8363
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8288
site Si1 (7.00,0.88,1.12): quality = 86.37%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.1548
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6565
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.7570
Decomposition of Ce3NiSi3#:
CeSi: 57.89%
CeNiSi#: 31.82%
CeSi2: 10.28%
Overall decomposition quality: 90.80%

--- Analysis of phase Ce5Ni2Si3 ---
site Ce1 (10.00,2.90,2.10): quality = 74.17%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.1870
 2: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 5.8243
 3: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 5.8776
site Ce2 (10.00,2.30,4.70): quality = 88.82%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2700
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.7313
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3585
site Ce3 (10.00,2.00,5.00): quality = 88.73%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2772
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6036
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3437
site Ce4 (8.00,4.20,7.80): quality = 94.51%
 1: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 1.7538
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 3.7050
 3: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.5249
site Ni1 (6.00,2.00,0.00): quality = 23.36%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.1245
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.1880
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 3.4397
site Mx1 (8.00,0.70,0.30): quality = 37.12%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.5349
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.3813
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4301
site Mx2 (6.00,0.30,2.70): quality = 87.24%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.1133
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.1334
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7948
site Si1 (7.00,1.40,0.60): quality = 80.97%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.3185
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.5510
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.6568
Decomposition of Ce5Ni2Si3:
CeSi: 79.43%
CeNiSi#: 13.93%
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CeSi2: 6.53%
Overall decomposition quality: 74.45%

--- Analysis of phase Ce6Ni2Si3# ---
site Ce1 (10.00,1.67,5.34): quality = 89.46%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2203
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.7885
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3669
site Ce2 (10.00,3.00,2.00): quality = 74.36%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.1765
 2: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 5.8471
 3: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 5.8922
site Mx1 (8.00,0.00,1.00): quality = 38.57%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.4822
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.3934
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4412
site Ni2 (6.00,2.00,0.00): quality = 23.34%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.1254
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.1894
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 3.4501
site Si2 (6.00,1.00,2.00): quality = 80.41%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.3345
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.3989
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8595
Decomposition of Ce6Ni2Si3#:
CeSi: 91.01%
CeNiSi#: 5.00%
CeSi2: 3.79%
Overall decomposition quality: 64.63%

--- Analysis of phase Ce6Ni7Si4 ---
site Ce1 (6.00,8.00,4.00): quality = 54.27%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 4.2782
 2: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 4.5412
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.3444
site Ce2 (7.00,7.00,4.00): quality = 56.69%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 4.1408
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.0961
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.9272
site Ce3 (8.00,5.00,4.00): quality = 72.74%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.2659
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.2884
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.5187
site Ce4 (8.00,8.00,4.00): quality = 85.61%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 2.4999
 2: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 3.7168
 3: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 5.6100
site Ni1 (6.00,2.00,1.00): quality = 65.24%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.7046
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.8492
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.5276
site Ni2 (6.00,1.00,3.00): quality = 33.40%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.6465
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6693
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 3.2869
site Ni3 (6.00,1.00,3.00): quality = 34.18%
 1: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.6158
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6364
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 3.2780
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site Ni4 (7.00,0.00,2.00): quality = 55.83%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.9447
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.7660
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.8333
site Si1 (6.00,4.00,0.00): quality = 41.69%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 2.3895
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.5756
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.5904
site Si2 (6.00,4.00,0.00): quality = 48.66%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 2.1754
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.5991
 3: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.6128
Decomposition of Ce6Ni7Si4:
CeSi2: 39.05%
CeSi: 37.59%
CeNiSi#: 13.32%
Overall decomposition quality: 51.91%

--- Analysis of phase Ce7Ni2Si5 ---
site Ce1 (10.00,2.00,5.00): quality = 83.67%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.6277
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.4147
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.5179
site Ce2 (9.00,2.00,6.00): quality = 68.23%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.5109
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.5958
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.9365
site Ce3 (9.00,2.00,6.00): quality = 77.19%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 3.0173
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.8023
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.0726
site Ce4 (10.00,2.00,5.00): quality = 87.99%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.3320
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.6902
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.4127
site Ce5 (11.00,1.00,5.00): quality = 83.43%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.6426
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.2941
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.3271
site Ce6 (11.00,1.00,5.00): quality = 81.37%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.7712
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.4027
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.2479
site Ce7 (10.00,2.00,5.00): quality = 89.09%
 1: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 2.2495
 2: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 5.7766
 3: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 6.1599
site Ni1 (6.00,0.00,3.00): quality = 80.72%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.3045
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.5069
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8066
site Ni2 (6.00,0.00,3.00): quality = 73.44%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.4981
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.5640
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.6900
site Si1 (7.00,2.00,0.00): quality = 69.80%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.6160
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.9664
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.0509
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site Si2 (7.00,1.00,1.00): quality = 75.88%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.4582
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.5292
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.6127
site Si3 (7.00,1.00,1.00): quality = 82.04%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 1.2878
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 2.7843
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 2.8814
site Si4 (8.00,1.00,0.00): quality = 38.06%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.5132
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.3373
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.4192
site Si5 (8.00,1.00,0.00): quality = 33.42%
 1: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.6884
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.4723
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.5491
Decomposition of Ce7Ni2Si5:
CeSi: 89.82%
CeSi2: 6.66%
CeNiSi#: 3.48%
Overall decomposition quality: 73.17%

--- Analysis of phase CeNi4Si ---
site Ce1 (2.00,14.00,4.00): quality = 99.01%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 0.9775
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 3.6373
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.4135
site Ni1 (3.00,7.00,2.00): quality = 94.22%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 0.8292
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 2.3017
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.2811
site Ni2 (4.00,6.00,2.00): quality = 90.27%
 1: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 1.0008
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.2016
 3: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.7154
site Si1 (4.00,8.00,0.00): quality = 81.88%
 1: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 1.2924
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.2767
 3: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.8280
Decomposition of CeNi4Si:
CeNi5: 99.89%
CeNi2Si2: 0.11%
CeNiSi#: 0.00%
Overall decomposition quality: 91.64%

--- Analysis of phase CeNi6Si6 ---
site Ce1 (0.00,12.00,12.00): quality = 31.25%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 5.8917
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 6.6327
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 8.1575
site Ce2 (0.00,12.00,12.00): quality = 31.23%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 5.8935
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 6.6345
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 8.1586
site Ni1 (2.00,2.00,7.00): quality = 16.52%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.6081
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.8112
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.9351
site Mx1 (2.00,4.50,4.50): quality = 17.84%
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 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.5268
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.7233
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.9791
site Ni3 (2.00,4.00,5.00): quality = 18.02%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.4842
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.6585
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.8974
site Si1 (2.00,7.00,2.00): quality = 17.41%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.5899
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.8155
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.9708
site Si3 (2.00,5.00,4.00): quality = 18.29%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.5195
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 3.7076
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.9046
Decomposition of CeNi6Si6:
CeNi5: 64.12%
CeNi2Si2: 21.61%
CeNiSi#: 7.01%
Overall decomposition quality: 18.70%

--- Analysis of phase CeNi8Si5# ---
site Ce1 (0.00,14.88,9.12): quality = 31.34%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 5.8828
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 6.6343
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 8.1575
site Mx1 (0.00,7.44,4.56): quality = 92.63%
 1: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 0.9098
 2: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 1.2815
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 4.4957
site Mx2 (2.00,6.20,3.80): quality = 13.43%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.9377
 2: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 4.2221
 3: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 4.2389
Decomposition of CeNi8Si5#:
CeNi5: 48.97%
Ni3Si: 37.85%
CeNi2Si2: 9.96%
Overall decomposition quality: 20.36%

--- Analysis of phase CeNi9Si4 ---
site Ce1 (0.00,16.00,8.00): quality = 31.31%
 1: site Ce1 in phase CeNi5 (2.00,18.00,0.00): distance = 5.8858
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 6.6348
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 8.1575
site Ni1 (2.00,6.00,4.00): quality = 12.07%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 4.0759
 2: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 4.0763
 3: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 4.0996
site Ni2 (2.00,7.00,4.00): quality = 13.54%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 3.9012
 2: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 4.2312
 3: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 4.2331
site Ni3 (0.00,8.00,4.00): quality = 92.19%
 1: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 0.9236
 2: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 1.2999
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 4.4683
site Si1 (2.00,9.00,1.00): quality = 12.78%
 1: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 4.0536
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 2: site Si1 in phase Ni3Si (0.00,12.00,0.00): distance = 4.0700
 3: site Ni1 in phase Ni3Si (0.00,8.00,4.00): distance = 4.0730
Decomposition of CeNi9Si4:
Ni3Si: 44.77%
CeNi5: 41.66%
CeNi2Si2: 9.01%
Overall decomposition quality: 19.79%

--- Analysis of phase CeNiSi ---
site Ce1 (8.00,6.00,6.00): quality = 94.53%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 1.7521
 2: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 3.1606
 3: site Ce1 in phase CeSi (10.00,0.00,7.00): distance = 5.8570
site Ni1 (6.00,0.00,3.00): quality = 97.80%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.5938
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.0412
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8038
site Si1 (6.00,3.00,0.00): quality = 90.03%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 1.0259
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.1131
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.8027
Decomposition of CeNiSi:
CeSi2: 85.54%
CeNiSi#: 14.44%
CeSi: 0.01%
Overall decomposition quality: 94.12%

--- Analysis of phase CeNiSi2 ---
site Ce1 (6.00,5.00,10.00): quality = 51.22%
 1: site Ce1 in phase CeSi2 (8.00,0.00,12.00): distance = 4.4564
 2: site Ce1 in phase CeNi2Si2 (4.00,8.00,10.00): distance = 5.2913
 3: site Ce1 in phase CeNiSi# (8.00,4.80,7.20): distance = 5.3379
site Ni1 (5.00,0.00,5.00): quality = 69.94%
 1: site Si1 in phase CeNi2Si2 (5.00,4.00,1.00): distance = 1.5867
 2: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 3.2231
 3: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 3.2321
site Si1 (6.00,1.00,2.00): quality = 92.36%
 1: site Si1 in phase CeSi2 (6.00,0.00,3.00): distance = 0.9308
 2: site Mx1 in phase CeNiSi# (6.00,1.20,1.80): distance = 1.1671
 3: site Si1 in phase CeSi (7.00,0.00,2.00): distance = 2.7194
site Si2 (4.00,4.00,4.00): quality = 77.67%
 1: site Ni1 in phase CeNi2Si2 (4.00,4.00,4.00): distance = 1.4102
 2: site Ni1 in phase CeNi5 (3.00,9.00,0.00): distance = 2.3395
 3: site Ni2 in phase CeNi5 (4.00,8.00,0.00): distance = 3.8482
Decomposition of CeNiSi2:
CeNi2Si2: 46.32%
CeSi2: 42.52%
CeNiSi#: 9.89%
Overall decomposition quality: 72.80%
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S4. Distance Matrix between All Ce-Ni-Si Ternary Phases

	Ce14Ni6Si11	**Ce15Ni4Si13**	**Ce2Ni15Si2#**	**Ce2Ni17Si5#**	**Ce2Ni3Si5**	**Ce3Ni2Si8**	**Ce3Ni4Si4**
Ce14Ni6Si11	0.000	0.783	2.406	2.450	1.960	1.713	1.382
Ce15Ni4Si13	0.783	0.000	2.416	2.459	1.979	1.773	1.428
Ce2Ni15Si2#	2.406	2.416	0.000	1.457	2.213	2.203	2.309
Ce2Ni17Si5#	2.450	2.459	1.457	0.000	2.330	2.352	2.452
Ce2Ni3Si5	1.960	1.979	2.213	2.330	0.000	1.082	1.324
Ce2Ni7	1.937	1.959	2.102	2.189	2.015	2.028	2.076
Ce2Si7	1.931	1.991	2.297	2.463	2.040	1.976	1.928
Ce3Ni2Si8	1.713	1.773	2.203	2.352	1.082	0.000	0.941
Ce3Ni4Si4	1.382	1.428	2.309	2.452	1.324	0.941	0.000
Ce3Ni6Si2	2.039	2.013	2.267	2.397	2.306	2.321	2.286
Ce3NiSi3#	0.344	0.657	2.381	2.372	1.869	1.660	1.382
Ce3Si2	1.266	1.207	2.176	2.233	2.196	2.099	1.978
Ce5Ni2Si3	0.665	0.695	2.368	2.393	2.017	1.811	1.523
Ce5Si3	1.327	1.347	2.367	2.411	2.343	2.201	2.140
Ce5Si4	1.080	1.128	2.299	2.362	2.134	2.067	1.999
Ce6Ni2Si3#	1.006	0.683	2.414	2.459	2.088	1.813	1.847
Ce6Ni7Si4	1.204	1.418	2.383	2.460	1.988	1.794	1.626
Ce7Ni2Si5	0.538	0.825	2.401	2.457	2.077	1.896	1.907
Ce7Ni3	1.351	1.130	2.224	2.239	2.191	2.054	2.084
CeNi	0.995	1.098	2.468	2.560	2.288	2.100	2.109
CeNi2	1.809	1.733	2.354	2.283	2.304	2.257	2.258
CeNi2Si2	2.087	2.073	2.141	2.290	1.122	1.011	1.299
CeNi3	1.930	1.958	2.185	2.345	2.011	2.043	2.048
CeNi4Si	2.431	2.206	1.626	1.992	1.819	1.989	2.145
CeNi5	2.320	2.154	1.643	1.998	1.684	1.839	2.047
CeNi6Si6	2.422	2.492	1.875	1.419	1.967	2.170	2.418
CeNi8Si5#	2.535	2.575	1.801	1.317	2.382	2.457	2.641
CeNi9Si4	2.473	2.538	1.788	1.467	2.450	2.516	2.607
CeNiSi#	0.683	0.520	2.384	2.362	1.665	1.416	0.682
CeNiSi	0.791	1.007	2.445	2.524	1.628	0.949	0.698
CeNiSi2	1.722	1.758	2.313	2.512	1.162	0.500	0.804
CeSi	0.720	0.804	2.277	2.400	2.012	1.953	1.997
CeSi2	0.835	1.074	2.275	2.430	1.572	1.134	0.790
CeSi5	2.066	1.940	1.992	2.071	2.089	2.050	1.994
Ni2Si	2.590	2.639	2.274	2.274	2.782	2.777	2.722
Ni3Si	2.738	2.796	1.918	1.690	2.999	3.011	2.936
NiSi	2.491	2.520	2.488	2.446	2.624	2.608	2.575
NiSi2	2.571	2.589	2.437	2.390	2.560	2.703	2.749

	Ce3Ni6Si2	**Ce3NiSi3#**	**Ce5Ni2Si3**	**Ce6Ni2Si3#**	**Ce6Ni7Si4**	**Ce7Ni2Si5**	**CeNi2Si2**
Ce14Ni6Si11	2.039	0.344	0.665	1.006	1.204	0.538	2.087
Ce15Ni4Si13	2.013	0.657	0.695	0.683	1.418	0.825	2.073
Ce2Ni15Si2#	2.267	2.381	2.368	2.414	2.383	2.401	2.141
Ce2Ni17Si5#	2.397	2.372	2.393	2.459	2.460	2.457	2.290
Ce2Ni3Si5	2.306	1.869	2.017	2.088	1.988	2.077	1.122
Ce2Ni7	1.515	1.951	1.857	1.893	1.915	1.845	1.893
Ce2Si7	1.914	1.854	1.963	2.093	1.825	1.999	1.970
Ce3Ni2Si8	2.321	1.660	1.811	1.813	1.794	1.896	1.011
Ce3Ni4Si4	2.286	1.382	1.523	1.847	1.626	1.907	1.299
Ce3Ni6Si2	0.000	2.113	2.051	2.053	1.902	2.098	2.445
Ce3NiSi3#	2.113	0.000	0.465	1.203	1.272	0.905	2.000
Ce3Si2	1.996	1.619	1.195	1.161	1.473	1.261	2.238
Ce5Ni2Si3	2.051	0.465	0.000	0.428	1.341	0.778	2.138
Ce5Si3	2.241	1.717	1.211	1.266	1.658	1.322	2.413
Ce5Si4	2.141	1.396	1.062	1.041	1.374	1.059	2.292
Ce6Ni2Si3#	2.053	1.203	0.428	0.000	1.461	0.885	2.353
Ce6Ni7Si4	1.902	1.272	1.341	1.461	0.000	1.218	1.981
Ce7Ni2Si5	2.098	0.905	0.778	0.885	1.218	0.000	2.221
Ce7Ni3	2.019	1.550	1.231	1.239	1.452	1.354	2.206
CeNi	2.185	1.299	1.056	1.131	1.160	0.977	2.224
CeNi2	1.747	1.898	1.699	1.694	1.799	1.788	2.393
CeNi2Si2	2.445	2.000	2.138	2.353	1.981	2.221	0.000
CeNi3	1.600	1.915	1.853	1.895	1.930	1.857	1.916
CeNi4Si	1.760	2.317	2.256	2.395	2.367	2.495	1.824
CeNi5	1.786	2.316	2.214	2.396	2.383	2.514	1.746
CeNi6Si6	2.620	2.428	2.447	2.462	2.377	2.403	2.256
CeNi8Si5#	2.585	2.497	2.516	2.565	2.533	2.508	2.472
CeNi9Si4	2.563	2.450	2.467	2.520	2.454	2.450	2.441
CeNiSi#	2.132	0.665	0.826	1.836	1.461	1.734	1.754
CeNiSi	2.304	0.997	1.074	1.466	1.188	1.380	2.025
CeNiSi2	2.319	1.666	1.813	1.818	1.747	1.896	1.382
CeSi	2.116	0.810	0.824	1.023	1.215	0.763	2.154
CeSi2	2.225	1.053	1.166	1.616	1.176	1.490	1.906
CeSi5	1.966	2.034	1.944	2.134	2.042	2.229	2.055
Ni2Si	2.636	2.598	2.552	2.586	2.640	2.550	2.793
Ni3Si	2.824	2.708	2.666	2.727	2.848	2.693	2.964
NiSi	2.783	2.498	2.491	2.499	2.539	2.480	2.667
NiSi2	2.667	2.578	2.494	2.482	2.667	2.522	2.751

	CeNi4Si	**CeNi6Si6**	**CeNi8Si5#**	**CeNi9Si4**	**CeNiSi#**	**CeNiSi**	**CeNiSi2**
Ce14Ni6Si11	2.431	2.422	2.535	2.473	0.683	0.791	1.722
Ce15Ni4Si13	2.206	2.492	2.575	2.538	0.520	1.007	1.758
Ce2Ni15Si2#	1.626	1.875	1.801	1.788	2.384	2.445	2.313
Ce2Ni17Si5#	1.992	1.419	1.317	1.467	2.362	2.524	2.512
Ce2Ni3Si5	1.819	1.967	2.382	2.450	1.665	1.628	1.162
Ce2Ni7	0.981	2.396	2.475	2.582	2.023	2.286	2.079
Ce2Si7	2.144	2.472	2.648	2.644	1.792	1.860	1.996
Ce3Ni2Si8	1.989	2.170	2.457	2.516	1.416	0.949	0.500
Ce3Ni4Si4	2.145	2.418	2.641	2.607	0.682	0.698	0.804
Ce3Ni6Si2	1.760	2.620	2.585	2.563	2.132	2.304	2.319
Ce3NiSi3#	2.317	2.428	2.497	2.450	0.665	0.997	1.666
Ce3Si2	2.220	2.431	2.371	2.346	1.953	2.065	2.097
Ce5Ni2Si3	2.256	2.447	2.516	2.467	0.826	1.074	1.813
Ce5Si3	2.383	2.569	2.421	2.401	2.076	2.154	2.219
Ce5Si4	2.364	2.341	2.391	2.338	2.030	1.927	2.066
Ce6Ni2Si3#	2.395	2.462	2.565	2.520	1.836	1.466	1.818
Ce6Ni7Si4	2.367	2.377	2.533	2.454	1.461	1.188	1.747
Ce7Ni2Si5	2.495	2.403	2.508	2.450	1.734	1.380	1.896
Ce7Ni3	2.275	2.306	2.269	2.243	2.116	2.090	2.058
CeNi	2.543	2.524	2.608	2.535	2.249	1.954	2.098
CeNi2	1.968	2.599	2.481	2.505	2.336	2.183	2.252
CeNi2Si2	1.824	2.256	2.472	2.441	1.754	2.025	1.382
CeNi3	1.397	2.443	2.574	2.570	1.946	2.260	2.039
CeNi4Si	0.000	2.193	2.212	2.404	2.041	2.378	2.158
CeNi5	0.504	2.244	2.300	2.325	2.019	2.348	2.020
CeNi6Si6	2.193	0.000	1.147	1.139	2.473	2.469	2.417
CeNi8Si5#	2.212	1.147	0.000	0.478	2.546	2.709	2.710
CeNi9Si4	2.404	1.139	0.478	0.000	2.503	2.651	2.660
CeNiSi#	2.041	2.473	2.546	2.503	0.000	0.978	1.423
CeNiSi	2.378	2.469	2.709	2.651	0.978	0.000	0.986
CeNiSi2	2.158	2.417	2.710	2.660	1.423	0.986	0.000
CeSi	2.394	2.363	2.413	2.324	2.088	1.941	1.950
CeSi2	2.232	2.412	2.603	2.556	1.014	0.560	1.180
CeSi5	1.833	2.414	2.292	2.281	1.873	2.247	2.165
Ni2Si	2.569	2.304	1.797	1.630	2.626	2.652	2.781
Ni3Si	2.681	2.617	0.705	0.695	2.696	2.898	3.065
NiSi	2.755	2.361	2.520	2.439	2.514	2.495	2.590
NiSi2	2.660	2.343	2.248	2.261	2.622	2.688	2.746