

Supporting Information

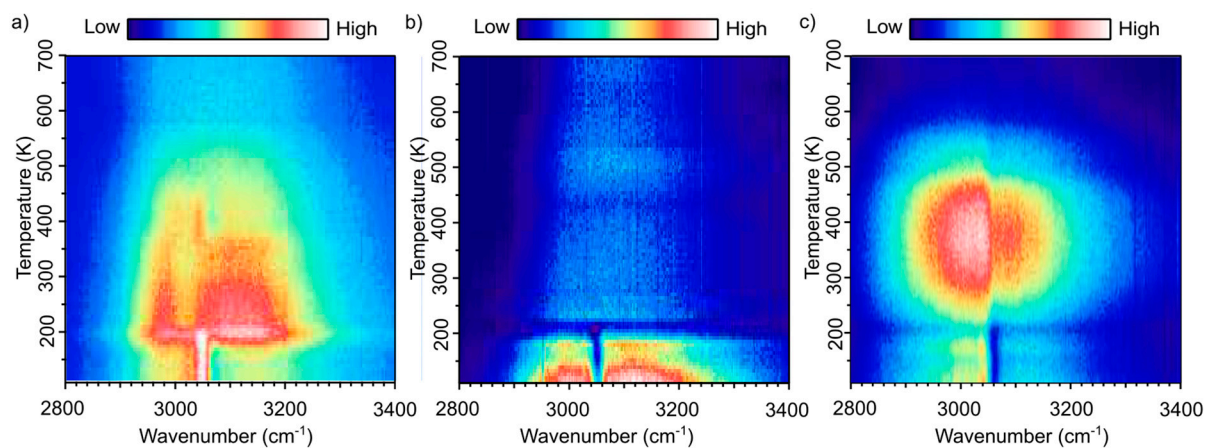


Figure S1, False color plot of temperature dependent SFG spectra recorded from a) Ni(111)-naphthalene, b) Ni(111)-O (2x2) naphthalene and c) Ni(111)-NiO-naphthalene. The slices presented in figure 3 are cut from the data in this figure.

Coordinates for optimized structures

Table S1. Naphthalene on Ni(111), ground state

i =	200, E = -24441.6135972239		
Ni	12.2813150153	11.3449928481	0.0000000000
Ni	12.2813150153	7.0906205301	0.0000000000
Ni	8.5969205107	4.9634343710	0.0000000000
Ni	11.0531835137	4.9634343710	0.0000000000
Ni	13.5094465168	4.9634343710	0.0000000000
Ni	7.3687890092	11.3449928481	0.0000000000
Ni	9.8250520122	7.0906205301	0.0000000000
Ni	14.7375780183	11.3449928481	0.0000000000
Ni	11.0531835137	9.2178066891	0.0000000000
Ni	14.7375780183	2.8362482120	0.0000000000
Ni	15.9657095198	4.9634343710	0.0000000000
Ni	14.7375780183	7.0906205301	0.0000000000
Ni	8.5969205107	9.2178066891	0.0000000000
Ni	6.1406575076	9.2178066891	0.0000000000
Ni	8.5969205107	0.7090620530	0.0000000000
Ni	6.1406575076	0.7090620530	0.0000000000
Ni	9.8250520122	11.3449928481	0.0000000000
Ni	9.8250520122	2.8362482120	0.0000000000
Ni	13.5094465168	9.2178066891	0.0000000000
Ni	17.1938410213	7.0906205301	0.0000000000
Ni	18.4219725229	9.2178066891	0.0000000000
Ni	19.6501040244	11.3449928481	0.0000000000
Ni	4.9125260061	2.8362482120	0.0000000000
Ni	11.0531835137	0.7090620530	0.0000000000
Ni	13.5094465168	0.7090620530	0.0000000000
Ni	12.2813150153	2.8362482120	0.0000000000
Ni	7.3687890092	2.8362482120	0.0000000000
Ni	1.2281315015	0.7090620530	0.0000000000
Ni	3.6843945046	0.7090620530	0.0000000000
Ni	7.3687890092	7.0906205301	0.0000000000
Ni	2.4562630031	2.8362482120	0.0000000000
Ni	6.1406575076	4.9634343710	0.0000000000
Ni	4.9125260061	7.0906205301	0.0000000000
Ni	17.1938410214	11.3449928481	0.0000000000
Ni	15.9657095198	9.2178066891	0.0000000000
Ni	3.6843945046	4.9634343710	0.0000000000
Ni	14.7375780183	4.2543723180	2.0052540942
Ni	15.9657095198	6.3815584771	2.0052540942
Ni	12.2813150153	4.2543723180	2.0052540942
Ni	13.5094465168	6.3815584771	2.0052540942
Ni	14.7375780183	8.5087446361	2.0052540942
Ni	2.4562630031	0.0000000000	2.0052540942
Ni	1.2281315015	2.1271861590	2.0052540942
Ni	18.4219725229	10.6359307951	2.0052540942
Ni	15.9657095198	10.6359307951	2.0052540942
Ni	12.2813150153	0.0000000000	2.0052540942
Ni	4.9125260061	0.0000000000	2.0052540942

Ni	11.0531835137	2.1271861590	2.0052540942
Ni	9.8250520122	0.0000000000	2.0052540942
Ni	13.5094465168	2.1271861590	2.0052540942
Ni	6.1406575076	6.3815584771	2.0052540942
Ni	2.4562630031	4.2543723180	2.0052540942
Ni	3.6843945046	6.3815584771	2.0052540942
Ni	4.9125260061	4.2543723180	2.0052540942
Ni	8.5969205107	10.6359307951	2.0052540942
Ni	0.0000000000	0.0000000000	2.0052540942
Ni	4.9125260061	8.5087446361	2.0052540942
Ni	6.1406575076	10.6359307951	2.0052540942
Ni	7.3687890092	8.5087446361	2.0052540942
Ni	8.5969205107	2.1271861590	2.0052540942
Ni	11.0531835137	6.3815584771	2.0052540942
Ni	8.5969205107	6.3815584771	2.0052540942
Ni	9.8250520122	4.2543723180	2.0052540942
Ni	12.2813150153	8.5087446361	2.0052540942
Ni	11.0531835137	10.6359307951	2.0052540942
Ni	9.8250520122	8.5087446361	2.0052540942
Ni	13.5094465168	10.6359307951	2.0052540942
Ni	17.1938410214	8.5087446361	2.0052540942
Ni	7.3687890092	0.0000000000	2.0052540942
Ni	6.1406575076	2.1271861590	2.0052540942
Ni	7.3687890092	4.2543723180	2.0052540942
Ni	3.6843945046	2.1271861590	2.0052540942
Ni	17.2018692797	9.9364669298	4.0221314960
Ni	18.4288977499	12.0572452027	4.0216296435
Ni	19.6600296120	9.9179226563	4.0235208224
Ni	11.0560233092	3.5528470899	4.0460342679
Ni	3.6873121878	3.5379598113	4.0224958924
Ni	6.1500806377	7.7840583932	4.0324147282
Ni	4.9011301166	5.6732248425	3.9850973503
Ni	8.5992632374	7.7768153941	4.0889849618
Ni	4.9182695490	1.4040445602	4.0228481615
Ni	12.2830843978	9.9127910721	4.0232884790
Ni	13.5181510073	12.0454089670	4.0219901729
Ni	14.7499646989	9.9319373038	4.0217727127
Ni	9.8165866502	9.8979690226	4.0383181829
Ni	8.6036452998	12.0373588302	4.0223903018
Ni	7.3877045273	9.8992582025	4.0392319347
Ni	11.0571183231	12.0354218057	4.0227805310
Ni	13.5244999985	7.7976521495	3.9876816932
Ni	9.8362425760	5.6625113505	4.0877610152
Ni	11.0518993962	7.7815917071	4.0231735531
Ni	12.2832701470	5.6494651401	4.0277375392
Ni	20.8872295679	12.0380166450	4.0224346475
Ni	9.8347810490	1.4451019448	4.0380972803
Ni	8.6064551676	3.5585537171	4.0373378974
Ni	7.3781093529	1.4183207126	4.0226605123
Ni	7.3801874859	5.6813461325	4.0362294923
Ni	14.7470263760	1.4046651608	4.0233854100

Ni	15.9780134086	12.0635260891	4.0221864617
Ni	18.4187591941	7.8064976017	4.0170052122
Ni	12.2892140524	1.4126219486	4.0222281397
Ni	13.5191725687	3.5338884285	4.0209458548
Ni	14.7488263570	5.6719562263	4.0179764120
Ni	17.1941216288	5.6756239309	4.0212547129
Ni	2.4633514262	1.4054927565	4.0238481544
Ni	6.1435218332	3.5373768775	4.0047124852
Ni	15.9736902883	3.5386647965	4.0231864003
Ni	15.9747996046	7.8088484944	4.0205951041
Ni	8.5216318900	4.9357674733	6.1013050176
Ni	11.1847817067	4.9281855302	6.1641515503
Ni	9.9123320503	7.0768336161	6.1033235188
Ni	14.7725348866	7.0852158100	6.0392792209
Ni	15.9898920979	4.9455226836	6.0439426946
Ni	9.8316094818	2.8405849784	6.1690292336
Ni	17.1848352054	7.0855948750	6.0433716999
Ni	2.4654725496	2.8109622215	6.0449681453
Ni	7.3392831982	2.8051383343	6.0307143867
Ni	8.6109157882	0.7016590901	6.0384335786
Ni	6.1509610877	0.6905670063	6.0419673541
Ni	17.2053412736	11.3457589789	6.0453583915
Ni	18.4125546679	9.2196403792	6.0440756674
Ni	15.9795536070	9.2185653264	6.0441673863
Ni	13.5948301113	4.9423509108	6.0301306346
Ni	12.3750479015	7.0858729811	5.9793506930
Ni	6.1118317376	9.2237935345	6.0353910911
Ni	8.6090082382	9.1955790404	6.2064484313
Ni	12.3309519379	2.7914362618	6.0343087160
Ni	13.5322825663	0.6858159327	6.0424994336
Ni	4.8464706047	7.0817875380	6.0251482562
Ni	6.0588140896	4.9380645244	5.9763290393
Ni	3.6613187676	4.9460975128	6.0392829929
Ni	11.0657030362	0.7004173984	6.0384534530
Ni	7.2643681831	7.0798135820	6.1638457325
Ni	9.8422845042	11.3279707486	6.0388802874
Ni	14.7559128753	11.3389852081	6.0436548930
Ni	13.5414936055	9.2108436055	6.0382726103
Ni	12.3019496762	11.3323760037	6.0421073594
Ni	14.7681066121	2.8098719289	6.0439911230
Ni	4.8983947727	2.8107193253	6.0398922860
Ni	1.2464923867	0.6848613631	6.0445627260
Ni	3.6980510569	0.6858864220	6.0438404186
Ni	7.3851472113	11.3285571595	6.0392679647
Ni	11.0999622006	9.2182861621	6.0341542709
Ni	19.6583540456	11.3409466800	6.0433327564
C	7.3534062099	6.4692157016	8.0888673752
C	7.4017996623	7.9001208160	8.1221281852
C	8.5802576071	5.6817892826	8.0155161140
C	9.8633035586	6.3916626298	8.0171194953
C	9.8901480286	7.8343371542	8.0642257674

C	8.6666436154	8.6145960919	8.1313061758
C	11.0906999594	5.6031216247	8.0797375807
C	11.0424471947	4.1723098348	8.1162796682
C	9.7771468718	3.4583652566	8.1064473563
C	8.5530274637	4.2385444222	8.0611382065
H	6.4401887468	5.9602012012	8.4084519512
H	6.5078692040	8.4415422261	8.4394630958
H	8.7036658361	9.5896362692	8.6246494878
H	10.8237764453	8.3186513341	8.3659200864
H	12.0044636840	6.1118248020	8.3987612521
H	11.9329920720	3.6288641009	8.4394299097
H	9.7405536284	2.4737615033	8.5809770389
H	7.6231922887	3.7526196462	8.3707068407

Table S2. Naphthalene on Ni(111)-O (2x2), ground state

i = 183, E = -24586.0534648148

Ni	12.2813150153	11.3449928481	0.0000000000
Ni	12.2813150153	7.0906205301	0.0000000000
Ni	8.5969205107	4.9634343710	0.0000000000
Ni	11.0531835137	4.9634343710	0.0000000000
Ni	13.5094465168	4.9634343710	0.0000000000
Ni	7.3687890092	11.3449928481	0.0000000000
Ni	9.8250520122	7.0906205301	0.0000000000
Ni	14.7375780183	11.3449928481	0.0000000000
Ni	11.0531835137	9.2178066891	0.0000000000
Ni	14.7375780183	2.8362482120	0.0000000000
Ni	15.9657095198	4.9634343710	0.0000000000
Ni	14.7375780183	7.0906205301	0.0000000000
Ni	8.5969205107	9.2178066891	0.0000000000
Ni	6.1406575076	9.2178066891	0.0000000000
Ni	8.5969205107	0.7090620530	0.0000000000
Ni	6.1406575076	0.7090620530	0.0000000000
Ni	9.8250520122	11.3449928481	0.0000000000
Ni	9.8250520122	2.8362482120	0.0000000000
Ni	13.5094465168	9.2178066891	0.0000000000
Ni	17.1938410213	7.0906205301	0.0000000000
Ni	18.4219725229	9.2178066891	0.0000000000
Ni	19.6501040244	11.3449928481	0.0000000000
Ni	4.9125260061	2.8362482120	0.0000000000
Ni	11.0531835137	0.7090620530	0.0000000000
Ni	13.5094465168	0.7090620530	0.0000000000
Ni	12.2813150153	2.8362482120	0.0000000000
Ni	7.3687890092	2.8362482120	0.0000000000
Ni	1.2281315015	0.7090620530	0.0000000000
Ni	3.6843945046	0.7090620530	0.0000000000
Ni	7.3687890092	7.0906205301	0.0000000000
Ni	2.4562630031	2.8362482120	0.0000000000
Ni	6.1406575076	4.9634343710	0.0000000000
Ni	4.9125260061	7.0906205301	0.0000000000
Ni	17.1938410214	11.3449928481	0.0000000000
Ni	15.9657095198	9.2178066891	0.0000000000
Ni	3.6843945046	4.9634343710	0.0000000000
Ni	14.7375780183	4.2543723180	2.0052540942
Ni	15.9657095198	6.3815584771	2.0052540942
Ni	12.2813150153	4.2543723180	2.0052540942
Ni	13.5094465168	6.3815584771	2.0052540942
Ni	14.7375780183	8.5087446361	2.0052540942
Ni	2.4562630031	0.0000000000	2.0052540942
Ni	1.2281315015	2.1271861590	2.0052540942
Ni	18.4219725229	10.6359307951	2.0052540942
Ni	15.9657095198	10.6359307951	2.0052540942
Ni	12.2813150153	0.0000000000	2.0052540942
Ni	4.9125260061	0.0000000000	2.0052540942
Ni	11.0531835137	2.1271861590	2.0052540942
Ni	9.8250520122	0.0000000000	2.0052540942

Ni	13.5094465168	2.1271861590	2.0052540942
Ni	6.1406575076	6.3815584771	2.0052540942
Ni	2.4562630031	4.2543723180	2.0052540942
Ni	3.6843945046	6.3815584771	2.0052540942
Ni	4.9125260061	4.2543723180	2.0052540942
Ni	8.5969205107	10.6359307951	2.0052540942
Ni	0.0000000000	0.0000000000	2.0052540942
Ni	4.9125260061	8.5087446361	2.0052540942
Ni	6.1406575076	10.6359307951	2.0052540942
Ni	7.3687890092	8.5087446361	2.0052540942
Ni	8.5969205107	2.1271861590	2.0052540942
Ni	11.0531835137	6.3815584771	2.0052540942
Ni	8.5969205107	6.3815584771	2.0052540942
Ni	9.8250520122	4.2543723180	2.0052540942
Ni	12.2813150153	8.5087446361	2.0052540942
Ni	11.0531835137	10.6359307951	2.0052540942
Ni	9.8250520122	8.5087446361	2.0052540942
Ni	13.5094465168	10.6359307951	2.0052540942
Ni	17.1938410214	8.5087446361	2.0052540942
Ni	7.3687890092	0.0000000000	2.0052540942
Ni	6.1406575076	2.1271861590	2.0052540942
Ni	7.3687890092	4.2543723180	2.0052540942
Ni	3.6843945046	2.1271861590	2.0052540942
Ni	17.1991275448	9.9097709095	4.0174118407
Ni	18.4219230931	12.0303670441	4.0177254374
Ni	19.6467664849	9.9082916699	4.0181209162
Ni	11.0521392957	3.5167828670	4.0903517767
Ni	3.6837303617	3.5198658933	4.0175093445
Ni	6.1416714357	7.7723578864	4.0231745707
Ni	4.9170974518	5.6541386779	4.0175321585
Ni	8.5896222318	7.7820612038	4.0903530646
Ni	4.9075027535	1.3999464648	4.0177432683
Ni	12.2837902712	9.9080160144	4.0195405025
Ni	13.5080369413	12.0284190101	4.0178867396
Ni	14.7337544018	9.9100121100	4.0176652712
Ni	9.8170490645	9.9058194489	4.0244317548
Ni	8.5962438455	12.0281654524	4.0178616951
Ni	7.3746050334	9.9080584518	4.0232197242
Ni	11.0516592436	12.0310805193	4.0830011278
Ni	13.5134473822	7.7817677261	4.0742135063
Ni	9.8294083108	5.6551996011	4.0167914072
Ni	11.0514450002	7.7753780690	4.0137648072
Ni	12.2763206925	5.6535227957	4.0143107986
Ni	20.8777615339	12.0328615381	4.0827977756
Ni	9.8193220508	1.4029809140	4.0233291768
Ni	8.5996443637	3.5199894659	4.0244725767
Ni	7.3727542317	1.4010012136	4.0173945213
Ni	7.3657033077	5.6577453163	4.0248983280
Ni	14.7320508746	1.4003778214	4.0182369720
Ni	15.9653961480	12.0332349903	4.0820392898
Ni	18.4219002318	7.7779518055	4.0822947563

Ni	12.2855564865	1.4028695747	4.0234842596
Ni	13.5050360696	3.5188884001	4.0244107655
Ni	14.7398003659	5.6539196147	4.0195278230
Ni	17.1880795254	5.6536920895	4.0181905357
Ni	2.4601457683	1.4001907166	4.0176827746
Ni	6.1418898018	3.5248854026	4.0820151272
Ni	15.9633257215	3.5237395050	4.0831272882
Ni	15.9663805338	7.7746683140	4.0173795963
Ni	8.6010823469	4.9377022844	5.9774182909
Ni	11.0540663798	4.8940296731	6.1004176385
Ni	9.7896419753	7.0843630660	6.0993455870
Ni	14.7157884597	7.0783028891	6.1075267091
Ni	15.9623124434	4.9045992540	6.1095048873
Ni	9.8514028386	2.8214360515	6.1531788370
Ni	17.2195270804	7.0775551544	6.1081251093
Ni	2.4294488349	2.8222877171	6.1075203875
Ni	7.3411261244	2.8225054069	6.1072480938
Ni	8.5938300097	0.6464484729	6.1066863526
Ni	6.1397907797	0.6815853290	5.9703352316
Ni	17.1687394286	11.3312606879	6.1073639643
Ni	18.4223515125	9.1599843896	6.1082905164
Ni	15.9684515674	9.1919729629	5.9704747987
Ni	13.5054730984	4.9356601777	5.9762042008
Ni	12.3274951506	7.0914266001	6.0914364562
Ni	6.1433952990	9.1884635342	5.9725089386
Ni	8.5918223730	9.1597872677	6.1529836765
Ni	12.2534477022	2.8186899097	6.1523739577
Ni	13.5089097975	0.6500776108	6.1096910724
Ni	4.8823237468	7.0761156662	6.1063181288
Ni	6.1399263923	4.9024791592	6.1078603404
Ni	3.6833484717	4.9360226262	5.9703432578
Ni	11.0522955237	0.6847540306	5.9724149934
Ni	7.3939008093	7.0778600192	6.1530179475
Ni	9.8507545574	11.3326943896	6.1093552480
Ni	14.7636324036	11.3316725323	6.1080191096
Ni	13.5120280837	9.1642481145	6.1084330913
Ni	12.2533391187	11.3300852561	6.1085971735
Ni	14.7631715946	2.8230055176	6.1098927031
Ni	4.9384006687	2.8230579441	6.1076444327
Ni	1.2279401762	0.6823991504	5.9702725605
Ni	3.6830003620	0.6508864793	6.1083745766
Ni	7.3421040387	11.3320154475	6.1084271348
Ni	11.0495173548	9.1899330205	5.9764664317
Ni	19.6768443835	11.3321467770	6.1074499471
O	3.6845721388	2.1001524555	7.1991166122
O	6.1133628912	6.3406863571	7.2109897167
O	8.5962290061	10.6324250167	7.2151992651
O	8.5729143483	2.0801138220	7.2108297726
O	11.0717726323	6.3654479278	7.1346181075
O	13.5092219998	10.6112592888	7.2019948353
O	13.5291617440	2.0868161399	7.2166634076

O	15.9668766852	6.3531230052	7.2016977657
O	18.4234967046	10.6090240190	7.1995696875
C	8.5811606473	6.4320603659	9.3599260822
C	8.6332444029	7.8148214576	9.3665750258
C	9.7606490381	5.6623249677	9.5386511474
C	11.0059874562	6.3406689233	9.7811926918
C	11.0152536748	7.7611816178	9.8290784439
C	9.8609359495	8.4843689066	9.6003479723
C	12.2045054625	5.5782742737	9.8289107984
C	12.1868209139	4.2167202265	9.5968869008
C	10.9593132025	3.5492666715	9.3568176451
C	9.7687788232	4.2550253992	9.3516768972
H	7.6372616631	5.9213742583	9.1647005510
H	7.7278586748	8.3953821628	9.1854066921
H	9.8872319145	9.5741330314	9.5811810490
H	11.9647496295	8.2759311225	9.9882080800
H	13.1515567275	6.0967949797	9.9904675172
H	13.1168280326	3.6481010283	9.5774957151
H	10.9556752447	2.4745647363	9.1707232429
H	8.8282703166	3.7388820559	9.1532238099

Table S3. Naphthalene on NiO

i = 50, E = -25592.5587255368

Ni	12.2813150153	11.3449928481	0.0000000000
Ni	12.2813150153	7.0906205301	0.0000000000
Ni	8.5969205107	4.9634343710	0.0000000000
Ni	11.0531835137	4.9634343710	0.0000000000
Ni	13.5094465168	4.9634343710	0.0000000000
Ni	7.3687890092	11.3449928481	0.0000000000
Ni	9.8250520122	7.0906205301	0.0000000000
Ni	14.7375780183	11.3449928481	0.0000000000
Ni	11.0531835137	9.2178066891	0.0000000000
Ni	14.7375780183	2.8362482120	0.0000000000
Ni	15.9657095198	4.9634343710	0.0000000000
Ni	14.7375780183	7.0906205301	0.0000000000
Ni	8.5969205107	9.2178066891	0.0000000000
Ni	6.1406575076	9.2178066891	0.0000000000
Ni	8.5969205107	0.7090620530	0.0000000000
Ni	6.1406575076	0.7090620530	0.0000000000
Ni	9.8250520122	11.3449928481	0.0000000000
Ni	9.8250520122	2.8362482120	0.0000000000
Ni	13.5094465168	9.2178066891	0.0000000000
Ni	17.1938410213	7.0906205301	0.0000000000
Ni	18.4219725229	9.2178066891	0.0000000000
Ni	19.6501040244	11.3449928481	0.0000000000
Ni	4.9125260061	2.8362482120	0.0000000000
Ni	11.0531835137	0.7090620530	0.0000000000
Ni	13.5094465168	0.7090620530	0.0000000000
Ni	12.2813150153	2.8362482120	0.0000000000
Ni	7.3687890092	2.8362482120	0.0000000000
Ni	1.2281315015	0.7090620530	0.0000000000
Ni	3.6843945046	0.7090620530	0.0000000000
Ni	7.3687890092	7.0906205301	0.0000000000
Ni	2.4562630031	2.8362482120	0.0000000000
Ni	6.1406575076	4.9634343710	0.0000000000
Ni	4.9125260061	7.0906205301	0.0000000000
Ni	17.1938410214	11.3449928481	0.0000000000
Ni	15.9657095198	9.2178066891	0.0000000000
Ni	3.6843945046	4.9634343710	0.0000000000
Ni	14.7375780183	4.2543723180	2.0052540942
Ni	15.9657095198	6.3815584771	2.0052540942
Ni	12.2813150153	4.2543723180	2.0052540942
Ni	13.5094465168	6.3815584771	2.0052540942
Ni	14.7375780183	8.5087446361	2.0052540942
Ni	2.4562630031	0.0000000000	2.0052540942
Ni	1.2281315015	2.1271861590	2.0052540942
Ni	18.4219725229	10.6359307951	2.0052540942
Ni	15.9657095198	10.6359307951	2.0052540942
Ni	12.2813150153	0.0000000000	2.0052540942
Ni	4.9125260061	0.0000000000	2.0052540942
Ni	11.0531835137	2.1271861590	2.0052540942
Ni	9.8250520122	0.0000000000	2.0052540942

Ni	13.5094465168	2.1271861590	2.0052540942
Ni	6.1406575076	6.3815584771	2.0052540942
Ni	2.4562630031	4.2543723180	2.0052540942
Ni	3.6843945046	6.3815584771	2.0052540942
Ni	4.9125260061	4.2543723180	2.0052540942
Ni	8.5969205107	10.6359307951	2.0052540942
Ni	0.0000000000	0.0000000000	2.0052540942
Ni	4.9125260061	8.5087446361	2.0052540942
Ni	6.1406575076	10.6359307951	2.0052540942
Ni	7.3687890092	8.5087446361	2.0052540942
Ni	8.5969205107	2.1271861590	2.0052540942
Ni	11.0531835137	6.3815584771	2.0052540942
Ni	8.5969205107	6.3815584771	2.0052540942
Ni	9.8250520122	4.2543723180	2.0052540942
Ni	12.2813150153	8.5087446361	2.0052540942
Ni	11.0531835137	10.6359307951	2.0052540942
Ni	9.8250520122	8.5087446361	2.0052540942
Ni	13.5094465168	10.6359307951	2.0052540942
Ni	17.1938410214	8.5087446361	2.0052540942
Ni	7.3687890092	0.0000000000	2.0052540942
Ni	6.1406575076	2.1271861590	2.0052540942
Ni	7.3687890092	4.2543723180	2.0052540942
Ni	3.6843945046	2.1271861590	2.0052540942
Ni	17.1345503862	9.8927082142	4.0282468403
Ni	18.3626022775	12.0200910068	4.0284923422
Ni	19.5909743749	9.8924889518	4.0285011791
Ni	10.9927990845	3.5107501291	4.0275305597
Ni	3.6253335099	3.5110513071	4.0282423108
Ni	6.0816100480	7.7652485925	4.0280262795
Ni	4.8533855921	5.6381525949	4.0281756931
Ni	8.5368916798	7.7648089267	4.0273260074
Ni	4.8534017138	1.3839637877	4.0282204377
Ni	12.2222998142	9.8924022929	4.0282559154
Ni	13.4502974395	12.0200670371	4.0281356220
Ni	14.6784560727	9.8929695588	4.0278729421
Ni	9.7659539115	9.8923920141	4.0276673932
Ni	8.5380251530	12.0198985598	4.0278032777
Ni	7.3096227250	9.8926356470	4.0276680713
Ni	10.9943888789	12.0195323639	4.0284065041
Ni	13.4506578418	7.7657590453	4.0282126040
Ni	9.7654687029	5.6380064172	4.0269887839
Ni	10.9944895960	7.7650783352	4.0279151171
Ni	12.2220848176	5.6389923699	4.0278522487
Ni	20.8189689864	12.0198293318	4.0280823610
Ni	9.7659305062	1.3841789025	4.0279815751
Ni	8.5369621645	3.5107308955	4.0272191197
Ni	7.3095712110	1.3839918124	4.0282352931
Ni	7.3088872060	5.6377859001	4.0272934531
Ni	14.6786202786	1.3842326251	4.0277979901
Ni	15.9063670892	12.0201599738	4.0283075246
Ni	18.3628990423	7.7653038177	4.0282552115

Ni	12.2221698563	1.3840513809	4.0275905346
Ni	13.4499617173	3.5114306546	4.0277847657
Ni	14.6782290431	5.6386284990	4.0281776741
Ni	17.1347721434	5.6382241685	4.0281383994
Ni	2.3973693311	1.3840767916	4.0284500288
Ni	6.0814713771	3.5110369667	4.0275695009
Ni	15.9064244876	3.5116066160	4.0284608563
Ni	15.9067709938	7.7654843352	4.0278865845
O	15.1917884402	4.5165533399	5.6898528070
O	16.4202584696	6.6440259279	5.6886588072
O	12.7378145430	4.5158034988	5.6909715855
O	13.9646386095	6.6434736928	5.6885950171
O	15.1917918166	8.7709439041	5.6906239459
O	2.9110219269	0.2627896180	5.6879771690
O	1.6830088877	2.3897395329	5.6877738232
O	18.8764851649	10.8983026726	5.6879056729
O	16.4202119156	10.8982244500	5.6884116961
O	12.7364846114	0.2620223940	5.6892635059
O	5.3672710873	0.2623956517	5.6890478656
O	11.5099525579	2.3880853705	5.6890399371
O	10.2794530604	0.2622622839	5.6878670167
O	13.9653858627	2.3884467668	5.6877886399
O	6.5938314818	6.6431058761	5.6872212474
O	2.9107096720	4.5170518613	5.6891333146
O	4.1386109270	6.6440968738	5.6891611034
O	5.3667717686	4.5168278612	5.6897628879
O	9.0512150572	10.9001701978	5.6880722599
O	0.4542791691	0.2622684119	5.6912369720
O	5.3668442487	8.7711343366	5.6882626997
O	6.5952158697	10.8990359922	5.6889719838
O	7.8232521394	8.7735329751	5.6884522378
O	9.0498730473	2.3889109590	5.6878091512
O	11.5090255327	6.6449400594	5.6800980587
O	9.0517617305	6.6483398056	5.6853381528
O	10.2839871866	4.5144635392	5.6831458612
O	12.7358029181	8.7720057953	5.6889825370
O	11.5074367245	10.8984502753	5.6893563578
O	10.2798747315	8.7734924267	5.6908203819
O	13.9640833855	10.8983880800	5.6886718127
O	17.6482273322	8.7711857736	5.6884509583
O	7.8232824445	0.2621698411	5.6892305311
O	6.5952095343	2.3894674859	5.6901573569
O	7.8221477502	4.5164816370	5.6874589635
O	4.1398058797	2.3901930839	5.6890084047
Ni2	9.0302936519	5.2137696654	6.9726316806
Ni2	11.4870330952	5.2143178646	6.9764791778
Ni2	10.2593782595	7.3413281909	6.9762985351
Ni2	15.1702862829	7.3402936058	6.9799624928
Ni2	16.3984768496	5.2134537985	6.9801495417
Ni2	10.2583685930	3.0846562351	6.9775151795
Ni2	17.6266113985	7.3406358845	6.9800938739

Ni2	2.8891505661	3.0860809962	6.9799700549
Ni2	7.8016381267	3.0859851718	6.9796472785
Ni2	9.0295652470	0.9589048347	6.9798603255
Ni2	6.5736391443	0.9588954427	6.9803702471
Ni2	17.6267163256	11.5948019487	6.9800425991
Ni2	18.8547013459	9.4677950120	6.9800037946
Ni2	16.3987532065	9.4677799698	6.9800554445
Ni2	13.9425599617	5.2136567899	6.9808817202
Ni2	12.7139212885	7.3403221079	6.9789746428
Ni2	6.5733889359	9.4685228180	6.9792213149
Ni2	9.0301595411	9.4691265175	6.9791138034
Ni2	12.7154321237	3.0858853929	6.9797483287
Ni2	13.9426465721	0.9590063496	6.9801046046
Ni2	5.3450615171	7.3403672098	6.9797169406
Ni2	6.5730501908	5.2136854257	6.9795439188
Ni2	4.1171974079	5.2134778759	6.9803067788
Ni2	11.4866445023	0.9583831799	6.9790927427
Ni2	7.8005730955	7.3418561286	6.9773344971
Ni2	10.2579102922	11.5953171202	6.9799478345
Ni2	15.1705459229	11.5948056369	6.9801496180
Ni2	13.9421048604	9.4677713328	6.9800400314
Ni2	12.7142650550	11.5948432522	6.9801650967
Ni2	15.1705401287	3.0859837411	6.9799421987
Ni2	5.3457134818	3.0864438055	6.9802621896
Ni2	1.6615293160	0.9593216689	6.9800129821
Ni2	4.1172717361	0.9591297574	6.9800146759
Ni2	7.8017995480	11.5951600786	6.9801786360
Ni2	11.4865806859	9.4680193517	6.9808365608
Ni2	20.0829533145	11.5948488098	6.9800651845
O	17.6156488510	10.1704055790	8.1281483879
O	18.8434414924	12.2981470826	8.1288188112
O	20.0722579808	10.1697641702	8.1287910734
O	11.4755496605	3.7907503355	8.1265105675
O	4.1065919503	3.7886594792	8.1292406986
O	6.5609592638	8.0464341343	8.1276048136
O	5.3336400472	5.9152424658	8.1316178441
O	9.0207356405	8.0436278704	8.1249913109
O	5.3344864743	1.6622158702	8.1292983569
O	12.7031095659	10.1700568617	8.1291253105
O	13.9314597914	12.2978357661	8.1284329698
O	15.1591537182	10.1704131408	8.1280223422
O	10.2461127405	10.1707914889	8.1305379558
O	9.0191072902	12.2975779703	8.1286603488
O	7.7909930906	10.1706202941	8.1302404882
O	11.4751271524	12.2976680638	8.1281648755
O	13.9302505080	8.0426602006	8.1291679136
O	10.2453451743	5.9157284110	8.1207024317
O	11.4752926044	8.0415536646	8.1311096296
O	12.7016100914	5.9168894132	8.1311496500
O	21.2998010667	12.2974710723	8.1286532900
O	10.2493534736	1.6584793019	8.1273806018

O	9.0203669096	3.7936331808	8.1232029077
O	7.7894154068	1.6614167279	8.1318601387
O	7.7947127516	5.9159451592	8.1241749623
O	15.1595489511	1.6620480313	8.1285997633
O	16.3876805165	12.2980082248	8.1296057191
O	18.8438821195	8.0433052608	8.1294704235
O	12.7037295581	1.6616255636	8.1302123161
O	13.9309182929	3.7881640398	8.1306795337
O	15.1590011543	5.9162318977	8.1290167233
O	17.6158568976	5.9160102397	8.1283299574
O	2.8782408264	1.6617330210	8.1279739491
O	6.5614176242	3.7884629990	8.1325534285
O	16.3875264297	3.7888158927	8.1280940695
O	16.3874319769	8.0428605183	8.1280025985
C	7.5053118990	5.8225587464	10.8809987344
C	7.5877840397	7.2139826830	10.8878419347
C	8.6755750143	5.0270469641	10.9348497216
C	9.9561418898	5.6752426023	10.9715591750
C	10.0089439782	7.0901511315	10.9548293172
C	8.8395257678	7.8472337158	10.9191055450
C	11.1285322132	4.8812657519	10.9574066518
C	11.0467604949	3.4907204742	10.9214270207
C	9.7961516550	2.8559152559	10.8871867049
C	8.6255904626	3.6134515788	10.8808548087
H	6.5351473023	5.3315027861	10.8010285958
H	6.6791213477	7.8086683185	10.8154651333
H	8.8990108640	8.9335564256	10.8720533816
H	10.9807288518	7.5837629643	10.9283382672
H	12.1009934625	5.3737919011	10.9320301057
H	11.9581939849	2.8966436237	10.8751593182
H	9.7380248265	1.7715283019	10.8141934302
H	7.6560890593	3.1214476536	10.7993161928

Table S4. Dissociated naphthalene on Ni(111)-O (2x2). Flat

i =	200,	E =	-24586.0165140281
Ni	12.2813150153	11.3449928481	0.0000000000
Ni	12.2813150153	7.0906205301	0.0000000000
Ni	8.5969205107	4.9634343710	0.0000000000
Ni	11.0531835137	4.9634343710	0.0000000000
Ni	13.5094465168	4.9634343710	0.0000000000
Ni	7.3687890092	11.3449928481	0.0000000000
Ni	9.8250520122	7.0906205301	0.0000000000
Ni	14.7375780183	11.3449928481	0.0000000000
Ni	11.0531835137	9.2178066891	0.0000000000
Ni	14.7375780183	2.8362482120	0.0000000000
Ni	15.9657095198	4.9634343710	0.0000000000
Ni	14.7375780183	7.0906205301	0.0000000000
Ni	8.5969205107	9.2178066891	0.0000000000
Ni	6.1406575076	9.2178066891	0.0000000000
Ni	8.5969205107	0.7090620530	0.0000000000
Ni	6.1406575076	0.7090620530	0.0000000000
Ni	9.8250520122	11.3449928481	0.0000000000
Ni	9.8250520122	2.8362482120	0.0000000000
Ni	13.5094465168	9.2178066891	0.0000000000
Ni	17.1938410213	7.0906205301	0.0000000000
Ni	18.4219725229	9.2178066891	0.0000000000
Ni	19.6501040244	11.3449928481	0.0000000000
Ni	4.9125260061	2.8362482120	0.0000000000
Ni	11.0531835137	0.7090620530	0.0000000000
Ni	13.5094465168	0.7090620530	0.0000000000
Ni	12.2813150153	2.8362482120	0.0000000000
Ni	7.3687890092	2.8362482120	0.0000000000
Ni	1.2281315015	0.7090620530	0.0000000000
Ni	3.6843945046	0.7090620530	0.0000000000
Ni	7.3687890092	7.0906205301	0.0000000000
Ni	2.4562630031	2.8362482120	0.0000000000
Ni	6.1406575076	4.9634343710	0.0000000000
Ni	4.9125260061	7.0906205301	0.0000000000
Ni	17.1938410214	11.3449928481	0.0000000000
Ni	15.9657095198	9.2178066891	0.0000000000
Ni	3.6843945046	4.9634343710	0.0000000000
Ni	14.7375780183	4.2543723180	2.0052540942
Ni	15.9657095198	6.3815584771	2.0052540942
Ni	12.2813150153	4.2543723180	2.0052540942
Ni	13.5094465168	6.3815584771	2.0052540942
Ni	14.7375780183	8.5087446361	2.0052540942
Ni	2.4562630031	0.0000000000	2.0052540942
Ni	1.2281315015	2.1271861590	2.0052540942
Ni	18.4219725229	10.6359307951	2.0052540942
Ni	15.9657095198	10.6359307951	2.0052540942
Ni	12.2813150153	0.0000000000	2.0052540942
Ni	4.9125260061	0.0000000000	2.0052540942
Ni	11.0531835137	2.1271861590	2.0052540942
Ni	9.8250520122	0.0000000000	2.0052540942

Ni	13.5094465168	2.1271861590	2.0052540942
Ni	6.1406575076	6.3815584771	2.0052540942
Ni	2.4562630031	4.2543723180	2.0052540942
Ni	3.6843945046	6.3815584771	2.0052540942
Ni	4.9125260061	4.2543723180	2.0052540942
Ni	8.5969205107	10.6359307951	2.0052540942
Ni	0.0000000000	0.0000000000	2.0052540942
Ni	4.9125260061	8.5087446361	2.0052540942
Ni	6.1406575076	10.6359307951	2.0052540942
Ni	7.3687890092	8.5087446361	2.0052540942
Ni	8.5969205107	2.1271861590	2.0052540942
Ni	11.0531835137	6.3815584771	2.0052540942
Ni	8.5969205107	6.3815584771	2.0052540942
Ni	9.8250520122	4.2543723180	2.0052540942
Ni	12.2813150153	8.5087446361	2.0052540942
Ni	11.0531835137	10.6359307951	2.0052540942
Ni	9.8250520122	8.5087446361	2.0052540942
Ni	13.5094465168	10.6359307951	2.0052540942
Ni	17.1938410214	8.5087446361	2.0052540942
Ni	7.3687890092	0.0000000000	2.0052540942
Ni	6.1406575076	2.1271861590	2.0052540942
Ni	7.3687890092	4.2543723180	2.0052540942
Ni	3.6843945046	2.1271861590	2.0052540942
Ni	17.2146368447	9.9404784409	4.0175023597
Ni	18.4368791569	12.0651504169	4.0181178735
Ni	19.6621078729	9.9390427333	4.0175807206
Ni	11.0474227491	3.5376773213	4.1506631620
Ni	3.7019236156	3.5497482523	4.0230987157
Ni	6.1579329787	7.8012848624	4.0135728686
Ni	4.9391379751	5.6829993773	4.0223524556
Ni	8.6138966634	7.8087441973	4.0862753375
Ni	4.9217541420	1.4331657248	4.0240211347
Ni	12.2996891699	9.9353576477	4.0172359051
Ni	13.5231187243	12.0575267925	4.0156477715
Ni	14.7482686773	9.9360356349	4.0149484407
Ni	9.8334228515	9.9342220387	4.0230207866
Ni	8.6116233148	12.0570853388	4.0181788299
Ni	7.3914773234	9.9357311257	4.0229518288
Ni	11.0675754437	12.0619801879	4.0826044353
Ni	13.5259055745	7.8052783957	4.0737375780
Ni	9.8380987692	5.6705735465	4.0302645287
Ni	11.0658660834	7.7964583719	4.0125538503
Ni	12.2752810936	5.6699670333	4.0238336491
Ni	20.8940369711	12.0621497142	4.0797327605
Ni	9.8256978005	1.4478168391	4.0381393674
Ni	8.6199984375	3.5444876920	4.0794802878
Ni	7.3877853583	1.4320600458	4.0148000957
Ni	7.3879174741	5.6741537465	4.0302591746
Ni	14.7463008441	1.4303688809	4.0118529514
Ni	15.9819279420	12.0630199932	4.0772157951
Ni	18.4380023905	7.8098374592	4.0802764360

Ni	12.2960051728	1.4346845467	4.0242723122
Ni	13.5083517032	3.5425641245	4.0250897889
Ni	14.7502173461	5.6797702317	4.0178706584
Ni	17.2060914098	5.6839725334	4.0160314947
Ni	2.4754611624	1.4312052645	4.0164879895
Ni	6.1534764774	3.5563352260	4.0884504791
Ni	15.9810933918	3.5580332506	4.0744859017
Ni	15.9801883501	7.8019909282	4.0164050972
Ni	8.6319418106	4.9677277755	6.0407421912
Ni	11.0848153652	4.9449053461	6.1553691730
Ni	9.8286289724	7.1227906351	6.1054390776
Ni	14.7389339584	7.1189316026	6.1059779628
Ni	15.9885002699	4.9524008911	6.1061252300
Ni	9.8785069644	2.8504669498	6.5322676978
Ni	17.2418397045	7.1244472790	6.1075085695
Ni	2.4488081529	2.8638569867	6.1034395400
Ni	7.3444414432	2.8331496986	6.1037082495
Ni	8.6041430776	0.6678847197	6.0914987145
Ni	6.1504924103	0.7052319949	5.9683492790
Ni	17.1898438392	11.3705845125	6.1066902445
Ni	18.4431376656	9.2067200000	6.1079363938
Ni	15.9902647478	9.2299051633	5.9698369629
Ni	13.5319726959	4.9741659603	5.9731753578
Ni	12.3515557441	7.1277494776	6.0973734212
Ni	6.1621455705	9.2322790954	5.9705525633
Ni	8.6181992216	9.1985821645	6.1505382644
Ni	12.2854629406	2.8611760387	6.1635353225
Ni	13.5327211357	0.6869174280	6.0994944272
Ni	4.9010707222	7.1281629028	6.1011969772
Ni	6.1494314787	4.9595133879	6.1526892014
Ni	3.6985197608	4.9846424892	5.9694533640
Ni	11.0542139988	0.7359037367	5.9668985038
Ni	7.4164452102	7.1251151713	6.0968212989
Ni	9.8692771786	11.3670291898	6.1089924719
Ni	14.7798660320	11.3576649657	6.1057989000
Ni	13.5345604866	9.2001615325	6.1041245331
Ni	12.2716857003	11.3647925384	6.1075712801
Ni	14.8042273666	2.8744767029	6.0948530735
Ni	4.9220246587	2.8516893350	6.1608224823
Ni	1.2467944585	0.7192661560	5.9682952133
Ni	3.6951422112	0.6842651120	6.1069580269
Ni	7.3644809474	11.3687602209	6.1085279346
Ni	11.0747932971	9.2249873811	5.9702155953
Ni	19.6973259916	11.3794395416	6.1071402618
O	3.6447554091	2.1040034916	7.2279351822
O	6.1509102587	6.4501571057	7.2102003262
O	8.6166983319	10.6612028898	7.2163938025
O	8.4461317858	1.9951187805	7.2875651607
O	11.1130921691	6.4521098159	7.1922280615
O	13.5264058338	10.6434280858	7.2004739748
O	13.6183096680	2.1159237304	7.1950714881

O	15.9912986560	6.3982229440	7.2010824463
O	18.4454396544	10.6537041029	7.2008043420
C	8.8747322396	5.1230308014	8.6343689942
C	8.5176016300	6.2990852436	9.2773731489
C	10.0418844776	4.3991515629	8.9960908725
C	10.7718120692	4.8425974292	10.1562655848
C	10.4063860553	6.0710595476	10.7658636178
C	9.3190783271	6.8005476444	10.3220887388
C	11.8116442692	4.0270922100	10.6745919126
C	12.0855174160	2.8015298839	10.1049027879
C	11.4259289140	2.4046053588	8.9185093902
C	10.5193923600	3.2514475616	8.2915552289
H	8.1461369830	4.6403572845	7.9558220846
H	7.6029971736	6.8112172428	8.9849706615
H	9.0532680304	7.7411509698	10.8046910643
H	10.9979066411	6.4252423962	11.6124854569
H	12.3601912079	4.3670403093	11.5545043059
H	12.8384127754	2.1405587164	10.5349115913
H	11.6745902653	1.4372078281	8.4822584309
H	6.1364505577	3.5513342448	7.0494193333

Table S5. Dissociated naphthalene on Ni(111)-O (2x2). Standing

i =	200,	E =	-24586.0256722785
Ni	12.2813150153	11.3449928481	0.0000000000
Ni	12.2813150153	7.0906205301	0.0000000000
Ni	8.5969205107	4.9634343710	0.0000000000
Ni	11.0531835137	4.9634343710	0.0000000000
Ni	13.5094465168	4.9634343710	0.0000000000
Ni	7.3687890092	11.3449928481	0.0000000000
Ni	9.8250520122	7.0906205301	0.0000000000
Ni	14.7375780183	11.3449928481	0.0000000000
Ni	11.0531835137	9.2178066891	0.0000000000
Ni	14.7375780183	2.8362482120	0.0000000000
Ni	15.9657095198	4.9634343710	0.0000000000
Ni	14.7375780183	7.0906205301	0.0000000000
Ni	8.5969205107	9.2178066891	0.0000000000
Ni	6.1406575076	9.2178066891	0.0000000000
Ni	8.5969205107	0.7090620530	0.0000000000
Ni	6.1406575076	0.7090620530	0.0000000000
Ni	9.8250520122	11.3449928481	0.0000000000
Ni	9.8250520122	2.8362482120	0.0000000000
Ni	13.5094465168	9.2178066891	0.0000000000
Ni	17.1938410213	7.0906205301	0.0000000000
Ni	18.4219725229	9.2178066891	0.0000000000
Ni	19.6501040244	11.3449928481	0.0000000000
Ni	4.9125260061	2.8362482120	0.0000000000
Ni	11.0531835137	0.7090620530	0.0000000000
Ni	13.5094465168	0.7090620530	0.0000000000
Ni	12.2813150153	2.8362482120	0.0000000000
Ni	7.3687890092	2.8362482120	0.0000000000
Ni	1.2281315015	0.7090620530	0.0000000000
Ni	3.6843945046	0.7090620530	0.0000000000
Ni	7.3687890092	7.0906205301	0.0000000000
Ni	2.4562630031	2.8362482120	0.0000000000
Ni	6.1406575076	4.9634343710	0.0000000000
Ni	4.9125260061	7.0906205301	0.0000000000
Ni	17.1938410214	11.3449928481	0.0000000000
Ni	15.9657095198	9.2178066891	0.0000000000
Ni	3.6843945046	4.9634343710	0.0000000000
Ni	14.7375780183	4.2543723180	2.0052540942
Ni	15.9657095198	6.3815584771	2.0052540942
Ni	12.2813150153	4.2543723180	2.0052540942
Ni	13.5094465168	6.3815584771	2.0052540942
Ni	14.7375780183	8.5087446361	2.0052540942
Ni	2.4562630031	0.0000000000	2.0052540942
Ni	1.2281315015	2.1271861590	2.0052540942
Ni	18.4219725229	10.6359307951	2.0052540942
Ni	15.9657095198	10.6359307951	2.0052540942
Ni	12.2813150153	0.0000000000	2.0052540942
Ni	4.9125260061	0.0000000000	2.0052540942
Ni	11.0531835137	2.1271861590	2.0052540942
Ni	9.8250520122	0.0000000000	2.0052540942

Ni	13.5094465168	2.1271861590	2.0052540942
Ni	6.1406575076	6.3815584771	2.0052540942
Ni	2.4562630031	4.2543723180	2.0052540942
Ni	3.6843945046	6.3815584771	2.0052540942
Ni	4.9125260061	4.2543723180	2.0052540942
Ni	8.5969205107	10.6359307951	2.0052540942
Ni	0.0000000000	0.0000000000	2.0052540942
Ni	4.9125260061	8.5087446361	2.0052540942
Ni	6.1406575076	10.6359307951	2.0052540942
Ni	7.3687890092	8.5087446361	2.0052540942
Ni	8.5969205107	2.1271861590	2.0052540942
Ni	11.0531835137	6.3815584771	2.0052540942
Ni	8.5969205107	6.3815584771	2.0052540942
Ni	9.8250520122	4.2543723180	2.0052540942
Ni	12.2813150153	8.5087446361	2.0052540942
Ni	11.0531835137	10.6359307951	2.0052540942
Ni	9.8250520122	8.5087446361	2.0052540942
Ni	13.5094465168	10.6359307951	2.0052540942
Ni	17.1938410214	8.5087446361	2.0052540942
Ni	7.3687890092	0.0000000000	2.0052540942
Ni	6.1406575076	2.1271861590	2.0052540942
Ni	7.3687890092	4.2543723180	2.0052540942
Ni	3.6843945046	2.1271861590	2.0052540942
Ni	17.2024880210	9.9245928310	4.0240470880
Ni	18.4212976866	12.0423664707	4.0226642705
Ni	19.6417865253	9.9158545906	4.0139668921
Ni	11.0730710925	3.5484519433	4.1467519849
Ni	3.6812228440	3.5242587176	4.0155063744
Ni	6.1324820751	7.7769699286	4.0269611353
Ni	4.9109216262	5.6635323456	4.0231015890
Ni	8.5755763474	7.7954740249	4.0802359023
Ni	4.9091636224	1.4040758407	4.0180535492
Ni	12.2863074631	9.9201178894	4.0240722292
Ni	13.5112010160	12.0335309870	4.0280238135
Ni	14.7402363187	9.9272242912	4.0230437937
Ni	9.8108076262	9.9179631854	4.0273505930
Ni	8.5959555368	12.0320642505	4.0229216280
Ni	7.3657169176	9.9168845726	4.0222379960
Ni	11.0523982030	12.0316515801	4.0933920462
Ni	13.5184900166	7.7947550542	4.0454776882
Ni	9.8462451737	5.6551841966	4.0351607082
Ni	11.0478916470	7.7880625662	3.9791002572
Ni	12.2684821540	5.6551675998	4.0342086122
Ni	20.8728027362	12.0417085771	4.0785682959
Ni	9.8207190292	1.4121281709	4.0076344787
Ni	8.5966465817	3.5357410921	3.9847447293
Ni	7.3785413890	1.4108221789	4.0239718354
Ni	7.3628923792	5.6678996189	4.0236796814
Ni	14.7275875793	1.4055529476	4.0107141576
Ni	15.9678122000	12.0443217285	4.0991806526
Ni	18.4199360855	7.7785764887	4.0867015459

Ni	12.2829578687	1.4343187007	4.0401525804
Ni	13.4979364709	3.5247901299	4.0415309727
Ni	14.7249065604	5.6521471174	4.0269882398
Ni	17.1803835037	5.6589805609	4.0145916062
Ni	2.4601050183	1.4020873630	4.0184991499
Ni	6.1337407854	3.5378906841	4.0776424973
Ni	15.9622712181	3.5284119046	4.0771643478
Ni	15.9650881046	7.7819340931	4.0171397091
Ni	8.5800638189	4.9526607168	5.9671795884
Ni	11.0106898304	4.9544122853	6.3485533951
Ni	9.7627825967	7.1300889701	6.0444232619
Ni	14.7106354824	7.0877265534	6.0994164402
Ni	15.9607650385	4.9075866405	6.1003082807
Ni	9.8087862800	2.8281309607	6.0388386003
Ni	17.2128433301	7.0779976598	6.1102337527
Ni	2.4303499609	2.8252743197	6.1066916427
Ni	7.3105494605	2.8590032019	6.0957570001
Ni	8.5716128840	0.6807112747	6.1592161364
Ni	6.1373329926	0.6932674798	5.9714735782
Ni	17.1816094955	11.3147436444	6.1622635491
Ni	18.4217771462	9.1460350615	6.1022808100
Ni	15.9736003112	9.1991404851	5.9710178280
Ni	13.4866996219	4.9482536316	6.0318000280
Ni	12.3216082356	7.1374309991	6.0376435002
Ni	6.1297307887	9.1925581893	5.9721919222
Ni	8.5719283734	9.1844287639	6.1508814057
Ni	12.2272972361	2.8087840405	6.4112495344
Ni	13.5072407481	0.6387089105	6.0888076697
Ni	4.8775831916	7.0766972824	6.1541918673
Ni	6.1199405916	4.9289611359	6.1130336478
Ni	3.6698451706	4.9433019809	5.9700391094
Ni	11.0551988392	0.6975032478	5.9761938219
Ni	7.3804864085	7.0905511275	6.1537906135
Ni	9.8490364927	11.3413047033	6.1551496165
Ni	14.7627254802	11.3408818260	6.1531604449
Ni	13.5245210573	9.1869328655	6.1044704982
Ni	12.2522406864	11.3394302377	6.1541648462
Ni	14.7753332517	2.8141968761	6.0890762730
Ni	4.9261441536	2.8363816752	6.1050959225
Ni	1.2275347430	0.6833621162	5.9703837063
Ni	3.6817060396	0.6562651340	6.1107437645
Ni	7.3441856949	11.3331557564	6.1090859523
Ni	11.0449343706	9.2125576150	5.9683471634
Ni	19.6776273917	11.3265950398	6.1062395363
O	3.6812149262	2.1064210070	7.2016740233
O	6.1330180170	6.3502052563	7.2435555836
O	8.5789795955	10.6329002947	7.2385340951
O	8.5475038761	2.1845179006	7.2053100599
O	11.0409534435	6.6193895906	7.1673082902
O	13.5097767475	10.6054591112	7.2358699516
O	13.6511618804	1.9979139533	7.2506557044

O	15.9539295404	6.3537781667	7.2009565863
O	18.4767185618	10.5507385046	7.2211628035
C	9.2806990453	5.4430111830	10.1178661262
C	9.1231827735	6.4943099600	11.0036905354
C	10.5523386967	5.1572144890	9.5693085769
C	11.6827807645	5.9534123199	9.9518296775
C	11.4935528593	7.0093365248	10.8736869107
C	10.2344608358	7.2800691548	11.3819966274
C	12.9573076247	5.6454530340	9.3953986016
C	13.0977109607	4.6678658357	8.4318210477
C	11.9485035210	3.9656870860	7.9122876342
C	10.7095690116	4.1456996777	8.5723093537
H	8.4221014852	4.8493085847	9.7987389050
H	8.1354659440	6.7263850241	11.4026193521
H	10.0955486552	8.1103868902	12.0750143448
H	12.3503620094	7.6200780582	11.1625033603
H	13.8381359024	6.1956360565	9.7313768205
H	14.1080281142	4.3756299126	8.1140848558
H	9.8786616086	0.0193475536	6.9566546087
H	9.8655230276	3.4819635422	8.3875631458