***Supporting Information***

**Hydrogen Transport through Different Crystal Phases**

Yuval Elbaz1, David Furman2,3, and Maytal Caspary Toroker1\*

1Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 3200003, Israel

2Fritz Haber Research Center for Molecular Dynamics, Institute of Chemistry, Hebrew University of Jerusalem, Jerusalem 91904, Israel

3Division of Chemistry, NRCN, P.O. Box 9001, Beer-Sheva 84190, Israel

**Nudged Elastic Band**

The Nudged Elastic Band (NEB) is a very popular method to find the minimum energy path (MEP) from known initial state to a known final state of a chemical reaction.

NEB is a method from the chain-of-states family. In this class of methods, a group of 'intermediates states', called images, are interpolated between a known initial and final states. An elastic force is added between every two adjacent images, thus creating an elastic band and keeps the continuity of the path. The MEP has a minimum energy in every directions perpendicular to the path and at least one first order saddle point.

The starting point for NEB calculation is an initial pathway connecting initial and final states of the atomic system. Usually, and in this work as well, a linear path (equally spaced images along one line) is the initial guess for the path. Two forces are acting on each image in the band, the true force from the potential energy surface (true force) and the virtual spring force between every two adjacent images. The relaxation process of the NEB takes only the perpendicular to the path component of the true force and the parallel component of the spring force. Thus, the force on image i is



Where  is the coordinates vector of image i and  is the unit tangent to the path. The perpendicular component of the true force is . This projection of the true and spring force is referred as nudging. Relaxed configuration to the MEP is achieved when for all i. The spring force is



The spring constant can be taken as an arbitrary value up to some level (-5 in this work. Negative value to turn on the nudging in VASP) because the spring force only influence the distribution of the images along the path.

NEB implementation in VASP

To do a NEB calculation one has to have an optimized initial and final structures of the system of interest. An initial guess of the path has to be made, meaning, creating multiple images along the guessed path. The initial path is usually linear and can be made using VTST scripts package. Number of images determine the resolution of the path.  
Two tags need to be added to the INCAR file:

*IMAGES = N #number of images in the initial path*

*SPRING = -5 #spring constant value*

The main job folder should contain the INCAR, POTCAR, KPOINTS, job submit file and sub folder for each image which contain the POSCAR file of the related image. The sub folder should be named 00,01,..N, where N is the number of images.

VTST scripts: http://theory.cm.utexas.edu/vtsttools/scripts.html

VASP manual: http://cms.mpi.univie.ac.at/vasp/guide/node140.html

**ZPE results**

|  |  |  |  |
| --- | --- | --- | --- |
| β-NiOOH |  |  |  |
| Vacancy | Mode # | IS [THz] | TS [THz] |
|  | 1 | 72.834 | 42.225 |
|  | 2 | 35.629 | 38.448 |
|  | 3 | 32.037 | 16.123 |
|  | 4 | 15.285 | 13.149 |
|  | 5 | 12.868 | 11.558 |
|  | 6 | 10.693 | - |
| Interstitial | Mode # | IS [Thz] | TS [Thz] |
|  | 1 | 100.469 | 48.165 |
|  | 2 | 30.149 | 36.889 |
|  | 3 | 27.281 | 19.413 |
|  | 4 | 15.527 | 14.089 |
|  | 5 | 15.360 | 13.198 |
|  | 6 | 13.926 | 10.848 |
|  | 7 | 11.780 | 10.276 |
|  | 8 | 11.583 | 9.059 |
|  | 9 | 11.255 | - |

|  |  |  |  |
| --- | --- | --- | --- |
| β-Ni(OH)2 |  |  |  |
| Vacancy | Mode # | IS [THz] | TS [THz] |
|  | 1 | 108.789 | 57.710 |
|  | 2 | 106.001 | 39.507 |
|  | 3 | 28.234 | 39.128 |
|  | 4 | 26.231 | 34.287 |
|  | 5 | 24.346 | 33.756 |
|  | 6 | 21.322 | 19.283 |
|  | 7 | 11.389 | 13.619 |
|  | 8 | 10.750 | 11.536 |
|  | 9 | 10.150 | 10.230 |
|  | 10 | 9.799 | 8.962 |
|  | 11 | 9.480 | 8.056 |
|  | 12 | 8.709 | - |
| Interstitial | Mode # | IS [Thz] | TS [Thz] |
|  | 1 | 110.625 | 109.682 |
|  | 2 | 110.026 | 109.339 |
|  | 3 | 29.867 | 28.625 |
|  | 4 | 25.322 | 27.988 |
|  | 5 | 23.652 | 24.514 |
|  | 6 | 23.013 | 23.314 |
|  | 7 | 21.760 | 23.040 |
|  | 8 | 15.181 | 14.412 |
|  | 9 | 13.360 | 11.820 |
|  | 10 | 11.146 | 10.290 |
|  | 11 | 9.965 | 10.029 |
|  | 12 | 9.605 | 9.180 |
|  | 13 | 9.158 | 9.072 |
|  | 14 | 8.227 | 7.378 |
|  | 15 | 8.132 | - |

|  |  |  |  |
| --- | --- | --- | --- |
| α-Ni(OH)2 |  |  |  |
| Vacancy | Mode # | IS [THz] | TS [THz] |
|  | 1 | 109.324 | 48.301 |
|  | 2 | 24.837 | 35.414 |
|  | 3 | 23.563 | 16.878 |
|  | 4 | 12.341 | 12.542 |
|  | 5 | 11.813 | 10.763 |
|  | 6 | 11.302 | 10.031 |
|  | 7 | 9.924 | 8.778 |
|  | 8 | 9.699 | 6.269 |
|  | 9 | 8.103 | - |

**Structures (VASP format)**

Structures and NEB results can also be found in the following link:

https://iochem-bd.bsc.es/browse/handle/100/192836

**β-NiOOH- Vacancy diffusion:**  
Image 0 (initial structure):  
**E=** **-232.26576748 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0016775813790630 0.4966994843915629 0.0932862375904406 T T T*

*0.0033937511612692 0.9945570680974072 0.0948020888357277 T T T*

*0.5019138468690443 0.4962258542583058 0.0944045091328221 T T T*

*0.5020998555749543 0.9945573945126612 0.0948020468302673 T T T*

*0.1708226939938911 0.1583691840184400 0.7588810661514742 T T T*

*0.1677997314436794 0.6639472917365410 0.7582511548809876 T T T*

*0.6701153133531506 0.1597944721575004 0.7645196581462912 T T T*

*0.6682629921226777 0.6639457613589244 0.7582488749217262 T T T*

*0.3304043282105908 0.3357350884197885 0.4254798801988926 T T T*

*0.3444194870829875 0.8111099619886346 0.4356292091021388 T T T*

*0.8338093704327889 0.3357325358647643 0.4254798329121243 T T T*

*0.8342156700492112 0.8315179055407427 0.4271052501599257 T T T*

*0.4967975306331951 0.0031686372153530 0.9054667777128600 T T T*

*0.4963924691366728 0.5071976487491483 0.9048153941232400 T T T*

*0.0000207388358504 0.0031681415114804 0.9054681746925936 T T T*

*0.9962902329443396 0.5074049425777858 0.9024349357762418 T T T*

*0.1622652805549336 0.1753826615530159 0.5724940654447295 T T T*

*0.1678769852913788 0.6656747630545183 0.5734374124195725 T T T*

*0.6524089238310182 0.1950853900754197 0.5606958798548050 T T T*

*0.6663715970872559 0.6656736674972592 0.5734371143411749 T T T*

*0.3302261663232358 0.3397289741109830 0.2379389095391033 T T T*

*0.3315348352529810 0.8369451545030415 0.2403719221357221 T T T*

*0.8300694311884627 0.3397287471764017 0.2379390630780094 T T T*

*0.8314980534842888 0.8370237003912990 0.2394545359018636 T T T*

*0.1654526631960280 0.1691334944117528 0.1647951121191298 T T T*

*0.1659207039585411 0.6671488899337916 0.1653921942839816 T T T*

*0.6664379484428125 0.1671648880833416 0.1651347993770571 T T T*

*0.6669701878479728 0.6671484704264117 0.1653927295411464 T T T*

*0.3355814565682920 0.3318598066399545 0.8313609799091566 T T T*

*0.3325418652038579 0.8349111864368979 0.8299319848693330 T T T*

*0.8325602811447936 0.3318603262372974 0.8313625508951290 T T T*

*0.8313557378550982 0.8372869274628556 0.8305450832627841 T T T*

*0.5002640791838786 0.0037630134407181 0.4988436728838437 T T T*

*0.5016570268503742 0.4966229781728089 0.4985681004318394 T T T*

*0.9959001196032632 0.0037634713011769 0.4988457285063603 T T T*

*0.9990767373438842 0.5017774062323994 0.4994354608443388 T T T*

*0.9991613273227102 0.5016849161554831 0.9813083727998516 T T T*

*0.0040674489658414 0.9952465772110344 0.9847447183335164 T T T*

*0.4995495995174934 0.5009020811159175 0.9837385724440466 T T T*

*0.5006939711443721 0.9952476699572016 0.9847433725275180 T T T*

*0.1665651337053760 0.1668212105107401 0.6542931006258428 T T T*

*0.1711330231999355 0.6602936508501429 0.6584606109198248 T T T*

*0.6685344148828989 0.6602917553347254 0.6584656573647649 T T T*

*0.3314084176483121 0.3369864235016706 0.3182271738178315 T T T*

*0.3406546510866093 0.8186729738971508 0.3163367235975656 T T T*

*0.8315952107820550 0.3369846603991533 0.3182278053680747 T T T*

*0.8342681996164956 0.8314502391143748 0.3207297123427182 T T T*

Image 1:

**E= -232.62387776 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0043844671502938 0.4887346082086792 0.0870086119125817 T T T*

*0.0059597002271989 0.9899087608813221 0.0945889471010700 T T T*

*0.4985370691536190 0.4993883346555597 0.0950594004782268 T T T*

*0.5028789129222243 0.9887302728984964 0.0924631474127323 T T T*

*0.1821438308110335 0.1396575690945968 0.7544959269361980 T T T*

*0.1708532181717421 0.6524989944011039 0.7583536652527034 T T T*

*0.6835358389843963 0.1303396894363542 0.7678662856086923 T T T*

*0.6659124864710950 0.6322646058827508 0.7536116065732801 T T T*

*0.3253962492711598 0.3388669911362242 0.4212808736279105 T T T*

*0.3386233979955821 0.8173086432175909 0.4324830872405813 T T T*

*0.8249731055054249 0.3388646708824025 0.4195317398248700 T T T*

*0.8320583825043053 0.8348309702131622 0.4237040969509299 T T T*

*0.5045683840038055 0.9827438694308913 0.9026321389905131 T T T*

*0.4985181263487568 0.4925633988755863 0.9048873183176960 T T T*

*0.0126565013727803 0.0006073300910868 0.9062867010234106 T T T*

*0.9956547447185811 0.5016413696986601 0.8923440931883529 T T T*

*0.1584763393623173 0.1794850037469379 0.5663727085745033 T T T*

*0.1615027868361732 0.6729546335612635 0.5691130907888392 T T T*

*0.6454925425321918 0.2047672840971949 0.5573778984103754 T T T*

*0.6655058429943392 0.6657324375501111 0.5652870090869659 T T T*

*0.3272939408242393 0.3412584391136548 0.2344619060176628 T T T*

*0.3278609929546882 0.8429816922914198 0.2411506489036830 T T T*

*0.8284898656298141 0.3421290727512488 0.2340788740554598 T T T*

*0.8308178149411050 0.8350373809710169 0.2326159488870742 T T T*

*0.1677244105114761 0.1626061899689792 0.1640088048539067 T T T*

*0.1636632533143889 0.6696994914579765 0.1631834278897343 T T T*

*0.6672660995948900 0.1629613013919395 0.1635069450234002 T T T*

*0.6639706310491952 0.6695774026280091 0.1627829670421134 T T T*

*0.3396526390269770 0.3183538404600528 0.8290027226475851 T T T*

*0.3375052513301735 0.8145754441660522 0.8294384520572191 T T T*

*0.8391000754011474 0.3150017783253279 0.8293640438194388 T T T*

*0.8404198884109102 0.8167074622651360 0.8300555419352966 T T T*

*0.4922240845023323 0.0098541940604751 0.4951290704690267 T T T*

*0.4971369431305597 0.5030282208560719 0.4938476675615201 T T T*

*0.9924224978586350 0.0129992096387607 0.4951522765228497 T T T*

*0.9949796048637624 0.4998610739788951 0.4949123793179085 T T T*

*0.0003823500744382 0.4954705235494853 0.0106345896131410 T T T*

*0.0166082319194165 0.9984181664050145 0.9844919084748013 T T T*

*0.4973488522972760 0.4943599350215399 0.9840700521426674 T T T*

*0.5054084765374163 0.9800782064517366 0.9824708681811625 T T T*

*0.1747977134416676 0.1531220082552155 0.6765152892034952 T T T*

*0.1690808188500448 0.6608003879676211 0.6474941025582969 T T T*

*0.6624335375939441 0.6355600589044442 0.6758416483679660 T T T*

*0.3261265991860657 0.3410581700652342 0.3158900650917582 T T T*

*0.3347917921829796 0.8293941789931201 0.3171569257118054 T T T*

*0.8257837069762886 0.3427638067558151 0.3155168097054490 T T T*

*0.8309497405525000 0.8372571733183755 0.3450153317760958 T T T*

Image 2:

**E= -232.51322827 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0042636248362039 0.4894607134545507 0.0875865714078230 T T T*

*0.0057159030819064 0.9902207684543557 0.0949142821954597 T T T*

*0.4980029290067291 0.4992824864723544 0.0956841618359043 T T T*

*0.5027494944834380 0.9875876369111419 0.0930051694674506 T T T*

*0.1877133276163222 0.1127395822634791 0.7521439163652748 T T T*

*0.1732786950159909 0.6267822238461699 0.7565157913522177 T T T*

*0.6879814967258275 0.1000867012193157 0.7668994272525823 T T T*

*0.6691379353123110 0.5978102031725829 0.7525058004187829 T T T*

*0.3227387017892012 0.3656419432286614 0.4224830414662542 T T T*

*0.3348029451068159 0.8455832915146280 0.4330423695992878 T T T*

*0.8217670962759346 0.3687042054489363 0.4199103408659440 T T T*

*0.8276528480846783 0.8655856933373525 0.4237944967281011 T T T*

*0.5080905268753535 0.9530894369639288 0.9012574213973968 T T T*

*0.5007418851608176 0.4641889116178096 0.9041392452197822 T T T*

*0.0163199558235781 0.9748467259293430 0.9049482414733421 T T T*

*0.9989465901718103 0.4743161470781556 0.8905958209742937 T T T*

*0.1558299422822336 0.2064941361292782 0.5672702058192285 T T T*

*0.1591124067211818 0.6997360191438643 0.5702686813117267 T T T*

*0.6433691540169532 0.2358222052456882 0.5583175326304807 T T T*

*0.6622066456566441 0.6936794157981073 0.5656006297550219 T T T*

*0.3268599337908627 0.3423097300907949 0.2346270052468240 T T T*

*0.3267768549683521 0.8434309760399848 0.2423755603546320 T T T*

*0.8278765094156317 0.3444236894448586 0.2338450241970836 T T T*

*0.8293104324026457 0.8379406812175855 0.2330956445528826 T T T*

*0.1676521211566419 0.1626776670853655 0.1644395645047489 T T T*

*0.1632577159536411 0.6706503181951146 0.1638464473493529 T T T*

*0.6666945491513611 0.1638842059574690 0.1636391155501195 T T T*

*0.6629034739174068 0.6705008531021981 0.1634430590324875 T T T*

*0.3435681099703529 0.2895269145088070 0.8280570801143010 T T T*

*0.3408000866354549 0.7849246127795579 0.8285349082384021 T T T*

*0.8433962501729999 0.2854670384184853 0.8282091590967040 T T T*

*0.8439674837967773 0.7877392935032699 0.8285215729983627 T T T*

*0.4890135949983841 0.0391927577353797 0.4959463153245275 T T T*

*0.4940688329119460 0.5320472423968299 0.4941134912080291 T T T*

*0.9886831381764876 0.0431723378791053 0.4952134440762649 T T T*

*0.9910154062889933 0.5297447272496407 0.4950562301451319 T T T*

*0.0015422284402763 0.4880034224141909 0.0110460136445412 T T T*

*0.0195510166590330 0.9833236168183949 0.9833805056426724 T T T*

*0.4973440193943761 0.4756914480989096 0.9833260225576987 T T T*

*0.5075769704608023 0.9598251992997893 0.9810015824681981 T T T*

*0.1786289495622476 0.1432172413877802 0.6765355838480936 T T T*

*0.1678401355156361 0.6696417942978485 0.6465056881055684 T T T*

*0.6641098767496424 0.6041938584703501 0.6766484979903650 T T T*

*0.3256732373342878 0.3505748036727025 0.3162149889801343 T T T*

*0.3323674119649855 0.8378354068001075 0.3197819197315698 T T T*

*0.8239391385257392 0.3559389913655563 0.3157509785595108 T T T*

*0.8270063335992832 0.8582471583133703 0.3436271626775688 T T T*

Image 3:

**E= -232.05787548 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0011658727541178 0.4951756944498072 0.0906253582633531 T T T*

*0.0025838637818316 0.9932716466080938 0.0930694964505206 T T T*

*0.4977062092134328 0.4983965846909680 0.0941794903086949 T T T*

*0.5038325900306617 0.9899899524337343 0.0916200781332724 T T T*

*0.1913915963827079 0.1032626246164247 0.7507044166876502 T T T*

*0.1729439115318448 0.6186603785225652 0.7547371540349765 T T T*

*0.6887751273751087 0.0907429105194565 0.7663910807637636 T T T*

*0.6705348527117755 0.5743876652625565 0.7513252588469934 T T T*

*0.3294854602006104 0.3699799026513380 0.4277137363176186 T T T*

*0.3287964809467427 0.8518524667416220 0.4266981423193348 T T T*

*0.8232939461908511 0.3855509381635081 0.4209657654993441 T T T*

*0.8223047435452854 0.8914783970750862 0.4276368370750815 T T T*

*0.5105044257714768 0.9397059841231079 0.8995553952969024 T T T*

*0.4963433473597945 0.4556280169726036 0.9041831038687222 T T T*

*0.0165615800066340 0.9679753490764067 0.9034033947832966 T T T*

*0.9979679569413598 0.4664417353936083 0.8897750845596817 T T T*

*0.1584245254394411 0.2179268758845105 0.5669830312379641 T T T*

*0.1611487696078985 0.7157866383477239 0.5713754159421475 T T T*

*0.6487622633385935 0.2676610893700462 0.5652597923490283 T T T*

*0.6537823027750016 0.7268678874008045 0.5613167370111901 T T T*

*0.3273795221486721 0.3391209689729988 0.2358911103396878 T T T*

*0.3304627955275533 0.8352831775402680 0.2374970974471546 T T T*

*0.8305562763595904 0.3411681563564372 0.2343405817452230 T T T*

*0.8268490563220968 0.8439159400758363 0.2372610481334661 T T T*

*0.1700419329622771 0.1578008879291432 0.1647501886276008 T T T*

*0.1660492983771006 0.6719063502643700 0.1639514221357301 T T T*

*0.6653724620797240 0.1668455317102783 0.1630103018421006 T T T*

*0.6589706475410809 0.6709377001492600 0.1638592303337443 T T T*

*0.3435725818580901 0.2796075061919224 0.8276057170452297 T T T*

*0.3414980567221306 0.7728684111199878 0.8273525604203309 T T T*

*0.8439709903467950 0.2750770075328758 0.8285713428177137 T T T*

*0.8445688257696223 0.7775721181166098 0.8262451201171401 T T T*

*0.4920030250855009 0.0548404411697205 0.4977387287367110 T T T*

*0.4965227910268031 0.5467398768630423 0.4946676241341082 T T T*

*0.9846570225106245 0.0620298923263508 0.4961489736074913 T T T*

*0.9889942563272480 0.5519680579993000 0.4950062493438488 T T T*

*0.9977758740044258 0.4929319778513870 0.0141201999543259 T T T*

*0.0182626057475718 0.9816923179173985 0.9824600040411391 T T T*

*0.4916055134882273 0.4718755095047900 0.9835460238568190 T T T*

*0.5102826333752321 0.9520846618559680 0.9797612473199669 T T T*

*0.1840071367533577 0.1384057513877140 0.6759608129861040 T T T*

*0.1675020888121995 0.6767159436523980 0.6463917813795266 T T T*

*0.6618202844749904 0.5263123314260778 0.6783197640454063 T T T*

*0.3314570255228255 0.3450525410270969 0.3151315965722958 T T T*

*0.3315885613936138 0.8319769944405849 0.3464283290569266 T T T*

*0.8254786323664127 0.3580260067363221 0.3159898365016674 T T T*

*0.8242861566408277 0.8622417819535255 0.3181331639263751 T T T*

Image 4:

**E= -231.58737796 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0009187263393196 0.4956102353987712 0.0910541362224218 T T T*

*0.0009275531053854 0.9960229702215712 0.0922535401375893 T T T*

*0.4972800429465709 0.4992261792078072 0.0947918252269365 T T T*

*0.5036563687842420 0.9914757268776303 0.0918554923319382 T T T*

*0.1993932364219382 0.0917835590896333 0.7484197345278848 T T T*

*0.1670083492279214 0.6168203183659368 0.7454949818591099 T T T*

*0.6880640217774323 0.0824862821912692 0.7647476997776579 T T T*

*0.6675898833664575 0.5489674345484349 0.7444173023378020 T T T*

*0.3394058698071434 0.3744925731050296 0.4345646453488763 T T T*

*0.3280929375328301 0.8565567608563102 0.4256552189407933 T T T*

*0.8278166187042132 0.3968015019167402 0.4259683752088340 T T T*

*0.8199910804444165 0.9129809591449691 0.4294728096096736 T T T*

*0.5156183073327456 0.9272525504884406 0.8979022091142758 T T T*

*0.4862089075976064 0.4526436421065899 0.9025338500147666 T T T*

*0.0180979174635915 0.9646703799119747 0.8988692566923939 T T T*

*0.9958086694814938 0.4621430434277458 0.8849298605694058 T T T*

*0.1644790238209909 0.2222986243536976 0.5703288569619536 T T T*

*0.1564431590202093 0.7330136109153158 0.5720281710742731 T T T*

*0.6497989849106568 0.3099863943157414 0.5803749442480737 T T T*

*0.6475666567215571 0.7569533722287017 0.5616559717484444 T T T*

*0.3279567465223734 0.3394808070823530 0.2375749099940112 T T T*

*0.3295407531604080 0.8369387024501681 0.2361727105785822 T T T*

*0.8314303655361094 0.3417799385496667 0.2363021405945489 T T T*

*0.8267572626590430 0.8462815771054349 0.2380417220253122 T T T*

*0.1699462579427365 0.1583590927561669 0.1653254779421241 T T T*

*0.1653444722340681 0.6739064635511002 0.1638501342947429 T T T*

*0.6655375222948010 0.1680225161979389 0.1637802453781673 T T T*

*0.6584638515482218 0.6723119349246073 0.1642427030489204 T T T*

*0.3440164409184781 0.2689235069264307 0.8260491470843001 T T T*

*0.3464124057646772 0.7616890142642458 0.8222259407610550 T T T*

*0.8421521793376003 0.2699131098379882 0.8254123630535274 T T T*

*0.8417427726855672 0.7702728885948036 0.8215310826753430 T T T*

*0.4927912819266799 0.0665850515530717 0.5001398895028044 T T T*

*0.4936946185692573 0.5680419342789440 0.4987176955287301 T T T*

*0.9864689971550062 0.0748844248797541 0.5008742432350910 T T T*

*0.9909611819006922 0.5677936746131648 0.4977499803732144 T T T*

*0.9965802935314135 0.4930810166279661 0.0150437911882082 T T T*

*0.0187005874781274 0.9817375376668254 0.9774625531324134 T T T*

*0.4810811048113700 0.4715490477861130 0.9809116014128623 T T T*

*0.5157668109154107 0.9418038437709314 0.9773454023179484 T T T*

*0.1948672233990637 0.1310422986324534 0.6738002984917062 T T T*

*0.1606176952464705 0.6691962687149167 0.6666022596736634 T T T*

*0.6588519340199236 0.4326159449312404 0.6621106384298018 T T T*

*0.3359083553901979 0.3434889878543047 0.3155024365100370 T T T*

*0.3296153216642150 0.8319614890013078 0.3469191466011942 T T T*

*0.8287418933481905 0.3600794294485662 0.3175926789477664 T T T*

*0.8237312336729549 0.8718127465632205 0.3190585609552383 T T T*

Image 5:

**E= -231.81031106 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0013903270043567 0.4961673787350678 0.0907225002425648 T T T*

*0.0004574863832378 0.9977775872818968 0.0920475373573219 T T T*

*0.4978398156140472 0.4996151908623476 0.0954461544768103 T T T*

*0.5036797263531780 0.9933385575741357 0.0924087500154419 T T T*

*0.1981259860207988 0.1015654832760262 0.7515270310570388 T T T*

*0.1664003843488077 0.6234269672439047 0.7497953227448884 T T T*

*0.6834267916752039 0.0995417598747174 0.7666957295185050 T T T*

*0.6702252405523885 0.5738408807519746 0.7567885295270828 T T T*

*0.3390710425590998 0.3662462548141318 0.4316024239014516 T T T*

*0.3405849838930000 0.8407591717539629 0.4206306712478653 T T T*

*0.8337218359718065 0.3796684318631363 0.4259587633713758 T T T*

*0.8222860846704783 0.9005381985122267 0.4266108039006771 T T T*

*0.5137894480046330 0.9464668211699732 0.9022286344039698 T T T*

*0.4796528647978867 0.4685918217967325 0.9054860667888256 T T T*

*0.0117837904949692 0.9810242146316719 0.8995720712721871 T T T*

*0.9975030188771660 0.4727460585528996 0.8909941743211612 T T T*

*0.1662972150458136 0.2097639521995782 0.5668695731091362 T T T*

*0.1541557126373472 0.7326512949112227 0.5654041524440109 T T T*

*0.6420549615544165 0.2941687830744756 0.5752525829581008 T T T*

*0.6490340225589341 0.7456848702477383 0.5593846168056067 T T T*

*0.3276975686495733 0.3402150361654483 0.2370722179718537 T T T*

*0.3296564423816079 0.8377560846982326 0.2353771150065456 T T T*

*0.8316756327080533 0.3422888332344808 0.2359939851023592 T T T*

*0.8269025926173492 0.8465070010308449 0.2368258412506532 T T T*

*0.1694211353624992 0.1602715495304830 0.1648335388607740 T T T*

*0.1651297613962971 0.6743201282684714 0.1633619388082722 T T T*

*0.6655805918933023 0.1690457140482219 0.1637805395159485 T T T*

*0.6592813119346410 0.6729041886862867 0.1636545463530709 T T T*

*0.3423938922032636 0.2810052612147373 0.8290753001821602 T T T*

*0.3465288501985209 0.7766112367657985 0.8273392505261866 T T T*

*0.8385559324510884 0.2871544117971608 0.8293846089850641 T T T*

*0.8380912859842362 0.7838677787486911 0.8256605718914048 T T T*

*0.4937416528952159 0.0546596240624924 0.4970999381786956 T T T*

*0.4933774868548614 0.5604270477566262 0.4949338639959607 T T T*

*0.9929285935818027 0.0585639454482379 0.4970153941477826 T T T*

*0.9926006783317191 0.5578249009600768 0.4954922346514002 T T T*

*0.9975562295737453 0.4947545799983621 0.0137216053136374 T T T*

*0.0115293735068879 0.9952053907784014 0.9782910337229549 T T T*

*0.4753213539386765 0.4835325212713026 0.9837284987523934 T T T*

*0.5150647694035777 0.9575997209997690 0.9821827721267081 T T T*

*0.2001213402885774 0.1277291512932199 0.6766540844480140 T T T*

*0.1574887688716909 0.6661565606659935 0.6762542215325343 T T T*

*0.6553236719489113 0.3716890746200523 0.6444488082638125 T T T*

*0.3352050621054111 0.3418284394617225 0.3151359760906438 T T T*

*0.3417327787074656 0.8203449184397250 0.3406309311525691 T T T*

*0.8325463897443679 0.3524203777248527 0.3162294777875403 T T T*

*0.8249119949998199 0.8674759472599313 0.3180548384980755 T T T*

Image 6:

**E= -232.00303802 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0019693335514790 0.4945278119074912 0.0909918389183855 T T T*

*0.0004645274748341 0.9956857602441306 0.0899557546288008 T T T*

*0.4991660898895495 0.4974298039526314 0.0940920227129835 T T T*

*0.5032337626449566 0.9934372423401630 0.0926807155064453 T T T*

*0.1850045958541557 0.1187600408807708 0.7542951600504575 T T T*

*0.1789936568581251 0.6251268443184899 0.7514517814685192 T T T*

*0.6751235978965227 0.1328475424222144 0.7632209391320642 T T T*

*0.6770341053897408 0.6184769535221464 0.7632419470539457 T T T*

*0.3371861355059550 0.3620545215118331 0.4299275631510316 T T T*

*0.3439092669608448 0.8342244272787460 0.4195363440396404 T T T*

*0.8344403779515710 0.3720430574484919 0.4255797983820304 T T T*

*0.8243727565073863 0.8916237262198851 0.4251693603276030 T T T*

*0.5027445289276602 0.9694491856185510 0.9041154897054966 T T T*

*0.4908116871430716 0.4787975985759165 0.9053714268646397 T T T*

*0.0042199873638866 0.9742387662397449 0.8987111256248766 T T T*

*0.0064059013356829 0.4713506513748352 0.8979432359008693 T T T*

*0.1665609929151350 0.2035501656024228 0.5659792296305146 T T T*

*0.1547860379689472 0.7274039354028089 0.5639385863479334 T T T*

*0.6419002842825302 0.2745332225080409 0.5708702223715384 T T T*

*0.6502175776285499 0.7384637386485194 0.5586642530845138 T T T*

*0.3281007838261170 0.3393301348553301 0.2366556073574919 T T T*

*0.3299560436051570 0.8366947131498511 0.2343809401535245 T T T*

*0.8316057267242652 0.3406224937369070 0.2353716918298379 T T T*

*0.8279025562075388 0.8451764905241888 0.2359854686699757 T T T*

*0.1690380999234073 0.1601633495255548 0.1639187222247105 T T T*

*0.1657888335457677 0.6724394008759690 0.1624873493956166 T T T*

*0.6657100387235810 0.1678866592701306 0.1631017965836767 T T T*

*0.6601755394532909 0.6714897014883462 0.1629626330602907 T T T*

*0.3422061563875155 0.2958786764427335 0.8300889163110836 T T T*

*0.3455185935737800 0.7934190187663981 0.8293307979652839 T T T*

*0.8381506133305732 0.3027641590043573 0.8310234552200915 T T T*

*0.8385733896261597 0.7950364834495057 0.8287218665666957 T T T*

*0.4947839732263573 0.0480786024616882 0.4957763321433986 T T T*

*0.4936956705909181 0.5537086640083829 0.4942821322054164 T T T*

*0.9954086026685519 0.0497774017806129 0.4955137867319539 T T T*

*0.9926743580648673 0.5515609367407184 0.4946393417847407 T T T*

*0.0022229310331817 0.4885544679401081 0.0119395880772140 T T T*

*0.0043141211065647 0.9819739469697284 0.9791588781059515 T T T*

*0.4881666831365892 0.4871098537290520 0.9845301029495767 T T T*

*0.5037402655731872 0.9742744080612844 0.9837072482863555 T T T*

*0.1869813609688869 0.1383339101594697 0.6783606795680613 T T T*

*0.1675426157174252 0.6608239423981800 0.6775747673538342 T T T*

*0.6426001848822522 0.3079940613553323 0.6455190570200396 T T T*

*0.3345087213727285 0.3407670283980466 0.3149872416923759 T T T*

*0.3443712947466106 0.8159715061524784 0.3392595011653041 T T T*

*0.8330743476990774 0.3484142852090932 0.3154564769018182 T T T*

*0.8264891642720131 0.8634647861149973 0.3171866308344750 T T T*

Image 7:

**E=-232.18577294 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0051795927875537 0.4907113136924562 0.0896355398951269 T T T*

*0.0033629927550150 0.9941041472016373 0.0906405426272914 T T T*

*0.4997734779736952 0.4983948157058814 0.0959527613733025 T T T*

*0.5021375325822732 0.9922935476247999 0.0931021790830887 T T T*

*0.1813680831226477 0.1330350058700988 0.7551609434052644 T T T*

*0.1793226213129800 0.6365699995663360 0.7532602724722933 T T T*

*0.6721212734592824 0.1514583669651582 0.7611496425319547 T T T*

*0.6757209480403001 0.6371100828186079 0.7638823713419676 T T T*

*0.3372066029274721 0.3511511755549087 0.4288699999086379 T T T*

*0.3386684453851175 0.8287860714752432 0.4228570502566686 T T T*

*0.8310118450936429 0.3652970686870333 0.4240722751368871 T T T*

*0.8275288112810993 0.8754006040098194 0.4210030246989896 T T T*

*0.5007910141354488 0.9862088017655299 0.9044381784930683 T T T*

*0.4920963572404886 0.4928342657414221 0.9060501146549398 T T T*

*0.0021828281134591 0.9863407717290086 0.8993556721902296 T T T*

*0.0060364367983678 0.4831843813561383 0.8985337734025431 T T T*

*0.1674976031168995 0.1928115914527899 0.5653923892010222 T T T*

*0.1558346144126538 0.7104351805131993 0.5649841839111108 T T T*

*0.6513469315025489 0.2442374385525047 0.5679067446128048 T T T*

*0.6512334214984630 0.7267852933082255 0.5582561618929319 T T T*

*0.3290214110074324 0.3399731447065260 0.2365205714657771 T T T*

*0.3274591334940569 0.8419520225981706 0.2391027644450099 T T T*

*0.8304931784055182 0.3413320676720126 0.2353174802815492 T T T*

*0.8299840292310274 0.8409013042192330 0.2327869223538087 T T T*

*0.1676178118967990 0.1633241707684371 0.1638920241896110 T T T*

*0.1639149196539083 0.6719886583782704 0.1629393178601974 T T T*

*0.6676629080549549 0.1647355198649754 0.1635192445134368 T T T*

*0.6638083539620153 0.6710376493144478 0.1633885499205906 T T T*

*0.3399772201294717 0.3122259671369697 0.8296343164866110 T T T*

*0.3441842223082410 0.8085291205587608 0.8301012929880001 T T T*

*0.8361745835872616 0.3186910759189429 0.8305138570043467 T T T*

*0.8374043433708027 0.8092863474665252 0.8295708409944486 T T T*

*0.4934909016815326 0.0357210496927976 0.4936931116152974 T T T*

*0.4923839159259248 0.5436851946546687 0.4944927157175198 T T T*

*0.9996214401667866 0.0365709272929586 0.4943184358947044 T T T*

*0.9938309168146311 0.5372187891479340 0.4944623770549258 T T T*

*0.0054811665336180 0.4877473075423906 0.0109667427468234 T T T*

*0.0035760989524756 0.9872947177071838 0.9793502776112349 T T T*

*0.4911910874586953 0.4954757360250218 0.9848723354594492 T T T*

*0.5012587299390263 0.9854795640693161 0.9838363244361640 T T T*

*0.1829715283299985 0.1450510848530115 0.6784518556552324 T T T*

*0.1717101168690431 0.6612856271796886 0.6773736118048185 T T T*

*0.6500651807841440 0.2499876374939242 0.6446570909266750 T T T*

*0.3338094111960954 0.3388595210321127 0.3149328997114023 T T T*

*0.3353587520490150 0.8251856747866853 0.3188424245509632 T T T*

*0.8315429320447008 0.3487083592455946 0.3163071677485917 T T T*

*0.8274297795880957 0.8658950058232140 0.3392401822371648 T T T*

Image 8:

**E= -232.36037330 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0047674555401001 0.4941388185626509 0.0901013428128478 T T T*

*0.0018201001769956 0.9962992159508088 0.0924908088621217 T T T*

*0.4996600509743014 0.5000712666962928 0.0972386851203076 T T T*

*0.5036219593467879 0.9945064896435443 0.0943024935314680 T T T*

*0.1816694494164353 0.1415543277177450 0.7557360990158803 T T T*

*0.1759459961227715 0.6446905765311861 0.7550126720818151 T T T*

*0.6700478848489697 0.1595322253292370 0.7595382324058758 T T T*

*0.6777821834457087 0.6396739936032142 0.7626215632193455 T T T*

*0.3408674592907263 0.3389525816439422 0.4321051665840141 T T T*

*0.3298471955679213 0.8596960050749957 0.4235041757277620 T T T*

*0.8278316877296351 0.3615578251001513 0.4236511554484618 T T T*

*0.8326977005300245 0.8627588923550631 0.4223791985664364 T T T*

*0.5033180530530836 0.9914536040754941 0.9023811905874950 T T T*

*0.4920324885722509 0.4995567312974080 0.9066238029501041 T T T*

*0.0007780209116361 0.9955532405952707 0.8990854605031421 T T T*

*0.0053364533205204 0.4880745012640422 0.9008625885370258 T T T*

*0.1642654175185848 0.1915947319721066 0.5663381913905025 T T T*

*0.1584801372566483 0.6996647125116103 0.5715223537520010 T T T*

*0.6587437142500937 0.2004425156919140 0.5706381265926227 T T T*

*0.6484360717135421 0.7254561819247145 0.5585747723296052 T T T*

*0.3281828162205963 0.3411318132693080 0.2379162527670505 T T T*

*0.3275728051039144 0.8445021013233787 0.2387962677584741 T T T*

*0.8311804109336773 0.3423778364958832 0.2366769816696148 T T T*

*0.8295972196597916 0.8423661095029339 0.2369952742738781 T T T*

*0.1673138264818098 0.1650394695266996 0.1643830344588422 T T T*

*0.1647429956242610 0.6733496058345387 0.1643854745611566 T T T*

*0.6669299867503811 0.1683187255773350 0.1648134938647441 T T T*

*0.6638611778730391 0.6712737007836630 0.1647574986853289 T T T*

*0.3364200068316080 0.3243954610449332 0.8290449813040334 T T T*

*0.3429841550070140 0.8138716447656289 0.8294002003791472 T T T*

*0.8352377943250554 0.3267882310584805 0.8300094579440460 T T T*

*0.8396612717850980 0.8146073371172420 0.8291024205081728 T T T*

*0.4955344751401305 0.0263618911268852 0.4950390149115292 T T T*

*0.4953328150968495 0.5331320667519998 0.4968510892020802 T T T*

*0.9966998496881621 0.0317765002126909 0.4955406193997540 T T T*

*0.9930941144740645 0.5298018188997307 0.4962633168108850 T T T*

*0.0056882051952509 0.4905819674429036 0.0093428079712121 T T T*

*0.0024429165616366 0.9937957376875193 0.9773691492302511 T T T*

*0.4913348335632317 0.4996254009614572 0.9842107483423737 T T T*

*0.5049390544032381 0.9883747117972757 0.9804357570061836 T T T*

*0.1808693530188180 0.1524671091540997 0.6794685210929694 T T T*

*0.1673207428501319 0.6741552348471525 0.6533018133028803 T T T*

*0.6619295640946171 0.1873344535767749 0.6498945030479374 T T T*

*0.3350826358599214 0.3321779257012724 0.3149255664741644 T T T*

*0.3291135944333716 0.8495998402407847 0.3203685571433532 T T T*

*0.8305843223525656 0.3489664290016060 0.3199062704291561 T T T*

*0.8302433993056383 0.8518679055025700 0.3233635661782794 T T T*

Image 9 (final structure):

**E= -232.37701316 eV**

*O Ni H*

*1.00000000000000*

*5.6249584429376300 0.0009925133028124 -0.0016687085156637*

*2.8116114436452397 5.3277490293928098 -0.0265931931402940*

*0.0046736821688241 -1.5930251140906500 13.1859794143861997*

*O Ni H*

*24 12 11*

*Selective dynamics*

*Direct*

*0.0032775095780266 0.4948707732952613 0.0918055662720221 T T T*

*0.0017095281659252 0.9964668487139504 0.0901364731302792 T T T*

*0.5017231353918419 0.4947142184066919 0.0935946998358119 T T T*

*0.5023075304214473 0.9954057134972132 0.0916143445173674 T T T*

*0.1744664771387292 0.1557474185669463 0.7565313197707582 T T T*

*0.1718999787085664 0.6542165107926365 0.7585074115882193 T T T*

*0.6679844625743172 0.1662923083056782 0.7609589257571443 T T T*

*0.6738598021583826 0.6522437821523752 0.7639244429670171 T T T*

*0.3440298021755908 0.3124485985552141 0.4320163785631408 T T T*

*0.3323498346622529 0.8367588325915492 0.4214294023445007 T T T*

*0.8312717226855071 0.3343359669519046 0.4238125767763066 T T T*

*0.8356138825849868 0.8368396623527588 0.4230291403869018 T T T*

*0.4975786030300071 0.0039653692275508 0.9031087016639034 T T T*

*0.4931515073238160 0.5053203579326180 0.9074292765230964 T T T*

*0.9981018226208960 0.0063832268416277 0.9009349440497160 T T T*

*0.0006013709459154 0.4996938938109068 0.9041653519885884 T T T*

*0.1661922388567163 0.1667252522230953 0.5665692273856209 T T T*

*0.1612560625969408 0.6770329910856319 0.5694279200171550 T T T*

*0.6618556330554668 0.1719248197718883 0.5703486040647974 T T T*

*0.6505815921254268 0.6982102419632952 0.5577307528155515 T T T*

*0.3315160844698752 0.3363796211257082 0.2377540302925567 T T T*

*0.3297451503989564 0.8407349402103677 0.2355675999179923 T T T*

*0.8313831286460882 0.3376506176904144 0.2363348525224822 T T T*

*0.8298076971056361 0.8402731297573851 0.2358431100991041 T T T*

*0.1662251791625664 0.1666033510782938 0.1625771135399887 T T T*

*0.1651573339182448 0.6694089995864445 0.1628140562086244 T T T*

*0.6671225341114067 0.1665935869377293 0.1627659357582942 T T T*

*0.6662571370422654 0.6675585742446941 0.1630227162685998 T T T*

*0.3350815993601088 0.3336885018706823 0.8302287214428077 T T T*

*0.3387728010991253 0.8249356590687782 0.8307911104419148 T T T*

*0.8305953072921710 0.3355409184359246 0.8309511262053704 T T T*

*0.8344678160725820 0.8288777249028456 0.8304976841664597 T T T*

*0.4985819929889956 0.9997727964688607 0.4947914296745566 T T T*

*0.4989089192750384 0.5066977378987900 0.4957147375290276 T T T*

*0.9995520175754464 0.0055109359326835 0.4953125142959607 T T T*

*0.9953055298826072 0.5038282047479328 0.4959161349151486 T T T*

*0.0031336548821770 0.4948488131057758 0.9855019075890540 T T T*

*0.9997508539015172 0.0024438723473779 0.9808871511283286 T T T*

*0.4959843467628389 0.4998076369522906 0.9873506571696424 T T T*

*0.5001715592654108 0.9994352497966617 0.9826853942814536 T T T*

*0.1742454967742191 0.1569141089746111 0.6782008440472467 T T T*

*0.1676682120737496 0.6657595355452841 0.6487498000727854 T T T*

*0.6648787689150737 0.1647567353342154 0.6490635371766800 T T T*

*0.3405523363521823 0.3181139872981333 0.3137456911551837 T T T*

*0.3320568936314388 0.8387514508113867 0.3166798235407526 T T T*

*0.8326966288615552 0.3337489691971811 0.3175491412436742 T T T*

*0.8321896087792382 0.8374888040292845 0.3168779238708552 T T T*

**β-NiOOH- Interstitial diffusion:**  
Image 0 (initial structure):

**E= -241.85460017 eV**

*O Ni H*

*1.00000000000000*

*5.6327090269547702 0.0008000542391262 -0.0011414832133461*

*2.8152908509052401 5.3966724341578098 -0.0178429094216550*

*0.0059602050226919 -1.5922106317759899 13.1580334283355995*

*O Ni H*

*24 12 13*

*Direct*

*0.9978288597886340 0.4996108449806720 0.0931590688572844*

*0.0001784634043782 0.9940132522461800 0.0883934211614041*

*0.5011928389257773 0.4926076436645204 0.0913250390279003*

*0.5003095141313701 0.9931840781652760 0.0894896297594268*

*0.1652898773254292 0.1387965101980531 0.7633399924785705*

*0.1707572730085692 0.6307801666952620 0.7570961623107010*

*0.6727480743549888 0.1136751842966292 0.7607629047259863*

*0.6703119178770697 0.6251612350952992 0.7548004393946119*

*0.3277060428315800 0.3654451529746919 0.4285252496804140*

*0.3168439762930815 0.8653059925451300 0.4223071700303369*

*0.8270336354942921 0.3734285080496889 0.4248781526456005*

*0.8344211823819774 0.8763552970605974 0.4254158761038149*

*0.5014478646606927 0.9667656099140982 0.9023166019086400*

*0.4997005841486536 0.4709658949793626 0.8988208522894182*

*0.9994278941137328 0.9709201944220006 0.9022187351151916*

*0.9954358494627780 0.4811094331054883 0.9065701084502710*

*0.1430405023306608 0.2189962792572014 0.5754717305353124*

*0.1552812657520958 0.7102927445686441 0.5711818597447677*

*0.6673413330024435 0.2383086517238454 0.5792503774320141*

*0.6501296811859829 0.7230095973870738 0.5678632559193852*

*0.3317770097902819 0.3344350779877995 0.2341347919067643*

*0.3264905717085670 0.8403245766050550 0.2322048110873017*

*0.8301599660451786 0.3350819003859927 0.2329482834380166*

*0.8286074207895626 0.8415281560955659 0.2348211839298895*

*0.1668251504434439 0.1617937021912934 0.1613413879164500*

*0.1594780442525727 0.6729652146804718 0.1616204943391259*

*0.6689694476593261 0.1574964284266759 0.1622186193380426*

*0.6631636526889044 0.6728633558322265 0.1622672072677811*

*0.3307456547238803 0.3044438713050447 0.8321112507170080*

*0.3366310265052261 0.7960645222631524 0.8298861922408697*

*0.8340079028191758 0.3032236676458619 0.8319097575733114*

*0.8388078507602081 0.7919421511082044 0.8308401232269222*

*0.4845485563119319 0.0524527542298572 0.4975105940885723*

*0.4875847341469084 0.5460549989880138 0.4934681798097598*

*0.9896926750422420 0.0521227026804095 0.4964544947144217*

*0.9907826591917506 0.5429759307201382 0.4967283939481192*

*0.9954717492923868 0.4912352760848047 0.9895621579619794*

*0.9994577873144970 0.9795064483099872 0.9857611393615932*

*0.5003673309866761 0.4869390311978429 0.0129225308649343*

*0.5022903385788818 0.9745221173097636 0.9848034812621768*

*0.1452801584448946 0.1940951453192690 0.6513323023682231*

*0.1640699613172592 0.6773152080109912 0.6479685591705514*

*0.6703308255271833 0.1063218349360111 0.6859539705965906*

*0.6572153265102283 0.6947417332303562 0.6441596849594972*

*0.3321913028599597 0.3388453734226577 0.3124098073905252*

*0.3152190452380668 0.8523115453926625 0.3423049194729632*

*0.8323667021901798 0.3430535213290028 0.3120200712318131*

*0.8393498882214708 0.8617532290720373 0.3452559471372139*

*0.6811308461649148 0.3454183359090797 0.6375330551085153*

Image 1:

**E= -241.92395607 eV**

*O Ni H*

*1.00000000000000*

*5.6327090268820204 0.0007111593236677 -0.0010146517451965*

*2.8153764280602100 5.3966310760291698 -0.0158603639303600*

*0.0056387778312817 -1.5968894180897699 13.1574597747315991*

*O Ni H*

*24 12 13*

*Direct*

*0.9934157013114586 0.4990702308171314 0.0935351072875157*

*0.9963431189868396 0.9935136786184424 0.0888621678100691*

*0.4971035834615007 0.4918608039602162 0.0913837046932121*

*0.4959693558603289 0.9933397150272131 0.0896079430349814*

*0.1734364422501302 0.1348803336464733 0.7631545586325329*

*0.1798717320288650 0.6254818531510798 0.7570918554630326*

*0.6860231157733093 0.1060205529086555 0.7603004849088613*

*0.6765811085619399 0.6231423089442197 0.7560534501916953*

*0.3053405755808181 0.3718202342801524 0.4270468674617826*

*0.2989955808751645 0.8690106247853933 0.4222712138179654*

*0.8078146489330837 0.3756288388582572 0.4249466399745795*

*0.8137193564589220 0.8790414103731715 0.4250772931724652*

*0.5085134675546874 0.9645934954090813 0.9026980671233341*

*0.5085967679119310 0.4651690849596265 0.8984994222842791*

*0.0082770519954392 0.9661230757276267 0.9026625754737262*

*0.0032690025450711 0.4767218447047142 0.9066121378819298*

*0.1223673195175667 0.2237217641577032 0.5750764773911776*

*0.1348367706363977 0.7158691471211880 0.5708687726387685*

*0.6358902247498072 0.2393955206337969 0.5762988339120640*

*0.6326081023356124 0.7222496167990506 0.5686165564197955*

*0.3262043286745109 0.3351411989727259 0.2339510393860331*

*0.3220988221325150 0.8400651002838386 0.2322389448645917*

*0.8248330326156021 0.3351382989666859 0.2332951571324285*

*0.8232662767587752 0.8412033272799944 0.2349357159781119*

*0.1620179244828280 0.1619930424442347 0.1616272605486116*

*0.1551171124482019 0.6723365349039359 0.1618601371994584*

*0.6641430808297430 0.1576423853438058 0.1624671846024624*

*0.6585118229773803 0.6723687685247572 0.1623092370164236*

*0.3399030585451883 0.2992421032961991 0.8315490953794359*

*0.3447149858689984 0.7922681065563630 0.8305686417950735*

*0.8430316915082217 0.2987621314689720 0.8316238893177683*

*0.8471554733198913 0.7876299181448365 0.8316980053589027*

*0.4632092737031710 0.0563399474237330 0.4968815632620037*

*0.4677308551556013 0.5494788076747463 0.4928485090169913*

*0.9681640471505397 0.0560072796395951 0.4965422666768736*

*0.9705005266452463 0.5465661425364681 0.4964961144108400*

*0.9983509493751310 0.4880659856079959 0.9891818441153813*

*0.0036962642405652 0.9764293398843950 0.9865319070968912*

*0.5007421753833066 0.4838949636177250 0.0128963659036228*

*0.5044268054687814 0.9746293130202821 0.9856970443479480*

*0.1335942242939195 0.1979685508339730 0.6506508330940278*

*0.1522297639363161 0.6810637287485261 0.6470942856284131*

*0.6924465055851236 0.0813860305358569 0.6856940647521963*

*0.6484973559895623 0.6891394801609919 0.6445080262684683*

*0.3204895013913398 0.3429686438675278 0.3128000313431893*

*0.3041486382347571 0.8542628951913270 0.3420201210048032*

*0.8223263264506349 0.3442378328216564 0.3125829595076360*

*0.8233617763441357 0.8617179901927114 0.3444818610927244*

*0.6156601685715563 0.3457260202077935 0.6399439464288604*

Image 2:

**E= -241.92643137 eV**

*O Ni H*

*1.00000000000000*

*5.6327090268092599 0.0006222644082093 -0.0008878202770470*

*2.8154620052151800 5.3965897179005200 -0.0138778184390650*

*0.0053173506398715 -1.6015682044035500 13.1568861211277000*

*O Ni H*

*24 12 13*

*Direct*

*0.9940105663231233 0.4991611767080996 0.0935653069897417*

*0.9971722683491810 0.9935067860847593 0.0895867092856209*

*0.4975627335414887 0.4919403107299358 0.0913852633461435*

*0.4966527506659472 0.9936050139430135 0.0888418215962737*

*0.1778401246231221 0.1349525956052109 0.7631565423743267*

*0.1863718095700982 0.6233513200136216 0.7561423547790749*

*0.6940550922015148 0.1060310285278131 0.7602523241877578*

*0.6809297412654526 0.6254099647257564 0.7571025473266826*

*0.3030013207356100 0.3755431008138632 0.4249491417885980*

*0.3181352126989164 0.8689618462138714 0.4222603301220016*

*0.8092534086018826 0.3719197127675525 0.4269818641848491*

*0.7938527171571126 0.8789944521975296 0.4250556708002341*

*0.5117216409508696 0.9661789907226317 0.9026804771268878*

*0.5123513137120915 0.4652034817420472 0.8984942366884371*

*0.0128868909021394 0.9648848474081249 0.9026909005366694*

*0.0061914717283199 0.4768078832249093 0.9066225435394197*

*0.1400121472328690 0.2237170955496118 0.5750698515171506*

*0.1314885309842352 0.7221283647254279 0.5686868256476445*

*0.6115738510845204 0.2394310475754781 0.5761544911841648*

*0.6355659755199479 0.7159673214315994 0.5708468121893245*

*0.3264539313826712 0.3352056101932105 0.2332986946705514*

*0.3241243717474941 0.8401904674138886 0.2322254289081685*

*0.8250381336646149 0.3352418072190658 0.2339532608528523*

*0.8220300331969100 0.8413271774138810 0.2349273083852030*

*0.1624272337105589 0.1621174686232278 0.1616191198574387*

*0.1555768539033462 0.6724662548076376 0.1622842346776560*

*0.6646713699687943 0.1577538011019901 0.1624539278352770*

*0.6590113336826757 0.6724319098348479 0.1618905032831963*

*0.3443483061136945 0.2988336216618497 0.8315999888661051*

*0.3491655592606592 0.7923754914559469 0.8305943304509190*

*0.8470063087692513 0.2993093572598718 0.8315374381244021*

*0.8513398289580355 0.7877458158216588 0.8317342873002280*

*0.4621940083315519 0.0559867131354097 0.4965343141472999*

*0.4691419041848459 0.5494588790466909 0.4928503839543078*

*0.9668057400003692 0.0563341490252264 0.4968645233359101*

*0.9693345276212187 0.5465502985805418 0.4965009910381628*

*0.9999319658946170 0.4881425430274059 0.9891334369893979*

*0.0070847091196649 0.9749526375599689 0.9856921459808234*

*0.5018010224813553 0.4839557884097562 0.0128973381928345*

*0.5061225779203463 0.9765333124997689 0.9866139178432625*

*0.1543017217755799 0.1980118611258949 0.6506476354504818*

*0.1487668134350528 0.6889344580913470 0.6445708348261463*

*0.7124338759746948 0.0805897492317319 0.6856470433819480*

*0.6529795684669278 0.6811268028594343 0.6470595552897253*

*0.3198349899177684 0.3442692382116211 0.3125858515845952*

*0.3276217199725350 0.8542303274018221 0.3420096466977764*

*0.8228987702262817 0.3430773671839243 0.3128207314054771*

*0.8017677838625140 0.8616843756997031 0.3444416703549022*

*0.5274043052955376 0.3453919985378029 0.6401256167707099*

Image 3:

**E= -241.79756922 eV**

*O Ni H*

*1.00000000000000*

*5.6327090267365101 0.0005333694927508 -0.0007609888088974*

*2.8155475823701601 5.3965483597718702 -0.0118952729477700*

*0.0049959234484613 -1.6062469907173300 13.1563124675236995*

*O Ni H*

*24 12 13*

*Direct*

*0.0019068163920537 0.4943056950592192 0.0908758224363848*

*0.0044383167446020 0.9895103198079926 0.0904185331327704*

*0.5022223946224151 0.4938288508470156 0.0903844587334954*

*0.5040419848052698 0.9905652239203973 0.0899764043921300*

*0.1914095364244608 0.1375767025379229 0.7613674075393322*

*0.2012347536399494 0.6260940194993665 0.7517854707240094*

*0.7068923393977712 0.1141207319041962 0.7621867979793346*

*0.6928349232618353 0.6302560877266243 0.7548159008168204*

*0.2967809874142234 0.3768535263196233 0.4245150050418193*

*0.3145238573507854 0.8686722695157544 0.4229607016247754*

*0.8038924027581612 0.3688839378022641 0.4280870311510268*

*0.7863875750390100 0.8794184537672582 0.4258023217310578*

*0.5271934371262350 0.9651800396050738 0.9012526825650072*

*0.5236488985859196 0.4716157307808578 0.9001749928793034*

*0.0288929164964257 0.9616666695867219 0.9011268375968051*

*0.0216209996812091 0.4765677628053248 0.9025666667823929*

*0.1353086552454558 0.2222638931104650 0.5754514184865165*

*0.1242755874515681 0.7257798058589418 0.5677100884968924*

*0.5918025471604664 0.2404107940916579 0.5794152916884889*

*0.6316792674470399 0.7127812339300474 0.5710906581892757*

*0.3312013976091202 0.3342101145477467 0.2328092584051737*

*0.3315650947134489 0.8366180009247064 0.2330087971599017*

*0.8317365327315612 0.3333287223245885 0.2336779854095453*

*0.8288342682207548 0.8369362047327255 0.2338734476837378*

*0.1709426711875386 0.1558445282308619 0.1625069326551936*

*0.1629724039504583 0.6713920002253253 0.1614662653515305*

*0.6710417147661167 0.1554280201083001 0.1627166195440704*

*0.6631795193321864 0.6716504774516249 0.1607897662249121*

*0.3564183260836459 0.3028172443102349 0.8311824867753739*

*0.3633888311934731 0.7936153041648919 0.8284406323686110*

*0.8612054145389350 0.3038353632393678 0.8313990486155947*

*0.8671585596631509 0.7863456718185429 0.8294890016268883*

*0.4552072618104795 0.0552604465545474 0.4968132659368714*

*0.4635503874778626 0.5491945952672059 0.4933762311367538*

*0.9598105359737352 0.0559782507487171 0.4979059671120350*

*0.9636239362259440 0.5459563608092747 0.4967068691609366*

*0.0078031790632462 0.4905683730952424 0.0096732485033963*

*0.0232252414816497 0.9669540255178083 0.9814572114963841*

*0.5080694712882423 0.4885986890855908 0.0098358619369939*

*0.5200168581105065 0.9711829145513028 0.9816014200685492*

*0.1574186137891242 0.1954438997903078 0.6517728272912445*

*0.1464187593114411 0.6963982355812299 0.6447749641394233*

*0.7160748885680202 0.1078102610712159 0.6873844190163434*

*0.6551976024166168 0.6786518038243926 0.6486613462888787*

*0.3203445145557222 0.3458118192024793 0.3124584816471057*

*0.3298974510456639 0.8531743530766964 0.3434384637036440*

*0.8252931560982180 0.3411342931732974 0.3125015295343221*

*0.7959006001066526 0.8622538880633503 0.3464964514931988*

*0.4704389347414094 0.3488845786077739 0.6374568039984905*

Image 4:

**E= -241.16535558 eV**

*O Ni H*

*1.00000000000000*

*5.6327090266637603 0.0004444745772923 -0.0006341573407478*

*2.8156331595251300 5.3965070016432302 -0.0099127274564750*

*0.0046744962570510 -1.6109257770311101 13.1557388139198004*

*O Ni H*

*24 12 13*

*Direct*

*0.0013936655427715 0.4954779571773728 0.0910283483655263*

*0.0038040396079400 0.9910092487152630 0.0905011246833253*

*0.5016452168162034 0.4953374802374155 0.0905138742317303*

*0.5034340475685538 0.9920668366645572 0.0898066830329914*

*0.1806918590794981 0.1554262327876953 0.7624440509893107*

*0.1868965158873034 0.6457910864150047 0.7534902634049323*

*0.6947476882648569 0.1365730113272275 0.7640127285797986*

*0.6816963149000328 0.6484917241061960 0.7557760282565363*

*0.3048524396154618 0.3570266485345908 0.4237705537635849*

*0.3239658467774396 0.8472058679557322 0.4214665274520167*

*0.8125817704470030 0.3477834906968286 0.4279105254607279*

*0.7951211889837235 0.8589401112028948 0.4246770194858662*

*0.5156275148820710 0.9844818760652082 0.9019909716886230*

*0.5113378563847456 0.4923363266155126 0.9013929253083036*

*0.0173069404230983 0.9816710190628327 0.9022020935031418*

*0.0101959208670763 0.4960225693983119 0.9035348384668200*

*0.1433641032686089 0.2014261060940450 0.5747747926936855*

*0.1316810926365001 0.7082790002590434 0.5664362464581045*

*0.5919775633472260 0.2226273654456216 0.5789869780106078*

*0.6393175519037539 0.6943706834042037 0.5697168181167369*

*0.3317218133242266 0.3335944228144700 0.2330337992956989*

*0.3315890719656521 0.8370036739131345 0.2328823167858008*

*0.8322939858388338 0.3325660206563870 0.2341179774924896*

*0.8290002116169527 0.8371707779573413 0.2337344305291685*

*0.1708470805480613 0.1564345341939229 0.1625794437827429*

*0.1628477252147212 0.6720446661947560 0.1615171212073209*

*0.6709073410738480 0.1560236298847719 0.1627826410078486*

*0.6629531775192806 0.6725006496534404 0.1607983032198202*

*0.3445138694942507 0.3232735580351646 0.8320755499931347*

*0.3511185182695228 0.8134117879210385 0.8290702587759715*

*0.8492938793720592 0.3243403443509996 0.8324947988986358*

*0.8547137090133881 0.8069346355822558 0.8303610306730589*

*0.4638449213196204 0.0328941468891417 0.4955100452407457*

*0.4717050808529576 0.5297081624822252 0.4926653200240475*

*0.9687787340719304 0.0347386147392922 0.4966059637237820*

*0.9721249160974850 0.5257091492225617 0.4962951903311102*

*0.0031754887564719 0.4987198802629322 0.0102301931947368*

*0.0157052684572822 0.9803445347024827 0.9822964868692998*

*0.5030817028363788 0.4974091500154617 0.0101252449881064*

*0.5123192979088032 0.9840080552299426 0.9822426913665113*

*0.1599235832347122 0.1844135381995262 0.6530535698670905*

*0.1471067519393658 0.6919663201800940 0.6454112680344294*

*0.7049449932852787 0.1310526889025163 0.6888754081268854*

*0.6564147760226593 0.6731530729832303 0.6494128693292094*

*0.3236680488968529 0.3381997914551904 0.3127147508097194*

*0.3358532939785981 0.8394074206353362 0.3419847710628762*

*0.8292036125750664 0.3326108669824832 0.3126543700723442*

*0.8022315579741737 0.8490914662630795 0.3454570004825747*

*0.4478842437533310 0.3295530656649566 0.6302239334844020*

Image 5:

**E= -241.68298830 eV**

*O Ni H*

*1.00000000000000*

*5.6327090265910105 0.0003555796618339 -0.0005073258725983*

*2.8157187366801102 5.3964656435145804 -0.0079301819651800*

*0.0043530690656408 -1.6156045633448799 13.1551651603158000*

*O Ni H*

*24 12 13*

*Direct*

*0.0019767181374470 0.4951096603371062 0.0912417405116632*

*0.0034253748417726 0.9929042009972167 0.0895159770494950*

*0.5024158263716637 0.4952782760101679 0.0912388495240738*

*0.5032661047348027 0.9937231654124469 0.0885423022129277*

*0.1718070731524375 0.1629215494957691 0.7587969614938851*

*0.1763267641823895 0.6552280558893898 0.7560365346632547*

*0.6807322450403384 0.1532075754077757 0.7641866721365450*

*0.6746228930764824 0.6553895806096934 0.7574362413251163*

*0.3188509301582330 0.3474548565293598 0.4220808337720016*

*0.3366213886855759 0.8348316350140241 0.4203031023163470*

*0.8238621457926213 0.3369929732042281 0.4277692969428335*

*0.8104900374404249 0.8477843851779444 0.4243088445614744*

*0.5048051441249132 0.9945431443848852 0.9017085300157148*

*0.5023217757468970 0.5012672059008116 0.9030284402871043*

*0.0078165531343626 0.9935214369279124 0.9020374974574052*

*0.0023041222533387 0.5032207617779612 0.9026723996452168*

*0.1599654801337454 0.1932475483012498 0.5728592496659125*

*0.1422261508885684 0.7006452282289980 0.5655392129912559*

*0.5924573225172348 0.2191714104452682 0.5811091797681227*

*0.6519826086118349 0.6846486044751333 0.5684524769326612*

*0.3329354233286437 0.3327930723661855 0.2330897854190407*

*0.3315028035464603 0.8384582175890175 0.2318059841365402*

*0.8335291208391645 0.3319240820721195 0.2345342866256032*

*0.8296066219048054 0.8383366270497458 0.2325833317160104*

*0.1714149521881620 0.1567998143454473 0.1623280877590886*

*0.1633167677797106 0.6726184879585502 0.1612219347399879*

*0.6712876161886826 0.1566513681992277 0.1624835280322842*

*0.6632077886115935 0.6734038301981815 0.1605870997382210*

*0.3353973245931193 0.3350799146746026 0.8315008919318606*

*0.3434564766441157 0.8193155018866880 0.8302298043038574*

*0.8372762170335643 0.3360730631917941 0.8318384968277434*

*0.8444631729852899 0.8180587149353800 0.8309117140295097*

*0.4766769157784694 0.0217083707125364 0.4931669718476998*

*0.4836422338067783 0.5199736079695479 0.4925821465628926*

*0.9826513384479263 0.0263652919227642 0.4961219045171301*

*0.9866816885918285 0.5123824543490060 0.4959658513505707*

*0.0007409915942077 0.5006537227539775 0.0118924070150999*

*0.0082787126313730 0.9901076171300386 0.9826674009576947*

*0.5006596007356173 0.5000991032371185 0.0115390426462760*

*0.5049655542293421 0.9919014730710515 0.9828253564226060*

*0.1645432172570072 0.1770303282431646 0.6767428156573480*

*0.1520532827867663 0.6897943077900358 0.6438026508190570*

*0.6801417650673075 0.1606133917930454 0.6879900857140078*

*0.6613258095461337 0.6688479407911712 0.6470398952866462*

*0.3289131743753351 0.3352380887576664 0.3137889345502246*

*0.3428916644546303 0.8322675816953125 0.3418594508848706*

*0.8336634150187213 0.3283229058085746 0.3131162522834680*

*0.8137327173990472 0.8422739269285903 0.3459805796952788*

*0.4141588812754172 0.3024374599458848 0.6165791058853326*

Image 6:

**E= -241.89553240 eV**

*O Ni H*

*1.00000000000000*

*5.6327090265182598 0.0002666847463754 -0.0003804944044487*

*2.8158043138350801 5.3964242853859297 -0.0059476364738850*

*0.0040316418742306 -1.6202833496586599 13.1545915067119008*

*O Ni H*

*24 12 13*

*Direct*

*0.0016357459980902 0.4953745618181986 0.0913898357415853*

*0.0032848166403573 0.9933201674518712 0.0899844390670110*

*0.5028499577100438 0.4953738870194554 0.0913920054555157*

*0.5028674809375214 0.9941133926902809 0.0887780184756944*

*0.1672987824116276 0.1625024834921089 0.7623546260754311*

*0.1702861298136605 0.6592840729549836 0.7573496081361910*

*0.6700641948022105 0.1625075867781298 0.7623263899848198*

*0.6707428241910088 0.6583637373479244 0.7575843014796949*

*0.3259757231292591 0.3480471983181974 0.4210968980740994*

*0.3382110709107087 0.8373488962716307 0.4215709983422322*

*0.8329556803924437 0.3341654276084268 0.4300607267768121*

*0.8245735502533817 0.8373314305871801 0.4215452690614702*

*0.5010706765282716 0.9976174044880289 0.9020631448431657*

*0.4967038882132266 0.5059857999971691 0.9035595170842662*

*0.0010751336752640 0.9976110903981500 0.9024717909170605*

*0.9970019472686462 0.5060055624772012 0.9035608577194200*

*0.1866698459205970 0.2093457866613610 0.5776154099399945*

*0.1483942800774713 0.7031861202042906 0.5664142410759984*

*0.6036307374371491 0.2092450613105707 0.5776210232482690*

*0.6593539342142585 0.6811216811269268 0.5686727048252447*

*0.3331876361161385 0.3333259000098081 0.2330144125613920*

*0.3312604343169367 0.8383089803991777 0.2322638129653057*

*0.8336878250240063 0.3323717147243351 0.2352592011949267*

*0.8301154089981783 0.8383567884513675 0.2322309556763422*

*0.1714613349111726 0.1570951587878413 0.1627405463382894*

*0.1636272628990212 0.6725482924675105 0.1611505383219494*

*0.6712299901418303 0.1571141338173931 0.1627308056640585*

*0.6630007959983241 0.6737603728789463 0.1607656391656998*

*0.3302465283011454 0.3392793555241330 0.8324063534852196*

*0.3384368682389343 0.8224179963927036 0.8309742679344727*

*0.8297613951815374 0.3402695210426754 0.8322640128902175*

*0.8389601069282840 0.8224116764820310 0.8309838180747352*

*0.4927307265780042 0.0144546932667977 0.4884785801297176*

*0.4917878280219284 0.5145452921650079 0.4953537186817384*

*0.9858903639089289 0.0284770258237714 0.4993357042721686*

*0.9936356200559512 0.5146185341878623 0.4953528452533325*

*0.9987778275765820 0.5015784308695931 0.0117681841853917*

*0.0035550533259221 0.9926896281674680 0.9827707668947097*

*0.4994731273097794 0.5015855909272982 0.0117546671313182*

*0.5030901281866058 0.9935532887902933 0.9830268606380270*

*0.1652608711476666 0.1767180490567658 0.6843698657068282*

*0.1561622407014957 0.6875023109342151 0.6441868112347191*

*0.6581024358166571 0.1766239392818146 0.6844095361704738*

*0.6658899192101421 0.6680377071825747 0.6478563021946915*

*0.3311798784293949 0.3373760924110388 0.3143083555605814*

*0.3404791187196518 0.8338037887610084 0.3429976892989707*

*0.8363662531983006 0.3270651997882498 0.3132647217300747*

*0.8256706022548712 0.8338036666670379 0.3429596259332822*

*0.3737178842935481 0.2530770384327406 0.5992497350163675*

Image 7:

**E= -241.93071429 eV**

*O Ni H*

*1.00000000000000*

*5.6327090264455100 0.0001777898309169 -0.0002536629362991*

*2.8158898909900500 5.3963829272572896 -0.0039650909825900*

*0.0037102146828204 -1.6249621359724400 13.1540178531079004*

*O Ni H*

*24 12 13*

*Direct*

*0.0020278923767571 0.4953394733082677 0.0912946021151109*

*0.0034082998578498 0.9930953204592640 0.0895891505261404*

*0.5027457564494392 0.4951590615228646 0.0912977547263826*

*0.5027728700115769 0.9938791109250794 0.0885760792772607*

*0.1658355517827405 0.1557418718237724 0.7641865499631029*

*0.1686720228210261 0.6567148129110519 0.7563808344264265*

*0.6658322404260383 0.1635360188337637 0.7593393924512906*

*0.6699690966977886 0.6566182780241653 0.7575757563393535*

*0.3325321551072218 0.3465290967657075 0.4218733212547611*

*0.3410382902865911 0.8456770601930055 0.4238823734151881*

*0.8386378221446452 0.3358130352793651 0.4279685318494355*

*0.8282942655930393 0.8334987477526443 0.4201682615364434*

*0.5004954988926587 0.9958425740023604 0.9018481881070185*

*0.4945536202111813 0.5044434966598209 0.9028855187357294*

*0.9987206177709648 0.9950375375435002 0.9021970031757703*

*0.9961892820151305 0.5029582634437979 0.9032672272167366*

*0.1880862740506614 0.2189172020413156 0.5811922757276766*

*0.1560715871028977 0.7000632595447579 0.5655607514085800*

*0.6440154140828516 0.1927790163733464 0.5724310801891803*

*0.6623559033021970 0.6836140422539310 0.5683820595102853*

*0.3338413476916708 0.3328748206443922 0.2331131168215269*

*0.3316221624592510 0.8383508411840027 0.2325326452862451*

*0.8341560919334811 0.3320178469707257 0.2346627073172620*

*0.8297375827475371 0.8385071887870585 0.2318119781471721*

*0.1717167544495949 0.1568032185513722 0.1625344549295850*

*0.1637633496717319 0.6726337291216778 0.1612159478042656*

*0.6714510609307952 0.1569272950393462 0.1624021929741290*

*0.6630857880995210 0.6734881025623832 0.1606202463740404*

*0.3293311588552877 0.3366749710239103 0.8317478601604615*

*0.3374105293992058 0.8196172767742125 0.8310194609553614*

*0.8268257848477861 0.3376369837463514 0.8320454031845340*

*0.8373246816520680 0.8205846929213182 0.8304366433076875*

*0.5007842614636768 0.0197473543474477 0.4923420260304635*

*0.4999506397033709 0.5113642320445502 0.4958541814534659*

*0.9901925006262117 0.0253745634869090 0.4961849569943039*

*0.9957831316132093 0.5187332070052595 0.4928653938524340*

*0.9989652151727714 0.5007121312631856 0.0116127859731858*

*0.0016352616711284 0.9911280004738612 0.9827986681660691*

*0.4985832524172708 0.5010611801479091 0.0119516448195609*

*0.5029218543252820 0.9926956248502546 0.9829737946424878*

*0.1588337446441725 0.1649331939461137 0.6878186719475022*

*0.1577385795408590 0.6891301604904586 0.6437907000677124*

*0.6587090051649367 0.1765934239079913 0.6782826384158784*

*0.6689827899686550 0.6687112137365948 0.6470420405660152*

*0.3349244497325660 0.3352107810584231 0.3139356854207579*

*0.3431499088559611 0.8405617606733407 0.3455018083932131*

*0.8376610701277157 0.3279516896974571 0.3131892025023127*

*0.8249919758289436 0.8314119192816498 0.3417460946193008*

*0.2950630864251722 0.2939267848340422 0.6137104775503870*

Image 8:

**E= -241.92561316 eV**

*O Ni H*

*1.00000000000000*

*5.6327090263727495 0.0000888949154585 -0.0001268314681496*

*2.8159754681450302 5.3963415691286398 -0.0019825454912950*

*0.0033887874914102 -1.6296409222862200 13.1534441995039995*

*O Ni H*

*24 12 13*

*Direct*

*0.0022488404474120 0.4958572406460445 0.0906035380857127*

*0.0044032423556342 0.9917049347075183 0.0905204937391118*

*0.5024937484965799 0.4958792297182057 0.0910721738036256*

*0.5037074310526967 0.9927154473900525 0.0897365804992030*

*0.1669945889531180 0.1439680219257342 0.7644814133656549*

*0.1667286473667448 0.6519446120270699 0.7541174206752368*

*0.6632522274804508 0.1605859056889501 0.7625230376136732*

*0.6689580092585506 0.6537626943395225 0.7560556467656309*

*0.3384216388728348 0.3512804096001925 0.4235893458389022*

*0.3460776210251071 0.8527193049879450 0.4242441962886286*

*0.8403074766412593 0.3415299378003350 0.4280221257289464*

*0.8293881460111767 0.8406024659199579 0.4209490408831441*

*0.4989727922507517 0.9900698147608930 0.9021979631019457*

*0.4927611304320190 0.5015164067697658 0.9037463562876528*

*0.9997599361693175 0.9877891327062763 0.9025015178044362*

*0.9950930512309382 0.4984132588796067 0.9018642314817785*

*0.1879949419043974 0.2181262305972124 0.5790865823990332*

*0.1598434320181466 0.7032678804766030 0.5661889493756359*

*0.6555891381788836 0.1949524399890583 0.5749026207894701*

*0.6662238975000643 0.6889531018290987 0.5693798718239942*

*0.3339604172458683 0.3335755190842612 0.2331541255077280*

*0.3328754758935995 0.8374534095314771 0.2336515445101530*

*0.8344244045284860 0.3325241628766036 0.2343382087600545*

*0.8305398097713239 0.8373356679121802 0.2328233995315609*

*0.1722819182188972 0.1564069189853835 0.1628339244921024*

*0.1643147761613056 0.6723961273740579 0.1615125121601634*

*0.6719425216848760 0.1567920966830221 0.1626291727153316*

*0.6637169337975974 0.6729398474575609 0.1607980058216368*

*0.3309234077197219 0.3294540407235379 0.8323166407782182*

*0.3371889026147604 0.8131298500354622 0.8305887602392611*

*0.8252071897191614 0.3304681189968274 0.8327594382096086*

*0.8345757392584892 0.8191647154048571 0.8293105088020282*

*0.5042278531497880 0.0258831930783663 0.4949616496167559*

*0.5025211887436483 0.5196655467325998 0.4962563836674875*

*0.9967233929166787 0.0284770369208134 0.4961843163090881*

*0.9988167417133484 0.5239772163269166 0.4926476155690607*

*0.9985700980932989 0.4999545247446488 0.0102653098328107*

*0.0029226764915868 0.9845683265683520 0.9824883719145465*

*0.4973920311727071 0.5009513889531775 0.0104453207522709*

*0.5029162209495263 0.9876922302695018 0.9824215855902992*

*0.1610809536228960 0.1406337373229530 0.6892266932481890*

*0.1599725631012290 0.6909905397601622 0.6456829884614435*

*0.6571814976597316 0.1806177204638046 0.6543065784370860*

*0.6699098157005920 0.6716925739552101 0.6496657167599686*

*0.3376881065951968 0.3362318306269786 0.3128650883197164*

*0.3479789032146232 0.8451132160145652 0.3450732481424033*

*0.8380467471335530 0.3302423830168256 0.3127331958309238*

*0.8248939977044718 0.8353050214158516 0.3415231539049340*

*0.2393797113066712 0.3213463446842485 0.6263935763917131*

Image 9 (final structure):

**E= -241.90953166 eV**

*O Ni H*

*1.00000000000000*

*5.6327090262999997 0.0000000000000000 0.0000000000000000*

*2.8160610453000001 5.3963002109999998 0.0000000000000000*

*0.0030673603000000 -1.6343197086000001 13.1528705459000008*

*O Ni H*

*24 12 13*

*Direct*

*0.0027356596123252 0.4903328303900839 0.0902484674753437*

*0.0050616630770767 0.9856095553268888 0.0905310405687955*

*0.5026720505340330 0.4906027550888747 0.0908180698535833*

*0.5043490824356502 0.9866827978796370 0.0899461003101545*

*0.1691321829949327 0.1274990559684147 0.7633485156194543*

*0.1656445384851825 0.6384869182148124 0.7527222007415921*

*0.6627542859126837 0.1492658146645990 0.7621588652574105*

*0.6687716620750704 0.6422841244364512 0.7553955445989176*

*0.3328667081713237 0.3675395536655250 0.4240273101868905*

*0.3411079644380440 0.8694253305555895 0.4251509140268185*

*0.8340772913917774 0.3591174660464808 0.4277786762541612*

*0.8236415621597726 0.8586982920967905 0.4221770213836447*

*0.4990259440962561 0.9773060325727868 0.9019154744901060*

*0.4930010549662375 0.4889855141728978 0.9032020322559092*

*0.0005827248707211 0.9738995690456134 0.9019683070897412*

*0.9957221303175192 0.4846124335306240 0.9008266820308418*

*0.1760881480173552 0.2315919680913447 0.5788754222706876*

*0.1555628943521667 0.7176397210660633 0.5669864888381987*

*0.6491692029201996 0.2131423210297344 0.5746395056700691*

*0.6614141431116287 0.7045767343731855 0.5703082264560507*

*0.3339611944871028 0.3295039921161129 0.2328182674338439*

*0.3335996247473264 0.8322286401887693 0.2338270655671016*

*0.8343594763814324 0.3285955808362833 0.2337336698164354*

*0.8311005097729252 0.8319853679441036 0.2329286779006208*

*0.1727529873448173 0.1510564211770606 0.1628090583347216*

*0.1648289304314600 0.6670171154530578 0.1614910952191536*

*0.6723343734296569 0.1514868224345962 0.1625972931735226*

*0.6643031290741213 0.6673545659191589 0.1607899508620204*

*0.3317776575189162 0.3157600709813912 0.8317492901370828*

*0.3377921776254983 0.7992885998154750 0.8301423386566724*

*0.8258514503353702 0.3168492146562468 0.8321244935704619*

*0.8344156234853722 0.8063784570543228 0.8288823300675897*

*0.4969334203936234 0.0449047610871111 0.4960328645660161*

*0.4968508527683253 0.5366464613350214 0.4963575674717414*

*0.9911969654086790 0.0460015136037865 0.4970891750242041*

*0.9935638702559848 0.5402293986213869 0.4928650813904640*

*0.9990661430002108 0.4915380635399040 0.0098943532114008*

*0.0036918436383997 0.9731427625073440 0.9820828899843952*

*0.4974331466079914 0.4932232851288067 0.0099681556064211*

*0.5029826490886247 0.9773561532175518 0.9820460330288614*

*0.1665668315647144 0.1188865132200250 0.6883996542878555*

*0.1582743133626016 0.6951059029137294 0.6450770984063330*

*0.6494608561438078 0.1922903162385707 0.6517282183103217*

*0.6669231153396928 0.6777721714858770 0.6490451683040379*

*0.3356416910343975 0.3394672163333153 0.3125345812428018*

*0.3463907632725389 0.8539147797377116 0.3457953013065337*

*0.8354096886416982 0.3345304316031543 0.3125660089906860*

*0.8213973572708094 0.8446841252048954 0.3425806676949269*

*0.1960679356339764 0.3406443524288481 0.6346589880554054*

**β-Ni(OH)2- Exchange diffusion:**  
Image 0 (initial structure):

**E= -194.35572870 eV**

*H O Ni*

*1.00000000000000*

*6.2244331736972303 0.0000000000008084 0.0000000000000000*

*-3.1122165868972300 5.3905172526041900 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209889636794*

*H O Ni*

*15 16 8*

*Direct*

*0.1666666420000027 0.3333332839999983 0.7187631235861858*

*0.1943344265249181 0.8471671462624641 0.2150495412655573*

*0.1833555194840031 0.8416776927420031 0.7102789604995650*

*0.6528327347375296 0.3056654994750829 0.2150495412655573*

*0.6583221882579977 0.3166444065159979 0.7102789604995650*

*0.6528327347375296 0.8471671462624712 0.2150495412655573*

*0.6583221882579977 0.8416776927420031 0.7102789604995650*

*0.2961318443521819 0.2038680816478191 0.2854578920652315*

*0.3278467269271843 0.1721531990728167 0.7855884948132399*

*0.2961318443521819 0.5922637477043651 0.2854578920652315*

*0.3278467269271843 0.6556935128543557 0.7855884948132399*

*0.9077361332956286 0.2038680816478191 0.2854578920652315*

*0.8443063681456451 0.1721531990728167 0.7855884948132399*

*0.8333332540000029 0.6666666269999979 0.2858442618406301*

*0.8333332540000029 0.6666666269999979 0.7957346806792174*

*0.1666666420000027 0.3333332839999983 0.1139561682097607*

*0.1666666420000027 0.3333332839999983 0.6137197007890336*

*0.1694646596081597 0.8347322628040743 0.1105211661322301*

*0.1713511277031117 0.8356754968515574 0.6054166550203419*

*0.6652676181959265 0.3305352663918484 0.1105211661322301*

*0.6643243841484434 0.3286487982968893 0.6054166550203419*

*0.6652676181959265 0.8347322628040743 0.1105211661322301*

*0.6643243841484434 0.8356754968515574 0.6054166550203419*

*0.3284199789161875 0.1715799470838135 0.3847090351033842*

*0.3328711843494574 0.1671287416505436 0.8906927741079258*

*0.3284199789161875 0.6568400168323905 0.3847090351033842*

*0.3328711843494574 0.6657424276989161 0.8906927741079258*

*0.8431598641676104 0.1715799470838135 0.3847090351033842*

*0.8342574533010847 0.1671287416505436 0.8906927741079258*

*0.8333332540000029 0.6666666269999979 0.3910569317121855*

*0.8333332540000029 0.6666666269999979 0.9012157169686644*

*0.0039080731638421 0.0078161463276700 0.0070557628820396*

*0.0009095572633626 0.0018191145267181 0.4991297480942762*

*0.0039080731638421 0.4960919268361579 0.0070557628820396*

*0.0009095572633626 0.4990904427366374 0.4991297480942762*

*0.5000000000000000 0.0000000000000000 0.9983956295771392*

*0.5000000000000000 0.0000000000000000 0.4865522076858042*

*0.4921838536723300 0.4960919268361579 0.0070557628820396*

*0.4981808854732819 0.4990904427366374 0.4991297480942762*

Image 1:

**E= -194.36268406 eV**

*H O Ni*

*1.00000000000000*

*6.2244331280177798 0.0000000000006467 0.0000000000000000*

*-3.1122165640377801 5.3905172130233501 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209824509406*

*H O Ni*

*15 16 8*

*Direct*

*0.1708518086844853 0.3387135032237246 0.7174158740880349*

*0.2051059153216379 0.8258551817739773 0.2174906118114110*

*0.1874365700786862 0.8398325508543969 0.7089042647042506*

*0.6573400790442017 0.3125156978554766 0.2179241827766774*

*0.6543337128430866 0.3187328382205131 0.7090461423769530*

*0.6439204376153670 0.8384795562621614 0.2172648940879591*

*0.6569990814460442 0.8417742422320389 0.7079395224713546*

*0.2966630047225013 0.1897059414825820 0.2840665395794434*

*0.3215423384737767 0.1671572167095667 0.7899074485809582*

*0.2846384528486188 0.5664204282200325 0.2841915307598905*

*0.3331845746792484 0.6588070199985134 0.7858917178043161*

*0.9010527248039178 0.1990517631856760 0.2846455250636490*

*0.8487517450216789 0.1776238849537236 0.7889592503941214*

*0.8424199421147234 0.6768815560920265 0.2849708065458703*

*0.8419415014731494 0.6687635690304500 0.7988921870629082*

*0.1702646402606978 0.3390313597172878 0.1163680935377401*

*0.1662615940616849 0.3336725931395383 0.6124122194194020*

*0.1731109756243877 0.8305417720356622 0.1143460199243620*

*0.1713496576149814 0.8347210402698926 0.6042909497096639*

*0.6671449977982721 0.3315079817768767 0.1129851269401783*

*0.6634374067678280 0.3299171080902756 0.6042015157276960*

*0.6673005086006136 0.8342619135577247 0.1130937331222888*

*0.6621155931715884 0.8350701686102675 0.6031050317925272*

*0.3282905934005486 0.1689498568564211 0.3853960841664176*

*0.3335232504135980 0.1669383826319842 0.8947833338275660*

*0.3236567722037655 0.6506772050936156 0.3792109608877708*

*0.3364132949364275 0.6667114573070076 0.8910131969039070*

*0.8406864829855474 0.1701564630411703 0.3846727832758199*

*0.8380306771794652 0.1692363952082626 0.8939889368088454*

*0.8336536675647190 0.6677895233032695 0.3900958264825830*

*0.8380288681991979 0.6675236733259645 0.9042719365768312*

*0.0071223957795671 0.0088941994808685 0.0122099458687230*

*0.0000035910850402 0.0013435718589100 0.4988679711913916*

*0.0068868143099999 0.4973334664253470 0.0087408568404183*

*1.0000084145127619 0.4986177917640799 0.4977299869920421*

*0.5026165194193357 1.0001217602475414 0.0005698931086157*

*0.4987499141760711 -0.0007727739221937 0.4852863539952160*

*0.4953693040261059 0.4977480457963148 0.0088718692812034*

*0.4967182015035164 0.4987476269159324 0.4966296369682314*

Image 2:

**E= -194.29383318 eV**

*H O Ni*

*1.00000000000000*

*6.2244330823383400 0.0000000000004850 0.0000000000000000*

*-3.1122165411783400 5.3905171734425101 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209759382106*

*H O Ni*

*15 16 8*

*Direct*

*0.1784495052046480 0.3452073224728429 0.7146031654299342*

*0.2139768768331397 0.8041877937527054 0.2193045341664234*

*0.1891837152654778 0.8381164801814465 0.7080663395126722*

*0.6601903771815660 0.3189249783937066 0.2210535495852325*

*0.6509750842332930 0.3204115559330296 0.7086959300390634*

*0.6383697349288400 0.8303202983149781 0.2185662569495764*

*0.6559692946937202 0.8380930235717506 0.7062181495741637*

*0.2992689927061652 0.1739843628219636 0.2828244537751601*

*0.3164140842931654 0.1619552590763772 0.7943848420118597*

*0.2739633167789674 0.5463732950694649 0.2813739832750918*

*0.3364971559908131 0.6636533661598267 0.7864856398003718*

*0.8915022383885490 0.1926792671601404 0.2838947791394009*

*0.8556966263648624 0.1875678906244636 0.7932684213590943*

*0.8515266078725809 0.6836721519763279 0.2841704697641710*

*0.8526117963870434 0.6667765365208843 0.8019566067102313*

*0.1705642040394773 0.3448851073579267 0.1184718992637354*

*0.1667557795320982 0.3342961050501297 0.6098675576872761*

*0.1760333293831826 0.8254425378733562 0.1189231547390430*

*0.1713507298125471 0.8337060720701900 0.6035996773897833*

*0.6672605503271081 0.3320485863114632 0.1158213261777142*

*0.6630581300774889 0.3312870436323350 0.6038966786213118*

*0.6693517064836639 0.8344687652128887 0.1147440517930528*

*0.6602630958751892 0.8337335542584121 0.6012753679010786*

*0.3286201281081017 0.1661648692849829 0.3859243195448929*

*0.3341223500058262 0.1665446022637891 0.8989592205376692*

*0.3184602155898762 0.6455876389093942 0.3725287502892439*

*0.3397908376120273 0.6689064182043380 0.8916184956844366*

*0.8375915727563261 0.1678800186649730 0.3850368210359150*

*0.8417014878911068 0.1734252616537054 0.8980495269739706*

*0.8336651425672864 0.6680483346667229 0.3889075946353159*

*0.8440884444656962 0.6673531656089541 0.9071703366760669*

*0.0098194755760736 0.0101853406560245 0.0165950358715694*

*0.9992101725836997 0.0004100204402804 0.4983012113240333*

*0.0091159849042013 0.4987954958007939 0.0108853326598480*

*0.9992876119325433 0.4982219897892136 0.4959250820482157*

*0.5045554312541268 0.0005253308039054 0.0036923896470553*

*0.4982734684891268 -0.0008825522153104 0.4857932434736996*

*0.4976672213837443 0.4993508586307938 0.0104010884707989*

*0.4955860386765652 0.4988846712303299 0.4932950963811591*

Image 3:

**E= -194.17499271 eV**

*H O Ni*

*1.00000000000000*

*6.2244330366588896 0.0000000000003234 0.0000000000000000*

*-3.1122165183188901 5.3905171338616800 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209694254701*

*H O Ni*

*15 16 8*

*Direct*

*0.1848672596436022 0.3510369495207436 0.7116393514792319*

*0.2201381943408091 0.7814227842669088 0.2217720827254756*

*0.1903279378561827 0.8371493813109867 0.7071038285385601*

*0.6619690311022965 0.3231270150284176 0.2235788426889601*

*0.6482968569215155 0.3205755573233683 0.7091997296848290*

*0.6365721257790444 0.8254712990627959 0.2188520667896820*

*0.6536956482991244 0.8336942065152217 0.7050292460973482*

*0.3029778050652993 0.1639143062682988 0.2821806059128548*

*0.3127270892689802 0.1579603974695104 0.7980770589152302*

*0.2636932141520591 0.5309106872215263 0.2759175204606112*

*0.3375593248675416 0.6669112865745870 0.7868369961771875*

*0.8835274320752065 0.1877413616845346 0.2833126316633133*

*0.8639129516240280 0.2006386238450264 0.7983522875376207*

*0.8579050639758981 0.6871591115453723 0.2838693244309662*

*0.8627769024420623 0.6618548110216830 0.8047039440444769*

*0.1639791333783971 0.3528705361995767 0.1192556741885302*

*0.1679306837569702 0.3361032091896091 0.6073415411283659*

*0.1757186223563358 0.8139933406403307 0.1235998202158895*

*0.1720094118588961 0.8334857852716175 0.6027767947292672*

*0.6656208360884637 0.3313925572482050 0.1181877104604662*

*0.6634114593644931 0.3321677845413123 0.6045872476245573*

*0.6718871368848314 0.8362709043733573 0.1153099770565395*

*0.6590531270698503 0.8326713953373336 0.6001594406353683*

*0.3293492337278497 0.1655053736142222 0.3859599680570863*

*0.3343154943204620 0.1656801416917472 0.9024185553476403*

*0.3116291090834932 0.6423232227693302 0.3635236368016362*

*0.3431119385278243 0.6714341070049794 0.8919562550685376*

*0.8349834558867579 0.1661132421662762 0.3852585240188006*

*0.8472591950499888 0.1825730987420899 0.9030664426074920*

*0.8329865336552120 0.6683481808301163 0.3880279126493096*

*0.8525572276987812 0.6641199632090103 0.9098851720022921*

*0.0115133072752795 0.0107835974844000 0.0201403663231387*

*0.9988686843142563 0.0001665367361946 0.4976627000222618*

*0.0114342382080296 0.5000985990955911 0.0130290659696319*

*0.9989520273972593 0.4985425495021867 0.4936640646101513*

*0.5051918543699837 0.0004614915510675 0.0070983740665612*

*0.4989757249106984 0.0004133617577546 0.4868866391130265*

*0.4991197090870661 0.5008035191550146 0.0116787780768249*

*0.4952454461900029 0.4998674373280181 0.4904653486481821*

Image 4:

**E= -193.90719919 eV**

*H O Ni*

*1.00000000000000*

*6.2244329909794498 0.0000000000001617 0.0000000000000000*

*-3.1122164954594500 5.3905170942808400 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209629127402*

*H O Ni*

*15 16 8*

*Direct*

*0.1867166549631950 0.3558517249121381 0.7083843464899943*

*0.2292707956708348 0.7621723118385941 0.2324762703305361*

*0.1899932238823653 0.8355418310660255 0.7061800444456016*

*0.6599903952235603 0.3251537609992329 0.2248358021877645*

*0.6483029178422257 0.3206487133969747 0.7105477513511977*

*0.6365276304044737 0.8226332231437438 0.2188070051383289*

*0.6515362698941749 0.8309696955777817 0.7040082874912130*

*0.3052040474803943 0.1609597258228442 0.2824721552084615*

*0.3107856854024090 0.1577973017982705 0.7990400319997835*

*0.2514084009486131 0.5136010855461264 0.2649010469191648*

*0.3391616352792590 0.6690294587820128 0.7867830575079737*

*0.8779244541974508 0.1846238684200106 0.2832907804701055*

*0.8675858509299609 0.2055965722087874 0.8024854008228297*

*0.8631570166338823 0.6884419606924611 0.2840118476164865*

*0.8643619508746870 0.6605838879985522 0.8050670372356914*

*0.1667843482698755 0.3573004686486766 0.1217360731568087*

*0.1708329956082158 0.3398550654214350 0.6040526536492580*

*0.1756446398866613 0.8078508566833089 0.1302576668491256*

*0.1727806061343518 0.8338689783447518 0.6018079984594391*

*0.6635653773632259 0.3314301640290453 0.1194704165765774*

*0.6647927006278772 0.3325382978597082 0.6059368643165770*

*0.6742850500201876 0.8378637359736827 0.1154760595243911*

*0.6580804190811482 0.8314885777735618 0.5990889928362156*

*0.3308336269609863 0.1672863850484504 0.3865234136537583*

*0.3347846283048905 0.1671568835547703 0.9032623029251926*

*0.2977155842719599 0.6426519532643784 0.3480152673099808*

*0.3458469627776131 0.6737427168011392 0.8918827730531448*

*0.8331054417513821 0.1652035857938150 0.3857110547718445*

*0.8512098099923296 0.1880174434777748 0.9072346199725556*

*0.8312003471012195 0.6690758938221303 0.3877156995372734*

*0.8539428318375408 0.6645420155643865 0.9102928292472130*

*0.0142007190441381 0.0106106895240806 0.0226107152588826*

*0.9992165053816909 0.0009546714247650 0.4969272966699685*

*0.0136627128145468 0.5039002885268064 0.0158394085051735*

*0.9986574372936330 0.4998421894244930 0.4911052910151041*

*0.5034395629911151 1.0001115168370012 0.0099617517112517*

*0.4999205047253089 0.0026177289888592 0.4882607805924548*

*0.5006232336298111 0.5026436364046679 0.0117954375971851*

*0.4974491056751281 0.5000193149997866 0.4900565124607990*

Image 5:

**E= -193.63524590 eV**

*H O Ni*

*1.00000000000000*

*6.2244329453000002 0.0000000000000000 0.0000000000000000*

*-3.1122164726000001 5.3905170547000001 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209563999996*

*H O Ni*

*15 16 8*

*Direct*

*0.1867620789188032 0.3569696560620166 0.7072698717845927*

*0.2414586114140913 0.7478243110526140 0.2544628248710397*

*0.1896882282891540 0.8351486872109549 0.7060056923615301*

*0.6594763967842934 0.3255130162775698 0.2248543881809373*

*0.6484409314704309 0.3207795580753932 0.7111594050749814*

*0.6375163912695374 0.8227026464690138 0.2185592644914910*

*0.6509888725496510 0.8304526981849549 0.7037183796700825*

*0.3057353514490059 0.1608701349081547 0.2824876291346917*

*0.3103817885628067 0.1586040698801575 0.7984988094443908*

*0.2437330594905827 0.5017051867038139 0.2537924557581493*

*0.3395406562489480 0.6691132827506642 0.7862703938699476*

*0.8768793519849128 0.1841896552992879 0.2832537269410927*

*0.8681992015805831 0.2060212348260915 0.8039445511788238*

*0.8645112919104436 0.6885072030118599 0.2838605499763844*

*0.8635714579960418 0.6600084423523381 0.8038043997343107*

*0.1710201016856666 0.3631581879568745 0.1266887106266933*

*0.1726187280539103 0.3419452932474338 0.6026491187399641*

*0.1701796859321341 0.8114482631548166 0.1244644833779007*

*0.1728931363473543 0.8338364063150228 0.6014738816345219*

*0.6627329283142341 0.3316076182452339 0.1196869302678535*

*0.6653808000599467 0.3320170618460603 0.6065101607495028*

*0.6743251460090535 0.8384172881824545 0.1153994126929521*

*0.6576644752730094 0.8306108860568636 0.5986636913750589*

*0.3312612453764044 0.1685333956502812 0.3867802759468346*

*0.3356160213731294 0.1693660100718977 0.9024623938071018*

*0.2889219956372004 0.6489164977147739 0.3383563988730991*

*0.3466218923891921 0.6738833104307895 0.8911768624750137*

*0.8332041923262393 0.1656458296965726 0.3859906607999430*

*0.8530124252505771 0.1896426160608748 0.9087135849174443*

*0.8304606730946260 0.6692678564473675 0.3876778048090170*

*0.8514812554005728 0.6638960642758430 0.9086707209686465*

*0.0156819086947091 0.0087078452344742 0.0232792453150081*

*-0.0005807666396743 0.0013231772791924 0.4966475311753941*

*0.0143073232228363 0.5084307025788055 0.0163788834459446*

*0.9973866233100457 0.5001659977298484 0.4910752712336780*

*0.5009661475022954 0.9994969888438977 0.0104998689506777*

*0.5004248093843837 0.0036648523581985 0.4890392763823525*

*0.5009436213387639 0.5034277830036065 0.0116556534833007*

*0.5012731271692198 0.4981793994313856 0.4925524628712196*

Image 6:

**E = -194.03739125 eV**

*H O Ni*

*1.00000000000000*

*6.2244329453000002 0.0000000000000000 0.0000000000000000*

*-3.1122164726000001 5.3905170547000001 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209563999996*

*H O Ni*

*15 16 8*

*Direct*

*0.1873473262287207 0.3563731276799222 0.7078478674692835*

*0.2536644544151418 0.7417213610500841 0.2701749449798485*

*0.1887804876287752 0.8372917769974804 0.7086704733318235*

*0.6609656656726919 0.3278174927476273 0.2243442382234534*

*0.6482148813926216 0.3207503435253018 0.7100467839355153*

*0.6357790945345366 0.8200078242452206 0.2188124296976506*

*0.6522326589592905 0.8301168055838754 0.7044400388705013*

*0.3044028384345481 0.1582622864779900 0.2823568948376252*

*0.3115100211775761 0.1602276211050044 0.7987867832312301*

*0.2279535997057407 0.4630736258494199 0.2266535931786886*

*0.3384373205109698 0.6688493990998048 0.7867691720241220*

*0.8732141094229531 0.1808090500436350 0.2834038399405779*

*0.8684969020268780 0.2052514349488431 0.8050963888381871*

*0.8674803064566963 0.6901039746257011 0.2838424064055044*

*0.8617092771379262 0.6601511342578987 0.8006391811898829*

*0.1765278006634733 0.3698364592722274 0.1291601954975616*

*0.1721577617579695 0.3416648530270051 0.6034093675916239*

*0.1649550392870690 0.8122052766021325 0.1188096850614275*

*0.1697523352846178 0.8345847960188046 0.6045272643733562*

*0.6643441369175759 0.3331086092331707 0.1189239255543574*

*0.6643693269510860 0.3311546023389357 0.6054450195863066*

*0.6733565313109113 0.8383024393739218 0.1153923210211946*

*0.6583294119083715 0.8301332019711851 0.5995633976481679*

*0.3301525649953826 0.1695915564388384 0.3864212678058204*

*0.3343176538081513 0.1706427349901268 0.9031104152376446*

*0.3041737034858238 0.6698495069020087 0.3546770118985959*

*0.3447128133065128 0.6727646710755267 0.8918986108821185*

*0.8345426631669202 0.1677234113130550 0.3862663314481692*

*0.8550997087363015 0.1910904240842037 0.9101713613374132*

*0.8310710594359569 0.6700739120280330 0.3872511031067293*

*0.8481429795964380 0.6639286226749493 0.9054850316835984*

*0.0125773801393959 1.0030545273971638 0.0211911421610353*

*0.9989590505876761 1.0017135662115249 0.4973214513280381*

*0.0127666685923763 0.5125611203027802 0.0143814029044819*

*0.9990994873635430 0.5027320095695731 0.4921032209477097*

*0.5000504784308006 0.9997066558871476 0.0106576947044827*

*0.4957410472639857 0.9978416625198248 0.4871545199071003*

*0.5042219972231049 0.5055177674293276 0.0098762032594927*

*0.5000509604703711 0.4996182713574167 0.4907978843536367*

Image 7:

**E= -194.24629765 eV**

*H O Ni*

*1.00000000000000*

*6.2244329453000002 0.0000000000000000 0.0000000000000000*

*-3.1122164726000001 5.3905170547000001 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209563999996*

*H O Ni*

*15 16 8*

*Direct*

*0.1866898438587800 0.3537617924109708 0.7090731285361126*

*0.2680487225162661 0.7339634280760947 0.2798742199926469*

*0.1807210327356292 0.8365811687578685 0.7132659989186838*

*0.6600720027589140 0.3307284508377455 0.2213545460050654*

*0.6512050102305142 0.3244826927738774 0.7091777314563915*

*0.6356495073198074 0.8140207958444321 0.2186233248526198*

*0.6547871806876394 0.8263342945601906 0.7061665916525784*

*0.2997278222266089 0.1411926947092138 0.2828281872577958*

*0.3155540483888633 0.1591043115417262 0.7948239345726547*

*0.2190734581712399 0.4237308376818418 0.2199070431769154*

*0.3365970334457724 0.6704984070994104 0.7862550182352840*

*0.8641076999102518 0.1750090099265770 0.2837926840286621*

*0.8571191766424513 0.1871721571155019 0.8018741225239514*

*0.8770581928599550 0.6939632648583329 0.2842914761648441*

*0.8519912292517923 0.6652951307356084 0.7942674524599697*

*0.1767170095552576 0.3537356185045130 0.1214165894258646*

*0.1710760088493686 0.3407159415833886 0.6044943759989576*

*0.1714404541558199 0.8255342474329925 0.1175833874839553*

*0.1672411749356326 0.8353719443530848 0.6086163857685534*

*0.6668813603102932 0.3334773818695284 0.1159463587238743*

*0.6633829529632059 0.3322120834610413 0.6043257059014140*

*0.6696070537323031 0.8358361188273943 0.1148563504752117*

*0.6595179527877020 0.8303356913824632 0.6011470891361744*

*0.3287950923733374 0.1680225320804927 0.3866022516925613*

*0.3338297676874531 0.1685459842093905 0.8994150379807572*

*0.3157245206429287 0.6764371545429971 0.3693721985658961*

*0.3402345909733664 0.6704510380383996 0.8913983921083900*

*0.8354552122435119 0.1693800672504744 0.3877154658088015*

*0.8457384799945362 0.1772771494449061 0.9070034530605560*

*0.8341656129473534 0.6712654350652059 0.3869831163915539*

*0.8411277739998738 0.6672609437050471 0.8991816315754578*

*0.0101162773772200 0.9996494730155669 0.0171826595095067*

*0.9989321519674520 1.0018594825777924 0.4984959208726846*

*0.0095970127997479 0.5103878835022836 0.0109344156854454*

*0.9993072939082314 0.5038581335926220 0.4953962999355499*

*0.4981686865467803 0.9983970753298910 0.0092255857214765*

*0.4953663570574436 0.9993098972376618 0.4909879414837712*

*0.5044043008754023 0.5040965589145885 0.0052420746642001*

*0.4981522034923862 0.5014878674299041 0.4883077396911864*

Image 8:

**E= -194.35244181 eV**

*H O Ni*

*1.00000000000000*

*6.2244329453000002 0.0000000000000000 0.0000000000000000*

*-3.1122164726000001 5.3905170547000001 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209563999996*

*H O Ni*

*15 16 8*

*Direct*

*0.1854828498506252 0.3486940538476905 0.7099273781975874*

*0.2815092077292870 0.7209116554787224 0.2842255614503024*

*0.1710307447152638 0.8342373181239564 0.7173501488690532*

*0.6568745527720998 0.3373754185495805 0.2175593032780780*

*0.6546701122261425 0.3322892947414730 0.7096839854543703*

*0.6405584145320987 0.8076700277790192 0.2168846818929831*

*0.6556625770908484 0.8198795428607063 0.7085278415815067*

*0.2964379394971731 0.1144534402243503 0.2842780898143363*

*0.3211222547986477 0.1565468177884950 0.7894521503458501*

*0.2070584526103609 0.3836820030146010 0.2172360400909273*

*0.3318174750156569 0.6716613134924919 0.7851501538890389*

*0.8488911643242116 0.1689485232913752 0.2850379789230300*

*0.8435908668566661 0.1720638119279992 0.7981570816035969*

*0.8919539226010156 0.6991171763308061 0.2851225030051127*

*0.8451156675413687 0.6688219411320410 0.7889418507682016*

*0.1727330958477285 0.3420844091725800 0.1146632618876372*

*0.1708022956513545 0.3386387740725789 0.6052556929846074*

*0.1706371005873429 0.8297091628210754 0.1153352664082109*

*0.1660248105916111 0.8347274100849941 0.6123813551211733*

*0.6664121222589265 0.3331040330409641 0.1123905058676400*

*0.6632640232426549 0.3342468851563881 0.6047509427108018*

*0.6663802177961226 0.8321042484254763 0.1126314411826595*

*0.6614806883696988 0.8297016772925272 0.6036444220745866*

*0.3280024440121472 0.1626351986452095 0.3861097910300491*

*0.3329566528887556 0.1658276639648749 0.8944173251947454*

*0.3225647829845271 0.6752253865948344 0.3786799589111784*

*0.3358243949378193 0.6679236911548316 0.8902863298964993*

*0.8343496071047225 0.1682021479521224 0.3898584154376081*

*0.8380648151630944 0.1691278482861322 0.9035333203761842*

*0.8384130020921556 0.6716390175240150 0.3862680074452679*

*0.8369525387603531 0.6671404053286624 0.8940723769679910*

*0.0068077854918472 0.9968217062523346 0.0120828079296022*

*0.9995192541228334 1.0007069088856559 0.4994935430237202*

*0.0064923151652488 0.5081360993448572 0.0080739435917029*

*0.9996861369635950 0.5032839966303496 0.4980308620298793*

*0.4949640857086056 0.9960942768354283 0.0075014333290721*

*0.4962227199217508 0.9998640948599687 0.4960055956809288*

*0.5019716625622317 0.5011081285866552 0.0007682852646618*

*0.4982036193617744 0.5015321008032970 0.4867035917781423*

Image 9 (final structure):

**E= -194.35385367 eV**

*H O Ni*

*1.00000000000000*

*6.2244329453000002 0.0000000000000000 0.0000000000000000*

*-3.1122164726000001 5.3905170547000001 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.2556209563999996*

*H O Ni*

*15 16 8*

*Direct*

*0.1821061522627758 0.3406737450441284 0.7109935448876641*

*0.2955234345985573 0.7037009905945411 0.2864842032220025*

*0.1655049643477184 0.8326153505121852 0.7203777852543993*

*0.6516927642343546 0.3480371009658754 0.2142073485955081*

*0.6588459225552583 0.3424606800580960 0.7111348672166642*

*0.6522293241676849 0.8040478971405065 0.2142220224433586*

*0.6586979881665229 0.8162007947208707 0.7111539486100327*

*0.2948858545536339 0.0903057801086931 0.2864544135922813*

*0.3276093540961469 0.1563444471834714 0.7845227840758469*

*0.1906498483038561 0.3446935930557160 0.2145868500221511*

*0.3271562618558548 0.6706974255381724 0.7846337768120080*

*0.8301393342652901 0.1651964382654896 0.2866139214416847*

*0.8313820064810784 0.1655664965375081 0.7946359059406731*

*0.9091090073623108 0.7043030643479327 0.2859735256435272*

*0.8423059980906515 0.6712069749766272 0.7844398113646633*

*0.1674033104431416 0.3336033157804152 0.1099888893041197*

*0.1707266176374418 0.3351497298207988 0.6061213079163821*

*0.1651170141491463 0.8326781579950975 0.1131607108705666*

*0.1660095921548290 0.8328092905317064 0.6152590480453242*

*0.6642253257950159 0.3340715310994185 0.1097878688380831*

*0.6639714052427834 0.3354393520974455 0.6062874205523912*

*0.6644340758106395 0.8301917554215947 0.1097765671802549*

*0.6639456527047614 0.8280865267352482 0.6062907449585921*

*0.3278277255123072 0.1560976760566035 0.3854158769206535*

*0.3310801173165245 0.1649142401344008 0.8897281146959557*

*0.3279394128490125 0.6711847989641058 0.3855993056501674*

*0.3310779038348741 0.6660100725154265 0.8898382890910810*

*0.8327435686899562 0.1662401535069904 0.3917808326724170*

*0.8315708796767893 0.1657920995784252 0.9001745837732926*

*0.8434879488047287 0.6715845642775093 0.3850313183529366*

*0.8331710932825658 0.6665503489467426 0.8896316673749567*

*0.0025721967060406 0.9956449698222798 0.0060972132929535*

*0.0004330302357971 0.9986558878598970 0.5000020083014149*

*0.0025545074187505 0.5068900682999242 0.0061808729823980*

*0.0004843085544053 0.5014248188324615 0.5000437200238323*

*0.4907426417432319 0.9953559472834356 0.0063317182595313*

*0.4977916535062477 0.9986761903474816 0.5003165390311395*

*0.4983712838454153 0.4991220653344257 0.9974091768476540*

*0.4996247777439535 0.4995541637083107 0.4866753829414279*

**β-Ni(OH)2- Interstitial diffusion:**  
Image 0 (initial structure):  
**E= -200.63653600 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1571961576108245 0.3272747822068114 0.2028211905902507*

*0.1648479106069235 0.3321042982339707 0.7200978534259913*

*0.1671479028567046 0.8328519910530406 0.2050545877032119*

*0.1660648171221141 0.8339350767876240 0.7222321069281602*

*0.6673121145532127 0.3326877943565231 0.2030598569128833*

*0.6663350987382829 0.3336648101714528 0.7205138236620815*

*0.6727251267029244 0.8428037362989207 0.2028211905902507*

*0.6678956106757651 0.8351519833028217 0.7200978534259913*

*0.3337737161043903 0.1691035927068195 0.2970859329702679*

*0.3351104697817390 0.1688106758490569 0.7797604483812891*

*0.3343461780481227 0.6656537308616131 0.2971311022300544*

*0.3346828577250418 0.6653170511846940 0.7801321437954689*

*0.8302497034014964 0.1697501905082488 0.2937462552857936*

*0.8323878793046796 0.1676120146050656 0.7769891739985628*

*0.8308963012029329 0.6662261928053526 0.2970859329702679*

*0.8311892180606884 0.6648894391279968 0.7797604483812891*

*0.5000115757693423 0.4999880276188832 0.2357176287471442*

*0.1593437269082602 0.3295027558835870 0.0982831713058474*

*0.1656219807790165 0.3337810344320705 0.6154990481164907*

*0.1666526465313018 0.8333472473784505 0.1006023860606178*

*0.1659720309346344 0.8340278629751108 0.6176423657259624*

*0.6698921494448308 0.3301077594649049 0.0985184507249069*

*0.6657447284772493 0.3342551804324865 0.6159105949958027*

*0.6704971530261488 0.8406561670014921 0.0982831713058474*

*0.6662188744776653 0.8343779131307215 0.6154990481164907*

*0.3305074867732778 0.1630479441642968 0.4015155363416066*

*0.3338999334892517 0.1677780976038696 0.8843985397925439*

*0.3302440591928175 0.6697558497169112 0.4015228684385588*

*0.3339313060663229 0.6660686028434200 0.8847654524957722*

*0.8323007490495824 0.1676991448601628 0.3981293554745763*

*0.8330003890465895 0.1669995048631558 0.8816088321939474*

*0.8369519497454413 0.6694924221364508 0.4015155363416066*

*0.8322217963058757 0.6660999754204913 0.8843985397925439*

*0.9999525219985500 0.0000474759111824 0.9906126072704874*

*0.9991139039626126 0.0008860939471271 0.5077892689589191*

*0.9999868860160256 0.5001594653484303 0.9911793856388236*

*0.9988882883238718 0.5004296785780721 0.5082199891451271*

*0.4998405325613094 0.0000131118937139 0.9911793856388236*

*0.4995703193316675 0.0011117095858678 0.5082199891451271*

*0.4999785527886957 0.5000214451210511 0.9938690953421240*

*0.4989750301704824 0.5010249677392571 0.5067293007494218*

Image 1:

**E= -200.57916696 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1378552162166235 0.3069864487301192 0.2019585215937216*

*0.1594149197749507 0.3272108381152919 0.7218476411120117*

*0.1724824202600244 0.8281710855118869 0.2047535305995222*

*0.1661044747905009 0.8361281118997502 0.7227420673086553*

*0.6636590330669841 0.3377671025658581 0.2042631191418976*

*0.6673236536881277 0.3356204934855943 0.7217337221696659*

*0.6823579409371303 0.8479839812757052 0.2016263345818321*

*0.6725463678066419 0.8397224250977842 0.7219453415012227*

*0.3352224977993776 0.1740876977379313 0.2971814121665718*

*0.3376314952956760 0.1689013610543996 0.7792530558198062*

*0.3420867326480948 0.6551482203811616 0.3026235946844961*

*0.3357111636913815 0.6607406487857387 0.7812832282111327*

*0.8207845033845456 0.1717210463541611 0.2945357225707450*

*0.8289360349070570 0.1677267700646260 0.7763285537945460*

*0.8317411068851283 0.6686653491807336 0.2967086157506705*

*0.8315114536452003 0.6622958289876975 0.7787676211486451*

*0.4620490213604354 0.5246311132187154 0.2149684056109575*

*0.1520410010686450 0.3194824644287252 0.0977024553140699*

*0.1635944373208424 0.3336401225532948 0.6173060313450948*

*0.1673056473487735 0.8299578118194585 0.1003181915113704*

*0.1655165822469445 0.8364340993480739 0.6181686877501105*

*0.6679701540941725 0.3299124023153361 0.0999894009421801*

*0.6656213541669879 0.3365173933805499 0.6171523839837900*

*0.6762453108213831 0.8430271929368967 0.0970714649127891*

*0.6677407393039112 0.8374421832487028 0.6173702940963803*

*0.3320114476847760 0.1684973367501230 0.4015747167364278*

*0.3345893713945796 0.1658684778745116 0.8839259788353163*

*0.3291860135626405 0.6723583860924236 0.4061665857280282*

*0.3341991033295562 0.6623791881927461 0.8859618525876395*

*0.8314466801597116 0.1696989008082042 0.3986249735749532*

*0.8315610443771985 0.1651446221883638 0.8809440620862570*

*0.8333351382076050 0.6700830291083624 0.4011290346094757*

*0.8322875252704504 0.6631012245874544 0.8834658764337503*

*1.0001894645478537 0.9966880132677121 0.9884388390902057*

*0.9991944983962909 0.0024682310871134 0.5075221668270928*

*0.9987596128771917 0.4970996941343713 0.9915407740683669*

*0.9977867247769064 0.5023827983048977 0.5090518678635395*

*0.4996624468506474 0.9980679766013419 0.9916422543456967*

*0.4996479154764059 0.0039312492254532 0.5093201673934061*

*0.5006607223486120 0.4972691465313833 0.9934377107218674*

*0.4979499683581522 0.5035563257550499 0.5096531850191565*

Image 2:

**E= -200.48926879 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1307154310575443 0.2951425202279022 0.2017761119373289*

*0.1567905344994037 0.3242609245654040 0.7230622310738092*

*0.1744590316601873 0.8248502572485485 0.2042106958045873*

*0.1646351505518703 0.8371528827390005 0.7234105506671366*

*0.6620890782857259 0.3391317726701504 0.2054022339467849*

*0.6665056923471668 0.3357148847534347 0.7221367021698175*

*0.6877503358631004 0.8492104501348301 0.2009000280114434*

*0.6743826089402891 0.8413147886597744 0.7232009727472513*

*0.3343465035224796 0.1728312840426449 0.2968091748413740*

*0.3385040743446323 0.1681483368317573 0.7788242583149630*

*0.3457262555686302 0.6499009433249174 0.3065355159401095*

*0.3351818416547715 0.6589223704532587 0.7821167408114342*

*0.8176538873299407 0.1724861527994110 0.2951981356298279*

*0.8273312405974268 0.1680932623327317 0.7766059864776462*

*0.8334192484227750 0.6698581470352510 0.2964541145195241*

*0.8314632991733667 0.6602911381187755 0.7779910354375634*

*0.4202542929942665 0.5596027564749602 0.1980870181960709*

*0.1493312720546078 0.3122938461399700 0.0977502712326801*

*0.1620256466341668 0.3327152315619274 0.6185956406705145*

*0.1673542526256817 0.8281379039137080 0.0998542702477157*

*0.1642298083516368 0.8374376992025422 0.6188603787823846*

*0.6659851370926547 0.3303717301803630 0.1011752443366199*

*0.6647232031686753 0.3369856645423689 0.6175840134631744*

*0.6812110669789136 0.8435126673205481 0.0963083665255961*

*0.6681866474451518 0.8385115637843384 0.6186742921927405*

*0.3319634106290352 0.1710231915751379 0.4011999173208702*

*0.3353773302169535 0.1647061895901216 0.8835217280135936*

*0.3282982835089164 0.6730985866912929 0.4105579279941203*

*0.3341862426875864 0.6604055535867333 0.8868417523589573*

*0.8305346175696076 0.1701664305331461 0.3991315579090243*

*0.8309789244841107 0.1642076895430283 0.8811934156713992*

*0.8308386943667102 0.6699488378688581 0.4008363566210338*

*0.8325083550338785 0.6610114757130057 0.8827141579818787*

*0.0007177665726128 0.9944405036344351 0.9869462849235652*

*0.9985051901919773 0.0027984670794575 0.5076794323683369*

*0.9982149628016537 0.4952269359548876 0.9921399138877589*

*0.9968095943699480 0.5028575656313431 0.5097598684503494*

*0.4998345479585442 0.9968492263991983 0.9921421349374264*

*0.4987917966912194 0.0047013147480327 0.5100534612260097*

*0.5018004959152296 0.4956899747502248 0.9923441897757523*

*0.4967464924665204 0.5045056655068164 0.5114133545569713*

Image 3:

**E= -200.48260641 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1336955269460549 0.2913929928425857 0.2024030625910375*

*0.1556299973911866 0.3224029448081149 0.7238030521849973*

*0.1738537091038479 0.8238153942400069 0.2033686218143453*

*0.1632020916120175 0.8375021619834816 0.7239542696321755*

*0.6622796491275901 0.3383870330986809 0.2062808558988229*

*0.6653079869533454 0.3356487281281321 0.7222621411441315*

*0.6879317725434899 0.8455272185871400 0.2014807152005383*

*0.6748610946947643 0.8412339223954024 0.7239486581891129*

*0.3337701009888427 0.1698283050883208 0.2964297157872564*

*0.3383688560403076 0.1670573062189600 0.7786036673200690*

*0.3416870768450143 0.6521814906477053 0.3068770869668952*

*0.3341173454583389 0.6581461485609780 0.7825226819140966*

*0.8174837866789726 0.1722766432910892 0.2956163083137648*

*0.8263159917471550 0.1677444685065035 0.7775910133997276*

*0.8351816857230061 0.6702271857345891 0.2961870099271244*

*0.8311197469572648 0.6591072505584658 0.7777726180256505*

*0.3772574162430498 0.5982472599208976 0.1839273492194983*

*0.1522255896443892 0.3103748700579815 0.0984447911826440*

*0.1611664142402269 0.3315793231545200 0.6193758531199756*

*0.1659662642456128 0.8281914763881337 0.0990938976793935*

*0.1631498631495336 0.8374330398623732 0.6194117828324920*

*0.6652076821614377 0.3296665012419892 0.1020198092422270*

*0.6640759912539727 0.3365623787667400 0.6177152503959783*

*0.6816665892851694 0.8393967945039207 0.0969169315664388*

*0.6681706533516840 0.8382891078699347 0.6194562064437743*

*0.3313479570345066 0.1707800901080607 0.4007983442056047*

*0.3354935102867413 0.1633613952632050 0.8833064163985781*

*0.3291436933173479 0.6713976553404823 0.4136132851457612*

*0.3336518799556509 0.6591668453568147 0.8872732849570845*

*0.8298246323309793 0.1698536619404045 0.3995804626747264*

*0.8306378860710038 0.1632296871594743 0.8821678018206724*

*0.8301701228643359 0.6695337787349576 0.4005268428565603*

*0.8322747585870162 0.6595146890557947 0.8824991094330642*

*0.0006246344964859 0.9930824604566866 0.9868772975954880*

*0.9976794762425758 0.0024282707419208 0.5079338750550403*

*0.9977577893593268 0.4939279326545625 0.9925066749470103*

*0.9966587396245786 0.5027369431355045 0.5104539757363531*

*0.4997468343734061 0.9955198549824708 0.9925994321938315*

*0.4978969736857243 0.0039076409889224 0.5106553366812147*

*0.5018347253946110 0.4939896543834560 0.9918612731121809*

*0.4963670571005196 0.5038662759814676 0.5118826696019462*

Image 4:

**E= -200.52318185 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1465309970789030 0.2993825126128989 0.2032321078317558*

*0.1579834574888742 0.3214725247548119 0.7240467710103116*

*0.1660307592659033 0.8289418691438575 0.2026011458786759*

*0.1624493868205523 0.8370138882397022 0.7242615540357313*

*0.6648465319308311 0.3356118101304362 0.2068619138398344*

*0.6654425055161499 0.3348668154820064 0.7223202426098986*

*0.6781070532798885 0.8365720613441003 0.2026273141679951*

*0.6741863835587922 0.8383739612827427 0.7242314559470691*

*0.3369154248800194 0.1674681267967965 0.2961558643449734*

*0.3380173564733611 0.1659126574051202 0.7785955705396367*

*0.3327688852114059 0.6584869056577981 0.3059399705153455*

*0.3314010073150672 0.6586457654911431 0.7824241330884238*

*0.8229502465276198 0.1695650980030738 0.2959885892409587*

*0.8261972320524744 0.1663718799633101 0.7785653463674657*

*0.8344811628000642 0.6681232706619681 0.2960439005780959*

*0.8298042112072991 0.6583604622095385 0.7780004422744058*

*0.3349268373116621 0.6347354384380934 0.1747850297847253*

*0.1563569720357773 0.3131155847463120 0.0989012792092582*

*0.1627570472918299 0.3300347684385823 0.6196062935915855*

*0.1610955611143263 0.8311590015174447 0.0981479335806843*

*0.1636257270079527 0.8359559710521951 0.6197154446231106*

*0.6644799741709074 0.3285132446399369 0.1024607026408726*

*0.6652181811235149 0.3346432863062916 0.6177673820665994*

*0.6760959300981995 0.8338621836927339 0.0980572920632591*

*0.6689080264285818 0.8361907849997416 0.6197204339424888*

*0.3323835964214997 0.1682706534299871 0.4004839355771718*

*0.3339552475885010 0.1623714366389748 0.8832745292868562*

*0.3317208323383544 0.6683059355179843 0.4143385655249025*

*0.3312547051600701 0.6592992266005236 0.8871733464786552*

*0.8310658962208527 0.1681902429073644 0.4001955055294087*

*0.8294588277635189 0.1624486519584551 0.8831882054196356*

*0.8318374368763659 0.6679092904116803 0.4004175202741947*

*0.8303627431828151 0.6588562722590308 0.8827172278038855*

*0.9980126775873721 0.9931385400835084 0.9877212262927302*

*0.9984877735687894 0.0009427438136642 0.5082019055989393*

*0.9958447488707283 0.4932774986004032 0.9925274459406045*

*0.9985536655201185 0.5012325476032561 0.5110587156942729*

*0.4983293124525652 0.9951056090098754 0.9927358009426486*

*0.4986582030963956 0.0013969580148392 0.5111850504777548*

*0.4994704932629696 0.4929817141255648 0.9923696338404501*

*0.4982718416916602 0.5014095836316078 0.5113526983840913*

Image 5:

**E= -200.50743988 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1532597394219866 0.2939958335576919 0.2029311355508693*

*0.1640718299731195 0.3218553721248463 0.7240297579809559*

*0.1571601768590136 0.8404113789263175 0.2020522458872478*

*0.1646312908528348 0.8398151084544480 0.7241905567145828*

*0.6728121008475552 0.3372560641736270 0.2065827087212418*

*0.6688128270351785 0.3353621842602181 0.7223538295602389*

*0.6549374573879944 0.8258745428231700 0.2027850332184556*

*0.6741496543756504 0.8376169787609382 0.7242085456898943*

*0.3499073644709459 0.1709857078650904 0.2958472163920691*

*0.3399205421656839 0.1669901750932024 0.7781872940366356*

*0.3180117351748341 0.6554750281774457 0.3063789566412510*

*0.3253508017390179 0.6582722972324945 0.7824474534007190*

*0.8318378837881598 0.1684671485188184 0.2963239043328236*

*0.8275474194185899 0.1666844060984193 0.7785574670532460*

*0.8334564076789325 0.6696126607623877 0.2961342043541613*

*0.8278216334031460 0.6587299288172066 0.7777929292998365*

*0.2658042491444819 0.6184829807716679 0.1780220378740622*

*0.1563260647847850 0.3116253989515733 0.0988168411959946*

*0.1678413960699233 0.3307490784498146 0.6195973798239272*

*0.1567835436058256 0.8361566717610798 0.0974784335283565*

*0.1677897709669103 0.8373469254295879 0.6196787782995591*

*0.6636719455236884 0.3290504258724389 0.1022466257521144*

*0.6700220335425333 0.3357188565916236 0.6178029752446549*

*0.6656578482755995 0.8296461720495988 0.0984471165782863*

*0.6725238845969552 0.8368555414941033 0.6196650328847698*

*0.3377142387944844 0.1691221759638728 0.3999429886637043*

*0.3321637469782006 0.1627691098989297 0.8827984692264695*

*0.3382137885626779 0.6697767264658776 0.4143468675817377*

*0.3261486985782327 0.6590503128210445 0.8872028527639667*

*0.8367119739276629 0.1696169176093342 0.4006697808213109*

*0.8275132010180376 0.1628640977531695 0.8832487565640113*

*0.8368341389697770 0.6688203677429591 0.4004915357115597*

*0.8272634034935522 0.6591382990322590 0.8825184411601775*

*0.9930824225279619 0.9929920291781205 0.9872985293743503*

*0.0026792306746088 0.0017435486000863 0.5081234616265972*

*0.9921083968426953 0.4934372149571440 0.9920249326753334*

*0.0043498385388354 0.5026862850412672 0.5116991285000672*

*0.4956622179996543 0.9951394296573791 0.9926604387053501*

*0.5034605033290546 0.0026957006753078 0.5110406933685204*

*0.4962373181416765 0.4935454350056038 0.9925108754526963*

*0.5034334465935706 0.5020822550737676 0.5108632090596670*

Image 6:

**E= -200.47308317 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1599044080523658 0.2910109254000104 0.2019875607606404*

*0.1663093891848569 0.3231014665289221 0.7236179945455470*

*0.1584345431904560 0.8476118815659904 0.2009473309115477*

*0.1660301318625645 0.8414857896249092 0.7237606037612849*

*0.6762249437247460 0.3390484879260057 0.2058947546223126*

*0.6686882219326472 0.3357006931975591 0.7222768688801544*

*0.6485676658299343 0.8238975542617332 0.2037528942747704*

*0.6731723794302876 0.8377020302062879 0.7237773756510421*

*0.3545737974898318 0.1724055805292795 0.2955186822107562*

*0.3404548568918272 0.1679202353378503 0.7770188994838373*

*0.3047252735733349 0.6500720238591970 0.3071519376024633*

*0.3233380785824952 0.6583191839287500 0.7823796382138620*

*0.8365892283591160 0.1715394926415157 0.2966554908787820*

*0.8282536079276280 0.1678180638364462 0.7786133628704129*

*0.8349389915848557 0.6703866173550005 0.2963580243059628*

*0.8275766050299261 0.6594432485887531 0.7777246025268104*

*0.1839027039731211 0.5804632823613161 0.1896740432372986*

*0.1594662292526252 0.3103429042975867 0.0980787670474958*

*0.1698747703604889 0.3321882848337400 0.6191808136591592*

*0.1588926409003450 0.8417231289083583 0.0963599495337810*

*0.1695418919470319 0.8386806135301599 0.6192506969477344*

*0.6641422673927337 0.3301766011873055 0.1016467236856729*

*0.6716745929653934 0.3369346071361672 0.6177324857278779*

*0.6603167833430653 0.8278277008388492 0.0994500602478335*

*0.6732365304735600 0.8376888546581647 0.6192341101347444*

*0.3391877893030908 0.1701840654882665 0.3994381009157263*

*0.3322636235919162 0.1636682870484442 0.8816076701915223*

*0.3429410566277393 0.6724993753324816 0.4125686570730339*

*0.3250494388422963 0.6595654221730718 0.8871276919382841*

*0.8387871112108248 0.1713701531975994 0.4010346180654358*

*0.8277675188309856 0.1640405037318392 0.8833174599297995*

*0.8387447915109086 0.6698853972858040 0.4007126352682419*

*0.8269759509069983 0.6600719294487948 0.8824561396781461*

*0.9921062154999182 0.9935565085600105 0.9866166070178295*

*0.0038658640301173 0.0028244208318041 0.5078859721395779*

*0.9921314066093886 0.4948242454755390 0.9918712707489039*

*0.0071911114220558 0.5044556175888729 0.5119158986640764*

*0.4956268095857318 0.9960879875402047 0.9923751326881910*

*0.5053491600141183 0.0045393823535607 0.5104626082699766*

*0.4958215577262385 0.4944232583484672 0.9923804383976975*

*0.5054875335879484 0.5030309604258553 0.5101848429953609*

Image 7:

**E= -200.51340526 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1653391625053725 0.2976706052997142 0.2016976330294881*

*0.1665663953273660 0.3250135586495738 0.7227683847392743*

*0.1619827495868220 0.8493002165938477 0.2009318242254936*

*0.1661906339793846 0.8409923602134661 0.7228838800496673*

*0.6759469972500574 0.3391136353358014 0.2050164270665374*

*0.6676651119678241 0.3357450036875989 0.7221177357326454*

*0.6506515829070860 0.8256915801660127 0.2043636504800687*

*0.6710570732117516 0.8371417976504876 0.7232098820353520*

*0.3532889426319601 0.1724680551098016 0.2950682463222759*

*0.3393000295345406 0.1679500661650039 0.7763833923138831*

*0.3039935130047264 0.6504597654866525 0.3057206450040596*

*0.3232979246919236 0.6592140737835864 0.7819036186626385*

*0.8379878001595985 0.1738236249302815 0.2969884222406699*

*0.8291030631744599 0.1686191746213660 0.7788895806116281*

*0.8357810849780402 0.6696746611821679 0.2966057105161293*

*0.8285055907186346 0.6607243366424703 0.7781295397692157*

*0.1121430107850923 0.5470475936614630 0.2032109108035690*

*0.1637453169897499 0.3139724257405804 0.0976338629288274*

*0.1696464091225579 0.3331147507499058 0.6182810851637125*

*0.1630693320751425 0.8438094221545483 0.0963535406834672*

*0.1692335039084410 0.8384470860451692 0.6183391093562882*

*0.6630196838542746 0.3303535820540536 0.1007956557993655*

*0.6709658403209886 0.3370257740123411 0.6175604731760339*

*0.6602762108564026 0.8285796463664026 0.0999818476943656*

*0.6715199168400627 0.8372780498563556 0.6186506604865102*

*0.3383162907378566 0.1702210661220432 0.3990168315991475*

*0.3325629654635492 0.1645064304919135 0.8809829053611252*

*0.3437025993375940 0.6731803168348455 0.4092041454490599*

*0.3259184992168447 0.6608580900249210 0.8866156664582810*

*0.8374084430607758 0.1706184972635590 0.4013820550559096*

*0.8290577928393753 0.1650684988620332 0.8835780004638795*

*0.8376187695084358 0.6701204060933275 0.4010029576803902*

*0.8283249504983333 0.6615633727193531 0.8828465470495364*

*0.9936277832678213 0.9950290548818570 0.9871961379099499*

*0.0030042906179833 0.0028756200361610 0.5076436674662008*

*0.9938462845755335 0.4961457127085394 0.9926479674197608*

*0.0063812410282788 0.5044859714713116 0.5110467162814417*

*0.4966243686729087 0.9972307734614601 0.9919494251607464*

*0.5045147921256659 0.0047461679562092 0.5098569411132732*

*0.4966010335271008 0.4957535404935394 0.9919519174705015*

*0.5047817941766857 0.5028823966672643 0.5095918093052920*

Image 8:

**E= -200.59894081 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1687598435259544 0.3102652073967573 0.2021240868374303*

*0.1666127832692415 0.3281088414051773 0.7215398165554711*

*0.1655589575929479 0.8468036881494522 0.2018957896433919*

*0.1661583926742115 0.8390225035308890 0.7216051284309414*

*0.6715538300470041 0.3369508237000987 0.2040181956719003*

*0.6668049139660980 0.3356134196294595 0.7215909693761133*

*0.6566829225983740 0.8292657074234357 0.2048444956081575*

*0.6686973682868119 0.8362089297585836 0.7225962149008786*

*0.3481167693090875 0.1713765069277348 0.2943623886385063*

*0.3370323134892603 0.1673678528050011 0.7763528460319846*

*0.3154373059988453 0.6570627601024603 0.3014630084042341*

*0.3250361177310915 0.6612580690852182 0.7810209273007707*

*0.8374707720103143 0.1741806136315722 0.2972542904337475*

*0.8306743634295005 0.1691393527706533 0.7793549899352302*

*0.8356416498446948 0.6684651749777213 0.2967569956182775*

*0.8304407052328364 0.6627595664203084 0.7789331364559938*

*0.0461696784856851 0.5177107774402386 0.2190713889601424*

*0.1671617248344805 0.3211804958223251 0.0978020831286507*

*0.1686855573122757 0.3340294067200988 0.6169853722409794*

*0.1665975808444443 0.8422207213356194 0.0973500936215679*

*0.1682522737695948 0.8371774008924467 0.6170148726881438*

*0.6603319368146767 0.3296162655729425 0.0996971366203982*

*0.6693018571932057 0.3364212089540654 0.6170033401171843*

*0.6623904362533559 0.8303955904364350 0.1003909623955662*

*0.6693069604190631 0.8364134340768026 0.6180172460363553*

*0.3366698803349636 0.1696890956661801 0.3985117474281515*

*0.3326454310111374 0.1651829009890493 0.8809782796923611*

*0.3412591025637390 0.6720880700204758 0.4051907743202310*

*0.3278895564339739 0.6627873778105564 0.8856915789161096*

*0.8345626486755620 0.1678032459808827 0.4016468082930211*

*0.8307886043176761 0.1660289288305653 0.8840255206697459*

*0.8348884078573271 0.6703192094239762 0.4011786419139184*

*0.8303924115932633 0.6634201892332801 0.8836231817652802*

*0.9961946030115882 0.9969870508722456 0.9888486759387660*

*0.0018825214646667 0.0025847946722258 0.5075134955736149*

*0.9963001276438923 0.4974738949584047 0.9936345441731435*

*0.0037447108557234 0.5033761931964500 0.5091626987270270*

*0.4976933573804876 0.9981657630802995 0.9915326047723074*

*0.5026246533581059 0.0037642177315225 0.5091136780918046*

*0.4975951240030740 0.4973861162971441 0.9914088882843750*

*0.5030019300802515 0.5024453893948166 0.5088925103559607*

Image 9 (final structure):

**E= -200.63767160 eV**

*H O Ni*

*1.0000000000000000*

*6.2916393279999996 0.0000000000000000 0.0000000000000000*

*-3.1458196639999998 5.4487194895000002 0.0000000000000000*

*0.0000000000000000 0.0000000000000000 9.3081312179999998*

*H O Ni*

*17 16 8*

*Direct*

*0.1665874021242715 0.3295943207641798 0.2028932098663603*

*0.1645109250236558 0.3329598876130078 0.7199730757895182*

*0.1693933378387626 0.8384797845575278 0.2024758586577065*

*0.1660399331338809 0.8332322932885603 0.7194343612334606*

*0.6616242309083091 0.3314975280005115 0.2029868510528701*

*0.6668053614649736 0.3340330990150733 0.7200864186508582*

*0.6683494297056285 0.8358658645850454 0.2060722928164722*

*0.6673675591478343 0.8351794462391027 0.7228398865450956*

*0.3329094735398428 0.1680502966019830 0.2933315136084360*

*0.3337617429887914 0.1676319499228711 0.7769048868506729*

*0.3349203567463164 0.6667382079804298 0.2968667458223848*

*0.3333114107873314 0.6657284952870057 0.7798466984021815*

*0.8315506821989089 0.1681687297723400 0.2970542959344229*

*0.8328586434965857 0.1679481936873302 0.7795918232730443*

*0.8318366467410385 0.6674747826801521 0.2967562442646638*

*0.8326779795562373 0.6659232270384692 0.7796714026816218*

*0.0003990567040120 0.5016143547440919 0.2396735329807242*

*0.1694918480725960 0.3295899534356721 0.0983398317116055*

*0.1656106534607815 0.3339219577577310 0.6153470491885003*

*0.1699395774438699 0.8401826637301113 0.0978899531370345*

*0.1656680903509340 0.8336322910868930 0.6147999091293812*

*0.6594833456957261 0.3300450546422340 0.0984387792230876*

*0.6659405368388036 0.3340117908108411 0.6154622069259119*

*0.6667232662941203 0.8336876901527006 0.1016178154128724*

*0.6660682240292104 0.8340741023751406 0.6182324279185138*

*0.3326201924197747 0.1676485732535440 0.3977424626146444*

*0.3332994984596596 0.1670614170792817 0.8815352182234477*

*0.3385534063511102 0.6698570996671904 0.4013216482906188*

*0.3326629069105564 0.6662405860780254 0.8845050379074593*

*0.8294604505889822 0.1619507302598251 0.4014834577278918*

*0.8333028609135624 0.1673434945518366 0.8842683955637654*

*0.8293031934392801 0.6700420798139675 0.4011912745166200*

*0.8330690159509402 0.6661715040066341 0.8843325423069501*

*0.9996579303157702 0.0000050550383790 0.9909788672236388*

*0.9995166637410976 0.0009119863816309 0.5078863225477264*

*0.9997341899273522 0.4999977294874185 0.9930721250077568*

*0.9990421374132340 0.5007107608944779 0.5058664167369997*

*0.4999635544138954 0.0001244437582244 0.9911867238454520*

*0.4987544187419815 0.0007832915140398 0.5080967790317459*

*0.4997470829049604 0.5001842927548168 0.9916978170490652*

*0.4989341752154459 0.5002177416917064 0.5082472393288171*

**α-Ni(OH)2- Vacancy diffusion:**Image 0 (initial structure):  
**E= -98.22908164 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.3049506271593714 0.0288152735244296 0.2526044515913171 T T T*

*0.7465468373332271 0.0703307402887248 0.7535683845316541 T T T*

*0.0858013796097055 0.3929775541475848 0.2483881272311024 T T T*

*0.0029815555714947 0.6336826604146992 0.7490667452099871 T T T*

*0.3867337896046550 0.2935892474039647 0.7420153224129180 T T T*

*0.3999907952858521 0.6815220674097517 0.6650691274727194 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.6937528803943920 0.0358890016231896 0.8764433789131729 T T T*

*0.9895414799391062 0.3475826789562646 0.1440396300813021 T T T*

*0.0104109697814110 0.6591425333154390 0.8732733425222321 T T T*

*0.6376073888885543 0.6607178562870075 0.1170729926514866 T T T*

*0.3539551629896351 0.3302785279418572 0.8640496744792969 T T T*

*0.4090348611576999 0.6735997941644172 0.5395255359013191 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3384418845670751 0.6757130635532533 0.9996666294775522 T T T*

*0.6587047618965443 0.3540366184010750 0.0022378289858693 T T T*

Image 1:

**E= -98.20824382 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.3159698005856487 0.0219525492943037 0.2516361906023629 T T T*

*0.7778918428261485 0.1103860095079141 0.7528778195919088 T T T*

*0.0851148149349904 0.3998698348178266 0.2468620977309062 T T T*

*0.0395713098832558 0.6490491880535936 0.7483738387550141 T T T*

*0.3803724862364745 0.3171928166274925 0.7437280953599246 T T T*

*0.4776397655640614 0.7432974712901294 0.6725622809462602 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7016561818634767 0.0448317043205469 0.8702501989826223 T T T*

*0.9844921599058097 0.3480616399906347 0.1440571786753194 T T T*

*0.0162964711365872 0.6661758097209065 0.8737044430223500 T T T*

*0.6360113336879734 0.6680945568668986 0.1158001313526302 T T T*

*0.3525060389509875 0.3363596974887221 0.8680101165192589 T T T*

*0.4165526240143826 0.6863944366868842 0.5565700714040211 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3355906187074887 0.6785036105463685 0.9984819278115152 T T T*

*0.6599530028610959 0.3584507120095461 0.0013633810890944 T T T*

Image 2:

**E= -98.06297417 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.3488383977468499 0.9814943215864053 0.2386171805537683 T T T*

*0.7812011813878580 0.1152164338435529 0.7461066498124974 T T T*

*0.0877955094525667 0.4146194621928513 0.2419831988543320 T T T*

*0.0616314990112938 0.6679940462193548 0.7480250154629883 T T T*

*0.3745288995251789 0.3425045252957071 0.7464955058181449 T T T*

*0.4996101015130565 0.7608759112892634 0.6715622585715443 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7070518479064652 0.0399010525193079 0.8617146383133905 T T T*

*0.9895681406337553 0.3619690235274898 0.1382348116213888 T T T*

*0.0323745328511008 0.6786721726439894 0.8735839860591674 T T T*

*0.6122768173580273 0.6993949600469126 0.1161967379464829 T T T*

*0.3518081720249712 0.3517470985418971 0.8715090019070464 T T T*

*0.4186780892582976 0.6904088912289867 0.5608770677788235 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3385203763288035 0.6886015146454736 0.9894193849382098 T T T*

*0.6604025122831262 0.3642046952649022 0.0059970930150632 T T T*

Image 3:

**E= -97.60597146 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.4016911678763462 0.9484592075874918 0.2008607019146782 T T T*

*0.7853718641292270 0.1199604724730931 0.7423191107766705 T T T*

*0.0824906870374203 0.4204310982913949 0.2380019328311770 T T T*

*0.0495479590290273 0.6669646496555709 0.7460285940708773 T T T*

*0.3785945813786067 0.3472560779131398 0.7473384601404340 T T T*

*0.5037706784801447 0.7652912630783780 0.6714947240871801 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7079144074109818 0.0400519038714220 0.8568966092563092 T T T*

*0.9845176446561225 0.3619326879763659 0.1337816745477618 T T T*

*0.0196428691134862 0.6752769545189994 0.8717583021711470 T T T*

*0.5943354996862997 0.7186316796396373 0.1210865431064143 T T T*

*0.3527008427969143 0.3559179780748992 0.8723937208247938 T T T*

*0.4167139871894528 0.6912206913110162 0.5627768884734887 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3279822727932314 0.6884758339431641 0.9828561739758941 T T T*

*0.6543748833030996 0.3604125848676274 0.0046838607915211 T T T*

Image 4:

**E= -96.99034751 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.4516757917846376 0.9186888776848112 0.1788521132166274 T T T*

*0.7894971982024911 0.1226801760607212 0.7396296622979974 T T T*

*0.0795978586730959 0.4225890665977289 0.2364436541057207 T T T*

*0.0439071400344004 0.6655818852900043 0.7458456311014854 T T T*

*0.3815732811296487 0.3522828871696329 0.7497211768047943 T T T*

*0.5053784277076128 0.7668573453495139 0.6717651586045951 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7097591879498661 0.0382323077906053 0.8528793660243422 T T T*

*0.9812491404235297 0.3612848819379243 0.1322394160793603 T T T*

*0.0080921317457329 0.6701137846786359 0.8715163755410653 T T T*

*0.5707665241547525 0.7583741880759246 0.1369694249497871 T T T*

*0.3560481674461700 0.3622993745018732 0.8748997616043307 T T T*

*0.4147709966798952 0.6916426794950695 0.5642444311589921 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3136000281320915 0.6906565475608725 0.9835912221790603 T T T*

*0.6493788680790656 0.3421363566206016 0.0006081630709145 T T T*

Image 5:

**E= -97.52039095 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.5242298883374524 0.8869950715832111 0.1992194810457820 T T T*

*0.7916684711803836 0.1243699253191842 0.7404365514599208 T T T*

*0.0752381720942475 0.4183052558467327 0.2398419489209097 T T T*

*0.0450491383833011 0.6651290335891404 0.7490508100721300 T T T*

*0.3809975245357871 0.3569764715730978 0.7518258706057276 T T T*

*0.5056157429630205 0.7670434777343229 0.6717770047246583 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7096801665291731 0.0359292795711778 0.8524769340678723 T T T*

*0.9772051587107115 0.3573616909724624 0.1357094729686492 T T T*

*0.0062506260423064 0.6688294856045900 0.8746921167643124 T T T*

*0.5826346440980595 0.7500586491478983 0.1372204631605430 T T T*

*0.3554753577209366 0.3669833569412667 0.8771334044142051 T T T*

*0.4155490525253999 0.6916917252953132 0.5639204362515324 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3125124382841926 0.6963388802900556 0.9900850757157442 T T T*

*0.6454623725328933 0.3331685323198341 0.0015390942094381 T T T*

Image 6:

**E= -97.80364959 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.5703004664129364 0.8385887234712112 0.2255808064373986 T T T*

*0.7885849173612309 0.1256542914117823 0.7446665214558635 T T T*

*0.0717956130708906 0.4109640237577529 0.2459166204573336 T T T*

*0.0489447091701109 0.6629732064921123 0.7528736946563201 T T T*

*0.3783409488310993 0.3594999395396995 0.7536745732636734 T T T*

*0.5082167860701132 0.7659955102844211 0.6704559615350694 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7076546573434005 0.0353582245294367 0.8562053430374604 T T T*

*0.9767673655309150 0.3538618415722884 0.1408692015237696 T T T*

*0.0099145484590858 0.6688781792850774 0.8781935141073322 T T T*

*0.6009335343565775 0.7257393552616709 0.1293501315272265 T T T*

*0.3535249303402614 0.3683768465477402 0.8788502836708439 T T T*

*0.4207967115563045 0.6915504893375566 0.5615701409690443 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3174319592916311 0.6989096444499391 0.9957819459117742 T T T*

*0.6447561816789006 0.3368070361158010 0.0075936831817873 T T T*

Image 7:

**E= -97.99573378 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.5950417532009029 0.7649779348009447 0.2448861568119906 T T T*

*0.7774645031211166 0.1194490944136962 0.7506413299358039 T T T*

*0.0695909729755261 0.4029872750865744 0.2509886871860412 T T T*

*0.0529505028013890 0.6610039656731523 0.7539827119796220 T T T*

*0.3732350326098600 0.3536050942704724 0.7530187308250424 T T T*

*0.5119954314793087 0.7575062793711966 0.6661558927984117 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7030471163728889 0.0313035143153517 0.8630290411146223 T T T*

*0.9814984672687663 0.3551620431384331 0.1437164757727416 T T T*

*0.0138007419648441 0.6686626296813771 0.8789686642261362 T T T*

*0.6173317430632259 0.7039517665615576 0.1262837936815890 T T T*

*0.3511430400854774 0.3643890770242124 0.8780490676505562 T T T*

*0.4292917125665858 0.6900326840731389 0.5555594272242359 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3219355242233831 0.6971258161635516 0.9999286338366214 T T T*

*0.6459735635676934 0.3421387236823276 0.0120037641017855 T T T*

Image 8:

**E= -98.07796452 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.6230898137545392 0.7178371866005603 0.2536179730500907 T T T*

*0.7863507607956999 0.1014851534357272 0.7543542067802799 T T T*

*0.0737998177998523 0.3752083037932119 0.2518811261084783 T T T*

*0.0401603765670261 0.6605880576201697 0.7527987276789192 T T T*

*0.3730026312263368 0.3082598131182707 0.7515885645828766 T T T*

*0.4978183947105004 0.7339907228074922 0.6623171252430555 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.7072119380602998 0.0235847821388894 0.8689619907479790 T T T*

*0.9861047195743539 0.3452178509598236 0.1458014421888635 T T T*

*0.0102766256846715 0.6673594623159438 0.8779883311608023 T T T*

*0.6374617245195171 0.6896775287014701 0.1293530060179190 T T T*

*0.3494769703101718 0.3385230530538320 0.8751895108172913 T T T*

*0.4338326285639796 0.6857527840983242 0.5465152995787337 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3261508276828298 0.6830890514721832 0.0027461550605071 T T T*

*0.6530587824175720 0.3407514248925390 0.0114069218470427 T T T*

Image 9 (final structure):

**E= -98.06715013 eV**

*H O Ni*

*1.00000000000000*

*5.4178834167702998 0.0018068709665042 0.3592927455615510*

*-2.6980566415456799 4.6549740619897300 -0.2270545498800670*

*0.5196987064184510 -0.0811684665641636 7.8198643353819097*

*H O Ni*

*9 8 3*

*Selective dynamics*

*Direct*

*0.6120745523356348 0.6824309126569688 0.2533858766948427 T T T*

*0.7455965336924564 0.0628749312430088 0.7540627929549046 T T T*

*0.0730048688476188 0.3699149964531472 0.2512440049040237 T T T*

*0.9966050448955528 0.6313875768978718 0.7509694066837369 T T T*

*0.3793433252623544 0.2885908726561013 0.7479435205194065 T T T*

*0.4157900375616350 0.6753515225146671 0.6584226599695029 T T T*

*0.4699685612933777 0.8716573952678175 0.5057139192974418 F F F*

*0.5427363121372366 0.3948800853860561 0.4659136283001288 F F F*

*0.7122539704205764 0.2806779428816810 0.3350161296406213 F F F*

*0.3064941985107410 0.0105443878390261 0.1275674635994974 F F F*

*0.6907022666474560 0.0187590279623180 0.8757260687506658 T T T*

*0.9871691084285530 0.3465857202435529 0.1451496620064603 T T T*

*0.9962699464548592 0.6533960202637061 0.8755762388998036 T T T*

*0.6327152899797781 0.6738695330566458 0.1282562501525888 T T T*

*0.3495746287484423 0.3329519627116753 0.8690927095849688 T T T*

*0.4191963367138740 0.6739327561270443 0.5332145230109617 T T T*

*0.5875614264943749 0.2379897032527438 0.4464404812470377 F F F*

*0.9971552325375370 0.0107370201785741 0.0031328272979820 F F F*

*0.3220736013186141 0.6781885430720109 0.0020079337493826 T T T*

*0.6444506920659734 0.3321547562483076 0.0092705732035654 T T T*

**γ-NiOOH:**

**E = -312.45371eV**

*gamma*

*1.00000000000000*

*4.9396681595998215 -0.0062114142560077 0.0336291725896149*

*-0.0112559782964949 8.3839560219648899 -0.0146961860617301*

*-3.4583804092534445 -0.0190279776467257 14.1199443792629360*

*H O Na Ni*

*16 32 4 12*

*Direct*

*0.1684121343776385 0.6356874635420224 0.5125858967538304*

*0.0778943683645085 0.6448209679211747 0.3988082686107692*

*0.0788099164372080 0.2909040634774306 0.4078697781102357*

*0.1506903038368252 0.2816203306531273 0.5193230389779204*

*0.6474683176158987 0.0643808726443419 0.5199561766213593*

*0.5858582838753531 0.0715393303526589 0.4058582224391464*

*0.5810695043418598 0.4246639956888673 0.4017057467714093*

*0.6458837356291708 0.4213636827922794 0.5135468096718848*

*0.6460764672771849 0.8095475059155955 0.0182442338749864*

*0.5975756308448248 0.7975930864852954 0.9042459742650267*

*0.5961394181837220 0.4593805271321130 0.9140920344197442*

*0.6096590319820941 0.4371847351853912 0.0235475702387443*

*0.1747157467141153 0.2203580567094758 0.0182264486888845*

*0.0947499551088662 0.2304792303931814 0.9049449955651008*

*0.0999057792696166 0.5663413468576209 0.9168768453132045*

*0.1353471680411548 0.5945578294018363 0.0258323396863006*

*0.0887099643037508 0.7053657328999401 0.4585213113387692*

*0.0202388017384686 0.2430568412850145 0.4616292866025702*

*0.5156021925283598 0.4629245432714301 0.4571040757263179*

*0.5831879019777234 0.8683415849576200 0.9575242158003199*

*0.5065232891762069 0.4053494595685418 0.9588373178283712*

*0.0961421621931753 0.1597779111892039 0.9593375760038918*

*0.0181161301413758 0.6221636643475156 0.9630629046264595*

*0.5929057987835037 0.7676840780622388 0.7789552925384151*

*0.0602503840609308 0.2714232757360838 0.7755339359720637*

*0.7723508390965876 0.7679540143098746 0.6353082727838594*

*0.3156561179349978 0.2715744317831087 0.6439850821652596*

*0.7766137584562276 0.1040321069277555 0.6375307872381637*

*0.3119392043853036 0.5991089734641492 0.6415947408932265*

*0.5949151557022230 0.1042011160279573 0.7808977072490912*

*0.0589317858912737 0.6017194610808220 0.7730366575609788*

*0.8105498554047273 0.4343823463201301 0.6412508236932748*

*0.5665824427275097 0.4377649258273256 0.7760525771455463*

*0.5849290309783940 0.7725917891816431 0.2824293762473667*

*0.0506063296827846 0.2702965554791063 0.2733883611032170*

*0.7667353293657782 0.7716779552382020 0.1390985047350889*

*0.3045269496093900 0.2658592884187271 0.1413970925787943*

*0.7965111973872596 0.1029200636543999 0.1400523008448337*

*0.3037789376210169 0.6020398076491463 0.1464154985267103*

*0.5525683806169501 0.1049548082644071 0.2765476669279616*

*0.0472376343750126 0.6067650616530561 0.2767824584636098*

*0.7712200480824644 0.4378232404198471 0.1392781818962272*

*0.5850268573535587 0.4337365250732664 0.2798484228869343*

*0.3096214050136685 0.9372011396087963 0.6424507519892426*

*0.0548127112629143 0.9346277563873735 0.7736168999745650*

*0.3005210964252808 0.9364324249754279 0.1436903394698504*

*0.0467476874780717 0.9425875967780905 0.2764577145675851*

*0.5837893506442842 0.0017218701499163 0.4601732289650368*

*0.1058554387677649 0.9770184778840419 0.4589215419081117*

*0.6152634347745509 0.1404899043440350 0.9520394683658719*

*0.0951012607567810 0.8868731181080409 0.9400792302385350*

*0.6124197163485053 0.7302031692728903 0.4610353700450836*

*0.6859275972654476 0.6036785123319069 0.7075882125327946*

*0.6869632604066480 0.2684029452041050 0.7093624822442829*

*0.6768415636623270 0.6045257391488321 0.2108132337458221*

*0.6762927230619139 0.2710603693882565 0.2082187697423732*

*0.1859619506860359 0.1023717641510292 0.7093050431174127*

*0.1833000754029009 0.7693529822496077 0.7070528990835361*

*0.1876750657199732 0.4361687954325967 0.7089581539386485*

*0.1748487050427291 0.1034126439512563 0.2083183991859135*

*0.1757829850613368 0.7714876711126256 0.2113277146094872*

*0.1776208740889540 0.4370933379440602 0.2098167887643272*

*0.6833403629612288 0.9358698588277120 0.7079783390066445*

*0.6745205456936176 0.9363073415063943 0.2097205471190390*