

**Supplementary Information for
Journal of Materials Chemistry A**

**Synergistic Core-shell Interactions Enable
Ultra-low Overpotentials for Enhanced CO₂
Electro-reduction Activity**

Rafia Ahmad and Abhishek K. Singh*

Materials Research Centre, Indian Institute of Science, Bangalore 560012, India

E-mail: abhishek@iisc.ac.in

*To whom correspondence should be addressed

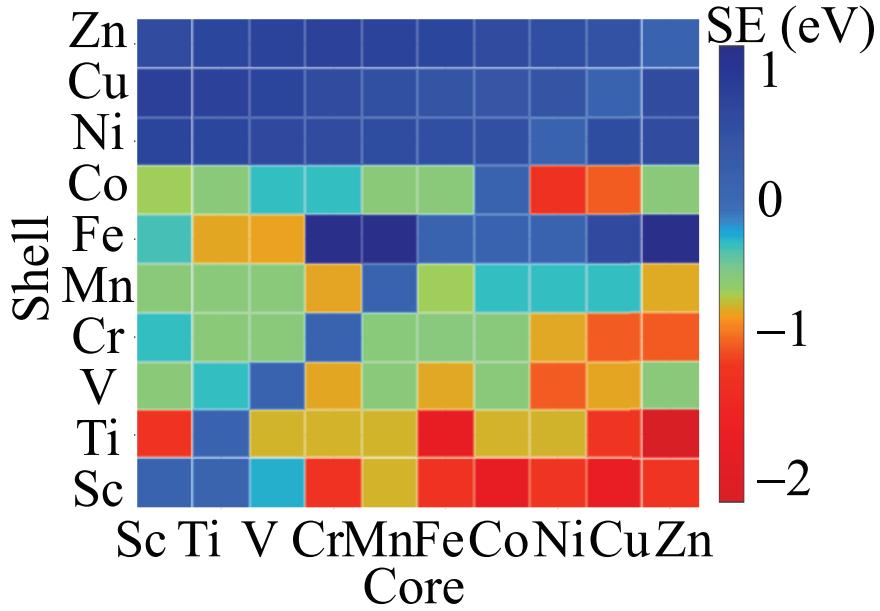


Figure S1: Color-coded matrix of segregation energies for impurity in 55-atom bimetallic core–shell nanoclusters ($\text{TM}_{13}@\text{TM}_{42}$) composed of 10 3d-TMs. The right diagonal represents the single component 55-atom cluster of TMs, thereby, showing zero segregation energy.

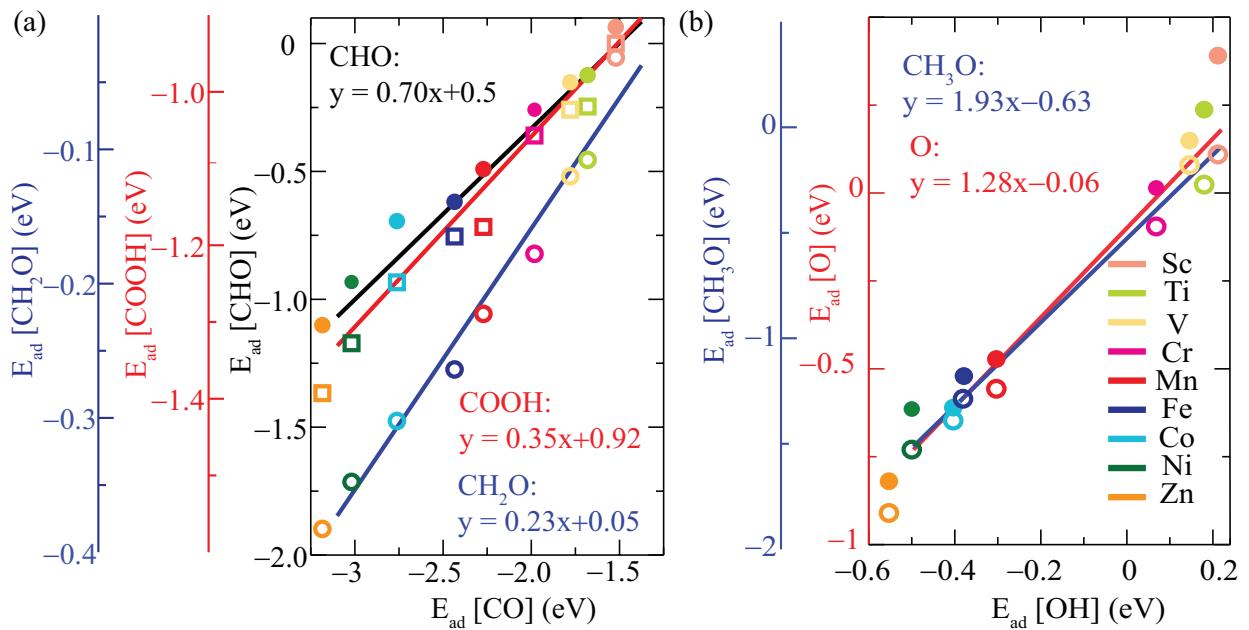


Figure S2: Adsorption energy correlation of (a) C bound intermediates with CO adsorption energy and (b) O bound intermediates with OH adsorption energy, for $\text{TM}_{13}@\text{Cu}_{42}$. The C and O bound intermediates correlate strongly with CO and OH adsorption energies. In (a) The filled circles, empty squares, and empty circles denote adsorption energies of CHO, COOH, and CH_2O , respectively. In (b) The filled circles and empty circles denote adsorption energies of O and CH_3O , respectively.

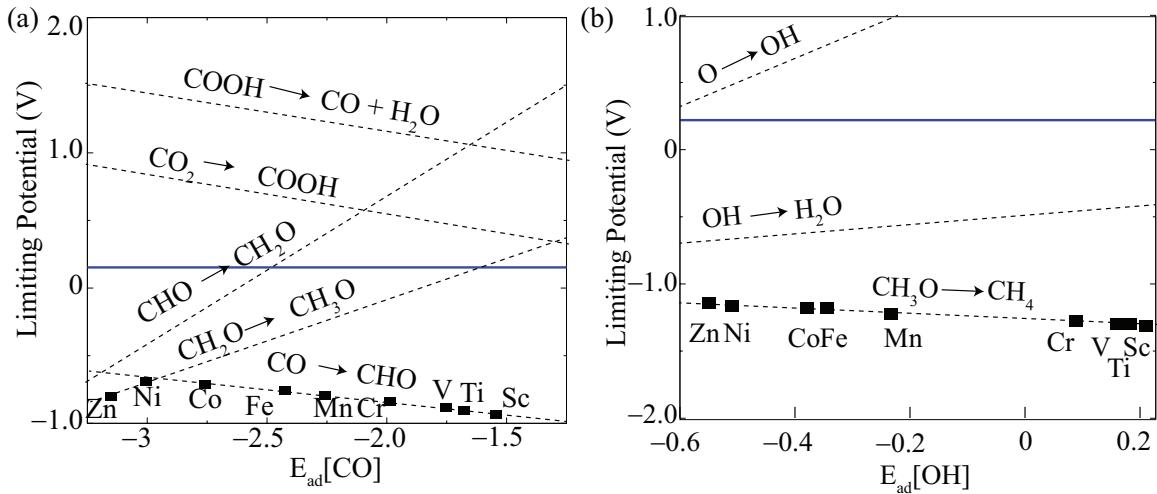


Figure S3: Limiting potentials for (a) C bound and (b) O bound intermediates reactions as a function of CO and OH adsorption energy, on $TM_{13}@\text{Cu}_{42}$.

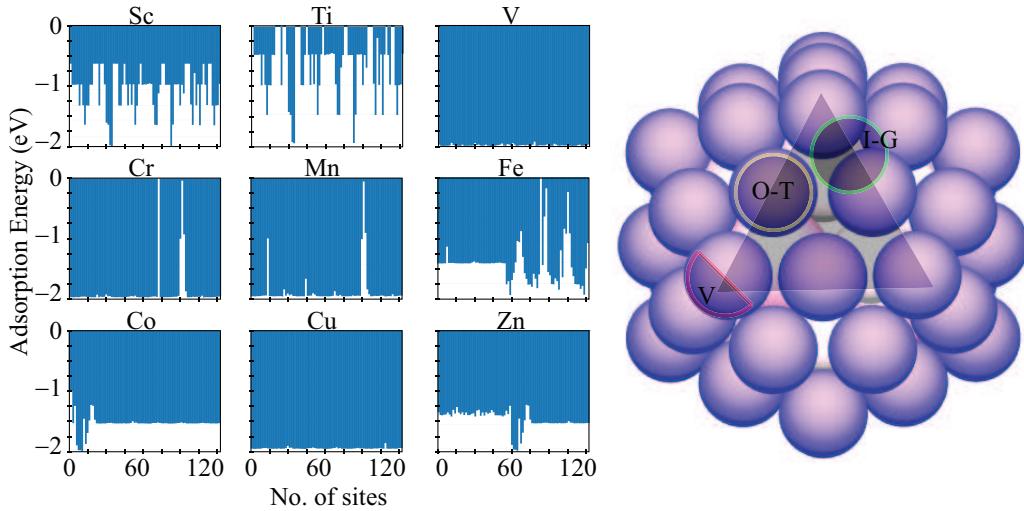


Figure S4: A complete scan of all the possible adsorption sites (on-top, interstitial, and vertex) of CO_2 for identifying the catalytically active sites on $\text{TM}_6\text{Ni}_7@\text{Cu}_{42}$. TM are all the 3d transition metals. It is seen that the adsorption energy for CO_2 is uniform for all the TMs except for Sc and Ti. Sc also, can be a good trimetallic component as it exhibits activity on all sites, where CO_2 adsorbs in the range of -0.5 to -2.0 eV. The structure is a representation of the general 55 atom icosahedral core–shell cluster. The gray shaded triangle represents one of the twenty fcc (111) surfaces of the cluster. The red, yellow, and green atoms depict vertex (V), on-top (O-T), and in-gap (I-G) type of adsorption sites.

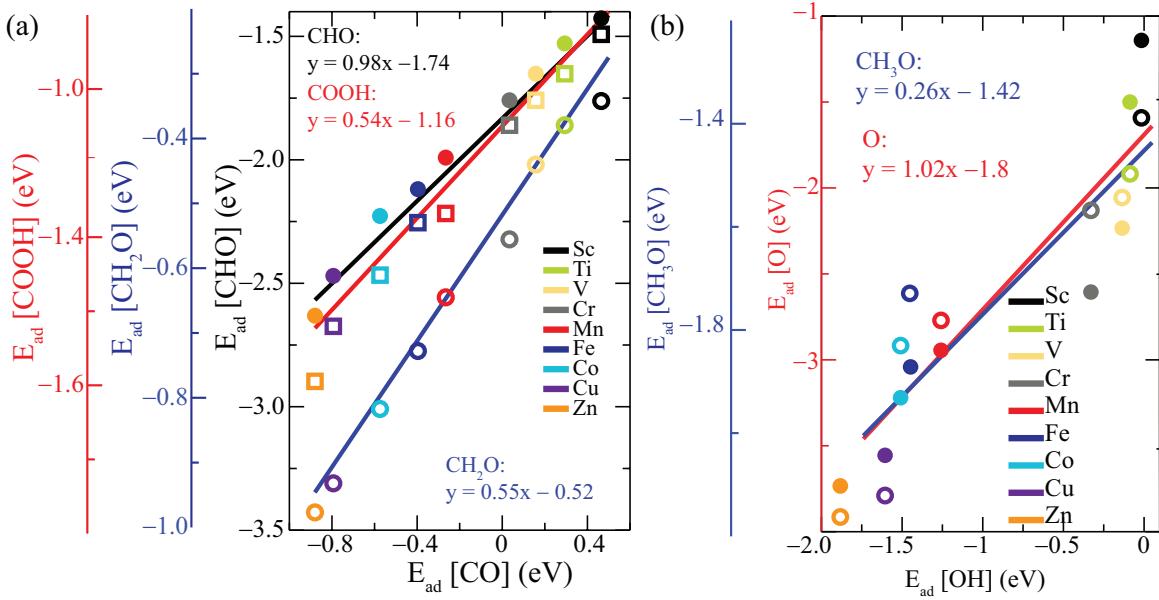


Figure S5: (a) Adsorption energy correlation for C bound intermediates as a function of CO adsorption energy on $\text{TM}_3\text{Ni}_{10}\text{@Cu}_{42}$. The filled circles, empty squares, and empty circles denote adsorption energies of CHO, COOH, and CH_2O , respectively. The C bound intermediates correlate strongly with CO adsorption energy. CO binds very weakly on the cluster as compared to CHO, which can be seen from the slope of the correlation line. (b) Adsorption energy correlation for O bound intermediates as a function of OH adsorption energy on $\text{TM}_3\text{Ni}_{10}\text{@Cu}_{42}$. The filled circles and empty circles denote adsorption energies of O and CH_3O , respectively. Intermediate range of adsorption energy dependence, shows that O bound intermediates will not be dominant descriptors of the energy profile.

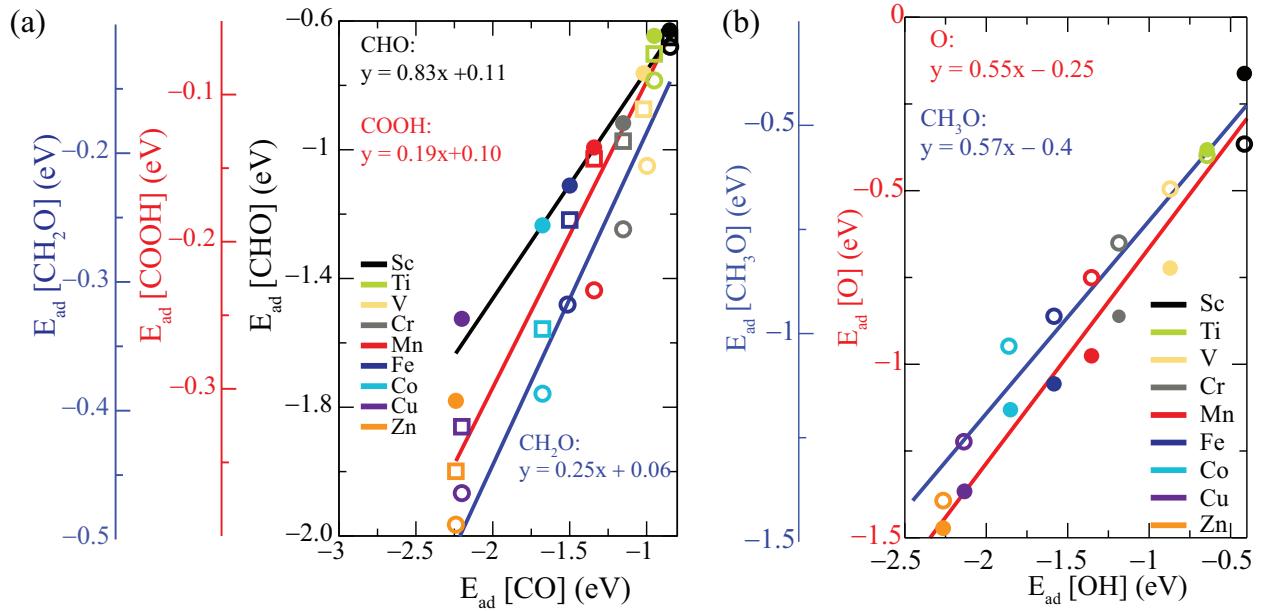


Figure S6: (a) Adsorption energy correlation for C bound intermediates as a function of CO adsorption energy $\text{TM}_9\text{Ni}_4@\text{Cu}_{42}$. The filled circles, empty squares, and empty circles denote adsorption energies of CHO, COOH, and CH_2O , respectively. The C bound intermediates correlate strongly with CO adsorption energy. CO binds very strongly on the cluster as compared to CHO, which can be seen from the slope of the correlation line. (b) Adsorption energy correlation for O bound intermediates as a function of OH adsorption energy on (b) $\text{TM}_9\text{Ni}_{10}@\text{Cu}_{42}$. The filled circles and empty circles denote adsorption energies of O and CH_3O , respectively.

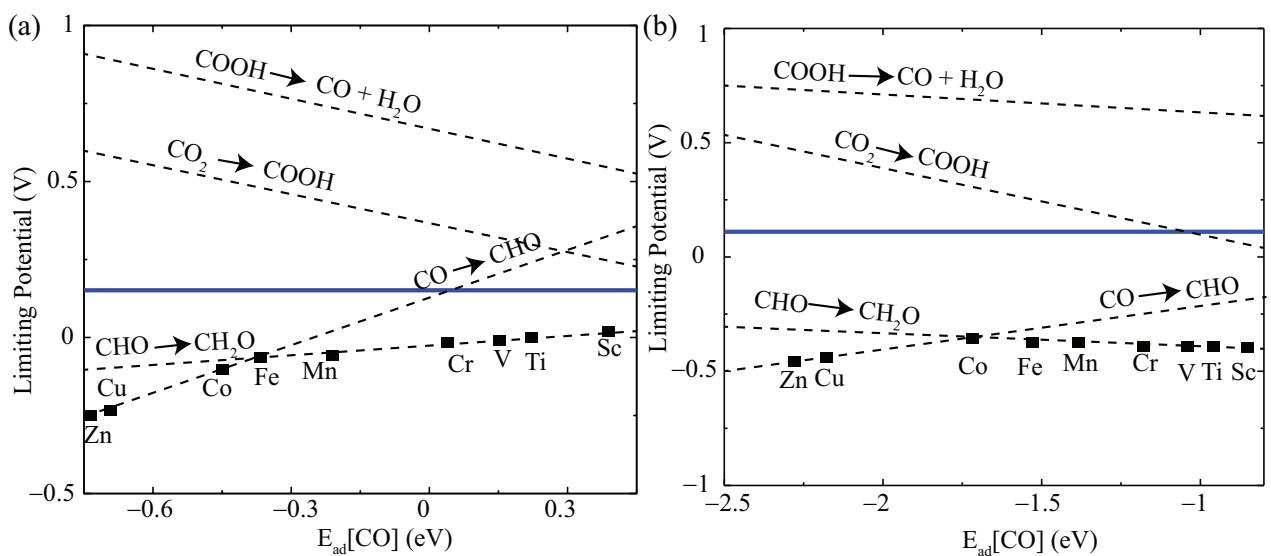


Figure S7: Limiting potentials for C bound intermediates reaction as a function of CO adsorption energy on (a) $\text{TM}_3\text{Ni}_{10}@\text{Cu}_{42}$ and (b) $\text{TM}_9\text{Ni}_4@\text{Cu}_{42}$.

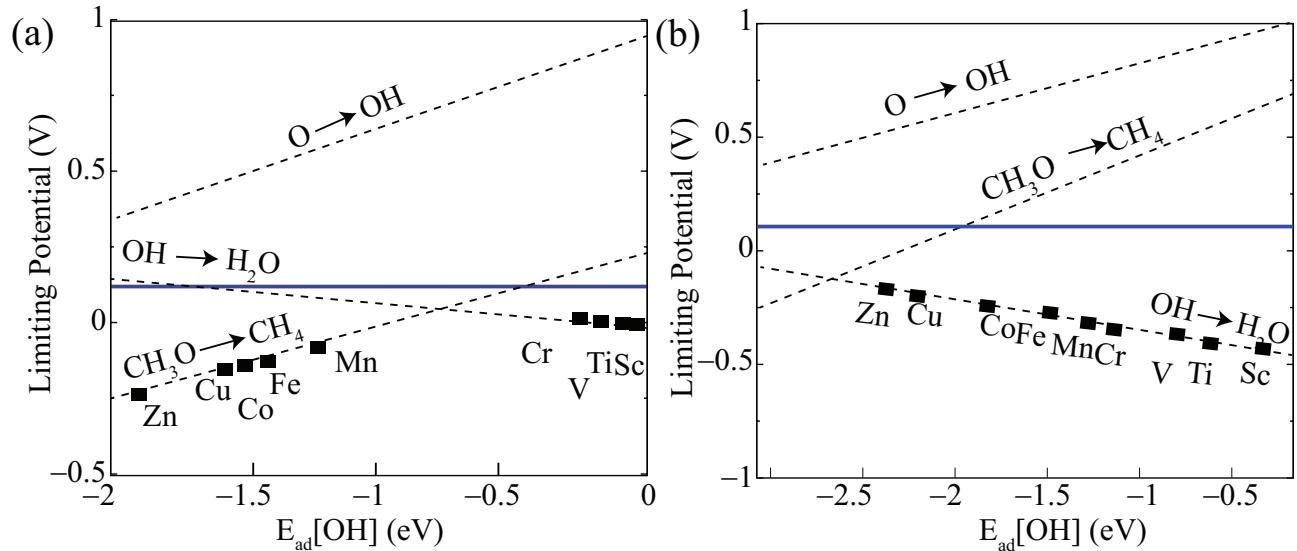


Figure S8: Limiting potentials for O bound intermediates reaction as a function of OH adsorption energy on (a) $\text{TM}_3\text{Ni}_{10}\text{@Cu}_{42}$, (b) $\text{TM}_6\text{Ni}_7\text{@Cu}_{42}$, and (c) $\text{TM}_9\text{Ni}_4\text{@Cu}_{42}$.

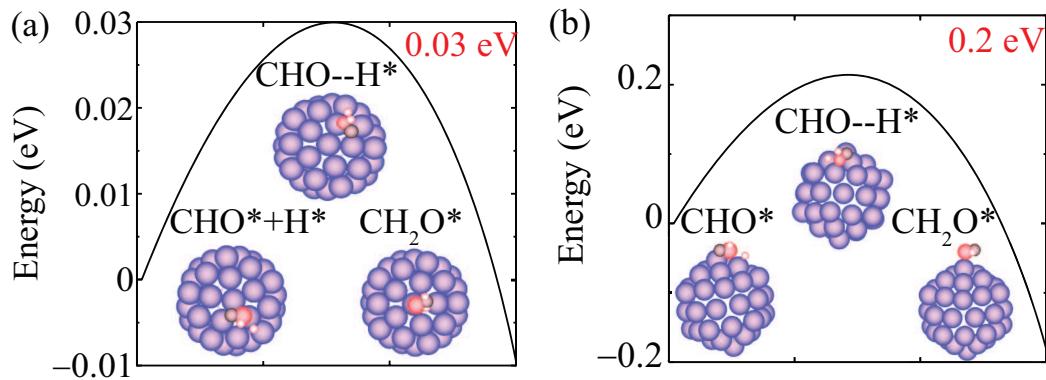


Figure S9: L-H mechanism reaction pathway and NEB barrier for CHO reduction on $\text{Sc}_3\text{Ni}_{10}\text{@Cu}_{42}$ and $\text{Sc}_9\text{Ni}_4\text{@Cu}_{42}$. IS is the starting point of reduction (referenced arbitrarily at zero). TS is the first transition state and FS is the final step. Purple, pink, red, and brown atoms represent Cu, H, O, and C, respectively.

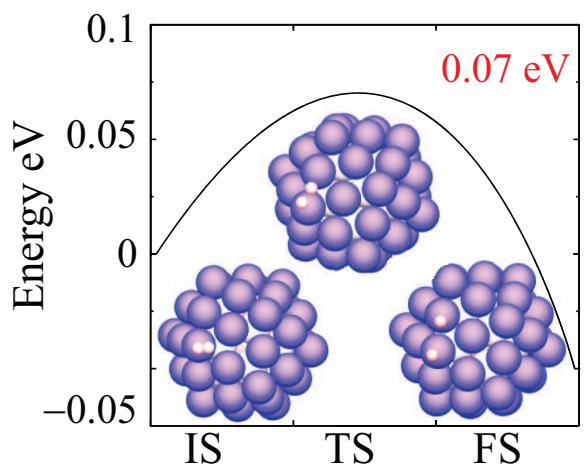


Figure S10: NEB reaction barrier with reaction profile of H₂ cleavage on Sc₆Ni₇–Cu₄₂. IS, TS, and FS denote initial, transition, and final structures. Purple and pink spheres depict Cu and H atoms, respectively.

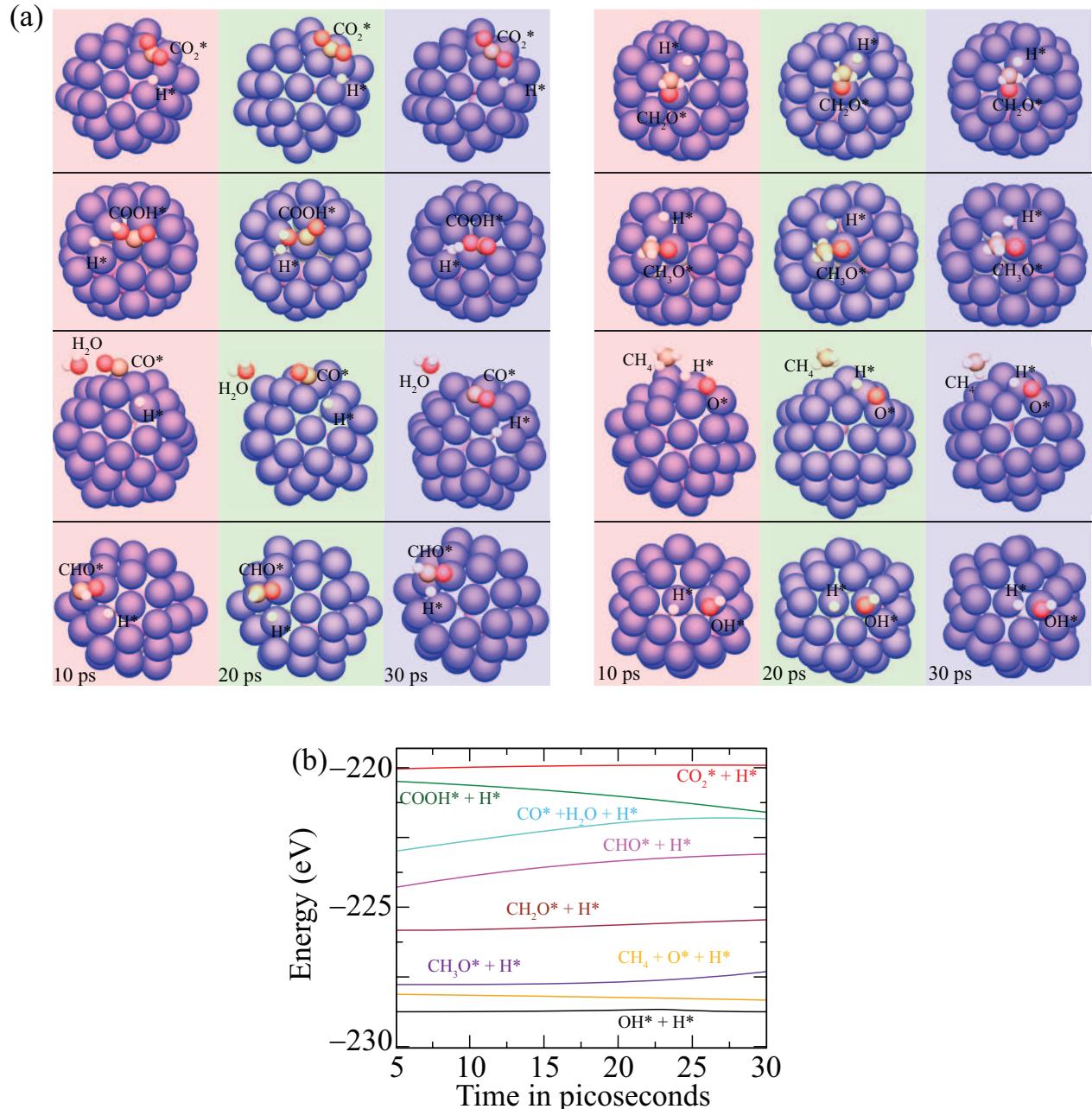


Figure S11: *Ab – initio* molecular dynamics (AIMD) calculations for CO_2 reduction reaction intermediates on $\text{Sc}_6\text{Ni}_7\text{–Cu}_{42}$. (a) Snapshots of intermediates reacting with an adsorbed proton at 10 ps (red panel), 20 ps (green panel), and 30 ps (blue panel). (b) Energy profile of the intermediate reaction steps with increasing time at 300 K.

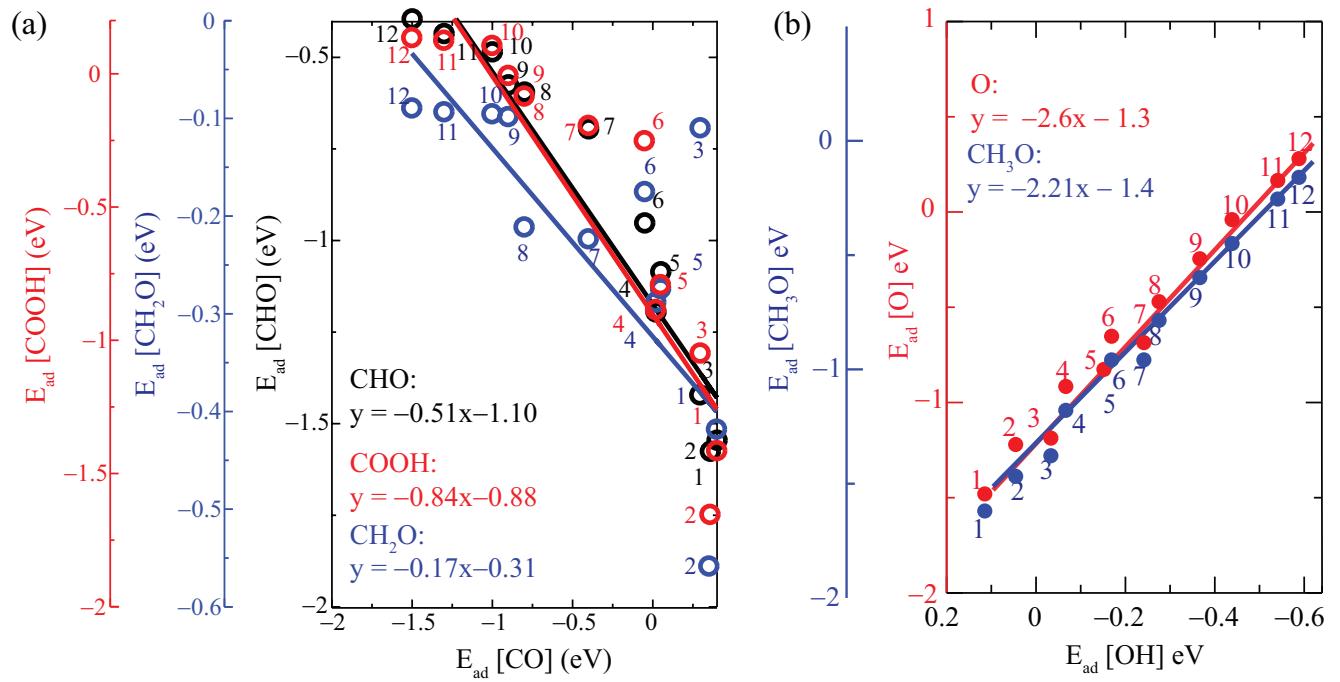


Figure S12: Adsorption energy correlation for (a) C and (b) O bound intermediates as a function of CO and OH adsorption energies on $\text{Sc}_x\text{Ni}_{13-x}@\text{Cu}_{42}$, respectively.

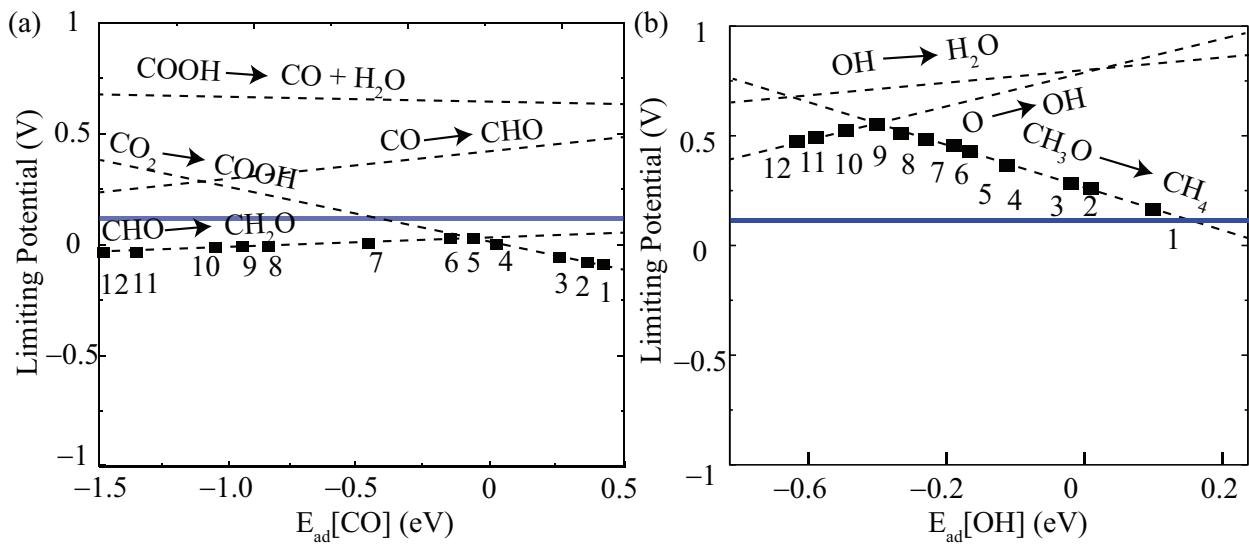


Figure S13: Limiting potential for $\text{Sc}_x\text{Ni}_{13-x}@\text{Cu}_{42}$ as a function of (a) CO and (b) OH adsorption energies for C and O bound intermediate reactions, respectively.

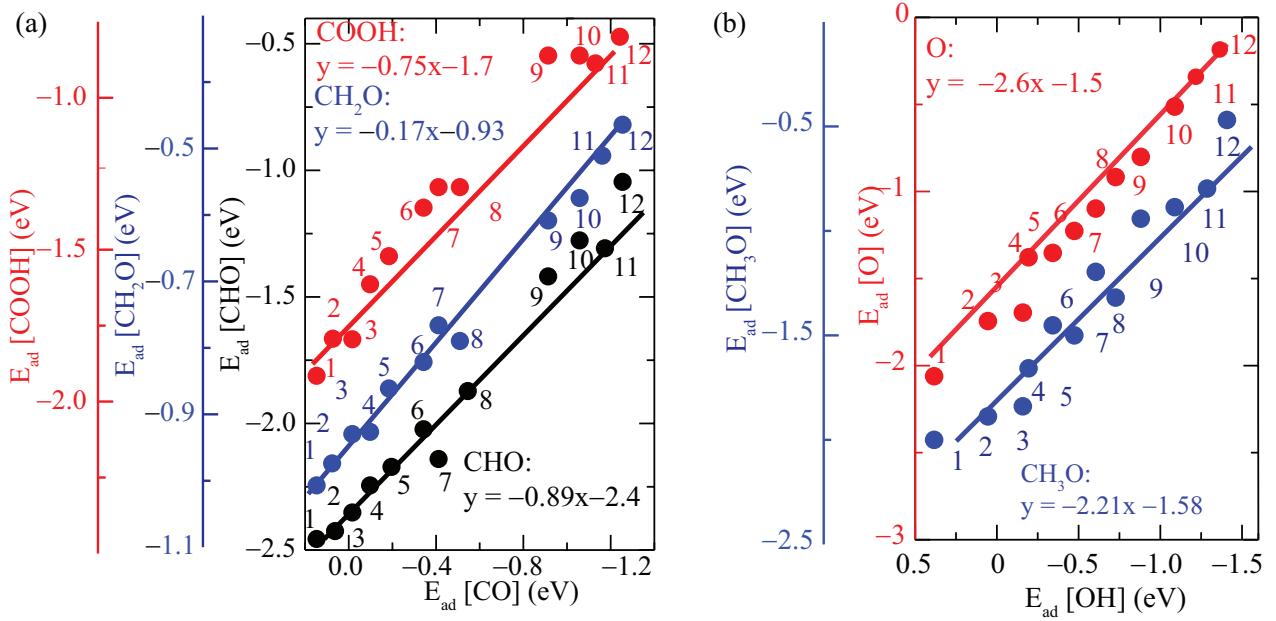


Figure S14: Adsorption energy correlation for C and O bound intermediates as a function of CO and OH adsorption energy on $\text{Sc}_x\text{Ni}_{13-x}\text{@Cu}_{42}$ in the presence of water.

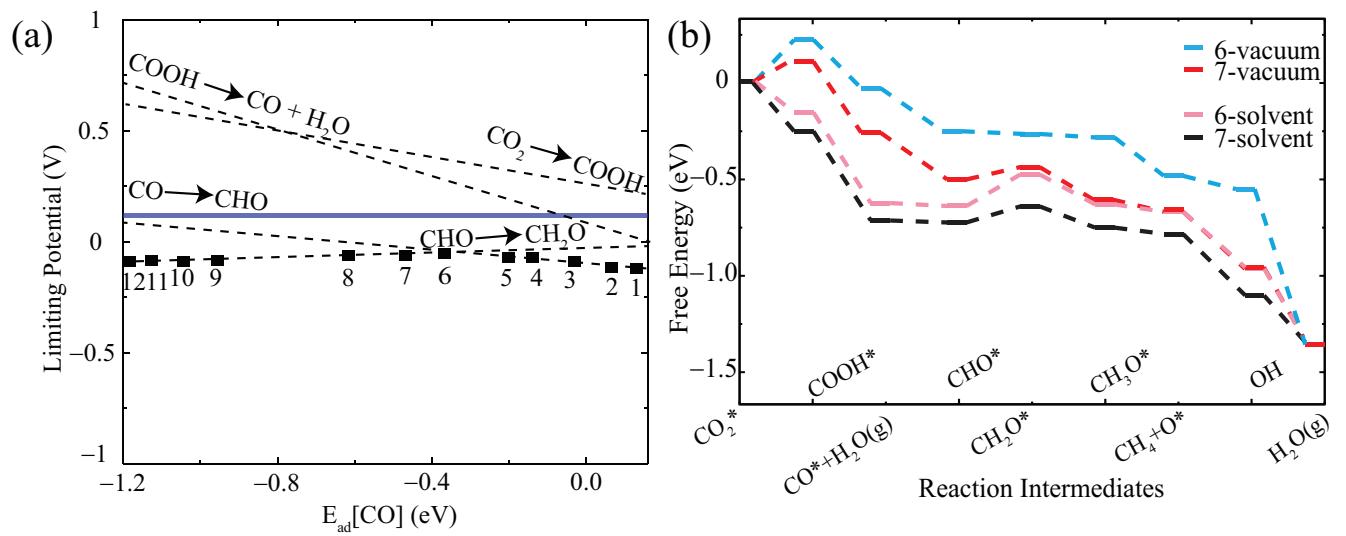


Figure S15: (a) Limiting potential for $\text{Sc}_x\text{Ni}_{13-x}\text{@Cu}_{42}$ as a function for CO adsorption energy for C bound intermediate reactions in the presence of a solvent. (b) Reaction energy profile for the complete electroreduction of CO_2 through eight protonation steps on $\text{Sc}_x\text{Ni}_{13-x}\text{@Cu}_{42}$ ($x = 4$ and 5) in the absence and presence of water, respectively.

Table S1: Adsorption energy of seven intermediates on $\text{Sc}_6\text{Ni}_7@\text{Cu}_{42}$ with varying GGA functionals

Functional:	CO	CHO	COOH	CH_2O	O	CH_3O	OH
GGA PBE	-0.11	-0.83	-0.15	-0.23	1.91	0.5	0.5
meta-GGA M06L	-0.4	-1.0	-0.51	-0.41	2.33	1.0	0.32
meta-GGA TPSS	-0.1	-0.7	-0.11	-0.21	1.98	0.6	0.55
meta-GGA rTPSS	-0.18	-0.98	-0.2	-0.23	1.9	0.76	0.58
meta-GGA MBJ	-0.17	-0.8	-0.1	-0.22	1.95	0.7	0.52

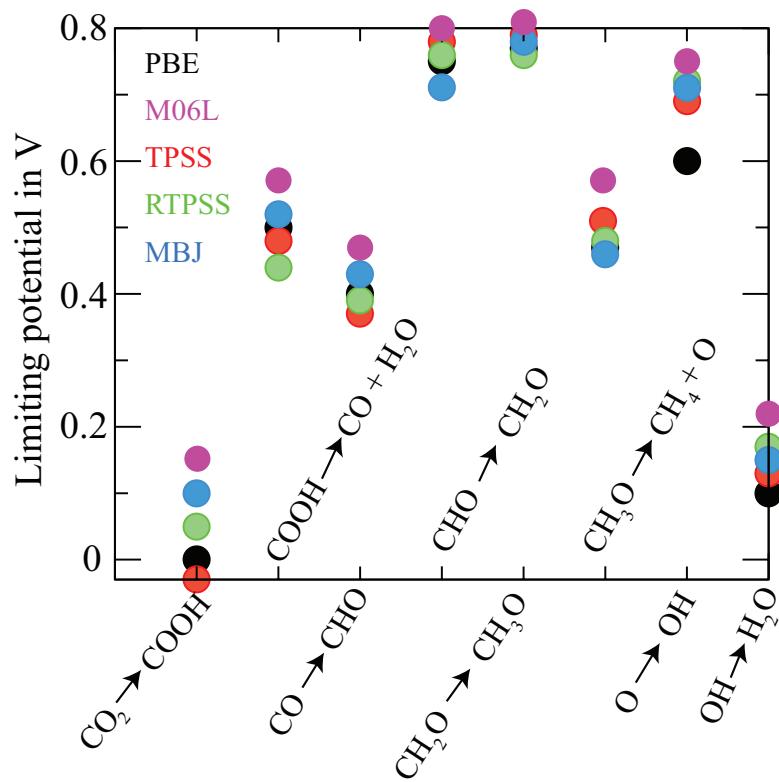


Figure S16: Comparison of performance of GGA functionals in predicting limiting potential values.

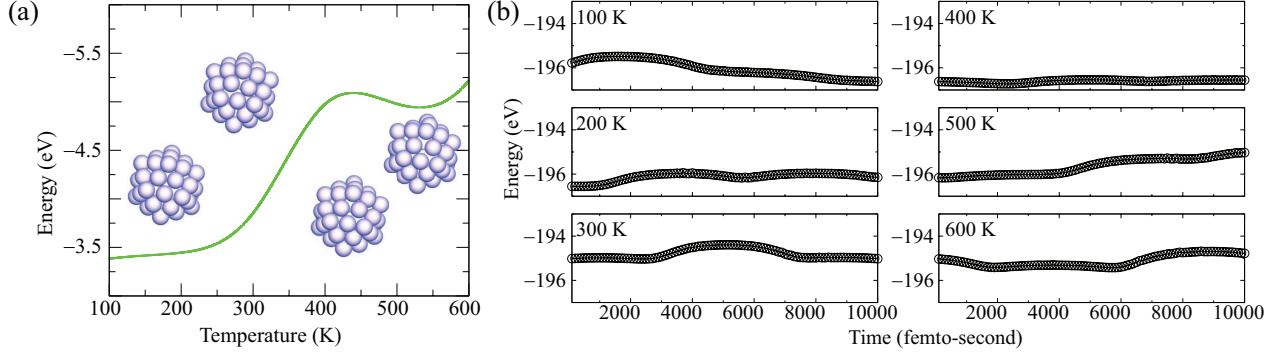


Figure S17: *Ab initio* molecular dynamics simulations of $\text{Sc}_6\text{Ni}_7@\text{Cu}_{42}$. (a) Energy change of $\text{Sc}_6\text{Ni}_7@\text{Cu}_{42}$ with varying temperature from 100 to 600 K. Insets are snapshots of $\text{Sc}_6\text{Ni}_7@\text{Cu}_{42}$ after 10 ps with respect to temperature. (b) Energy change of $\text{Sc}_6\text{Ni}_7@\text{Cu}_{42}$ with temperature and time.

1 Statistical coverage of CHO

The random occupation of the sites gives rise to different configurations that can be taken into account through a configurational entropy term. $q(i, j)$, is the partition function, where i CO molecules and j CHO species are bound to a given site pair, with the restriction ($i + j \leq 2$). The possible partition functions are

$$q(0, 0) = 1, \quad (\text{S1})$$

$$q(i, 0) = e^{-U_{i\text{CO}}/kT} \prod_{n=1}^6 q_{\nu_{(n)\text{CO}}^i}, \quad (\text{S2})$$

$$q(0, j) = e^{-U_{j\text{CHO}}/kT} \prod_{m=1}^6 q_{\nu_{(m)\text{CHO}}^j}, \quad (\text{S3})$$

for $i, j = 1$ or 2 ; and

$$q(1, 1) = 2e^{-U_{\text{CO+CHO}}/kT} \prod_{n=1}^6 q_{\nu_{(n)\text{CO}}} \prod_{m=1}^6 q_{\nu_{(m)\text{CHO}}}, \quad (\text{S4})$$

where $U_{i\text{CO}}$, $U_{j\text{CHO}}$ represent the binding energies of the adsorbed molecules, and $q_{\nu_{(n)\text{CO}}}$ and $q_{\nu_{(m)\text{CHO}}}$ correspond to the harmonic partitions functions of the n th and m th normal modes calculated according to

$$q_{\nu_{(j)S}} = \frac{e^{\frac{\hbar\nu}{2kT}}}{1 - e^{\frac{\hbar\nu}{kT}}} \quad (\text{S5})$$

$\nu_{(j)S}$ represents the vibrational frequency of the j th normal mode corresponding to the adsorbed species of type S = CO and CHO. The grand canonical partition function for each double adsorption site is given by

$$\begin{aligned} Q = & q(0, 0) + q(1, 0)\lambda_{\text{CO}} + q(0, 1)\lambda_{\text{CHO}} + q(2, 0)\lambda_{\text{CO}}^2 \\ & + q(1, 1)\lambda_{\text{CO}}\lambda_{\text{CHO}} + q(0, 2)\lambda_{\text{CHO}}^2 \end{aligned} \quad (\text{S6})$$

where, $\lambda_{\text{CO}} = e^{\mu_{\text{CO(ads)}}/kT}$, $\lambda_{\text{CHO}} = e^{\mu_{\text{CHO(ads)}}/kT}$, and $\mu_{\text{CO(ads)}}$ and $\mu_{\text{CHO(ads)}}$ are the chemical potentials for CO and CHO, respectively. The average numbers of molecules per (double) site can be calculated from

$$\bar{s}_{\text{CO}} = \frac{q(1, 0)\lambda_{\text{CO}} + 2q(2, 0)\lambda_{\text{CO}}^2 + q(1, 1)\lambda_{\text{CO}}\lambda_{\text{CHO}}}{Q} \quad (\text{S7})$$

$$\bar{s}_{\text{CHO}} = \frac{q(0, 1)\lambda_{\text{CHO}} + 2q(0, 2)\lambda_{\text{CHO}}^2 + q(1, 1)\lambda_{\text{CO}}\lambda_{\text{CHO}}}{Q} \quad (\text{S8})$$

The degree of CO coverage is given by;

$$\theta_{\text{CO}} = \bar{s}_{\text{CO}}/2. \quad (\text{S9})$$

Within the ideal diatomic gas approximation, the chemical potential of the gaseous species CO at the pressure p_{gas} can be written as

$$\mu_{\text{gas}}(T) = \mu_{\text{gas}}^0(T) + kT \ln p_{\text{gas}} \quad (\text{S10})$$

where,

$$\mu_{\text{gas}}^0(T) = -\ln \left[\frac{4\pi m k T}{h^2} \right] kT - \ln \frac{8\pi^2 I k T}{\sigma h^2}$$

$$+\frac{h\nu}{2kT} + \ln \left[1 - \exp \left(\frac{-h\nu}{kT} \right) \right], \quad (\text{S11})$$

where m is the atomic mass of the atoms that compose the molecule, I is the moment of inertia, and $\sigma = 3$, since we are dealing with asymmetric molecules. Eqs. S8, S9, and S10 were employed to evaluate the degree of CHO coverage as a function of the CO partial pressure p_{CO} .

1. Relaxed structures of 3, 6, 9 TM for $\text{TM}_x\text{Ni}_{13-x}\text{@Cu}_{42}$

2. Relaxed structures of $\text{Sc}_x\text{Ni}_{13-x}\text{-Cu}_{42}$ for $x = 1$ to 12

3. Relaxed structures of intermediates on $\text{TM}_x\text{Ni}_{13-x}\text{-Cu}_{42}$

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Co Ni
42 3 10

Direct

0.3886174834174045 0.4863133879153179 0.4076910428731138
0.6113778187550606 0.5136852249270319 0.5923161550171200
0.4298717039525167 0.5508700989978783 0.4032308944084980
0.5701030566343007 0.4491660027979456 0.5967306696604814
0.3804338294508240 0.5367025560290373 0.4648969851426753
0.6196181003503894 0.4632683373493622 0.5351114034703857
0.3792569789723862 0.4575228456477773 0.4780642307797729
0.6207460418695401 0.5424829121867658 0.5219616761718526
0.4279198077532215 0.4226923485082456 0.4244955920009518
0.5720910992378461 0.5773107208046614 0.5754917505534543
0.4591871248811745 0.4803238156023562 0.3782819279217313
0.5407900112931568 0.5196645107515174 0.6217185162572282
0.5060826347593903 0.5456687548199904 0.3784161029024993
0.4939147331912132 0.4543853491405088 0.6215348325978460
0.4778606902339940 0.6104164105401938 0.4081887383576440
0.5221223837428403 0.3895977498584491 0.5918127586890178
0.4272971469334747 0.6019412511618125 0.4651639457784281
0.5727258090433579 0.3980635091710328 0.5348094392353683
0.3837994628301610 0.5834044770355197 0.5254789051862649
0.6162089501575454 0.4165761591123225 0.4745331471385134
0.3766791245302972 0.5084653318755761 0.5400135694998062
0.6233817143709809 0.4914967407921986 0.4599647772339399
0.3815234545855797 0.4327016273131851 0.5505701885677875
0.6184942096649498 0.5673100598224098 0.4494287338767881
0.4242066913148207 0.3945990048002359 0.4996196164214627
0.5757920645224814 0.6054127267925690 0.5004038053776509
0.4741262470492091 0.3665849684346701 0.4486170257004246
0.5258687025000681 0.6334136623680079 0.5513897938874535
0.5041152694976777 0.4174061598242807 0.3997967707677038
0.4958657228817908 0.5825762688748308 0.6002057762704274
0.5336267775259679 0.4763620165399549 0.3606495737786802
0.4663724850277259 0.5236311547520374 0.6393317654830717
0.5506454141116648 0.5933785071647518 0.4251350040037117
0.4493493569043124 0.4066733607873084 0.5748130217338593
0.5018784572724253 0.6281769308910435 0.4787542022151011
0.4981127041284332 0.3718771780151889 0.5212247567501964
0.4525191580076933 0.6139710472553116 0.5404158873094822
0.5475148368128944 0.3859805211315378 0.4595735038748088
0.4212412519301756 0.5562479907629700 0.5866379306825975
0.5788209087172331 0.4437155145893057 0.4133418772371122
0.4200806711982410 0.4770748195540288 0.5997872045523276

0.5799294637068817 0.5229279046377789 0.4002001368369725
0.5000471796728602 0.5000164692244008 0.4999364894621509
0.4886600819994439 0.5564256353795795 0.4531323755027067
0.5593698032727297 0.4573589132558946 0.4869552424957062
0.4426346763478922 0.4930387741401014 0.4524953152023183
0.5574514654485637 0.5069861073875365 0.5473932605815957
0.5115101810188125 0.4431956939084100 0.5470974353300302
0.4402832852017918 0.5429741020067133 0.5130317056324788
0.4389412565988291 0.4653643049231867 0.5260348267162013
0.5608449587965756 0.5344915186683131 0.4739875345218119
0.4868716834919263 0.4313344184429577 0.4735917922928157
0.5132168725084068 0.5686896948608808 0.5262955394172529
0.5172789402304486 0.4879216930305521 0.4284278350056250
0.4827200616904183 0.5121627554345650 0.5718170116350932

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu Co Ni
42 3 10

Direct

0.3983720630453246 0.4876292398469552 0.4158020790359865
0.6016176070663271 0.5124017301580706 0.5842668848179808
0.4377727690422001 0.5454276464606199 0.4139925646782713
0.5621272778509362 0.4546463143469370 0.5859316291612198
0.3937404844095050 0.5327313505338571 0.4687379190290445
0.6061549989481199 0.4672813315173837 0.5312862636634385
0.3925761528905610 0.4621303554814221 0.4806871216737621
0.6071641747819982 0.5378497320841733 0.5193539459193446
0.4360426879971205 0.4315234660276806 0.4328947560611513
0.5638584507292217 0.5685174628266930 0.5670995335414616
0.4636600045367046 0.4827420888976780 0.3918261990157042
0.5362089488554452 0.5172610505909211 0.6081243112780947
0.5052622742049995 0.5408012259936906 0.3917170983052884
0.4946451236371614 0.4592810926791867 0.6080943325955590
0.4799429566074511 0.6006204903309839 0.4165094576318149
0.5201762924098449 0.3988377936924204 0.5839130069998788
0.4355373877068663 0.5906484853323569 0.4689056768018098
0.5643736406526897 0.4094317221071250 0.5309903769394434
0.3940333836518708 0.5762666893706653 0.5233609175908890
0.6059555992262021 0.4237190010693870 0.4766336507070492
0.3903624525737551 0.5075114808250220 0.5353660094511972
0.6094950712063886 0.4924656394643960 0.4646887301438611
0.3919899473327594 0.4388523822762593 0.5461179133492842
0.6086373468461616 0.5614787996439823 0.4536960453898769
0.4324158742872082 0.4062814470401074 0.4996940877390869
0.5674202122569936 0.5936498056534175 0.5003381122137458
0.4762272612721851 0.3781408201239454 0.4530578944324792
0.5236739590476960 0.6218966338120726 0.5469189244206786
0.5036112021359275 0.4267186630827757 0.4109620086338198

0.4962319294338101 0.5733441772984043 0.5889839469825139
 0.5307223422396598 0.4784331373428938 0.3728076211593483
 0.4691760235295347 0.5215773194852409 0.6271693556901932
 0.5452667907255739 0.5832838380137323 0.4330425367783483
 0.4545825781994648 0.4168164312254033 0.5668677181580603
 0.5018740911398313 0.6139856812462011 0.4810361047458258
 0.4979898910929001 0.3861395891845848 0.5188793867626754
 0.4579169869517141 0.6013132671160663 0.5358898196088825
 0.5420028367890424 0.3986789678189810 0.4641310610284108
 0.4300299781266604 0.5499551864281009 0.5767787998366641
 0.5698623004382555 0.4500895144913987 0.4232251792169804
 0.4287319072319650 0.4795302240342791 0.5887323529031699
 0.5711007912721212 0.5204521044667350 0.4112593520372433
 0.5001485802381183 0.4999706179839916 0.5000501242248429
 0.4903049253971218 0.5498334945774148 0.4585907172064349
 0.4467345705959769 0.4695191067166144 0.5229296996392490
 0.4491326077047221 0.4940170269666407 0.4581174769858719
 0.5511881284812095 0.5061106963157770 0.5422390964990846
 0.5097460667741447 0.4491306491260908 0.5421948927636653
 0.4469802715028284 0.5380879379669062 0.5114661373176744
 0.5533252942179103 0.4616566849006648 0.4883993505946265
 0.5542210034620380 0.5312239310174642 0.4763813206398659
 0.4881363008157428 0.4389681891233858 0.4764627804431977
 0.5117418948624777 0.5610827028583605 0.5234524585659072
 0.5153278483065967 0.4895168929140360 0.4361303291919890
 0.4844684552609558 0.5105386901104432 0.5638149297980518

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Co Ni
 42 6 7

Direct

0.3984981496748129 0.4877020519487079 0.4156392892207019
 0.6015327099319271 0.5120855575617710 0.5843635560701835
 0.4374917026627257 0.5458135674911414 0.4128612001139919
 0.5625126887711561 0.4542077052464832 0.5863949328139103
 0.3934837604571188 0.5330182846081368 0.4680769010067257
 0.6072108245700841 0.4668433823363467 0.5315634282636097
 0.3922396499938382 0.4623898560847931 0.4799367682656175
 0.6078477673297606 0.5378162936896709 0.5199612558878852
 0.4357842858605055 0.4315154499664452 0.4325230913872802
 0.5641675115364547 0.5681505223166384 0.5672937146719164
 0.4637550377407362 0.4824577047922839 0.3911480269171361
 0.5366294370862306 0.5169996439404003 0.6085592259236976
 0.5057642673792703 0.5406921236435657 0.3914947045834467
 0.4946237453805248 0.4593496975517132 0.6081658051328979
 0.4803663480865010 0.6009316413425074 0.4164536116887132
 0.5195780179376780 0.3987066241553213 0.5839159998182744
 0.4356325975881707 0.5909048818563094 0.4685278637155311

0.6067048952967533 0.4661748519558983 0.5309302080732756
0.3917352484121890 0.4624963421103687 0.4800303924600406
0.6080473176112272 0.5373958326195534 0.5191672155571928
0.4354822646400276 0.4314921890683401 0.4324853383819702
0.5642269707501659 0.5686187976168423 0.5674515428868362
0.4633746977592738 0.4826743369836636 0.3910577259260006
0.5353738855192312 0.5172698720711608 0.6092734526065282
0.5053582257687856 0.5407909479136097 0.3913670727150387
0.4939367326147195 0.4592916921719766 0.6084894120447665
0.4806260266184576 0.6007973993502361 0.4162615649198693
0.5192771541085960 0.3992605858487434 0.5836901092944583
0.4358238487549592 0.5912474911018704 0.4685661664833816
0.5639288629501671 0.4085865390952564 0.5311668876738322
0.3946679986197493 0.5766066450934910 0.5228903181714398
0.6059662164633051 0.4230519103442107 0.4767775806787909
0.3899349282502233 0.5084091233458367 0.5352237981428081
0.6099382408135284 0.4917107875960539 0.4644022546025306
0.3916494634542935 0.4396768088247390 0.5457759301580498
0.6092564908516376 0.5607087647206142 0.4538397867269720
0.4321255762222236 0.4069288644052003 0.4994714617751059
0.5679986990790783 0.5934530939057653 0.5001912433536368
0.4758377867013508 0.3783218461991402 0.4530081699542090
0.5244952930983711 0.6208751197866770 0.5466561646448873
0.5034640965340766 0.4265791062600924 0.4106881335491329
0.4961916003833465 0.5738056504468819 0.5891804841218830
0.53067973738742877 0.4784860905488425 0.3735565129232871
0.4688674031076867 0.5220087467931958 0.6277984612233571
0.5456579195472052 0.5824154992268825 0.4332854641151886
0.4542777930742996 0.4178800024595332 0.5665499175096842
0.5025972016422556 0.6135077203638475 0.4811005094227460
0.4973514427673685 0.3866493685147749 0.5189082998841350
0.4585361110421332 0.6014139931010202 0.5355735958167469
0.5415723313346588 0.3986795459849963 0.4640739288771070
0.4300706225965251 0.5505754996734759 0.5766000824158430
0.5693066929111100 0.4499181821803583 0.4234965609998991
0.4284588879161566 0.4804515440414827 0.5882802612909851
0.5710476532808068 0.5200570409458565 0.4115166750645409
0.4991580807936320 0.5000414811683628 0.4994886840893671
0.4488773204360758 0.4939978661293610 0.4576574457679407
0.5495556030182109 0.5055706955012872 0.5419596214341735
0.4902240440799767 0.5498633184067018 0.4583151803359383
0.5101274617211752 0.4504010239689112 0.5419544463942668
0.4474179011413667 0.5381415242272816 0.5109925491779910
0.4457682959648374 0.4703191170736356 0.5222445505452447
0.5124165028791678 0.5595998863102940 0.5235700072966624
0.5144500311187393 0.4898423881619817 0.4368948082452442
0.5535824292452521 0.4613807817118486 0.4890548444218815
0.5549999168835437 0.5304635191650521 0.4772849289090108
0.4880719394917106 0.4392402634318331 0.4761448653722014
0.4846048381745027 0.5110061155774169 0.5644448778529764

vasp

1.00000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Cr Ni

42 3 10

Direct

0.3977584854216527 0.4875416452523982 0.4149712739218134
0.6021174648313280 0.5122692311674315 0.5840314135955293
0.4369295375639416 0.5457753835384894 0.4129352184614040
0.5621079965392396 0.4547953880361587 0.5859830758826565
0.3921762713876259 0.5328742828886248 0.4682156173477661
0.6064542444564112 0.4669932406949919 0.5312955794370646
0.3910488240593641 0.4619765192093498 0.4800355525872404
0.6075657478591013 0.5380285760135388 0.5194501488873496
0.4350436227713072 0.4306840244124095 0.4320671295285629
0.5637733395779411 0.5683838422445906 0.5673715382832053
0.4631729832519749 0.4824571184764901 0.3903610184758255
0.5367658540693930 0.5175164019801342 0.6095252000080987
0.5051155889710335 0.5404394353359003 0.3920786027444049
0.4946836284084629 0.4591703303787323 0.6093044940734244
0.4803075612443538 0.6012939013035362 0.4163022653297343
0.5202859510944573 0.3987468638877836 0.5836545812929098
0.4355202510418062 0.5902359413052823 0.4689137996099647
0.5646047471082528 0.4092638963656151 0.5309655399701336
0.3940176939028180 0.5765437997934106 0.5232865842707813
0.6065793098695897 0.4233739139633473 0.4766457137323571
0.3907295853696668 0.5076624842904981 0.5351426176028071
0.6098210220021482 0.4922824982283928 0.4647158686520469
0.3915495342998944 0.4384681886419181 0.5461914203424777
0.6089994128769390 0.5615251552836347 0.4536916341215828
0.4325878379513109 0.4067089785926769 0.4993318386911157
0.5676067960916221 0.5936426855524434 0.5003831529794626
0.4765608983905462 0.3778209804909805 0.4531276883005574
0.5241247321896306 0.6221963210651084 0.5466612398931574
0.5035388418603237 0.4267319964667070 0.4109044498876126
0.4962125729828222 0.5743164409549173 0.5901818831053989
0.5312664385986363 0.4784056496635943 0.3727793717233460
0.4692840713560285 0.5218154690399913 0.6280481005376207
0.5454194248872908 0.5829877985416261 0.4332538315578954
0.4548632883362889 0.4175130277044524 0.5668511392207620
0.5018030440395557 0.6138547346343260 0.4812742046467661
0.4978438306057669 0.3861721744990835 0.5188912112159227
0.4581027022950044 0.6010825668358373 0.5361843760616247
0.5422338107720690 0.3984846833188304 0.4640391798858013
0.4291167977092601 0.5504802308481422 0.5780975479201094
0.5702319519554491 0.4496948385850907 0.4231381361084611
0.4280035619592311 0.4796651859866314 0.5898501511757617
0.5713906910589117 0.5205055331537897 0.4112582104795702
0.5013858717935883 0.4999179108270048 0.4995264246200098
0.4491838989877861 0.4937366110826718 0.4577220310689629
0.4846074644224210 0.5107991276690542 0.5635939129417816

0.5512881651637950 0.5061126622582289 0.5422051041309963
 0.4898578176569114 0.5504679505078048 0.4578442882515084
 0.5100133665395369 0.4495279061758991 0.5421877682897166
 0.4467206675305915 0.5381439230551794 0.5115805205749483
 0.5536866805152848 0.4613789937124779 0.4883059695817120
 0.4456372326648573 0.4693632850080128 0.5231009955635573
 0.5547625024073014 0.5309796066557304 0.4765293682095723
 0.4881509079653884 0.4390483638776443 0.4760630261652589
 0.5118124120634034 0.5609477380782111 0.5239858035267555
 0.5155730612706828 0.4891945624651919 0.4359631855251327

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Cr Ni
42 6 7

Direct

0.3989781490442091 0.4874238566987148 0.4157150791025621
 0.6010772684669015 0.5128275406454262 0.5845151639745184
 0.4369101196849335 0.5459392397122325 0.4128194690429335
 0.5630612398071579 0.4552123687823695 0.5864277405498528
 0.3938576788327456 0.5321286426396876 0.4680881318908308
 0.6061895749405265 0.4672747866008837 0.5311403315351544
 0.3912451675694220 0.4617721666227653 0.4802884290166135
 0.6078515166994699 0.5376929011532746 0.5205386029818517
 0.4351796907653011 0.4309619472302835 0.4321990642658411
 0.5651042980125919 0.5696037966268552 0.5681505007921004
 0.4628888401273386 0.4823707682990612 0.3909142074269525
 0.5371526312938484 0.5176769742482025 0.6098019802742997
 0.5050967718984277 0.5410814455380170 0.3914557070682338
 0.4945691591629166 0.4598266376219612 0.6073275347936323
 0.4802649136548092 0.6015704104414785 0.4163541830470984
 0.5201874498358944 0.3991729746880062 0.5837809539693012
 0.4355423488852557 0.5912863530149667 0.4684995793265707
 0.5652120026890362 0.4090917295616250 0.5302788627676781
 0.3944834107534753 0.5762285259076113 0.5237647210205111
 0.6059171724213880 0.4235301629725541 0.4762584412050442
 0.3898401366081133 0.5070384482203847 0.5358042242890581
 0.6099006295625429 0.4915033096590765 0.4644398108425044
 0.3918221601425255 0.4384811411478228 0.5468635816132642
 0.6082655035016287 0.5614100007699270 0.4540027949241526
 0.4320502263701094 0.4059823053856964 0.4998877186760675
 0.5668188468396260 0.5932517462324671 0.5004522757658451
 0.4764013638998246 0.3778609806433474 0.4531915027577864
 0.5233248481152767 0.6223607596410149 0.5472676958669893
 0.5038230350905438 0.4271535746852131 0.4116901378639031
 0.4965975075382362 0.5731574740970978 0.5889722325374701
 0.5309356033200079 0.4784008741679929 0.3725956530270726
 0.4689526226038800 0.5220790959144738 0.6276837081456939
 0.5455437039231540 0.5839744572058342 0.4326100008401764

0.4542218724871386	0.4159307084135715	0.5672096221103382
0.5016895505955771	0.6158812053454458	0.4809314440786397
0.4982194199155682	0.3868221878383732	0.5186984018465538
0.4580203896627149	0.6010296021425683	0.5356225886162819
0.5429037059892464	0.3971576123744118	0.4636198921164643
0.4301433706895802	0.5495935368950894	0.5766154254263214
0.5710970193472529	0.4492633841161515	0.4219658378773243
0.4277740756857475	0.4794005417837152	0.5900649006599913
0.5705434488932128	0.5202641821321244	0.4119215312435422
0.5003485800431372	0.4998509420263643	0.5002167875535324
0.4509003074033792	0.4947881153496839	0.4603923973911705
0.5498991785717391	0.5046863467081480	0.5396885512124870
0.4883923186678498	0.5493364226849028	0.4572657475387557
0.5528342281578001	0.4627285146543459	0.4893041013132718
0.4451505632455233	0.4694532404109867	0.5211765681926801
0.5101664504578316	0.4493666032627420	0.5425179120116048
0.4464957826513771	0.5389460582155159	0.5121705483512914
0.5545454991029811	0.5312214313857865	0.4769943779095699
0.4886608030149492	0.4382460793355516	0.4761060579974263
0.5122258476909406	0.5612518027178072	0.5238487436427008
0.5160292314794654	0.4887742386578954	0.4356799942299553
0.4846927641858697	0.5106798467724930	0.5642085474785324

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu	Cr	Ni
42	9	4

Direct

0.3987267855039652	0.4876161777992205	0.4166109151378085
0.6004471128302539	0.5115579046262559	0.5839298449343269
0.4359481542791840	0.5461102577948931	0.4121978816209979
0.5628408294563682	0.4538105885292679	0.5881174151197357
0.3941472462910783	0.5336702024629730	0.4694237591837097
0.6057191763444129	0.4670204815942818	0.5310839572033873
0.3897801214291972	0.4611786280409493	0.4793307301423807
0.6072872449335788	0.5381254155377878	0.5198637189509577
0.4364995322527900	0.4310383523559599	0.4331230884074737
0.5640278709293696	0.5691314299027975	0.5674544168533870
0.4638950264070531	0.4823565231914435	0.3923083662209122
0.5354069903974165	0.5184246514576377	0.6086690075896486
0.5054716953500319	0.5400878597471057	0.3921419310469257
0.4948483481927503	0.4606609224165126	0.6085391426632540
0.4794383378650177	0.5996677625532869	0.4167626541907077
0.5194173641929644	0.3997228368854304	0.5833877491758114
0.4351509243252051	0.5910321412727223	0.4705064890188908
0.5638189816704583	0.4096138848107014	0.5307295975395734
0.3947958977981196	0.5767120141468307	0.5246519823330263
0.6075576671622226	0.4219384647791999	0.4759634691912275
0.3895641201731721	0.5073790528394668	0.5352596471522331

0.6101852768104161 0.4915682093816000 0.4640303840389951
 0.3935024416981272 0.4379596197776593 0.5444934077884187
 0.6086142547061016 0.5616617526755144 0.4539398340231605
 0.4328495848895835 0.4041101502223885 0.4982112146251896
 0.5689002602183612 0.5954255358885040 0.5002433632230285
 0.4768932477798993 0.3762743403436936 0.4517844570359552
 0.5249972116790927 0.6252956659467402 0.5474956042223872
 0.5047503726329169 0.4243496422373429 0.4086842582252510
 0.4965911418468614 0.5762165104684386 0.5899496460118664
 0.5312849697171425 0.4772802377199352 0.3703416786099316
 0.4688929999717054 0.5231361612107399 0.6268252332395143
 0.5451348518265280 0.5831186446774407 0.4338604866459033
 0.4541022502641202 0.4148301803776281 0.5681265047373344
 0.5018166673450919 0.6144540613641412 0.4813569949882617
 0.4978902227094766 0.3862609706983591 0.5181885391350424
 0.4583709746267542 0.6042969817401526 0.5373066873285668
 0.5435381355311244 0.3960180797762202 0.4622784601972779
 0.4238381092886139 0.5554012549982764 0.5843087820208466
 0.5712174608961422 0.4481545232356373 0.4213604946047665
 0.4286999524738255 0.4793908310628383 0.5887560554326043
 0.5718281730001515 0.5194647833269268 0.4104690060087610
 0.5039339534441720 0.5001374317197361 0.4971016635031682
 0.4501602587357396 0.4951408283220516 0.4611619736278242
 0.5470780890903091 0.5041941163124805 0.5416505498728881
 0.4874904457086094 0.5470750674390152 0.4598802622931503
 0.5076268325157692 0.4528458708649891 0.5414242173320833
 0.4504853704240389 0.5359204927405008 0.5233268894265491
 0.4485721704315748 0.4678666698699903 0.5194331014582605
 0.5534920074977929 0.5296496394211492 0.4770549195063308
 0.4769883763114889 0.5172903003611568 0.5589348794098103
 0.5548198477974630 0.4593074046580266 0.4865483146930589
 0.4900804130172858 0.4370736354237463 0.4741004944090025
 0.5137998463856469 0.5647336870112749 0.5238763043290515
 0.5167844009434647 0.4872411659809804 0.4334395743193822

vasp

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

Cu Cu Ni
42 3 10

Direct

0.3983978473838113 0.4878702341137359 0.4156841440633438
 0.6016039546326634 0.5121071459159562 0.5843786440881334
 0.4378739030958624 0.5455624219728245 0.4137571537739602
 0.5619301401114000 0.4543245057968066 0.5862146754905944
 0.3940711077196132 0.5330523105793896 0.4686073702877091
 0.6060451002417963 0.4669406686504176 0.5313299412413173
 0.3925539070749655 0.4624669489076354 0.4806185401321812
 0.6073016235047540 0.5374568144557037 0.5194349821574032
 0.4358429027498723 0.4313239017288093 0.4326059139343525

0.5642405901211193 0.5686246518523871 0.5673797029592504
0.4638285688676772 0.4826879197643714 0.3918105955725765
0.5362357321484642 0.5172615906604615 0.6083524266688398
0.5055225999118739 0.5405352782882014 0.3916453099302786
0.4943725271912046 0.4592931298310922 0.6085792806765699
0.4802030393383424 0.6015811073412647 0.4156347210343758
0.5194737330366295 0.3985725610069549 0.5842277306148622
0.4358493308502637 0.5912719677694022 0.4688932735689540
0.5638746228103236 0.4092059515351292 0.5312005980274375
0.3943748598333432 0.5768654105731681 0.5231807157676618
0.6056309552201824 0.4231070054820343 0.4769693695600771
0.3903567742092797 0.5080006498721661 0.5354288659027375
0.6096445545886149 0.4918193897733060 0.4645915329133528
0.3912430925244104 0.4389383301172948 0.5463050278366054
0.6087380227827300 0.5610229395947561 0.4536660024292153
0.4323709087415153 0.4066352201873840 0.4995579010830327
0.5679092765841018 0.5937521950008687 0.5001374127881989
0.4757063373872447 0.3776103919955064 0.4529785792294093
0.5244364210276573 0.6226802239289926 0.5469033066841683
0.5035846552515191 0.4259458991633212 0.4106357212430524
0.4965210728793774 0.5738731082378256 0.5892197388902970
0.5307481975841997 0.4781654977189543 0.3727755508529002
0.4692914165416429 0.5219235860628808 0.6272596292704946
0.5456943631251612 0.5830079526550836 0.4329192802785619
0.4542173614730939 0.4170434653822848 0.5671224815988990
0.5025072936474805 0.6146776906657234 0.4808097750783940
0.4974960415783240 0.3861721877919395 0.5188644711343108
0.4582483587899134 0.6020252389208102 0.5357919308722228
0.5417098773589484 0.3981857857406589 0.4640433023742503
0.4302566430807849 0.5504730667588025 0.5769583944090199
0.5699704136431056 0.4493784678848449 0.4230735488829131
0.4286057318794286 0.4799485694494840 0.5889769522056578
0.5712681792355192 0.5199483991895252 0.4111550191367952
0.5000285106648469 0.4998310136704298 0.5000269578459945
0.4901452323675042 0.5511605559763906 0.4575334155277154
0.5121455574882754 0.5617631385344386 0.5237163607381443
0.4485870088194803 0.4936950336288177 0.4575932143992416
0.5513301301372587 0.5058328863625776 0.5425675562684589
0.5096065052658600 0.4488691267708499 0.5429238887580451
0.4465068324286994 0.5387491417694525 0.5117914885013695
0.5532884114025566 0.4612716767379657 0.4883166388286778
0.4454797192028443 0.4692006225351403 0.5236888778855038
0.5549081554270905 0.5308214733088956 0.4763454870122074
0.4881131111506758 0.4381808762906103 0.4756616409918923
0.5157071299200764 0.4886268177012509 0.4359165508382354
0.4844016559666169 0.5106578543950204 0.5642384077601471

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Cu Ni
42 6 7

Direct

0.3979493269692337 0.4880276353893238 0.4149450687173096
0.6021833397568778 0.5120647950826840 0.5850511224786459
0.4378138770590316 0.5458612789723207 0.4129578282821503
0.5620741360141627 0.4543485258492117 0.5866311316507323
0.3937297647332195 0.5334157922332786 0.4680363250411981
0.6063960338757548 0.4666669659447494 0.5320087748920148
0.3916655129882515 0.4625149418110970 0.4799822337709565
0.6080831722904394 0.5373751686235780 0.5197774393106288
0.4350485776616775 0.4312857824645489 0.4324515653744200
0.5646257805395235 0.5686668368177848 0.5673545945065323
0.4638401619392130 0.4826561303982128 0.3914310093468157
0.5363329411087132 0.5173898028787877 0.6086217361203199
0.5058531690289491 0.5403383947041225 0.3915766599843828
0.4941591026109650 0.4597552692625025 0.6082826504175468
0.4807605677109854 0.6013346016900907 0.4154602593951752
0.5190392044482434 0.3986357000921467 0.5844367762924394
0.4360074480790320 0.5913682940700957 0.4682397289369277
0.5638757921494576 0.4086515591819187 0.5317487194736259
0.3942681798936901 0.5771659555853427 0.5224391610947706
0.6056933383173563 0.4227369761836997 0.4775863317315823
0.3901604931533091 0.5085063572553106 0.5349892975078318
0.6096770880878425 0.4914969149567997 0.4650504922980703
0.3906310801651621 0.4392337533137514 0.5460982170755344
0.6092543422094099 0.5607069723701070 0.4538246931333081
0.4314166404727928 0.4062806949287371 0.4995667656999190
0.5680444433377398 0.5931323120901835 0.5003689401568767
0.4751978063615681 0.3776638350802467 0.4531587258455717
0.5246148934962858 0.6223169991994034 0.5467098013103658
0.5034315697029342 0.4259998219176450 0.4108747662186948
0.4966362734407302 0.5739966809138158 0.5890182679348527
0.5308974075458199 0.4778580821565985 0.3728833353319717
0.4690896436129053 0.5221811623718783 0.6271599958722337
0.5461591758947967 0.5827264159463337 0.4330068317527087
0.4539527342135264 0.4171828692088240 0.5669389416717608
0.5027637618289673 0.6142549209432211 0.4808410629437153
0.4971423043296317 0.3858583105985033 0.5192759931824356
0.4584878131164508 0.6020520508007385 0.5354046358348146
0.5416426781435831 0.3978553829450716 0.4644766008201766
0.4302605294853778 0.5507810760929491 0.5764030683189586
0.5698789173846469 0.4492428654115601 0.4237703553601231
0.4283401241842748 0.4803421717119150 0.5887874106052728
0.5716301369400225 0.5198326643225301 0.4113578020697208
0.5002866501710671 0.5000653022187228 0.5002383239279795
0.4485148913289880 0.4940123382671368 0.4570709900866397
0.5515708452741203 0.5061532384247556 0.5428837890523210
0.4904312927099512 0.5510308504410564 0.4574152907909306
0.4450389117277577 0.4694020539669588 0.5233034357618006
0.4878262601120741 0.4383740084126078 0.4762846003239912
0.5097535972692577 0.4485036639649915 0.54313112112172

```

0.4464452381496133 0.5392626048202476 0.5110600232668924
0.5535601548335211 0.4607046358795148 0.4891809694966398
0.5554653173668289 0.5306563897501244 0.4764474435801141
0.5120918321428728 0.5620459277859780 0.5239728640073474
0.5159345179820423 0.4886912276987854 0.4356661775703425
0.4843712066493514 0.5113350365975011 0.5643596631606902

```

vasp

1.00000000000000

Cu Cu Ni
42 9 4

Direct

0.3980120297376192	0.4879919570010329	0.4152580970585206
0.6019955792701470	0.5120900759126997	0.5847038697379533
0.4375533002032276	0.5458364026069880	0.4131023368016944
0.5623602079661181	0.4541310316582743	0.5869017535522647
0.3933053528330979	0.5333905797579750	0.4682565359569102
0.6063856087348682	0.4667024198848589	0.5314362216044831
0.3919424692227785	0.4625446718219698	0.4804124162459261
0.6083882661620659	0.5375612872277200	0.5197901653969739
0.4351513335184951	0.4310499472728592	0.4323900026637947
0.5649956630979380	0.5688608973963443	0.5675985817371836
0.4637573707533698	0.4826364510412033	0.3913481772852095
0.5362566248209616	0.5174147574466825	0.6086324464494730
0.5056836333336824	0.5404179931946812	0.3913027208807910
0.4943433451302278	0.4595482125419155	0.6087097433477167
0.4805452459822736	0.6013279334864892	0.4157808079064824
0.5194531007876417	0.3987752496536453	0.5842656638116299
0.4356648922316645	0.5914731958259899	0.4686506821296901
0.5641420711803488	0.4089867361629212	0.5312785810794783
0.3940568977930046	0.5771347404829561	0.5230653150335787
0.6062051706217050	0.4227369854097408	0.4768332726657759
0.3898117157819783	0.5081442951546786	0.5353615582516029
0.6101514156799018	0.4915678406612013	0.4646104785616959
0.3906131916883783	0.4390262565734555	0.5463680635432069
0.6091542453535026	0.5608709697357347	0.4537047927873179
0.4318892933319985	0.4065236111347759	0.4996916902364287
0.5683542054199254	0.5938065717256097	0.5003235381120354
0.4755414341145248	0.3777303031673077	0.4530467088576715
0.5244915896803339	0.6223075962521204	0.5469144336503802
0.5035013879991467	0.4260546775453214	0.4106365654378440
0.4965312978185638	0.5738104861815514	0.5893821182525215
0.5310133189950219	0.4778617857869198	0.3719928456139759
0.4689992992802495	0.5221447828088791	0.6280181760576287
0.5460817437920669	0.5832424647154879	0.4328967303666241
0.4539776235035225	0.4170206669528427	0.5670158871611289
0.5026339144684461	0.6145858560674354	0.4808426380031156
0.4973898016871753	0.3854660606621518	0.5191522516614758
0.4581065034998413	0.6024554134046670	0.5358026786368365

0.5418571192526018 0.3978762562595081 0.4642352012480398
 0.4298920473310228 0.5508146379328078 0.5773313394699803
 0.5699917555115441 0.4492699295378593 0.4230254214548614
 0.4285141019074126 0.4800060875149216 0.5888933235229271
 0.5715788186718834 0.5199851080862489 0.4107454790332650
 0.4999632342578009 0.4999050942559193 0.5000258494389993
 0.4484840924550106 0.4938339056626238 0.4572478263898794
 0.5514715260911875 0.5059912696792409 0.5427658097938550
 0.4902077555902323 0.5510555914286643 0.4572419407338656
 0.5095878947794324 0.4490876812883453 0.5426292386048287
 0.4464304242721762 0.5387080847126815 0.5119066038223896
 0.5550285213006531 0.5305253752240645 0.4764460041851527
 0.4879840895398244 0.4384439808896425 0.4760889442232711
 0.5121227673600893 0.5617137513465398 0.5239687375350329
 0.5541351803517879 0.4606870032353520 0.4881233458366009
 0.4443117909065403 0.4688969669662034 0.5238338026640655
 0.5160550213917792 0.4887346735381304 0.4347142277670565
 0.4839437135532070 0.5112334381241573 0.5652983577389088

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Fe Ni
42 3 10

Direct

0.3984945062360145 0.4876470480108632 0.4157113575557688
 0.6021681860755472 0.5124224512473129 0.5846483545874411
 0.4373606426305885 0.5453423613023771 0.4135614364400380
 0.5622858968232611 0.4547978321715302 0.5861255982391652
 0.3933887745811309 0.5327737922530570 0.4683841746008885
 0.6061444097492743 0.4673769718995277 0.5315976861647296
 0.3921331097163487 0.4620966143543968 0.4801427051331753
 0.6072800484915893 0.5378106243811044 0.5198016078619626
 0.4356274505414943 0.4312681904139864 0.4324342855627771
 0.5639474647241213 0.5684772858238948 0.5674247108099052
 0.4633721077495033 0.4825340453843980 0.3909820799006244
 0.5365643492634462 0.5174289427019174 0.6090159564958493
 0.5051482328536665 0.5404103562673889 0.3918334305887283
 0.4947620938774707 0.4594248991331186 0.6086078524619950
 0.4799172429988449 0.6009089785279420 0.4161940209932288
 0.5202088945422830 0.3990531871048202 0.5837763096444155
 0.4355336951957306 0.5904574049432378 0.4690089116372398
 0.5644233828663789 0.4095368867968550 0.5310140643975304
 0.3941440263323107 0.5763412817960542 0.5233063185578783
 0.6058325295475748 0.4238654146052783 0.4767478802845478
 0.3907758429415012 0.5076037677784506 0.5351523303800445
 0.6093766742913806 0.4923752236624171 0.4648300307873229
 0.3917028947379649 0.4385809311511475 0.5461248568975664
 0.6082331154890122 0.5611936967985498 0.4539120306244538
 0.4326400657840253 0.4064942207180103 0.4994859819164213

0.5672961936013569 0.5934979664811137 0.5005242146417046
 0.4763320377034558 0.3781333122144149 0.4529644063528951
 0.5238035862322907 0.6218736171770254 0.5469795754820587
 0.5035916459321207 0.4266702567489321 0.4106887867663174
 0.4962853615632401 0.5736184799671118 0.5895790411086310
 0.5309550124782071 0.4783357038324006 0.3722584358307193
 0.4694005626625107 0.5215394521706941 0.6269581869952593
 0.5450911410719890 0.5828654898612406 0.4333240066309497
 0.4548378414284228 0.4171558216405692 0.5667123307545159
 0.5017323019625514 0.6137539434168042 0.4812698915039434
 0.4979243510234583 0.3862700521793658 0.5188303173846627
 0.4579851484255723 0.6013262239589600 0.5360111781054296
 0.5419795149934794 0.3987109791619450 0.4640411117512391
 0.4299296815931076 0.5502258117988228 0.5773947938002121
 0.5697409687542025 0.4499941489952152 0.4229692374216310
 0.4287667222416774 0.4796416749365958 0.5891096347669366
 0.5709405876833397 0.5202849896007105 0.4112505693338359
 0.5003285446640884 0.4999679094691074 0.4998848979849183
 0.4498733517936433 0.4938936834154215 0.4583642193385363
 0.4849626303822919 0.5105423488356794 0.5627624732229667
 0.5511908020205919 0.5062575566683903 0.5427527116619199
 0.4898856587461368 0.5504898153141927 0.4579038078097143
 0.5100390598506689 0.4495034228127035 0.5421135619121992
 0.4470839202476790 0.5381767206554091 0.5115658706018302
 0.5531504499586595 0.4617717014420424 0.4884330481149897
 0.4460064858665702 0.4692325982140103 0.5230133999502983
 0.5541751258494656 0.5308521599643701 0.4768553492187059
 0.4882520032879081 0.4390664905458793 0.4761484585743051
 0.5117176444372694 0.5609395806968834 0.5238440571859880
 0.5152760255035802 0.4891856785963528 0.4356684532689882

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Fe Ni
42 6 7

Direct

0.3982976424636105 0.4875988419321823 0.4155315141170714
 0.6016765094989797 0.5122609958556198 0.5843101932586796
 0.4369250793399954 0.5458492373094067 0.4126855106588155
 0.5624415243037170 0.4543452347795167 0.5863969758872273
 0.3933030579152665 0.5331114542985985 0.4687987673356658
 0.6082201445648653 0.4667183723986000 0.5317069013671185
 0.3911660451426104 0.4619050948121645 0.4801081770800029
 0.6078499707969867 0.5379503106313679 0.5195465266431459
 0.4361415787882813 0.4315558227235285 0.4326635120408235
 0.5642663444281314 0.5683689250239611 0.5671604501045834
 0.4637457000135990 0.4825158629120845 0.3917878471755158
 0.5365493645325310 0.5170162871316273 0.6082610247499119
 0.5053411647178814 0.5405400668089159 0.3916273803749494

0.4944091778910834 0.4592428010810541 0.6081009527128065
0.4799244121022836 0.6006350775594613 0.4164513693030043
0.5196894164960558 0.3986710804256994 0.5841419404013051
0.4353306754197835 0.5908791862263256 0.4690042744171405
0.5644254997921437 0.4092307318502487 0.5311583152118985
0.3937413053108437 0.5769996839807842 0.5240537790754706
0.6058832496482258 0.4237929256811245 0.4768480796956569
0.3900950904667865 0.5078268267098163 0.5354946299089016
0.6097577086030673 0.4925104810866094 0.4645251527822108
0.3918248438905417 0.4390146278551167 0.5459725220032794
0.6085758899598230 0.5618455720916354 0.4536003151085341
0.4323698021260219 0.4063148437196434 0.4994822633940514
0.5673938113367311 0.5936975023363682 0.5003694061750622
0.4763953974905496 0.3780723771624922 0.4530609810840080
0.5237913069961727 0.6216585390785337 0.5470204529131388
0.5038949667545003 0.4263849967087857 0.4109101343315228
0.4964090426239086 0.5733180768802782 0.5891795226313220
0.5310065371370136 0.4782199146817070 0.3728594637725954
0.4693549312972378 0.5214879491315936 0.6270488015312132
0.5451440895146135 0.5832831431269693 0.4328441687626868
0.4542575446275264 0.4168394238583327 0.5667427214342157
0.5016997106197628 0.6134671579749648 0.4812227836136317
0.4978285445422914 0.3862206093756352 0.5189459878381429
0.4579600735216631 0.6016889175132534 0.5364485086700840
0.5423798595768548 0.3983772515198024 0.4643095592158560
0.4301320122401225 0.5502896168344604 0.5773226261484842
0.5704715578940410 0.4498265839088982 0.4231715175509724
0.4288428342847841 0.4798622346065562 0.5883092592783293
0.5710844915972321 0.5204513701583160 0.4113596084869329
0.4998842277214240 0.4999621871124609 0.4998137587446362
0.4486253582676341 0.4946656138787595 0.4583932521495903
0.5515009783329965 0.5049058148933835 0.5409714586653597
0.4892140717665013 0.5488586235515593 0.4581268379679591
0.5530592798015149 0.4627851653661602 0.4895194406563185
0.4462976673961055 0.4699692031432097 0.5214203953517919
0.5094550967809426 0.4491224106625138 0.5424806029587369
0.4463829143738015 0.5391005651896091 0.5122434095460893
0.5541163894971204 0.5316425346320561 0.4764170380808084
0.4887947446692432 0.4389840740632132 0.4763057902985807
0.5118308904098360 0.5606273954131133 0.5237709736015367
0.5158552097238767 0.4888070275300713 0.4364375539948611
0.4849852609908810 0.5107233748218492 0.5635556097377615

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu Fe Ni
42 9 4

Direct

0.3984559838965647 0.4877419116126462 0.4152014241873342

0.6021469586091807 0.5122780683598246 0.5840093381265793
0.4370959690738024 0.5462044924646015 0.4134043657632125
0.5628229426570319 0.4544299772207981 0.5871530481130803
0.3916045025540352 0.5332054881974405 0.4678504457127147
0.6063679981617975 0.4669379172823980 0.5312661891117851
0.3918929958238006 0.4624449691728803 0.4802339084321589
0.6085212449955061 0.5381566766996567 0.5196451356205479
0.4358903151443583 0.4318968704623450 0.4327539159949054
0.5641061144414382 0.5685560071820923 0.5675167324213709
0.4637644641783999 0.4828685413969306 0.3912604797887599
0.5371722289649830 0.5174321582726228 0.6092130693607830
0.5053822180283624 0.5405103570382103 0.3917291117861939
0.4948346985905520 0.4584725644770128 0.6099125642991596
0.4805130581353421 0.6010328747856273 0.4161465836245709
0.5203287667850309 0.3988578437138492 0.5836049271106131
0.4352844932628845 0.5917081171206501 0.4685592840503094
0.5646788055348895 0.4091343678901221 0.5310002988988274
0.3940947694546951 0.5763121040084141 0.5229696834114120
0.6061032816326873 0.4231429149915392 0.4760823624121113
0.3888223421539247 0.5080820582963291 0.5357720135975190
0.6096777161379309 0.4921921101561885 0.4646815307880932
0.3912161380372937 0.4389159850848977 0.5462676636422293
0.6081687880342269 0.5610157163322506 0.4539975139307357
0.4324309943052342 0.4073463618540842 0.4998423453352767
0.5672850887606542 0.5935635418711251 0.5007836858428432
0.4759452203897829 0.3786242928408202 0.4532864640493454
0.5234687055402543 0.6218923003878153 0.5474152354039141
0.5035954872567393 0.4263422876673026 0.4107366013219539
0.4962709048116020 0.5729497158539892 0.5894757827212375
0.5311294082260395 0.4778542338225638 0.3722911013875090
0.4695876500034342 0.5213298817389702 0.6271470910641991
0.5459064934992310 0.5836079787144253 0.4329212582629194
0.4545566451924585 0.4168974704502104 0.5670910475209200
0.5020442781683629 0.6140064126575965 0.4813121370467529
0.4978741619173685 0.3864877557606856 0.5189452624740702
0.4575607239027132 0.6011588929023752 0.5356635006609065
0.5418317929921821 0.3984174697068330 0.4638632054320667
0.4309086762362503 0.5494019427713644 0.5759592072091445
0.5702652942631738 0.4494328601667197 0.4225803346694518
0.4281263551905490 0.4794618927557088 0.5899903541892341
0.5712380062771146 0.5202392314006364 0.4113070799739075
0.5009833981028011 0.5002145708386231 0.4993919523022167
0.4492096146827764 0.4953223781138507 0.4582407996745035
0.5509015049044402 0.5060333626523582 0.5417903681302122
0.4903615253736323 0.5502374388197921 0.4582788200329979
0.5101651519158968 0.4508493516699947 0.5425968729446564
0.4463465414400862 0.5367945502470893 0.5091091556255452
0.4454535613790520 0.4711619174683802 0.5242066534782707
0.5533112630264803 0.5307155863106143 0.4776340814817472
0.4858983493228165 0.5081135204719357 0.5635653966546514
0.5534803908717552 0.4609828978578410 0.4879912813648164
0.4882104296020444 0.4395379718863510 0.4764524656738226

0.5110101544690911 0.5608789850389678 0.5244158898101321
0.5156954336872641 0.4886128530816466 0.4354829780757679

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu Sc Ni
42 10 3

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
0.6131999999999991 0.5138999999999996 0.5938000000000017
0.4286999999999992 0.5516999999999967 0.4016000000000020
0.5713000000000008 0.4483000000000033 0.5983999999999980
0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015

0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.4827000000000012 0.5122000000000000 0.5718999999999994
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5172999999999988 0.4878000000000000 0.4281000000000006

vasp

1.00000000000000
 35.00000000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.00000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.000000000000000000

Cu Sc Ni
 42 1 12

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980
 0.3783999999999992 0.5373000000000019 0.4643000000000015
 0.6216000000000008 0.4626999999999981 0.5356999999999985
 0.3772000000000020 0.4568000000000012 0.4776999999999987
 0.6227999999999980 0.5431999999999988 0.5223000000000013
 0.4266999999999967 0.4213999999999984 0.4232000000000014
 0.5733000000000033 0.5786000000000016 0.5767999999999986
 0.4585000000000008 0.4799999999999969 0.3761999999999972
 0.5414999999999992 0.5200000000000031 0.6238000000000028
 0.5061999999999998 0.5463999999999984 0.3763999999999967
 0.4938000000000002 0.4536000000000016 0.6236000000000033
 0.4774999999999991 0.6122000000000014 0.4067000000000007
 0.5225000000000009 0.3877999999999986 0.5932999999999993
 0.4260999999999981 0.6036000000000001 0.4645999999999972
 0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011
 0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995

0.4958000000000027 0.584000000000032 0.601900000000005
 0.534199999999985 0.475999999999991 0.3584000000000032
 0.4658000000000015 0.524000000000009 0.641599999999968
 0.551499999999972 0.594900000000026 0.4239000000000033
 0.4485000000000028 0.405099999999974 0.576099999999967
 0.501899999999991 0.630299999999983 0.478400000000006
 0.498100000000009 0.369700000000017 0.521599999999994
 0.4517000000000024 0.615900000000034 0.541100000000001
 0.548299999999976 0.384099999999966 0.458899999999999
 0.419899999999984 0.557200000000017 0.588099999999972
 0.580100000000016 0.442799999999983 0.411900000000028
 0.418700000000012 0.476700000000010 0.601500000000015
 0.581299999999988 0.523299999999990 0.398499999999985
 0.440100000000010 0.542999999999993 0.513199999999977
 0.500000000000000 0.500000000000000 0.500000000000000
 0.4425000000000026 0.492899999999988 0.452399999999972
 0.557499999999974 0.507100000000012 0.547600000000028
 0.485999999999981 0.556899999999988 0.452700000000001
 0.511400000000019 0.443100000000012 0.547299999999999
 0.559899999999990 0.457000000000007 0.486800000000023
 0.438899999999967 0.465299999999992 0.526099999999996
 0.561100000000033 0.534700000000008 0.473900000000004
 0.486699999999990 0.431199999999969 0.473500000000014
 0.513300000000010 0.568800000000031 0.526499999999986
 0.517299999999988 0.487800000000000 0.428100000000006
 0.482700000000012 0.512200000000000 0.57189999999994

vasp

1.00000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.0000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

Cu Sc Ni
 42 11 2

Direct

0.386800000000009 0.486100000000004 0.406199999999983
 0.613199999999991 0.513899999999996 0.5938000000000017
 0.428699999999992 0.551699999999967 0.4016000000000020
 0.571300000000008 0.448300000000033 0.598399999999980
 0.378399999999992 0.537300000000019 0.4643000000000015
 0.621600000000008 0.462699999999981 0.535699999999985
 0.3772000000000020 0.456800000000012 0.477699999999987
 0.622799999999980 0.543199999999988 0.522300000000013
 0.426699999999967 0.421399999999984 0.423200000000014
 0.573300000000033 0.578600000000016 0.576799999999986
 0.458500000000008 0.479999999999969 0.376199999999972
 0.541499999999992 0.520000000000031 0.6238000000000028
 0.506199999999998 0.546399999999984 0.376399999999967
 0.493800000000002 0.453600000000016 0.623600000000033
 0.477499999999991 0.612200000000014 0.406700000000007
 0.522500000000009 0.387799999999986 0.593299999999993
 0.426099999999981 0.603600000000001 0.464599999999972

0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011
 0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.5514999999999972 0.5949000000000026 0.4239000000000033
 0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.5718999999999994
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999

vasp

1.00000000000000
 35.000000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni
 42 2 11

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980
 0.3783999999999992 0.5373000000000019 0.4643000000000015

0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.3984999999999985
0.4425000000000026 0.4928999999999988 0.4523999999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.5472999999999999
0.4401000000000010 0.5429999999999993 0.5131999999999977
0.5598999999999990 0.4570000000000007 0.4868000000000023
0.4388999999999967 0.4652999999999992 0.526099999999996
0.5611000000000033 0.5347000000000008 0.4739000000000004
0.4866999999999990 0.4311999999999969 0.4735000000000014
0.5133000000000010 0.5688000000000031 0.5264999999999986
0.5172999999999988 0.4878000000000000 0.4281000000000006
0.4827000000000012 0.5122000000000000 0.5718999999999994

vasp

1.00000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni

42 3 10

Direct

0.3944235625601286 0.4860853384089390 0.4126085327566774
0.6042772856102432 0.5124759759917787 0.5865552000415915
0.4362077506359087 0.5463943387539379 0.4116643570094914
0.5627897902314214 0.4542408560246560 0.5872430274319116
0.3911269849745586 0.5341300622144342 0.4670202874880395
0.6070530401874952 0.4668854658559447 0.5313627696222916
0.3839526183407466 0.4600106076272100 0.4808097413683004
0.6089891528457367 0.5379839087825955 0.5203463415341761
0.4327982038274480 0.4251125782749263 0.4274566995564581
0.5658806966088835 0.5692459875703156 0.5680248233229206
0.4622920758636864 0.4828016442600771 0.3887353768890583
0.5365036497239186 0.5178117503785705 0.6094011889214607
0.5042589517980803 0.5413400091437427 0.3890335894724796
0.4942656050901206 0.4592996199004963 0.6092985447911177
0.4802853961791158 0.6051942968979845 0.4136029017335563
0.5202825251918211 0.3966273653025454 0.5859791115664609
0.4331771512464860 0.5924479473998447 0.4671850888535641
0.5647777218108937 0.4084017750029856 0.5311564098382932
0.3935765096287235 0.5768206305418383 0.5238436231179876
0.6079474009907887 0.4219930189241559 0.4758430102188635
0.3904785028481934 0.5074932740742747 0.5334160964856443
0.6110309385069074 0.4912339334083291 0.4634236594119486
0.3906503840801986 0.4381480266518473 0.5474064868898637
0.6106701362774395 0.5607116787861429 0.4535816528499146
0.4314535287834792 0.4082156680458461 0.4974013719881449
0.5662204387651004 0.5936875215096356 0.4986009556971228
0.4766835306204109 0.3760760987123031 0.4532155458729390
0.5248113092624991 0.6229302579552780 0.5484690927952175
0.5020047976316814 0.4271518805692249 0.4107299871962692
0.4959002029856046 0.5745180488636202 0.5904805323901594
0.5310755430991403 0.4779235154788182 0.3721444914061072
0.4682879698820959 0.5224839625858911 0.6298645990758794
0.5503883933969578 0.5879412300913255 0.4286789123388224
0.4543188832467479 0.4158633452733650 0.5674600980633587
0.5022408469322537 0.6225767200718849 0.4817146649515381
0.4976696747192325 0.3848706137696517 0.5197921413433106
0.4584901077873468 0.6019121648958077 0.5339291286994315
0.5430424512272057 0.3973517975955465 0.4630192374970247
0.4295564104319311 0.5508155147174253 0.5770237937584471
0.5698384448777071 0.4497630973847036 0.4223598330467676
0.4276401232793364 0.4803133099751597 0.5900599773307886
0.5696826218764840 0.5215392238676274 0.4111633306482106
0.5040430692324561 0.4971209518242265 0.5055828319797732
0.4447248970494568 0.4867596185039857 0.4586667885242692
0.4954772945318914 0.5567889962622179 0.4589775665021688

0.5544718410542405 0.5067148588012087 0.5454212570693644
 0.5105984454247684 0.4461449591286380 0.5452589755256912
 0.4463915492093014 0.5392201703897739 0.5107108100345337
 0.5559178252278405 0.4594672541046671 0.4875298010131643
 0.4445379540696682 0.4680827253486823 0.5252964038907009
 0.5573086064241796 0.5306710355524760 0.4767141727834845
 0.4889475075238370 0.4361698478941708 0.4761225888100698
 0.5127986248468100 0.5627483502438129 0.5259086024250761
 0.5144476197413638 0.4896603096624860 0.4352536018521336
 0.4833334518000264 0.5116268607429685 0.5674503843179599

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni
42 4 9

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980
 0.3783999999999992 0.5373000000000019 0.4643000000000015
 0.6216000000000008 0.4626999999999981 0.5356999999999985
 0.3772000000000020 0.4568000000000012 0.4776999999999987
 0.6227999999999980 0.5431999999999988 0.5223000000000013
 0.4266999999999967 0.4213999999999984 0.4232000000000014
 0.5733000000000033 0.5786000000000016 0.5767999999999986
 0.4585000000000008 0.4799999999999969 0.376199999999972
 0.5414999999999992 0.5200000000000031 0.6238000000000028
 0.5061999999999998 0.5463999999999984 0.3763999999999967
 0.4938000000000002 0.4536000000000016 0.6236000000000033
 0.4774999999999991 0.6122000000000014 0.4067000000000007
 0.5225000000000009 0.3877999999999986 0.5932999999999993
 0.4260999999999981 0.6036000000000001 0.4645999999999972
 0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011
 0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.551499999999972 0.5949000000000026 0.4239000000000033

0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994

vasp

1.00000000000000
 35.00000000000000 0.00000000000000 0.00000000000000
 0.00000000000000 35.00000000000000 0.00000000000000
 0.00000000000000 0.00000000000000 35.00000000000000

Cu Sc Ni
42 5 8

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980
 0.3783999999999992 0.5373000000000019 0.4643000000000015
 0.6216000000000008 0.4626999999999981 0.5356999999999985
 0.3772000000000020 0.4568000000000012 0.4776999999999987
 0.6227999999999980 0.5431999999999988 0.5223000000000013
 0.4266999999999967 0.4213999999999984 0.4232000000000014
 0.5733000000000033 0.5786000000000016 0.5767999999999986
 0.4585000000000008 0.4799999999999969 0.3761999999999972
 0.5414999999999992 0.5200000000000031 0.6238000000000028
 0.5061999999999998 0.5463999999999984 0.3763999999999967
 0.4938000000000002 0.4536000000000016 0.6236000000000033
 0.4774999999999991 0.6122000000000014 0.4067000000000007
 0.5225000000000009 0.3877999999999986 0.5932999999999993
 0.4260999999999981 0.6036000000000001 0.4645999999999972
 0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011

0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.5514999999999972 0.5949000000000026 0.4239000000000033
 0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Sc Ni
42 6 7

Direct

0.3893597821437082 0.4881529909825601 0.4112737455794644
 0.6082853542152191 0.5169279264783964 0.5887645840741438
 0.4333982365097058 0.5506374564917823 0.4091290296904900
 0.5665313319358293 0.4546931685630134 0.5934209986793304
 0.3891801346559072 0.5426861321608865 0.4634457838619447
 0.6132506829298759 0.4648244534186043 0.5369629417298720
 0.3829212506812339 0.4515002135737891 0.4769102001155465
 0.6168208533543111 0.5411813740491791 0.5206191344851058
 0.4294471715967685 0.4253018140291291 0.4270727775593189

0.5674587100446481 0.5748046119831873 0.5709272492614079
0.4581552183495423 0.4880312564561972 0.3881198188095396
0.5396724618583022 0.5203269898112687 0.6123381843714029
0.5038313380945887 0.5447416688329813 0.3841786520764210
0.5006193257508582 0.4619615765604397 0.6185412070015691
0.4812284861254217 0.6086473240941132 0.4123882644603982
0.5187560496251756 0.3928678995868443 0.5923053912894476
0.4344853887233085 0.5963182141207390 0.4669847709368031
0.5672811918438512 0.4080712514767600 0.5399558563691913
0.3931761208526324 0.5780755652868745 0.5247795438951330
0.6076931755668993 0.4225131491134386 0.4788598250018484
0.3885500031301516 0.5067174818235344 0.5258483933978283
0.6096733422150621 0.4912889414447934 0.4690108294840725
0.3907853179648414 0.4390891496455715 0.5459894144536286
0.6098341378596852 0.5599199859840882 0.4529707811894062
0.4363411139887187 0.4074107419821268 0.4963575407236497
0.5681938561735903 0.5923976735294326 0.5000984924292086
0.4774095299805605 0.3720872254293662 0.4485064586949075
0.5243040147742587 0.6243955536581983 0.5469158018106788
0.4925598122676565 0.4272188625340476 0.3969799907269361
0.4965590458467110 0.5748668989142718 0.5892209088081090
0.5301523787694856 0.4792175882742162 0.3708119420390849
0.4682368706925618 0.5242300563991843 0.6288232770705219
0.5498481426914946 0.5890227835935127 0.4289448575192737
0.4484119175609269 0.4046258376553448 0.5672008852821484
0.5035852382695993 0.6212328314994577 0.4802921602074225
0.4967206366317325 0.3762906338031132 0.5214885857870640
0.4579861073609124 0.6027437089050177 0.5346554180158088
0.5489357388069247 0.3857330330932404 0.4754617938944280
0.4303198195152553 0.5464814740917922 0.5746976406958877
0.5656500182927942 0.4505819232804523 0.4271941860671485
0.4350771633084485 0.4734476524105071 0.5907456607615347
0.5678839216422051 0.5218586449092887 0.4105777913452789
0.4990786438979712 0.5012448970642673 0.5016870833134395
0.4366225501329356 0.4904745062574997 0.4583114802044163
0.5585327781437514 0.5102809396586866 0.5432330711311260
0.4929175816023535 0.5564045429904690 0.4537970267222430
0.5038848666198193 0.4429492807408020 0.5508346908824631
0.4992722971976633 0.4326203035644401 0.4657076511996411
0.4444281780297924 0.5412512666954337 0.5086294296536130
0.5560407345678511 0.4571391462804981 0.4952051888533153
0.4442630481844347 0.4679996819329590 0.5243644662472288
0.5560404992574494 0.5311124992982675 0.4753392049419329
0.5127773866790905 0.5644219136006725 0.5241731009378219
0.5100937399923486 0.4905159628591559 0.4310645391790734
0.4874773030931759 0.5104613391261053 0.5678822970812772

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni
42 7 6

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
0.6131999999999991 0.5138999999999996 0.5938000000000017
0.4286999999999992 0.5516999999999967 0.4016000000000020
0.5713000000000008 0.4483000000000033 0.5983999999999980
0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.3984999999999985
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4425000000000026 0.4928999999999988 0.4523999999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.5472999999999999
0.5172999999999988 0.4878000000000000 0.4281000000000006
0.4827000000000012 0.5122000000000000 0.5718999999999994

0.440100000000010	0.5429999999999993	0.513199999999977
0.5598999999999990	0.4570000000000007	0.486800000000023
0.4388999999999967	0.4652999999999992	0.526099999999996
0.561100000000033	0.5347000000000008	0.473900000000004
0.4866999999999990	0.4311999999999969	0.473500000000014
0.513300000000010	0.5688000000000031	0.5264999999999986

vasp

1.00000000000000

Cu	Sc	Ni
42	8	5

Direct

0.3868000000000009 0.4861000000000004 0.406199999999998
0.6131999999999991 0.5138999999999996 0.5938000000000017
0.4286999999999992 0.5516999999999967 0.4016000000000020
0.5713000000000008 0.4483000000000033 0.5983999999999980
0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001

0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.419899999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.398499999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.5133000000000010 0.5688000000000031 0.526499999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Sc Ni
42 9 4

Direct

0.3960961357071711 0.4874720120368708 0.4115506626090277
 0.5963493963301035 0.4814810542660640 0.5950539468469161
 0.4446912880031582 0.5406491647430430 0.4122652172749094
 0.5666531377169035 0.4226680984395207 0.6059705990024928
 0.3954458232808331 0.5321696870817909 0.4615404412534649
 0.6029347122432256 0.4548342103509282 0.5335583146055743
 0.3841345539312342 0.4630453749678647 0.4768619503532830
 0.5993493043111863 0.5171937338398663 0.5055140520828911
 0.4155041273806884 0.4244035482249562 0.4307741090206224
 0.5542678418397629 0.6188027680035649 0.5537291575725183
 0.4575483906811086 0.4675581326008366 0.3880786529325427
 0.5339181710495691 0.4897144462366231 0.6219457095692359
 0.5041012660817267 0.5833352021669673 0.3763590715654743
 0.4895971105199715 0.4361546501146101 0.6162543441564124
 0.4587476483317356 0.6070429091257551 0.4204999248708851
 0.5168211935956354 0.3866016313050094 0.5807521032695133
 0.4505537280776634 0.5702691042741495 0.4797118973722925
 0.5619680089576355 0.3973489684573088 0.5323090458170888
 0.3883401251390709 0.5783130756826390 0.5114981164157102
 0.6047321338719590 0.4128555706060375 0.4809516274425285
 0.3874174800682000 0.5118696759600770 0.5247022664253598
 0.6272475061625890 0.4734734241146832 0.4582398127342895
 0.3869381804463757 0.4461424806611969 0.5474344938437585
 0.6216991859891031 0.5421689926132837 0.4427329894882132
 0.4292949473855939 0.4166952943025823 0.5019248331352782

0.5731284989671805 0.5801824184214226 0.5027128449691072
 0.4718144730739125 0.3966148475093389 0.4536517310646341
 0.4897167811018676 0.6492356649349880 0.5508759463275265
 0.5105735726451708 0.4390956164764606 0.4202020070486877
 0.5031486518861239 0.5960217408722134 0.5916890017146866
 0.5473541603991745 0.4572104762619557 0.3682671835407541
 0.4625601739708332 0.4987992656570539 0.6152287657739519
 0.5708142993088403 0.5670754411840819 0.3919923659971537
 0.4526171975772126 0.4049220917920754 0.5652187924534411
 0.4741558288130925 0.6389780659569543 0.4794650776381069
 0.4950017047088532 0.3839237717932758 0.5169344244197829
 0.4317936250545033 0.6248500775092651 0.5277668752169020
 0.5404402145422446 0.3948846370935813 0.4661524794415507
 0.3967613793939893 0.5017188739473127 0.5898308972859221
 0.5833713923941477 0.4261416395789566 0.4178967516644707
 0.4210943718316528 0.4430000198218858 0.6091195912241600
 0.5882730113209895 0.4967131135986141 0.4037518884703004
 0.5117939486775589 0.5269538742339276 0.5034226033764849
 0.4522960276877823 0.4820877914543666 0.4579098402113122
 0.5687206339210610 0.5453752974538963 0.5692550459423467
 0.5230460029223535 0.5956200203092752 0.4480535197075521
 0.5326699199782778 0.4596712034926124 0.5578015084386413
 0.4414430114183572 0.5619214152505628 0.5600042398472979
 0.5572612323735326 0.4670518242133193 0.4699284020440873
 0.4508493782756607 0.4763170774921681 0.5470571944978331
 0.5151123589796613 0.5167232931957486 0.4004781130875485
 0.5595077769554203 0.5379325504542225 0.4514345626550174
 0.4949963597791808 0.4464432378439158 0.4964488180031214
 0.5012886154088263 0.5911392119502086 0.5232221980847300
 0.5040439995303380 0.5311322300701082 0.5740139901926041

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Ti Ni
 42 3 10

Direct

0.3958519618604779 0.4876744490786117 0.4142451363193776
 0.6022864825839002 0.5129317215456560 0.5856213280623557
 0.4356802207687911 0.5464213115301129 0.4115380378541789
 0.5630414841675145 0.4543213635201118 0.5855915644333446
 0.3905544607205609 0.5334018467569251 0.4678020333900605
 0.6094704760457612 0.4666113180736640 0.5320683893466877
 0.3895247758749964 0.4612255265422802 0.4796220270709241
 0.6079327704233587 0.5371508038758573 0.5194819111925760
 0.4336830808405440 0.4292449647339061 0.4306612323902669
 0.5644828063332215 0.5690833536637782 0.5674075556500786
 0.4621446638269331 0.4819868108645566 0.3884616861686816
 0.5363999560120084 0.5172822873843538 0.6090198115023971
 0.5043390922790499 0.5400347076448740 0.3923217236793973

0.4946225531336528 0.4591989299029731 0.6086592703036823
 0.4802586163706094 0.6015268291286764 0.4161344653463905
 0.5197986060572967 0.3987639040076151 0.5842577321633780
 0.4346979598455930 0.5900943502069080 0.4686137192336128
 0.5668172450858061 0.4068953017922902 0.5316509894795810
 0.3932444825947269 0.5771952468723590 0.5241190342387644
 0.6085361190784333 0.4225393192005990 0.4765453391280434
 0.3900003961686002 0.5075862549270401 0.5345689498500098
 0.6128360625626377 0.4919300157737109 0.4634842278954348
 0.3914433962852235 0.4383253034477654 0.5467016958109862
 0.6085938560356318 0.5619730925966326 0.4536482693035339
 0.4323603825642255 0.4071565706541539 0.4988909066446431
 0.5678075209904621 0.5940795446663045 0.5002873946685105
 0.4762333147459499 0.3782010688601388 0.4532912958258002
 0.5243241529802767 0.6239469722896082 0.5472631761207820
 0.5034846214827537 0.4274005498858555 0.4115690781155193
 0.4962557165936162 0.5742033432114159 0.5897698119652272
 0.5306872662476746 0.4787298540798683 0.3729241583824849
 0.4686802001702543 0.5218498573637653 0.6294864103228074
 0.5451888469961051 0.5823409301002750 0.4330735625900238
 0.4549470542250271 0.4169646634605687 0.5662660614314566
 0.5020173422569594 0.6143946800923682 0.4810001639601235
 0.4991891819071525 0.3866649182342007 0.5184214811941152
 0.4577046879261591 0.6020891994900417 0.5359918281126422
 0.5436829599113852 0.3955479819060306 0.4626542364988209
 0.4293987775207142 0.5502278219900997 0.5774915290730659
 0.5721764116609911 0.4480736610886656 0.4205782844695623
 0.4284715491224336 0.4795129183053958 0.5891908098811000
 0.5713535100559538 0.5193982933807146 0.4120080681121053
 0.4998264201052239 0.5040447246669467 0.5049860903406704
 0.4476993538169631 0.4931811665990444 0.4560525566958221
 0.5546159635241563 0.4603055052530812 0.4874735171854939
 0.5522748964833526 0.5061472952245852 0.5432050149157351
 0.4888808291011431 0.5507620361479794 0.4575751827198525
 0.5111843789631835 0.4490356052882697 0.5421952958827800
 0.4455961869188945 0.5390062991834021 0.5117566010815543
 0.4448229654613490 0.4693889001822469 0.5226927845384995
 0.5552782376732056 0.5303170288644125 0.4771198763445794
 0.4884276671038013 0.4394625212119989 0.4762733115375022
 0.5122598650137125 0.5637268039252441 0.5247155792197361
 0.5152193347524950 0.4891082441891572 0.4367561564842012
 0.4837088787690977 0.5113320271329039 0.5668136458710390

vasp

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

Cu Ti Ni
42 6 7

Direct

0.3977258719790326 0.4864513863616919 0.4132097767450476

0.6018872697222654 0.5128102888533973 0.5851152882442272
0.4384850862565318 0.5468108560483471 0.4117827327408374
0.5626601085828793 0.4541660639133230 0.5887349067052241
0.3936509690016884 0.5329099577292739 0.4686755949582745
0.6073786715698413 0.4670813806100665 0.5318349118826535
0.3909263255719433 0.4607390830412164 0.4817539037610704
0.6090598273743630 0.5396479873025783 0.5202530513773047
0.4334131870419720 0.4274409134896646 0.4309457007278125
0.5657273457952655 0.5710896819625945 0.5687338409749031
0.4637740610452133 0.4826201431446650 0.3868014854610397
0.5368548628078840 0.5179891529655749 0.6114679595615401
0.5046527760211778 0.5415468896237956 0.3859870177171626
0.4925138761752320 0.4581445380339143 0.6085072018013744
0.4831662706238550 0.6049239831591942 0.4120106240493074
0.5207592151062389 0.3974465173954775 0.5845885604263985
0.4361297395721324 0.5917172207711667 0.4671913098780618
0.5644758515857639 0.4095877297568305 0.5311346927240520
0.3934625555670372 0.5784384317788523 0.5251353787792602
0.6057396602604779 0.4230565032781915 0.4758626877339173
0.3895227649232430 0.5061533891824785 0.5366177207809815
0.6095404821053810 0.4922971322220889 0.4649826834313779
0.3901085660842525 0.4331713317230527 0.5501090955731994
0.6099195763487369 0.5615607690842357 0.4529924332126871
0.4283491392253197 0.4022302711863936 0.4977298800285125
0.5667556573006484 0.5951832688659242 0.4976846740148491
0.4772307427603857 0.3751081222349364 0.4527622688581364
0.5249138346441063 0.6234932168578282 0.5466938801595294
0.5025186503811822 0.4272859836279504 0.4109822281591102
0.4955351437456210 0.5732284781622916 0.5881992091855275
0.5331709878555049 0.4775187666733200 0.3704819403504320
0.4691262808144623 0.5212392630658567 0.6294299851187574
0.5510605115828389 0.5908130207177609 0.4280690258576216
0.4526313587102090 0.4096132325924064 0.5745941128689943
0.5009398624870578 0.6196432878321325 0.4802655347888421
0.4948135414986226 0.3850636233416232 0.5206858995562549
0.4574832667276185 0.6064923280044962 0.5366671658509770
0.5416897279639622 0.3979281913162287 0.4643310436991394
0.4269194345611691 0.5506660566222642 0.5813716936856268
0.5703663903954707 0.4502870644244147 0.4224590641598595
0.4247572131752956 0.4791140852376119 0.5932891524705408
0.5702729656311860 0.5237756988536844 0.4093959197248683
0.4990706112729085 0.4982650798107128 0.4972729098584239
0.4500829715654353 0.4908058436232988 0.4547976964324144
0.5492168637807360 0.5070050284504845 0.5424200813795828
0.4989479809095059 0.5559742153322323 0.4535988360229797
0.4478853318969847 0.5413284801164349 0.5161339741948007
0.4468182240146838 0.4606137528363770 0.5303464833514581
0.5099960053488336 0.4474804318634422 0.5435816041818016
0.5533937787340836 0.4610289154132625 0.4879590688840493
0.5559951102482485 0.5318315551633992 0.4756866635826217
0.4860050160664152 0.4351940217391803 0.4765476860952851
0.5127656395361031 0.5635198366821595 0.5233529584840022

0.5164633113402303 0.4903414101439745 0.4322655182524419
0.4832895247027653 0.5101261377762443 0.5665152814948465

vasp

1.000000000000000

Cu Ti Ni

42 9 4

Direct

0.3935285035705987	0.4886021210640245	0.4133568495463706
0.6032462805136839	0.5163809564296959	0.5871025126549313
0.4401905889654691	0.5464860421118387	0.4094440146296934
0.5636066151418470	0.4552601041271520	0.5835259094688150
0.3894715507090031	0.5326215007302961	0.4715355535014633
0.6106132379777488	0.4704903838315801	0.5323048820178669
0.3893198841189139	0.4603949014699663	0.4800833530492198
0.6121995866415092	0.5405253210864757	0.5198703068553715
0.4318396830023802	0.4282387772012226	0.4295269406521126
0.5677900152893099	0.5755965824093238	0.5719796289133514
0.4616885473450620	0.479926667800017	0.3865445171960091
0.5374558076820062	0.5171918833783734	0.6126074486441196
0.5080152830918321	0.5432762816444625	0.3873704276779613
0.4933922986717256	0.4584114435266225	0.6138070924941030
0.4811675911186674	0.6055934478186650	0.4152979262808293
0.5180690248079342	0.3969277408818728	0.5884397446196041
0.4336137431755762	0.5880095466383490	0.4690371520284299
0.5617271142079733	0.4041316077838185	0.5312130679424552
0.3917318907999102	0.5776717400444460	0.5271629256160340
0.6113115117177430	0.4218486033936398	0.4778597286904629
0.3853470162311675	0.5071785769108274	0.5380006502713911
0.6130428830075119	0.4928588041446938	0.4628273997472094
0.3895250883924119	0.4376987742474290	0.5481570375779040
0.6102027141710538	0.5641652079458580	0.4537570025006230
0.4303941792158164	0.4041914556111907	0.4997416549056301
0.5676574416329792	0.5945676549920751	0.5013614051783167
0.4742121235341092	0.3707810441774738	0.4501619060900134
0.5233637692277918	0.6232809105128392	0.5485336059478183
0.5041458949918693	0.4215433914244897	0.4042136012518449
0.4960170648575666	0.5738575548328271	0.5895782762400319
0.5341247060564444	0.4779294605047691	0.3653899490559255
0.4691061847935823	0.5228835735941250	0.6290395601306004
0.5493984325244224	0.5880664801066645	0.4297770575469254
0.4501778833704669	0.4118515812847673	0.5702717494512863
0.5028221114896910	0.6197267240962692	0.4814218358074006
0.4956850425941881	0.3807501543805161	0.5202537516422210
0.4563275711194651	0.6053181006013423	0.5364840554164850
0.5454733500619544	0.3945788897532364	0.4599825278245090
0.4252523549433613	0.5528140166470171	0.5843446326122730
0.5750331287970132	0.4481224538165771	0.4196757833134132
0.4285151021781047	0.4799731301754079	0.5894933645630349

0.5737680654638913	0.5215038469892939	0.4094942068368876
0.5002675929265797	0.4959322599088031	0.4952136749987762
0.4448610710718544	0.4943154728206969	0.4547529855512352
0.5517643819462418	0.5156489123164899	0.5442261155320318
0.4954677704963781	0.5560292279864364	0.4569370942159995
0.5039103117512824	0.4468312422651993	0.5469078749207146
0.4456035390031792	0.5381183601380081	0.5212775382709302
0.5577152673181508	0.4589665540612639	0.4889516670464810
0.4878515044031254	0.4314216470056785	0.4718845495273996
0.5168449529367173	0.4865341583677716	0.4282696565142067
0.4421767408524891	0.4678747524489925	0.5245573273733078
0.5575781745743678	0.5328129688625386	0.4759591102910055
0.5110318996511753	0.5637150047330047	0.5241898376205812
0.4853559258646993	0.5105719999836033	0.5668415717463801

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu V Ni
42 3 10

Direct

0.3975015278802655 0.4881927935381856 0.4152174610628692
0.6024120311736620 0.5124919619242667 0.5850519002419012
0.4370089472500112 0.5458922394113321 0.4118485319313683
0.5625100117045777 0.4545207260572796 0.5861809022906017
0.3914431308734108 0.5330131171821644 0.4683499847550548
0.6065765458456721 0.4671108076509861 0.5317006622775033
0.3911508765020984 0.4617450089174733 0.4800378916698391
0.6079995046301611 0.5377301590567858 0.5195830460484828
0.4335763294280675 0.4290452725668369 0.4310397719358914
0.5644725011318381 0.5688988798512333 0.5674962564541184
0.4630279521849993 0.4821365726957880 0.3905211838132444
0.5364319617522518 0.5173126973294744 0.6087972258322286
0.5050532526034306 0.5403898053036617 0.3920811226397930
0.4944987392521265 0.4594056573587379 0.6078498199559521
0.4804702416484984 0.6015734698660867 0.4162978659351960
0.5203889102770305 0.3991636079520173 0.5843197082262980
0.4349796627180008 0.5903443311064643 0.4683346317747795
0.5641228716308966 0.4087005678527411 0.5306431287521859
0.3941403093336004 0.5771220506935734 0.5236688028112312
0.6067480764116493 0.4238621639220098 0.4771073497981912
0.3904545454492725 0.5078965910346535 0.5347508108592828
0.6096231351725834 0.4921437708094634 0.4646266539761135
0.3916087372240706 0.4393095711936567 0.5470168007116407
0.6093072857619620 0.5615543817101003 0.4534886511838207
0.4315725905077029 0.4051250074737951 0.4996858165526420
0.5679238120592683 0.5940027036864155 0.5001337330570749
0.4764413028231164 0.3770478549332041 0.4532486998343731
0.5243974558100331 0.6228283944416159 0.5471066593106571
0.5034771540857731 0.4254066139617665 0.4101570922213713

0.4962994878749601 0.5739816631318261 0.5893064423190340
 0.5315099757728953 0.4788271431753421 0.3729922314879712
 0.4690311117546370 0.5219262349266227 0.6281128082397909
 0.5453319175018601 0.5827884776148367 0.4330336885710385
 0.4548205929357405 0.4169714891101060 0.5664566432687881
 0.5020342745313522 0.6142544826272001 0.4811113089860604
 0.4974030148707984 0.3838121475410805 0.5194308952404063
 0.4581259763360667 0.6020147212463283 0.5358561378128777
 0.5428068209307848 0.3969878485894089 0.4630924474944455
 0.4299176595108219 0.5501029127656623 0.5767067875357221
 0.5697132839856597 0.4496953495575319 0.4234592838758970
 0.4287197249912899 0.4798688884010909 0.5889881692480341
 0.5714638617460402 0.5203185531681314 0.4111667552718091
 0.5029410082006179 0.5031853456751106 0.5030915937223623
 0.4491970913895140 0.4934994797443010 0.4578923600239103
 0.4877318185986836 0.4391880198694054 0.4764302905218689
 0.5521852818407404 0.5064558641179456 0.5433021400628333
 0.4890101488758556 0.5505709193679889 0.4577129764316234
 0.5100941135282685 0.4485333642580406 0.5412721872139916
 0.4464378019530792 0.5387390342714171 0.5107116181728975
 0.5529825299822224 0.4608450762311551 0.4886287709960032
 0.4457716786770901 0.4693701333002961 0.5229761466283945
 0.5552210565143989 0.5313482300944627 0.4764136374545949
 0.5123917642285545 0.5624862481995114 0.5241357167215339
 0.5151293622615788 0.4890278011406826 0.4364558613193530
 0.4844092380804586 0.5112337923927464 0.5649209354650505

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu V Ni
 42 6 7

Direct

0.3992461017459327 0.4865779963749144 0.4162387154984681
 0.6006219802088022 0.5121649205703060 0.5833416976334778
 0.4374260642511054 0.5459022825183339 0.4137632215040940
 0.5627517465356437 0.4540682058464121 0.5871258142340171
 0.3935665218665868 0.5333230427846569 0.4687905051220322
 0.6075021175455440 0.4668202895588298 0.5312866404850103
 0.3915177627824103 0.4621963246145627 0.4807188142213552
 0.6076318994268194 0.5379781908588298 0.5196290662920213
 0.4351643357768519 0.4287548150972214 0.4318440686329035
 0.5644031766007533 0.5697823719804168 0.5674574634665090
 0.4636530622643744 0.4825720221744152 0.3907356414570852
 0.5364824884985793 0.5176940885732538 0.6084935996563776
 0.5058499288369454 0.5403589290586951 0.3920103489195788
 0.4948634970057477 0.4589451148475138 0.6078306228574631
 0.4809702881413282 0.6025145552756340 0.4139961105676800
 0.5203864594341344 0.3971971837974885 0.5841871269327382
 0.4337669822243820 0.5952350375999864 0.4687217386943009

0.5655129158559444	0.4082797017855105	0.5315543425869510
0.3918665819625167	0.5773119517422122	0.5250902946415634
0.6066694546738267	0.4217680956735264	0.4764501761044579
0.3905996419954960	0.5078346842768996	0.5358238494004288
0.6095236979761411	0.4915321744414435	0.4646024378038842
0.3916277057868736	0.4373028951890949	0.5470717853030130
0.6093208086361720	0.5603027273606747	0.4531494542996991
0.4321094109825160	0.4054951663375770	0.4994396566678604
0.5676239928013685	0.5942712273325670	0.4998131436733733
0.4767466209016760	0.3749822579795649	0.4534128132392772
0.5245532570572844	0.6251991012112972	0.5474027921662956
0.5035477474369842	0.4250929673141428	0.4107236056365366
0.4959962644890140	0.5742108944093943	0.5888825484707221
0.5319522379668045	0.4766097867961299	0.3723566865757613
0.4690621378704322	0.5206623654525488	0.6278381037816558
0.5463867634875433	0.5850364233983973	0.4323155330728532
0.4548818400120954	0.4158861681513154	0.5672101360266948
0.5020675026377838	0.6213570613222976	0.4795056651146238
0.4981355604441839	0.3839955886313665	0.5192849653769824
0.4551320441139954	0.6082396975733825	0.5380169222527513
0.5426457226317265	0.3965409603430624	0.4639743899232835
0.4287712194747140	0.5519777209931793	0.5791513672925919
0.5707821264624660	0.4485719362143011	0.4228403062668043
0.4281402710400173	0.4796612133657069	0.5890602727237054
0.5713644786524039	0.5201805685525824	0.4104480456787790
0.5006910714183660	0.4965330497059607	0.4997940061697845
0.4522732848333707	0.4917095624410002	0.4598093691422239
0.5471191287364242	0.5055858684800552	0.5390774421110159
0.4901140315265858	0.5542656683834525	0.4596321401891279
0.4478923986804251	0.5424328160127423	0.5129249452116340
0.5084790202514310	0.5657076996570888	0.5214592130563614
0.5109083001035077	0.4471962596598157	0.5427194886637225
0.5543668606557082	0.4597265603808009	0.4885711613932323
0.4453493219053594	0.4676208327678312	0.5240011105765340
0.5545059551338937	0.5309029447261234	0.4753231893857622
0.4878304050161974	0.4356591815806539	0.4756041865081039
0.5163427359566898	0.4876440687382954	0.4351538936442987
0.4833030672861199	0.5106267800865343	0.5643393636925353

vasp

1.00000000000000

35.000000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	35.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	35.0000000000000000

Cu V Ni
42 9 4

Direct

```

0.4000660753173164 0.4881904724456814 0.4179749300822059
0.5990117934469206 0.5110523250506049 0.5807817114092295
0.4378566243623553 0.5471595313076048 0.4140580816184501
0.5612814957843552 0.4523004096698464 0.5851034740368490
0.3900300711789390 0.5352804031740914 0.4687162971470951

```

0.6076149568857497 0.4658006356743408 0.5293384229550255
0.3901084816471566 0.4613618950449482 0.4814332698257350
0.6062894459404183 0.5386652832620010 0.5166614715304046
0.4376555651255105 0.4316538307223023 0.4356385838142158
0.5632013071378603 0.5683631099637304 0.5667176667769979
0.4643553670645416 0.4837010848050030 0.3952862148524597
0.5355732741852238 0.5167694297531044 0.6071418866543562
0.5066509134168669 0.5415389184613518 0.3917694990807064
0.4939682263723763 0.4588001308749129 0.6085489912982449
0.4794749773886978 0.6040184715104100 0.4143888897887728
0.5194407351718948 0.3950819127525113 0.5859819741311038
0.4335403881524282 0.5947363648386607 0.4680659220535385
0.5643438219213680 0.4064934497132780 0.5311159539534769
0.3929217393193267 0.5794524973155564 0.5241481580832781
0.6098909727999376 0.4217631457957876 0.4747506795903255
0.3891498476779844 0.5089921748477431 0.5368905128722328
0.6090214981866292 0.4926797382339436 0.4619906214846686
0.3898340949970569 0.4380186556003050 0.5476605360372343
0.6093987696551936 0.5637353421894561 0.4509781479190067
0.4332935232641233 0.4028843228410445 0.5014923692015300
0.5671456783578156 0.5959559966546338 0.4988052426055691
0.4779270475731345 0.3754021589150829 0.4524552121052755
0.5247844060276358 0.6246140750563042 0.5487348244517223
0.5035889212767866 0.4250555259935702 0.4109878451217741
0.4955819031489086 0.5744196330490811 0.5896561685992981
0.5297770371790075 0.4776344343398393 0.3734876493897169
0.4687703704229421 0.5222185238951419 0.6285812164929657
0.5471997986188504 0.5906498552443029 0.4284880023294267
0.4507783634609002 0.4125608955106270 0.5727272547519264
0.5009428600779466 0.6190169710677482 0.4809028515591587
0.4998335717709355 0.3764735625377180 0.5192077311918377
0.4564017171200138 0.6053553152436948 0.5374213829761668
0.5454398196294850 0.3925116880456521 0.4619888448896146
0.4281327742795011 0.5520698768776677 0.5779824965255804
0.5707510589303888 0.4483963687907143 0.4208133475483709
0.4271801916659192 0.4787615972357820 0.5905546871986562
0.5735056065324516 0.5205286341290584 0.4061477373311921
0.5120879923467944 0.5008232901678227 0.5081012947088369
0.4504585434489569 0.4973095940007791 0.4653860757282756
0.5467061644784020 0.5034391531756194 0.5354904044629499
0.4929504931440618 0.5550470527106460 0.4578911519332601
0.5043127434218441 0.4420734833318393 0.5413775135072656
0.4466078020238359 0.5402638919281193 0.5098888219106170
0.4457791621354016 0.4673744805352879 0.5237993445873832
0.5524483168541280 0.5352812295262759 0.4688845771381087
0.4927844925120902 0.4356120559228165 0.4803870175891828
0.5562490150281140 0.4553533244388899 0.4853561632128065
0.5099802527240705 0.5667494528504885 0.5240780298290365
0.5170003603500406 0.4883980883140583 0.4382966176511151
0.4809195690594088 0.5121562546625213 0.5654862264757677

vasp

1.00000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Zn Ni

42 3 10

Direct

0.3978742150180190 0.4874977374466959 0.4152821124399261
0.6021257849819809 0.5125022625533040 0.5847178875600735
0.4376272418978465 0.5453612899264418 0.4139738334242042
0.5623727581021533 0.4546387100735583 0.5860261665757958
0.3928894393749048 0.5328056425135687 0.4682744525840449
0.6071105606250954 0.4671943574864317 0.5317255474159552
0.3925758086998344 0.4622046955842563 0.4805257657865153
0.6074241913001658 0.5377953044157434 0.5194742342134847
0.4357647453530469 0.4311480749752894 0.4325989634654626
0.5642352546469535 0.5688519250247105 0.5674010365345374
0.4634487298903587 0.4826366933165778 0.3912903590826140
0.5365512701096415 0.5173633066834223 0.6087096409173862
0.5052474039831896 0.5407330929579306 0.3915063145670735
0.4947525960168102 0.4592669070420691 0.6084936854329261
0.4798200825377533 0.6014022771392069 0.4158675704419575
0.5201799174622470 0.3985977228607931 0.5841324295580425
0.4351517845643902 0.5914307447221503 0.4687085295213357
0.5648482154356097 0.4085692552778496 0.5312914704786643
0.3934321053729090 0.5765646713473948 0.5235432862881561
0.6065678946270914 0.4234353286526049 0.4764567137118440
0.3895761609391906 0.5073870844956049 0.5357966738009714
0.6104238390608094 0.4926129155043950 0.4642033261990287
0.3911678421006176 0.4383171184428730 0.5463659772879759
0.6088321578993825 0.5616828815571271 0.4536340227120240
0.4322987108538831 0.4060996005441616 0.4996222431620695
0.5677012891461171 0.5939003994558386 0.5003777568379306
0.4759837583220484 0.3776056339419429 0.4529562007501988
0.5240162416779514 0.6223943660580574 0.5470437992498013
0.5036499952434433 0.4264742268718415 0.4108521799677396
0.4963500047565567 0.5735257731281584 0.5891478200322604
0.5307219778554748 0.4783818916012655 0.3722180879598324
0.4692780221445254 0.5216181083987348 0.6277819120401676
0.5453442486381176 0.5832900380594193 0.4330503740216605
0.4546557513618825 0.4167099619405810 0.5669496259783394
0.5019364516410586 0.6139493420447113 0.4811784317107554
0.4980635483589413 0.3860506579552886 0.5188215682892445
0.4578221366579948 0.6022504395572653 0.5364268626379655
0.5421778633420054 0.3977495604427346 0.4635731373620344
0.4296259335970839 0.5502759505959257 0.5778798771559115
0.5703740664029163 0.4497240494040742 0.4221201228440887
0.4289040692598438 0.4796062008925525 0.5888050843137589
0.5710959307401562 0.5203937991074473 0.4111949156862412
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4465082080872168 0.5384194104295184 0.5117946074598605
0.5534917919127832 0.4615805895704821 0.4882053925401394

0.4481696472709559 0.4934829861791613 0.4569358065803495
 0.5518303527290445 0.5065170138208387 0.5430641934196505
 0.4899367785765239 0.5514063672634013 0.4570869194712803
 0.5100632214234763 0.4485936327365986 0.5429130805287197
 0.4450865538514349 0.4684030571291731 0.5237677462203392
 0.5549134461485649 0.5315969428708271 0.4762322537796612
 0.4878580139527562 0.4379601871302463 0.4760536723974811
 0.5121419860472437 0.5620398128697538 0.5239463276025187
 0.5153187571241956 0.4891513394120748 0.4350346330263210
 0.4846812428758043 0.5108486605879250 0.5649653669736789

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Zn Ni
42 6 7

Direct

0.3972238993618444 0.4875376146828483 0.4142823348311881
 0.6035944314460396 0.5121165867086097 0.5844186563436122
 0.4372717220932488 0.5462908992815390 0.4122001550344989
 0.5629749194164468 0.4546503615338648 0.5873858475762973
 0.3925943367468860 0.5326042174054803 0.4678457799440701
 0.6084999596209255 0.4663265989521119 0.5307814426070998
 0.3900185763383913 0.4610628699063304 0.4795676704934549
 0.6100144116866720 0.5381750810998051 0.5189622725039166
 0.4344380028584583 0.4298600480418286 0.4319164734530204
 0.5654793357684549 0.5689599747175664 0.5680904320720250
 0.4631695938453474 0.4824383238885011 0.3894846452504097
 0.5378578147574351 0.5180031717698843 0.6100210082513843
 0.5053762498036309 0.5411716984602405 0.3908151677343590
 0.4947306311778658 0.4598973073241933 0.6098754407040340
 0.4802764077003470 0.6020385100638306 0.4162674889146034
 0.5199780835337140 0.3991350329412408 0.5845110253885610
 0.4352370366684121 0.5912084248006972 0.4685857373687264
 0.5641246270389040 0.4098225046837012 0.5312767316640419
 0.3938691102611394 0.5762124818371170 0.5229618066299077
 0.6057463983242259 0.4227541072387901 0.4760624191047849
 0.3890567750759244 0.5072997021421887 0.5354480831950158
 0.6099294621679361 0.4917672539055075 0.4640351814672953
 0.3902410822414681 0.4380985373874936 0.5465121110146925
 0.6095007916721744 0.5613505653582623 0.4533032336424038
 0.4309582969916869 0.4044931651001294 0.4994305039829069
 0.5680814346283473 0.5934519145951427 0.5005780724373373
 0.4758802482185523 0.3774617748058436 0.453241125682111
 0.5242519903438478 0.6221488503615987 0.5473663520916403
 0.5031771824633079 0.4264637445131080 0.4108673683629784
 0.4968058547181490 0.5749050319815376 0.5908422056884536
 0.5307875800809995 0.4781607344221656 0.3720275657129970
 0.4689356825803289 0.5225915591095096 0.6285929385402063
 0.5466240607768135 0.5842515850900906 0.4324920408490134

0.4540623936718469	0.4164313530812541	0.5683235481240351
0.5026864808010595	0.6158265343501289	0.4816794733511938
0.4974561105725138	0.3867301107345361	0.5193948644724975
0.4581477992543950	0.6007916212900907	0.5361255923338777
0.5416127527428510	0.3982012434709555	0.4639092686680432
0.4285905328089073	0.5504794478889049	0.5775627013019778
0.5696164270720666	0.4495290852811799	0.4226650100024936
0.4273377002141265	0.4796659087556732	0.5905048644144759
0.5712489985105810	0.5203016989575053	0.4107929875413461
0.5011835177894204	0.4993838360932706	0.4993706792050687
0.4481319798870423	0.4929542197829543	0.4556633284971872
0.5536925779321984	0.5060245334765735	0.5415688336445619
0.4915217986043654	0.5523528471622230	0.4583182311216106
0.4445793275181426	0.4674749559824740	0.5236301305673646
0.4841630603974401	0.5123100113789143	0.5653034670038590
0.5096122445064939	0.4496066410527560	0.5443678340004314
0.4454474204369926	0.5378231205130328	0.5111635213145621
0.5540629745574452	0.4606924359793453	0.4880413972266069
0.5560156401635584	0.5316085834921082	0.4758875515007899
0.4866994323331122	0.4378191279175997	0.4760862981677771
0.5124755600708540	0.5618366445160402	0.5252086679001816
0.5149492797466626	0.4894458047317205	0.4343824442169119

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu Zn Ni
42 9 4

Direct

0.3956402138754160	0.4863555993825392	0.4144987503351793
0.6039962537133980	0.5119202239599729	0.5862564996071252
0.4357327046356880	0.5449905922902837	0.4125913550449669
0.5635065160037234	0.4530313595740516	0.5883120373231822
0.3908484503309407	0.5327338555658065	0.4683057632558699
0.6087352583402578	0.4668157516712954	0.5321381097086246
0.3891845904708014	0.4612815950460018	0.4805639851258753
0.6102417893097155	0.5387214840792466	0.5207424198639056
0.4344500675131966	0.4290246166550430	0.4306052750164877
0.5667377649074565	0.5700105539771658	0.5685992222770433
0.4623127961533060	0.4816751903597952	0.3895554474714232
0.5378155234320647	0.5177459013610330	0.6104676654810691
0.5047616899323433	0.5398807576474993	0.3901025752433506
0.4952831368725656	0.4592185653377834	0.6088095151540042
0.4786542702307767	0.6020018355765274	0.4146356316259791
0.5194701545404742	0.3980581998733583	0.5837779323346298
0.4332866280950860	0.5911772465767529	0.4691248846213904
0.5651337988872064	0.4091142268871300	0.5316001446361696
0.3918103509046379	0.5765473076247785	0.5246762962985549
0.6064385838241143	0.4236708645102733	0.4770389271799671
0.3869717273805868	0.5074072127793086	0.5363044966331976

0.6126856761969343 0.4919531585348938 0.4640700830022888
0.3911451626909327 0.4386957059229867 0.5465930051116586
0.6106301182202116 0.5617838720835950 0.4534511258447757
0.4322124117499314 0.4066700518671615 0.4991209702996752
0.5689772115285979 0.5950214032093017 0.5005100602191762
0.4763804313848565 0.3777404398600882 0.4527404955747679
0.5247344837844113 0.6238848005862193 0.5478448295527958
0.5032713982412426 0.4243566930487222 0.4082796893066964
0.4968597323261862 0.5751862742574169 0.5915397225398547
0.5311052302989164 0.4771229544488516 0.3708403084690229
0.4700474098372265 0.5216451853027259 0.6277332052329593
0.5461524652608265 0.5840151355603570 0.4321089002504304
0.4535532290918064 0.4161077417227006 0.5673463740807350
0.5017025587291712 0.6162553907859664 0.4809553441874850
0.4976499324758165 0.3841709568346117 0.5184560717775016
0.4567322071477902 0.6036905243535821 0.5368987881946349
0.5422992052830091 0.3992932338839367 0.4636654301915576
0.4295100348874981 0.5518249798379207 0.5797003101514865
0.5725419621584728 0.4491647996800548 0.4216762743827507
0.4291540693191535 0.4806776667238280 0.5884703985303578
0.5726062325419266 0.5203706754474142 0.4091075101448894
0.4995896529440710 0.4999224628546282 0.4997679610763127
0.4456469251582255 0.4910410665987319 0.4566484282352168
0.5534093013767082 0.5054305521261415 0.5447995815615415
0.4890457701377695 0.5530630503911561 0.4558061590844645
0.5083582372268237 0.4476593926618166 0.5416130534198214
0.4438615436885379 0.5383678015827397 0.5144208878296965
0.5576484959862771 0.5311915742143242 0.4759674014576724
0.5123647687293037 0.5638018267092397 0.5257686303299178
0.5166693990601492 0.4862859497274575 0.4339856901740554
0.5550145145284984 0.4623854146407574 0.4885988156685876
0.4436880972739290 0.4695233130384585 0.5231042964750012
0.4877419486196832 0.4381536086556295 0.4746118580481901
0.4859979127613498 0.5121594021109362 0.5650914053560273

vasp

1.000000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.00000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.00000000000000

Cu	Sc	Ni
42	10	3

Direct

0.3868000000000009	0.4861000000000004	0.4061999999999983
0.6131999999999991	0.5138999999999996	0.5938000000000017
0.4286999999999992	0.5516999999999967	0.4016000000000020
0.5713000000000008	0.4483000000000033	0.5983999999999980
0.3783999999999992	0.5373000000000019	0.4643000000000015
0.6216000000000008	0.4626999999999981	0.5356999999999985
0.3772000000000020	0.4568000000000012	0.4776999999999987
0.6227999999999980	0.5431999999999988	0.5223000000000013

0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.3984999999999985
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4425000000000026 0.4928999999999988 0.4523999999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.5472999999999999
0.4401000000000010 0.5429999999999993 0.5131999999999977
0.5611000000000033 0.5347000000000008 0.4739000000000004
0.4866999999999990 0.4311999999999969 0.4735000000000014
0.5133000000000010 0.5688000000000031 0.5264999999999986
0.4827000000000012 0.5122000000000000 0.5718999999999994
0.5598999999999990 0.4570000000000007 0.4868000000000023
0.4388999999999967 0.4652999999999992 0.526099999999996
0.5172999999999988 0.4878000000000000 0.4281000000000006

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000

0.000000000000000 0.000000000000000 35.000000000000000

Cu Sc Ni
42 1 12

Direct

0.3868000000000009 0.4861000000000004 0.406199999999983
0.6131999999999991 0.5138999999999996 0.5938000000000017
0.4286999999999992 0.5516999999999967 0.4016000000000020
0.5713000000000008 0.4483000000000033 0.598399999999980
0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.535699999999985
0.3772000000000020 0.4568000000000012 0.477699999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.576799999999986
0.4585000000000008 0.4799999999999969 0.376199999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.376399999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.593299999999993
0.4260999999999981 0.6036000000000001 0.464599999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.459299999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.448599999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.500399999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.552199999999991
0.504199999999973 0.4159999999999968 0.398099999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.641599999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.576099999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.521599999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.458899999999999
0.4198999999999984 0.5572000000000017 0.588099999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.398499999999985
0.4401000000000010 0.5429999999999993 0.513199999999977
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4425000000000026 0.4928999999999988 0.452399999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.547299999999999

0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.526499999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.57189999999994

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni
42 11 2

Direct

0.3868000000000009 0.4861000000000004 0.406199999999983
 0.613199999999991 0.513899999999996 0.5938000000000017
 0.428699999999992 0.551699999999997 0.4016000000000020
 0.5713000000000008 0.448300000000033 0.598399999999980
 0.378399999999992 0.537300000000019 0.4643000000000015
 0.6216000000000008 0.462699999999981 0.535699999999985
 0.3772000000000020 0.456800000000012 0.477699999999987
 0.622799999999980 0.543199999999988 0.5223000000000013
 0.426699999999967 0.421399999999984 0.4232000000000014
 0.5733000000000033 0.578600000000016 0.576799999999986
 0.4585000000000008 0.479999999999969 0.376199999999972
 0.541499999999992 0.520000000000031 0.6238000000000028
 0.506199999999998 0.546399999999984 0.376399999999967
 0.4938000000000002 0.453600000000016 0.6236000000000033
 0.477499999999991 0.612200000000014 0.4067000000000007
 0.5225000000000009 0.387799999999986 0.593299999999993
 0.426099999999981 0.603600000000001 0.464599999999972
 0.5739000000000019 0.396399999999999 0.5354000000000028
 0.3819000000000017 0.584800000000013 0.5259000000000000
 0.618099999999983 0.415199999999987 0.4741000000000000
 0.3746000000000009 0.508600000000013 0.5407000000000011
 0.625399999999991 0.491399999999987 0.459299999999989
 0.3796000000000035 0.431600000000031 0.5514000000000010
 0.620399999999965 0.568399999999969 0.448599999999990
 0.422899999999985 0.392800000000011 0.4996000000000009
 0.5771000000000015 0.607199999999989 0.500399999999991
 0.4737000000000009 0.364400000000034 0.4478000000000009
 0.526299999999991 0.635599999999966 0.552199999999991
 0.504199999999973 0.415999999999968 0.398099999999995
 0.4958000000000027 0.584000000000032 0.6019000000000005
 0.534199999999985 0.475999999999991 0.3584000000000032
 0.4658000000000015 0.524000000000009 0.641599999999968
 0.551499999999972 0.594900000000026 0.4239000000000033
 0.4485000000000028 0.405099999999974 0.576099999999967
 0.501899999999991 0.630299999999983 0.4784000000000006
 0.4981000000000009 0.369700000000017 0.521599999999994

0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.3984999999999985
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4425000000000026 0.4928999999999988 0.4523999999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.4401000000000010 0.5429999999999993 0.5131999999999977
0.5598999999999990 0.4570000000000007 0.4868000000000023
0.4388999999999967 0.4652999999999992 0.5260999999999996
0.5611000000000033 0.5347000000000008 0.4739000000000004
0.4866999999999990 0.4311999999999969 0.4735000000000014
0.5133000000000010 0.5688000000000031 0.5264999999999986
0.5172999999999988 0.4878000000000000 0.4281000000000006
0.4827000000000012 0.5122000000000000 0.5718999999999994
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.5472999999999999

vasp

1.00000000000000

Cu	Sc	Ni
42	2	11

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
0.6131999999999991 0.5138999999999996 0.5938000000000017
0.4286999999999992 0.5516999999999967 0.4016000000000020
0.5713000000000008 0.4483000000000033 0.5983999999999980
0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990

0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.5514999999999972 0.5949000000000026 0.4239000000000033
 0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.5260999999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994

vasp

1.00000000000000		
35.00000000000000	0.00000000000000	0.00000000000000
0.00000000000000	35.00000000000000	0.00000000000000
0.00000000000000	0.00000000000000	35.00000000000000

Cu Sc Ni
42 3 10

Direct

0.3944235625601286 0.4860853384089390 0.4126085327566774
 0.6042772856102432 0.5124759759917787 0.5865552000415915
 0.4362077506359087 0.5463943387539379 0.4116643570094914
 0.5627897902314214 0.4542408560246560 0.5872430274319116
 0.3911269849745586 0.5341300622144342 0.4670202874880395
 0.6070530401874952 0.4668854658559447 0.5313627696222916
 0.3839526183407466 0.4600106076272100 0.4808097413683004
 0.6089891528457367 0.5379839087825955 0.5203463415341761
 0.4327982038274480 0.4251125782749263 0.4274566995564581
 0.5658806966088835 0.5692459875703156 0.5680248233229206
 0.4622920758636864 0.4828016442600771 0.3887353768890583
 0.5365036497239186 0.5178117503785705 0.6094011889214607

0.5042589517980803 0.5413400091437427 0.3890335894724796
0.4942656050901206 0.4592996199004963 0.6092985447911177
0.4802853961791158 0.6051942968979845 0.4136029017335563
0.5202825251918211 0.3966273653025454 0.5859791115664609
0.4331771512464860 0.5924479473998447 0.4671850888535641
0.5647777218108937 0.4084017750029856 0.5311564098382932
0.3935765096287235 0.5768206305418383 0.5238436231179876
0.6079474009907887 0.4219930189241559 0.4758430102188635
0.3904785028481934 0.5074932740742747 0.5334160964856443
0.6110309385069074 0.4912339334083291 0.4634236594119486
0.3906503840801986 0.4381480266518473 0.5474064868898637
0.6106701362774395 0.5607116787861429 0.4535816528499146
0.4314535287834792 0.4082156680458461 0.4974013719881449
0.5662204387651004 0.5936875215096356 0.4986009556971228
0.4766835306204109 0.3760760987123031 0.4532155458729390
0.5248113092624991 0.6229302579552780 0.5484690927952175
0.5020047976316814 0.4271518805692249 0.4107299871962692
0.4959002029856046 0.5745180488636202 0.5904805323901594
0.5310755430991403 0.4779235154788182 0.3721444914061072
0.4682879698820959 0.5224839625858911 0.6298645990758794
0.5503883933969578 0.5879412300913255 0.4286789123388224
0.4543188832467479 0.4158633452733650 0.5674600980633587
0.5022408469322537 0.6225767200718849 0.4817146649515381
0.4976696747192325 0.3848706137696517 0.5197921413433106
0.4584901077873468 0.6019121648958077 0.5339291286994315
0.5430424512272057 0.3973517975955465 0.4630192374970247
0.4295564104319311 0.5508155147174253 0.5770237937584471
0.5698384448777071 0.4497630973847036 0.4223598330467676
0.4276401232793364 0.4803133099751597 0.5900599773307886
0.5696826218764840 0.5215392238676274 0.4111633306482106
0.5040430692324561 0.4971209518242265 0.5055828319797732
0.4447248970494568 0.4867596185039857 0.4586667885242692
0.4954772945318914 0.5567889962622179 0.4589775665021688
0.5544718410542405 0.5067148588012087 0.5454212570693644
0.5105984454247684 0.4461449591286380 0.5452589755256912
0.4463915492093014 0.5392201703897739 0.5107108100345337
0.5559178252278405 0.4594672541046671 0.4875298010131643
0.4445379540696682 0.4680827253486823 0.5252964038907009
0.5573086064241796 0.5306710355524760 0.4767141727834845
0.4889475075238370 0.4361698478941708 0.4761225888100698
0.5127986248468100 0.5627483502438129 0.5259086024250761
0.5144476197413638 0.4896603096624860 0.4352536018521336
0.4833334518000264 0.5116268607429685 0.5674503843179599

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu Sc Ni

42 4 9

Direct

0.3868000000000009 0.486100000000004 0.406199999999983
0.613199999999991 0.513899999999996 0.5938000000000017
0.428699999999992 0.5516999999999967 0.4016000000000020
0.571300000000008 0.448300000000033 0.598399999999980
0.378399999999992 0.537300000000019 0.4643000000000015
0.621600000000008 0.462699999999981 0.535699999999985
0.3772000000000020 0.456800000000012 0.477699999999987
0.622799999999980 0.543199999999988 0.5223000000000013
0.426699999999967 0.421399999999984 0.4232000000000014
0.5733000000000033 0.578600000000016 0.576799999999986
0.4585000000000008 0.479999999999969 0.376199999999972
0.541499999999992 0.520000000000031 0.6238000000000028
0.506199999999998 0.546399999999984 0.376399999999967
0.4938000000000002 0.453600000000016 0.6236000000000033
0.477499999999991 0.612200000000014 0.4067000000000007
0.5225000000000009 0.387799999999986 0.593299999999993
0.426099999999981 0.603600000000001 0.464599999999972
0.5739000000000019 0.396399999999999 0.5354000000000028
0.3819000000000017 0.584800000000013 0.5259000000000000
0.618099999999983 0.415199999999987 0.4741000000000000
0.3746000000000009 0.508600000000013 0.5407000000000011
0.625399999999991 0.491399999999987 0.459299999999989
0.3796000000000035 0.431600000000031 0.5514000000000010
0.620399999999965 0.568399999999969 0.448599999999990
0.422899999999985 0.392800000000011 0.4996000000000009
0.5771000000000015 0.607199999999989 0.500399999999991
0.4737000000000009 0.364400000000034 0.4478000000000009
0.526299999999991 0.635599999999966 0.552199999999991
0.504199999999973 0.415999999999968 0.398099999999995
0.4958000000000027 0.584000000000032 0.6019000000000005
0.534199999999985 0.475999999999991 0.3584000000000032
0.4658000000000015 0.524000000000009 0.641599999999968
0.551499999999972 0.594900000000026 0.4239000000000033
0.4485000000000028 0.405099999999974 0.576099999999967
0.501899999999991 0.630299999999983 0.4784000000000006
0.4981000000000009 0.369700000000017 0.521599999999994
0.4517000000000024 0.615900000000034 0.5411000000000001
0.548299999999976 0.384099999999966 0.458899999999999
0.419899999999984 0.557200000000017 0.588099999999972
0.5801000000000016 0.442799999999983 0.4119000000000028
0.4187000000000012 0.476700000000010 0.6015000000000015
0.581299999999988 0.523299999999990 0.398499999999985
0.500000000000000 0.500000000000000 0.500000000000000
0.4425000000000026 0.492899999999988 0.452399999999972
0.488599999999981 0.556899999999988 0.4527000000000001
0.5611000000000033 0.534700000000008 0.4739000000000004
0.557499999999974 0.507100000000012 0.5476000000000028
0.5114000000000019 0.443100000000012 0.547299999999999
0.4401000000000010 0.542999999999993 0.513199999999977
0.559899999999990 0.457000000000007 0.4868000000000023
0.438899999999967 0.465299999999992 0.526099999999996
0.486699999999990 0.431199999999969 0.4735000000000014

0.5133000000000010 0.5688000000000031 0.5264999999999986
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994

vasp
1.000000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.00000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.00000000000000

Cu Sc Ni
42 5 8

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980
 0.3783999999999992 0.5373000000000019 0.4643000000000015
 0.6216000000000008 0.4626999999999981 0.5356999999999985
 0.3772000000000020 0.4568000000000012 0.4776999999999987
 0.6227999999999980 0.5431999999999988 0.5223000000000013
 0.4266999999999967 0.4213999999999984 0.4232000000000014
 0.5733000000000033 0.5786000000000016 0.5767999999999986
 0.4585000000000008 0.4799999999999969 0.3761999999999972
 0.5414999999999992 0.5200000000000031 0.6238000000000028
 0.5061999999999998 0.5463999999999984 0.3763999999999967
 0.4938000000000002 0.4536000000000016 0.6236000000000033
 0.4774999999999991 0.6122000000000014 0.4067000000000007
 0.5225000000000009 0.3877999999999986 0.5932999999999993
 0.4260999999999981 0.6036000000000001 0.4645999999999972
 0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011
 0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.5514999999999972 0.5949000000000026 0.4239000000000033
 0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028

0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.581299999999988 0.523299999999990 0.398499999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.492899999999988 0.452399999999972
 0.557499999999974 0.5071000000000012 0.5476000000000028
 0.4401000000000010 0.542999999999993 0.513199999999977
 0.486699999999990 0.431199999999969 0.4735000000000014
 0.488599999999981 0.556899999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.547299999999999
 0.559899999999990 0.4570000000000007 0.4868000000000023
 0.438899999999967 0.465299999999992 0.526099999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.5133000000000010 0.5688000000000031 0.526499999999986
 0.517299999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.57189999999994

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Sc Ni
42 6 7

Direct

0.3893597821437082 0.4881529909825601 0.4112737455794644
 0.6082853542152191 0.5169279264783964 0.5887645840741438
 0.4333982365097058 0.5506374564917823 0.4091290296904900
 0.5665313319358293 0.4546931685630134 0.5934209986793304
 0.3891801346559072 0.5426861321608865 0.4634457838619447
 0.6132506829298759 0.4648244534186043 0.5369629417298720
 0.3829212506812339 0.4515002135737891 0.4769102001155465
 0.6168208533543111 0.5411813740491791 0.5206191344851058
 0.4294471715967685 0.4253018140291291 0.4270727775593189
 0.5674587100446481 0.5748046119831873 0.5709272492614079
 0.4581552183495423 0.4880312564561972 0.3881198188095396
 0.5396724618583022 0.5203269898112687 0.6123381843714029
 0.5038313380945887 0.5447416688329813 0.3841786520764210
 0.5006193257508582 0.4619615765604397 0.6185412070015691
 0.4812284861254217 0.6086473240941132 0.4123882644603982
 0.5187560496251756 0.3928678995868443 0.5923053912894476
 0.4344853887233085 0.5963182141207390 0.4669847709368031
 0.5672811918438512 0.4080712514767600 0.5399558563691913
 0.3931761208526324 0.5780755652868745 0.5247795438951330
 0.6076931755668993 0.4225131491134386 0.4788598250018484
 0.3885500031301516 0.5067174818235344 0.5258483933978283
 0.6096733422150621 0.4912889414447934 0.4690108294840725
 0.3907853179648414 0.4390891496455715 0.5459894144536286
 0.6098341378596852 0.5599199859840882 0.4529707811894062
 0.4363411139887187 0.4074107419821268 0.4963575407236497
 0.5681938561735903 0.5923976735294326 0.5000984924292086
 0.4774095299805605 0.3720872254293662 0.4485064586949075
 0.5243040147742587 0.6243955536581983 0.5469158018106788

0.4925598122676565 0.4272188625340476 0.3969799907269361
 0.4965590458467110 0.5748668989142718 0.5892209088081090
 0.5301523787694856 0.4792175882742162 0.3708119420390849
 0.4682368706925618 0.5242300563991843 0.6288232770705219
 0.5498481426914946 0.5890227835935127 0.4289448575192737
 0.4484119175609269 0.4046258376553448 0.5672008852821484
 0.5035852382695993 0.6212328314994577 0.4802921602074225
 0.4967206366317325 0.3762906338031132 0.5214885857870640
 0.4579861073609124 0.6027437089050177 0.5346554180158088
 0.5489357388069247 0.3857330330932404 0.4754617938944280
 0.4303198195152553 0.5464814740917922 0.5746976406958877
 0.5656500182927942 0.4505819232804523 0.4271941860671485
 0.4350771633084485 0.4734476524105071 0.5907456607615347
 0.5678839216422051 0.5218586449092887 0.4105777913452789
 0.4990786438979712 0.5012448970642673 0.5016870833134395
 0.4366225501329356 0.4904745062574997 0.4583114802044163
 0.5585327781437514 0.5102809396586866 0.5432330711311260
 0.4929175816023535 0.5564045429904690 0.4537970267222430
 0.5038848666198193 0.4429492807408020 0.5508346908824631
 0.4992722971976633 0.4326203035644401 0.4657076511996411
 0.4444281780297924 0.5412512666954337 0.5086294296536130
 0.5560407345678511 0.4571391462804981 0.4952051888533153
 0.4442630481844347 0.4679996819329590 0.5243644662472288
 0.5560404992574494 0.5311124992982675 0.4753392049419329
 0.5127773866790905 0.5644219136006725 0.5241731009378219
 0.5100937399923486 0.4905159628591559 0.4310645391790734
 0.4874773030931759 0.5104613391261053 0.5678822970812772

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu Sc Ni
42 7 6

Direct

0.386800000000009 0.486100000000004 0.406199999999983
 0.613199999999991 0.513899999999996 0.5938000000000017
 0.428699999999992 0.5516999999999967 0.4016000000000020
 0.571300000000008 0.448300000000033 0.598399999999980
 0.378399999999992 0.537300000000019 0.4643000000000015
 0.621600000000008 0.462699999999981 0.535699999999985
 0.377200000000020 0.456800000000012 0.477699999999987
 0.622799999999980 0.543199999999988 0.5223000000000013
 0.426699999999967 0.421399999999984 0.4232000000000014
 0.573300000000033 0.578600000000016 0.576799999999986
 0.458500000000008 0.479999999999969 0.376199999999972
 0.541499999999992 0.520000000000031 0.6238000000000028
 0.506199999999998 0.546399999999984 0.376399999999967
 0.493800000000002 0.453600000000016 0.6236000000000033
 0.477499999999991 0.612200000000014 0.4067000000000007
 0.522500000000009 0.387799999999986 0.593299999999993

0.4260999999999981 0.6036000000000001 0.4645999999999972
 0.5739000000000019 0.3963999999999999 0.5354000000000028
 0.3819000000000017 0.5848000000000013 0.5259000000000000
 0.6180999999999983 0.4151999999999987 0.4741000000000000
 0.3746000000000009 0.5086000000000013 0.5407000000000011
 0.6253999999999991 0.4913999999999987 0.4592999999999989
 0.3796000000000035 0.4316000000000031 0.5514000000000010
 0.6203999999999965 0.5683999999999969 0.4485999999999990
 0.4228999999999985 0.3928000000000011 0.4996000000000009
 0.5771000000000015 0.6071999999999989 0.5003999999999991
 0.4737000000000009 0.3644000000000034 0.4478000000000009
 0.5262999999999991 0.6355999999999966 0.5521999999999991
 0.5041999999999973 0.4159999999999968 0.3980999999999995
 0.4958000000000027 0.5840000000000032 0.6019000000000005
 0.5341999999999985 0.4759999999999991 0.3584000000000032
 0.4658000000000015 0.5240000000000009 0.6415999999999968
 0.5514999999999972 0.5949000000000026 0.4239000000000033
 0.4485000000000028 0.4050999999999974 0.5760999999999967
 0.5018999999999991 0.6302999999999983 0.4784000000000006
 0.4981000000000009 0.3697000000000017 0.5215999999999994
 0.4517000000000024 0.6159000000000034 0.5411000000000001
 0.5482999999999976 0.3840999999999966 0.4588999999999999
 0.4198999999999984 0.5572000000000017 0.5880999999999972
 0.5801000000000016 0.4427999999999983 0.4119000000000028
 0.4187000000000012 0.4767000000000010 0.6015000000000015
 0.5812999999999988 0.5232999999999990 0.3984999999999985
 0.5000000000000000 0.5000000000000000 0.5000000000000000
 0.4425000000000026 0.4928999999999988 0.4523999999999972
 0.5574999999999974 0.5071000000000012 0.5476000000000028
 0.4885999999999981 0.5568999999999988 0.4527000000000001
 0.5114000000000019 0.4431000000000012 0.5472999999999999
 0.5172999999999988 0.4878000000000000 0.4281000000000006
 0.4827000000000012 0.5122000000000000 0.571899999999994
 0.4401000000000010 0.5429999999999993 0.5131999999999977
 0.5598999999999990 0.4570000000000007 0.4868000000000023
 0.4388999999999967 0.4652999999999992 0.526099999999996
 0.5611000000000033 0.5347000000000008 0.4739000000000004
 0.4866999999999990 0.4311999999999969 0.4735000000000014
 0.5133000000000010 0.5688000000000031 0.5264999999999986

vasp

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

Cu Sc Ni
42 8 5

Direct

0.3868000000000009 0.4861000000000004 0.4061999999999983
 0.6131999999999991 0.5138999999999996 0.5938000000000017
 0.4286999999999992 0.5516999999999967 0.4016000000000020
 0.5713000000000008 0.4483000000000033 0.5983999999999980

0.3783999999999992 0.5373000000000019 0.4643000000000015
0.6216000000000008 0.4626999999999981 0.5356999999999985
0.3772000000000020 0.4568000000000012 0.4776999999999987
0.6227999999999980 0.5431999999999988 0.5223000000000013
0.4266999999999967 0.4213999999999984 0.4232000000000014
0.5733000000000033 0.5786000000000016 0.5767999999999986
0.4585000000000008 0.4799999999999969 0.3761999999999972
0.5414999999999992 0.5200000000000031 0.6238000000000028
0.5061999999999998 0.5463999999999984 0.3763999999999967
0.4938000000000002 0.4536000000000016 0.6236000000000033
0.4774999999999991 0.6122000000000014 0.4067000000000007
0.5225000000000009 0.3877999999999986 0.5932999999999993
0.4260999999999981 0.6036000000000001 0.4645999999999972
0.5739000000000019 0.3963999999999999 0.5354000000000028
0.3819000000000017 0.5848000000000013 0.5259000000000000
0.6180999999999983 0.4151999999999987 0.4741000000000000
0.3746000000000009 0.5086000000000013 0.5407000000000011
0.6253999999999991 0.4913999999999987 0.4592999999999989
0.3796000000000035 0.4316000000000031 0.5514000000000010
0.6203999999999965 0.5683999999999969 0.4485999999999990
0.4228999999999985 0.3928000000000011 0.4996000000000009
0.5771000000000015 0.6071999999999989 0.5003999999999991
0.4737000000000009 0.3644000000000034 0.4478000000000009
0.5262999999999991 0.6355999999999966 0.5521999999999991
0.5041999999999973 0.4159999999999968 0.3980999999999995
0.4958000000000027 0.5840000000000032 0.6019000000000005
0.5341999999999985 0.4759999999999991 0.3584000000000032
0.4658000000000015 0.5240000000000009 0.6415999999999968
0.5514999999999972 0.5949000000000026 0.4239000000000033
0.4485000000000028 0.4050999999999974 0.5760999999999967
0.5018999999999991 0.6302999999999983 0.4784000000000006
0.4981000000000009 0.3697000000000017 0.5215999999999994
0.4517000000000024 0.6159000000000034 0.5411000000000001
0.5482999999999976 0.3840999999999966 0.4588999999999999
0.4198999999999984 0.5572000000000017 0.5880999999999972
0.5801000000000016 0.4427999999999983 0.4119000000000028
0.4187000000000012 0.4767000000000010 0.6015000000000015
0.5812999999999988 0.5232999999999990 0.3984999999999985
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.4425000000000026 0.4928999999999988 0.4523999999999972
0.5574999999999974 0.5071000000000012 0.5476000000000028
0.4885999999999981 0.5568999999999988 0.4527000000000001
0.5114000000000019 0.4431000000000012 0.5472999999999999
0.4388999999999967 0.4652999999999992 0.5260999999999996
0.5611000000000033 0.5347000000000008 0.4739000000000004
0.4866999999999990 0.4311999999999969 0.4735000000000014
0.4401000000000010 0.5429999999999993 0.5131999999999977
0.5598999999999990 0.4570000000000007 0.4868000000000023
0.5133000000000010 0.5688000000000031 0.5264999999999986
0.5172999999999988 0.4878000000000000 0.4281000000000006
0.4827000000000012 0.5122000000000000 0.571899999999994

vasp
1.00000000000000

35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni
42 9 4

Direct

0.3960961357071711 0.4874720120368708 0.4115506626090277
0.5963493963301035 0.4814810542660640 0.5950539468469161
0.4446912880031582 0.5406491647430430 0.4122652172749094
0.5666531377169035 0.4226680984395207 0.6059705990024928
0.3954458232808331 0.5321696870817909 0.4615404412534649
0.6029347122432256 0.4548342103509282 0.5335583146055743
0.3841345539312342 0.4630453749678647 0.4768619503532830
0.5993493043111863 0.5171937338398663 0.5055140520828911
0.4155041273806884 0.4244035482249562 0.4307741090206224
0.5542678418397629 0.6188027680035649 0.5537291575725183
0.4575483906811086 0.4675581326008366 0.3880786529325427
0.5339181710495691 0.4897144462366231 0.6219457095692359
0.5041012660817267 0.5833352021669673 0.3763590715654743
0.4895971105199715 0.4361546501146101 0.6162543441564124
0.4587476483317356 0.6070429091257551 0.4204999248708851
0.5168211935956354 0.3866016313050094 0.5807521032695133
0.4505537280776634 0.5702691042741495 0.4797118973722925
0.5619680089576355 0.3973489684573088 0.5323090458170888
0.3883401251390709 0.5783130756826390 0.5114981164157102
0.6047321338719590 0.4128555706060375 0.4809516274425285
0.3874174800682000 0.5118696759600770 0.5247022664253598
0.6272475061625890 0.4734734241146832 0.4582398127342895
0.3869381804463757 0.4461424806611969 0.5474344938437585
0.6216991859891031 0.5421689926132837 0.4427329894882132
0.4292949473855939 0.4166952943025823 0.5019248331352782
0.5731284989671805 0.5801824184214226 0.5027128449691072
0.4718144730739125 0.3966148475093389 0.4536517310646341
0.4897167811018676 0.6492356649349880 0.5508759463275265
0.5105735726451708 0.4390956164764606 0.4202020070486877
0.5031486518861239 0.5960217408722134 0.5916890017146866
0.5473541603991745 0.4572104762619557 0.3682671835407541
0.4625601739708332 0.4987992656570539 0.6152287657739519
0.5708142993088403 0.5670754411840819 0.3919923659971537
0.4526171975772126 0.4049220917920754 0.5652187924534411
0.4741558288130925 0.6389780659569543 0.4794650776381069
0.4950017047088532 0.3839237717932758 0.5169344244197829
0.4317936250545033 0.6248500775092651 0.5277668752169020
0.5404402145422446 0.3948846370935813 0.4661524794415507
0.3967613793939893 0.5017188739473127 0.5898308972859221
0.5833713923941477 0.4261416395789566 0.4178967516644707
0.4210943718316528 0.4430000198218858 0.6091195912241600
0.5882730113209895 0.4967131135986141 0.4037518884703004
0.5117939486775589 0.5269538742339276 0.5034226033764849
0.4522960276877823 0.4820877914543666 0.4579098402113122

0.5687206339210610 0.5453752974538963 0.5692550459423467
 0.5230460029223535 0.5956200203092752 0.4480535197075521
 0.5326699199782778 0.4596712034926124 0.5578015084386413
 0.4414430114183572 0.5619214152505628 0.5600042398472979
 0.5572612323735326 0.4670518242133193 0.4699284020440873
 0.4508493782756607 0.4763170774921681 0.5470571944978331
 0.5151123589796613 0.5167232931957486 0.4004781130875485
 0.5595077769554203 0.5379325504542225 0.4514345626550174
 0.4949963597791808 0.4464432378439158 0.4964488180031214
 0.5012886154088263 0.5911392119502086 0.5232221980847300
 0.5040439995303380 0.5311322300701082 0.5740139901926041

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Sc Ni C H O
 42 3 10 1 1 1

Direct

0.3953881447538964 0.4868336525378471 0.4122784816824765
 0.6117896004477942 0.5130479164335914 0.5865894498027271
 0.4354218434978309 0.5472234379214704 0.4134841444911447
 0.5657922864859437 0.4530314010645424 0.5899397896232357
 0.3867056937110425 0.5339923076064041 0.4676022779206028
 0.6114220748396583 0.4651046909210429 0.5312427520759702
 0.3855949269010539 0.4607611700530060 0.4797612757591168
 0.6122577761398766 0.5403102070311266 0.5187506217371299
 0.4333215122293181 0.4289675608389993 0.4326705382344187
 0.5680662267019575 0.5715002439017773 0.5703532342838261
 0.4623417514632657 0.4820168043838141 0.3880564293330504
 0.5375502538426027 0.5180867606672467 0.6112025504327379
 0.5055768001098606 0.5417811048729922 0.3867664687096072
 0.4930625563616606 0.4580414087567430 0.6105702540449250
 0.4801502135019109 0.6049383851802966 0.4118372819451446
 0.5227829566861096 0.3946979586505193 0.5879074976112206
 0.4287951802214079 0.6006142732018155 0.4631259424760975
 0.5680052023689389 0.4048564664727898 0.5317117087265175
 0.3866395457653679 0.5835682381115741 0.5243094539086646
 0.6128227362718939 0.4188045552309605 0.4747404346336291
 0.3835178448725827 0.5081040324344018 0.5375459336200419
 0.6142661685316519 0.4920129219414330 0.4626540072975509
 0.3844841685630221 0.4323597252404660 0.5500756834312686
 0.6147963018189696 0.5651247707037653 0.4499747542517569
 0.4253684678453276 0.3955286985326918 0.4970496059696959
 0.5707742854053002 0.5982311812305899 0.4996134317704231
 0.4764906191254488 0.3728437109819403 0.4502250503255837
 0.5266386838827074 0.6272748097278368 0.5495242987223435
 0.5034508536603806 0.4239102790299203 0.4063353822130472
 0.4950581360650035 0.5759655060975536 0.5911752939528296
 0.5321449266391853 0.4771642031943704 0.3658375939815053

0.4692871814590808 0.5228182331001536 0.6322509256728307
 0.5475669501787619 0.5867831694200439 0.4304477175326555
 0.4523409299776350 0.4082579860402133 0.5756478958004854
 0.4992278053159141 0.6162580809789194 0.4820418129681209
 0.4956512010837616 0.3843054116477241 0.5202127405488510
 0.455397008237156 0.6127457331441293 0.5419644322419506
 0.5446499962501316 0.3938238578784815 0.4624837658375921
 0.4251685656705678 0.5526782642033741 0.5812958242143921
 0.5726040943494702 0.4478160938242996 0.4195856700685666
 0.4240755983158632 0.4794896227234046 0.5939209505708858
 0.5740254262827426 0.5209154753637918 0.4073513069366306
 0.5078966815093573 0.4995997126627092 0.4981309166395576
 0.4460542477749170 0.5478887942373603 0.5101693744079893
 0.4447197696880901 0.4598431924767525 0.5250317350463000
 0.4466580535089347 0.4934678572261461 0.4571642900511886
 0.5576654597816406 0.5068263952771980 0.5463297694903737
 0.4909355241656552 0.5536868067718510 0.4542200287441998
 0.5133749863706754 0.4463838872408157 0.5454819812497546
 0.5593524655661730 0.4572597355837665 0.4870261781801384
 0.5603933521651273 0.5343499490043865 0.4741230494783036
 0.4891493726720627 0.4348520092463689 0.4738396675599976
 0.5151480339990394 0.5650103466385432 0.5258972291285646
 0.5168114874033458 0.4883638781577964 0.4302955671293539
 0.4828596550102241 0.5113891943025113 0.5661251501664949
 0.6593353168086749 0.5074381350904904 0.6135420799396202
 0.6848932285333638 0.5218180152521141 0.6001130674976505
 0.6637357723151577 0.4892317795532063 0.6426710633323058

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

Cu	Ti	Ni	C	H	O
42	3	10	1	1	1

Direct

0.3961776165351643 0.4870040011487107 0.4142080335925952
 0.6100461974402823 0.5128226359213418 0.5869637719549402
 0.4357817028528044 0.5469027552947275 0.4135514709638222
 0.5648798378169454 0.4532767780926387 0.5884879071293005
 0.3878775140867530 0.5347883500316347 0.4685425468859089
 0.6115669332273805 0.4655147807761465 0.5312779393763349
 0.3868853819735710 0.4593003848382178 0.4806375345550135
 0.6123552683788369 0.5401343382520939 0.5189211681912981
 0.4340929925597783 0.4294056963105258 0.4324571880788252
 0.5673165951279528 0.5710704169741029 0.5690217286390591
 0.4623846959859403 0.4825847069532772 0.3896547351648404
 0.5373293587914268 0.5178368307817783 0.6097493459748050
 0.5055316296133536 0.5418390026340333 0.3881679219289497
 0.4937681491307778 0.4583782996311888 0.6100641850668512
 0.4804103434327991 0.6045475105757834 0.4123983600875185
 0.5229741416779882 0.3954024224945721 0.5870860646955064

0.4298749682313929 0.5982827256211741 0.4649923709177870
0.5678431128900306 0.4057284322175178 0.5316393577722206
0.3889067267008717 0.5820122907206263 0.5239234776511488
0.6118132861398223 0.4196340211250691 0.4748578495992495
0.3861369417476386 0.5079759420154133 0.5366374663969478
0.6146234006966858 0.4920409690489405 0.4626071548966916
0.3867061847866403 0.4332589289420766 0.5485252912191452
0.6140318648073538 0.5645053304707336 0.4505268822544681
0.4265660756972363 0.3979387297431352 0.4982137316022722
0.5706227994723341 0.5976717330888243 0.4997025110910156
0.4766752566070632 0.3735187444558415 0.4510612492686458
0.5264941630358707 0.6263949743516899 0.5487032392428033
0.5032372998528620 0.4245031191174967 0.4080378244237423
0.4963438029012386 0.5752718513584916 0.5909720621137537
0.5313565060739537 0.4773201481526066 0.3672066273623344
0.4691362625547308 0.5222392169349910 0.6302245496034414
0.5474249011022834 0.5861627301380257 0.4309600723267396
0.4524322457698758 0.4105287450777370 0.5737676979703557
0.4995747053199012 0.6172715939187308 0.4817138831742885
0.4961738438247258 0.3832425276639506 0.5204940604406977
0.4555346851427668 0.6096743392854568 0.5408516853190664
0.5442823414977255 0.3950300214799890 0.4627743322157549
0.4256957073952504 0.5529072091839442 0.5802116447681711
0.5725433722601176 0.4480730736863344 0.4199964162524835
0.4245891266416033 0.4781764765247961 0.5923472186656062
0.5740203415985908 0.5209232427976007 0.4077778275561673
0.5072534025349585 0.4995603097842340 0.4978817056564733
0.4466961833731580 0.5456233785266164 0.5104067678449187
0.4452976619488723 0.4621094317869271 0.5244956978455556
0.4470188211889300 0.4940653401632389 0.4601620949824668
0.5565212427127844 0.5067837170714742 0.5445790307697459
0.4901311912047345 0.5536667247828568 0.4564751115525920
0.5113010857853588 0.4468549075111328 0.5438254120820597
0.5583577062043633 0.4591252959614040 0.4874855900298264
0.5594608139848605 0.5330784861603737 0.4749852468519273
0.4880612609775830 0.4355540878668911 0.4762516524257733
0.5132739319814719 0.5642147989084512 0.5241635099916685
0.5168332725709167 0.4886708807108872 0.4322170293798566
0.4820118874845181 0.5109493723683833 0.5633871417411853
0.6583791420139293 0.5074121458166182 0.6128214107506091
0.6837441536664843 0.5220367437152588 0.5992992105888406
0.6630958646777318 0.4891983510334756 0.6419228145191601

vasp

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000

Cu V Ni C H O
42 3 10 1 1 1

Direct

0.3962860728492518 0.4868566983674503 0.4127831445257522

0.6105353509630390 0.5128247380949440 0.5861079134490846
0.4360128057568523 0.5466739420021964 0.4122733145960597
0.5644210181480352 0.4534205958763872 0.5880372560948562
0.3890896290496284 0.5339969661400973 0.4679291447383616
0.6109082763094277 0.4657862763873146 0.5312869457601089
0.3877552042360650 0.4606906278935500 0.4800236829806891
0.6119300119227334 0.5397939186541686 0.5188729064426307
0.4339747577739474 0.4292449927467575 0.4316819516748582
0.5668215120121918 0.5707831176980196 0.5686069955662304
0.4629245717557638 0.4821612448376018 0.3883748660409116
0.5385206202922866 0.5178908510128475 0.6110188173348481
0.5059433838505243 0.5415092657816681 0.3888862807636561
0.4943633140974761 0.4585564312905830 0.6107807447509349
0.4801982011221567 0.6037022641151349 0.4132228891400279
0.5214681965750005 0.3961300723155952 0.5865956935021037
0.4321376680444503 0.5946594956926776 0.4672808550938874
0.5669745294214261 0.4064218064418477 0.5318480048571510
0.3904467634977878 0.5798787820930756 0.5239098587946981
0.6107145548492017 0.4202986093826763 0.4754511238954662
0.3837763331739610 0.5084072455762776 0.5378179764485735
0.6142791673684024 0.4919260052453694 0.4629989352354528
0.3876372473258733 0.4360251336766615 0.5477745457084457
0.6131119164003742 0.5638676324754055 0.4513602268683564
0.4287843176903579 0.4020825598589973 0.4995289728077148
0.5700123599386058 0.5968272599810475 0.4998409204201196
0.4761231028901076 0.3742164591851764 0.4516981690144023
0.5253292156819387 0.6256466225146343 0.5479677126741067
0.5032796025635009 0.4246463678304345 0.4084519000315618
0.4969199495749937 0.5754252180642822 0.5914429943641306
0.5320735434787836 0.4774837274705995 0.3678470781052608
0.4699966077272424 0.5225016847593755 0.6314555802943083
0.5470898979325399 0.5855751541417256 0.4311368096635446
0.4526990343121990 0.4140091021556945 0.5700711427945689
0.5011984502587942 0.6170513471799755 0.4806989964610723
0.4972691219590878 0.3831129015185026 0.5200754769420149
0.4560050926726086 0.6057217355342615 0.5384009122636101
0.5435872037218089 0.3955792962649368 0.4632275230756234
0.4273313949095248 0.5523632548439971 0.5803203581959514
0.5725348469123914 0.4480775471721458 0.4203199143443853
0.4256565170284760 0.4793364344998370 0.5921562901796366
0.5741689289606157 0.5207039825496675 0.4081038244731846
0.5053699043053040 0.4996231105025803 0.4984421103691703
0.4453314618708448 0.5385268755252869 0.5121811076219783
0.4440022915072545 0.4694731096978397 0.5236195950483363
0.4481351856952246 0.4935396785992072 0.4569908492336003
0.5552709685911141 0.5067753346894454 0.5444500481398891
0.4895113925252690 0.5524387790633407 0.4574626004915783
0.5099934223379378 0.4480598275993020 0.5430830054897893
0.5568406938733678 0.4599662764627900 0.4878052956348022
0.5579086685317534 0.5320820988566675 0.4756361529260561
0.4873045807420033 0.4368608643811833 0.4767682929900121
0.5119517969109213 0.5629173609462740 0.5238676184610460

0.5169785702088291 0.4885604444949435 0.4332782609838127
 0.4845573343706764 0.5111785957805126 0.5650534509483890
 0.6587620460868782 0.5072304988733074 0.6125345370494784
 0.6843732261527408 0.5221259360303303 0.5998482808169034
 0.6628740649715138 0.4887738391733143 0.6415859568298047

vasp

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
Cu Mn Ni C H O		
42 3 10 1 1 1		

Direct

0.3951863066868172 0.4870715730530333 0.4135975936660140
 0.6081923488914193 0.5121821703599752 0.5863508407044695
 0.4360315498625867 0.5468605692394689 0.4124528535162542
 0.5646080893051261 0.4532792955374704 0.5882460326340082
 0.3898520061930012 0.5342750891132889 0.4682319704073631
 0.6100839783695181 0.4657375181645163 0.5311328946906347
 0.3884393983432289 0.4604823558590663 0.4803104475153450
 0.6112411443370079 0.5393239053778084 0.5189718258625450
 0.4340308697785807 0.4291324523364802 0.4318891654211589
 0.5671567049097549 0.5706466293536145 0.5687513942890408
 0.4627399682888299 0.4822072020809163 0.3889354873191914
 0.5384527842845863 0.5178785771243497 0.6108563569464600
 0.5061852842563119 0.5414659175904839 0.3887367640670279
 0.4946577319749719 0.4584628437487802 0.6107725393097464
 0.4801359587267633 0.6038576919577489 0.4131124479426984
 0.5215433887221399 0.3959456594152833 0.5866993329755227
 0.4328927262832773 0.5953380212659052 0.4670153635422010
 0.5672913395588906 0.4063497469513266 0.5316065164578347
 0.3910034994747673 0.5802910399626777 0.5243327777286884
 0.6103822063956785 0.4205252716617812 0.4753365611387483
 0.3867603749212863 0.5082626438962987 0.5366641813349872
 0.6137827078017835 0.4919444116694720 0.4631531838130699
 0.3879361443790627 0.4360772302175188 0.5481330087536199
 0.6128664763469132 0.5636308469739468 0.4515678939743965
 0.4295443082871437 0.4015744476732871 0.4997136008309322
 0.5704741880481889 0.5966944477896307 0.4996615888541115
 0.4759496842309599 0.3741042664845864 0.4519264178364437
 0.5257630424759020 0.6256906830214779 0.5479060615256203
 0.5034489851654885 0.4246203964495043 0.4084859844980537
 0.4971334007625884 0.5754522875778627 0.5913102096583330
 0.5316261458395246 0.4774793816104967 0.3688294617985656
 0.4695321309554727 0.5226146182453358 0.6311491595374346
 0.5473326153298508 0.5855520124842467 0.4311349235773944
 0.4532728339963753 0.4134774790082854 0.5702358498276334
 0.5020857997674184 0.6167441479029694 0.4804704813478248
 0.4978437857094116 0.3832450613340249 0.5200026618641476
 0.4571628318609506 0.6063888319329592 0.5380316645372072
 0.5438539519524537 0.3955414500486337 0.4632714438730737

0.4282308762136855 0.5522305972223881 0.5796563150349537
 0.5721758609730866 0.4484618782492042 0.4208795604998463
 0.4264880246652140 0.4793952110159678 0.5917559621542601
 0.5736766235654979 0.5206706238851557 0.4086201928529303
 0.5006466826124533 0.4998766029681091 0.4994765830967592
 0.4470649982151673 0.5415140695360635 0.5113083998643880
 0.4455460674877217 0.4665044726599226 0.5239036185163645
 0.4473670336307143 0.4935564349201328 0.4568655403428016
 0.5539618669748274 0.5065666057731082 0.5437896933340280
 0.4903259825233346 0.5523006345536100 0.4564897732962813
 0.5113666492807841 0.4478947511468476 0.5434141970038671
 0.5561615842938866 0.4602233404243667 0.4879441502039891
 0.5573776376429089 0.5318140126130417 0.4758675432690997
 0.4882162714699093 0.4366807452788693 0.4760709257632312
 0.5134504774543451 0.5629004407256466 0.5240348020544318
 0.5160161079197776 0.4888066504593278 0.4345334249874962
 0.4847795529311682 0.5111336298710513 0.5652883198941446
 0.6567508175315850 0.5072209853537953 0.6119142656082110
 0.6816390226469868 0.5224582082391219 0.5982903251957552
 0.6617370731839323 0.4893819306297665 0.6411852768523304

vasp

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 Cu Cr Ni C H O
 42 3 10 1 1 1

Direct

0.3962237606944508 0.4868321949064695 0.4135158896478660
 0.6090320619450281 0.5126322667793449 0.5860691123304743
 0.4360471021601532 0.5468500531010616 0.4127050844901027
 0.5646692577478477 0.4534585661135326 0.5882680454005272
 0.3898191158916421 0.5340651025493819 0.4683023914475731
 0.6101064983631291 0.4659373938515766 0.5310213754842937
 0.3884165247048103 0.4605971326141703 0.4803649614199110
 0.6113500379108289 0.5393815046833011 0.5187552012180459
 0.4341419393323163 0.4290215735857223 0.4320400359235250
 0.5671062270641700 0.5706714893963725 0.5687837639295108
 0.4629815270913037 0.4821910276936334 0.3890587907834609
 0.5383667551683590 0.5178094618759936 0.6106369848938622
 0.5061449740657494 0.5414965128684417 0.3885841959020126
 0.4941630045976743 0.4584136458595618 0.6105592605381049
 0.4801659043034712 0.6038079158925643 0.4130489745999905
 0.5219335246478766 0.3961154501289548 0.5867613639163213
 0.4327736632749493 0.5955429115243206 0.4672459782154142
 0.5670509082439267 0.4065689788408303 0.5315780183788419
 0.3906045222995016 0.5803295880583762 0.5242027363127804
 0.6100482259356561 0.4209293496833070 0.4753959366339358
 0.3863094477774562 0.5082339173331075 0.5368156588695669
 0.6138894998430644 0.4919675359747949 0.4629014398827210
 0.3875398531999570 0.4358290427142595 0.5480327262782568

0.6125406166881825	0.5635069863250239	0.4514514109605156
0.4294649678043613	0.4013068624838640	0.4999660051353151
0.5702327384002097	0.5966931801432372	0.4997101115399214
0.4761595785829207	0.3740259047096578	0.4517343182711405
0.5257284416991063	0.6256302391025783	0.5480980519890931
0.5035146989797716	0.4245594734262271	0.4083810605886967
0.4969313124883000	0.5753930383997573	0.5912841058328573
0.5317161288829371	0.4774311400768774	0.3684852091333390
0.4697255759400628	0.5225181623140012	0.6312142777322783
0.5471408101890809	0.5854955252523306	0.4311601805041627
0.4530680336108868	0.4131139311898044	0.5702938342829106
0.5019066821066356	0.6166254552413479	0.4806379742698949
0.4978438557359861	0.3833786656122870	0.5200011917254742
0.4566588012582130	0.6065945322706849	0.5381369440932652
0.5437509612980281	0.3955909533397231	0.4632194434025282
0.4277140157278375	0.5521983006853528	0.5799585484085292
0.5722606153597292	0.4483367996722699	0.4205791923623848
0.4258816165412134	0.4794649482268993	0.5919744167548191
0.5738171658363819	0.5205875152339670	0.4083676154540833
0.5021807021564541	0.4998461131713720	0.4991658234404486
0.4466730618355486	0.5416179801671046	0.5115380485682500
0.4452375787747723	0.4663105441610603	0.5242424518162959
0.4479712747307331	0.4935084669845399	0.4575858984369097
0.5541578242926063	0.5065863516551123	0.5438293103567319
0.4901319639938309	0.5521600911127854	0.4566035849439672
0.5110916114955926	0.4481960827048173	0.5434059747659010
0.5556578143995194	0.4607301949833831	0.4878370574550122
0.5570015263091265	0.5315195505517836	0.4759314401393673
0.4880405265952082	0.4367633384511777	0.4760983953736602
0.5130989402643125	0.5627234605824590	0.5241070881687534
0.5165230133556725	0.4887974273039270	0.4342627024628716
0.4841414675209698	0.5111257021554042	0.5648164984687372
0.6576073181418352	0.5073513649533389	0.6118204346550351
0.6828794304021343	0.5223571650258014	0.5986896680680168
0.6621208960294935	0.4892719363013325	0.6410396173451489

vasp

1.00000000000000

Cu Fe Ni C H O
42 3 10 1 1 1

Direct

0.3953606035695769	0.4871938059305894	0.4129340105690452
0.6083752014228203	0.5124681275486490	0.5860920178842345
0.4359591232497737	0.5467449613580250	0.4118691623905137
0.5644654496777040	0.4531397803155300	0.5879012598082674
0.3901924664719064	0.5338538114081687	0.4679441200782326
0.6104995680203088	0.4656390066378198	0.5310276849173535
0.3886450476985460	0.4614098183237194	0.4800221165916119
0.6117773714495369	0.5395266108903238	0.5187022948817372

0.4335827843903193 0.4294013891072470 0.4315019511163951
0.5670350812287137 0.5708303530256807 0.5685298477667791
0.4626972651574905 0.4822761595946942 0.3885668077763807
0.5387717584617874 0.5179387161398313 0.6111536422469771
0.5060648569777336 0.5415540208227552 0.3889470819937788
0.4951196848520491 0.4584965257299847 0.6114608625148945
0.4799059632174320 0.6037563861884724 0.4135376553454364
0.5208856404405399 0.3960262926517249 0.5867454452373315
0.4335199823358591 0.5937740287910351 0.4681957088036892
0.5666937823645040 0.4063881000615696 0.5318007773529803
0.3913965943164199 0.5788956923907993 0.5244960861765877
0.6098814644476643 0.4200793222888966 0.4753303279667510
0.3853956467332680 0.5082502700378467 0.5372798948373256
0.6139218777872711 0.4918621568526906 0.4629484949920148
0.3886083875168962 0.4370749345743971 0.5480416764089066
0.6126804705246289 0.5637893470632617 0.4511238105913830
0.4298063977919350 0.4031455469221074 0.5000901353307993
0.5702364903222891 0.5967443467229434 0.4997355209187856
0.4753207320804925 0.3745316148432131 0.4522739248240646
0.5253000061387821 0.6256699332032902 0.5479288305999809
0.5032224063234407 0.4246885560842859 0.4085855272983843
0.4972585912206482 0.5755821112055871 0.5916009563274538
0.5317297989637931 0.4774465462558870 0.3681573819489241
0.4699629065624426 0.5225937466039728 0.6316356282612789
0.5469837304389380 0.5854850955892638 0.4311997607655165
0.4532501262284472 0.4144931110347386 0.5693790813255396
0.5024420787339123 0.6170380720570789 0.4803743420043297
0.4979854674334817 0.3831647629916967 0.5199143104010800
0.4571168916534999 0.6045938821523675 0.5373259414672347
0.5431609058137467 0.3956535587593799 0.4632369369795937
0.4286143290360644 0.5518709794406401 0.5799960056333509
0.5722223318861918 0.4481488336131976 0.4203748743498057
0.4272286278788343 0.4796185668470459 0.5918574117403561
0.5739221215836553 0.5205332178355511 0.4082273733272445
0.5033438424906433 0.4997442534002923 0.4988452295623150
0.4461278227484984 0.5378192343129664 0.5124010083971393
0.4448049424929200 0.4696604207214195 0.5236787277086156
0.4478872143801670 0.4936244253918217 0.4567486621816177
0.5546815524563105 0.5066270937008215 0.5437842957917830
0.4895908554203555 0.5521659980327448 0.4571304515758230
0.5103578932676939 0.4481411951057962 0.5435269872667148
0.5564724917140978 0.4599722115361846 0.4877965994544798
0.5577206634499812 0.5320075177523446 0.4756396821780763
0.4872255350308879 0.4371908523962665 0.4764018126833854
0.5127899787945118 0.5627960775108490 0.5241425604434458
0.5166230241691079 0.4886743282775535 0.4334972627501433
0.4855017284686174 0.5111985299461264 0.5656665269542169
0.6563708036073092 0.5072952743089703 0.6125000896555174
0.6812857267200469 0.5225746754260097 0.5989354517262295
0.6614718160764193 0.4891358122837940 0.6415337833214232

vasp

1.00000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 Cu Co Ni C H O
 42 3 10 1 1 1
 Direct
 0.3954778358434108 0.4872565151980612 0.4134720904785176
 0.6080312556646981 0.5125647812079337 0.5857675355494629
 0.4361864562650522 0.5466961014677417 0.4116357179585741
 0.5643601648440244 0.4531239072250484 0.5875768908170910
 0.3908588250167768 0.5338198203232963 0.4683125595257698
 0.6101468871508112 0.4656910919210697 0.5309321262272222
 0.3895768811969907 0.4612367034696780 0.4803274087036603
 0.6115107247304378 0.5393276727584351 0.5185521217628754
 0.4339578001993945 0.4292588818177610 0.4311773000680134
 0.5668666799192585 0.5707674288733718 0.5683717037824729
 0.4627833377076464 0.4822419650846093 0.3886190197915567
 0.5388330688642440 0.5178903075648457 0.6111909394261329
 0.5061933529627979 0.5416023712070560 0.3890307554341274
 0.4954320623595062 0.4585162799256778 0.6116411547601468
 0.4798160419356188 0.6037844061561367 0.4136546666989580
 0.5207737347514512 0.3960108271192441 0.5865622673249008
 0.4338290392080326 0.5929026542343641 0.4685440770251669
 0.5664445403630309 0.4064704148764194 0.5315767683785872
 0.3918704112086960 0.5785578115534161 0.5244204549523822
 0.6094190909882299 0.4203304824389625 0.4752664595150390
 0.3862663500302431 0.5081611834005707 0.5370899826194662
 0.6137255032783885 0.4918696427445596 0.4630186295211586
 0.3892093762661309 0.4372641283562941 0.5479193414760751
 0.6123637164040738 0.5636192444211109 0.4513309290984518
 0.4302593239486767 0.4039034773980942 0.5001097111324511
 0.5701475664770386 0.5966859935006429 0.4997667988232516
 0.4753018781738604 0.3745207317496715 0.4522876839049934
 0.5252163305260705 0.6256164736467716 0.5478568267976124
 0.5033114615382860 0.4247304767508295 0.4086025558412047
 0.4973540776060270 0.5755792889878967 0.5916853446712710
 0.5316291528730497 0.4775407876723708 0.3686606434097719
 0.4697839864978040 0.5226958349427460 0.6316906881669123
 0.5469835968932607 0.5854892980292009 0.4312731664136518
 0.4535001591419513 0.4150253200122063 0.5691220428234021
 0.5023630607591253 0.6172628820779823 0.4803628104314447
 0.4977763795197477 0.3828103638715389 0.5198813946022343
 0.4572740287155070 0.6040469621397567 0.5373007163790077
 0.5431092190895924 0.3957227758161450 0.4631811739740345
 0.4289326988238067 0.5516282035344577 0.5796471530726197
 0.5721280835019792 0.4483618298545088 0.4205829616006475
 0.4276818020069393 0.4794272212190470 0.5916669768609060
 0.5737991126805362 0.5205793003915431 0.4084232446213661
 0.5007715387314491 0.4999281397115660 0.4995917209783538
 0.4464645752754583 0.5373578020606495 0.5126067932644731
 0.4452296391619474 0.4704042455713348 0.5237522169343980

0.4480255543821415	0.4935764412164303	0.4566426477332186
0.5542085636818614	0.5066049615237042	0.5434389782992064
0.4899769032570666	0.5521863809863512	0.4570470361837699
0.5104286090186921	0.4480068055910600	0.5432622693140630
0.5557840909887009	0.4605000586829368	0.4878502824232845
0.5571858688363198	0.5316983725358537	0.4759314833146793
0.4875823341707846	0.4370989548409046	0.4763688877814718
0.5128443452757051	0.5628025821679609	0.5239124353016730
0.5164429494092297	0.4888485497397081	0.4342378710038940
0.4857898997133775	0.5111858064947296	0.5660464322398228
0.6561107012388697	0.5074159230132973	0.6119936112014360
0.6810981476258942	0.5225336778019536	0.5984283916280714
0.6610271269913125	0.4892594531204683	0.6410719613785701

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu	Ni	Ni	C	H	O
42	3	10	1	1	1

Direct

0.3922075808823266 0.4867485578584924 0.4106318849972847
0.6125412395591008 0.5122243261268871 0.5890103563202836
0.4331410988474965 0.5486051996864462 0.4076772747418984
0.5661984361772577 0.4511405620981352 0.5923050756665139
0.3858403249063930 0.5350767885404560 0.4665217013345904
0.6148564394331744 0.4648967654601407 0.5332566458246630
0.3847307705587119 0.4593708578954082 0.4791545817970605
0.6152035706353175 0.5406943298188971 0.5208108922786704
0.4312596044948367 0.4262517993192303 0.4279354581125712
0.5685965441036435 0.5736202797270620 0.5720157367583496
0.4610413239052322 0.4811862328123255 0.3838347789377631
0.5392280438221543 0.5188179213856019 0.6158679304041581
0.5059747593111380 0.5435635629124638 0.3840405098759551
0.4939415311733720 0.4564095206325426 0.6160296053303806
0.4785273900142531 0.6067985818904083 0.4110784556665257
0.5214800859980019 0.3931159624171487 0.5889977827300689
0.4306508001888180 0.5972487104281061 0.4667784970332372
0.5693893838013739 0.4028377496986846 0.5332504734869511
0.3874805535002729 0.5807171160298078 0.5245977953967634
0.6125394010458549 0.4192211306586565 0.4753626896571762
0.3823096267976185 0.5081074626539914 0.5384369578330009
0.6176791400399647 0.4919009216928839 0.4615270729112878
0.3852915916453429 0.4348229801808686 0.5489689536371205
0.6147201171861909 0.5651754415315633 0.4510523827292722
0.4276379021119737 0.3993477996979591 0.4996638918086704
0.5723745401411187 0.6006117695934239 0.5003306601129147
0.4749406924287909 0.3708307947534959 0.4502490952780884
0.5251121451430146 0.6291616984169970 0.5498143675468884
0.5039298907033916 0.4211552216915095 0.4043193183785486
0.4960689115253195 0.5788512618400710 0.5956977123540399

0.5325491773978736	0.4771071522523777	0.3650228646112672
0.4675379965010234	0.5228962848010660	0.6350114578349249
0.5483679140081251	0.5890268907174374	0.4284694940453380
0.4516156004813437	0.4109979184090072	0.5714936281371352
0.5017915294823831	0.6222799449655357	0.4798144296689560
0.4981511825756582	0.3777197316302446	0.5200956482688182
0.4546750038359715	0.6087729021033870	0.5386936276604222
0.5453004941739636	0.3912509748007799	0.4612413047103302
0.4247299281638438	0.5536823805809393	0.5825867295953603
0.5752098305522427	0.4462515711399366	0.4173729933528044
0.4236566524209117	0.4780778351849200	0.5952418951515064
0.5762769261803636	0.5220001504916763	0.4046972309783237
0.4999333365421079	0.4999899167058895	0.4999819222464549
0.4418442598437676	0.5419454639245884	0.5129715533083995
0.4406523923823270	0.4662487513497713	0.5254248275594062
0.4437402789594869	0.4931782147442879	0.4533721810298496
0.5563591766438133	0.5070907879404705	0.5468085635464891
0.4890084586195061	0.5554180756048884	0.4538957035083612
0.5110208098853791	0.4446006803047097	0.5461567637927157
0.5585018986332475	0.4582316535889848	0.4872831327341094
0.5595401159485689	0.5336807557765358	0.4747002844007282
0.4870774827485125	0.4331033166899674	0.4742571491847550
0.5127930222231556	0.5669641128762383	0.5256772397769545
0.5169574571238597	0.4879582251864827	0.4301914369310751
0.4829516904122744	0.5120344622674377	0.5699072662998550
0.6689860208772991	0.5074494136223893	0.6077135862320232
0.7019550111697394	0.5222509100604359	0.6082057502503326
0.6533788158228032	0.4912802148299633	0.6347686096456068

vasp

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Cu Cu Ni C H O
42 3 10 1 1 1

Direct

0.3947120018074398	0.4872433885382166	0.4130536403583304
0.6075455041587289	0.5120129757800065	0.5859036966763104
0.4359858073191303	0.5468137631575044	0.4115506963178085
0.5647641246579552	0.4529172418587498	0.5881525432078394
0.3905804468276367	0.5338758770850021	0.4679571250568521
0.6104404766564879	0.4655875823198760	0.5310328748786385
0.3893607485983278	0.4616784737826379	0.4800165293237680
0.6116584425515222	0.5394665983341282	0.5186048342651712
0.4337450524787549	0.4294011821922624	0.4313280687363569
0.5675107291307129	0.5709724662150976	0.5686643063288415
0.4626496125954567	0.4822590049751108	0.3884607814111383
0.5389886872835413	0.5178877447396564	0.6113448910838062
0.5061302859442764	0.5415527722478874	0.3885565223915574
0.4953324323269798	0.4582817638892924	0.6118369084361206
0.4798300561837252	0.6037837882526577	0.4135265112623120

0.5209051661329284 0.3957356168757717 0.5869075667590420
 0.4340607790366739 0.5935290494507306 0.4681927391059846
 0.5671551142402470 0.4058229966273307 0.5320389167565120
 0.3910772572515686 0.5792750699986965 0.5246035207395475
 0.6097696191626351 0.4202108520025640 0.4753465582178313
 0.3865121182791426 0.5082454945471948 0.5368255731694523
 0.6135457464607770 0.4918458612035604 0.4631240557240898
 0.3880896811044162 0.4370181776133162 0.5481082441663314
 0.6124886931027903 0.5636104071661507 0.4511000748085050
 0.4304158060970202 0.4036024490476994 0.5001126360401340
 0.5705761382838969 0.5970962852585850 0.4996251539410068
 0.4752923581099157 0.3745332927745765 0.4523676214644192
 0.5253348653304417 0.6257375126932689 0.5478946330925348
 0.5032902406931927 0.4245798661815806 0.4085182847775599
 0.4974295594717069 0.5755805275222734 0.5916457585441793
 0.5316220749681514 0.4774255052687861 0.3689516987665282
 0.4695599234587266 0.5226494553698172 0.6317042529990845
 0.5471070158316380 0.5856421321528763 0.4309426594796789
 0.4536867893789141 0.4147306160726766 0.5690779929606898
 0.5026062274420543 0.6171678670773293 0.4802752535482619
 0.4981420886370158 0.3830340478313124 0.5199380065995375
 0.4576431869403630 0.6044162344359995 0.5370750606476911
 0.5433386882585757 0.3953967749709181 0.4631988581042300
 0.4289228076556738 0.5514772034808243 0.5796484058553524
 0.5720301997232282 0.4483949058014928 0.4209336833484362
 0.4274968557451301 0.4796081688098713 0.5916997020276039
 0.5736795330660616 0.5205826345596718 0.4083668337321201
 0.5007617601800320 0.4999277921391189 0.4998526236880131
 0.4454838794999531 0.5396402463686966 0.5123661835598615
 0.4441597918029178 0.4684858319613418 0.5243835805516012
 0.4471360788003680 0.4937301230575945 0.4556019073431977
 0.5542811100157049 0.5066378774981675 0.5434571477462565
 0.4904153855603668 0.5522372795306869 0.4562603093080672
 0.5115382322846038 0.4476750168368769 0.5440253350518893
 0.5560277989986749 0.4596908037517697 0.4884613401663281
 0.5573711358085418 0.5321214630463568 0.4757954281723752
 0.4879712450649467 0.4368772708191357 0.4758147138796765
 0.5139918059989451 0.5631500947771481 0.5243014163441001
 0.5161628083672420 0.4888719335616695 0.4343576792571733
 0.4858902523653860 0.5111989988998734 0.5668172886178874
 0.6556828695051270 0.5072264364572553 0.6118898316260374
 0.6802734020600842 0.5222126581898829 0.5974980780018764
 0.6612954049946562 0.4896325449413373 0.6411792749773381

vasp

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

Cu Zn Ni C H O
 42 3 10 1 1 1

Direct

0.3945601432115863 0.4871477711290622 0.4132170061842184
0.6073096350658003 0.5123340664521091 0.5861174642707621
0.4359687505603450 0.5469346434652979 0.4120790038192244
0.5648669426403631 0.4528392526140733 0.5883936885750892
0.3897331387666504 0.5341718547075178 0.4679718384981081
0.6108677899852244 0.4653175708915783 0.5314603307449098
0.3882346780096551 0.4607647415984819 0.4798993942659825
0.6118361716235007 0.5394768146928447 0.5187590608032202
0.4338776427250502 0.4292406349466323 0.4316616490538583
0.5676074681397451 0.5709972986225607 0.5689225956159231
0.4625416575449945 0.4824148968182598 0.3891592737555841
0.5382210985209990 0.5177474945627971 0.6107555264497327
0.5059928578510755 0.5416860313269730 0.3882945650085252
0.4950056095558186 0.4581760913695876 0.6115206871556165
0.4797942077069675 0.6046929346379059 0.4130206500455475
0.5210221561797530 0.3952262525256055 0.5871938052605092
0.4336087696620568 0.5952747349709850 0.4670900879340411
0.5671908401203719 0.4057739277110334 0.5319841142338994
0.3913334176634417 0.5801024879686159 0.5246252376837670
0.6101307100143628 0.4200056141225947 0.4753811545763311
0.3865879125741372 0.5082578431436983 0.5366438806705912
0.6139703631967186 0.4918360184683475 0.4631724415645918
0.3881446809672418 0.4364256221756398 0.5481705468951492
0.6127441998894234 0.5638083873159511 0.4510832030758428
0.4300489273579198 0.4016546193628494 0.4996660562181939
0.5707432247117822 0.5971300564209820 0.4997451158612921
0.4756612380484795 0.3736917900792470 0.4518343347834435
0.5258985100511477 0.6264707000743736 0.5485878323194566
0.5033681417180244 0.4245619556805513 0.4082680225574554
0.4972151115279486 0.5755960755257127 0.5916095581761242
0.5315820434603296 0.4774397196947204 0.3681108257744987
0.4691712238505649 0.5225241785741997 0.6318265571554196
0.5471601389683342 0.5856148380669264 0.4310380795920498
0.4536412850710712 0.4134852546664124 0.5698812383106729
0.5029124291568967 0.6172537834726192 0.4803881945360935
0.4982581435378092 0.3828003474243512 0.5199233376822444
0.4580336405666324 0.6063150452617960 0.5376067321363075
0.5435740241578196 0.3954509638315261 0.4633521085596923
0.4283670862932448 0.5520341262815300 0.5800353050758831
0.5721172616063868 0.4483640605119333 0.4207719073381385
0.4267605317347713 0.4793994842101469 0.5919732966341931
0.5738580029715658 0.5204634587023326 0.4083697459160857
0.5021882150639153 0.4997341353823186 0.4988804378379975
0.4467628021550961 0.5415346495964224 0.5116331317608709
0.4451293658222749 0.4665977921083544 0.5239916481197106
0.4460032536424955 0.4936625456786598 0.4569147875969831
0.5546247732281897 0.5064619172519959 0.5435658190831932
0.4899615474716271 0.5531850450256093 0.4556205238422271
0.5116897840660258 0.4471272301940086 0.5445607712506821
0.5570193536538155 0.4597867323040112 0.4883348802913409
0.5580418149309150 0.5322434637313284 0.4757340636772464
0.4877688380654074 0.4357232958153995 0.4755174059825738

0.5141975683609975 0.5640535562935788 0.5249602706781291
 0.5163794673773487 0.4887262421220591 0.4328911510535646
 0.4843129748491917 0.5112078012213997 0.5666445954746651
 0.6552797270343990 0.5072765116140004 0.6121541731047107
 0.6799630383943658 0.5222162321803516 0.5979021352774483
 0.6606115726091263 0.4895594054000721 0.6414045636030852

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Sc
 1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511
 0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093
 0.4257849678501046 0.5971843911863962 0.5587682477032310
 0.5732856100339081 0.3861121456696936 0.5178866030464339
 0.4617792912002723 0.6005336702018357 0.4937629545277189
 0.5364005247444733 0.3872098918791446 0.5801227938240562
 0.4930348404685829 0.6043420957278490 0.4310799230154365
 0.5309952836979567 0.4475125045440733 0.6199152142184708
 0.4978035903338358 0.5533983515900252 0.3824983707176304
 0.5220397280956448 0.5174509235122763 0.6488932678900868
 0.5048179920747644 0.4787628296167423 0.3570925292592017
 0.4998442820943942 0.6070583114105093 0.5564470311933010
 0.5271381796045747 0.3880150233648889 0.4496470543811366
 0.5347272693884709 0.6108491808402140 0.4870886141035011

0.4989420329914552 0.3841870378204137 0.5182627628108848
 0.5599193518024095 0.5884123450732816 0.4150266825591807
 0.4717811541623304 0.4188034734493732 0.5828950793929381
 0.5675703513400806 0.5158699791478590 0.3918030504795775
 0.4603629970435845 0.4841122233022239 0.6165156690251775
 0.5541439038779801 0.4426189693874140 0.4041177007753957
 0.4729132924384511 0.5586946480496960 0.6077928844360877
 0.2927837911408216 0.4775294688895357 0.4515767337234892
 0.2852894161421514 0.5281686521156205 0.4579773266513435
 0.5782384423573470 0.4959641704414688 0.5313207897253848
 0.4429786503353321 0.5015264317809685 0.4791456768797655
 0.5449859257592128 0.5606793094201545 0.5356494118493789
 0.4833261763333588 0.4415948577305505 0.4796238498333665
 0.4569982882570157 0.4752366677373885 0.5451482275647933
 0.4669554062184572 0.5489429868255215 0.5394763713102301
 0.5241373335250599 0.4433953974297727 0.5445675730906232
 0.5209384125934406 0.5301252299288740 0.4561273268338138
 0.5205506450248886 0.5075401343933150 0.5794474395781177
 0.4968599886243143 0.4927258324265706 0.4247822523169529
 0.3380150405587863 0.5188745765317422 0.4001761527807525
 0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Sc
 1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511

0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093
 0.4257849678501046 0.5971843911863962 0.5587682477032310
 0.5732856100339081 0.3861121456696936 0.5178866030464339
 0.4617792912002723 0.6005336702018357 0.4937629545277189
 0.5364005247444733 0.3872098918791446 0.5801227938240562
 0.4930348404685829 0.6043420957278490 0.4310799230154365
 0.5309952836979567 0.4475125045440733 0.6199152142184708
 0.4978035903338358 0.5533983515900252 0.3824983707176304
 0.5220397280956448 0.5174509235122763 0.6488932678900868
 0.5048179920747644 0.4787628296167423 0.3570925292592017
 0.4998442820943942 0.6070583114105093 0.5564470311933010
 0.5271381796045747 0.3880150233648889 0.4496470543811366
 0.5347272693884709 0.6108491808402140 0.4870886141035011
 0.4989420329914552 0.3841870378204137 0.5182627628108848
 0.5599193518024095 0.5884123450732816 0.4150266825591807
 0.4717811541623304 0.4188034734493732 0.5828950793929381
 0.5675703513400806 0.5158699791478590 0.3918030504795775
 0.4603629970435845 0.4841122233022239 0.6165156690251775
 0.5541439038779801 0.4426189693874140 0.4041177007753957
 0.4729132924384511 0.5586946480496960 0.6077928844360877
 0.2927837911408216 0.4775294688895357 0.4515767337234892
 0.2852894161421514 0.5281686521156205 0.4579773266513435
 0.5782384423573470 0.4959641704414688 0.5313207897253848
 0.4429786503353321 0.5015264317809685 0.4791456768797655
 0.5449859257592128 0.5606793094201545 0.5356494118493789
 0.4833261763333588 0.4415948577305505 0.4796238498333665
 0.4569982882570157 0.4752366677373885 0.5451482275647933
 0.4669554062184572 0.5489429868255215 0.5394763713102301
 0.5241373335250599 0.4433953974297727 0.5445675730906232
 0.5209384125934406 0.5301252299288740 0.4561273268338138
 0.5205506450248886 0.5075401343933150 0.5794474395781177
 0.4968599886243143 0.4927258324265706 0.4247822523169529
 0.3380150405587863 0.5188745765317422 0.4001761527807525
 0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000
 C Cu H Ni O Sc
 1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211

0.4216728403116562 0.4452985869093634 0.4468838760477263
0.6387694044876243 0.5172420165363314 0.4949726631458777
0.3914762083297880 0.4788014964741549 0.5177209666138497
0.6261496732469048 0.4453658797971391 0.5053971160713022
0.4067977616106873 0.5543247832344517 0.5039234664552771
0.5877477556936557 0.4386305980243673 0.5707728382716245
0.4413555387372207 0.5575673553952437 0.4363264279969088
0.5866814367651708 0.5036625474379380 0.6100397149112371
0.4292765228027315 0.4981532450378733 0.3971195582604697
0.5499758852399371 0.5723385155426441 0.6049516233268996
0.4811063962364906 0.4239660708099836 0.4071777839624231
0.5719261171149872 0.6190281495989748 0.5502755877624668
0.4549080585032683 0.3827574005198018 0.4614153955274179
0.6082119506383177 0.5971824661862516 0.4920042829572453
0.4302183594242659 0.4161788373541528 0.5195498702331950
0.6276388657507826 0.5518663671070854 0.4273620740738511
0.4055949459205679 0.4490338600901938 0.5799970852861056
0.6116441300217919 0.4775717375457150 0.4376205337106883
0.4146040071468167 0.5228238088836493 0.5727873565243482
0.6008763433716312 0.4013724369935392 0.4499050887878093
0.4257849678501046 0.5971843911863962 0.5587682477032310
0.5732856100339081 0.3861121456696936 0.5178866030464339
0.4617792912002723 0.6005336702018357 0.4937629545277189
0.5364005247444733 0.3872098918791446 0.5801227938240562
0.4930348404685829 0.6043420957278490 0.4310799230154365
0.5309952836979567 0.4475125045440733 0.6199152142184708
0.4978035903338358 0.5533983515900252 0.3824983707176304
0.5220397280956448 0.5174509235122763 0.6488932678900868
0.5048179920747644 0.4787628296167423 0.3570925292592017
0.4998442820943942 0.6070583114105093 0.5564470311933010
0.5271381796045747 0.3880150233648889 0.4496470543811366
0.5347272693884709 0.6108491808402140 0.4870886141035011
0.4989420329914552 0.3841870378204137 0.5182627628108848
0.5599193518024095 0.5884123450732816 0.4150266825591807
0.4717811541623304 0.4188034734493732 0.5828950793929381
0.5675703513400806 0.5158699791478590 0.3918030504795775
0.4603629970435845 0.4841122233022239 0.6165156690251775
0.5541439038779801 0.4426189693874140 0.4041177007753957
0.4729132924384511 0.5586946480496960 0.6077928844360877
0.2927837911408216 0.4775294688895357 0.4515767337234892
0.2852894161421514 0.5281686521156205 0.4579773266513435
0.5782384423573470 0.4959641704414688 0.5313207897253848
0.4429786503353321 0.5015264317809685 0.4791456768797655
0.5449859257592128 0.5606793094201545 0.5356494118493789
0.4833261763333588 0.4415948577305505 0.4796238498333665
0.4569982882570157 0.4752366677373885 0.5451482275647933
0.4669554062184572 0.5489429868255215 0.5394763713102301
0.5241373335250599 0.4433953974297727 0.5445675730906232
0.5209384125934406 0.5301252299288740 0.4561273268338138
0.5205506450248886 0.5075401343933150 0.5794474395781177
0.4968599886243143 0.4927258324265706 0.4247822523169529
0.3380150405587863 0.5188745765317422 0.4001761527807525

0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.000000000000000		
35.0000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

C Cu H Ni O Sc
1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511
 0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093
 0.4257849678501046 0.5971843911863962 0.5587682477032310
 0.5732856100339081 0.3861121456696936 0.5178866030464339
 0.4617792912002723 0.6005336702018357 0.4937629545277189
 0.5364005247444733 0.3872098918791446 0.5801227938240562
 0.4930348404685829 0.6043420957278490 0.4310799230154365
 0.5309952836979567 0.4475125045440733 0.6199152142184708
 0.4978035903338358 0.5533983515900252 0.3824983707176304
 0.5220397280956448 0.5174509235122763 0.6488932678900868
 0.5048179920747644 0.4787628296167423 0.3570925292592017
 0.4998442820943942 0.6070583114105093 0.5564470311933010
 0.5271381796045747 0.3880150233648889 0.4496470543811366
 0.5347272693884709 0.6108491808402140 0.4870886141035011
 0.4989420329914552 0.3841870378204137 0.5182627628108848
 0.5599193518024095 0.5884123450732816 0.4150266825591807
 0.4717811541623304 0.4188034734493732 0.5828950793929381
 0.5675703513400806 0.5158699791478590 0.3918030504795775

0.4603629970435845 0.4841122233022239 0.6165156690251775
 0.5541439038779801 0.4426189693874140 0.4041177007753957
 0.4729132924384511 0.5586946480496960 0.6077928844360877
 0.2927837911408216 0.4775294688895357 0.4515767337234892
 0.2852894161421514 0.5281686521156205 0.4579773266513435
 0.5782384423573470 0.4959641704414688 0.5313207897253848
 0.4429786503353321 0.5015264317809685 0.4791456768797655
 0.5449859257592128 0.5606793094201545 0.5356494118493789
 0.4833261763333588 0.4415948577305505 0.4796238498333665
 0.4569982882570157 0.4752366677373885 0.5451482275647933
 0.4669554062184572 0.5489429868255215 0.5394763713102301
 0.5241373335250599 0.4433953974297727 0.5445675730906232
 0.5209384125934406 0.5301252299288740 0.4561273268338138
 0.5205506450248886 0.5075401343933150 0.5794474395781177
 0.4968599886243143 0.4927258324265706 0.4247822523169529
 0.3380150405587863 0.5188745765317422 0.4001761527807525
 0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

```

1.0000000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000
C Cu H Ni O Sc
 1  42   2   7   1   6

```

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511
 0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093

0.4257849678501046	0.5971843911863962	0.5587682477032310
0.5732856100339081	0.3861121456696936	0.5178866030464339
0.4617792912002723	0.6005336702018357	0.4937629545277189
0.5364005247444733	0.3872098918791446	0.5801227938240562
0.4930348404685829	0.6043420957278490	0.4310799230154365
0.5309952836979567	0.4475125045440733	0.6199152142184708
0.4978035903338358	0.5533983515900252	0.3824983707176304
0.5220397280956448	0.5174509235122763	0.6488932678900868
0.5048179920747644	0.4787628296167423	0.3570925292592017
0.4998442820943942	0.6070583114105093	0.5564470311933010
0.5271381796045747	0.3880150233648889	0.4496470543811366
0.5347272693884709	0.6108491808402140	0.4870886141035011
0.4989420329914552	0.3841870378204137	0.5182627628108848
0.5599193518024095	0.5884123450732816	0.4150266825591807
0.4717811541623304	0.4188034734493732	0.5828950793929381
0.5675703513400806	0.5158699791478590	0.3918030504795775
0.4603629970435845	0.4841122233022239	0.6165156690251775
0.5541439038779801	0.4426189693874140	0.4041177007753957
0.4729132924384511	0.5586946480496960	0.6077928844360877
0.2927837911408216	0.4775294688895357	0.4515767337234892
0.2852894161421514	0.5281686521156205	0.4579773266513435
0.5782384423573470	0.4959641704414688	0.5313207897253848
0.4429786503353321	0.5015264317809685	0.4791456768797655
0.5449859257592128	0.5606793094201545	0.5356494118493789
0.4833261763333588	0.4415948577305505	0.4796238498333665
0.4569982882570157	0.4752366677373885	0.5451482275647933
0.4669554062184572	0.5489429868255215	0.5394763713102301
0.5241373335250599	0.4433953974297727	0.5445675730906232
0.5209384125934406	0.5301252299288740	0.4561273268338138
0.5205506450248886	0.5075401343933150	0.5794474395781177
0.4968599886243143	0.4927258324265706	0.4247822523169529
0.3380150405587863	0.5188745765317422	0.4001761527807525
0.5058680308543726	0.5079135416367551	0.5050033012179531
0.5733166524557535	0.5394289806155496	0.4694232603678968
0.5564476917141106	0.4470547507080826	0.4818887869822548

POSCAR

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

C Cu H Ni O Sc
1 42 2 7 1 6

Direct

0.3023213428350320	0.5062946603603229	0.4425227446654854
0.6384171687972533	0.4891297074307798	0.5619880735005651
0.3824978835516402	0.5091013259902806	0.4529446549147964
0.6092568833239977	0.5543791773540137	0.5554903219268211
0.4216728403116562	0.4452985869093634	0.4468838760477263
0.6387694044876243	0.5172420165363314	0.4949726631458777
0.3914762083297880	0.4788014964741549	0.5177209666138497
0.6261496732469048	0.4453658797971391	0.5053971160713022

0.4067977616106873 0.5543247832344517 0.5039234664552771
0.5877477556936557 0.4386305980243673 0.5707728382716245
0.4413555387372207 0.5575673553952437 0.4363264279969088
0.5866814367651708 0.5036625474379380 0.6100397149112371
0.4292765228027315 0.4981532450378733 0.3971195582604697
0.5499758852399371 0.5723385155426441 0.6049516233268996
0.4811063962364906 0.4239660708099836 0.4071777839624231
0.5719261171149872 0.6190281495989748 0.5502755877624668
0.4549080585032683 0.3827574005198018 0.4614153955274179
0.6082119506383177 0.5971824661862516 0.4920042829572453
0.4302183594242659 0.4161788373541528 0.5195498702331950
0.6276388657507826 0.5518663671070854 0.4273620740738511
0.4055949459205679 0.4490338600901938 0.5799970852861056
0.6116441300217919 0.4775717375457150 0.4376205337106883
0.4146040071468167 0.5228238088836493 0.5727873565243482
0.6008763433716312 0.4013724369935392 0.4499050887878093
0.4257849678501046 0.5971843911863962 0.5587682477032310
0.5732856100339081 0.3861121456696936 0.5178866030464339
0.4617792912002723 0.6005336702018357 0.4937629545277189
0.5364005247444733 0.3872098918791446 0.5801227938240562
0.4930348404685829 0.6043420957278490 0.4310799230154365
0.5309952836979567 0.4475125045440733 0.6199152142184708
0.4978035903338358 0.5533983515900252 0.3824983707176304
0.5220397280956448 0.5174509235122763 0.6488932678900868
0.5048179920747644 0.4787628296167423 0.3570925292592017
0.4998442820943942 0.6070583114105093 0.5564470311933010
0.5271381796045747 0.3880150233648889 0.4496470543811366
0.5347272693884709 0.6108491808402140 0.4870886141035011
0.4989420329914552 0.3841870378204137 0.5182627628108848
0.5599193518024095 0.5884123450732816 0.4150266825591807
0.4717811541623304 0.4188034734493732 0.5828950793929381
0.5675703513400806 0.5158699791478590 0.3918030504795775
0.4603629970435845 0.4841122233022239 0.6165156690251775
0.5541439038779801 0.4426189693874140 0.4041177007753957
0.4729132924384511 0.5586946480496960 0.6077928844360877
0.2927837911408216 0.4775294688895357 0.4515767337234892
0.2852894161421514 0.5281686521156205 0.4579773266513435
0.5782384423573470 0.4959641704414688 0.5313207897253848
0.4429786503353321 0.5015264317809685 0.4791456768797655
0.5449859257592128 0.5606793094201545 0.5356494118493789
0.4833261763333588 0.4415948577305505 0.4796238498333665
0.4569982882570157 0.4752366677373885 0.5451482275647933
0.4669554062184572 0.5489429868255215 0.5394763713102301
0.5241373335250599 0.4433953974297727 0.5445675730906232
0.5209384125934406 0.5301252299288740 0.4561273268338138
0.5205506450248886 0.5075401343933150 0.5794474395781177
0.4968599886243143 0.4927258324265706 0.4247822523169529
0.3380150405587863 0.5188745765317422 0.4001761527807525
0.5058680308543726 0.5079135416367551 0.5050033012179531
0.5733166524557535 0.5394289806155496 0.4694232603678968
0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.000000000000000
 35.0000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000
 C Cu H Ni O Sc
 1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511
 0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093
 0.4257849678501046 0.5971843911863962 0.5587682477032310
 0.5732856100339081 0.3861121456696936 0.5178866030464339
 0.4617792912002723 0.6005336702018357 0.4937629545277189
 0.5364005247444733 0.3872098918791446 0.5801227938240562
 0.4930348404685829 0.6043420957278490 0.4310799230154365
 0.5309952836979567 0.4475125045440733 0.6199152142184708
 0.4978035903338358 0.5533983515900252 0.3824983707176304
 0.5220397280956448 0.5174509235122763 0.6488932678900868
 0.5048179920747644 0.4787628296167423 0.3570925292592017
 0.4998442820943942 0.6070583114105093 0.5564470311933010
 0.5271381796045747 0.3880150233648889 0.4496470543811366
 0.5347272693884709 0.6108491808402140 0.4870886141035011
 0.4989420329914552 0.3841870378204137 0.5182627628108848
 0.5599193518024095 0.5884123450732816 0.4150266825591807
 0.4717811541623304 0.4188034734493732 0.5828950793929381
 0.5675703513400806 0.5158699791478590 0.3918030504795775
 0.4603629970435845 0.4841122233022239 0.6165156690251775
 0.5541439038779801 0.4426189693874140 0.4041177007753957
 0.4729132924384511 0.5586946480496960 0.6077928844360877
 0.2927837911408216 0.4775294688895357 0.4515767337234892

0.2852894161421514 0.5281686521156205 0.4579773266513435
 0.5782384423573470 0.4959641704414688 0.5313207897253848
 0.4429786503353321 0.5015264317809685 0.4791456768797655
 0.5449859257592128 0.5606793094201545 0.5356494118493789
 0.4833261763333588 0.4415948577305505 0.4796238498333665
 0.4569982882570157 0.4752366677373885 0.5451482275647933
 0.4669554062184572 0.5489429868255215 0.5394763713102301
 0.5241373335250599 0.4433953974297727 0.5445675730906232
 0.5209384125934406 0.5301252299288740 0.4561273268338138
 0.5205506450248886 0.5075401343933150 0.5794474395781177
 0.4968599886243143 0.4927258324265706 0.4247822523169529
 0.3380150405587863 0.5188745765317422 0.4001761527807525
 0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Sc		
1 42 2 7 1 6		

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371
 0.4292765228027315 0.4981532450378733 0.3971195582604697
 0.5499758852399371 0.5723385155426441 0.6049516233268996
 0.4811063962364906 0.4239660708099836 0.4071777839624231
 0.5719261171149872 0.6190281495989748 0.5502755877624668
 0.4549080585032683 0.3827574005198018 0.4614153955274179
 0.6082119506383177 0.5971824661862516 0.4920042829572453
 0.4302183594242659 0.4161788373541528 0.5195498702331950
 0.6276388657507826 0.5518663671070854 0.4273620740738511
 0.4055949459205679 0.4490338600901938 0.5799970852861056
 0.6116441300217919 0.4775717375457150 0.4376205337106883
 0.4146040071468167 0.5228238088836493 0.5727873565243482
 0.6008763433716312 0.4013724369935392 0.4499050887878093
 0.4257849678501046 0.5971843911863962 0.5587682477032310
 0.5732856100339081 0.3861121456696936 0.5178866030464339
 0.4617792912002723 0.6005336702018357 0.4937629545277189
 0.5364005247444733 0.3872098918791446 0.5801227938240562

0.4930348404685829 0.6043420957278490 0.4310799230154365
 0.5309952836979567 0.4475125045440733 0.6199152142184708
 0.4978035903338358 0.5533983515900252 0.3824983707176304
 0.5220397280956448 0.5174509235122763 0.6488932678900868
 0.5048179920747644 0.4787628296167423 0.3570925292592017
 0.4998442820943942 0.6070583114105093 0.5564470311933010
 0.5271381796045747 0.3880150233648889 0.4496470543811366
 0.5347272693884709 0.6108491808402140 0.4870886141035011
 0.4989420329914552 0.3841870378204137 0.5182627628108848
 0.5599193518024095 0.5884123450732816 0.4150266825591807
 0.4717811541623304 0.4188034734493732 0.5828950793929381
 0.5675703513400806 0.5158699791478590 0.3918030504795775
 0.4603629970435845 0.4841122233022239 0.6165156690251775
 0.5541439038779801 0.4426189693874140 0.4041177007753957
 0.4729132924384511 0.5586946480496960 0.6077928844360877
 0.2927837911408216 0.4775294688895357 0.4515767337234892
 0.2852894161421514 0.5281686521156205 0.4579773266513435
 0.5782384423573470 0.4959641704414688 0.5313207897253848
 0.4429786503353321 0.5015264317809685 0.4791456768797655
 0.5449859257592128 0.5606793094201545 0.5356494118493789
 0.4833261763333588 0.4415948577305505 0.4796238498333665
 0.4569982882570157 0.4752366677373885 0.5451482275647933
 0.4669554062184572 0.5489429868255215 0.5394763713102301
 0.5241373335250599 0.4433953974297727 0.5445675730906232
 0.5209384125934406 0.5301252299288740 0.4561273268338138
 0.5205506450248886 0.5075401343933150 0.5794474395781177
 0.4968599886243143 0.4927258324265706 0.4247822523169529
 0.3380150405587863 0.5188745765317422 0.4001761527807525
 0.5058680308543726 0.5079135416367551 0.5050033012179531
 0.5733166524557535 0.5394289806155496 0.4694232603678968
 0.5564476917141106 0.4470547507080826 0.4818887869822548

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

C Cu H Ni O Sc
1 42 2 7 1 6

Direct

0.3023213428350320 0.5062946603603229 0.4425227446654854
 0.6384171687972533 0.4891297074307798 0.5619880735005651
 0.3824978835516402 0.5091013259902806 0.4529446549147964
 0.6092568833239977 0.5543791773540137 0.5554903219268211
 0.4216728403116562 0.4452985869093634 0.4468838760477263
 0.6387694044876243 0.5172420165363314 0.4949726631458777
 0.3914762083297880 0.4788014964741549 0.5177209666138497
 0.6261496732469048 0.4453658797971391 0.5053971160713022
 0.4067977616106873 0.5543247832344517 0.5039234664552771
 0.5877477556936557 0.4386305980243673 0.5707728382716245
 0.4413555387372207 0.5575673553952437 0.4363264279969088
 0.5866814367651708 0.5036625474379380 0.6100397149112371

0.4292765228027315	0.4981532450378733	0.3971195582604697
0.5499758852399371	0.5723385155426441	0.6049516233268996
0.4811063962364906	0.4239660708099836	0.4071777839624231
0.5719261171149872	0.6190281495989748	0.5502755877624668
0.4549080585032683	0.3827574005198018	0.4614153955274179
0.6082119506383177	0.5971824661862516	0.4920042829572453
0.4302183594242659	0.4161788373541528	0.5195498702331950
0.6276388657507826	0.5518663671070854	0.4273620740738511
0.4055949459205679	0.4490338600901938	0.5799970852861056
0.6116441300217919	0.4775717375457150	0.4376205337106883
0.4146040071468167	0.5228238088836493	0.5727873565243482
0.6008763433716312	0.4013724369935392	0.4499050887878093
0.4257849678501046	0.5971843911863962	0.5587682477032310
0.5732856100339081	0.3861121456696936	0.5178866030464339
0.4617792912002723	0.6005336702018357	0.4937629545277189
0.5364005247444733	0.3872098918791446	0.5801227938240562
0.4930348404685829	0.6043420957278490	0.4310799230154365
0.5309952836979567	0.4475125045440733	0.6199152142184708
0.4978035903338358	0.5533983515900252	0.3824983707176304
0.5220397280956448	0.5174509235122763	0.6488932678900868
0.5048179920747644	0.4787628296167423	0.3570925292592017
0.4998442820943942	0.6070583114105093	0.5564470311933010
0.5271381796045747	0.3880150233648889	0.4496470543811366
0.5347272693884709	0.6108491808402140	0.4870886141035011
0.4989420329914552	0.3841870378204137	0.5182627628108848
0.5599193518024095	0.5884123450732816	0.4150266825591807
0.4717811541623304	0.4188034734493732	0.5828950793929381
0.5675703513400806	0.5158699791478590	0.3918030504795775
0.4603629970435845	0.4841122233022239	0.6165156690251775
0.5541439038779801	0.4426189693874140	0.4041177007753957
0.4729132924384511	0.5586946480496960	0.6077928844360877
0.2927837911408216	0.4775294688895357	0.4515767337234892
0.2852894161421514	0.5281686521156205	0.4579773266513435
0.5782384423573470	0.4959641704414688	0.5313207897253848
0.4429786503353321	0.5015264317809685	0.4791456768797655
0.5449859257592128	0.5606793094201545	0.5356494118493789
0.4833261763333588	0.4415948577305505	0.4796238498333665
0.4569982882570157	0.4752366677373885	0.5451482275647933
0.4669554062184572	0.5489429868255215	0.5394763713102301
0.5241373335250599	0.4433953974297727	0.5445675730906232
0.5209384125934406	0.5301252299288740	0.4561273268338138
0.5205506450248886	0.5075401343933150	0.5794474395781177
0.4968599886243143	0.4927258324265706	0.4247822523169529
0.3380150405587863	0.5188745765317422	0.4001761527807525
0.5058680308543726	0.5079135416367551	0.5050033012179531
0.5733166524557535	0.5394289806155496	0.4694232603678968
0.5564476917141106	0.4470547507080826	0.4818887869822548

POSCAR

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000	0.0000000000000000	35.0000000000000000
C Cu H Ni O Sc		
1 42 2 7 1 6		
Direct		
0.3023213428350320	0.5062946603603229	0.4425227446654854
0.6384171687972533	0.4891297074307798	0.5619880735005651
0.3824978835516402	0.5091013259902806	0.4529446549147964
0.6092568833239977	0.5543791773540137	0.5554903219268211
0.4216728403116562	0.4452985869093634	0.4468838760477263
0.6387694044876243	0.5172420165363314	0.4949726631458777
0.3914762083297880	0.4788014964741549	0.5177209666138497
0.6261496732469048	0.4453658797971391	0.5053971160713022
0.4067977616106873	0.5543247832344517	0.5039234664552771
0.5877477556936557	0.4386305980243673	0.5707728382716245
0.4413555387372207	0.5575673553952437	0.4363264279969088
0.5866814367651708	0.5036625474379380	0.6100397149112371
0.4292765228027315	0.4981532450378733	0.3971195582604697
0.5499758852399371	0.5723385155426441	0.6049516233268996
0.4811063962364906	0.4239660708099836	0.4071777839624231
0.5719261171149872	0.6190281495989748	0.5502755877624668
0.4549080585032683	0.3827574005198018	0.4614153955274179
0.6082119506383177	0.5971824661862516	0.4920042829572453
0.4302183594242659	0.4161788373541528	0.5195498702331950
0.6276388657507826	0.5518663671070854	0.4273620740738511
0.4055949459205679	0.4490338600901938	0.5799970852861056
0.6116441300217919	0.4775717375457150	0.4376205337106883
0.4146040071468167	0.5228238088836493	0.5727873565243482
0.6008763433716312	0.4013724369935392	0.4499050887878093
0.4257849678501046	0.5971843911863962	0.5587682477032310
0.5732856100339081	0.3861121456696936	0.5178866030464339
0.4617792912002723	0.6005336702018357	0.4937629545277189
0.5364005247444733	0.3872098918791446	0.5801227938240562
0.4930348404685829	0.6043420957278490	0.4310799230154365
0.5309952836979567	0.4475125045440733	0.6199152142184708
0.4978035903338358	0.5533983515900252	0.3824983707176304
0.5220397280956448	0.5174509235122763	0.6488932678900868
0.5048179920747644	0.4787628296167423	0.3570925292592017
0.4998442820943942	0.6070583114105093	0.5564470311933010
0.5271381796045747	0.3880150233648889	0.4496470543811366
0.5347272693884709	0.6108491808402140	0.4870886141035011
0.4989420329914552	0.3841870378204137	0.5182627628108848
0.5599193518024095	0.5884123450732816	0.4150266825591807
0.4717811541623304	0.4188034734493732	0.5828950793929381
0.5675703513400806	0.5158699791478590	0.3918030504795775
0.4603629970435845	0.4841122233022239	0.6165156690251775
0.5541439038779801	0.4426189693874140	0.4041177007753957
0.4729132924384511	0.5586946480496960	0.6077928844360877
0.2927837911408216	0.4775294688895357	0.4515767337234892
0.2852894161421514	0.5281686521156205	0.4579773266513435
0.5782384423573470	0.4959641704414688	0.5313207897253848
0.4429786503353321	0.5015264317809685	0.4791456768797655
0.5449859257592128	0.5606793094201545	0.5356494118493789

0.4833261763333588	0.4415948577305505	0.4796238498333665
0.4569982882570157	0.4752366677373885	0.5451482275647933
0.4669554062184572	0.5489429868255215	0.5394763713102301
0.5241373335250599	0.4433953974297727	0.5445675730906232
0.5209384125934406	0.5301252299288740	0.4561273268338138
0.5205506450248886	0.5075401343933150	0.5794474395781177
0.4968599886243143	0.4927258324265706	0.4247822523169529
0.3380150405587863	0.5188745765317422	0.4001761527807525
0.5058680308543726	0.5079135416367551	0.5050033012179531
0.5733166524557535	0.5394289806155496	0.4694232603678968
0.5564476917141106	0.4470547507080826	0.4818887869822548

POSCAR

1.00000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Ti
 1 42 2 7 1 6

Direct
0.3036041813367280 0.5054781576784461 0.4550273796650818
0.6385977689057917 0.4890151547104086 0.5613506176404321
0.3884113731044395 0.5099679832337438 0.4486514033292938
0.6080603144450346 0.5537557268929693 0.5556012640726447
0.4207428928765099 0.4446910979001141 0.4516543367014254
0.6350438274493775 0.5186716709488440 0.4949916845415483
0.3948031064513852 0.4794760511560222 0.5139562629886383
0.6239255552455203 0.4450500374220348 0.5053493979905010
0.4081161739227480 0.5542303598803255 0.5026323550921999
0.5891304347405633 0.4370282284266774 0.5713105154613362
0.4392298793966560 0.5621274550138319 0.4363522283039659
0.5841764782739367 0.5032126222355765 0.6067794871996842
0.4419306720802986 0.4968838779473193 0.4015972539534010
0.5487764945499610 0.5710315014861510 0.6007754383252336
0.4803911947531764 0.4294122805372517 0.4099020658795965
0.5721010616752498 0.6181215720298022 0.5484935388472301
0.4549256358434372 0.3821690606185207 0.4612634977870539
0.6013562429358456 0.5894959791885004 0.4886215900867270
0.4303395341482565 0.4151729857806491 0.5195455676066245
0.6228974253717452 0.5493729512956589 0.4298359271668071
0.4065792357788717 0.4503747794930964 0.5784068991714623
0.6120704858386206 0.4763587943812199 0.4383662524242410
0.4161440627117908 0.5228714344271970 0.5704873811196944
0.6001076752259407 0.4033112785875038 0.4501051381967303
0.4276907065637495 0.5955961317993728 0.5585447297130228
0.5715772942861664 0.3889190295031209 0.5166900113818121
0.4587654771752243 0.6051229825993457 0.4933274133960538
0.5368708540811887 0.3866416231991746 0.5802401906818768
0.4904744611582413 0.6104789356186100 0.4305293476053499
0.5303247971041440 0.4493769090795736 0.6161006782510864
0.4969718917436942 0.5521715444532418 0.3884033512022373
0.5213010540329355 0.5173837052937226 0.6439637561721953

0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678
 0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049
 0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Ti		
1 42 2 7 1 6		

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010
 0.4081161739227480 0.5542303598803255 0.5026323550921999
 0.5891304347405633 0.4370282284266774 0.5713105154613362
 0.4392298793966560 0.5621274550138319 0.4363522283039659
 0.5841764782739367 0.5032126222355765 0.6067794871996842
 0.4419306720802986 0.4968838779473193 0.4015972539534010
 0.5487764945499610 0.5710315014861510 0.6007754383252336
 0.4803911947531764 0.4294122805372517 0.4099020658795965
 0.5721010616752498 0.6181215720298022 0.5484935388472301

0.4549256358434372 0.3821690606185207 0.4612634977870539
 0.6013562429358456 0.5894959791885004 0.4886215900867270
 0.4303395341482565 0.4151729857806491 0.5195455676066245
 0.6228974253717452 0.5493729512956589 0.4298359271668071
 0.4065792357788717 0.4503747794930964 0.5784068991714623
 0.6120704858386206 0.4763587943812199 0.4383662524242410
 0.4161440627117908 0.5228714344271970 0.5704873811196944
 0.6001076752259407 0.4033112785875038 0.4501051381967303
 0.4276907065637495 0.5955961317993728 0.5585447297130228
 0.5715772942861664 0.3889190295031209 0.5166900113818121
 0.4587654771752243 0.6051229825993457 0.4933274133960538
 0.5368708540811887 0.3866416231991746 0.5802401906818768
 0.4904744611582413 0.6104789356186100 0.4305293476053499
 0.5303247971041440 0.4493769090795736 0.6161006782510864
 0.4969718917436942 0.5521715444532418 0.3884033512022373
 0.5213010540329355 0.5173837052937226 0.6439637561721953
 0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678
 0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049
 0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

C Cu H Ni O Ti
 1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
0.6385977689057917 0.4890151547104086 0.5613506176404321
0.3884113731044395 0.5099679832337438 0.4486514033292938
0.6080603144450346 0.5537557268929693 0.5556012640726447
0.4207428928765099 0.4446910979001141 0.4516543367014254
0.6350438274493775 0.5186716709488440 0.4949916845415483
0.3948031064513852 0.4794760511560222 0.5139562629886383
0.6239255552455203 0.4450500374220348 0.5053493979905010
0.4081161739227480 0.5542303598803255 0.5026323550921999
0.5891304347405633 0.4370282284266774 0.5713105154613362
0.4392298793966560 0.5621274550138319 0.4363522283039659
0.5841764782739367 0.5032126222355765 0.6067794871996842
0.4419306720802986 0.4968838779473193 0.4015972539534010
0.5487764945499610 0.5710315014861510 0.6007754383252336
0.4803911947531764 0.4294122805372517 0.4099020658795965
0.5721010616752498 0.6181215720298022 0.5484935388472301
0.4549256358434372 0.3821690606185207 0.4612634977870539
0.6013562429358456 0.5894959791885004 0.4886215900867270
0.4303395341482565 0.4151729857806491 0.5195455676066245
0.6228974253717452 0.5493729512956589 0.4298359271668071
0.4065792357788717 0.4503747794930964 0.5784068991714623
0.6120704858386206 0.4763587943812199 0.4383662524242410
0.4161440627117908 0.5228714344271970 0.5704873811196944
0.6001076752259407 0.4033112785875038 0.4501051381967303
0.4276907065637495 0.5955961317993728 0.5585447297130228
0.5715772942861664 0.3889190295031209 0.5166900113818121
0.4587654771752243 0.6051229825993457 0.4933274133960538
0.5368708540811887 0.3866416231991746 0.5802401906818768
0.4904744611582413 0.6104789356186100 0.4305293476053499
0.5303247971041440 0.4493769090795736 0.6161006782510864
0.4969718917436942 0.5521715444532418 0.3884033512022373
0.5213010540329355 0.5173837052937226 0.6439637561721953
0.5056536818962678 0.4807879240627962 0.3636332940859567
0.5003430489758749 0.6069991905278587 0.5538678754843314
0.5278532514079322 0.3891798388529084 0.4521389533409145
0.5321073627382545 0.6154200126427055 0.4873044934507678
0.4973075057987665 0.3827213850180751 0.5197878344528253
0.5580996295831260 0.5865626330795476 0.4230449769181316
0.4722020246454268 0.4179687772087972 0.5809778417240564
0.5659570938979271 0.5161265833753590 0.3939051803000049
0.4627623223099753 0.4838004362359217 0.6141367493446492
0.5540067997976925 0.4414548218965934 0.4054880711422289
0.4738602425937604 0.5579854506695565 0.6049415625975100
0.2920625822924532 0.4774707085403189 0.4454534381001980
0.2834636265093087 0.5298442365139604 0.4498427137052367
0.5770164988339307 0.4941726336447064 0.5326000491525930
0.4481567291290724 0.5030911001096524 0.4757611524880543
0.5448173362441722 0.5592774302290756 0.5310574897082717
0.4855523747723344 0.4403517498486183 0.4801695668347027
0.4592024951009945 0.4749278201838289 0.5433034728461154
0.4698908807134987 0.5477950907502359 0.5351791822996977
0.5259229559884970 0.4428972271010679 0.5429070106653766

0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Ti
 1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010
 0.4081161739227480 0.5542303598803255 0.5026323550921999
 0.5891304347405633 0.4370282284266774 0.5713105154613362
 0.4392298793966560 0.5621274550138319 0.4363522283039659
 0.5841764782739367 0.5032126222355765 0.6067794871996842
 0.4419306720802986 0.4968838779473193 0.4015972539534010
 0.5487764945499610 0.5710315014861510 0.6007754383252336
 0.4803911947531764 0.4294122805372517 0.4099020658795965
 0.5721010616752498 0.6181215720298022 0.5484935388472301
 0.4549256358434372 0.3821690606185207 0.4612634977870539
 0.6013562429358456 0.5894959791885004 0.4886215900867270
 0.4303395341482565 0.4151729857806491 0.5195455676066245
 0.6228974253717452 0.5493729512956589 0.4298359271668071
 0.4065792357788717 0.4503747794930964 0.5784068991714623
 0.6120704858386206 0.4763587943812199 0.4383662524242410
 0.4161440627117908 0.5228714344271970 0.5704873811196944
 0.6001076752259407 0.4033112785875038 0.4501051381967303
 0.4276907065637495 0.5955961317993728 0.5585447297130228
 0.5715772942861664 0.3889190295031209 0.5166900113818121
 0.4587654771752243 0.6051229825993457 0.4933274133960538
 0.5368708540811887 0.3866416231991746 0.5802401906818768
 0.4904744611582413 0.6104789356186100 0.4305293476053499
 0.5303247971041440 0.4493769090795736 0.6161006782510864
 0.4969718917436942 0.5521715444532418 0.3884033512022373
 0.5213010540329355 0.5173837052937226 0.6439637561721953
 0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678

0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049
 0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

C	Cu	H	Ni	O	Ti
1	42	2	7	1	6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010
 0.4081161739227480 0.5542303598803255 0.5026323550921999
 0.5891304347405633 0.4370282284266774 0.5713105154613362
 0.4392298793966560 0.5621274550138319 0.4363522283039659
 0.5841764782739367 0.5032126222355765 0.6067794871996842
 0.4419306720802986 0.4968838779473193 0.4015972539534010
 0.5487764945499610 0.5710315014861510 0.6007754383252336
 0.4803911947531764 0.4294122805372517 0.4099020658795965
 0.5721010616752498 0.6181215720298022 0.5484935388472301
 0.4549256358434372 0.3821690606185207 0.4612634977870539
 0.6013562429358456 0.5894959791885004 0.4886215900867270
 0.4303395341482565 0.4151729857806491 0.5195455676066245
 0.6228974253717452 0.5493729512956589 0.4298359271668071

0.4065792357788717 0.4503747794930964 0.5784068991714623
 0.6120704858386206 0.4763587943812199 0.4383662524242410
 0.4161440627117908 0.5228714344271970 0.5704873811196944
 0.6001076752259407 0.4033112785875038 0.4501051381967303
 0.4276907065637495 0.5955961317993728 0.5585447297130228
 0.5715772942861664 0.3889190295031209 0.5166900113818121
 0.4587654771752243 0.6051229825993457 0.4933274133960538
 0.5368708540811887 0.3866416231991746 0.5802401906818768
 0.4904744611582413 0.6104789356186100 0.4305293476053499
 0.5303247971041440 0.4493769090795736 0.6161006782510864
 0.4969718917436942 0.5521715444532418 0.3884033512022373
 0.5213010540329355 0.5173837052937226 0.6439637561721953
 0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678
 0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049
 0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Ti
 1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447

0.4207428928765099 0.4446910979001141 0.4516543367014254
0.6350438274493775 0.5186716709488440 0.4949916845415483
0.3948031064513852 0.4794760511560222 0.5139562629886383
0.623925552455203 0.4450500374220348 0.5053493979905010
0.4081161739227480 0.5542303598803255 0.5026323550921999
0.5891304347405633 0.4370282284266774 0.5713105154613362
0.4392298793966560 0.5621274550138319 0.4363522283039659
0.5841764782739367 0.5032126222355765 0.6067794871996842
0.4419306720802986 0.4968838779473193 0.4015972539534010
0.5487764945499610 0.5710315014861510 0.6007754383252336
0.4803911947531764 0.4294122805372517 0.4099020658795965
0.5721010616752498 0.6181215720298022 0.5484935388472301
0.4549256358434372 0.3821690606185207 0.4612634977870539
0.6013562429358456 0.5894959791885004 0.4886215900867270
0.4303395341482565 0.4151729857806491 0.5195455676066245
0.6228974253717452 0.5493729512956589 0.4298359271668071
0.4065792357788717 0.4503747794930964 0.5784068991714623
0.6120704858386206 0.4763587943812199 0.4383662524242410
0.4161440627117908 0.5228714344271970 0.5704873811196944
0.6001076752259407 0.4033112785875038 0.4501051381967303
0.4276907065637495 0.5955961317993728 0.5585447297130228
0.5715772942861664 0.3889190295031209 0.5166900113818121
0.4587654771752243 0.6051229825993457 0.4933274133960538
0.5368708540811887 0.3866416231991746 0.5802401906818768
0.4904744611582413 0.6104789356186100 0.4305293476053499
0.5303247971041440 0.4493769090795736 0.6161006782510864
0.4969718917436942 0.5521715444532418 0.3884033512022373
0.5213010540329355 0.5173837052937226 0.6439637561721953
0.5056536818962678 0.4807879240627962 0.3636332940859567
0.5003430489758749 0.6069991905278587 0.5538678754843314
0.5278532514079322 0.3891798388529084 0.4521389533409145
0.5321073627382545 0.6154200126427055 0.4873044934507678
0.4973075057987665 0.3827213850180751 0.5197878344528253
0.5580996295831260 0.5865626330795476 0.4230449769181316
0.4722020246454268 0.4179687772087972 0.5809778417240564
0.5659570938979271 0.5161265833753590 0.3939051803000049
0.4627623223099753 0.4838004362359217 0.6141367493446492
0.5540067997976925 0.4414548218965934 0.4054880711422289
0.4738602425937604 0.5579854506695565 0.6049415625975100
0.2920625822924532 0.4774707085403189 0.4454534381001980
0.2834636265093087 0.5298442365139604 0.4498427137052367
0.5770164988339307 0.4941726336447064 0.5326000491525930
0.4481567291290724 0.5030911001096524 0.4757611524880543
0.5448173362441722 0.5592774302290756 0.5310574897082717
0.4855523747723344 0.4403517498486183 0.4801695668347027
0.4592024951009945 0.4749278201838289 0.5433034728461154
0.4698908807134987 0.5477950907502359 0.5351791822996977
0.5259229559884970 0.4428972271010679 0.5429070106653766
0.5155873336502210 0.5370778519647652 0.4614739498171530
0.5204511019655126 0.5092596294389422 0.5760750767049900
0.5058464697800708 0.4935754655866855 0.4307482454085797
0.3326082472033348 0.5170802703710735 0.4117954387905362

0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000		
35.0000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

C Cu H Ni O Ti
1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010
 0.4081161739227480 0.5542303598803255 0.5026323550921999
 0.5891304347405633 0.4370282284266774 0.5713105154613362
 0.4392298793966560 0.5621274550138319 0.4363522283039659
 0.5841764782739367 0.5032126222355765 0.6067794871996842
 0.4419306720802986 0.4968838779473193 0.4015972539534010
 0.5487764945499610 0.5710315014861510 0.6007754383252336
 0.4803911947531764 0.4294122805372517 0.4099020658795965
 0.5721010616752498 0.6181215720298022 0.5484935388472301
 0.4549256358434372 0.3821690606185207 0.4612634977870539
 0.6013562429358456 0.5894959791885004 0.4886215900867270
 0.4303395341482565 0.4151729857806491 0.5195455676066245
 0.6228974253717452 0.5493729512956589 0.4298359271668071
 0.4065792357788717 0.4503747794930964 0.5784068991714623
 0.6120704858386206 0.4763587943812199 0.4383662524242410
 0.4161440627117908 0.5228714344271970 0.5704873811196944
 0.6001076752259407 0.4033112785875038 0.4501051381967303
 0.4276907065637495 0.5955961317993728 0.5585447297130228
 0.5715772942861664 0.3889190295031209 0.5166900113818121
 0.4587654771752243 0.6051229825993457 0.4933274133960538
 0.5368708540811887 0.3866416231991746 0.5802401906818768
 0.4904744611582413 0.6104789356186100 0.4305293476053499
 0.5303247971041440 0.4493769090795736 0.6161006782510864
 0.4969718917436942 0.5521715444532418 0.3884033512022373
 0.5213010540329355 0.5173837052937226 0.6439637561721953
 0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678
 0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049

0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000		
35.0000000000000000000000	0.000000000000000000000000	0.000000000000000000000000
0.000000000000000000000000	35.0000000000000000000000	0.000000000000000000000000
0.000000000000000000000000	0.000000000000000000000000	35.0000000000000000000000
C Cu H Ni O Ti		
1 42 2 7 1 6		

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010
 0.4081161739227480 0.5542303598803255 0.5026323550921999
 0.5891304347405633 0.4370282284266774 0.5713105154613362
 0.4392298793966560 0.5621274550138319 0.4363522283039659
 0.5841764782739367 0.5032126222355765 0.6067794871996842
 0.4419306720802986 0.4968838779473193 0.4015972539534010
 0.5487764945499610 0.5710315014861510 0.6007754383252336
 0.4803911947531764 0.4294122805372517 0.4099020658795965
 0.5721010616752498 0.6181215720298022 0.5484935388472301
 0.4549256358434372 0.3821690606185207 0.4612634977870539
 0.6013562429358456 0.5894959791885004 0.4886215900867270
 0.4303395341482565 0.4151729857806491 0.5195455676066245
 0.6228974253717452 0.5493729512956589 0.4298359271668071
 0.4065792357788717 0.4503747794930964 0.5784068991714623
 0.6120704858386206 0.4763587943812199 0.4383662524242410
 0.4161440627117908 0.5228714344271970 0.5704873811196944
 0.6001076752259407 0.4033112785875038 0.4501051381967303

0.4276907065637495 0.5955961317993728 0.5585447297130228
 0.5715772942861664 0.3889190295031209 0.5166900113818121
 0.4587654771752243 0.6051229825993457 0.4933274133960538
 0.5368708540811887 0.3866416231991746 0.5802401906818768
 0.4904744611582413 0.6104789356186100 0.4305293476053499
 0.5303247971041440 0.4493769090795736 0.6161006782510864
 0.4969718917436942 0.5521715444532418 0.3884033512022373
 0.5213010540329355 0.5173837052937226 0.6439637561721953
 0.5056536818962678 0.4807879240627962 0.3636332940859567
 0.5003430489758749 0.6069991905278587 0.5538678754843314
 0.5278532514079322 0.3891798388529084 0.4521389533409145
 0.5321073627382545 0.6154200126427055 0.4873044934507678
 0.4973075057987665 0.3827213850180751 0.5197878344528253
 0.5580996295831260 0.5865626330795476 0.4230449769181316
 0.4722020246454268 0.4179687772087972 0.5809778417240564
 0.5659570938979271 0.5161265833753590 0.3939051803000049
 0.4627623223099753 0.4838004362359217 0.6141367493446492
 0.5540067997976925 0.4414548218965934 0.4054880711422289
 0.4738602425937604 0.5579854506695565 0.6049415625975100
 0.2920625822924532 0.4774707085403189 0.4454534381001980
 0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000		
35.0000000000000000000000	0.000000000000000000000000	0.000000000000000000000000
0.000000000000000000000000	35.000000000000000000000000	0.000000000000000000000000
0.000000000000000000000000	0.000000000000000000000000	35.000000000000000000000000

C Cu H Ni O Ti
 1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
 0.6385977689057917 0.4890151547104086 0.5613506176404321
 0.3884113731044395 0.5099679832337438 0.4486514033292938
 0.6080603144450346 0.5537557268929693 0.5556012640726447
 0.4207428928765099 0.4446910979001141 0.4516543367014254
 0.6350438274493775 0.5186716709488440 0.4949916845415483
 0.3948031064513852 0.4794760511560222 0.5139562629886383
 0.6239255552455203 0.4450500374220348 0.5053493979905010

0.4081161739227480 0.5542303598803255 0.5026323550921999
0.5891304347405633 0.4370282284266774 0.5713105154613362
0.4392298793966560 0.5621274550138319 0.4363522283039659
0.5841764782739367 0.5032126222355765 0.6067794871996842
0.4419306720802986 0.4968838779473193 0.4015972539534010
0.5487764945499610 0.5710315014861510 0.6007754383252336
0.4803911947531764 0.4294122805372517 0.4099020658795965
0.5721010616752498 0.6181215720298022 0.5484935388472301
0.4549256358434372 0.3821690606185207 0.4612634977870539
0.6013562429358456 0.5894959791885004 0.4886215900867270
0.4303395341482565 0.4151729857806491 0.5195455676066245
0.6228974253717452 0.5493729512956589 0.4298359271668071
0.4065792357788717 0.4503747794930964 0.5784068991714623
0.6120704858386206 0.4763587943812199 0.4383662524242410
0.4161440627117908 0.5228714344271970 0.5704873811196944
0.6001076752259407 0.4033112785875038 0.4501051381967303
0.4276907065637495 0.5955961317993728 0.5585447297130228
0.5715772942861664 0.3889190295031209 0.5166900113818121
0.4587654771752243 0.6051229825993457 0.4933274133960538
0.5368708540811887 0.3866416231991746 0.5802401906818768
0.4904744611582413 0.6104789356186100 0.4305293476053499
0.5303247971041440 0.4493769090795736 0.6161006782510864
0.4969718917436942 0.5521715444532418 0.3884033512022373
0.5213010540329355 0.5173837052937226 0.6439637561721953
0.5056536818962678 0.4807879240627962 0.3636332940859567
0.5003430489758749 0.6069991905278587 0.5538678754843314
0.5278532514079322 0.3891798388529084 0.4521389533409145
0.5321073627382545 0.6154200126427055 0.4873044934507678
0.4973075057987665 0.3827213850180751 0.5197878344528253
0.5580996295831260 0.5865626330795476 0.4230449769181316
0.4722020246454268 0.4179687772087972 0.5809778417240564
0.5659570938979271 0.5161265833753590 0.3939051803000049
0.4627623223099753 0.4838004362359217 0.6141367493446492
0.5540067997976925 0.4414548218965934 0.4054880711422289
0.4738602425937604 0.5579854506695565 0.6049415625975100
0.2920625822924532 0.4774707085403189 0.4454534381001980
0.2834636265093087 0.5298442365139604 0.4498427137052367
0.5770164988339307 0.4941726336447064 0.5326000491525930
0.4481567291290724 0.5030911001096524 0.4757611524880543
0.5448173362441722 0.5592774302290756 0.5310574897082717
0.4855523747723344 0.4403517498486183 0.4801695668347027
0.4592024951009945 0.4749278201838289 0.5433034728461154
0.4698908807134987 0.5477950907502359 0.5351791822996977
0.5259229559884970 0.4428972271010679 0.5429070106653766
0.5155873336502210 0.5370778519647652 0.4614739498171530
0.5204511019655126 0.5092596294389422 0.5760750767049900
0.5058464697800708 0.4935754655866855 0.4307482454085797
0.3326082472033348 0.5170802703710735 0.4117954387905362
0.5078837708809031 0.5022297917192283 0.5059301659410993
0.5693872561568906 0.5303539550750422 0.4691117325504098
0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.000000000000000
35.0000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000
C Cu H Ni O Ti
1 42 2 7 1 6

Direct

0.3036041813367280 0.5054781576784461 0.4550273796650818
0.6385977689057917 0.4890151547104086 0.5613506176404321
0.3884113731044395 0.5099679832337438 0.4486514033292938
0.6080603144450346 0.5537557268929693 0.5556012640726447
0.4207428928765099 0.4446910979001141 0.4516543367014254
0.6350438274493775 0.5186716709488440 0.4949916845415483
0.3948031064513852 0.4794760511560222 0.5139562629886383
0.6239255552455203 0.4450500374220348 0.5053493979905010
0.4081161739227480 0.5542303598803255 0.5026323550921999
0.5891304347405633 0.4370282284266774 0.5713105154613362
0.4392298793966560 0.5621274550138319 0.4363522283039659
0.5841764782739367 0.5032126222355765 0.6067794871996842
0.4419306720802986 0.4968838779473193 0.4015972539534010
0.5487764945499610 0.5710315014861510 0.6007754383252336
0.4803911947531764 0.4294122805372517 0.4099020658795965
0.5721010616752498 0.6181215720298022 0.5484935388472301
0.4549256358434372 0.3821690606185207 0.4612634977870539
0.6013562429358456 0.5894959791885004 0.4886215900867270
0.4303395341482565 0.4151729857806491 0.5195455676066245
0.6228974253717452 0.5493729512956589 0.4298359271668071
0.4065792357788717 0.4503747794930964 0.5784068991714623
0.6120704858386206 0.4763587943812199 0.4383662524242410
0.4161440627117908 0.5228714344271970 0.5704873811196944
0.6001076752259407 0.4033112785875038 0.4501051381967303
0.4276907065637495 0.5955961317993728 0.5585447297130228
0.5715772942861664 0.3889190295031209 0.5166900113818121
0.4587654771752243 0.6051229825993457 0.4933274133960538
0.5368708540811887 0.3866416231991746 0.5802401906818768
0.4904744611582413 0.6104789356186100 0.4305293476053499
0.5303247971041440 0.4493769090795736 0.6161006782510864
0.4969718917436942 0.5521715444532418 0.3884033512022373
0.5213010540329355 0.5173837052937226 0.6439637561721953
0.5056536818962678 0.4807879240627962 0.3636332940859567
0.5003430489758749 0.6069991905278587 0.5538678754843314
0.5278532514079322 0.3891798388529084 0.4521389533409145
0.5321073627382545 0.6154200126427055 0.4873044934507678
0.4973075057987665 0.3827213850180751 0.5197878344528253
0.5580996295831260 0.5865626330795476 0.4230449769181316
0.4722020246454268 0.4179687772087972 0.5809778417240564
0.5659570938979271 0.5161265833753590 0.3939051803000049
0.4627623223099753 0.4838004362359217 0.6141367493446492
0.5540067997976925 0.4414548218965934 0.4054880711422289
0.4738602425937604 0.5579854506695565 0.6049415625975100
0.2920625822924532 0.4774707085403189 0.4454534381001980

0.2834636265093087 0.5298442365139604 0.4498427137052367
 0.5770164988339307 0.4941726336447064 0.5326000491525930
 0.4481567291290724 0.5030911001096524 0.4757611524880543
 0.5448173362441722 0.5592774302290756 0.5310574897082717
 0.4855523747723344 0.4403517498486183 0.4801695668347027
 0.4592024951009945 0.4749278201838289 0.5433034728461154
 0.4698908807134987 0.5477950907502359 0.5351791822996977
 0.5259229559884970 0.4428972271010679 0.5429070106653766
 0.5155873336502210 0.5370778519647652 0.4614739498171530
 0.5204511019655126 0.5092596294389422 0.5760750767049900
 0.5058464697800708 0.4935754655866855 0.4307482454085797
 0.3326082472033348 0.5170802703710735 0.4117954387905362
 0.5078837708809031 0.5022297917192283 0.5059301659410993
 0.5693872561568906 0.5303539550750422 0.4691117325504098
 0.5566591489265689 0.4485160975346802 0.4806075391904099

POSCAR

1.0000000000000000		
35.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	35.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	35.0000000000000000
C Cu H Ni O Cr		
1 42 2 7 1 6		

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.5532277773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049
 0.4454455295156791 0.4968002718195332 0.4051004232023184
 0.5476757566882242 0.5694687507241936 0.5990213554163978
 0.4807548919739799 0.4304936561515663 0.4114879905411332
 0.571723322039549 0.6173384602142707 0.5485796693146120
 0.4559850703546380 0.3830326105509780 0.4611183712771826
 0.5989214163059439 0.5867145232691900 0.4891755138305232
 0.4306458169311455 0.4154260083211325 0.5197910179775906
 0.6209094349787511 0.5486824484630553 0.4306073365066626
 0.4082250835804340 0.4514170618247466 0.5782403147686865
 0.6109876052272792 0.4767284182259738 0.4386254323961656
 0.4168356238704340 0.5231570832724521 0.5704218739201927
 0.5986727556925938 0.4053612587800817 0.4503334782564189
 0.4291405640246626 0.5938830326433044 0.5584023491331827
 0.5699379994792326 0.3929218412896489 0.5152869125269955
 0.4598689607884331 0.6035826729183160 0.4934287550395620
 0.5371844257657453 0.3869735885155572 0.5797409806968457

0.4911483164150884 0.6090226414061379 0.4304464102411961
 0.5300277776531137 0.4510173690756221 0.6135207492209885
 0.4982025712036929 0.5498095176656037 0.3923286540633994
 0.5212096515639840 0.5172521548605937 0.6409270262673683
 0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623
 0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842
 0.4633353508527396 0.4842475390396247 0.6128171142498114
 0.5544069090707989 0.4416068118999035 0.4049078947104687
 0.4744141790753252 0.5575580086968187 0.6033777336983154
 0.2923136946705203 0.4770029991766063 0.4516746682012835
 0.2829513659401132 0.5288144561136719 0.4569213144182909
 0.5769298465303094 0.4943992471055524 0.5317614616182595
 0.4507818760953542 0.5039817999638145 0.4764072233766172
 0.5440293354586166 0.5591155524323022 0.5298387410664294
 0.4846310633404934 0.4412967802343833 0.4818480410777378
 0.4606602572875949 0.4757798190767325 0.5422533074763368
 0.4711653010796484 0.5468085876547932 0.5336895558760969
 0.5260686693542846 0.4427806005514729 0.5423734990313870
 0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000

C Cu H Ni O Cr
 1 42 2 7 1 6

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.553227773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049

0.4454455295156791 0.4968002718195332 0.4051004232023184
0.5476757566882242 0.5694687507241936 0.5990213554163978
0.4807548919739799 0.4304936561515663 0.4114879905411332
0.571723322039549 0.6173384602142707 0.5485796693146120
0.4559850703546380 0.3830326105509780 0.4611183712771826
0.5989214163059439 0.5867145232691900 0.4891755138305232
0.4306458169311455 0.4154260083211325 0.5197910179775906
0.6209094349787511 0.5486824484630553 0.4306073365066626
0.4082250835804340 0.4514170618247466 0.5782403147686865
0.6109876052272792 0.4767284182259738 0.4386254323961656
0.4168356238704340 0.5231570832724521 0.5704218739201927
0.5986727556925938 0.4053612587800817 0.4503334782564189
0.4291405640246626 0.5938830326433044 0.5584023491331827
0.5699379994792326 0.3929218412896489 0.5152869125269955
0.4598689607884331 0.6035826729183160 0.4934287550395620
0.5371844257657453 0.3869735885155572 0.5797409806968457
0.4911483164150884 0.6090226414061379 0.4304464102411961
0.5300277776531137 0.4510173690756221 0.6135207492209885
0.4982025712036929 0.5498095176656037 0.3923286540633994
0.5212096515639840 0.5172521548605937 0.6409270262673683
0.5060663875441083 0.4821379738884364 0.3678520329288624
0.5002498965221114 0.6069598539016724 0.5541240039644177
0.5276768483309037 0.3908583809991849 0.4534980247105933
0.5317773414895878 0.6143377570302024 0.4875137972772623
0.4969137981270976 0.3829752812043803 0.5201254565292458
0.5581000916860696 0.5856480407357736 0.4245195617037240
0.4723333505996675 0.4181705758094839 0.5806562786482145
0.5655336065863676 0.5162905232667430 0.3948901148079842
0.4633353508527396 0.4842475390396247 0.6128171142498114
0.5544069090707989 0.4416068118999035 0.4049078947104687
0.4744141790753252 0.5575580086968187 0.6033777336983154
0.2923136946705203 0.4770029991766063 0.4516746682012835
0.2829513659401132 0.5288144561136719 0.4569213144182909
0.5769298465303094 0.4943992471055524 0.5317614616182595
0.4507818760953542 0.5039817999638145 0.4764072233766172
0.5440293354586166 0.5591155524323022 0.5298387410664294
0.4846310633404934 0.4412967802343833 0.4818480410777378
0.4606602572875949 0.4757798190767325 0.5422533074763368
0.4711653010796484 0.5468085876547932 0.5336895558760969
0.5260686693542846 0.4427806005514729 0.5423734990313870
0.5132287325585768 0.5350709479666903 0.4654902755404757
0.5175688085772299 0.5089132795333076 0.5718265893701560
0.5112338393191765 0.4908967750609645 0.4358548727062133
0.3362250419920369 0.5181724265378230 0.4065262881045078
0.5121072623733978 0.5002219564490065 0.5065230328721276
0.5663369852456326 0.5289192665881183 0.4673593159069731
0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000	0.0000000000000000	35.0000000000000000
C Cu H Ni O Cr		
1 42 2 7 1 6		
Direct		
0.3006444754137268	0.5063011145701837	0.4437061395246031
0.6381589639026403	0.4889052300444562	0.5608441396800031
0.3890929714957376	0.5101136481021240	0.4499861250164660
0.6074618538602923	0.5537782538418276	0.5554353263894990
0.4210736466415820	0.4452790042320877	0.4524886946346022
0.6324730922516321	0.5191822117441021	0.4952174622557374
0.3962878774196554	0.4801134418966374	0.5141171224736897
0.6213937502486735	0.4459312687004766	0.5050127610255752
0.4083005281610361	0.5532277773914320	0.5032328787930529
0.5891534456284411	0.4372224290296955	0.5712206782216505
0.4397115311076667	0.5615463306409738	0.4374050518856695
0.5816737542987828	0.5034877803696726	0.6038855833515049
0.4454455295156791	0.4968002718195332	0.4051004232023184
0.5476757566882242	0.5694687507241936	0.5990213554163978
0.4807548919739799	0.4304936561515663	0.4114879905411332
0.5717233222039549	0.6173384602142707	0.5485796693146120
0.4559850703546380	0.3830326105509780	0.4611183712771826
0.5989214163059439	0.5867145232691900	0.4891755138305232
0.4306458169311455	0.4154260083211325	0.5197910179775906
0.6209094349787511	0.5486824484630553	0.4306073365066626
0.4082250835804340	0.4514170618247466	0.5782403147686865
0.6109876052272792	0.4767284182259738	0.4386254323961656
0.4168356238704340	0.5231570832724521	0.5704218739201927
0.5986727556925938	0.4053612587800817	0.4503334782564189
0.4291405640246626	0.5938830326433044	0.5584023491331827
0.5699379994792326	0.3929218412896489	0.5152869125269955
0.4598689607884331	0.6035826729183160	0.4934287550395620
0.5371844257657453	0.3869735885155572	0.5797409806968457
0.4911483164150884	0.6090226414061379	0.4304464102411961
0.5300277776531137	0.4510173690756221	0.6135207492209885
0.4982025712036929	0.5498095176656037	0.3923286540633994
0.5212096515639840	0.5172521548605937	0.6409270262673683
0.5060663875441083	0.4821379738884364	0.3678520329288624
0.5002498965221114	0.6069598539016724	0.5541240039644177
0.5276768483309037	0.3908583809991849	0.4534980247105933
0.5317773414895878	0.6143377570302024	0.4875137972772623
0.4969137981270976	0.3829752812043803	0.5201254565292458
0.5581000916860696	0.5856480407357736	0.4245195617037240
0.4723333505996675	0.4181705758094839	0.5806562786482145
0.5655336065863676	0.5162905232667430	0.3948901148079842
0.4633353508527396	0.4842475390396247	0.6128171142498114
0.5544069090707989	0.4416068118999035	0.4049078947104687
0.4744141790753252	0.5575580086968187	0.6033777336983154
0.2923136946705203	0.4770029991766063	0.4516746682012835
0.2829513659401132	0.5288144561136719	0.4569213144182909
0.5769298465303094	0.4943992471055524	0.5317614616182595
0.4507818760953542	0.5039817999638145	0.4764072233766172
0.5440293354586166	0.5591155524323022	0.5298387410664294

0.4846310633404934	0.4412967802343833	0.4818480410777378
0.4606602572875949	0.4757798190767325	0.5422533074763368
0.4711653010796484	0.5468085876547932	0.5336895558760969
0.5260686693542846	0.4427806005514729	0.5423734990313870
0.5132287325585768	0.5350709479666903	0.4654902755404757
0.5175688085772299	0.5089132795333076	0.5718265893701560
0.5112338393191765	0.4908967750609645	0.4358548727062133
0.3362250419920369	0.5181724265378230	0.4065262881045078
0.5121072623733978	0.5002219564490065	0.5065230328721276
0.5663369852456326	0.5289192665881183	0.4673593159069731
0.5541317106453725	0.4527629135269202	0.4763332412787238

POSCAR

```

1.000000000000000
35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

C Cu H Ni O Cr
 1 42 2 7 1 6

```

Direct
0.3006444754137268 0.5063011145701837 0.4437061395246031
0.6381589639026403 0.4889052300444562 0.5608441396800031
0.3890929714957376 0.5101136481021240 0.4499861250164660
0.6074618538602923 0.5537782538418276 0.5554353263894990
0.4210736466415820 0.4452790042320877 0.4524886946346022
0.6324730922516321 0.5191822117441021 0.4952174622557374
0.3962878774196554 0.4801134418966374 0.5141171224736897
0.6213937502486735 0.4459312687004766 0.5050127610255752
0.4083005281610361 0.5532277773914320 0.5032328787930529
0.5891534456284411 0.4372224290296955 0.5712206782216505
0.4397115311076667 0.5615463306409738 0.4374050518856695
0.5816737542987828 0.5034877803696726 0.6038855833515049
0.4454455295156791 0.4968002718195332 0.4051004232023184
0.5476757566882242 0.5694687507241936 0.5990213554163978
0.4807548919739799 0.4304936561515663 0.4114879905411332
0.5717233222039549 0.6173384602142707 0.5485796693146120
0.4559850703546380 0.3830326105509780 0.4611183712771826
0.5989214163059439 0.5867145232691900 0.4891755138305232
0.4306458169311455 0.4154260083211325 0.5197910179775906
0.6209094349787511 0.5486824484630553 0.4306073365066626
0.4082250835804340 0.4514170618247466 0.5782403147686865
0.6109876052272792 0.4767284182259738 0.4386254323961656
0.4168356238704340 0.5231570832724521 0.5704218739201927
0.5986727556925938 0.4053612587800817 0.4503334782564189
0.4291405640246626 0.5938830326433044 0.5584023491331827
0.5699379994792326 0.3929218412896489 0.5152869125269955
0.4598689607884331 0.6035826729183160 0.4934287550395620
0.5371844257657453 0.3869735885155572 0.5797409806968457
0.4911483164150884 0.6090226414061379 0.4304464102411961
0.5300277776531137 0.4510173690756221 0.6135207492209885
0.4982025712036929 0.5498095176656037 0.3923286540633994
0.5212096515639840 0.5172521548605937 0.6409270262673683

0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623
 0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842
 0.4633353508527396 0.4842475390396247 0.6128171142498114
 0.5544069090707989 0.4416068118999035 0.4049078947104687
 0.4744141790753252 0.5575580086968187 0.6033777336983154
 0.2923136946705203 0.4770029991766063 0.4516746682012835
 0.2829513659401132 0.5288144561136719 0.4569213144182909
 0.5769298465303094 0.4943992471055524 0.5317614616182595
 0.4507818760953542 0.5039817999638145 0.4764072233766172
 0.5440293354586166 0.5591155524323022 0.5298387410664294
 0.4846310633404934 0.4412967802343833 0.4818480410777378
 0.4606602572875949 0.4757798190767325 0.5422533074763368
 0.4711653010796484 0.5468085876547932 0.5336895558760969
 0.5260686693542846 0.4427806005514729 0.5423734990313870
 0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Cr		
1 42 2 7 1 6		

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.5532277773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049
 0.4454455295156791 0.4968002718195332 0.4051004232023184
 0.5476757566882242 0.5694687507241936 0.5990213554163978
 0.4807548919739799 0.4304936561515663 0.4114879905411332
 0.571723322039549 0.6173384602142707 0.5485796693146120

0.4559850703546380 0.3830326105509780 0.4611183712771826
 0.5989214163059439 0.5867145232691900 0.4891755138305232
 0.4306458169311455 0.4154260083211325 0.5197910179775906
 0.6209094349787511 0.5486824484630553 0.4306073365066626
 0.4082250835804340 0.4514170618247466 0.5782403147686865
 0.6109876052272792 0.4767284182259738 0.4386254323961656
 0.4168356238704340 0.5231570832724521 0.5704218739201927
 0.5986727556925938 0.4053612587800817 0.4503334782564189
 0.4291405640246626 0.5938830326433044 0.5584023491331827
 0.5699379994792326 0.3929218412896489 0.5152869125269955
 0.4598689607884331 0.6035826729183160 0.4934287550395620
 0.5371844257657453 0.3869735885155572 0.5797409806968457
 0.4911483164150884 0.6090226414061379 0.4304464102411961
 0.5300277776531137 0.4510173690756221 0.6135207492209885
 0.4982025712036929 0.5498095176656037 0.3923286540633994
 0.5212096515639840 0.5172521548605937 0.6409270262673683
 0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623
 0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842
 0.4633353508527396 0.4842475390396247 0.6128171142498114
 0.5544069090707989 0.4416068118999035 0.4049078947104687
 0.4744141790753252 0.5575580086968187 0.6033777336983154
 0.2923136946705203 0.4770029991766063 0.4516746682012835
 0.2829513659401132 0.5288144561136719 0.4569213144182909
 0.5769298465303094 0.4943992471055524 0.5317614616182595
 0.4507818760953542 0.5039817999638145 0.4764072233766172
 0.5440293354586166 0.5591155524323022 0.5298387410664294
 0.4846310633404934 0.4412967802343833 0.4818480410777378
 0.4606602572875949 0.4757798190767325 0.5422533074763368
 0.4711653010796484 0.5468085876547932 0.5336895558760969
 0.5260686693542846 0.4427806005514729 0.5423734990313870
 0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

C Cu H Ni O Cr
1 42 2 7 1 6

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
0.6381589639026403 0.4889052300444562 0.5608441396800031
0.3890929714957376 0.5101136481021240 0.4499861250164660
0.6074618538602923 0.5537782538418276 0.5554353263894990
0.4210736466415820 0.4452790042320877 0.4524886946346022
0.6324730922516321 0.5191822117441021 0.4952174622557374
0.3962878774196554 0.4801134418966374 0.5141171224736897
0.6213937502486735 0.4459312687004766 0.5050127610255752
0.4083005281610361 0.5532277773914320 0.5032328787930529
0.5891534456284411 0.4372224290296955 0.5712206782216505
0.4397115311076667 0.5615463306409738 0.4374050518856695
0.5816737542987828 0.5034877803696726 0.6038855833515049
0.4454455295156791 0.4968002718195332 0.4051004232023184
0.5476757566882242 0.5694687507241936 0.5990213554163978
0.4807548919739799 0.4304936561515663 0.4114879905411332
0.571723322039549 0.6173384602142707 0.5485796693146120
0.4559850703546380 0.3830326105509780 0.4611183712771826
0.5989214163059439 0.5867145232691900 0.4891755138305232
0.4306458169311455 0.4154260083211325 0.5197910179775906
0.6209094349787511 0.5486824484630553 0.4306073365066626
0.4082250835804340 0.4514170618247466 0.5782403147686865
0.6109876052272792 0.4767284182259738 0.4386254323961656
0.4168356238704340 0.5231570832724521 0.5704218739201927
0.5986727556925938 0.4053612587800817 0.4503334782564189
0.4291405640246626 0.5938830326433044 0.5584023491331827
0.5699379994792326 0.3929218412896489 0.5152869125269955
0.4598689607884331 0.6035826729183160 0.4934287550395620
0.5371844257657453 0.3869735885155572 0.5797409806968457
0.4911483164150884 0.6090226414061379 0.4304464102411961
0.5300277776531137 0.4510173690756221 0.6135207492209885
0.4982025712036929 0.5498095176656037 0.3923286540633994
0.5212096515639840 0.5172521548605937 0.6409270262673683
0.5060663875441083 0.4821379738884364 0.3678520329288624
0.5002498965221114 0.6069598539016724 0.5541240039644177
0.5276768483309037 0.3908583809991849 0.4534980247105933
0.5317773414895878 0.6143377570302024 0.4875137972772623
0.4969137981270976 0.3829752812043803 0.5201254565292458
0.5581000916860696 0.5856480407357736 0.4245195617037240
0.4723333505996675 0.4181705758094839 0.5806562786482145
0.5655336065863676 0.5162905232667430 0.3948901148079842
0.4633353508527396 0.4842475390396247 0.6128171142498114
0.5544069090707989 0.4416068118999035 0.4049078947104687
0.4744141790753252 0.5575580086968187 0.6033777336983154
0.2923136946705203 0.4770029991766063 0.4516746682012835
0.2829513659401132 0.5288144561136719 0.4569213144182909
0.5769298465303094 0.4943992471055524 0.5317614616182595
0.4507818760953542 0.5039817999638145 0.4764072233766172
0.5440293354586166 0.5591155524323022 0.5298387410664294
0.4846310633404934 0.4412967802343833 0.4818480410777378
0.4606602572875949 0.4757798190767325 0.5422533074763368
0.4711653010796484 0.5468085876547932 0.5336895558760969
0.5260686693542846 0.4427806005514729 0.5423734990313870

0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.528919266581183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Cr
 1 42 2 7 1 6

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.5532277773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049
 0.4454455295156791 0.4968002718195332 0.4051004232023184
 0.5476757566882242 0.5694687507241936 0.5990213554163978
 0.4807548919739799 0.4304936561515663 0.4114879905411332
 0.571723322039549 0.6173384602142707 0.5485796693146120
 0.4559850703546380 0.3830326105509780 0.4611183712771826
 0.5989214163059439 0.5867145232691900 0.4891755138305232
 0.4306458169311455 0.4154260083211325 0.5197910179775906
 0.6209094349787511 0.5486824484630553 0.4306073365066626
 0.4082250835804340 0.4514170618247466 0.5782403147686865
 0.6109876052272792 0.4767284182259738 0.4386254323961656
 0.4168356238704340 0.5231570832724521 0.5704218739201927
 0.5986727556925938 0.4053612587800817 0.4503334782564189
 0.4291405640246626 0.5938830326433044 0.5584023491331827
 0.5699379994792326 0.3929218412896489 0.5152869125269955
 0.4598689607884331 0.6035826729183160 0.4934287550395620
 0.5371844257657453 0.3869735885155572 0.5797409806968457
 0.4911483164150884 0.6090226414061379 0.4304464102411961
 0.5300277776531137 0.4510173690756221 0.6135207492209885
 0.4982025712036929 0.5498095176656037 0.3923286540633994
 0.5212096515639840 0.5172521548605937 0.6409270262673683
 0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623

0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842
 0.4633353508527396 0.4842475390396247 0.6128171142498114
 0.5544069090707989 0.4416068118999035 0.4049078947104687
 0.4744141790753252 0.5575580086968187 0.6033777336983154
 0.2923136946705203 0.4770029991766063 0.4516746682012835
 0.2829513659401132 0.5288144561136719 0.4569213144182909
 0.5769298465303094 0.4943992471055524 0.5317614616182595
 0.4507818760953542 0.5039817999638145 0.4764072233766172
 0.5440293354586166 0.5591155524323022 0.5298387410664294
 0.4846310633404934 0.4412967802343833 0.4818480410777378
 0.4606602572875949 0.4757798190767325 0.5422533074763368
 0.4711653010796484 0.5468085876547932 0.5336895558760969
 0.5260686693542846 0.4427806005514729 0.5423734990313870
 0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000

C	Cu	H	Ni	O	Cr
1	42	2	7	1	6

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.5532277773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049
 0.4454455295156791 0.4968002718195332 0.4051004232023184
 0.5476757566882242 0.5694687507241936 0.5990213554163978
 0.4807548919739799 0.4304936561515663 0.4114879905411332
 0.571723322039549 0.6173384602142707 0.5485796693146120
 0.4559850703546380 0.3830326105509780 0.4611183712771826
 0.5989214163059439 0.5867145232691900 0.4891755138305232
 0.4306458169311455 0.4154260083211325 0.5197910179775906
 0.6209094349787511 0.5486824484630553 0.4306073365066626

0.4082250835804340 0.4514170618247466 0.5782403147686865
 0.6109876052272792 0.4767284182259738 0.4386254323961656
 0.4168356238704340 0.5231570832724521 0.5704218739201927
 0.5986727556925938 0.4053612587800817 0.4503334782564189
 0.4291405640246626 0.5938830326433044 0.5584023491331827
 0.5699379994792326 0.3929218412896489 0.5152869125269955
 0.4598689607884331 0.6035826729183160 0.4934287550395620
 0.5371844257657453 0.3869735885155572 0.5797409806968457
 0.4911483164150884 0.6090226414061379 0.4304464102411961
 0.5300277776531137 0.4510173690756221 0.6135207492209885
 0.4982025712036929 0.5498095176656037 0.3923286540633994
 0.5212096515639840 0.5172521548605937 0.6409270262673683
 0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623
 0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842
 0.4633353508527396 0.4842475390396247 0.6128171142498114
 0.5544069090707989 0.4416068118999035 0.4049078947104687
 0.4744141790753252 0.5575580086968187 0.6033777336983154
 0.2923136946705203 0.4770029991766063 0.4516746682012835
 0.2829513659401132 0.5288144561136719 0.4569213144182909
 0.5769298465303094 0.4943992471055524 0.5317614616182595
 0.4507818760953542 0.5039817999638145 0.4764072233766172
 0.5440293354586166 0.5591155524323022 0.5298387410664294
 0.4846310633404934 0.4412967802343833 0.4818480410777378
 0.4606602572875949 0.4757798190767325 0.5422533074763368
 0.4711653010796484 0.5468085876547932 0.5336895558760969
 0.5260686693542846 0.4427806005514729 0.5423734990313870
 0.5132287325585768 0.5350709479666903 0.4654902755404757
 0.5175688085772299 0.5089132795333076 0.5718265893701560
 0.5112338393191765 0.4908967750609645 0.4358548727062133
 0.3362250419920369 0.5181724265378230 0.4065262881045078
 0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Cr		
1 42 2 7 1 6		

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990

0.4210736466415820 0.4452790042320877 0.4524886946346022
0.6324730922516321 0.5191822117441021 0.4952174622557374
0.3962878774196554 0.4801134418966374 0.5141171224736897
0.6213937502486735 0.4459312687004766 0.5050127610255752
0.4083005281610361 0.5532277773914320 0.5032328787930529
0.5891534456284411 0.4372224290296955 0.5712206782216505
0.4397115311076667 0.5615463306409738 0.4374050518856695
0.5816737542987828 0.5034877803696726 0.6038855833515049
0.4454455295156791 0.4968002718195332 0.4051004232023184
0.5476757566882242 0.5694687507241936 0.5990213554163978
0.4807548919739799 0.4304936561515663 0.4114879905411332
0.571723322039549 0.6173384602142707 0.5485796693146120
0.4559850703546380 0.3830326105509780 0.4611183712771826
0.5989214163059439 0.5867145232691900 0.4891755138305232
0.4306458169311455 0.4154260083211325 0.5197910179775906
0.6209094349787511 0.5486824484630553 0.4306073365066626
0.4082250835804340 0.4514170618247466 0.5782403147686865
0.6109876052272792 0.4767284182259738 0.4386254323961656
0.4168356238704340 0.5231570832724521 0.5704218739201927
0.5986727556925938 0.4053612587800817 0.4503334782564189
0.4291405640246626 0.5938830326433044 0.5584023491331827
0.5699379994792326 0.3929218412896489 0.5152869125269955
0.4598689607884331 0.6035826729183160 0.4934287550395620
0.5371844257657453 0.3869735885155572 0.5797409806968457
0.4911483164150884 0.6090226414061379 0.4304464102411961
0.5300277776531137 0.4510173690756221 0.6135207492209885
0.4982025712036929 0.5498095176656037 0.3923286540633994
0.5212096515639840 0.5172521548605937 0.6409270262673683
0.5060663875441083 0.4821379738884364 0.3678520329288624
0.5002498965221114 0.6069598539016724 0.5541240039644177
0.5276768483309037 0.3908583809991849 0.4534980247105933
0.5317773414895878 0.6143377570302024 0.4875137972772623
0.4969137981270976 0.3829752812043803 0.5201254565292458
0.5581000916860696 0.5856480407357736 0.4245195617037240
0.4723333505996675 0.4181705758094839 0.5806562786482145
0.5655336065863676 0.5162905232667430 0.3948901148079842
0.4633353508527396 0.4842475390396247 0.6128171142498114
0.5544069090707989 0.4416068118999035 0.4049078947104687
0.4744141790753252 0.5575580086968187 0.6033777336983154
0.2923136946705203 0.4770029991766063 0.4516746682012835
0.2829513659401132 0.5288144561136719 0.4569213144182909
0.5769298465303094 0.4943992471055524 0.5317614616182595
0.4507818760953542 0.5039817999638145 0.4764072233766172
0.5440293354586166 0.5591155524323022 0.5298387410664294
0.4846310633404934 0.4412967802343833 0.4818480410777378
0.4606602572875949 0.4757798190767325 0.5422533074763368
0.4711653010796484 0.5468085876547932 0.5336895558760969
0.5260686693542846 0.4427806005514729 0.5423734990313870
0.5132287325585768 0.5350709479666903 0.4654902755404757
0.5175688085772299 0.5089132795333076 0.5718265893701560
0.5112338393191765 0.4908967750609645 0.4358548727062133
0.3362250419920369 0.5181724265378230 0.4065262881045078

0.5121072623733978 0.5002219564490065 0.5065230328721276
 0.5663369852456326 0.5289192665881183 0.4673593159069731
 0.5541317106453725 0.4527629135269202 0.4763332412787238

POSCAR

1.000000000000000		
35.0000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Cr		
1 42 2 7 1 6		

Direct

0.3006444754137268 0.5063011145701837 0.4437061395246031
 0.6381589639026403 0.4889052300444562 0.5608441396800031
 0.3890929714957376 0.5101136481021240 0.4499861250164660
 0.6074618538602923 0.5537782538418276 0.5554353263894990
 0.4210736466415820 0.4452790042320877 0.4524886946346022
 0.6324730922516321 0.5191822117441021 0.4952174622557374
 0.3962878774196554 0.4801134418966374 0.5141171224736897
 0.6213937502486735 0.4459312687004766 0.5050127610255752
 0.4083005281610361 0.5532277773914320 0.5032328787930529
 0.5891534456284411 0.4372224290296955 0.5712206782216505
 0.4397115311076667 0.5615463306409738 0.4374050518856695
 0.5816737542987828 0.5034877803696726 0.6038855833515049
 0.4454455295156791 0.4968002718195332 0.4051004232023184
 0.5476757566882242 0.5694687507241936 0.5990213554163978
 0.4807548919739799 0.4304936561515663 0.4114879905411332
 0.571723322039549 0.6173384602142707 0.5485796693146120
 0.4559850703546380 0.3830326105509780 0.4611183712771826
 0.5989214163059439 0.5867145232691900 0.4891755138305232
 0.4306458169311455 0.4154260083211325 0.5197910179775906
 0.6209094349787511 0.5486824484630553 0.4306073365066626
 0.4082250835804340 0.4514170618247466 0.5782403147686865
 0.6109876052272792 0.4767284182259738 0.4386254323961656
 0.4168356238704340 0.5231570832724521 0.5704218739201927
 0.5986727556925938 0.4053612587800817 0.4503334782564189
 0.4291405640246626 0.5938830326433044 0.5584023491331827
 0.5699379994792326 0.3929218412896489 0.5152869125269955
 0.4598689607884331 0.6035826729183160 0.4934287550395620
 0.5371844257657453 0.3869735885155572 0.5797409806968457
 0.4911483164150884 0.6090226414061379 0.4304464102411961
 0.5300277776531137 0.4510173690756221 0.6135207492209885
 0.4982025712036929 0.5498095176656037 0.3923286540633994
 0.5212096515639840 0.5172521548605937 0.6409270262673683
 0.5060663875441083 0.4821379738884364 0.3678520329288624
 0.5002498965221114 0.6069598539016724 0.5541240039644177
 0.5276768483309037 0.3908583809991849 0.4534980247105933
 0.5317773414895878 0.6143377570302024 0.4875137972772623
 0.4969137981270976 0.3829752812043803 0.5201254565292458
 0.5581000916860696 0.5856480407357736 0.4245195617037240
 0.4723333505996675 0.4181705758094839 0.5806562786482145
 0.5655336065863676 0.5162905232667430 0.3948901148079842

0.4633353508527396	0.4842475390396247	0.6128171142498114
0.5544069090707989	0.4416068118999035	0.4049078947104687
0.4744141790753252	0.5575580086968187	0.6033777336983154
0.2923136946705203	0.4770029991766063	0.4516746682012835
0.2829513659401132	0.5288144561136719	0.4569213144182909
0.5769298465303094	0.4943992471055524	0.5317614616182595
0.4507818760953542	0.5039817999638145	0.4764072233766172
0.5440293354586166	0.5591155524323022	0.5298387410664294
0.4846310633404934	0.4412967802343833	0.4818480410777378
0.4606602572875949	0.4757798190767325	0.5422533074763368
0.4711653010796484	0.5468085876547932	0.5336895558760969
0.5260686693542846	0.4427806005514729	0.5423734990313870
0.5132287325585768	0.5350709479666903	0.4654902755404757
0.5175688085772299	0.5089132795333076	0.5718265893701560
0.5112338393191765	0.4908967750609645	0.4358548727062133
0.3362250419920369	0.5181724265378230	0.4065262881045078
0.5121072623733978	0.5002219564490065	0.5065230328721276
0.5663369852456326	0.5289192665881183	0.4673593159069731
0.5541317106453725	0.4527629135269202	0.4763332412787238

POSCAR

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

C	Cu	H	Ni	O	Fe
1	42	2	7	1	6

Direct

0.2954705818043527	0.5051355283572435	0.4574655652027443
0.6476592270665971	0.4879396554237083	0.5651968510197141
0.3820583630665713	0.5109525002378987	0.4438253520724803
0.6167957852193879	0.5591685495527250	0.5609787243985560
0.4115966341677952	0.4397227471990416	0.4475137020957465
0.6438425999599448	0.5203196071742313	0.4947287760121097
0.3845947227631105	0.4785628663384900	0.5137953171763038
0.6318882478586505	0.4406182942196961	0.5057898206390287
0.3964639369010118	0.5583052682630524	0.5027006726079182
0.5975647952325349	0.4301763350147779	0.5788038312248246
0.4306501232934270	0.5687139359347344	0.4296632411748543
0.5883453318713208	0.5033896919856954	0.6129261819627440
0.4400550601352461	0.4955489441675471	0.3954800709869655
0.5506791567355342	0.5752285747278663	0.6055552311485510
0.4777271562672804	0.4236659342350536	0.4029475097709363
0.5759739642322315	0.6244898818639908	0.5511273569836984
0.4522936799766305	0.3744227503503412	0.4573668775876218
0.6061550290584534	0.5920968773296152	0.4872371388242863
0.4222330054824817	0.4068418571686108	0.5211347932206722
0.6273443221830526	0.5506568817889725	0.4252543104344300
0.4009725714966696	0.4482788656512133	0.5832259854283443
0.6212554430533126	0.4734974169049200	0.4321488938628373
0.4072179252796815	0.5253986977756584	0.5763217345913864
0.6047276852704050	0.3988990560951795	0.4461747085274613

0.4236982044238159 0.5999611793896060 0.562279698889479
0.5749716984580333 0.3833960091813215 0.5162716269600016
0.4532748407760575 0.6155202352324670 0.4922893876662723
0.5395152313884846 0.3790876420563937 0.5851327124045862
0.4888936778696976 0.6197948817038074 0.4233776301520969
0.5314296785260858 0.4461864762636217 0.6233823838036725
0.4969608221254892 0.5527049386897646 0.3850448724550508
0.5217586818559760 0.5185405380020512 0.6499488460172514
0.5066038570092535 0.4803617196776644 0.3584406571963292
0.4990575064057209 0.6179630134101637 0.5593646061386225
0.5292454654878257 0.3809245113152390 0.4490000663641504
0.5334705394659406 0.6284762325386318 0.4862971985199961
0.4948832202320053 0.3705112930576669 0.5221308774790222
0.5604107311981884 0.5896126313225317 0.4200541567575485
0.4679821584077760 0.4093416123936993 0.5882647196067378
0.5697033775046165 0.5162749206674285 0.3860955309947874
0.4586940164635895 0.4825581692504113 0.6223938026231608
0.5577605214158076 0.4365854062937245 0.3970677677026591
0.4705496136830897 0.5622737811092792 0.6114313572787683
0.3040326704303435 0.4812128788913750 0.4396213639286462
0.2905390880165470 0.5326599830392245 0.4481108110203021
0.5821453189222173 0.4935156763910507 0.5352948795175345
0.4462993614169569 0.5053875871375358 0.4732189185524869
0.5455998430261316 0.5630619853797304 0.5280826728713405
0.4827165944457095 0.4358625526564063 0.4803894510026141
0.4566548375794122 0.4734629678000419 0.5444577284785604
0.4681293687631784 0.5505452359367289 0.5338167196539874
0.5270155529393643 0.4382313767623086 0.5453621999152792
0.5014169823552947 0.5603020944106075 0.4632134297342598
0.5180783188584972 0.5090783964840553 0.5782244467408575
0.5103130420353309 0.4897415078850790 0.4302099133972111
0.3289796284935130 0.5113646874300285 0.4214410120843095
0.5139954405347757 0.4995011334430449 0.5043193859336887
0.5715806329007540 0.5253817660573851 0.4640218045462344
0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.000000000000000					
35.000000000000000	0.000000000000000	0.000000000000000			
0.000000000000000	35.000000000000000	0.000000000000000			
0.000000000000000	0.000000000000000	35.000000000000000			
C_s	C_p	H_s	Ni_s	O_s	Fe_s

C	Cu	H	N ₁	O	Fe
1	42	2	7	1	6

Direct

0.2954705818043527	0.5051355283572435	0.4574655652027443
0.6476592270665971	0.4879396554237083	0.5651968510197141
0.3820583630665713	0.5109525002378987	0.4438253520724803
0.6167957852193879	0.5591685495527250	0.5609787243985560
0.4115966341677952	0.4397227471990416	0.4475137020957465
0.6438425999599448	0.5203196071742313	0.4947287760121097
0.3845947227631105	0.4785628663384900	0.5137953171763038
0.6318882478586505	0.4406182942196961	0.5057898206390287

0.3964639369010118 0.5583052682630524 0.5027006726079182
0.5975647952325349 0.4301763350147779 0.5788038312248246
0.4306501232934270 0.5687139359347344 0.4296632411748543
0.5883453318713208 0.5033896919856954 0.6129261819627440
0.4400550601352461 0.4955489441675471 0.3954800709869655
0.5506791567355342 0.5752285747278663 0.6055552311485510
0.4777271562672804 0.4236659342350536 0.4029475097709363
0.5759739642322315 0.6244898818639908 0.5511273569836984
0.4522936799766305 0.3744227503503412 0.4573668775876218
0.6061550290584534 0.5920968773296152 0.4872371388242863
0.4222330054824817 0.4068418571686108 0.5211347932206722
0.6273443221830526 0.5506568817889725 0.4252543104344300
0.4009725714966696 0.4482788656512133 0.5832259854283443
0.6212554430533126 0.4734974169049200 0.4321488938628373
0.4072179252796815 0.5253986977756584 0.5763217345913864
0.6047276852704050 0.3988990560951795 0.4461747085274613
0.4236982044238159 0.5999611793896060 0.5622796988889479
0.5749716984580333 0.3833960091813215 0.5162716269600016
0.4532748407760575 0.6155202352324670 0.4922893876662723
0.5395152313884846 0.3790876420563937 0.5851327124045862
0.4888936778696976 0.6197948817038074 0.4233776301520969
0.5314296785260858 0.4461864762636217 0.6233823838036725
0.4969608221254892 0.5527049386897646 0.3850448724550508
0.5217586818559760 0.5185405380020512 0.6499488460172514
0.5066038570092535 0.4803617196776644 0.3584406571963292
0.4990575064057209 0.6179630134101637 0.5593646061386225
0.5292454654878257 0.3809245113152390 0.4490000663641504
0.5334705394659406 0.6284762325386318 0.4862971985199961
0.4948832202320053 0.3705112930576669 0.5221308774790222
0.5604107311981884 0.5896126313225317 0.4200541567575485
0.4679821584077760 0.4093416123936993 0.5882647196067378
0.5697033775046165 0.5162749206674285 0.3860955309947874
0.4586940164635895 0.4825581692504113 0.6223938026231608
0.5577605214158076 0.4365854062937245 0.3970677677026591
0.4705496136830897 0.5622737811092792 0.6114313572787683
0.3040326704303435 0.4812128788913750 0.4396213639286462
0.2905390880165470 0.5326599830392245 0.4481108110203021
0.5821453189222173 0.4935156763910507 0.5352948795175345
0.4462993614169569 0.5053875871375358 0.4732189185524869
0.5455998430261316 0.5630619853797304 0.5280826728713405
0.4827165944457095 0.4358625526564063 0.4803894510026141
0.4566548375794122 0.4734629678000419 0.5444577284785604
0.4681293687631784 0.5505452359367289 0.5338167196539874
0.5270155529393643 0.4382313767623086 0.5453621999152792
0.5014169823552947 0.5603020944106075 0.4632134297342598
0.5180783188584972 0.5090783964840553 0.5782244467408575
0.5103130420353309 0.4897415078850790 0.4302099133972111
0.3289796284935130 0.5113646874300285 0.4214410120843095
0.5139954405347757 0.4995011334430449 0.5043193859336887
0.5715806329007540 0.5253817660573851 0.4640218045462344
0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.000000000000000
35.0000000000000000 0.000000000000000 0.000000000000000
0.000000000000000 35.000000000000000 0.000000000000000
0.000000000000000 0.000000000000000 35.000000000000000
C Cu H Ni O Fe
1 42 2 7 1 6

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
0.6476592270665971 0.4879396554237083 0.5651968510197141
0.3820583630665713 0.5109525002378987 0.4438253520724803
0.6167957852193879 0.5591685495527250 0.5609787243985560
0.4115966341677952 0.4397227471990416 0.4475137020957465
0.6438425999599448 0.5203196071742313 0.4947287760121097
0.3845947227631105 0.4785628663384900 0.5137953171763038
0.6318882478586505 0.4406182942196961 0.5057898206390287
0.3964639369010118 0.5583052682630524 0.5027006726079182
0.5975647952325349 0.4301763350147779 0.5788038312248246
0.4306501232934270 0.5687139359347344 0.4296632411748543
0.5883453318713208 0.5033896919856954 0.6129261819627440
0.4400550601352461 0.4955489441675471 0.3954800709869655
0.5506791567355342 0.5752285747278663 0.6055552311485510
0.4777271562672804 0.4236659342350536 0.4029475097709363
0.5759739642322315 0.6244898818639908 0.5511273569836984
0.4522936799766305 0.3744227503503412 0.4573668775876218
0.6061550290584534 0.5920968773296152 0.4872371388242863
0.4222330054824817 0.4068418571686108 0.5211347932206722
0.6273443221830526 0.5506568817889725 0.4252543104344300
0.4009725714966696 0.4482788656512133 0.5832259854283443
0.6212554430533126 0.4734974169049200 0.4321488938628373
0.4072179252796815 0.5253986977756584 0.5763217345913864
0.6047276852704050 0.3988990560951795 0.4461747085274613
0.4236982044238159 0.5999611793896060 0.5622796988889479
0.5749716984580333 0.3833960091813215 0.5162716269600016
0.4532748407760575 0.6155202352324670 0.4922893876662723
0.5395152313884846 0.3790876420563937 0.5851327124045862
0.4888936778696976 0.6197948817038074 0.4233776301520969
0.5314296785260858 0.4461864762636217 0.6233823838036725
0.4969608221254892 0.5527049386897646 0.3850448724550508
0.5217586818559760 0.5185405380020512 0.6499488460172514
0.5066038570092535 0.4803617196776644 0.3584406571963292
0.4990575064057209 0.6179630134101637 0.5593646061386225
0.5292454654878257 0.3809245113152390 0.4490000663641504
0.5334705394659406 0.6284762325386318 0.4862971985199961
0.4948832202320053 0.3705112930576669 0.5221308774790222
0.5604107311981884 0.5896126313225317 0.4200541567575485
0.4679821584077760 0.4093416123936993 0.5882647196067378
0.5697033775046165 0.5162749206674285 0.3860955309947874
0.4586940164635895 0.4825581692504113 0.6223938026231608
0.5577605214158076 0.4365854062937245 0.3970677677026591
0.4705496136830897 0.5622737811092792 0.6114313572787683
0.3040326704303435 0.4812128788913750 0.4396213639286462

0.2905390880165470	0.5326599830392245	0.4481108110203021
0.5821453189222173	0.4935156763910507	0.5352948795175345
0.4462993614169569	0.5053875871375358	0.4732189185524869
0.5455998430261316	0.5630619853797304	0.5280826728713405
0.4827165944457095	0.4358625526564063	0.4803894510026141
0.4566548375794122	0.4734629678000419	0.5444577284785604
0.4681293687631784	0.5505452359367289	0.5338167196539874
0.5270155529393643	0.4382313767623086	0.5453621999152792
0.5014169823552947	0.5603020944106075	0.4632134297342598
0.5180783188584972	0.5090783964840553	0.5782244467408575
0.5103130420353309	0.4897415078850790	0.4302099133972111
0.3289796284935130	0.5113646874300285	0.4214410120843095
0.5139954405347757	0.4995011334430449	0.5043193859336887
0.5715806329007540	0.5253817660573851	0.4640218045462344
0.5601741432088304	0.4484842759796693	0.4746847356588114

POSCAR

1.00000000000000			
35.00000000000000	0.00000000000000	0.00000000000000	
0.00000000000000	35.00000000000000	0.00000000000000	
0.00000000000000	0.00000000000000	35.00000000000000	
C Cu H Ni O Fe			
1 42 2 7 1 6			

Direct

0.2954705818043527	0.5051355283572435	0.4574655652027443
0.6476592270665971	0.4879396554237083	0.5651968510197141
0.3820583630665713	0.5109525002378987	0.4438253520724803
0.6167957852193879	0.5591685495527250	0.5609787243985560
0.4115966341677952	0.4397227471990416	0.4475137020957465
0.6438425999599448	0.5203196071742313	0.4947287760121097
0.3845947227631105	0.4785628663384900	0.5137953171763038
0.6318882478586505	0.4406182942196961	0.5057898206390287
0.3964639369010118	0.5583052682630524	0.5027006726079182
0.5975647952325349	0.4301763350147779	0.5788038312248246
0.4306501232934270	0.5687139359347344	0.4296632411748543
0.5883453318713208	0.5033896919856954	0.6129261819627440
0.4400550601352461	0.4955489441675471	0.3954800709869655
0.5506791567355342	0.5752285747278663	0.6055552311485510
0.4777271562672804	0.4236659342350536	0.4029475097709363
0.5759739642322315	0.6244898818639908	0.5511273569836984
0.4522936799766305	0.3744227503503412	0.4573668775876218
0.6061550290584534	0.5920968773296152	0.4872371388242863
0.4222330054824817	0.4068418571686108	0.5211347932206722
0.6273443221830526	0.5506568817889725	0.4252543104344300
0.4009725714966696	0.4482788656512133	0.5832259854283443
0.6212554430533126	0.4734974169049200	0.4321488938628373
0.4072179252796815	0.5253986977756584	0.5763217345913864
0.6047276852704050	0.3988990560951795	0.4461747085274613
0.4236982044238159	0.5999611793896060	0.5622796988889479
0.5749716984580333	0.3833960091813215	0.5162716269600016
0.4532748407760575	0.6155202352324670	0.4922893876662723
0.5395152313884846	0.3790876420563937	0.5851327124045862

0.4888936778696976 0.6197948817038074 0.4233776301520969
 0.5314296785260858 0.4461864762636217 0.6233823838036725
 0.4969608221254892 0.5527049386897646 0.3850448724550508
 0.5217586818559760 0.5185405380020512 0.6499488460172514
 0.5066038570092535 0.4803617196776644 0.3584406571963292
 0.4990575064057209 0.6179630134101637 0.5593646061386225
 0.5292454654878257 0.3809245113152390 0.4490000663641504
 0.5334705394659406 0.6284762325386318 0.4862971985199961
 0.4948832202320053 0.3705112930576669 0.5221308774790222
 0.5604107311981884 0.5896126313225317 0.4200541567575485
 0.4679821584077760 0.4093416123936993 0.5882647196067378
 0.5697033775046165 0.5162749206674285 0.3860955309947874
 0.4586940164635895 0.4825581692504113 0.6223938026231608
 0.5577605214158076 0.4365854062937245 0.3970677677026591
 0.4705496136830897 0.5622737811092792 0.6114313572787683
 0.3040326704303435 0.4812128788913750 0.4396213639286462
 0.2905390880165470 0.5326599830392245 0.4481108110203021
 0.5821453189222173 0.4935156763910507 0.5352948795175345
 0.4462993614169569 0.5053875871375358 0.4732189185524869
 0.5455998430261316 0.5630619853797304 0.5280826728713405
 0.4827165944457095 0.4358625526564063 0.4803894510026141
 0.4566548375794122 0.4734629678000419 0.5444577284785604
 0.4681293687631784 0.5505452359367289 0.5338167196539874
 0.5270155529393643 0.4382313767623086 0.5453621999152792
 0.5014169823552947 0.5603020944106075 0.4632134297342598
 0.5180783188584972 0.5090783964840553 0.5782244467408575
 0.5103130420353309 0.4897415078850790 0.4302099133972111
 0.3289796284935130 0.5113646874300285 0.4214410120843095
 0.5139954405347757 0.4995011334430449 0.5043193859336887
 0.5715806329007540 0.5253817660573851 0.4640218045462344
 0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.0000000000000000		
35.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	35.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	35.0000000000000000

C Cu H Ni O Fe
 1 42 2 7 1 6

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
 0.6476592270665971 0.4879396554237083 0.5651968510197141
 0.3820583630665713 0.5109525002378987 0.4438253520724803
 0.6167957852193879 0.5591685495527250 0.5609787243985560
 0.4115966341677952 0.4397227471990416 0.4475137020957465
 0.6438425999599448 0.5203196071742313 0.4947287760121097
 0.3845947227631105 0.4785628663384900 0.5137953171763038
 0.6318882478586505 0.4406182942196961 0.5057898206390287
 0.3964639369010118 0.5583052682630524 0.5027006726079182
 0.5975647952325349 0.4301763350147779 0.5788038312248246
 0.4306501232934270 0.5687139359347344 0.4296632411748543
 0.5883453318713208 0.5033896919856954 0.6129261819627440

0.4400550601352461	0.4955489441675471	0.3954800709869655
0.5506791567355342	0.5752285747278663	0.6055552311485510
0.4777271562672804	0.4236659342350536	0.4029475097709363
0.5759739642322315	0.6244898818639908	0.5511273569836984
0.4522936799766305	0.3744227503503412	0.4573668775876218
0.6061550290584534	0.5920968773296152	0.4872371388242863
0.4222330054824817	0.4068418571686108	0.5211347932206722
0.6273443221830526	0.5506568817889725	0.4252543104344300
0.4009725714966696	0.4482788656512133	0.5832259854283443
0.6212554430533126	0.4734974169049200	0.4321488938628373
0.4072179252796815	0.5253986977756584	0.5763217345913864
0.6047276852704050	0.3988990560951795	0.4461747085274613
0.4236982044238159	0.5999611793896060	0.5622796988889479
0.5749716984580333	0.3833960091813215	0.5162716269600016
0.4532748407760575	0.6155202352324670	0.4922893876662723
0.5395152313884846	0.3790876420563937	0.5851327124045862
0.4888936778696976	0.6197948817038074	0.4233776301520969
0.5314296785260858	0.4461864762636217	0.6233823838036725
0.4969608221254892	0.5527049386897646	0.3850448724550508
0.5217586818559760	0.5185405380020512	0.6499488460172514
0.5066038570092535	0.4803617196776644	0.3584406571963292
0.4990575064057209	0.6179630134101637	0.5593646061386225
0.5292454654878257	0.3809245113152390	0.4490000663641504
0.5334705394659406	0.6284762325386318	0.4862971985199961
0.4948832202320053	0.3705112930576669	0.5221308774790222
0.5604107311981884	0.5896126313225317	0.4200541567575485
0.4679821584077760	0.4093416123936993	0.5882647196067378
0.5697033775046165	0.5162749206674285	0.3860955309947874
0.4586940164635895	0.4825581692504113	0.6223938026231608
0.5577605214158076	0.4365854062937245	0.3970677677026591
0.4705496136830897	0.5622737811092792	0.6114313572787683
0.3040326704303435	0.4812128788913750	0.4396213639286462
0.2905390880165470	0.5326599830392245	0.4481108110203021
0.5821453189222173	0.4935156763910507	0.5352948795175345
0.4462993614169569	0.5053875871375358	0.4732189185524869
0.5455998430261316	0.5630619853797304	0.5280826728713405
0.4827165944457095	0.4358625526564063	0.4803894510026141
0.4566548375794122	0.4734629678000419	0.5444577284785604
0.4681293687631784	0.5505452359367289	0.5338167196539874
0.5270155529393643	0.4382313767623086	0.5453621999152792
0.5014169823552947	0.5603020944106075	0.4632134297342598
0.5180783188584972	0.5090783964840553	0.5782244467408575
0.5103130420353309	0.4897415078850790	0.4302099133972111
0.3289796284935130	0.5113646874300285	0.4214410120843095
0.5139954405347757	0.4995011334430449	0.5043193859336887
0.5715806329007540	0.5253817660573851	0.4640218045462344
0.5601741432088304	0.4484842759796693	0.4746847356588114

POSCAR

1.00000000000000
35.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 35.0000000000000000 0.0000000000000000

0.0000000000000000	0.0000000000000000	35.0000000000000000
C Cu H Ni O Fe		
1 42 2 7 1 6		
Direct		
0.2954705818043527	0.5051355283572435	0.4574655652027443
0.6476592270665971	0.4879396554237083	0.5651968510197141
0.3820583630665713	0.5109525002378987	0.4438253520724803
0.6167957852193879	0.5591685495527250	0.5609787243985560
0.4115966341677952	0.4397227471990416	0.4475137020957465
0.6438425999599448	0.5203196071742313	0.4947287760121097
0.3845947227631105	0.4785628663384900	0.5137953171763038
0.6318882478586505	0.4406182942196961	0.5057898206390287
0.3964639369010118	0.5583052682630524	0.5027006726079182
0.5975647952325349	0.4301763350147779	0.5788038312248246
0.4306501232934270	0.5687139359347344	0.4296632411748543
0.5883453318713208	0.5033896919856954	0.6129261819627440
0.4400550601352461	0.4955489441675471	0.3954800709869655
0.5506791567355342	0.5752285747278663	0.6055552311485510
0.4777271562672804	0.4236659342350536	0.4029475097709363
0.5759739642322315	0.6244898818639908	0.5511273569836984
0.4522936799766305	0.3744227503503412	0.4573668775876218
0.6061550290584534	0.5920968773296152	0.4872371388242863
0.4222330054824817	0.4068418571686108	0.5211347932206722
0.6273443221830526	0.5506568817889725	0.4252543104344300
0.4009725714966696	0.4482788656512133	0.5832259854283443
0.6212554430533126	0.4734974169049200	0.4321488938628373
0.4072179252796815	0.5253986977756584	0.5763217345913864
0.6047276852704050	0.3988990560951795	0.4461747085274613
0.4236982044238159	0.5999611793896060	0.5622796988889479
0.5749716984580333	0.3833960091813215	0.5162716269600016
0.4532748407760575	0.6155202352324670	0.4922893876662723
0.5395152313884846	0.3790876420563937	0.5851327124045862
0.4888936778696976	0.6197948817038074	0.4233776301520969
0.5314296785260858	0.4461864762636217	0.6233823838036725
0.4969608221254892	0.5527049386897646	0.3850448724550508
0.5217586818559760	0.5185405380020512	0.6499488460172514
0.5066038570092535	0.4803617196776644	0.3584406571963292
0.4990575064057209	0.6179630134101637	0.5593646061386225
0.5292454654878257	0.3809245113152390	0.4490000663641504
0.5334705394659406	0.6284762325386318	0.4862971985199961
0.4948832202320053	0.3705112930576669	0.5221308774790222
0.5604107311981884	0.5896126313225317	0.4200541567575485
0.4679821584077760	0.4093416123936993	0.5882647196067378
0.5697033775046165	0.5162749206674285	0.3860955309947874
0.4586940164635895	0.4825581692504113	0.6223938026231608
0.5577605214158076	0.4365854062937245	0.3970677677026591
0.4705496136830897	0.5622737811092792	0.6114313572787683
0.3040326704303435	0.4812128788913750	0.4396213639286462
0.2905390880165470	0.5326599830392245	0.4481108110203021
0.5821453189222173	0.4935156763910507	0.5352948795175345
0.4462993614169569	0.5053875871375358	0.4732189185524869
0.5455998430261316	0.5630619853797304	0.5280826728713405

0.4827165944457095	0.4358625526564063	0.4803894510026141
0.4566548375794122	0.4734629678000419	0.5444577284785604
0.4681293687631784	0.5505452359367289	0.5338167196539874
0.5270155529393643	0.4382313767623086	0.5453621999152792
0.5014169823552947	0.5603020944106075	0.4632134297342598
0.5180783188584972	0.5090783964840553	0.5782244467408575
0.5103130420353309	0.4897415078850790	0.4302099133972111
0.3289796284935130	0.5113646874300285	0.4214410120843095
0.5139954405347757	0.4995011334430449	0.5043193859336887
0.5715806329007540	0.5253817660573851	0.4640218045462344
0.5601741432088304	0.4484842759796693	0.4746847356588114

POSCAR

1.000000000000000			
35.000000000000000	0.000000000000000	0.000000000000000	
0.000000000000000	35.000000000000000	0.000000000000000	
0.000000000000000	0.000000000000000	35.000000000000000	
C Cu H Ni O Fe			
1 42 2 7 1 6			

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
0.6476592270665971 0.4879396554237083 0.5651968510197141
0.3820583630665713 0.5109525002378987 0.4438253520724803
0.6167957852193879 0.5591685495527250 0.5609787243985560
0.4115966341677952 0.4397227471990416 0.4475137020957465
0.6438425999599448 0.5203196071742313 0.4947287760121097
0.3845947227631105 0.4785628663384900 0.5137953171763038
0.6318882478586505 0.4406182942196961 0.5057898206390287
0.3964639369010118 0.5583052682630524 0.5027006726079182
0.5975647952325349 0.4301763350147779 0.5788038312248246
0.4306501232934270 0.5687139359347344 0.4296632411748543
0.5883453318713208 0.5033896919856954 0.6129261819627440
0.4400550601352461 0.4955489441675471 0.3954800709869655
0.5506791567355342 0.5752285747278663 0.6055552311485510
0.4777271562672804 0.4236659342350536 0.4029475097709363
0.5759739642322315 0.6244898818639908 0.5511273569836984
0.4522936799766305 0.3744227503503412 0.4573668775876218
0.6061550290584534 0.5920968773296152 0.4872371388242863
0.4222330054824817 0.4068418571686108 0.5211347932206722
0.6273443221830526 0.5506568817889725 0.4252543104344300
0.4009725714966696 0.4482788656512133 0.5832259854283443
0.6212554430533126 0.4734974169049200 0.4321488938628373
0.4072179252796815 0.5253986977756584 0.5763217345913864
0.6047276852704050 0.3988990560951795 0.4461747085274613
0.4236982044238159 0.5999611793896060 0.562279698889479
0.5749716984580333 0.3833960091813215 0.5162716269600016
0.4532748407760575 0.6155202352324670 0.4922893876662723
0.5395152313884846 0.3790876420563937 0.5851327124045862
0.4888936778696976 0.6197948817038074 0.4233776301520969
0.5314296785260858 0.4461864762636217 0.6233823838036725
0.4969608221254892 0.5527049386897646 0.3850448724550508
0.5217586818559760 0.5185405380020512 0.6499488460172514

0.5066038570092535 0.4803617196776644 0.3584406571963292
 0.4990575064057209 0.6179630134101637 0.5593646061386225
 0.5292454654878257 0.3809245113152390 0.4490000663641504
 0.5334705394659406 0.6284762325386318 0.4862971985199961
 0.4948832202320053 0.3705112930576669 0.5221308774790222
 0.5604107311981884 0.5896126313225317 0.4200541567575485
 0.4679821584077760 0.4093416123936993 0.5882647196067378
 0.5697033775046165 0.5162749206674285 0.3860955309947874
 0.4586940164635895 0.4825581692504113 0.6223938026231608
 0.5577605214158076 0.4365854062937245 0.3970677677026591
 0.4705496136830897 0.5622737811092792 0.6114313572787683
 0.3040326704303435 0.4812128788913750 0.4396213639286462
 0.2905390880165470 0.5326599830392245 0.4481108110203021
 0.5821453189222173 0.4935156763910507 0.5352948795175345
 0.4462993614169569 0.5053875871375358 0.4732189185524869
 0.5455998430261316 0.5630619853797304 0.5280826728713405
 0.4827165944457095 0.4358625526564063 0.4803894510026141
 0.4566548375794122 0.4734629678000419 0.5444577284785604
 0.4681293687631784 0.5505452359367289 0.5338167196539874
 0.5270155529393643 0.4382313767623086 0.5453621999152792
 0.5014169823552947 0.5603020944106075 0.4632134297342598
 0.5180783188584972 0.5090783964840553 0.5782244467408575
 0.5103130420353309 0.4897415078850790 0.4302099133972111
 0.3289796284935130 0.5113646874300285 0.4214410120843095
 0.5139954405347757 0.4995011334430449 0.5043193859336887
 0.5715806329007540 0.5253817660573851 0.4640218045462344
 0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.000000000000000		
35.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	35.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	35.000000000000000
C Cu H Ni O Fe		
1 42 2 7 1 6		

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
 0.6476592270665971 0.4879396554237083 0.5651968510197141
 0.3820583630665713 0.5109525002378987 0.4438253520724803
 0.6167957852193879 0.5591685495527250 0.5609787243985560
 0.4115966341677952 0.4397227471990416 0.4475137020957465
 0.6438425999599448 0.5203196071742313 0.4947287760121097
 0.3845947227631105 0.4785628663384900 0.5137953171763038
 0.6318882478586505 0.4406182942196961 0.5057898206390287
 0.3964639369010118 0.5583052682630524 0.5027006726079182
 0.5975647952325349 0.4301763350147779 0.5788038312248246
 0.4306501232934270 0.5687139359347344 0.4296632411748543
 0.5883453318713208 0.5033896919856954 0.6129261819627440
 0.4400550601352461 0.4955489441675471 0.3954800709869655
 0.5506791567355342 0.5752285747278663 0.6055552311485510
 0.4777271562672804 0.4236659342350536 0.4029475097709363
 0.5759739642322315 0.6244898818639908 0.5511273569836984

0.4522936799766305 0.3744227503503412 0.4573668775876218
 0.6061550290584534 0.5920968773296152 0.4872371388242863
 0.4222330054824817 0.4068418571686108 0.5211347932206722
 0.6273443221830526 0.5506568817889725 0.4252543104344300
 0.4009725714966696 0.4482788656512133 0.5832259854283443
 0.6212554430533126 0.4734974169049200 0.4321488938628373
 0.4072179252796815 0.5253986977756584 0.5763217345913864
 0.6047276852704050 0.3988990560951795 0.4461747085274613
 0.4236982044238159 0.5999611793896060 0.5622796988889479
 0.5749716984580333 0.3833960091813215 0.5162716269600016
 0.4532748407760575 0.6155202352324670 0.4922893876662723
 0.5395152313884846 0.3790876420563937 0.5851327124045862
 0.4888936778696976 0.6197948817038074 0.4233776301520969
 0.5314296785260858 0.4461864762636217 0.6233823838036725
 0.4969608221254892 0.5527049386897646 0.3850448724550508
 0.5217586818559760 0.5185405380020512 0.6499488460172514
 0.5066038570092535 0.4803617196776644 0.3584406571963292
 0.4990575064057209 0.6179630134101637 0.5593646061386225
 0.5292454654878257 0.3809245113152390 0.4490000663641504
 0.5334705394659406 0.6284762325386318 0.4862971985199961
 0.4948832202320053 0.3705112930576669 0.5221308774790222
 0.5604107311981884 0.5896126313225317 0.4200541567575485
 0.4679821584077760 0.4093416123936993 0.5882647196067378
 0.5697033775046165 0.5162749206674285 0.3860955309947874
 0.4586940164635895 0.4825581692504113 0.6223938026231608
 0.5577605214158076 0.4365854062937245 0.3970677677026591
 0.4705496136830897 0.5622737811092792 0.6114313572787683
 0.3040326704303435 0.4812128788913750 0.4396213639286462
 0.2905390880165470 0.5326599830392245 0.4481108110203021
 0.5821453189222173 0.4935156763910507 0.5352948795175345
 0.4462993614169569 0.5053875871375358 0.4732189185524869
 0.5455998430261316 0.5630619853797304 0.5280826728713405
 0.4827165944457095 0.4358625526564063 0.4803894510026141
 0.4566548375794122 0.4734629678000419 0.5444577284785604
 0.4681293687631784 0.5505452359367289 0.5338167196539874
 0.5270155529393643 0.4382313767623086 0.5453621999152792
 0.5014169823552947 0.5603020944106075 0.4632134297342598
 0.5180783188584972 0.5090783964840553 0.5782244467408575
 0.5103130420353309 0.4897415078850790 0.4302099133972111
 0.3289796284935130 0.5113646874300285 0.4214410120843095
 0.5139954405347757 0.4995011334430449 0.5043193859336887
 0.5715806329007540 0.5253817660573851 0.4640218045462344
 0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.000000000000000
 35.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 35.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 35.000000000000000

C Cu H Ni O Fe
 1 42 2 7 1 6

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
0.6476592270665971 0.4879396554237083 0.5651968510197141
0.3820583630665713 0.5109525002378987 0.4438253520724803
0.6167957852193879 0.5591685495527250 0.5609787243985560
0.4115966341677952 0.4397227471990416 0.4475137020957465
0.6438425999599448 0.5203196071742313 0.4947287760121097
0.3845947227631105 0.4785628663384900 0.5137953171763038
0.6318882478586505 0.4406182942196961 0.5057898206390287
0.3964639369010118 0.5583052682630524 0.5027006726079182
0.5975647952325349 0.4301763350147779 0.5788038312248246
0.4306501232934270 0.5687139359347344 0.4296632411748543
0.5883453318713208 0.5033896919856954 0.6129261819627440
0.4400550601352461 0.4955489441675471 0.3954800709869655
0.5506791567355342 0.5752285747278663 0.6055552311485510
0.4777271562672804 0.4236659342350536 0.4029475097709363
0.5759739642322315 0.6244898818639908 0.5511273569836984
0.4522936799766305 0.3744227503503412 0.4573668775876218
0.6061550290584534 0.5920968773296152 0.4872371388242863
0.4222330054824817 0.4068418571686108 0.5211347932206722
0.6273443221830526 0.5506568817889725 0.4252543104344300
0.4009725714966696 0.4482788656512133 0.5832259854283443
0.6212554430533126 0.4734974169049200 0.4321488938628373
0.4072179252796815 0.5253986977756584 0.5763217345913864
0.6047276852704050 0.3988990560951795 0.4461747085274613
0.4236982044238159 0.5999611793896060 0.5622796988889479
0.5749716984580333 0.3833960091813215 0.5162716269600016
0.4532748407760575 0.6155202352324670 0.4922893876662723
0.5395152313884846 0.3790876420563937 0.5851327124045862
0.4888936778696976 0.6197948817038074 0.4233776301520969
0.5314296785260858 0.4461864762636217 0.6233823838036725
0.4969608221254892 0.5527049386897646 0.3850448724550508
0.5217586818559760 0.5185405380020512 0.6499488460172514
0.5066038570092535 0.4803617196776644 0.3584406571963292
0.4990575064057209 0.6179630134101637 0.5593646061386225
0.5292454654878257 0.3809245113152390 0.4490000663641504
0.5334705394659406 0.6284762325386318 0.4862971985199961
0.4948832202320053 0.3705112930576669 0.5221308774790222
0.5604107311981884 0.5896126313225317 0.4200541567575485
0.4679821584077760 0.4093416123936993 0.5882647196067378
0.5697033775046165 0.5162749206674285 0.3860955309947874
0.4586940164635895 0.4825581692504113 0.6223938026231608
0.5577605214158076 0.4365854062937245 0.3970677677026591
0.4705496136830897 0.5622737811092792 0.6114313572787683
0.3040326704303435 0.4812128788913750 0.4396213639286462
0.2905390880165470 0.5326599830392245 0.4481108110203021
0.5821453189222173 0.4935156763910507 0.5352948795175345
0.4462993614169569 0.5053875871375358 0.4732189185524869
0.5455998430261316 0.5630619853797304 0.5280826728713405
0.4827165944457095 0.4358625526564063 0.4803894510026141
0.4566548375794122 0.4734629678000419 0.5444577284785604
0.4681293687631784 0.5505452359367289 0.5338167196539874
0.5270155529393643 0.4382313767623086 0.5453621999152792

0.5014169823552947 0.5603020944106075 0.4632134297342598
 0.5180783188584972 0.5090783964840553 0.5782244467408575
 0.5103130420353309 0.4897415078850790 0.4302099133972111
 0.3289796284935130 0.5113646874300285 0.4214410120843095
 0.5139954405347757 0.4995011334430449 0.5043193859336887
 0.5715806329007540 0.5253817660573851 0.4640218045462344
 0.5601741432088304 0.4484842759796693 0.4746847356588114

POSCAR

1.0000000000000000
 35.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 35.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.0000000000000000
 C Cu H Ni O Fe
 1 42 2 7 1 6

Direct

0.2954705818043527 0.5051355283572435 0.4574655652027443
 0.6476592270665971 0.4879396554237083 0.5651968510197141
 0.3820583630665713 0.5109525002378987 0.4438253520724803
 0.6167957852193879 0.5591685495527250 0.5609787243985560
 0.4115966341677952 0.4397227471990416 0.4475137020957465
 0.6438425999599448 0.5203196071742313 0.4947287760121097
 0.3845947227631105 0.4785628663384900 0.5137953171763038
 0.6318882478586505 0.4406182942196961 0.5057898206390287
 0.3964639369010118 0.5583052682630524 0.5027006726079182
 0.5975647952325349 0.4301763350147779 0.5788038312248246
 0.4306501232934270 0.5687139359347344 0.4296632411748543
 0.5883453318713208 0.5033896919856954 0.6129261819627440
 0.4400550601352461 0.4955489441675471 0.3954800709869655
 0.5506791567355342 0.5752285747278663 0.6055552311485510
 0.4777271562672804 0.4236659342350536 0.4029475097709363
 0.5759739642322315 0.6244898818639908 0.5511273569836984
 0.4522936799766305 0.3744227503503412 0.4573668775876218
 0.6061550290584534 0.5920968773296152 0.4872371388242863
 0.4222330054824817 0.4068418571686108 0.5211347932206722
 0.6273443221830526 0.5506568817889725 0.4252543104344300
 0.4009725714966696 0.4482788656512133 0.5832259854283443
 0.6212554430533126 0.4734974169049200 0.4321488938628373
 0.4072179252796815 0.5253986977756584 0.5763217345913864
 0.6047276852704050 0.3988990560951795 0.4461747085274613
 0.4236982044238159 0.5999611793896060 0.5622796988889479
 0.5749716984580333 0.3833960091813215 0.5162716269600016
 0.4532748407760575 0.6155202352324670 0.4922893876662723
 0.5395152313884846 0.3790876420563937 0.5851327124045862
 0.4888936778696976 0.6197948817038074 0.4233776301520969
 0.5314296785260858 0.4461864762636217 0.6233823838036725
 0.4969608221254892 0.5527049386897646 0.3850448724550508
 0.5217586818559760 0.5185405380020512 0.6499488460172514
 0.5066038570092535 0.4803617196776644 0.3584406571963292
 0.4990575064057209 0.6179630134101637 0.5593646061386225
 0.5292454654878257 0.3809245113152390 0.4490000663641504
 0.5334705394659406 0.6284762325386318 0.4862971985199961

0.4948832202320053 0.3705112930576669 0.5221308774790222
 0.5604107311981884 0.5896126313225317 0.4200541567575485
 0.4679821584077760 0.4093416123936993 0.5882647196067378
 0.5697033775046165 0.5162749206674285 0.3860955309947874
 0.4586940164635895 0.4825581692504113 0.6223938026231608
 0.5577605214158076 0.4365854062937245 0.3970677677026591
 0.4705496136830897 0.5622737811092792 0.6114313572787683
 0.3040326704303435 0.4812128788913750 0.4396213639286462
 0.2905390880165470 0.5326599830392245 0.4481108110203021
 0.5821453189222173 0.4935156763910507 0.5352948795175345
 0.4462993614169569 0.5053875871375358 0.4732189185524869
 0.5455998430261316 0.5630619853797304 0.5280826728713405
 0.4827165944457095 0.4358625526564063 0.4803894510026141
 0.4566548375794122 0.4734629678000419 0.5444577284785604
 0.4681293687631784 0.5505452359367289 0.5338167196539874
 0.5270155529393643 0.4382313767623086 0.5453621999152792
 0.5014169823552947 0.5603020944106075 0.4632134297342598
 0.5180783188584972 0.5090783964840553 0.5782244467408575
 0.5103130420353309 0.4897415078850790 0.4302099133972111
 0.3289796284935130 0.5113646874300285 0.4214410120843095
 0.5139954405347757 0.4995011334430449 0.5043193859336887
 0.5715806329007540 0.5253817660573851 0.4640218045462344
 0.5601741432088304 0.4484842759796693 0.4746847356588114

Absolute energies of $\text{TM}_x\text{Ni}_{13-x}\text{-Cu}_{42}$ structures in eV:

$\text{TM}=$	X=3	X=6	X=9
Sc	-218.895726577	-225.515075698	-226.252075456
Ti	-223.2533250585	-234.6970403855	-241.9877368865
V	-222.7764779955	-235.0496408095	-245.89427401
Cr	-223.4855316595	-235.0680686475	-243.2853583765
Mn	-222.8493969185	-234.488688555	-243.084624266
Fe	-219.1577096665	-227.378548408	-235.4282537365
Co	-214.499220309	-218.526539638	-219.195827818
Cu	-205.2124384255	-201.158654895	-197.0328761775
Zn	-199.614908537	-188.6181773355	-176.5961312995

Absolute energies of $\text{Sc}_x\text{Ni}_{13-x}\text{-Cu}_{42}$ in eV:

x=	
1	-217.8613517795
2	-219.0001906675
3	-218.895726577
4	-225.2415329395
5	-225.2476866365
6	-225.515075698
7	-225.2394786675
8	-224.199728698
9	-226.252075456
10	-226.381324037
11	-227.30237486
12	-226.422412359