

Supporting Information  
For  
**Toward a Deeper Understanding of H–Ni<sub>3</sub>C Interactions: Rule-Based Insights**

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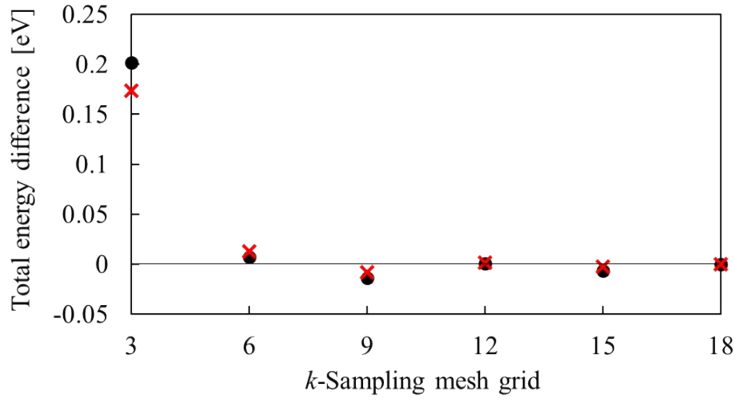
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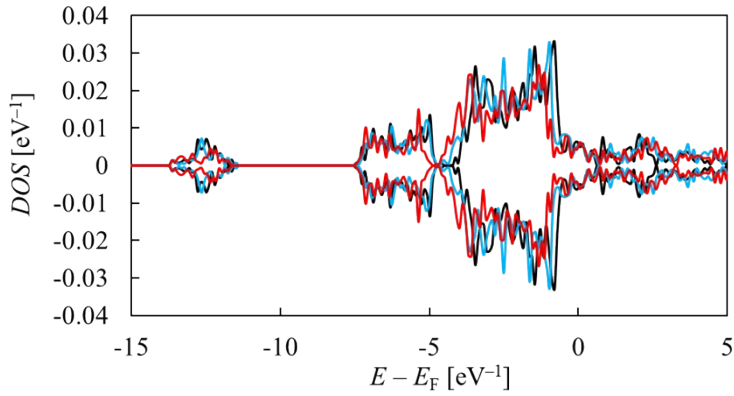
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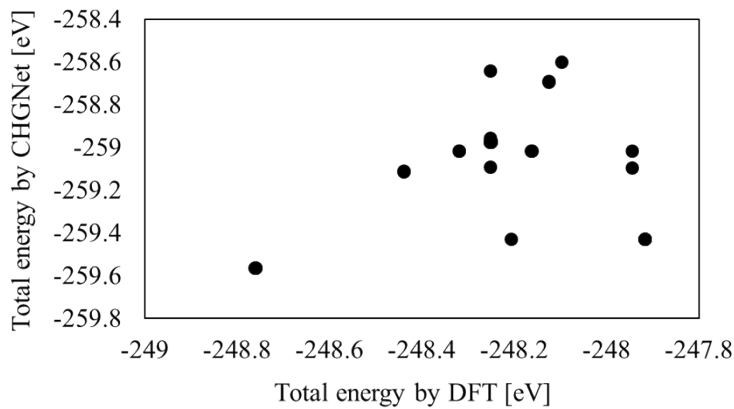
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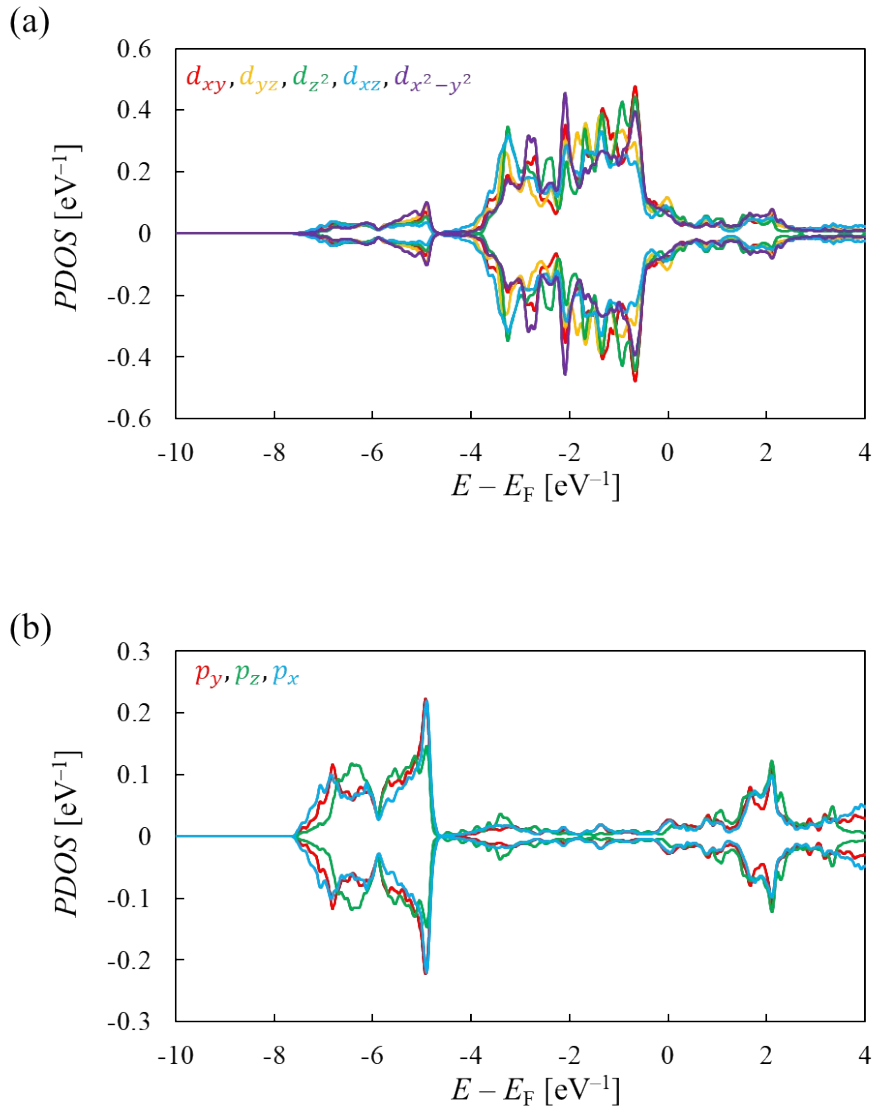
**Fig. S1** Total energy-dependence of  $\text{Ni}_3\text{C}$  bulk on  $k$ -point sampling mesh. The vertical axis shows the total energy difference relative to the  $18 \times 18 \times 6$  mesh. The horizontal axis indicates the number of mesh points along the  $a$  ( $= b$ ) axis of  $\text{Ni}_3\text{C}$ ; the mesh points along the  $c$  axis are one-third of this value. Black circles and red crosses represent results from DFT and DFT-D3 calculations, respectively.



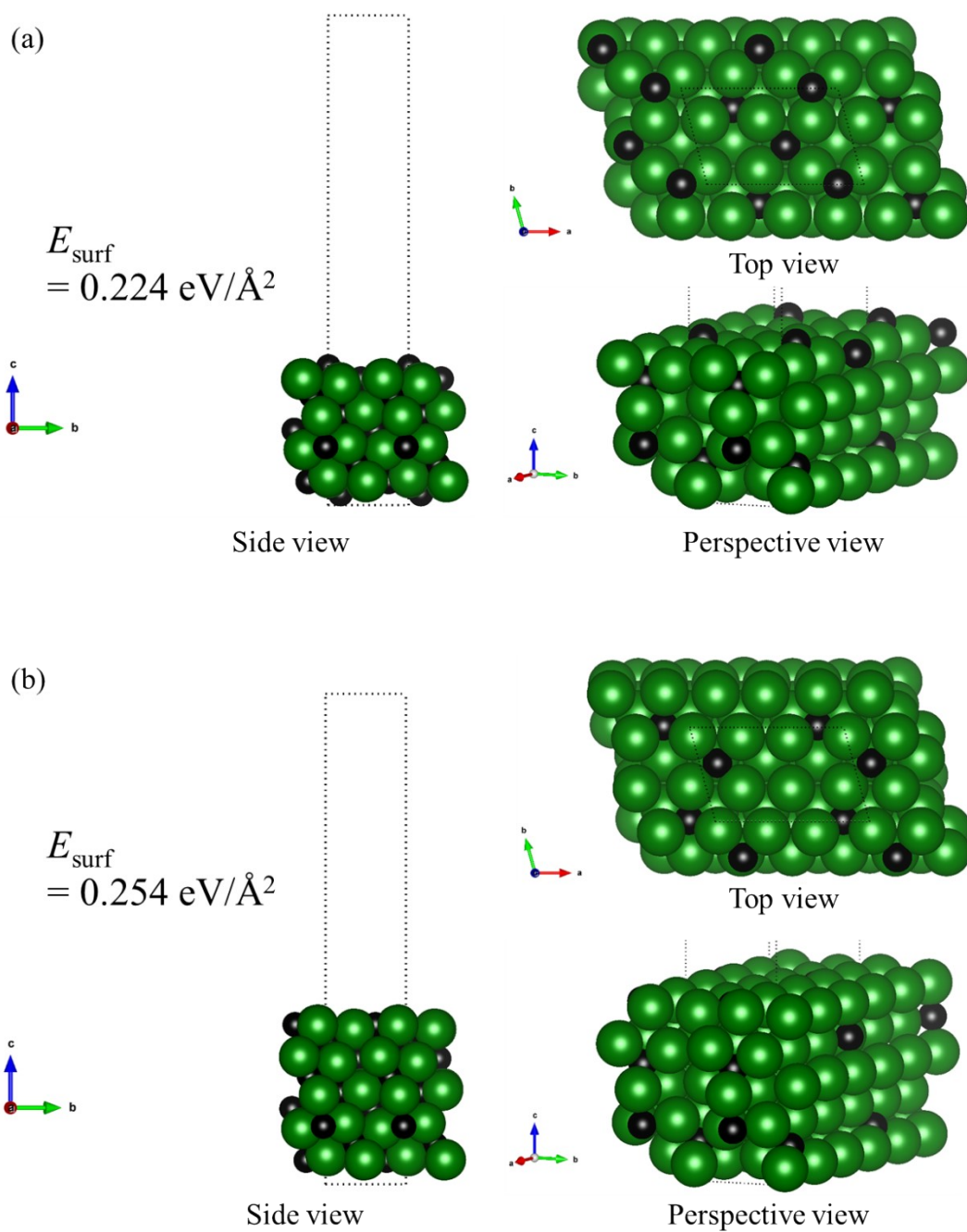
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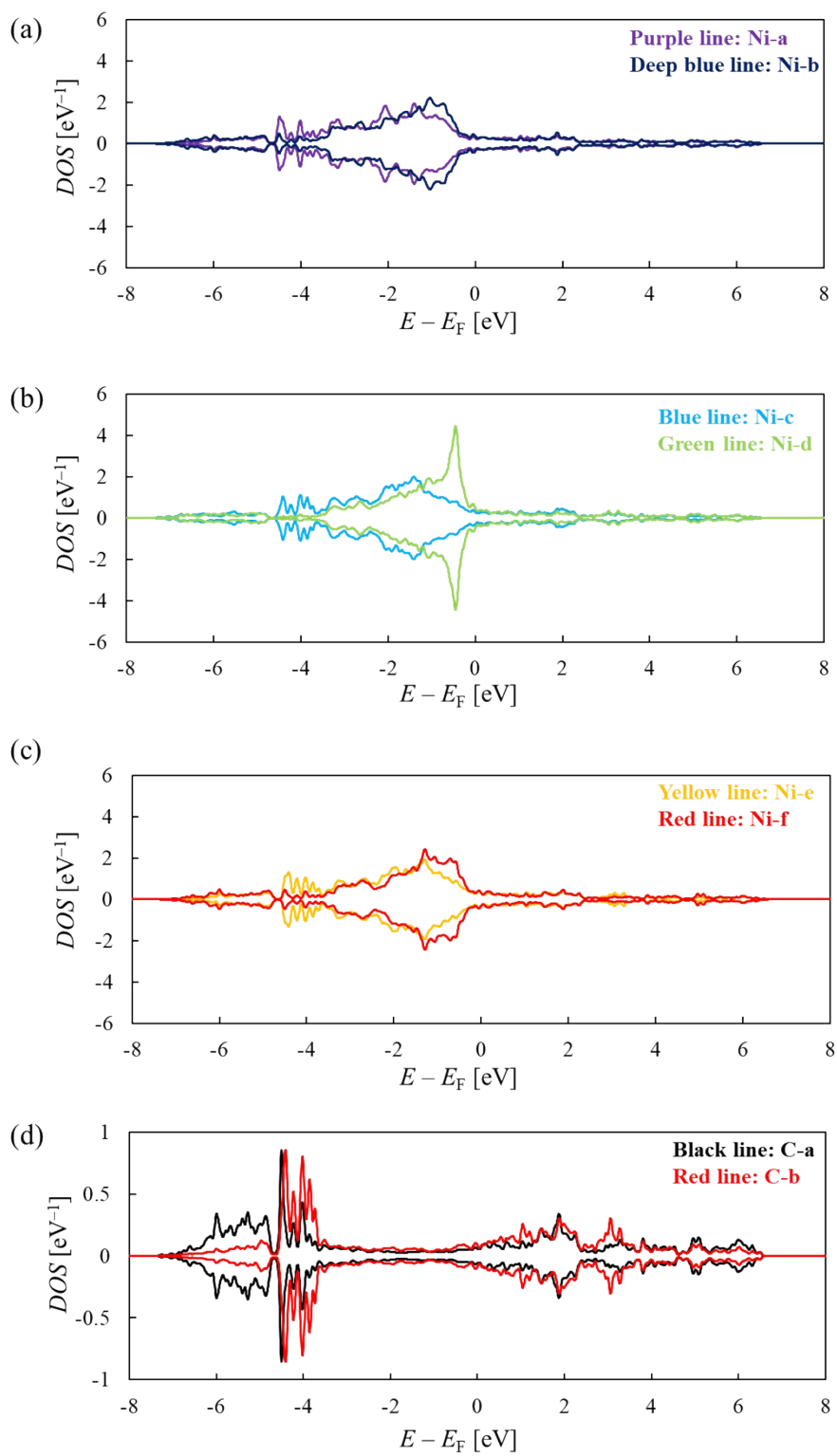
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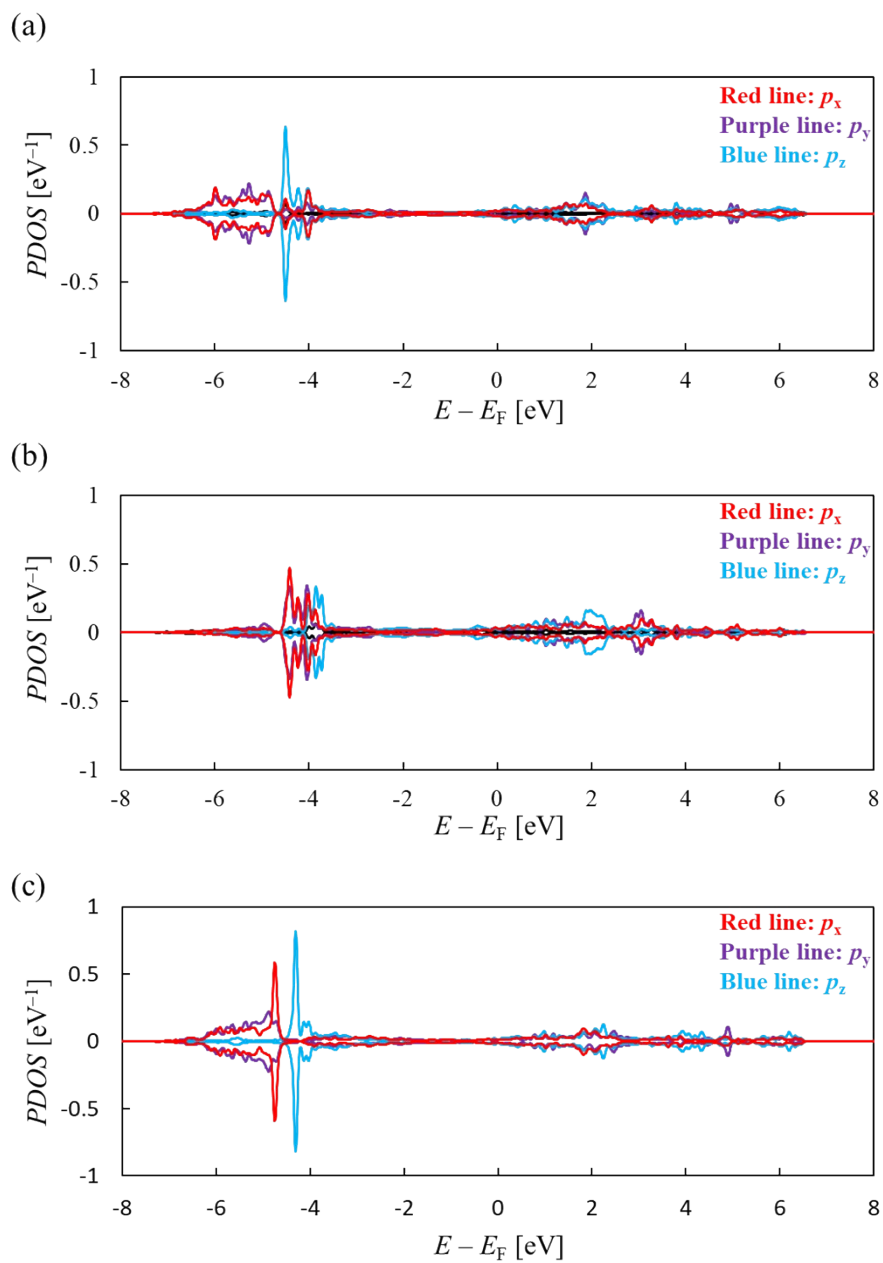
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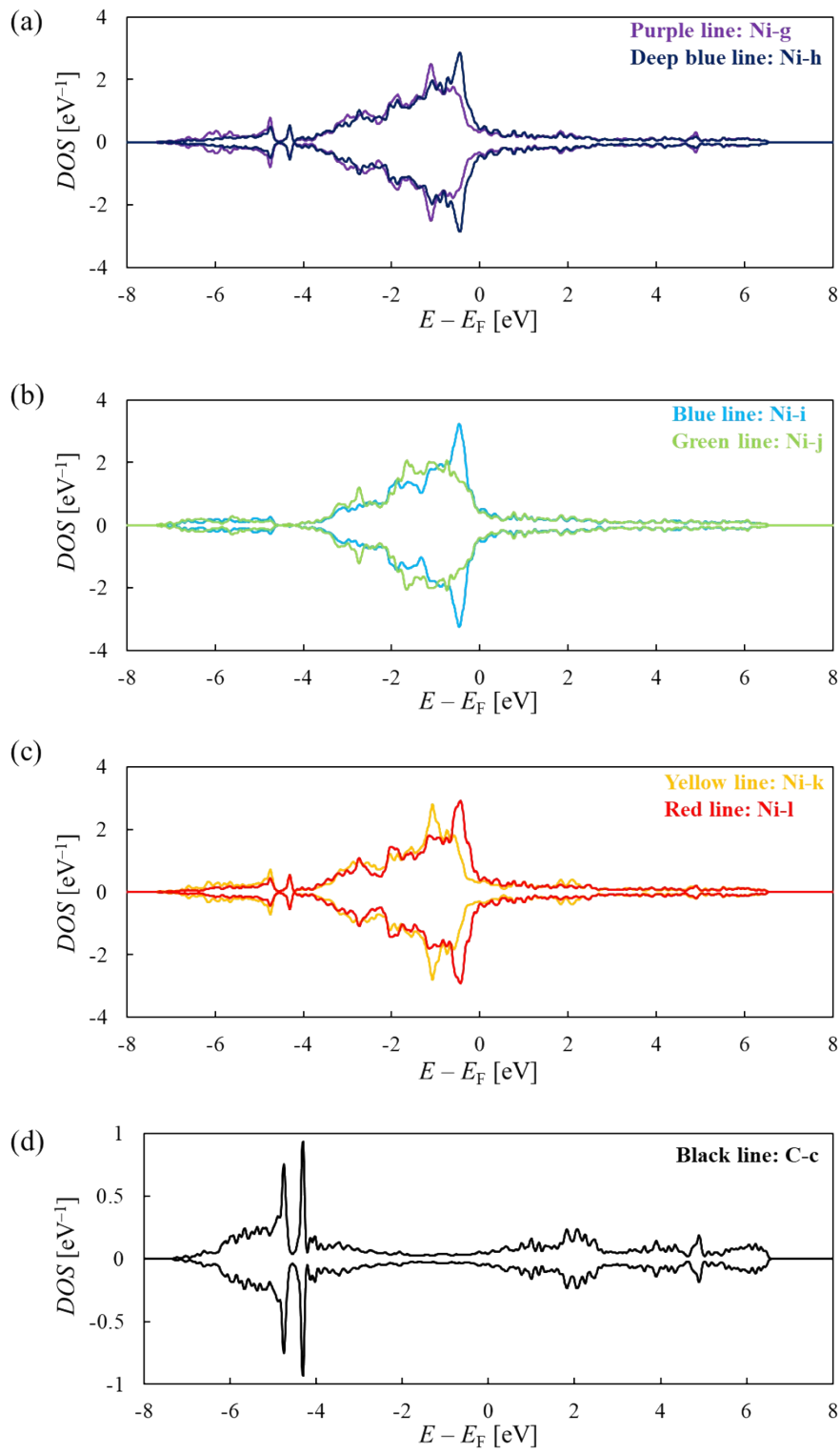
**Fig. S5** Optimised structures and surface energies ( $E_{\text{surf}}$ ) of dual-slab models of C-terminated (a) and Ni-terminated (b)  $\text{Ni}_3\text{C}$  (113) surfaces. The scheme used to estimate  $E_{\text{surf}}$  is described in the Supplementary Note. Green and black balls represent Ni and C atoms, respectively.



**Fig. S6** Projected DOS of Ni atoms (a-c) and C atoms (d) in C-terminated  $\text{Ni}_3\text{C}$  (113).  $E_F$  is the Fermi energy.

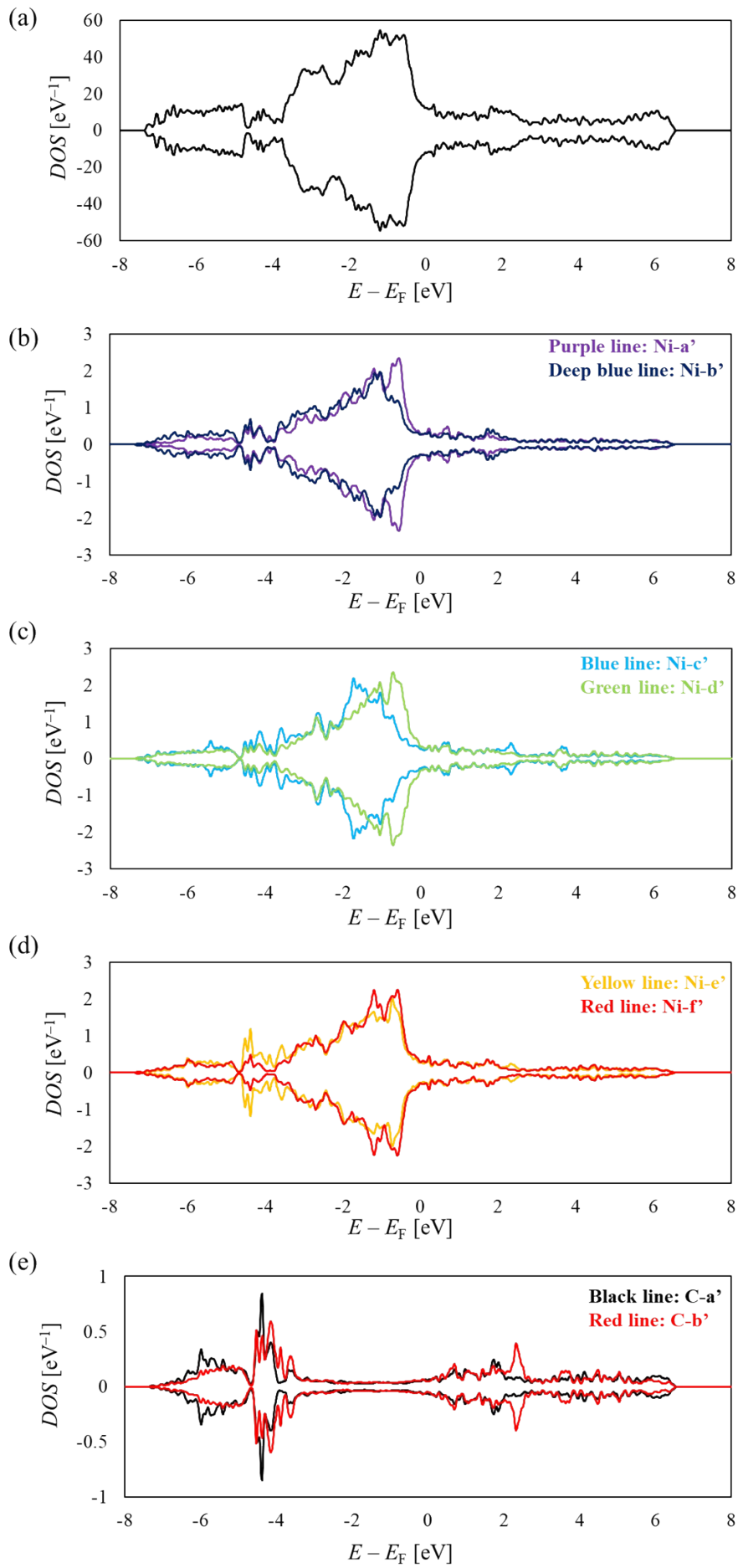


**Fig. S7** Projected DOS of C atoms in Ni<sub>3</sub>C (113): (a) C-a, (b) C-b, and (c) C-c.  $E_F$  is the Fermi energy.

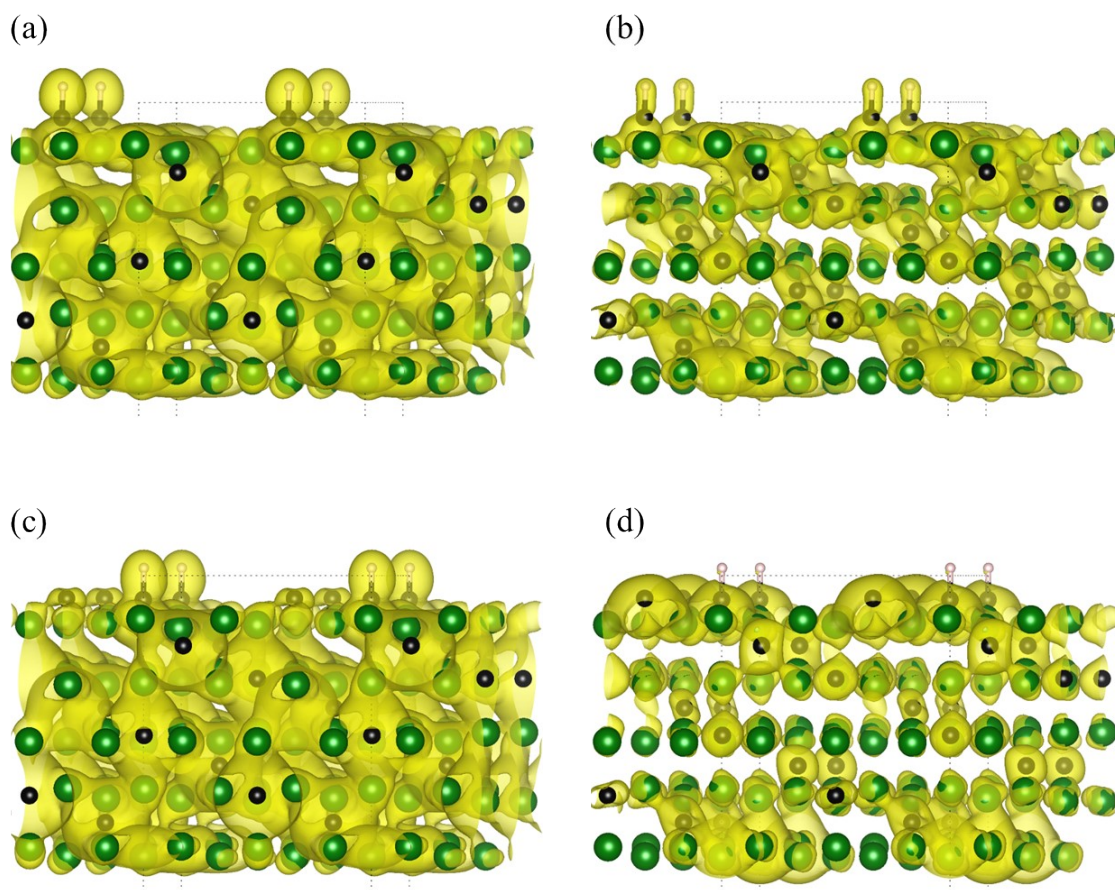


**Fig. S8** Projected DOS of Ni (a) and C atoms (b) in C-terminated  $\text{Ni}_3\text{C}$  (113).  $E_F$  is the Fermi energy.

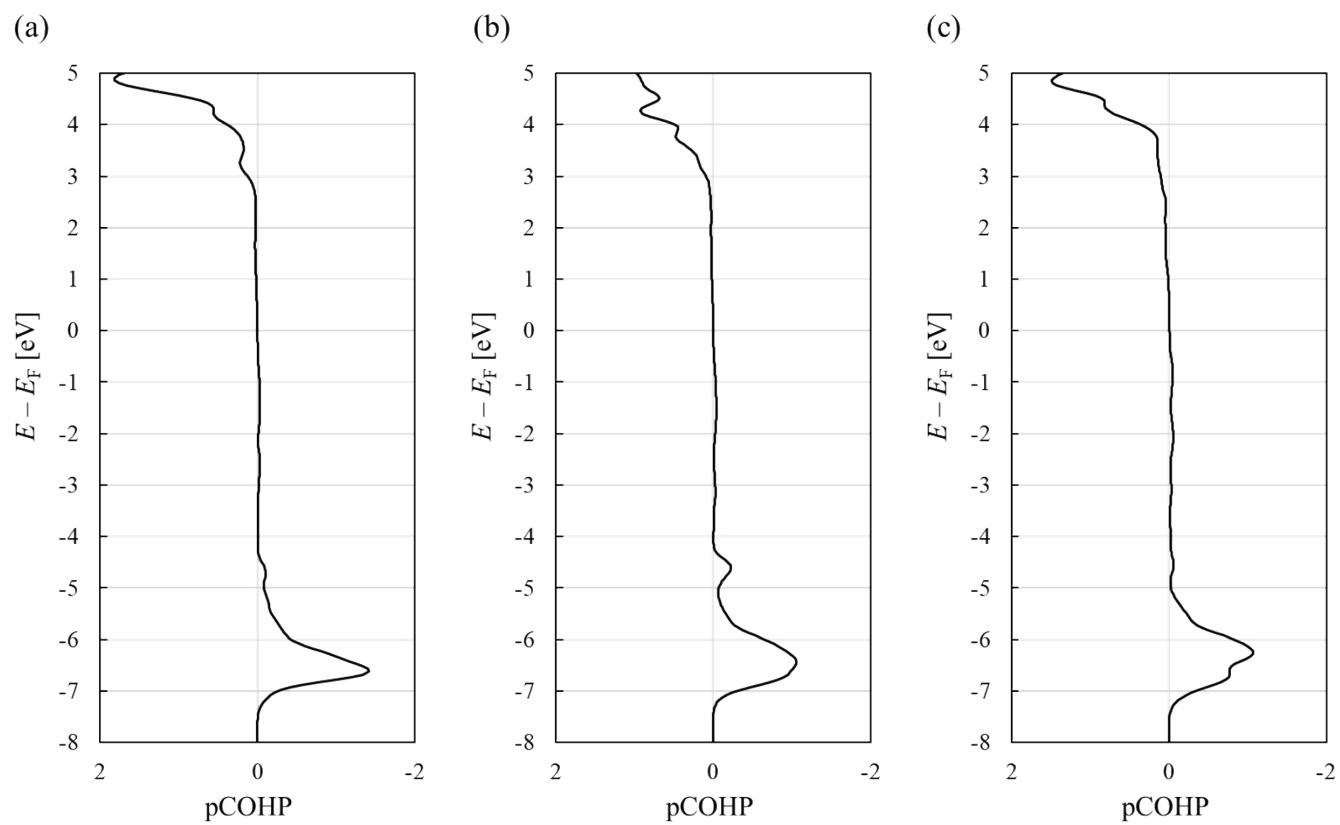




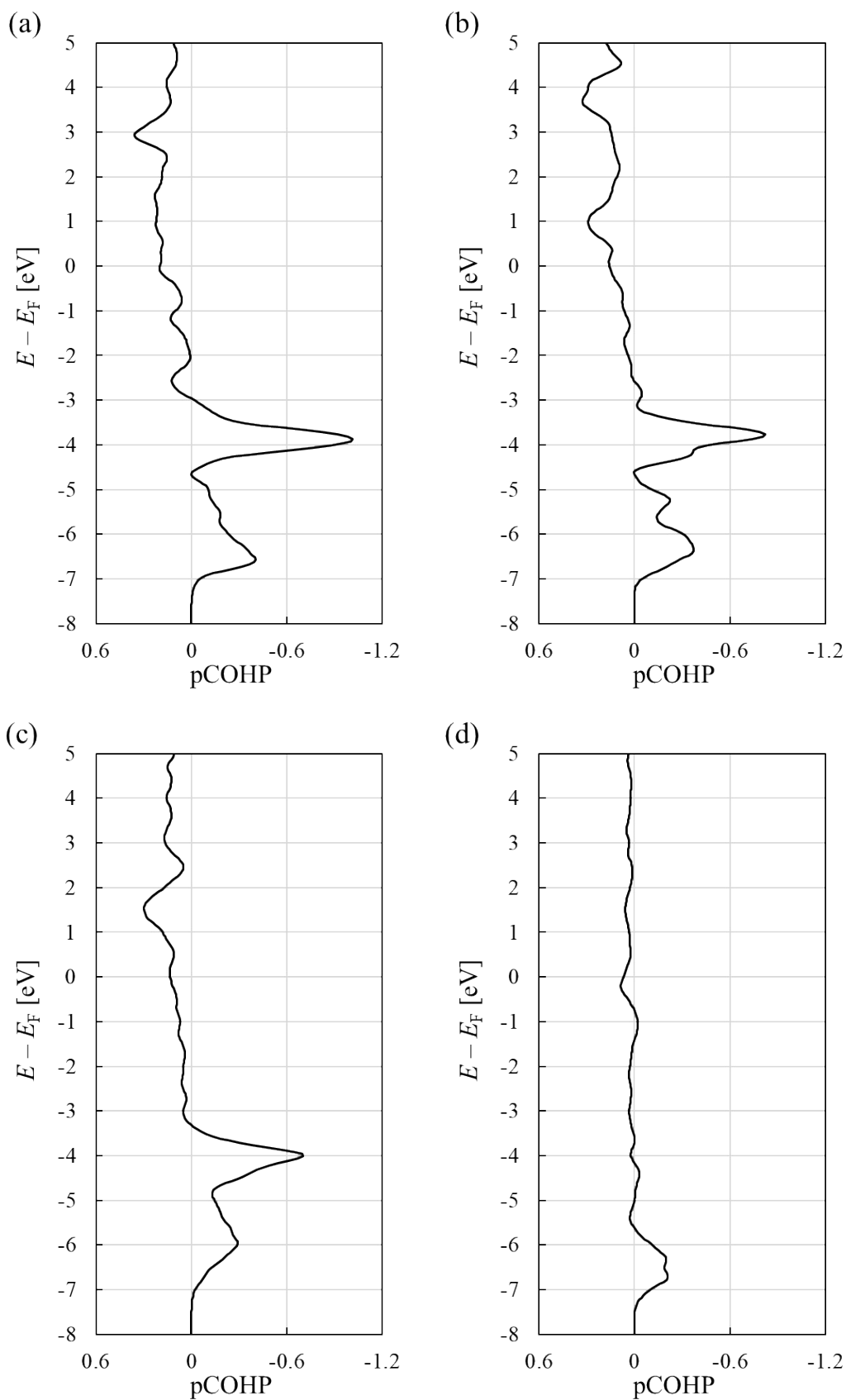
**Fig. S9** DOS of reconstructed  $\text{Ni}_3\text{C}$  (113). (a) Total DOS, (b–d) PDOS of exposed Ni atoms, and (e) PDOS of exposed C atoms.



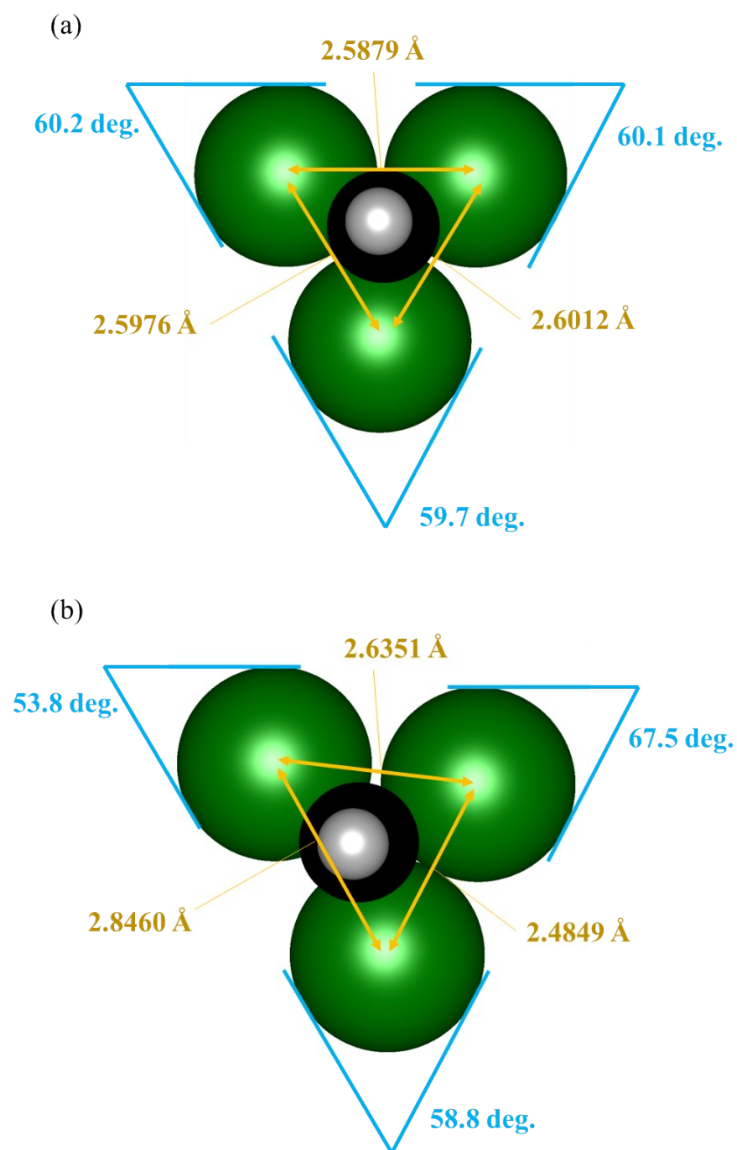
**Fig. S10** Partial charge density distributions of 1-C and 10-C structures. (a) Distribution of 1-C in energy range of  $-7.5$  to  $-5.0$  eV (threshold is 0.01 a.u.), (b) distribution of 1-C in energy range of  $-5.0$  to  $-4.5$  eV (threshold is 0.005 a.u.), (c) distribution of 10-C in energy range of  $-7.0$  to  $-5.0$  eV (threshold is 0.01 a.u.), and (d) distribution of 10-C in energy range of  $-5.0$  to  $-3.0$  eV (threshold is 0.01 a.u.). Reference for energies is the Fermi energy.



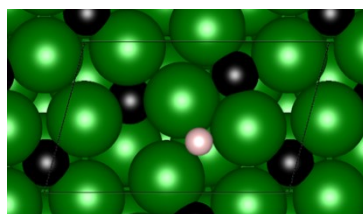
**Fig. S11** Projected COHP results for C-H interaction in the 1-C (a), 5-C (b), and 10-C (c) structures.



**Fig. S12** Projected COHP results for C-Ni interaction. (a) H-adsorbing C and its nearest neighbouring Ni in 1-C structure, (b) H-adsorbing C and its nearest neighbouring Ni in 5-C structure, (c) H-adsorbing C and its nearest neighbouring Ni in 10-C structure, and (d) H-adsorbing C and Ni in its axial position in 10-C structure.



**Fig. S13** Comparison of geometry of 1-C (a) and 5-C (b) structures. Green, black, and white balls represent Ni, C, and H atoms, respectively.

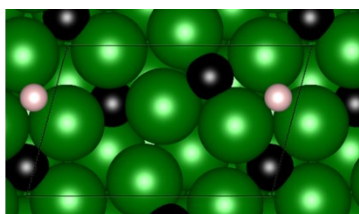


2-C

$$E_{\text{ads}} = -0.41 \text{ eV}$$

$$E_{\text{dis}} = 0.11 \text{ eV}$$

$$E_{\text{int}} = -2.79 \text{ eV}$$

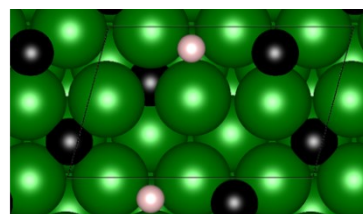


3-C

$$E_{\text{ads}} = -0.29 \text{ eV}$$

$$E_{\text{dis}} = 0.15 \text{ eV}$$

$$E_{\text{int}} = -2.71 \text{ eV}$$

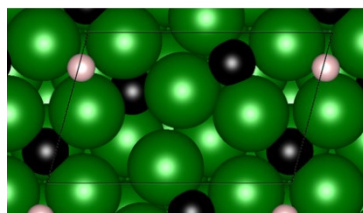


4-C

$$E_{\text{ads}} = -0.22 \text{ eV}$$

$$E_{\text{dis}} = 0.35 \text{ eV}$$

$$E_{\text{int}} = -2.85 \text{ eV}$$

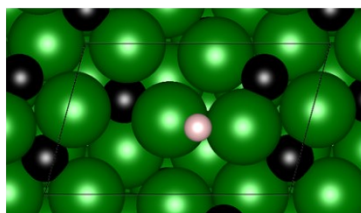


6-C

$$E_{\text{ads}} = -0.13 \text{ eV}$$

$$E_{\text{dis}} = 0.17 \text{ eV}$$

$$E_{\text{int}} = -2.57 \text{ eV}$$

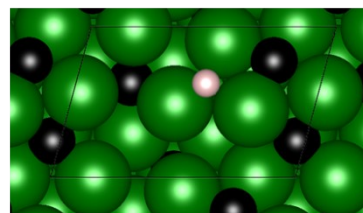


7-C

$$E_{\text{ads}} = -0.10 \text{ eV}$$

$$E_{\text{dis}} = 0.55 \text{ eV}$$

$$E_{\text{int}} = -2.92 \text{ eV}$$

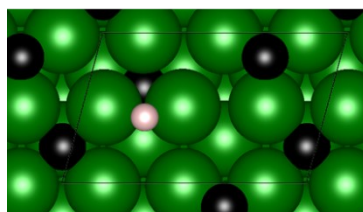


8-C

$$E_{\text{ads}} = -0.07 \text{ eV}$$

$$E_{\text{dis}} = 0.60 \text{ eV}$$

$$E_{\text{int}} = -2.94 \text{ eV}$$



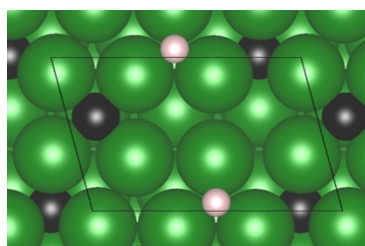
9-C

$$E_{\text{ads}} = 0.08 \text{ eV}$$

$$E_{\text{dis}} = 0.41 \text{ eV}$$

$$E_{\text{int}} = -2.60 \text{ eV}$$

**Fig. S14** Optimised structures of H/C-terminated  $\text{Ni}_3\text{C}$  (113) surfaces with H atom interacting with Ni atoms. The adsorption energies ( $E_{\text{ads}}$ ), surface distortion energies ( $E_{\text{dis}}$ ), and H- $\text{Ni}_3\text{C}$  interaction energies ( $E_{\text{int}}$ ) are also provided. Green, black, and white balls represent Ni, C, and H atoms, respectively.

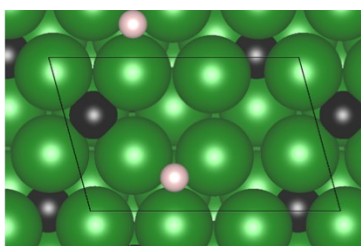


1-Ni

$$E_{\text{ads}} = -0.69 \text{ eV}$$

$$E_{\text{dis}} = 0.11 \text{ eV}$$

$$E_{\text{int}} = -3.07 \text{ eV}$$

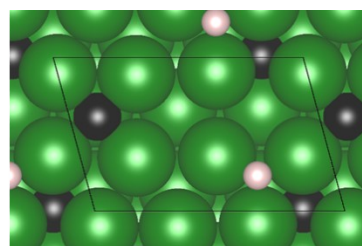


2-Ni

$$E_{\text{ads}} = -0.60 \text{ eV}$$

$$E_{\text{dis}} = 0.12 \text{ eV}$$

$$E_{\text{int}} = -2.99 \text{ eV}$$

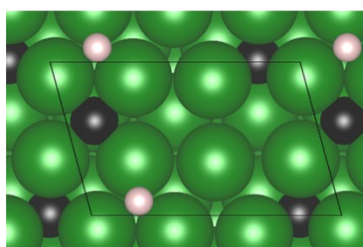


3-Ni

$$E_{\text{ads}} = -0.51 \text{ eV}$$

$$E_{\text{dis}} = 0.16 \text{ eV}$$

$$E_{\text{int}} = -2.94 \text{ eV}$$

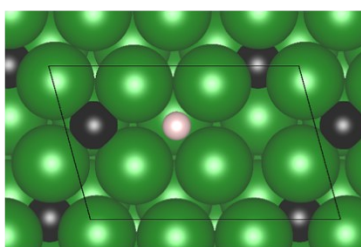


4-Ni

$$E_{\text{ads}} = -0.46 \text{ eV}$$

$$E_{\text{dis}} = 0.12 \text{ eV}$$

$$E_{\text{int}} = -2.85 \text{ eV}$$



5-Ni

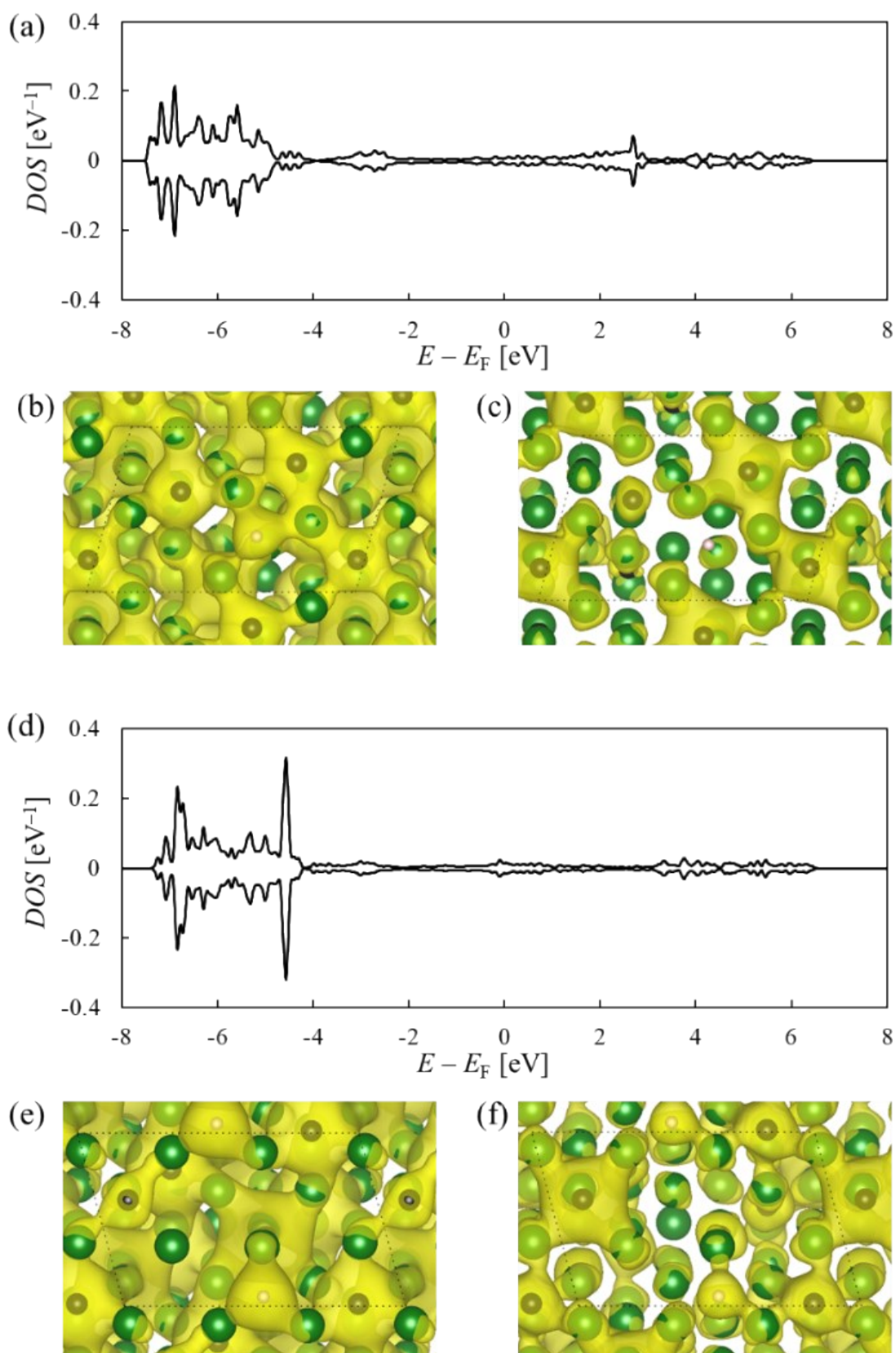
$$E_{\text{ads}} = -0.40 \text{ eV}$$

$$E_{\text{dis}} = 0.13 \text{ eV}$$

$$E_{\text{int}} = -2.80 \text{ eV}$$

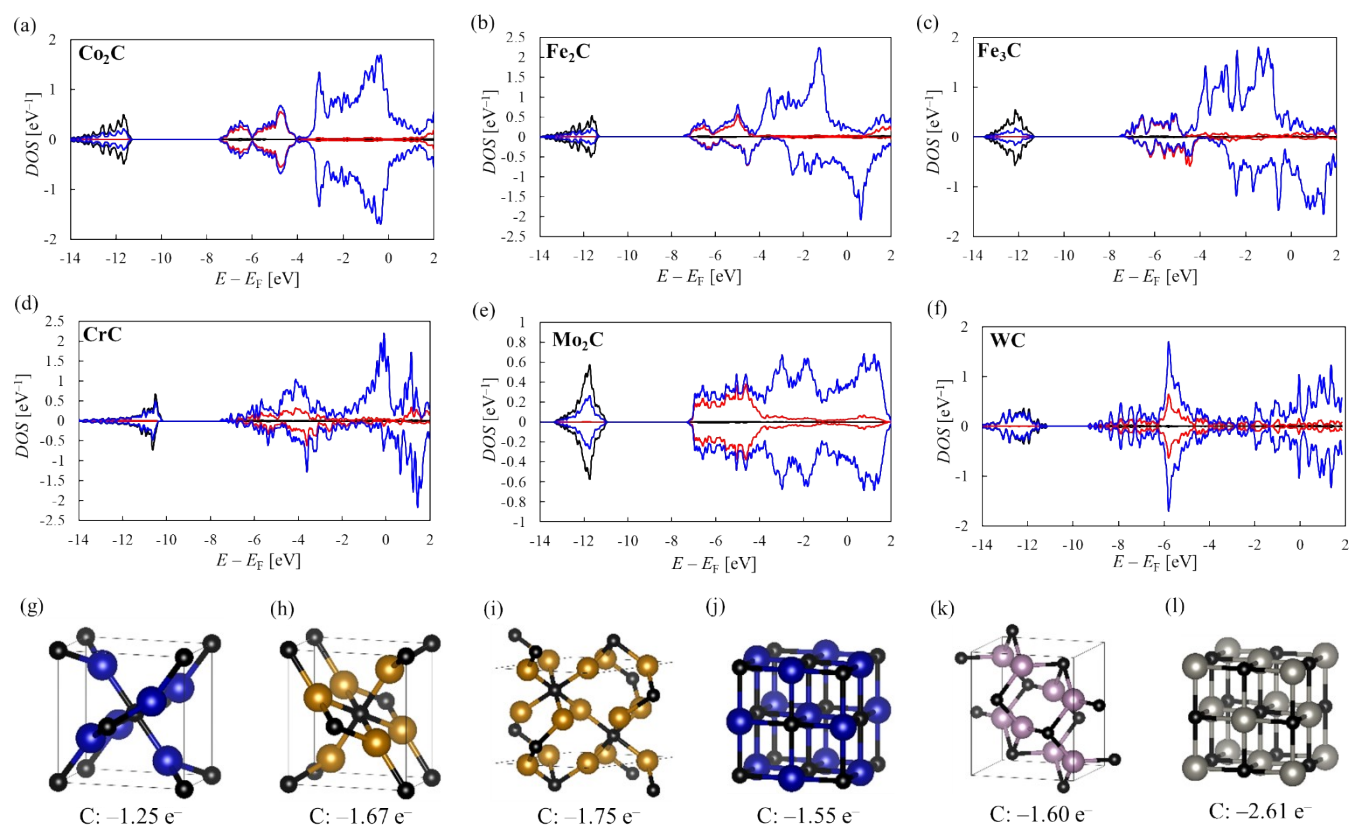
**Fig. S15** Optimised structures of H/Ni-terminated  $\text{Ni}_3\text{C}$  (113) where H atom interacts with Ni atoms. The adsorption energies ( $E_{\text{ads}}$ ), surface distortion energies ( $E_{\text{dis}}$ ), and H- $\text{Ni}_3\text{C}$  interaction energies ( $E_{\text{int}}$ ) are also shown. Green, black, and white balls represent Ni, C, and H atoms, respectively.





**Fig. S16** (a) PDOS of H, (b) partial charge density distribution in energy range of  $-7.5$  to  $-4.7$  eV (threshold is  $0.03$  a.u.), and (c) partial charge density distribution in energy range of  $-4.7$  to  $-4.0$  eV (threshold is  $0.01$  a.u.) for 2-C structure. (d) PDOS of H, (e) partial charge density distribution in energy range of  $-7.5$  to  $-6.0$  eV (threshold is  $0.01$  a.u.), (f) partial charge density distribution in energy range of  $-5.0$  to  $-4.0$  eV (threshold is  $0.01$  a.u.) for 1-Ni structure.





**Fig. S17** (a–f) PDOS of several metal carbides with their unit cell structures: (a)  $\text{Co}_2\text{C}$ , (b)  $\text{Fe}_2\text{C}$ , (c)  $\text{Fe}_3\text{C}$ , (d)  $\text{CrC}$ , (e)  $\text{Mo}_2\text{C}$ , and (f)  $\text{WC}$ . Blue, red, and black lines represent PDOS of metal species, carbon p orbitals, and carbon s orbitals. (g–l) Perspective views of calculated cells and estimated atomic charges for C: (g)  $\text{Co}_2\text{C}$ , (h)  $\text{Fe}_2\text{C}$ , (i)  $\text{Fe}_3\text{C}$ , (j)  $\text{CrC}$ , (k)  $\text{Mo}_2\text{C}$ , and (l)  $\text{WC}$ .

**Table S1.** Comparison of population analysis methods. The values are estimated numbers of valence electrons of atoms in the compounds.

| Atom | Compound                  | Bader [ $e^-$ ] | Mulliken [ $e^-$ ] | Löwdin [ $e^-$ ] |
|------|---------------------------|-----------------|--------------------|------------------|
| Ni   | Ni <sub>3</sub> C bulk    | 9.58            | 9.58               | 9.60             |
| Ni   | Ni bulk                   | 10.00           | 10.00              | 10.00            |
| Ni   | NiO bulk                  | 8.96            | 8.92               | 8.96             |
| C    | Ni <sub>3</sub> C bulk    | 5.28            | 5.26               | 5.16             |
| C    | CH <sub>4</sub>           | 4.04            | 5.03               | 4.69             |
| C    | CO                        | 2.17            | 3.60               | 3.81             |
| H    | CH <sub>4</sub>           | 0.98            | 0.74               | 0.82             |
| H    | H/Ni <sub>3</sub> C (1-C) | 0.95            | 0.66               | 0.78             |
| H    | H/Ni <sub>3</sub> C (2-C) | 1.28            | 1.42               | 1.32             |

**Table S2.** Lattice parameters of Ni<sub>3</sub>C. The units of distance and angle are Å and degree.

|          | DFT       |        |        | Exp.  |        |
|----------|-----------|--------|--------|-------|--------|
|          | This work | [35]   | [53]   | [51]  | [52]   |
| a        | 4.59535   | 4.553  | 4.604  | 4.553 | 4.60   |
| b        | 4.59535   | 4.553  | 4.604  | 4.553 | 4.60   |
| c        | 12.99523  | 12.920 | 13.022 | 12.92 | 13.016 |
| $\alpha$ | 90.0      | 90.0   | 90.0   | 90.0  | 90.0   |
| $\beta$  | 90.0      | 90.0   | 90.0   | 90.0  | 90.0   |
| $\gamma$ | 120.0     | 120.0  | 120.0  | 120.0 | 120.0  |

**Table S3.** Atomic charges of Ni and C atoms in Ni<sub>3</sub>C (113) model. Ni-d has one fewer bond to C than the other Ni atoms; hence, its charge is less cationic. Similarly, because the number of Ni–C bonds is less than that of bulk Ni<sub>3</sub>C, C-b, which is three-coordinate, and C-a, which is five-coordinate, are less anionic than the C atoms in the bulk, and the charge on C-b is more neutral than that on C-a. The four Ni atoms (Ni-h, Ni-i, Ni-j, and Ni-l) with one bond to C-c in the Ni-terminated surface are more electron-rich than the Ni atoms in bulk Ni<sub>3</sub>C, as is Ni-d on the C-terminated surface, and C-c is more electron-rich than the C-b atom in bulk Ni<sub>3</sub>C.

| Atom | Charge [e <sup>-</sup> ] | Atom | Charge [e <sup>-</sup> ] |
|------|--------------------------|------|--------------------------|
| Ni-a | 0.46                     | Ni-g | 0.46                     |
| Ni-b | 0.45                     | Ni-h | 0.20                     |
| Ni-c | 0.43                     | Ni-i | 0.23                     |
| Ni-d | 0.29                     | Ni-j | 0.17                     |
| Ni-e | 0.46                     | Ni-k | 0.46                     |
| N-f  | 0.51                     | Ni-l | 0.25                     |
| C-a  | -1.13                    | C-c  | -1.11                    |
| C-b  | -0.80                    |      |                          |

**Table S4.** Proportionality constant (a), intercept (b), and coefficient of determination ( $R^2$ ) for regression lines shown in Fig. 14

|            | a      | b       | $R^2$  |
|------------|--------|---------|--------|
| Fig. 14(a) | 0.7834 | −0.0995 | 0.4713 |
| Fig. 14(b) | 0.4950 | 0.1413  | 0.8117 |
| Fig. 14(c) | 1.2269 | 0.6996  | 0.9704 |
| Fig. 14(d) | 1.2540 | 0.0491  | 0.9712 |
| Fig. 14(e) | 0.8319 | −0.1461 | 0.9437 |
| Fig. 14(f) | 1.1396 | −0.1114 | 0.9995 |
| Fig. 14(g) | 0.7392 | −0.7516 | 0.4882 |
| Fig. 14(h) | 1.1944 | 0.0381  | 0.9865 |

# Supplementary Note 1:

## Scheme for estimating surface energy

Because dual-sided models of  $\text{Ni}_3\text{C}$  (113) cannot be constructed using the stoichiometric ratio of  $\text{Ni}_3\text{C}$ , the calculated composition is denoted as  $\text{Ni}_x\text{C}_y$ . The calculated composition of the reference bulk  $\text{Ni}_3\text{C}$  was denoted as  $\text{Ni}_{3z}\text{C}_z$ .  $E_{\text{surf}}$  is then calculated by

$$E_{\text{surf}} = \frac{1}{2A} \left( E(\text{Ni}_3\text{C}(113): \text{Ni}_x\text{C}_y) - \frac{y}{z} E(\text{bulk Ni}_3\text{C}: \text{Ni}_{3z}\text{C}_z) - \frac{(x-3y)}{4} E(\text{Ni metal}: \text{Ni}_4) \right), \quad (\text{s1})$$

where  $A$  is the surface area of  $\text{Ni}_3\text{C}$  (113) per cell. A value of  $39.00 \text{ \AA}^2$  was estimated from the optimised lattice constants of bulk  $\text{Ni}_3\text{C}$ . The number of Ni atoms in the unit cell of Ni metal is four; hence,  $E(\text{Ni metal})$  is divided into four. The dual-sided model comprised C-terminated  $\text{Ni}_{24}\text{C}_9$  and Ni-terminated  $\text{Ni}_{30}\text{C}_9$ . The calculated composition of bulk  $\text{Ni}_3\text{C}$  was  $\text{Ni}_{18}\text{C}_6$ .

Although it is difficult to estimate the surface energies from a single-sided model, the energy difference between surface configurations can still be evaluated using the following approach: The surface energy of the C-terminated surface in the single-sided model is denoted as  $E'_{\text{surf}}(\text{C})$  and that of the reconstructed surface in the single-sided model is denoted as  $E_{\text{surf}}(\text{R})$ . The counterparts of the C-terminated and reconstructed surfaces are the same: Ni-terminated surface with bulk structure. The surface energy of this Ni-terminated counterpart is denoted as  $E'_{\text{surf}}(\text{N})$ , therefore,

$$(E'_{\text{surf}}(\text{C}) + E'_{\text{surf}}(\text{N})) \times 2A = E(\text{C\_slab}) - n E(\text{bulk Ni}_3\text{C}), \quad (\text{s2})$$

$$(E_{\text{surf}}(\text{R}) + E'_{\text{surf}}(\text{N})) \times 2A = E(\text{R\_slab}) - n E(\text{bulk Ni}_3\text{C}). \quad (\text{s3})$$

$E(\text{C\_slab})$ ,  $E(\text{R\_slab})$ , and  $E(\text{bulk Ni}_3\text{C})$  are the total energies of the single-sided C-terminated slab, single-sided restricted slab, and bulk  $\text{Ni}_3\text{C}$ , respectively. Because the composition of the single-sided model was  $\text{Ni}_{30}\text{C}_{10}$  and that of bulk  $\text{Ni}_3\text{C}$  was  $\text{Ni}_{18}\text{C}_6$ , the  $n$  values in Eqs. (s2) and (s3) is  $5/3$ . From Eqs. (s2) and (s3), the difference between the surface energies of the C-terminated and reconstructed surfaces is.

$$\Delta E_{\text{surf}} \equiv E'_{\text{surf}}(\text{C}) - E_{\text{surf}}(\text{R}) = (E(\text{C\_slab}) - E(\text{R\_slab}))/2A. \quad (\text{s4})$$

The surface energies of the C-terminated surfaces estimated for the single-sided ( $E'_{\text{surf}}(\text{C})$ ) and dual-sided ( $E_{\text{surf}}(\text{C})$ ) models were assumed to be identical (Eq. (s5)). Thus, the energy of the reconstructed surface can be estimated using Eqs. (s6).

$$E'_{\text{surf}}(\text{C}) \approx E_{\text{surf}}(\text{C}) \quad (\text{s5})$$

$$E_{\text{surf}}(\text{R}) = E_{\text{surf}}(\text{C}) - (E(\text{C\_slab}) - E(\text{R\_slab}))/2A \quad (\text{s6})$$

## Supplementary Note 2:

### Specific coordinates of optimised structures

Here we summarise the specific atomic positions in the optimised structures of Ni<sub>3</sub>C bulk, Ni<sub>3</sub>C (113) slab models, H/Ni<sub>3</sub>C model systems. The atomic coordinates are supplied in a direct coordination to the lattice vectors. The lattice vectors of Ni<sub>3</sub>C bulk are summarised in Table S1, and those of other models are (7.97347811 Å, 0.00000000 Å, 0.00000000 Å), (−1.32891302 Å, 4.89112746 Å, 0.00000000 Å), and (0.00000000 Å, 0.00000000 Å, 29.82589270 Å).

#### Ni<sub>3</sub>C bulk

|      |            |            |            |
|------|------------|------------|------------|
| Ni1  | 1.00000000 | 0.67080414 | 0.25000000 |
| Ni2  | 0.67080414 | 0.00000000 | 0.25000000 |
| Ni3  | 0.32919583 | 0.32919583 | 0.25000000 |
| Ni4  | 0.99586248 | 0.33333334 | 0.08333333 |
| Ni5  | 0.33747083 | 0.00413749 | 0.08333333 |
| Ni6  | 0.66666669 | 0.66252917 | 0.08333333 |
| Ni7  | 0.66666669 | 0.00413749 | 0.58333331 |
| Ni8  | 0.33747083 | 0.33333334 | 0.58333331 |
| Ni9  | 0.99586248 | 0.66252917 | 0.58333331 |
| Ni10 | 0.66252917 | 0.66666669 | 0.41666666 |
| Ni11 | 0.00413749 | 0.33747083 | 0.41666666 |
| Ni12 | 0.33333334 | 0.99586248 | 0.41666666 |
| Ni13 | 0.33333334 | 0.33747083 | 0.91666669 |
| Ni14 | 0.00413749 | 0.66666669 | 0.91666669 |
| Ni15 | 0.66252917 | 0.99586248 | 0.91666669 |
| Ni16 | 0.32919583 | 0.00000000 | 0.75000000 |
| Ni17 | 0.67080415 | 0.67080414 | 0.75000000 |
| Ni18 | 1.00000000 | 0.32919583 | 0.75000000 |
| C1   | 0.00000000 | 0.00000000 | 0.00000000 |
| C2   | 0.33333334 | 0.66666669 | 0.16666667 |
| C3   | 0.66666669 | 0.33333334 | 0.33333334 |
| C4   | 0.00000000 | 0.00000000 | 0.50000000 |
| C5   | 0.33333334 | 0.66666669 | 0.66666669 |
| C6   | 0.66666669 | 0.33333334 | 0.83333331 |

#### C-terminated Ni<sub>3</sub>C (113)

|     |            |            |            |
|-----|------------|------------|------------|
| Ni1 | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2 | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3 | 0.64789318 | 0.90021698 | 0.32856616 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44622150 | 0.68490437 | 0.26395350 |
| Ni8  | 0.78294530 | 0.68255160 | 0.25999851 |
| Ni9  | 0.10909226 | 0.68619619 | 0.26066237 |
| Ni10 | 0.02900546 | 0.14958852 | 0.25016044 |
| Ni11 | 0.35578106 | 0.14545218 | 0.25265604 |
| Ni12 | 0.69324232 | 0.14717008 | 0.24878066 |
| Ni13 | 0.91365934 | 0.46597571 | 0.19443941 |
| Ni14 | 0.24865823 | 0.46431822 | 0.19322777 |
| Ni15 | 0.57586146 | 0.46478778 | 0.19425627 |
| Ni16 | 0.49019720 | 0.92929104 | 0.18337135 |
| Ni17 | 0.82184248 | 0.92905913 | 0.18311299 |
| Ni18 | 0.15871985 | 0.92781160 | 0.18108568 |
| Ni19 | 0.37335947 | 0.24419635 | 0.12641977 |
| Ni20 | 0.70944221 | 0.24085367 | 0.12737934 |
| Ni21 | 0.04144682 | 0.24232126 | 0.12498723 |
| Ni22 | 0.95269939 | 0.70947687 | 0.11455408 |
| Ni23 | 0.28234554 | 0.70759948 | 0.11420895 |
| Ni24 | 0.61932228 | 0.70883103 | 0.11468007 |
| Ni25 | 0.83367092 | 0.01886233 | 0.05732863 |
| Ni26 | 0.16866928 | 0.01222711 | 0.05953249 |
| Ni27 | 0.50206211 | 0.01818800 | 0.05692056 |
| Ni28 | 0.42788885 | 0.49414107 | 0.05032680 |
| Ni29 | 0.74863772 | 0.49001816 | 0.05002841 |
| Ni30 | 0.06760871 | 0.47683687 | 0.04864246 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56901213 | 0.41469387 | 0.25749479 |
| C4   | 0.30170809 | 0.80544872 | 0.22252128 |
| C5   | 0.03550082 | 0.19640885 | 0.18735602 |
| C6   | 0.76591149 | 0.58677821 | 0.15453881 |
| C7   | 0.49541783 | 0.97556715 | 0.12033938 |
| C8   | 0.23265653 | 0.36732213 | 0.08340545 |
| C9   | 0.96015438 | 0.75824573 | 0.04950593 |
| C10  | 0.69100387 | 0.16294208 | 0.02474091 |

**Ni-terminated Ni<sub>3</sub>C (113)**

|     |            |            |            |
|-----|------------|------------|------------|
| Ni1 | 0.00371475 | 0.90673542 | 0.32394357 |
| Ni2 | 0.31662412 | 0.90165831 | 0.32283209 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni3  | 0.62977993 | 0.89011970 | 0.32327145 |
| Ni4  | 0.54964433 | 0.35460106 | 0.31545649 |
| Ni5  | 0.89856724 | 0.37516934 | 0.31487767 |
| Ni6  | 0.22839718 | 0.35550134 | 0.31525925 |
| Ni7  | 0.44454241 | 0.67859992 | 0.26003150 |
| Ni8  | 0.78257161 | 0.68076881 | 0.26006945 |
| Ni9  | 0.11165518 | 0.67639103 | 0.25898114 |
| Ni10 | 0.02228549 | 0.14169219 | 0.24879550 |
| Ni11 | 0.35414632 | 0.14337847 | 0.24873656 |
| Ni12 | 0.69500260 | 0.14460917 | 0.24819852 |
| Ni13 | 0.91005657 | 0.46038873 | 0.19317149 |
| Ni14 | 0.24553376 | 0.45829416 | 0.19080958 |
| Ni15 | 0.57530570 | 0.45993413 | 0.19219523 |
| Ni16 | 0.49046841 | 0.92464578 | 0.18133101 |
| Ni17 | 0.81888640 | 0.92309648 | 0.18147126 |
| Ni18 | 0.15583953 | 0.92340313 | 0.17886434 |
| Ni19 | 0.37373456 | 0.23899866 | 0.12474358 |
| Ni20 | 0.71022542 | 0.23739936 | 0.12485260 |
| Ni21 | 0.04047586 | 0.23907542 | 0.12348360 |
| Ni22 | 0.95444843 | 0.70141002 | 0.11349215 |
| Ni23 | 0.28333192 | 0.70253536 | 0.11248183 |
| Ni24 | 0.61840317 | 0.69986931 | 0.11175205 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11619984 | 0.62259408 | 0.32446335 |
| C2   | 0.83234333 | 0.01896185 | 0.29234704 |
| C3   | 0.56980507 | 0.41068146 | 0.25531928 |
| C4   | 0.29839525 | 0.80022809 | 0.21968540 |
| C5   | 0.03197330 | 0.19056845 | 0.18621724 |
| C6   | 0.76399761 | 0.58178805 | 0.15258479 |
| C7   | 0.49711840 | 0.97031765 | 0.11864535 |
| C8   | 0.23151978 | 0.36077478 | 0.08238482 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

**reconstructed Ni<sub>3</sub>C (113)**

|     |            |            |            |
|-----|------------|------------|------------|
| Ni1 | 0.98384405 | 0.90306438 | 0.32944171 |
|-----|------------|------------|------------|



|      |            |            |            |
|------|------------|------------|------------|
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44837305 | 0.68688893 | 0.26425787 |
| Ni8  | 0.78477089 | 0.68320609 | 0.26010697 |
| Ni9  | 0.11104558 | 0.68810406 | 0.26082019 |
| Ni10 | 0.02900207 | 0.15065387 | 0.25015867 |
| Ni11 | 0.35714881 | 0.14820830 | 0.25280960 |
| Ni12 | 0.69503235 | 0.14897787 | 0.24854391 |
| Ni13 | 0.91489075 | 0.46825378 | 0.19435557 |
| Ni14 | 0.25035818 | 0.46540364 | 0.19445992 |
| Ni15 | 0.57963108 | 0.46675770 | 0.19417126 |
| Ni16 | 0.49310192 | 0.93277953 | 0.18340352 |
| Ni17 | 0.82397769 | 0.93217307 | 0.18277861 |
| Ni18 | 0.15890586 | 0.93074616 | 0.18207534 |
| Ni19 | 0.37562916 | 0.24432240 | 0.12823472 |
| Ni20 | 0.71123299 | 0.24422506 | 0.12446825 |
| Ni21 | 0.04686117 | 0.25482272 | 0.12477938 |
| Ni22 | 0.95709667 | 0.72456642 | 0.11500735 |
| Ni23 | 0.28338701 | 0.70663428 | 0.11801219 |
| Ni24 | 0.62133599 | 0.70769168 | 0.11525450 |
| Ni25 | 0.83314301 | 0.07753725 | 0.05384886 |
| Ni26 | 0.17841479 | 0.03573126 | 0.06179582 |
| Ni27 | 0.47969921 | 0.91019784 | 0.05555799 |
| Ni28 | 0.45900442 | 0.39309203 | 0.05076130 |
| Ni29 | 0.76804871 | 0.55280371 | 0.04642240 |
| Ni30 | 0.08134442 | 0.51566969 | 0.05123828 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.57087401 | 0.41635036 | 0.25741352 |
| C4   | 0.30475156 | 0.80866106 | 0.22282147 |
| C5   | 0.03699582 | 0.20014483 | 0.18713728 |
| C6   | 0.76943706 | 0.58749599 | 0.15421235 |
| C7   | 0.49611341 | 0.97433060 | 0.11977487 |
| C8   | 0.25010351 | 0.39227334 | 0.08271673 |
| C9   | 0.96998976 | 0.81004570 | 0.05093880 |
| C10  | 0.63626030 | 0.21201762 | 0.03789523 |

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.68834091 | 0.13852981 | 0.98157976 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44681031 | 0.68690170 | 0.26421242 |
| Ni8  | 0.78380186 | 0.68316649 | 0.26008258 |
| Ni9  | 0.11020597 | 0.68810633 | 0.26069511 |
| Ni10 | 0.02957389 | 0.15176085 | 0.25029400 |
| Ni11 | 0.35654285 | 0.14862948 | 0.25254471 |
| Ni12 | 0.69433704 | 0.14957666 | 0.24875858 |
| Ni13 | 0.91529411 | 0.46993012 | 0.19453239 |
| Ni14 | 0.25054511 | 0.46825727 | 0.19340701 |
| Ni15 | 0.57686440 | 0.46809093 | 0.19421993 |
| Ni16 | 0.49172215 | 0.93239588 | 0.18330068 |
| Ni17 | 0.82365171 | 0.93318504 | 0.18348104 |
| Ni18 | 0.16165790 | 0.93344639 | 0.18129586 |
| Ni19 | 0.37455025 | 0.24994563 | 0.12623114 |
| Ni20 | 0.71288934 | 0.24436420 | 0.12775559 |
| Ni21 | 0.04448560 | 0.25102785 | 0.12538570 |
| Ni22 | 0.95395718 | 0.72143649 | 0.11517918 |
| Ni23 | 0.28514631 | 0.71568277 | 0.11308019 |
| Ni24 | 0.61851576 | 0.71150996 | 0.11515473 |
| Ni25 | 0.82601110 | 0.01753317 | 0.05617623 |
| Ni26 | 0.16532898 | 0.01653702 | 0.05945003 |
| Ni27 | 0.50261134 | 0.03108435 | 0.05710149 |
| Ni28 | 0.43164508 | 0.50205772 | 0.05028062 |
| Ni29 | 0.74924022 | 0.48214928 | 0.05130630 |
| Ni30 | 0.06401902 | 0.48018479 | 0.04983997 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56962518 | 0.41683310 | 0.25747983 |
| C4   | 0.30315718 | 0.80830765 | 0.22265264 |
| C5   | 0.03753681 | 0.20064653 | 0.18755724 |
| C6   | 0.76752398 | 0.59187381 | 0.15467728 |
| C7   | 0.49811416 | 0.98338282 | 0.12049201 |
| C8   | 0.23415380 | 0.37238091 | 0.08265624 |
| C9   | 0.95318985 | 0.76114430 | 0.04985084 |
| C10  | 0.68803436 | 0.16604816 | 0.01819204 |

**2-C**

|      |            |            |            |
|------|------------|------------|------------|
| H    | 0.57639306 | 0.66242699 | 0.02599079 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44773628 | 0.68538117 | 0.26442885 |
| Ni8  | 0.78404975 | 0.68315558 | 0.25991139 |
| Ni9  | 0.10893840 | 0.68606102 | 0.26082271 |
| Ni10 | 0.02851616 | 0.15068017 | 0.25012220 |
| Ni11 | 0.35652314 | 0.14729736 | 0.25270250 |
| Ni12 | 0.69472837 | 0.14796488 | 0.24862284 |
| Ni13 | 0.91210067 | 0.46342031 | 0.19360127 |
| Ni14 | 0.24915812 | 0.46289213 | 0.19478495 |
| Ni15 | 0.58122853 | 0.46301603 | 0.19393389 |
| Ni16 | 0.49239944 | 0.92911678 | 0.18399030 |
| Ni17 | 0.82363845 | 0.92885943 | 0.18233670 |
| Ni18 | 0.15725591 | 0.92713705 | 0.18224266 |
| Ni19 | 0.37284272 | 0.24220998 | 0.12911087 |
| Ni20 | 0.70362962 | 0.24881347 | 0.11836016 |
| Ni21 | 0.04531532 | 0.25401881 | 0.12477320 |
| Ni22 | 0.95512038 | 0.72277278 | 0.11370447 |
| Ni23 | 0.28032004 | 0.70582174 | 0.11770796 |
| Ni24 | 0.61871012 | 0.70738934 | 0.11676207 |
| Ni25 | 0.85047603 | 0.08654900 | 0.05363604 |
| Ni26 | 0.17990620 | 0.03682629 | 0.06150929 |
| Ni27 | 0.48437863 | 0.90726733 | 0.05556047 |
| Ni28 | 0.46062237 | 0.38885379 | 0.05134660 |
| Ni29 | 0.76395559 | 0.57217896 | 0.03993506 |
| Ni30 | 0.08258379 | 0.51323098 | 0.05030593 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.57064228 | 0.41548446 | 0.25730788 |
| C4   | 0.30294335 | 0.80634048 | 0.22316719 |
| C5   | 0.03583404 | 0.19725096 | 0.18704637 |
| C6   | 0.76948706 | 0.58231107 | 0.15318994 |
| C7   | 0.49165525 | 0.97056538 | 0.12116803 |
| C8   | 0.24912481 | 0.39031576 | 0.08329191 |
| C9   | 0.97408768 | 0.80311166 | 0.04956910 |

|     |            |            |            |
|-----|------------|------------|------------|
| C10 | 0.65080116 | 0.21798491 | 0.04561721 |
|-----|------------|------------|------------|

**3-C**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.91980878 | 0.34585286 | 0.01849922 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44816664 | 0.68599766 | 0.26421513 |
| Ni8  | 0.78365845 | 0.68270556 | 0.26002034 |
| Ni9  | 0.10990457 | 0.68602509 | 0.26081063 |
| Ni10 | 0.02840911 | 0.14916590 | 0.25016818 |
| Ni11 | 0.35676587 | 0.14670293 | 0.25275047 |
| Ni12 | 0.69416131 | 0.14741394 | 0.24850202 |
| Ni13 | 0.91219950 | 0.46569429 | 0.19415050 |
| Ni14 | 0.24857188 | 0.46295487 | 0.19467407 |
| Ni15 | 0.57770032 | 0.46422325 | 0.19383170 |
| Ni16 | 0.49220216 | 0.92741041 | 0.18302212 |
| Ni17 | 0.82228940 | 0.92919233 | 0.18270474 |
| Ni18 | 0.15839486 | 0.92943090 | 0.18244076 |
| Ni19 | 0.37357177 | 0.24012278 | 0.12861036 |
| Ni20 | 0.70896230 | 0.24414150 | 0.12362855 |
| Ni21 | 0.04230336 | 0.24940034 | 0.12494311 |
| Ni22 | 0.95634141 | 0.72181364 | 0.11536727 |
| Ni23 | 0.28108270 | 0.70109163 | 0.11827410 |
| Ni24 | 0.62762778 | 0.71437533 | 0.11317085 |
| Ni25 | 0.82181749 | 0.06304263 | 0.04880589 |
| Ni26 | 0.17511144 | 0.03194837 | 0.06201165 |
| Ni27 | 0.46543670 | 0.90628116 | 0.05562855 |
| Ni28 | 0.45972578 | 0.40439653 | 0.05191082 |
| Ni29 | 0.77665801 | 0.53045026 | 0.03952996 |
| Ni30 | 0.08085564 | 0.51457198 | 0.05095334 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.57035386 | 0.41494910 | 0.25734243 |
| C4   | 0.30417867 | 0.80666106 | 0.22292961 |
| C5   | 0.03516801 | 0.19796359 | 0.18715317 |
| C6   | 0.76653390 | 0.58464738 | 0.15381603 |
| C7   | 0.49512567 | 0.97093664 | 0.11966731 |

|     |            |            |            |
|-----|------------|------------|------------|
| C8  | 0.24627430 | 0.38547223 | 0.08357222 |
| C9  | 0.96342112 | 0.80913910 | 0.05290497 |
| C10 | 0.61727400 | 0.20518808 | 0.03714011 |

#### 4-C

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.36155703 | 0.14370774 | 0.02613091 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44731192 | 0.68736247 | 0.26388645 |
| Ni8  | 0.78386088 | 0.68341969 | 0.26000336 |
| Ni9  | 0.10993753 | 0.68791203 | 0.26072200 |
| Ni10 | 0.02912067 | 0.15147895 | 0.25028223 |
| Ni11 | 0.35634858 | 0.14853623 | 0.25270336 |
| Ni12 | 0.69420664 | 0.14953697 | 0.24868158 |
| Ni13 | 0.91415418 | 0.46985999 | 0.19413807 |
| Ni14 | 0.24874647 | 0.46837363 | 0.19333769 |
| Ni15 | 0.57678489 | 0.46866734 | 0.19408364 |
| Ni16 | 0.49136155 | 0.93270008 | 0.18309066 |
| Ni17 | 0.82145208 | 0.93204918 | 0.18282525 |
| Ni18 | 0.15970826 | 0.93184689 | 0.18148664 |
| Ni19 | 0.37438644 | 0.24553107 | 0.12752445 |
| Ni20 | 0.71027432 | 0.24497399 | 0.12682691 |
| Ni21 | 0.04123946 | 0.24439632 | 0.12532567 |
| Ni22 | 0.95628405 | 0.71481697 | 0.11500604 |
| Ni23 | 0.28545925 | 0.71198945 | 0.11437825 |
| Ni24 | 0.61863441 | 0.71017589 | 0.11383423 |
| Ni25 | 0.84100860 | 0.02352719 | 0.05894547 |
| Ni26 | 0.17633783 | 0.02155808 | 0.05777755 |
| Ni27 | 0.51271954 | 0.01854565 | 0.05487157 |
| Ni28 | 0.42165242 | 0.46996458 | 0.04934830 |
| Ni29 | 0.75389794 | 0.49873184 | 0.04974136 |
| Ni30 | 0.07147468 | 0.48202142 | 0.04881939 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56984875 | 0.41666865 | 0.25743790 |
| C4   | 0.30302454 | 0.80873244 | 0.22258838 |
| C5   | 0.03548671 | 0.19913189 | 0.18777237 |

|     |            |            |            |
|-----|------------|------------|------------|
| C6  | 0.76589160 | 0.59032223 | 0.15415850 |
| C7  | 0.49729705 | 0.97969630 | 0.11963874 |
| C8  | 0.23109794 | 0.37111420 | 0.08544821 |
| C9  | 0.96641603 | 0.76365162 | 0.05033950 |
| C10 | 0.70857272 | 0.17212363 | 0.02474878 |

## 5-C

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.96499841 | 0.91478689 | 0.98053214 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44741276 | 0.68700367 | 0.26403588 |
| Ni8  | 0.78270022 | 0.68191587 | 0.26045981 |
| Ni9  | 0.10829970 | 0.68611343 | 0.26077805 |
| Ni10 | 0.02772388 | 0.14991789 | 0.24996746 |
| Ni11 | 0.35481794 | 0.14902623 | 0.25266440 |
| Ni12 | 0.69156953 | 0.14723131 | 0.24919284 |
| Ni13 | 0.90676719 | 0.46210197 | 0.19510633 |
| Ni14 | 0.24674047 | 0.46613374 | 0.19412053 |
| Ni15 | 0.57628466 | 0.46697305 | 0.19324798 |
| Ni16 | 0.49009136 | 0.93058904 | 0.18349150 |
| Ni17 | 0.82076845 | 0.93506282 | 0.18411641 |
| Ni18 | 0.15749195 | 0.93102811 | 0.18231498 |
| Ni19 | 0.35538015 | 0.22739570 | 0.12693058 |
| Ni20 | 0.69257028 | 0.27604606 | 0.11834292 |
| Ni21 | 0.03423559 | 0.24766251 | 0.12405471 |
| Ni22 | 0.96517706 | 0.71352662 | 0.11938921 |
| Ni23 | 0.28249750 | 0.69382094 | 0.11542051 |
| Ni24 | 0.64245856 | 0.75608761 | 0.11425462 |
| Ni25 | 0.82237541 | 0.11130061 | 0.04968711 |
| Ni26 | 0.12955473 | 0.01388963 | 0.05834806 |
| Ni27 | 0.47904540 | 0.97812350 | 0.05824943 |
| Ni28 | 0.46388828 | 0.46833875 | 0.05452773 |
| Ni29 | 0.80558911 | 0.61479159 | 0.04913827 |
| Ni30 | 0.09350553 | 0.52555608 | 0.04936121 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56873126 | 0.41586413 | 0.25703571 |

|     |            |            |            |
|-----|------------|------------|------------|
| C4  | 0.30196143 | 0.80788082 | 0.22312219 |
| C5  | 0.03397882 | 0.20157838 | 0.18658638 |
| C6  | 0.76856992 | 0.59494046 | 0.15438599 |
| C7  | 0.48792259 | 0.97397363 | 0.12118129 |
| C8  | 0.23614125 | 0.36405523 | 0.08051909 |
| C9  | 0.94994650 | 0.90021978 | 0.01722530 |
| C10 | 0.64263494 | 0.29184141 | 0.04428682 |

## **6-C**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.01140984 | 0.23434405 | 0.02251933 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44806375 | 0.68740303 | 0.26409704 |
| Ni8  | 0.78381217 | 0.68297264 | 0.25996858 |
| Ni9  | 0.10983226 | 0.68670373 | 0.26083289 |
| Ni10 | 0.02792227 | 0.15088339 | 0.25017445 |
| Ni11 | 0.35627810 | 0.14847430 | 0.25269222 |
| Ni12 | 0.69374459 | 0.14805849 | 0.24857619 |
| Ni13 | 0.91162564 | 0.46844030 | 0.19391216 |
| Ni14 | 0.24807924 | 0.46506411 | 0.19449691 |
| Ni15 | 0.57677782 | 0.46442810 | 0.19381819 |
| Ni16 | 0.49070319 | 0.92995784 | 0.18273489 |
| Ni17 | 0.82094738 | 0.93171640 | 0.18235143 |
| Ni18 | 0.15638679 | 0.93035380 | 0.18272587 |
| Ni19 | 0.36837434 | 0.23726478 | 0.12779015 |
| Ni20 | 0.70739303 | 0.24234852 | 0.12399433 |
| Ni21 | 0.04246185 | 0.25334349 | 0.12510496 |
| Ni22 | 0.95533520 | 0.72922438 | 0.11528183 |
| Ni23 | 0.27654201 | 0.70765078 | 0.11810990 |
| Ni24 | 0.61918996 | 0.70778407 | 0.11418539 |
| Ni25 | 0.82549382 | 0.06818104 | 0.04928982 |
| Ni26 | 0.15622087 | 0.05723643 | 0.05480365 |
| Ni27 | 0.46744276 | 0.89904625 | 0.05494122 |
| Ni28 | 0.44957427 | 0.38512741 | 0.05062494 |
| Ni29 | 0.75693328 | 0.53980626 | 0.04593707 |
| Ni30 | 0.08138869 | 0.51993540 | 0.05016334 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |

|     |            |            |            |
|-----|------------|------------|------------|
| C2  | 0.83699679 | 0.02198082 | 0.28913693 |
| C3  | 0.57006218 | 0.41603459 | 0.25730328 |
| C4  | 0.30381738 | 0.80831321 | 0.22289708 |
| C5  | 0.03423355 | 0.19999128 | 0.18725099 |
| C6  | 0.76536714 | 0.58580279 | 0.15372616 |
| C7  | 0.49186332 | 0.97152807 | 0.11908351 |
| C8  | 0.24597400 | 0.39130862 | 0.08407310 |
| C9  | 0.95766045 | 0.79015917 | 0.05233086 |
| C10 | 0.62334433 | 0.20099518 | 0.03737137 |

### 7-C

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.55185864 | 0.55692019 | 0.00792431 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44830162 | 0.68648184 | 0.26375490 |
| Ni8  | 0.78449032 | 0.68252682 | 0.26013034 |
| Ni9  | 0.11308710 | 0.68849193 | 0.26061792 |
| Ni10 | 0.03105554 | 0.14868434 | 0.25068090 |
| Ni11 | 0.35721843 | 0.14693467 | 0.25249647 |
| Ni12 | 0.69417521 | 0.14730668 | 0.24859522 |
| Ni13 | 0.91672324 | 0.46691407 | 0.19552425 |
| Ni14 | 0.25274423 | 0.46829871 | 0.19238408 |
| Ni15 | 0.57645755 | 0.46432215 | 0.19425722 |
| Ni16 | 0.49121913 | 0.93173805 | 0.18190219 |
| Ni17 | 0.82587454 | 0.93190058 | 0.18310282 |
| Ni18 | 0.16382179 | 0.93125018 | 0.18089203 |
| Ni19 | 0.37259112 | 0.24103286 | 0.12334671 |
| Ni20 | 0.71188838 | 0.24243299 | 0.12928934 |
| Ni21 | 0.04775488 | 0.24651254 | 0.12621557 |
| Ni22 | 0.96047141 | 0.69634104 | 0.11631977 |
| Ni23 | 0.28545386 | 0.70640446 | 0.11231169 |
| Ni24 | 0.61692941 | 0.70249420 | 0.11584566 |
| Ni25 | 0.83956764 | 0.99501218 | 0.06920533 |
| Ni26 | 0.17243348 | 0.00653465 | 0.05984152 |
| Ni27 | 0.54477475 | 0.07474088 | 0.05626953 |
| Ni28 | 0.42891208 | 0.50503095 | 0.05087025 |
| Ni29 | 0.73730607 | 0.55254542 | 0.03240886 |



|      |            |            |            |
|------|------------|------------|------------|
| Ni30 | 0.02156117 | 0.43806437 | 0.04829700 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.57035308 | 0.41539483 | 0.25750119 |
| C4   | 0.30617452 | 0.80802872 | 0.22205377 |
| C5   | 0.04041268 | 0.19880911 | 0.18838916 |
| C6   | 0.76892827 | 0.58892599 | 0.15528746 |
| C7   | 0.49819049 | 0.97872308 | 0.11758189 |
| C8   | 0.22035667 | 0.37004185 | 0.07995988 |
| C9   | 0.96235414 | 0.75966766 | 0.05104230 |
| C10  | 0.76972400 | 0.22511891 | 0.03484184 |

### **8-C**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.53084531 | 0.37502882 | 0.01633450 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44846064 | 0.68587431 | 0.26382692 |
| Ni8  | 0.78457155 | 0.68216231 | 0.26019673 |
| Ni9  | 0.11376572 | 0.68763365 | 0.26057885 |
| Ni10 | 0.03141463 | 0.14811238 | 0.25083985 |
| Ni11 | 0.35767362 | 0.14609666 | 0.25248179 |
| Ni12 | 0.69401151 | 0.14677611 | 0.24854803 |
| Ni13 | 0.91704397 | 0.46608822 | 0.19557629 |
| Ni14 | 0.25266680 | 0.46780954 | 0.19243866 |
| Ni15 | 0.57628998 | 0.46402921 | 0.19420086 |
| Ni16 | 0.49146738 | 0.93055638 | 0.18144168 |
| Ni17 | 0.82568891 | 0.93031169 | 0.18322796 |
| Ni18 | 0.16369470 | 0.93019577 | 0.18116887 |
| Ni19 | 0.37380979 | 0.23956839 | 0.12400129 |
| Ni20 | 0.71269554 | 0.24038687 | 0.12956591 |
| Ni21 | 0.04803076 | 0.24279849 | 0.12643857 |
| Ni22 | 0.96090241 | 0.69315651 | 0.11646560 |
| Ni23 | 0.28576825 | 0.70676124 | 0.11308533 |
| Ni24 | 0.61864081 | 0.70360799 | 0.11544829 |
| Ni25 | 0.84119570 | 0.99188202 | 0.06937987 |
| Ni26 | 0.17509990 | 0.00737945 | 0.06019114 |
| Ni27 | 0.55360158 | 0.09040343 | 0.05470786 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni28 | 0.42752084 | 0.51166321 | 0.05173149 |
| Ni29 | 0.74279647 | 0.54820976 | 0.03318874 |
| Ni30 | 0.02741365 | 0.43697594 | 0.04786122 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.57056168 | 0.41499889 | 0.25747669 |
| C4   | 0.30739554 | 0.80775830 | 0.22196690 |
| C5   | 0.04034600 | 0.19745939 | 0.18863154 |
| C6   | 0.76884086 | 0.58740636 | 0.15537612 |
| C7   | 0.49938904 | 0.97898854 | 0.11621283 |
| C8   | 0.22269539 | 0.36954117 | 0.08116135 |
| C9   | 0.96614034 | 0.75822667 | 0.05146512 |
| C10  | 0.78415815 | 0.22579978 | 0.03381755 |

### **9-C**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.26541067 | 0.56180946 | 0.01348403 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44703457 | 0.68610102 | 0.26405159 |
| Ni8  | 0.78377597 | 0.68303742 | 0.25994584 |
| Ni9  | 0.10951643 | 0.68502711 | 0.26064822 |
| Ni10 | 0.02896822 | 0.14985735 | 0.25026379 |
| Ni11 | 0.35644074 | 0.14682461 | 0.25259182 |
| Ni12 | 0.69445146 | 0.14859357 | 0.24864802 |
| Ni13 | 0.91372905 | 0.46784517 | 0.19394176 |
| Ni14 | 0.24876722 | 0.46394798 | 0.19344885 |
| Ni15 | 0.57672679 | 0.46693011 | 0.19409893 |
| Ni16 | 0.49101910 | 0.92995226 | 0.18351751 |
| Ni17 | 0.82193759 | 0.92938370 | 0.18245263 |
| Ni18 | 0.15750851 | 0.92821673 | 0.18169876 |
| Ni19 | 0.37567157 | 0.24497780 | 0.12643664 |
| Ni20 | 0.70905371 | 0.24028564 | 0.12711433 |
| Ni21 | 0.03747402 | 0.24201480 | 0.12490897 |
| Ni22 | 0.95407454 | 0.70773133 | 0.11393799 |
| Ni23 | 0.28256659 | 0.70634567 | 0.11643810 |
| Ni24 | 0.61709351 | 0.70438933 | 0.11368440 |
| Ni25 | 0.83472465 | 0.01834493 | 0.05769132 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni26 | 0.16921654 | 0.01574132 | 0.05909527 |
| Ni27 | 0.50062268 | 0.02058817 | 0.05690555 |
| Ni28 | 0.40938671 | 0.49330055 | 0.04693488 |
| Ni29 | 0.75158617 | 0.48855088 | 0.04962718 |
| Ni30 | 0.08850225 | 0.49634455 | 0.04523762 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56985472 | 0.41553536 | 0.25740963 |
| C4   | 0.30254002 | 0.80604163 | 0.22263911 |
| C5   | 0.03501299 | 0.19761541 | 0.18762011 |
| C6   | 0.76541504 | 0.58696451 | 0.15387562 |
| C7   | 0.49590906 | 0.97377232 | 0.12033565 |
| C8   | 0.22961378 | 0.36469312 | 0.08589254 |
| C9   | 0.96185727 | 0.75787652 | 0.04931906 |
| C10  | 0.69151990 | 0.15985452 | 0.02514602 |

#### **10-C**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.96827081 | 0.79911666 | 0.99111353 |
| Ni1  | 0.98384405 | 0.90306438 | 0.32944171 |
| Ni2  | 0.31884581 | 0.90021698 | 0.32856616 |
| Ni3  | 0.64789318 | 0.90021698 | 0.32856616 |
| Ni4  | 0.56301050 | 0.36520516 | 0.31780098 |
| Ni5  | 0.89205787 | 0.36520516 | 0.31780098 |
| Ni6  | 0.22705959 | 0.36235756 | 0.31692543 |
| Ni7  | 0.44659619 | 0.68563061 | 0.26400672 |
| Ni8  | 0.78319974 | 0.68198235 | 0.26043461 |
| Ni9  | 0.10934513 | 0.68622956 | 0.26071115 |
| Ni10 | 0.02920732 | 0.14938943 | 0.25010343 |
| Ni11 | 0.35564044 | 0.14662792 | 0.25246413 |
| Ni12 | 0.69300346 | 0.14695892 | 0.24887108 |
| Ni13 | 0.91207174 | 0.46348009 | 0.19541573 |
| Ni14 | 0.24852404 | 0.46551143 | 0.19307068 |
| Ni15 | 0.57624823 | 0.46652243 | 0.19416252 |
| Ni16 | 0.49042240 | 0.92670811 | 0.18337375 |
| Ni17 | 0.82231990 | 0.93087156 | 0.18336181 |
| Ni18 | 0.15983786 | 0.92944353 | 0.18116978 |
| Ni19 | 0.37194572 | 0.24274120 | 0.12622568 |
| Ni20 | 0.70908534 | 0.24273598 | 0.12732265 |
| Ni21 | 0.04161289 | 0.23966373 | 0.12451192 |
| Ni22 | 0.95365837 | 0.70783471 | 0.11654398 |
| Ni23 | 0.28237587 | 0.70727035 | 0.11329496 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni24 | 0.62533410 | 0.71487106 | 0.11452908 |
| Ni25 | 0.83510850 | 0.01798887 | 0.05607696 |
| Ni26 | 0.15470439 | 0.00494871 | 0.06113498 |
| Ni27 | 0.50221690 | 0.01866825 | 0.05757088 |
| Ni28 | 0.43789405 | 0.49584586 | 0.05147350 |
| Ni29 | 0.76424768 | 0.50562623 | 0.05070022 |
| Ni30 | 0.06998648 | 0.49679961 | 0.05072002 |
| C1   | 0.10545183 | 0.63271097 | 0.32318355 |
| C2   | 0.83699679 | 0.02198082 | 0.28913693 |
| C3   | 0.56898842 | 0.41526183 | 0.25740080 |
| C4   | 0.30186363 | 0.80561992 | 0.22266153 |
| C5   | 0.03607719 | 0.19802555 | 0.18703108 |
| C6   | 0.76825972 | 0.58773778 | 0.15502277 |
| C7   | 0.49554280 | 0.97506277 | 0.12067224 |
| C8   | 0.23557307 | 0.36495465 | 0.08196800 |
| C9   | 0.96321844 | 0.78153005 | 0.02815234 |
| C10  | 0.69232384 | 0.17823251 | 0.02665322 |

### **1-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.50412626 | 0.05578568 | 0.35118107 |
| Ni1  | 0.00443911 | 0.89955227 | 0.32375263 |
| Ni2  | 0.31754059 | 0.89048946 | 0.32386140 |
| Ni3  | 0.63242366 | 0.88809440 | 0.32371685 |
| Ni4  | 0.54706052 | 0.34252785 | 0.31578825 |
| Ni5  | 0.89908951 | 0.36811338 | 0.31451297 |
| Ni6  | 0.22748588 | 0.34765658 | 0.31492201 |
| Ni7  | 0.44404112 | 0.66806619 | 0.25955747 |
| Ni8  | 0.78011164 | 0.67201832 | 0.26112797 |
| Ni9  | 0.11124594 | 0.67136121 | 0.25894703 |
| Ni10 | 0.02234973 | 0.13670717 | 0.24853865 |
| Ni11 | 0.35240005 | 0.13713921 | 0.24791660 |
| Ni12 | 0.69462740 | 0.13707005 | 0.24765172 |
| Ni13 | 0.90907149 | 0.45694942 | 0.19319104 |
| Ni14 | 0.24404216 | 0.45347833 | 0.19022336 |
| Ni15 | 0.57492532 | 0.45488224 | 0.19210738 |
| Ni16 | 0.48957051 | 0.91849826 | 0.18120201 |
| Ni17 | 0.81767787 | 0.91875252 | 0.18136334 |
| Ni18 | 0.15450323 | 0.91872754 | 0.17898268 |
| Ni19 | 0.37320044 | 0.23680726 | 0.12473402 |
| Ni20 | 0.70972948 | 0.23406364 | 0.12468947 |
| Ni21 | 0.04001719 | 0.23663554 | 0.12331676 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni22 | 0.95378560 | 0.69920063 | 0.11342172 |
| Ni23 | 0.28276264 | 0.70149555 | 0.11244190 |
| Ni24 | 0.61772378 | 0.69725886 | 0.11163193 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11571767 | 0.61447059 | 0.32417936 |
| C2   | 0.83395876 | 0.01309309 | 0.29173101 |
| C3   | 0.56830103 | 0.40041316 | 0.25522177 |
| C4   | 0.29796908 | 0.79318304 | 0.21974299 |
| C5   | 0.03039773 | 0.18642301 | 0.18595145 |
| C6   | 0.76333718 | 0.57816790 | 0.15245177 |
| C7   | 0.49666476 | 0.96797989 | 0.11858305 |
| C8   | 0.23135602 | 0.36026449 | 0.08232914 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

## **2-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.37267448 | 0.21719232 | 0.34742320 |
| Ni1  | 0.00253829 | 0.90585713 | 0.32413284 |
| Ni2  | 0.31736013 | 0.90482114 | 0.32360692 |
| Ni3  | 0.63352647 | 0.88975791 | 0.32368733 |
| Ni4  | 0.55479196 | 0.35177170 | 0.31580386 |
| Ni5  | 0.90081101 | 0.37308291 | 0.31460257 |
| Ni6  | 0.23333711 | 0.36179050 | 0.31736117 |
| Ni7  | 0.44628358 | 0.67964942 | 0.25976015 |
| Ni8  | 0.78108775 | 0.67478283 | 0.26092564 |
| Ni9  | 0.11171032 | 0.67354327 | 0.25905881 |
| Ni10 | 0.02250936 | 0.13988872 | 0.24870728 |
| Ni11 | 0.35240095 | 0.14251192 | 0.24795849 |
| Ni12 | 0.69346651 | 0.14134940 | 0.24814308 |
| Ni13 | 0.90894596 | 0.45878630 | 0.19315850 |
| Ni14 | 0.24464056 | 0.45755363 | 0.19054383 |
| Ni15 | 0.57433058 | 0.45876818 | 0.19209000 |
| Ni16 | 0.48998182 | 0.92283510 | 0.18109522 |
| Ni17 | 0.81820589 | 0.92220585 | 0.18149720 |
| Ni18 | 0.15482790 | 0.92162681 | 0.17891258 |
| Ni19 | 0.37363011 | 0.23865027 | 0.12475416 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni20 | 0.70980339 | 0.23708471 | 0.12480927 |
| Ni21 | 0.04038146 | 0.23872982 | 0.12345057 |
| Ni22 | 0.95381775 | 0.70139342 | 0.11351628 |
| Ni23 | 0.28301016 | 0.70255885 | 0.11239174 |
| Ni24 | 0.61843844 | 0.69948627 | 0.11155939 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11612704 | 0.62471729 | 0.32424965 |
| C2   | 0.83280342 | 0.01663687 | 0.29184664 |
| C3   | 0.56783647 | 0.40690631 | 0.25500414 |
| C4   | 0.29816368 | 0.79813700 | 0.21973252 |
| C5   | 0.03128077 | 0.18958129 | 0.18623501 |
| C6   | 0.76328277 | 0.58124927 | 0.15261092 |
| C7   | 0.49706856 | 0.96963343 | 0.11854363 |
| C8   | 0.23161851 | 0.36071348 | 0.08237101 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

### **3-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.68890364 | 0.23079411 | 0.34808040 |
| Ni1  | 0.00120209 | 0.89755041 | 0.32371879 |
| Ni2  | 0.31353220 | 0.89131683 | 0.32326253 |
| Ni3  | 0.63820170 | 0.91328334 | 0.32438509 |
| Ni4  | 0.54845395 | 0.35747357 | 0.31626767 |
| Ni5  | 0.89191311 | 0.36094995 | 0.31787751 |
| Ni6  | 0.22477137 | 0.34787125 | 0.31499922 |
| Ni7  | 0.44488129 | 0.67324104 | 0.26068091 |
| Ni8  | 0.78090569 | 0.67684961 | 0.25958371 |
| Ni9  | 0.10969799 | 0.66852272 | 0.25919915 |
| Ni10 | 0.02382290 | 0.14023278 | 0.24854955 |
| Ni11 | 0.35363493 | 0.13865275 | 0.24943498 |
| Ni12 | 0.69582315 | 0.14234313 | 0.24686242 |
| Ni13 | 0.91050696 | 0.45884686 | 0.19297845 |
| Ni14 | 0.24552210 | 0.45704240 | 0.19076985 |
| Ni15 | 0.57478731 | 0.45727789 | 0.19224150 |
| Ni16 | 0.48895693 | 0.92133479 | 0.18144989 |
| Ni17 | 0.81927071 | 0.92111793 | 0.18102983 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni18 | 0.15628367 | 0.92110698 | 0.17927390 |
| Ni19 | 0.37322358 | 0.23779486 | 0.12478774 |
| Ni20 | 0.70948815 | 0.23573309 | 0.12486186 |
| Ni21 | 0.04042949 | 0.23818628 | 0.12335107 |
| Ni22 | 0.95431838 | 0.70080976 | 0.11345143 |
| Ni23 | 0.28300517 | 0.70172586 | 0.11247256 |
| Ni24 | 0.61806616 | 0.69883078 | 0.11179963 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11229649 | 0.61396083 | 0.32441360 |
| C2   | 0.83603693 | 0.01451226 | 0.29011657 |
| C3   | 0.56908173 | 0.40508898 | 0.25539322 |
| C4   | 0.29838172 | 0.79684943 | 0.22037851 |
| C5   | 0.03232922 | 0.18905963 | 0.18586370 |
| C6   | 0.76374676 | 0.57959784 | 0.15252021 |
| C7   | 0.49660656 | 0.96907963 | 0.11869367 |
| C8   | 0.23155973 | 0.36064065 | 0.08230429 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

#### **4-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.20484565 | 0.09398639 | 0.35058549 |
| Ni1  | 0.00641505 | 0.90487448 | 0.32490895 |
| Ni2  | 0.31491118 | 0.89769922 | 0.32401955 |
| Ni3  | 0.63017402 | 0.88276626 | 0.32314183 |
| Ni4  | 0.55325284 | 0.34767013 | 0.31544842 |
| Ni5  | 0.89739118 | 0.36850698 | 0.31448670 |
| Ni6  | 0.23264492 | 0.35814429 | 0.31601152 |
| Ni7  | 0.44463283 | 0.67211702 | 0.26018674 |
| Ni8  | 0.78420204 | 0.67433346 | 0.26052159 |
| Ni9  | 0.11095071 | 0.66628017 | 0.25844069 |
| Ni10 | 0.02296067 | 0.13513409 | 0.24856120 |
| Ni11 | 0.35478099 | 0.13637440 | 0.24852170 |
| Ni12 | 0.69546733 | 0.13719831 | 0.24810754 |
| Ni13 | 0.91001531 | 0.45510272 | 0.19285064 |
| Ni14 | 0.24610929 | 0.45310793 | 0.19064895 |
| Ni15 | 0.57621148 | 0.45516992 | 0.19244962 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni16 | 0.49078970 | 0.92030759 | 0.18118238 |
| Ni17 | 0.81881480 | 0.91843851 | 0.18141385 |
| Ni18 | 0.15611220 | 0.91805286 | 0.17888213 |
| Ni19 | 0.37407961 | 0.23743085 | 0.12471550 |
| Ni20 | 0.71019703 | 0.23384721 | 0.12478467 |
| Ni21 | 0.04097114 | 0.23701435 | 0.12348502 |
| Ni22 | 0.95412380 | 0.69963783 | 0.11345078 |
| Ni23 | 0.28320847 | 0.70157513 | 0.11240016 |
| Ni24 | 0.61802669 | 0.69672636 | 0.11169798 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11345617 | 0.61623192 | 0.32312863 |
| C2   | 0.83327111 | 0.01111996 | 0.29233067 |
| C3   | 0.57059205 | 0.40335549 | 0.25545673 |
| C4   | 0.29918219 | 0.79418851 | 0.21966717 |
| C5   | 0.03230293 | 0.18549719 | 0.18617548 |
| C6   | 0.76367492 | 0.57798410 | 0.15247796 |
| C7   | 0.49721191 | 0.96787811 | 0.11855311 |
| C8   | 0.23184200 | 0.36015101 | 0.08236438 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

### **5-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.44631879 | 0.60920698 | 0.33340989 |
| Ni1  | 0.00974147 | 0.90214897 | 0.32385692 |
| Ni2  | 0.32204968 | 0.88254065 | 0.32419383 |
| Ni3  | 0.63452649 | 0.88692208 | 0.32350618 |
| Ni4  | 0.55321380 | 0.35149201 | 0.31579443 |
| Ni5  | 0.90206356 | 0.36418488 | 0.31484970 |
| Ni6  | 0.23387659 | 0.35082214 | 0.31730032 |
| Ni7  | 0.44895688 | 0.67217559 | 0.25903719 |
| Ni8  | 0.78551445 | 0.67252937 | 0.25992292 |
| Ni9  | 0.11363107 | 0.66779389 | 0.25915114 |
| Ni10 | 0.02687969 | 0.13767147 | 0.24874705 |
| Ni11 | 0.35533708 | 0.13454480 | 0.24945409 |
| Ni12 | 0.69668657 | 0.13639247 | 0.24856054 |
| Ni13 | 0.91223708 | 0.45625756 | 0.19305608 |



|      |            |            |            |
|------|------------|------------|------------|
| Ni14 | 0.24776463 | 0.45302883 | 0.19063625 |
| Ni15 | 0.57691705 | 0.45322482 | 0.19209498 |
| Ni16 | 0.49150893 | 0.92098592 | 0.18124944 |
| Ni17 | 0.81997631 | 0.91917377 | 0.18148181 |
| Ni18 | 0.15726451 | 0.91843951 | 0.17908665 |
| Ni19 | 0.37442692 | 0.23696038 | 0.12458894 |
| Ni20 | 0.71105350 | 0.23437990 | 0.12466669 |
| Ni21 | 0.04125357 | 0.23778408 | 0.12354551 |
| Ni22 | 0.95518736 | 0.69951299 | 0.11344872 |
| Ni23 | 0.28402658 | 0.70107437 | 0.11246710 |
| Ni24 | 0.61930852 | 0.69759432 | 0.11187798 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11537625 | 0.61420292 | 0.32453408 |
| C2   | 0.83766965 | 0.00949818 | 0.29177818 |
| C3   | 0.57264162 | 0.40091298 | 0.25491511 |
| C4   | 0.29993985 | 0.79394024 | 0.21975902 |
| C5   | 0.03357348 | 0.18607636 | 0.18618336 |
| C6   | 0.76537913 | 0.57770940 | 0.15260083 |
| C7   | 0.49787581 | 0.96805906 | 0.11857556 |
| C8   | 0.23179533 | 0.36021421 | 0.08232841 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |

## **6-Ni**

|      |            |            |            |
|------|------------|------------|------------|
| H1   | 0.11511135 | 0.59403163 | 0.37650872 |
| Ni1  | 0.00411102 | 0.90343513 | 0.32238162 |
| Ni2  | 0.31175533 | 0.89357466 | 0.32214308 |
| Ni3  | 0.62514524 | 0.88407307 | 0.32251664 |
| Ni4  | 0.54400954 | 0.34657115 | 0.31490571 |
| Ni5  | 0.90258946 | 0.37821119 | 0.31284130 |
| Ni6  | 0.22395287 | 0.35734688 | 0.31420473 |
| Ni7  | 0.44034230 | 0.67190300 | 0.26005834 |
| Ni8  | 0.78272559 | 0.67689405 | 0.26080109 |
| Ni9  | 0.11402625 | 0.67368548 | 0.25877953 |
| Ni10 | 0.02210752 | 0.14455959 | 0.24872470 |
| Ni11 | 0.35246353 | 0.13977764 | 0.24785946 |

|      |            |            |            |
|------|------------|------------|------------|
| Ni12 | 0.69232874 | 0.14012351 | 0.24787308 |
| Ni13 | 0.90926645 | 0.45882069 | 0.19320274 |
| Ni14 | 0.24496010 | 0.45429983 | 0.19023927 |
| Ni15 | 0.57433024 | 0.45967837 | 0.19209624 |
| Ni16 | 0.48913275 | 0.91991780 | 0.18118456 |
| Ni17 | 0.81792456 | 0.92051357 | 0.18175096 |
| Ni18 | 0.15420894 | 0.92097863 | 0.17865874 |
| Ni19 | 0.37395595 | 0.23847102 | 0.12454540 |
| Ni20 | 0.71012141 | 0.23567347 | 0.12499188 |
| Ni21 | 0.03956487 | 0.23738565 | 0.12334669 |
| Ni22 | 0.95392160 | 0.70002294 | 0.11344054 |
| Ni23 | 0.28314858 | 0.70195743 | 0.11235725 |
| Ni24 | 0.61834804 | 0.69908797 | 0.11162699 |
| Ni25 | 0.83620369 | 0.01722221 | 0.05706870 |
| Ni26 | 0.17120541 | 0.01437460 | 0.05619315 |
| Ni27 | 0.50025278 | 0.01437460 | 0.05619315 |
| Ni28 | 0.41537012 | 0.47936289 | 0.04542798 |
| Ni29 | 0.74441749 | 0.47936289 | 0.04542798 |
| Ni30 | 0.07941921 | 0.47651529 | 0.04455243 |
| C1   | 0.11262205 | 0.61234973 | 0.33912001 |
| C2   | 0.82908694 | 0.01767958 | 0.29256541 |
| C3   | 0.56881200 | 0.40769880 | 0.25502099 |
| C4   | 0.29576408 | 0.79545256 | 0.21927699 |
| C5   | 0.03055952 | 0.18829410 | 0.18613006 |
| C6   | 0.76356827 | 0.58027489 | 0.15253709 |
| C7   | 0.49706270 | 0.96929551 | 0.11860338 |
| C8   | 0.23136333 | 0.36044903 | 0.08236338 |
| C9   | 0.95781144 | 0.74686870 | 0.05081058 |
| C10  | 0.68935642 | 0.13613855 | 0.01676396 |