

Supporting information to

Self-assembly and coverage dependent thermally induced conformational changes of Ni(II)-*meso*-tetrakis (4-*tert*-butylphenyl) benzoporphyrin on Cu(111)

Liang Zhang^{1,2}, Michael Lepper^{1,2}, Michael Stark^{1,2}, Dominik Lungerich^{2,3}, Norbert Jux^{2,3},
Wolfgang Hieringer^{2,4}
Hans-Peter Steinrück^{1,2}, and Hubertus Marbach^{1,2*}

Affiliations:

¹Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany.

²Interdisciplinary Center for Molecular Materials (ICMM) Universität Erlangen-Nürnberg, Germany.

³Lehrstuhl für Organische Chemie II, Universität Erlangen-Nürnberg, Henkestr. 42, 91054 Erlangen, Germany.

⁴Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany.

*Correspondence to: hubertus.marbach@fau.de

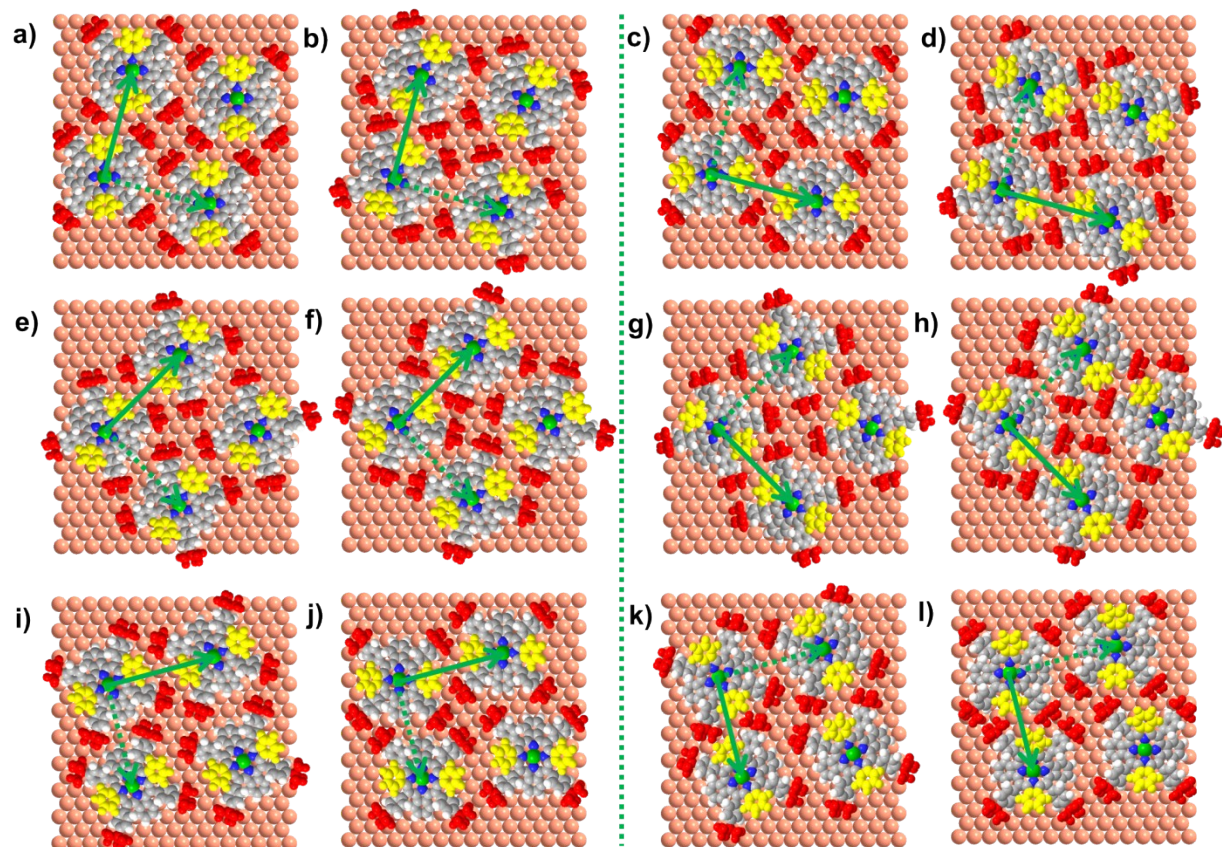


Figure S1. Models of twelve different domains for Ni-TTBPP on Cu(111).

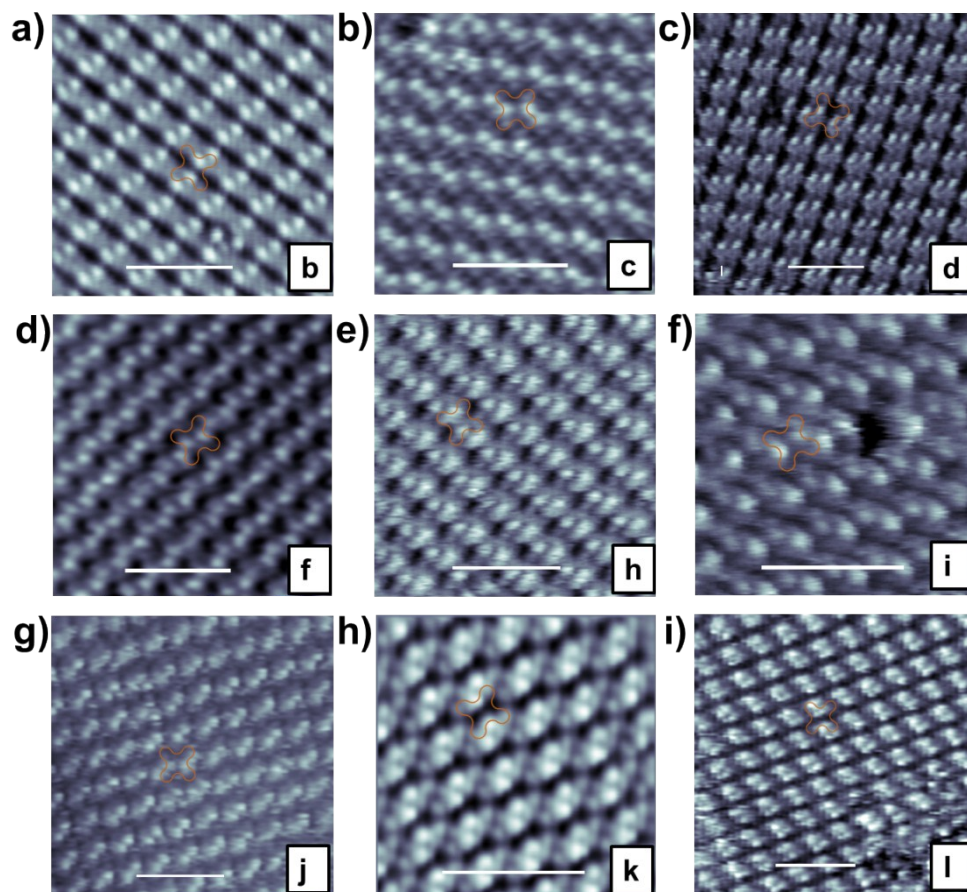


Figure S2. Constant current STM images of different domains for Ni-TTBPP on Cu(111). The orange profiles indicate the structure of individual molecules in each domain. The letters in each image correspond to the domain models in Figure S1. The scale bar is 5 Å. It is worth to note that not all the twelve domain structures are observed in the STM images because of the large area of each domain. The substrate orientation in each image is same to that in Figure S1.

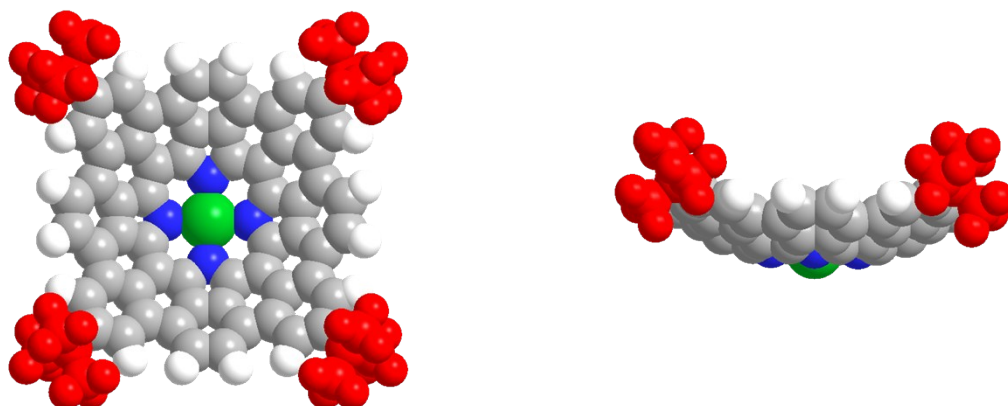


Figure S3. Top view (left) and side view (right) of the gas-phase bowl-like structure for Ni-TTBPP after annealing. In this structure, the partial dehydrogenation occurs to the four benzene rings and phenyl rings and intramolecular C-C bonds form between the four benzene rings and phenyl rings.

Computational Details

The general aspects of the DFT calculations performed in the paper are summarized in the main text. The following are the atomic Cartesian coordinates for the gas-phase model structures of Ni-TTBPP and its dehydrogenated congeners.

Ni-TTBPP (motif 1, cf. Figure 6a)

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Energy = -4662.628733609

C -5.5215958 -5.4322794 0.0364254

C -5.5860403 -4.2910932 -0.7985813

C -4.5839278 -3.3139324 -0.7881557

C -3.4625965 -3.4418317 0.0581892

C -3.3824660 -4.5757088 0.8880981

C -4.3951386 -5.5488697 0.8787866

C -2.3993198 -2.3974915 0.0739724

C	-2.7061743	-1.1192789	0.5685982
C	-3.9483618	-0.7118936	1.2191333
C	-3.9483618	0.7118936	1.2191333
C	-2.7061743	1.1192789	0.5685982
N	-1.9251415	0.0000000	0.3163233
C	-2.3993198	2.3974915	0.0739724
C	-3.4625965	3.4418317	0.0581892
C	-4.5839278	3.3139324	-0.7881557
C	-5.5860403	4.2910932	-0.7985813
C	-5.5215958	5.4322794	0.0364254
C	-4.3951386	5.5488697	0.8787866
C	-3.3824660	4.5757088	0.8880981
C	-1.1194883	2.7064826	-0.4137797
C	-0.7119543	3.9444178	-1.0723572
C	0.7119543	3.9444178	-1.0723572
C	1.1194883	2.7064826	-0.4137797
N	0.0000000	1.9277157	-0.1547029
C	2.3993198	2.3974915	0.0739724
C	3.4625965	3.4418317	0.0581892
C	4.5839278	3.3139324	-0.7881557
C	5.5860403	4.2910932	-0.7985813
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C	3.9483618	0.7118936	1.2191333

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C	2.3993198	-2.3974915	0.0739724
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C	4.5839278	-3.3139324	-0.7881557
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C	5.5215958	-5.4322794	0.0364254
C	4.3951386	-5.5488697	0.8787866
C	3.3824660	-4.5757088	0.8880981
C	1.1194883	-2.7064826	-0.4137797
C	0.71119543	-3.9444178	-1.0723572
C	-0.71119543	-3.9444178	-1.0723572
C	-1.1194883	-2.7064826	-0.4137797
N	0.0000000	-1.9277157	-0.1547029
C	-5.0015742	-1.4289942	1.8298503
C	-5.0015742	1.4289942	1.8298503
C	-1.4289962	4.9923658	-1.6920071
C	1.4289962	4.9923658	-1.6920071
C	5.0015742	1.4289942	1.8298503
C	5.0015742	-1.4289942	1.8298503
C	1.4289962	-4.9923658	-1.6920071
C	-1.4289962	-4.9923658	-1.6920071
H	4.6653888	-2.4292274	-1.4402252
H	2.5098996	-4.6948900	1.5507927
H	6.4446094	-4.1525077	-1.4764822

H	4.2888333	-6.4137982	1.5499022
C	6.6561372	-6.4749444	0.0001459
H	4.6653888	2.4292274	-1.4402252
H	2.5098996	4.6948900	1.5507927
H	6.4446094	4.1525077	-1.4764822
H	4.2888333	6.4137982	1.5499022
C	6.6561372	6.4749444	0.0001459
H	-4.6653888	2.4292274	-1.4402252
H	-2.5098996	4.6948900	1.5507927
H	-6.4446094	4.1525077	-1.4764822
H	-4.2888333	6.4137982	1.5499022
C	-6.6561372	6.4749444	0.0001459
H	-4.6653888	-2.4292274	-1.4402252
H	-2.5098996	-4.6948900	1.5507927
H	-6.4446094	-4.1525077	-1.4764822
H	-4.2888333	-6.4137982	1.5499022
C	-6.6561372	-6.4749444	0.0001459
Ni	0.0000000	0.0000000	0.0815870
C	6.0411214	0.7076979	2.4298585
C	6.0411214	-0.7076979	2.4298585
C	-6.0411214	0.7076979	2.4298585
C	-6.0411214	-0.7076979	2.4298585
C	-0.7076828	6.0270358	-2.3004849
C	0.7076828	6.0270358	-2.3004849
C	-0.7076828	-6.0270358	-2.3004849
C	0.7076828	-6.0270358	-2.3004849

H	2.5272993	-4.9938457	-1.7200709
H	1.2522065	-6.8465738	-2.7984770
H	-1.2522065	-6.8465738	-2.7984770
H	-2.5272993	-4.9938457	-1.7200709
H	-5.0039644	-2.5273527	1.8568415
H	-6.8650933	-1.2522434	2.9204476
H	-6.8650933	1.2522434	2.9204476
H	-5.0039644	2.5273527	1.8568415
H	-2.5272993	4.9938457	-1.7200709
H	-1.2522065	6.8465738	-2.7984770
H	1.2522065	6.8465738	-2.7984770
H	2.5272993	4.9938457	-1.7200709
H	6.8650933	1.2522434	2.9204476
H	5.0039644	2.5273527	1.8568415
H	6.8650933	-1.2522434	2.9204476
H	5.0039644	-2.5273527	1.8568415
C	6.4033269	-7.6517200	0.9654936
C	6.7818750	-7.0452512	-1.4359159
C	7.9869119	-5.7908894	0.4063457
H	7.2438033	-8.3781737	0.9022967
H	6.3355724	-7.3133397	2.0229729
H	5.4691887	-8.2012298	0.7139445
H	7.5966998	-7.8034218	-1.4836109
H	5.8338445	-7.5353802	-1.7506957
H	7.0165138	-6.2534684	-2.1798657
H	8.8241530	-6.5254451	0.3882243

H	8.2533668	-4.9597390	-0.2822577
H	7.9173442	-5.3699229	1.4340292
C	-7.9869119	-5.7908894	0.4063457
C	-6.7818750	-7.0452512	-1.4359159
C	-6.4033269	-7.6517200	0.9654936
H	-8.8241530	-6.5254451	0.3882243
H	-7.9173442	-5.3699229	1.4340292
H	-8.2533668	-4.9597390	-0.2822577
H	-7.2438033	-8.3781737	0.9022967
H	-5.4691887	-8.2012298	0.7139445
H	-6.3355724	-7.3133397	2.0229729
H	-7.5966998	-7.8034218	-1.4836109
H	-7.0165138	-6.2534684	-2.1798657
H	-5.8338445	-7.5353802	-1.7506957
C	-6.4033269	7.6517200	0.9654936
C	-6.7818750	7.0452512	-1.4359159
C	-7.9869119	5.7908894	0.4063457
H	-8.8241530	6.5254451	0.3882243
H	-8.2533668	4.9597390	-0.2822577
H	-7.9173442	5.3699229	1.4340292
H	-7.2438033	8.3781737	0.9022967
H	-6.3355724	7.3133397	2.0229729
H	-5.4691887	8.2012298	0.7139445
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H	-7.0165138	6.2534684	-2.1798657

C	6.4033269	7.6517200	0.9654936
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C	6.7818750	7.0452512	-1.4359159
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H	8.2533668	4.9597390	-0.2822577
H	7.5966998	7.8034218	-1.4836109
H	7.0165138	6.2534684	-2.1798657
H	5.8338445	7.5353802	-1.7506957
H	7.2438033	8.3781737	0.9022967
H	5.4691887	8.2012298	0.7139445
H	6.3355724	7.3133397	2.0229729

Dehydrogenated Ni-TTBPP (motif 2, cf. Figure 6b)

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Energy = -4660.263872525

C	-5.7005376	-5.2489726	0.2191708
C	-5.9138986	-3.8654033	0.1033539
C	-4.8682338	-2.9251985	-0.0297196
C	-3.4930396	-3.3947355	-0.1172217
C	-3.2941042	-4.7824852	0.0861080
C	-4.3531285	-5.6815821	0.2407230
C	-2.3453561	-2.4734473	-0.3065222
C	-2.6162839	-1.1187512	-0.0906555
C	-3.9688432	-0.7057719	0.0499105
C	-3.9697305	0.6849581	0.0495773

C	-2.6177379	1.0997838	-0.0907289
N	-1.7896614	-0.0089624	-0.1837888
C	-2.3479790	2.4551185	-0.3042455
C	-3.4973239	3.3747002	-0.1156203
C	-4.8720074	2.9031636	-0.0300113
C	-5.9192860	3.8417375	0.1020306
C	-5.7082402	5.2255384	0.2190343
C	-4.3614949	5.6600038	0.2431892
C	-3.3009251	4.7625845	0.0894110
C	-1.0151866	2.7878671	-0.6731251
C	-0.5263406	3.9657212	-1.3724722
C	0.8948742	3.9282336	-1.2835336
C	1.2211730	2.7084206	-0.5552472
N	0.0594490	1.9688555	-0.3420257
C	2.4571299	2.3862741	0.0263003
C	3.5242235	3.4259094	0.0684438
C	4.7123921	3.2714630	-0.6767333
C	5.7040282	4.2588214	-0.6509084
C	5.5630677	5.4360152	0.1230184
C	4.3738105	5.5747551	0.8703003
C	3.3708807	4.5920155	0.8413423
C	2.7259861	1.1093027	0.5522262
C	3.9180280	0.7002491	1.2869852
C	3.9205821	-0.7246154	1.2772696
C	2.7292092	-1.1279558	0.5382402
N	1.9677327	-0.0085853	0.2381528

C	2.4615492	-2.4002173	0.0002134
C	3.5320514	-3.4368186	0.0277535
C	4.7162546	-3.2711167	-0.7212140
C	5.7120999	-4.2545118	-0.7081111
C	5.5793687	-5.4388057	0.0563700
C	4.3938367	-5.5889680	0.8073727
C	3.3867659	-4.6101975	0.7912022
C	1.2233489	-2.7202953	-0.5774605
C	0.8947719	-3.9368343	-1.3101728
C	-0.5269568	-3.9777655	-1.3884284
C	-1.0135644	-2.8038202	-0.6808687
N	0.0613686	-1.9843514	-0.3525649
C	-5.1251887	-1.4838915	-0.0027031
C	-5.1270828	1.4615400	-0.0031780
C	-1.1711157	4.9515639	-2.1539033
C	1.6771590	4.9124447	-1.9301356
C	4.9254233	1.4144953	1.9738358
C	4.9309517	-1.4443933	1.9539798
C	1.6748259	-4.9155113	-1.9677468
C	-1.1749767	-4.9620883	-2.1691018
H	4.8490784	-2.3554610	-1.3197931
H	2.4657132	-4.7575597	1.3780600
H	6.6191061	-4.0884134	-1.3125148
H	4.2341497	-6.4865427	1.4224743
C	6.7041928	-6.4924053	0.0416790
H	4.8516280	2.3615954	-1.2826382

H	2.4466412	4.7305511	1.4253427
H	6.6142452	4.1017805	-1.2529159
H	4.2076353	6.4663136	1.4924129
C	6.6832713	6.4946317	0.1216167
H	-2.2749282	5.1516020	0.1549695
H	-6.9474491	3.4474578	0.1451682
H	-4.1191385	6.7213864	0.3979169
C	-6.9084912	6.1839295	0.3502060
H	-2.2672952	-5.1698564	0.1494175
H	-6.9425950	-3.4727203	0.1483069
H	-4.1090718	-6.7427830	0.3939718
C	-6.8991732	-6.2092301	0.3515723
Ni	0.0802467	-0.0082844	-0.1280931
C	5.9224002	0.6903499	2.6385821
C	5.9252133	-0.7256644	2.6286023
C	-6.3364954	0.6957536	-0.0207708
C	-6.3355872	-0.7196848	-0.0205346
C	-0.3871147	5.9162252	-2.7952438
C	1.0246967	5.9025628	-2.6742357
C	-0.3932446	-5.9215430	-2.8209623
C	1.0194414	-5.9040737	-2.7113603
H	2.7728322	-4.8913952	-1.9270270
H	1.6148590	-6.6656244	-3.2418790
H	-0.8821873	-6.6900943	-3.4422912
H	-2.2687613	-4.9607987	-2.2854537
H	-7.3105186	-1.2329211	-0.0579892

H	-7.3120955	1.2077047	-0.0583593
H	-2.2639400	4.9474389	-2.2789573
H	-0.8733374	6.6860040	-3.4171969
H	1.6219946	6.6685036	-3.1962691
H	2.7748671	4.8915559	-1.8807334
H	6.7096914	1.2322377	3.1885573
H	4.9229673	2.5130088	2.0072389
H	6.7147714	-1.2720827	3.1707941
H	4.9329679	-2.5432617	1.9720358
C	6.3768201	-7.7138347	0.9256279
C	6.9181181	-6.9896972	-1.4110872
C	8.0120406	-5.8478097	0.5685202
H	7.2134324	-8.4463195	0.8819152
H	6.2400369	-7.4296017	1.9924230
H	5.4573161	-8.2387155	0.5837291
H	7.7269051	-7.7549916	-1.4452884
H	5.9880448	-7.4502611	-1.8120777
H	7.2087358	-6.1636042	-2.0958967
H	8.8405423	-6.5922021	0.5677309
H	8.3330236	-4.9868475	-0.0575812
H	7.8789222	-5.4784192	1.6095360
C	-7.7168535	-5.8428271	1.6166761
C	-7.7972520	-6.0741601	-0.9048479
C	-6.4555593	-7.6825922	0.4729631
H	-8.5836066	-6.5324884	1.7321492
H	-7.0870906	-5.9200244	2.5306691

H	-8.1161937	-4.8062243	1.5683515
H	-7.3494725	-8.3404365	0.5501775
H	-5.8732942	-8.0137865	-0.4153782
H	-5.8362591	-7.8561175	1.3808577
H	-8.6725869	-6.7593306	-0.8344467
H	-8.1874341	-5.0400550	-1.0252046
H	-7.2292189	-6.3302128	-1.8267080
C	-6.4672259	7.6578866	0.4729239
C	-7.8045932	6.0481243	-0.9075439
C	-7.7274024	5.8156856	1.6139853
H	-8.5953495	6.5039909	1.7285783
H	-8.1251146	4.7785057	1.5645778
H	-7.0990274	5.8933560	2.5288919
H	-7.3622166	8.3143792	0.5490626
H	-5.8495635	7.8319296	1.3818413
H	-5.8840851	7.9903018	-0.4143866
H	-8.6810286	6.7319718	-0.8380611
H	-7.2356286	6.3054334	-1.8284806
H	-8.1930785	5.0135019	-1.0289351
C	6.3473554	7.7068600	1.0149675
C	7.9921424	5.8513004	0.6474829
C	6.9000802	7.0054654	-1.3260133
H	8.8172912	6.5993646	0.6561067
H	7.8570734	5.4723590	1.6848191
H	8.3191669	4.9972332	0.0151082
H	7.7054390	7.7747550	-1.3506476

H	7.1968603	6.1866746	-2.0169002
H	5.9693334	7.4652457	-1.7263216
H	7.1808992	8.4434001	0.9809196
H	5.4268635	8.2307422	0.6742243
H	6.2078231	7.4125671	2.0786403

Dehydrogenated Ni-TTBPP (motif 3, cf. Figure 6c)

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Energy = -4657.899334523

C	-5.7247550	-5.2521138	0.2677111
C	-5.9427524	-3.8660156	0.1930641
C	-4.9059200	-2.9238721	0.0163896
C	-3.5393491	-3.3920541	-0.1607401
C	-3.3305285	-4.7838743	-0.0016283
C	-4.3796923	-5.6860117	0.1970708
C	-2.4013141	-2.4683344	-0.3993473
C	-2.6596277	-1.1168410	-0.1404787
C	-4.0014165	-0.7057006	0.0845689
C	-4.0030710	0.6861342	0.0890151
C	-2.6622578	1.1018920	-0.1333267
N	-1.8430077	-0.0060576	-0.2771892
C	-2.4071868	2.4556488	-0.3834504
C	-3.5473764	3.3751094	-0.1387270
C	-4.9128349	2.9025464	0.0351468
C	-5.9519865	3.8410208	0.2176329

C	-5.7373316	5.2271106	0.3014498
C	-4.3932923	5.6646583	0.2338823
C	-3.3419236	4.7663630	0.0294851
C	-1.1093600	2.8025652	-0.8463030
C	-0.7008487	3.9675579	-1.6094868
C	0.7242107	3.9691797	-1.6078548
C	1.1336419	2.8051705	-0.8436725
N	0.0127255	2.0214003	-0.5577938
C	2.4311923	2.4613365	-0.3777421
C	3.5686086	3.3835078	-0.1303902
C	4.9347436	2.9141683	0.0470128
C	5.9711818	3.8551212	0.2320978
C	5.7530242	5.2407142	0.3150835
C	4.4081214	5.6750752	0.2441896
C	3.3594147	4.7742738	0.0372078
C	2.6888487	1.1082062	-0.1268845
C	4.0300391	0.6956266	0.0990899
C	4.0316531	-0.6962004	0.0948954
C	2.6914486	-1.1105370	-0.1336952
N	1.8725928	-0.0016880	-0.2727865
C	2.4370424	-2.4626684	-0.3930735
C	3.5765817	-3.3837020	-0.1512442
C	4.9415173	-2.9122504	0.0297791
C	5.9800862	-3.8518588	0.2097142
C	5.7652566	-5.2384816	0.2836809
C	4.4214753	-5.6756429	0.2088858

C	3.3706976	-4.7760367	0.0072246
C	1.1403821	-2.8065591	-0.8614101
C	0.7337549	-3.9666370	-1.6330306
C	-0.6913002	-3.9682885	-1.6349310
C	-1.1026358	-2.8091832	-0.8642947
N	0.0175914	-2.0272493	-0.5706741
C	-5.1600949	-1.4827486	0.0805209
C	-5.1635905	1.4604399	0.0898077
C	-1.4167519	4.8931032	-2.4046013
C	1.4398577	4.8963556	-2.4012975
C	5.1887277	1.4726390	0.1027491
C	5.1921344	-1.4705373	0.0942573
C	1.4516901	-4.8868013	-2.4325492
C	-1.4049202	-4.8903163	-2.4361627
H	2.3435525	-5.1677263	-0.0064928
H	7.0023567	-3.4577299	0.3278817
H	4.1729086	-6.7407712	0.3221643
C	6.9566991	-6.1972025	0.4761215
H	2.3313251	5.1635135	0.0263761
H	6.9945126	3.4627532	0.3468288
H	4.1570148	6.7388019	0.3647953
C	6.9423648	6.2011877	0.5116481
H	-2.3147525	5.1580926	0.0211350
H	-6.9746937	3.4462045	0.3295230
H	-4.1450131	6.7289967	0.3549678
C	-6.9294262	6.1847209	0.4953192

H	-2.3024025	-5.1730465	-0.0125521
H	-6.9663757	-3.4744077	0.3078272
H	-4.1288629	-6.7504898	0.3114026
C	-6.9144860	-6.2137803	0.4560457
Ni	0.0149040	-0.0035860	-0.3591815
C	6.3983968	0.7102855	0.1486386
C	6.4000397	-0.7056652	0.1444887
C	-6.3715924	0.6952405	0.1319745
C	-6.3699115	-0.7207044	0.1275786
C	-0.6980260	5.8180437	-3.1680917
C	0.7208053	5.8196605	-3.1664549
C	-0.6839167	-5.8081909	-3.2060209
C	0.7349092	-5.8065336	-3.2041319
H	2.5507960	-4.8597309	-2.4739904
H	1.2802601	-6.5211860	-3.8424282
H	-1.2258931	-6.5237867	-3.8461326
H	-2.5039889	-4.8661894	-2.4801107
H	-7.3451686	-1.2346328	0.1334954
H	-7.3480700	1.2068116	0.1408143
H	-2.5157381	4.8662993	-2.4490817
H	-1.2417676	6.5370404	-3.8028775
H	1.2643698	6.5398491	-3.8000403
H	2.5390029	4.8720012	-2.4432343
H	7.3736553	1.2241057	0.1607847
H	7.3764821	-1.2173011	0.1531792
C	6.5140123	-7.6749421	0.5277130

C	7.9416388	-6.0266692	-0.7087779
C	7.6795769	-5.8597706	1.8053794
H	7.4040544	-8.3311628	0.6498975
H	5.8340959	-7.8750761	1.3852316
H	5.9968876	-7.9845371	-0.4074574
H	8.8125087	-6.7113082	-0.5931007
H	7.4426469	-6.2607057	-1.6753235
H	8.3355263	-4.9890846	-0.7744713
H	8.5411165	-6.5473229	1.9639845
H	8.0732110	-4.8199447	1.8124155
H	6.9874530	-5.9653868	2.6700493
C	-7.6438209	-5.8772273	1.7819956
C	-7.8948746	-6.0466904	-0.7331181
C	-6.4681654	-7.6903204	0.5107005
H	-8.5039535	-6.5671892	1.9377235
H	-6.9549598	-5.9799443	2.6496216
H	-8.0406317	-4.8385958	1.7864355
H	-7.3569740	-8.3487495	0.6300037
H	-5.9466329	-7.9994712	-0.4221715
H	-5.7910465	-7.8878547	1.3710334
H	-8.7646642	-6.7332018	-0.6203940
H	-8.2907717	-5.0100400	-0.8014726
H	-7.3913027	-6.2805356	-1.6973362
C	-6.4864088	7.6617304	0.5624044
C	-7.9071480	6.0247834	-0.6970229
C	-7.6606239	5.8363282	1.8171794

H	-8.5223896	6.5233972	1.9766374
H	-8.0555328	4.7969666	1.8128012
H	-6.9736421	5.9335865	2.6869289
H	-7.3768018	8.3172396	0.6858631
H	-5.8107567	7.8537833	1.4251423
H	-5.9644335	7.9795611	-0.3672815
H	-8.7786399	6.7085212	-0.5807219
H	-7.4022185	6.2671765	-1.6584195
H	-8.3005669	4.9877970	-0.7741534
C	6.4957057	7.6771687	0.5772054
C	7.6711421	5.8549054	1.8353881
C	7.9233847	6.0432239	-0.6782381
H	8.5310271	6.5439076	1.9966419
H	6.9818711	5.9510407	2.7034542
H	8.0682856	4.8163928	1.8323850
H	8.7928951	6.7291647	-0.5600422
H	8.3195998	5.0071978	-0.7540077
H	7.4202261	6.2839995	-1.6409668
H	7.3842366	8.3348234	0.7027239
H	5.9752825	7.9934976	-0.3538611
H	5.8174692	7.8678774	1.4381999

Dehydrogenated Ni-TTBPP (bowl structure, cf. Figure S3)

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Energy = -4653.181453951

C	5.1552277	-5.2111268	0.7855188
C	5.5355660	-3.8813852	0.4947956
C	4.6593422	-2.9411675	-0.0804206
C	3.3137397	-3.3765727	-0.4253632
C	2.8779621	-4.7108285	-0.0496199
C	3.8221571	-5.5875867	0.5295068
C	2.3682411	-2.4344677	-1.0145631
C	2.7241364	-1.1031480	-1.2037491
C	4.0387447	-0.7134472	-0.8505630
C	4.0415998	0.6850543	-0.8507858
C	2.7286057	1.0800164	-1.2041256
N	1.8994688	-0.0099040	-1.4208642
C	2.3781656	2.4128618	-1.0154330
C	3.3275670	3.3512740	-0.4266089
C	4.6713771	2.9104785	-0.0815259
C	5.5515057	3.8473418	0.4931899
C	5.1766943	5.1788147	0.7832162
C	3.8451560	5.5606237	0.5271942
C	2.8972940	4.6874599	-0.0513807
C	1.0438356	2.7700253	-1.1782043
C	0.6594810	4.0784853	-0.7988668
C	-0.7387464	4.0817352	-0.7804787
C	-1.1387715	2.7748623	-1.1489098
N	-0.0523446	1.9486958	-1.3933999
C	-2.4693693	2.4230796	-0.9480881
C	-3.3982676	3.3656992	-0.3337706

C	-4.7328668	2.9298212	0.0513691
C	-5.5926854	3.8705584	0.6498358
C	-5.2073557	5.2030548	0.9205157
C	-3.8827887	5.5804194	0.6248302
C	-2.9532717	4.7012904	0.0257747
C	-2.8299250	1.0913827	-1.1249558
C	-4.1335824	0.7017192	-0.7334141
C	-4.1364259	-0.6966791	-0.7331957
C	-2.8343827	-1.0917775	-1.1246597
N	-2.0118393	-0.0019124	-1.3654055
C	-2.4792863	-2.4249103	-0.9475104
C	-3.4120858	-3.3635625	-0.3330391
C	-4.7448629	-2.9221183	0.0520450
C	-5.6086134	-3.8592359	0.6505170
C	-5.2289228	-5.1933942	0.9210427
C	-3.9058987	-5.5762487	0.6255187
C	-2.9726399	-4.7009531	0.0266540
C	-1.1501462	-2.7821819	-1.1482383
C	-0.7554863	-4.0905887	-0.7794435
C	0.6427456	-4.0929912	-0.7975656
C	1.0324622	-2.7862229	-1.1772515
N	-0.0603257	-1.9605053	-1.3928207
C	5.0191993	-1.5111015	-0.2465171
C	5.0253370	1.4788829	-0.2470389
C	1.4661945	5.0493767	-0.1911962
C	-1.5247341	5.0566241	-0.1522934

C	-5.0966288	1.4994468	-0.1022649
C	-5.1027308	-1.4902907	-0.1018379
C	-1.5455255	-5.0621268	-0.1511497
C	1.4454230	-5.0669798	-0.1895055
H	-6.6211856	-3.5216998	0.9236834
H	-3.5640151	-6.5912374	0.8728372
C	-6.2525235	-6.1595473	1.5534788
H	-6.6066972	3.5373049	0.9229367
H	-3.5366609	6.5939281	0.8722855
C	-6.2267352	6.1734039	1.5533137
H	6.5733085	3.5115064	0.7316723
H	3.5084724	6.5734584	0.7897753
C	6.2186157	6.1473101	1.3810131
H	6.5587425	-3.5496062	0.7330923
H	3.4812877	-6.5988801	0.7926104
C	6.1930064	-6.1836339	1.3839816
Ni	-0.0575398	-0.0059166	-1.4866520
C	-6.1660307	0.7190801	0.4523041
C	-6.1689442	-0.7054112	0.4524960
C	6.1067446	0.6940101	0.2770937
C	6.1038141	-0.7304887	0.2773553
C	0.6922955	6.1273624	0.3580202
C	-0.7316078	6.1308797	0.3764063
C	0.6670709	-6.1416888	0.3598433
C	-0.7568415	-6.1394437	0.3779740
H	-1.2516197	-6.9787101	0.8947459

H	1.1722184	-6.9825709	0.8637761
H	6.9491551	-1.2319424	0.7775322
H	6.9541671	1.1921445	0.7770682
H	1.2009575	6.9662935	0.8616663
H	-1.2228659	6.9723052	0.8930290
H	-6.9972211	1.2208199	0.9753620
H	-7.0022136	-1.2035754	0.9756687
C	6.7494268	-5.5998662	2.7079449
C	5.5914098	-7.5723157	1.6869354
C	7.3515525	-6.3671027	0.3699429
C	-5.6777453	-7.5785466	1.7495998
C	-6.6813457	-5.6146459	2.9402339
C	-7.4919850	-6.2652385	0.6285958
C	-6.6586146	5.6294457	2.9395065
C	-5.6454889	7.5895868	1.7508509
C	-7.4653085	6.2855599	0.6280193
C	5.6230459	7.5389124	1.6824952
C	6.7720598	5.5623370	2.7057078
C	7.3782558	6.3247750	0.3671847
H	-6.4563646	-8.2425178	2.1859402
H	-5.3553135	-8.0304966	0.7856217
H	-4.8101814	-7.5843225	2.4459683
H	-8.2449532	-6.9595576	1.0658457
H	-7.9887109	-5.2813935	0.4823130
H	-7.2056576	-6.6514389	-0.3747504
H	-7.4175352	-6.3012201	3.4164679

H	-5.8028637	-5.5237426	3.6167671
H	-7.1562963	-4.6118969	2.8662721
H	-6.4212341	8.2567785	2.1874029
H	-4.7782460	7.5907129	2.4476403
H	-5.3205521	8.0409296	0.7874303
H	-8.2153400	6.9828093	1.0656511
H	-7.1768582	6.6714612	-0.3748355
H	-7.9664046	5.3041061	0.4805163
H	-7.3918689	6.3190106	3.4159503
H	-7.1381098	4.6289330	2.8646748
H	-5.7808155	5.5340914	3.6163109
H	7.5116539	6.2611213	3.1580686
H	5.9531947	5.3992568	3.4410578
H	7.2865503	4.5891172	2.5503389
H	8.1497599	7.0165358	0.7755038
H	7.8792145	5.3589576	0.1372114
H	7.0047008	6.7481347	-0.5914397
H	6.4117442	8.2024704	2.1010360
H	5.2290283	8.0296929	0.7653689
H	4.8020825	7.4846264	2.4313312
H	8.1202246	-7.0617887	0.7786381
H	6.9758260	-6.7897490	-0.5881470
H	7.8565677	-5.4036534	0.1389105
H	6.3772763	-8.2388789	2.1060261
H	4.7707829	-7.5137342	2.4358251
H	5.1951609	-8.0623198	0.7703542

H	7.4857318	-6.3016726	3.1609960
H	7.2686093	-4.6293269	2.5514027
H	5.9314916	-5.4319908	3.4432608