Supplementary Material (ESI) for Chemical Communications

Supporting Information

A manipulation of electronic structure via supporting ligands: a charge disproportionate model within the linear metal framework of asymmetric nickel string $[Ni_7(phdptrany)_4Cl](PF_6)$

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Experimental Section

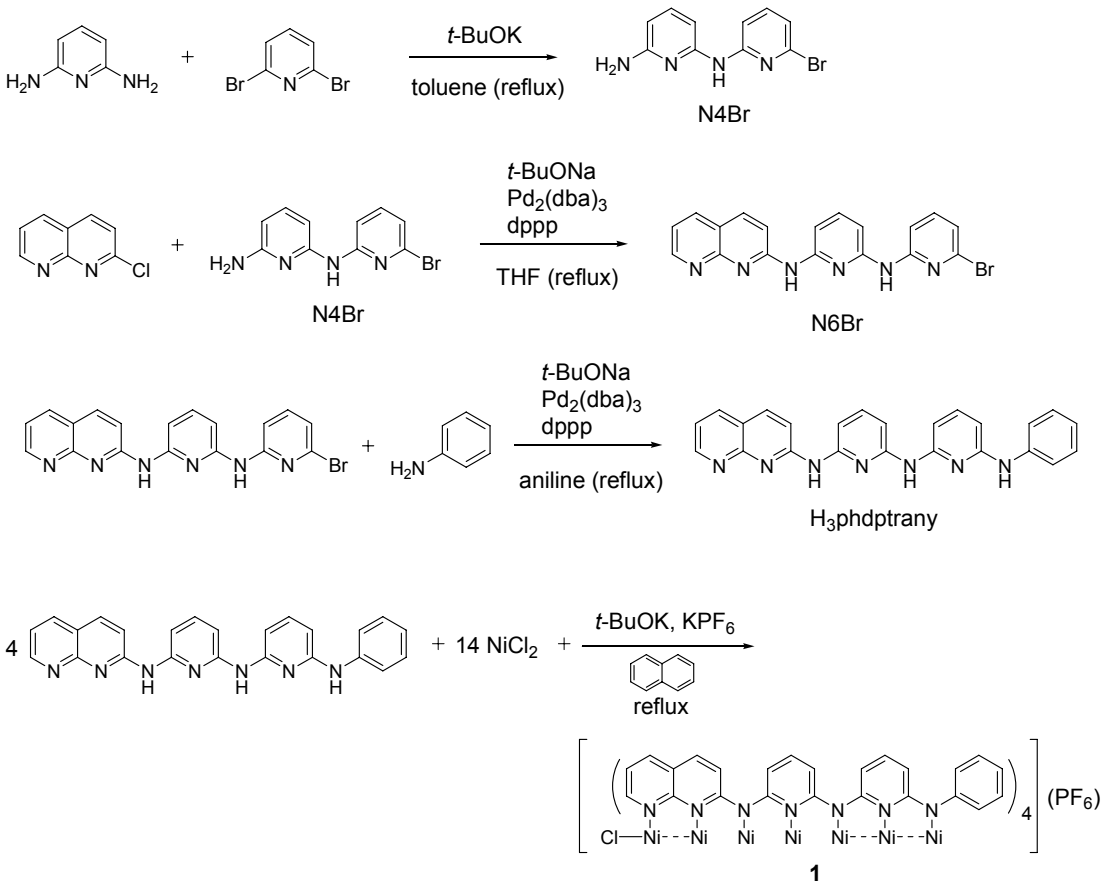
Computational Method: Calculations and full geometry optimizations on complex **1** were carried out by assuming *C*4 symmetry and using the density functional theory (DFT) formalism with the spin-unrestricted option, as implemented in the Gaussian03 software,[1] with the B3LYP exchange-correlation functional. The phenyl groups were replaced by hydrogen atom for simplicity. All electron valence double-ζ basis sets (D95V) were used to describe carbon, nitrogen and hydrogen. Los Alamos core potentials were used to model the neon core of nickel and chlorine. The valence shell of all types of metal atoms was described at the double-ζ level (LanL2DZ basis).

Materials: All reagents and solvents were purchased from commercial sources and were used as received unless otherwise noted. The precursor, 2-chloro-1,8-naphthyridine were prepared according to the literature procedures.[2]

Physical Measurements: Absorption spectra were recorded with a Shimadzu UV-3600 spectrophotometer. IR spectra were obtained with a Nicolet Fourier-Transform in the range 500–4000 cm^{-1}. FAB mass spectra were obtained with a JEOL HX-110 HF double-focusing spectrometer operating in the positive ion detection mode. Magnetic susceptibility values were collected with a Quantum external magnetic field of 2000 G.

Synthesis:

Scheme S1. Synthesis of ligand and complex **1**.



Bromo-H_3dpda (N_4Br):

A mixture of 2,6-diaminopyridine (10 g, 0.1 mol), 2,6-dibromopyridine (19.4 g, 0.08 mol) and *t*-BuONa (22.3 g, 0.23 mol) were placed in a flame-dried flask. The mixture was stirred and refluxed in toluene (500mL) for 48 h. After cooling to room temperature, the solvent was removed using a rotary evaporator. The residue was washed with water to remove unreacted 2,6-diaminopyridine. The resulting dark solid was chromatographed on silica gel using EA–hexane (1: 4) as the eluent to afford H_4Br as a white powder. (14.95 g, 94% Yield); ^{1}H NMR (400 MHz ; [D]DMSO): δ = 9.54 (s, 1H), 8.03 (d, 1H, J = 8.4 Hz), 7.49 (t, 1H, J = 8.0 Hz), 7.25 (t, J = 8.0 Hz, 1H), 6.96 (d, J = 7.2 Hz, 1H), 6.54 (d, J = 7.6 Hz, 1H), 5.97 (d, J = 8.0 Hz, 1H), 5.77 ppm (s, 2H); MS (ESI): *m/z* = 274 $[M+H]^+$.

2-(bromodopyridyldiamino)-1,8-naphthyridine (N_6Br):

A mixture of 2-chloro-1,8-naphthyridine (13.9 g, 84 mmol), Bromo-H_3dpda (15 g, 57 mmol), *t*-BuONa (6.52 g, 68 mmol), Pd_2 (dba)$_3$ (1.035 g, 1.1 mmol) and dppp (0.933 g, 2.2 mmol) were placed in a flame-dried flask under argon. The mixture was stirred and refluxed in THF (150mL) for 48 h. After cooling to room temperature, the solvent was removed using a rotary evaporator. The mixture was washed with water. The resulting dark solid was chromatographed on silica gel using CH_2Cl_2–acetone (4: 1) as the eluent to afford N_6Br as a yellow powder. (18 g, 81%Yield); ^{1}H NMR (400 MHz ; [D]DMSO): δ = 9.99 (s, 1H), 9.89 (s, 1H), 8.82 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.20 (dd, *J* = 8.0, 2.0 Hz, 1H), 8.17 (d, *J* = 9.2 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.63 (m, 3H), 7.34 (dd, *J* = 8.0, 4.4 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 7.05 ppm (d, *J* = 7.6 Hz, 1H); MS (ESI): *m/z* = 393 $[M+H]^+$.

2-(phenyldipyridyltriamino)-1,8-naphthyridine (H_3phdptrany):

A mixture of N_6Br (8 g , 20.4 mmol), *t*-BuONa (3.92 g , 40.8 mmol), Pd_2(dba)$_3$ (0.374 g , 0.4 mmol), dppp (0.337 g , 0.8 mmol) and aniline 20mL (219 mmol) were placed in a flame-dried flask under argon. The mixture was stirred and refluxed for 48 h. After cooling to room temperature, ether was added to the mixture and the solution was then filtered. The resulting dark solid was chromatographed on silica gel using CH_2Cl_2–acetone (4: 1) as the eluent to afford H_3phdptrany as a yellow powder. (4.13 g, 50%Yield); ^{1}H NMR (400 MHz ; [D]DMSO): δ 9.93 (s, 1H), 9.10 (s, 1H), 8.81 (dd, *J* = 4.4, *J'* = 2.0 Hz, 1H), 8.20 (dd, *J* = 7.8, *J'* = 2 Hz, 1H), 8.16 (d, *J* = 9.2 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.33 (dd, *J* = 7.6, *J'* = 4.4Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.34 (d, *J* = 7.2 Hz, 1H); MS (ESI): *m/z* = 406 $[M+H]^+$.

[Ni_7(phdptrany)$_4$Cl](PF_6) (1):

A mixture of H_3phdptrany (200 mg, 0.5 mmol), $NiCl_2$ (227 mg, 1.75 mmol) and naphthalene (20 g) in a 125-mL round-bottomed flask was gently refluxed for 24 h (about 220 °C), and then *t*-BuOK (200 mg, 1.8 mmol) in *t*-BuOH (5 mL) was slowly added to the solution. The resulting solution immediately turned to dark brown. The mixture was heated

for another 5 h and then KPF_6 (200 mg) was added to this solution as the source of counter anions. After 1 h, this solution was cooled to ca. 50 °C, and hexane (300 mL) was added. The mixture was then filtered and the solid was washed with hexane (3×100 mL) to remove naphthalene. The solid was dissolved in CH_2Cl_2 (200 mL) and the solution was filtered. The filtrate was then condensed to 10 mL under reduced pressure. Hexane (20 mL) was added to the CH_2Cl_2 solution prior to filtration. The solid was dissolved in CH_2Cl_2 layered by hexane. After two weeks, deep brown crystals were obtained. (40.74 mg, 15 % Yield); IR (KBr): $\tilde{\nu}$ = 1602, 1580, 1548, 1522, 1492, 1447, 1415, 1375, 1332, 1251, 1221, 1135, 837, 790, 642, 440 cm^{-1}; MS (FAB): *m/z* = 2054 $[M+H]^+$; UV/Vis (CH_2Cl_2): $\lambda_{max}(\varepsilon)$ = 332 (4.55×10^4), 388 (6.01×10^4), 656 (7.16×10^3), 1198 (6.52×10^3) , 1700 (2.89×10^3); Elemental analysis (%)$[Ni_7(phdptrany)_4Cl](PF_6)\cdot2CH_2Cl\cdot C_6H_{14}$: calcd. C 50.84, H 3.36, N 15.96; found: C 51.13, H 3.41, N 15.54.

X-ray Structure Determinations:

Crystallographic data were collected at 150(2) K on a NONIUS Kappa CCD diffractometer using graphite-monochromatized Mo-Kα radiation (λ = 0.71073 Å). Cell parameters were retrieved and refined using *DENZO-SMN* software on all observed reflections. Data reduction was performed with the *DENZO-SMN* software.[3] An empirical absorption was based on the symmetry-equivalent reflection and absorption corrections were applied with the SORTAV program.[4] The structures were solved and refined with *SHELX* programs.[5] The hydrogen atoms were included in calculated positions and refined using a riding mode.

Table S1.

Total Energies and Cartesian Coordinates Obtained from DFT/B3LYP Calculations

$Ni_7(phdptrany)_4Cl$ (156 atoms, C_4 symmetry)

^5A state E = −149752.1525 eV ; $<S^2>$ = 6.00116

	X	Y	Z	SPIN	Charge
Ni	0.00000	0.00000	7.75014	0.17981	0.24111
Ni	0.00000	0.00000	5.39800	0.38534	0.13328
Ni	0.00000	0.00000	3.11234	0.27230	0.06818
Ni	0.00000	0.00000	0.82286	0.07264	-0.24361
Ni	0.00000	0.00000	-1.49726	-0.02097	0.07576
Ni	0.00000	0.00000	-3.84578	1.21441	0.34112
Ni	0.00000	0.00000	-6.20513	1.41396	-0.04665
Cl	0.00000	0.00000	-8.69304	0.05079	-0.40765
N	-1.10535	1.53984	7.64878	0.01523	-0.27418
N	-0.64297	1.82089	5.36874	0.00081	-0.25730
N	-0.07724	1.91175	3.08675	0.00255	-0.25413
N	0.59196	1.83354	0.83505	0.00324	-0.25017
N	1.17557	1.53412	-1.43536	-0.00005	-0.24567
N	-1.20807	1.66500	-3.69752	0.05306	-0.18447
N	-0.81929	1.99172	-5.99103	0.04952	-0.14382
C	-1.22962	2.28811	6.53703	-0.00406	0.37589
C	-1.93667	3.53803	6.49254	0.00357	-0.32302
C	-2.00309	4.24213	5.29856	-0.00248	-0.16392
C	-1.37104	3.75808	4.12916	0.00289	-0.33299
C	-0.68098	2.53473	4.18851	-0.00065	0.33807
C	0.43992	2.57275	1.99798	-0.00154	0.32064
C	0.87062	3.93026	2.00683	0.00117	-0.30369
C	1.36281	4.49861	0.83297	-0.00101	-0.19918
C	1.46702	3.74373	-0.34909	0.00174	-0.31534
C	1.11342	2.37733	-0.32041	-0.00069	0.29156
C	-1.73160	2.03306	-2.49450	-0.00676	0.23537
C	-2.38287	3.32164	-2.36369	0.00467	-0.25697
C	-2.48591	4.15542	-3.45199	-0.00504	-0.33418
C	-1.32927	2.47029	-4.79974	-0.00543	-0.08791
C	-1.97301	3.75044	-4.72897	0.00616	0.47685
C	-2.05081	4.54114	-5.90305	-0.00574	-0.32667
C	-1.51151	4.05059	-7.09005	0.00493	-0.20414

C	-0.91198	2.76704	-7.09137	-0.01025	-0.17439
N	1.53984	1.10535	7.64878	0.01523	-0.54723
N	1.82089	0.64297	5.36874	0.00081	-0.25730
N	1.91175	0.07724	3.08675	0.00255	-0.25413
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N	1.99172	0.81929	-5.99103	0.04952	-0.14382
C	2.28811	1.22962	6.53703	-0.00406	0.37589
C	3.53803	1.93667	6.49254	0.00357	-0.32302
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C	3.75808	1.37104	4.12916	0.00289	-0.33299
C	2.53473	0.68098	4.18851	-0.00065	0.33807
C	2.57275	-0.43992	1.99798	-0.00154	0.32064
C	3.93026	-0.87062	2.00683	0.00117	-0.30369
C	4.49861	-1.36281	0.83297	-0.00101	-0.19918
C	3.74373	-1.46702	-0.34909	0.00174	-0.31534
C	2.37733	-1.11342	-0.32041	-0.00069	0.29156
C	2.03306	1.73160	-2.49450	-0.00676	0.23537
C	3.32164	2.38287	-2.36369	0.00467	-0.25697
C	4.15542	2.48591	-3.45199	-0.00504	-0.33418
C	2.47029	1.32927	-4.79974	-0.00543	-0.08791
C	3.75044	1.97301	-4.72897	0.00616	0.47685
C	4.54114	2.05081	-5.90305	-0.00574	-0.32667
C	4.05059	1.51151	-7.09005	0.00493	-0.20414
C	2.76704	0.91198	-7.09137	-0.01025	-0.17439
N	1.10535	-1.53984	7.64878	0.01523	-0.54723
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C	-3.93026	0.87062	2.00683	0.00117	-0.30369
C	-4.49861	1.36281	0.83297	-0.00101	-0.19918
C	-3.74373	1.46702	-0.34909	0.00174	-0.31534
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C	-2.03306	-1.73160	-2.49450	-0.00676	0.23537
C	-3.32164	-2.38287	-2.36369	0.00467	-0.25697
C	-4.15542	-2.48591	-3.45199	-0.00504	-0.33418
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C	-4.54114	-2.05081	-5.90305	-0.00574	-0.32667
C	-4.05059	-1.51151	-7.09005	0.00493	-0.20414
C	-2.76704	-0.91198	-7.09137	-0.01025	-0.17439
H	-0.51496	2.33069	-8.00257	0.00173	0.29427
H	-1.54940	4.61828	-8.01321	0.00003	0.24647
H	-2.53026	5.51662	-5.86492	0.00057	0.25128
H	-2.94264	5.13718	-3.35020	0.00055	0.25067
H	-2.73789	3.63352	-1.38970	0.00057	0.27813
H	-4.20531	1.78717	-1.27427	-0.00011	0.26213

H	-5.54131	1.67060	0.83054	0.00002	0.23798
H	-4.49592	0.82646	2.92771	-0.00011	0.27876
H	-4.29013	-1.45781	3.19116	-0.00016	0.25617
H	-5.18018	-2.55171	5.25559	0.00015	0.22803
H	-3.90730	-2.40497	7.39970	-0.00033	0.21949
H	0.51496	-2.33069	-8.00257	0.00173	0.29427
H	1.54940	-4.61828	-8.01321	0.00003	0.24647
H	2.53026	-5.51662	-5.86492	0.00057	0.25128
H	2.94264	-5.13718	-3.35020	0.00055	0.25067
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H	5.54131	-1.67060	0.83054	0.00002	0.23798
H	4.49592	-0.82646	2.92771	-0.00011	0.27876
H	1.45781	-4.29013	3.19116	-0.00016	0.25617
H	2.55171	-5.18018	5.25559	0.00015	0.22803
H	2.40497	-3.90730	7.39970	-0.00033	0.21949
H	4.29013	1.45781	3.19116	-0.00016	0.25617
H	5.18018	2.55171	5.25559	0.00015	0.22803
H	3.90730	2.40497	7.39970	-0.00033	0.21949
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H	1.78717	4.20531	-1.27427	-0.00011	0.26213
H	1.67060	5.54131	0.83054	0.00002	0.23798
H	0.82646	4.49592	2.92771	-0.00011	0.27876
H	-1.45781	4.29013	3.19116	-0.00016	0.25617
H	-2.55171	5.18018	5.25559	0.00015	0.22803
H	-2.40497	3.90730	7.39970	-0.00033	0.21949
H	-2.33069	-0.51496	-8.00257	0.00173	0.29427
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H	-5.51662	-2.53026	-5.86492	0.00057	0.25128
H	-5.13718	-2.94264	-3.35020	0.00055	0.25067
H	-3.63352	-2.73789	-1.38970	0.00057	0.27813
H	-1.78717	-4.20531	-1.27427	-0.00011	0.26213
H	-1.67060	-5.54131	0.83054	0.00002	0.23798
H	-0.82646	-4.49592	2.92771	-0.00011	0.27876
H	-1.68391	1.82013	8.43731	-0.00084	0.27305
H	-1.82013	-1.68391	8.43731	-0.00084	0.27305
H	1.68391	-1.82013	8.43731	-0.00084	0.27305

H	1.82013	1.68391	8.43731	-0.00084	0.27305

^{3}B state E = −149751.5183 eV ; $<S^2>$ = 2.00057

	X	Y	Z	SPIN	Charge
Ni	0.00000	0.00000	7.815132	0.000484	0.202901
Ni	0.00000	0.00000	5.425976	0.001787	0.188039
Ni	0.00000	0.00000	3.109782	0.002993	0.155609
Ni	0.00000	0.00000	0.825078	0.005616	-0.32806
Ni	0.00000	0.00000	-1.476695	0.019658	0.286124
Ni	0.00000	0.00000	-3.799698	0.045265	-0.013424
Ni	0.00000	0.00000	-6.250501	1.603435	-0.047729
Cl	0.00000	0.00000	-8.665204	0.098487	-0.342776
N	1.620348	1.004221	7.683616	0.000279	-0.529146
N	1.847949	0.588404	5.378896	0.000078	-0.25152
N	1.922515	0.085221	3.069516	0.00008	-0.242103
N	1.847204	-0.567430	0.812193	0.00016	-0.251614
N	1.570826	-1.094939	-1.477577	0.000678	-0.232781
N	1.603398	1.106385	-3.718638	0.0018	-0.230645
N	2.012059	0.612812	-5.989585	0.056791	-0.175031
C	2.345065	1.132978	6.561335	-0.000072	0.344635
C	3.613034	1.820642	6.51645	0.000054	-0.322223
C	4.294581	1.928989	5.315923	-0.000043	-0.173079
C	3.778174	1.344296	4.132601	0.000043	-0.347189
C	2.554307	0.656365	4.20021	-0.000006	0.310692
C	2.581297	-0.408713	1.987556	-0.000143	0.289258
C	3.956171	-0.824620	1.977371	0.00065	-0.287132
C	4.534681	-1.282975	0.803343	-0.000303	-0.204099
C	3.781647	-1.371906	-0.392043	0.000637	-0.335167
C	2.416732	-1.050063	-0.342127	-0.000286	0.295123
C	1.941701	1.718775	-2.523154	-0.000057	0.285292
C	3.218273	2.403408	-2.423466	0.000772	-0.250366
C	4.083043	2.430047	-3.484199	-0.000614	-0.330335
C	2.442580	1.173474	-4.81139	-0.00141	0.006257
C	3.719559	1.820738	-4.733961	0.002686	0.474889
C	4.556694	1.814699	-5.873328	-0.004051	-0.327819
C	4.120598	1.194870	-7.04608	0.003871	-0.20381
C	2.834633	0.617859	-7.065	-0.008188	-0.156335
N	1.004221	-1.620348	7.683616	0.000279	-0.529146
N	0.588404	-1.847949	5.378896	0.000078	-0.25152
N	0.085221	-1.922515	3.069516	0.00008	-0.242103

N	-0.567430	-1.847204	0.812193	0.00016	-0.251614
N	-1.094939	-1.570826	-1.477577	0.000678	-0.232781
N	1.106385	-1.603398	-3.718638	0.0018	-0.230645
N	0.612812	-2.012059	-5.989585	0.056791	-0.175031
C	1.132978	-2.345065	6.561335	-0.000072	0.344635
C	1.820642	-3.613034	6.51645	0.000054	-0.322223
C	1.928989	-4.294581	5.315923	-0.000043	-0.173079
C	1.344296	-3.778174	4.132601	0.000043	-0.347189
C	0.656365	-2.554307	4.20021	-0.000006	0.310692
C	-0.408713	-2.581297	1.987556	-0.000143	0.289258
C	-0.824620	-3.956171	1.977371	0.00065	-0.287132
C	-1.282975	-4.534681	0.803343	-0.000303	-0.204099
C	-1.371906	-3.781647	-0.392043	0.000637	-0.335167
C	-1.050063	-2.416732	-0.342127	-0.000286	0.295123
C	1.718775	-1.941701	-2.523154	-0.000057	0.285292
C	2.403408	-3.218273	-2.423466	0.000772	-0.250366
C	2.430047	-4.083043	-3.484199	-0.000614	-0.330335
C	1.173474	-2.442580	-4.81139	-0.00141	0.006257
C	1.820738	-3.719559	-4.733961	0.002686	0.474889
C	1.814699	-4.556694	-5.873328	-0.00018	-0.327819
C	1.194870	-4.120598	-7.04608	0.003871	-0.20381
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N	-1.620348	-1.004221	7.683616	0.000279	-0.529146
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N	-1.922515	-0.085221	3.069516	0.00008	-0.242103
N	-1.847204	0.567430	0.812193	0.00016	-0.251614
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C	-3.781647	1.371906	-0.392043	0.000637	-0.335167
C	-2.416732	1.050063	-0.342127	-0.000286	0.295123
C	-1.941701	-1.718775	-2.523154	-0.000057	0.285292
C	-3.218273	-2.403408	-2.423466	0.000772	-0.250366

C	-4.083043	-2.430047	-3.484199	-0.000614	-0.330335
C	-2.442580	-1.173474	-4.81139	-0.00141	0.006257
C	-3.719559	-1.820738	-4.733961	0.002686	0.474889
C	-4.556694	-1.814699	-5.873328	-0.004051	-0.327819
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C	-0.656365	2.554307	4.20021	-0.000006	0.310692
C	0.408713	2.581297	1.987556	-0.000143	0.289258
C	0.824620	3.956171	1.977371	0.00065	-0.287132
C	1.282975	4.534681	0.803343	-0.000303	-0.204099
C	1.371906	3.781647	-0.392043	0.000637	-0.335167
C	1.050063	2.416732	-0.342127	-0.000286	0.295123
C	-1.718775	1.941701	-2.523154	-0.000057	0.285292
C	-2.403408	3.218273	-2.423466	0.000772	-0.250366
C	-2.430047	4.083043	-3.484199	-0.000614	-0.330335
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C	-1.820738	3.719559	-4.733961	0.002686	0.474889
C	-1.814699	4.556694	-5.873328	-0.004051	-0.327819
C	-1.194870	4.120598	-7.04608	0.003871	-0.20381
C	-0.617859	2.834633	-7.065	-0.008188	-0.156335
H	2.426617	0.176203	-7.967347	0.001563	0.290505
H	4.732850	1.165597	-7.940156	0.000142	0.251105
H	5.531150	2.294395	-5.823173	0.00018	0.2568
H	5.060871	2.894642	-3.385081	0.000362	0.256784
H	3.493619	2.828289	-1.467321	0.000001	0.290222
H	1.656812	4.251457	-1.325094	-0.000045	0.258248
H	1.581712	5.579949	0.800442	0.000014	0.237497
H	0.788275	4.518748	2.900533	-0.000043	0.285949
H	-1.468232	4.288323	3.186195	0.00000	0.248931
H	-2.470932	5.237028	5.275072	0.000005	0.221329

H	-2.252965	4.003585	7.433172	-0.000002	0.212992
H	-2.426617	-0.176203	-7.967347	0.001563	0.290505
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H	-5.531150	-2.294395	-5.823173	0.00018	0.2568
H	-5.060871	-2.894642	-3.385081	0.000362	0.256784
H	-3.493619	-2.828289	-7.789229	0.000001	0.290222
H	-1.656812	-4.251457	-7.233363	-0.000045	0.258248
H	-1.581712	-5.579949	0.800442	0.000014	0.237497
H	-0.788275	-4.518748	2.900533	-0.000043	0.285949
H	-4.288323	-1.468232	3.186195	0.00000	0.248931
H	-5.237028	-2.470932	5.275072	0.000005	0.221329
H	-4.003585	-2.252965	7.433172	-0.000002	0.212992
H	1.468232	-4.288323	3.186195	0.00000	0.248931
H	2.470932	-5.237028	5.275072	0.000005	0.221329
H	2.252965	-4.003585	7.433172	-0.000002	0.212992
H	0.176203	-2.426617	-7.967347	0.001563	0.290505
H	1.165597	-4.732850	-7.940156	0.000142	0.251105
H	2.294395	-5.531150	-5.823173	0.00018	0.2568
H	2.894642	-5.060871	-3.385081	0.000362	0.256784
H	2.828289	-3.493619	-1.467321	0.000001	0.290222
H	4.251457	-1.656812	-1.325094	-0.000045	0.258248
H	5.579949	-1.581712	0.800442	0.000014	0.237497
H	4.518748	-0.788275	2.900533	-0.000043	0.285949
H	4.288323	1.468232	3.186195	0.00000	0.248931
H	5.237028	2.470932	5.275072	0.000005	0.221329
H	4.003585	2.252965	7.433172	-0.000002	0.212992
H	-0.176203	2.426617	-7.967347	0.001563	0.290505
H	-1.165597	4.732850	-7.940156	0.000142	0.251105
H	-2.294395	5.531150	-5.823173	0.00018	0.2568
H	-2.894642	5.060871	-3.385081	0.000362	0.256784
H	-2.828289	3.493619	-1.467321	0.000001	0.290222
H	-4.251457	1.656812	-1.325094	-0.000045	0.258248
H	-5.579949	1.581712	0.800442	0.000014	0.237497
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H	-1.516134	1.979954	8.487149	-0.000015	0.258717
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H	1.516134	-1.979954	8.487149	-0.000015	0.258717

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