One Step Conversion of 1,5-*bis*(Dimethylamino)naphthalene to Salts of "Back to Back" *bis*-Acridine Derivatives.

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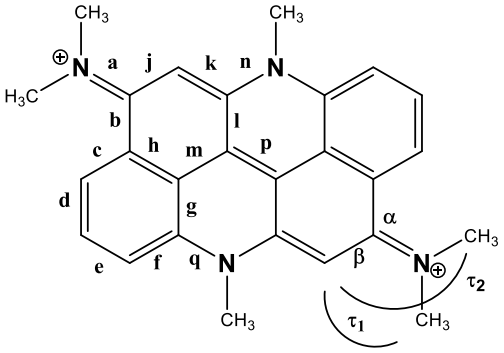
Supplementary Information.

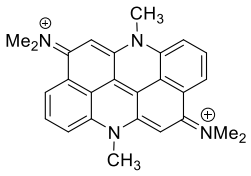
Tables of experimental and calculated bond lengths for $\mathbf{9}^{2+}$, $\mathbf{10}^{+}$,$\mathbf{12}^{+\cdot}$, **13**.

Details of X-ray Crystallography, for **9**$(I_3)_2$, **9**$(TCNQ)_4$ and **10**.TCNQ-F_4.

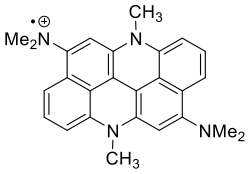
Coordinates for calculated structures.

Table S1. Selected Bond Lengths, Angles and Torsion Angles for dication **9**, radical cation **11**, and neutral heterocycle **12** for structures calculated at the (UB3LYP/6-31g(d,p)) level, and for dication **9** from the crystal structure of its triiodide and tetrakis(TCNQ) salts.

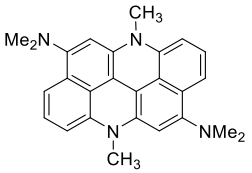




9



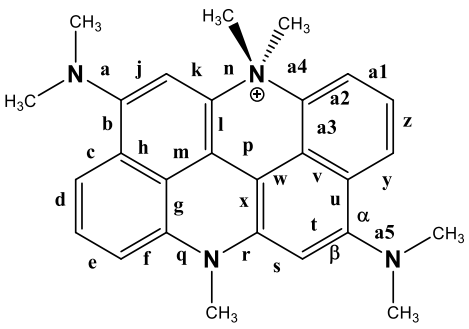
11

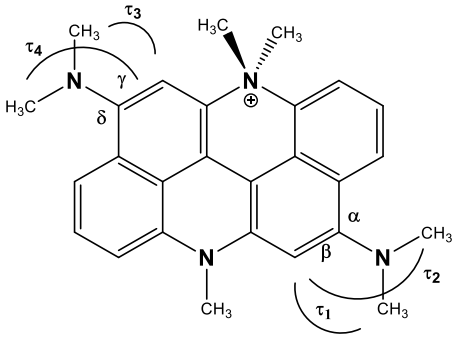


12

Distances (Å), Angles (°)	**9^{2+}** experimental from **9**.$(I_3)_2$	**9^{2+}** experimental from **9**.$(TCNQ)_4$	**9^{2+}** calculated	**$12^{+\cdot}$** calculated	**13** calculated
a	1.337(7)	1.347(3)	1.351	1.386	1.423
b	1.470(8)	1.462(3)	1.473	1.453	1.434
c	1.386(7)	1.393(3)	1.398	1.410	1.423
d	1.388(8)	1.389(3)	1.398	1.385	1.374
e	1.366(8)	1.364(3)	1.386	1.398	1.412
f	1.406(7)	1.405(3)	1.407	1.399	1.392
g	1.409(7)	1.410(3)	1.421	1.427	1.434
h	1.406(7)	1.416(3)	1.426	1.424	1.426
j	1.394(8)	1.395(3)	1.411	1.394	1.387
k	1.381(8)	1.380(3)	1.395	1.410	1.414
l	1.441(7)	1.439(3)	1.444	1.416	1.396
m	1.418(7)	1.419(3)	1.424	1.422	1.423
n	1.368(7)	1.367(3)	1.374	1.387	1.406
p	1.372(11)	1.377(4)	1.389	1.415	1.439
q	1.394(7)	1.394(3)	1.397	1.401	1.404
α /°	121.3(5)	121.72(19)	121.9	119.7	118.3
β /°	120.1(5)	118.39(19)	119.5	120.9	121.7
$(H_3C\text{-})_2N$=	1.469(7) 1.455(7)	1.468(3) 1.458(3)	1.474 1.470	1.470 1.458	1.465 1.454
H_3C-N	1.467(7)	1.474(3)	1.475	1.465	1.453
Σangles /°	357.5(14)	357.7(3)	358.6	351.9	343.4
T_1 /°	-13.4(7)	-12.8(3)	-15.5	-18.2	-24.9
T_2 /°	147.3(5)	148.8(2)	149.9	128.1	108.7

Table S2. Selected Bond Lengths, Angles and Torsion Angles for cation **10** from the crystal structure of its TCNQ-F_4 salt and from calculation on the isolated cation at the (UB3LYP/6-31g(d,p)) level.





Distances (Å), Angles (°)	**10**$^+$ experimental	**10**$^+$ calculated.
a	1.419(2)	1.410
b	1.438(2)	1.445
c	1.413(2)	1.413
d	1.365(2)	1.380
e	1.389(3)	1.403
f	1.390(2)	1.393
g	1.428(2)	1.430
h	1.414(2)	1.427
j	1.374(2)	1.384
k	1.406(2)	1.413
l	1.372(2)	1.381
m	1.430(2)	1.430
n	1.5098(19)	1.514
p	1.433(2)	1.436
q	1.395(2)	1.406
r	1.392(2)	1.387
s	1.419(2)	1.422
t	1.371(2)	1.383
u	1.438(2)	1.448
v	1.416(2)	1.431
w	1.416(2)	1.418
x	1.390(2)	1.398
y	1.406(2)	1.410
z	1.365(2)	1.380
a1	1.394(2)	1.404
a2	1.374(2)	1.383
a3	1.412(2)	1.417
a4	1.509(2)	1.519

a5	1.405(2)	1.403
N-CH_3	1.464(2)	1.463
$N^+(-CH_3)_2$	1.514(2) 1.518(2)	1.522 1.523
2 x $N(CH_3)_2$	1.455(2)-1.471(2)	1.456-1.471
α /º	117.92(15)	118.7
β /º	122.59(15)	122.0
γ /º	122.91(16)	122.2
δ /º	117.19(14)	118.8
Σ angles /º	338.7(3), 341.8(3)	345.0, 346.5
τ_1 /º	-13.0(2)	-21.3
τ_2 /º	118.42(19)	116.1
τ_3 /º	20.6(2)	23.5
τ_4 /º	-107.20(18)	-112.2

X-Ray Crystallography.

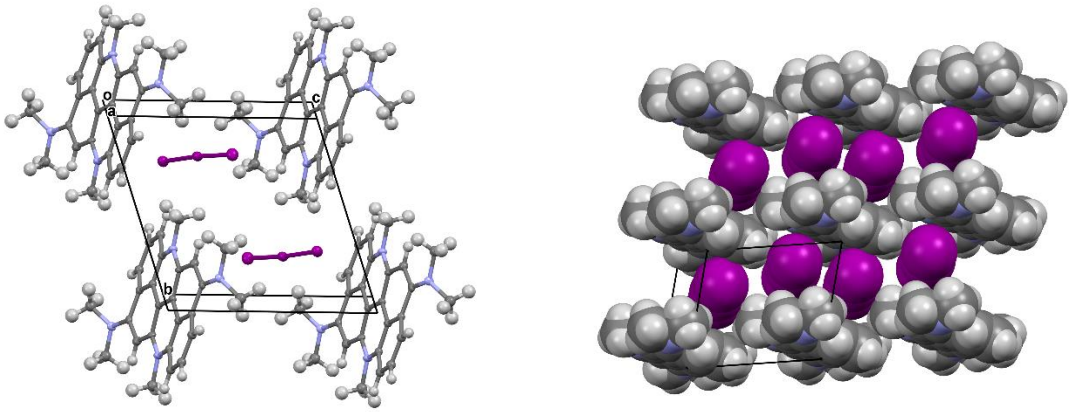


Fig. S1. Crystal structure of **9**.$(I_3)_2$ viewed down the *a* axis (a) showing the two centrosymmetrically related triiodide anions and the dications which are located on centres of symmetry, *c* axis horizontal (left), and (b) showing the layer structure with gaps between triiodide ions, *b* axis horizontal (right).

Table S3. Crystallographic data.

	9.$(I_3)_2$	**9.$(TNCQ)_4$**	**10.TCNQ-F_4**
Formula	$C_{26}H_{26}N_4.(I_3)_2$	$C_{26}H_{26}N_4.$ $(C_{12}H_4N_4)_4$	$C_{27}H_{29}N_4.$ $C_{12}F_4N_4$
Formula weight	1,155.9	1,211.3	685.70
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1
a[Å]	9.0754(6)	7.2711(4)	11.4701(4)
b[Å]	9.9135(7)	13.2126(7)	11.7251(4)
c[Å]	7.3890(4)	15.6117(7)	13.1590(4)
α[°]	69.799(6)	86.844(4)	74.899(3)
β [°]	77.933(6)	77.551(4)	67.021(3)
γ[°]	67.701(6)	80.640(4)	86.962(2)
V [Å^3]	772.34(10)	1444.74(13)	1570.67(10)
Z	1	1	2
ρ [g cm^{-3}]	2.48	1.392	1.450
T [*K*]	150	150	150
μ (mm^{-1})	6.06	0.088	0.106
unique refl.	3560	5898	7821
Refl, I > 2σI	2700	3626	5110
R_1	0.039	0.059	0.052
wR_2	0.084	0.144	0.132
$\Delta\rho$(r) [e Å^{-3}]	0.875 / -1.093	0.216/ -0.302	0.305/ -0.237
Cryst. Solvent.	DMF/ether	CH_3CN	CH_3CN

Single crystal X-ray diffraction data were measured using MoKα radiation on an Agilent Xcalibur diffractometer equipped with a Sapphire detector and an 700 series Cryostream low temperature system at Nottingham Trent University using the CrysAlis-Pro software package.[S1] Structures were solved by direct methods and refined using the SHELXS and SHELXL suite of programs[S2] operated through the XSEED interface.[S3] Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed in calculated positions, and refined with isotropic displacement parameters linked to the connected carbon atom. Molecular illustrations were made with Mercury.[S4]

Calculations on 9^{2+}, 10^{+}, $12^{+\cdot}$ and 13.

Calculations on these four species were carried out at the UB3LYP/6-31g(d,p) level. In the case of dication $\mathbf{9}^{2+}$ the energies of both the singlet and triplet states were separately calculated, and the singlet found to be 1.29 eV more stable.

Table S4. Summary of results of calculations on $\mathbf{9}^{2+}$, and its reduction products $\mathbf{12}^{+\cdot}$ and **13**, and also on cation $\mathbf{10}^{+}$.

	Charge	Multiplicity	Energy (a.u.)	dE (eV)	C(Ar)-NMe_2 (Å)
$\mathbf{9}^{2+}$	2	1	-1225.022546	0.000	1.351
	2	3	-1224.975101	1.291	1.366
$\mathbf{12}^{+\cdot}$	1	2	-1225.317765	-8.033	1.386
13	0	1	-1225.493738	-12.822	1.423
$\mathbf{10}^{+}$	1	1	-1265.182866		

Coordinates for the calculated structures.

Structure 9^{2+}

Dication singlet

56

E(UB3LYP/6-31G(d,p)) = -1225.022546

C	-1.62870900	-0.86650500	-0.32146500
C	-2.85979500	-0.65251400	-1.00832200
H	-4.20671700	-1.42823400	-3.22781300
C	-3.93996900	-1.48945000	-0.71443700
H	-4.92165900	-1.28994700	-1.11906100
H	-5.73806300	-0.51683300	-3.08651700
C	-4.23536800	1.93214500	-3.44145400
H	-4.12253200	2.74746800	-2.72581100
H	-5.26818300	1.93043800	-3.79185100
N	-3.96920300	0.63860700	-2.79666500
N	0.21370400	2.26606800	-1.08028400

C	-2.95014300	0.50008100	-1.92060900
C	-1.94247600	1.48642500	-1.86413400
H	-2.01350200	2.32549400	-2.53573300
C	-0.78257500	1.32050700	-1.10733000
C	-0.58230000	0.09835800	-0.36503300
C	-4.69775600	-0.47810000	-3.42451100
H	-4.69716400	-0.31102900	-4.50519300
H	-3.57847400	2.09774400	-4.30422000
C	-0.04390600	3.58381000	-1.69140500
H	0.16518500	3.57332400	-2.76528300
H	0.56974600	4.33645800	-1.20379600
H	-1.08537600	3.85277700	-1.52030300
C	1.45797500	2.01725900	-0.49509900
C	2.55616000	2.86532900	-0.72646000
H	2.47953800	3.71336000	-1.39302000
C	3.78371400	2.57455800	-0.15224900
H	4.63884500	3.20023400	-0.38348200
C	-1.45797500	-2.01725900	0.49509900
C	-2.55616000	-2.86532900	0.72646000
H	-2.47953800	-3.71336000	1.39302000
C	-3.78371400	-2.57455800	0.15224900
H	-4.63884500	-3.20023400	0.38348200
N	3.96920300	-0.63860700	2.79666500
N	-0.21370400	-2.26606800	1.08028400
C	2.95014300	-0.50008100	1.92060900
C	1.94247600	-1.48642500	1.86413400
H	2.01350200	-2.32549400	2.53573300
C	0.78257500	-1.32050700	1.10733000
C	0.58230000	-0.09835800	0.36503300
C	4.69775600	0.47810000	3.42451100
H	4.69716400	0.31102900	4.50519300

H	5.73806300	0.51683300	3.08651700
C	4.23536800	-1.93214500	3.44145400
H	4.12253200	-2.74746800	2.72581100
H	5.26818300	-1.93043800	3.79185100
H	3.57847400	-2.09774400	4.30422000
C	0.04390600	-3.58381000	1.69140500
H	-0.16518500	-3.57332400	2.76528300
H	-0.56974600	-4.33645800	1.20379600
H	1.08537600	-3.85277700	1.52030300
C	1.62870900	0.86650500	0.32146500
C	2.85979500	0.65251400	1.00832200
H	4.20671700	1.42823400	3.22781300
C	3.93996900	1.48945000	0.71443700
H	4.92165900	1.28994700	1.11906100

Structure 9^{2+}

Dication triplet

56

E(UB3LYP/6-31G(d,p)) = -1224.975101

C	-1.63726900	-0.85049500	-0.31197300
C	-2.86594000	-0.65163800	-1.01268100
H	-4.15685500	-1.41488400	-3.28262300
C	-3.94692600	-1.50985000	-0.73093300
H	-4.92635400	-1.31526100	-1.14435200
H	-5.71517800	-0.55443900	-3.13502400
C	-4.29477900	1.95004600	-3.38687500
H	-4.14832300	2.74473000	-2.65509200
H	-5.34609300	1.95026000	-3.68034200
N	-3.98440700	0.64108200	-2.80096400

N	0.23793900	2.26092600	-1.10990300
C	-2.95571900	0.48560600	-1.91565500
C	-1.93262700	1.46040800	-1.88536900
H	-2.00654200	2.29706900	-2.56188500
C	-0.77448600	1.29973900	-1.11433900
C	-0.59829500	0.10854800	-0.37087000
C	-4.67375100	-0.47460300	-3.46452100
H	-4.67465400	-0.27865100	-4.54110400
H	-3.69128800	2.14671600	-4.28221400
C	-0.00415200	3.57011200	-1.74054000
H	0.27560500	3.56586200	-2.79866200
H	0.56433200	4.33469400	-1.21559800
H	-1.05567500	3.83026300	-1.63700900
C	1.46765700	2.01012400	-0.51690900
C	2.56538000	2.86600000	-0.73039000
H	2.49030900	3.71202500	-1.39913800
C	3.78968500	2.59054100	-0.13495900
H	4.64010900	3.22647700	-0.35534300
C	-1.46765700	-2.01012400	0.51690900
C	-2.56538000	-2.86600000	0.73039000
H	-2.49030900	-3.71202500	1.39913800
C	-3.78968500	-2.59054100	0.13495900
H	-4.64010900	-3.22647700	0.35534300
N	3.98440700	-0.64108200	2.80096400
N	-0.23793900	-2.26092600	1.10990300
C	2.95571900	-0.48560600	1.91565500
C	1.93262700	-1.46040800	1.88536900
H	2.00654200	-2.29706900	2.56188500
C	0.77448600	-1.29973900	1.11433900
C	0.59829500	-0.10854800	0.37087000
C	4.67375100	0.47460300	3.46452100

H	4.67465400	0.27865100	4.54110400
H	5.71517800	0.55443900	3.13502400
C	4.29477900	-1.95004600	3.38687500
H	4.14832300	-2.74473000	2.65509200
H	5.34609300	-1.95026000	3.68034200
H	3.69128800	-2.14671600	4.28221400
C	0.00415200	-3.57011200	1.74054000
H	-0.27560500	-3.56586200	2.79866200
H	-0.56433200	-4.33469400	1.21559800
H	1.05567500	-3.83026300	1.63700900
C	1.63726900	0.85049500	0.31197300
C	2.86594000	0.65163800	1.01268100
H	4.15685500	1.41488400	3.28262300
C	3.94692600	1.50985000	0.73093300
H	4.92635400	1.31526100	1.14435200

Structure $12^{+\cdot}$

Cation doublet

56

E(UB3LYP/6-31G(d,p)) = -1225.317765

C	-1.64806800	-0.84700400	-0.28557600
C	-2.87687400	-0.64192700	-0.97572300
H	-4.12778100	-1.40763900	-3.23003800
C	-3.96386900	-1.49556700	-0.69822600
H	-4.93468100	-1.29003100	-1.12941700
H	-5.63126400	-0.51989200	-3.55857300
C	-4.39781100	1.95243900	-3.23676200
H	-4.27158800	2.72441200	-2.47498200
H	-5.44288600	1.95696100	-3.55696800

N	-4.09281300	0.63988800	-2.68079900
N	0.23791300	2.23238000	-1.14467600
C	-2.96753000	0.48709700	-1.88583500
C	-1.94049400	1.42962300	-1.91065200
H	-2.01236900	2.24782900	-2.61045800
C	-0.77058700	1.27969700	-1.13875800
C	-0.59351000	0.10333400	-0.37058300
C	-4.53859600	-0.45464400	-3.55547200
H	-4.20176000	-0.27385800	-4.58591500
H	-3.77859200	2.20341900	-4.11254300
C	-0.00443100	3.53309500	-1.77481700
H	0.27648300	3.53550100	-2.83380100
H	0.56500700	4.29883000	-1.25032000
H	-1.05895200	3.78762500	-1.68044000
C	1.48529700	1.98870600	-0.55497800
C	2.57877900	2.83171300	-0.78048200
H	2.50653200	3.66849800	-1.46188100
C	3.80832500	2.56240700	-0.17184900
H	4.65680100	3.19923100	-0.39924400
C	-1.48529700	-1.98870600	0.55497800
C	-2.57877900	-2.83171300	0.78048200
H	-2.50653200	-3.66849800	1.46188100
C	-3.80832500	-2.56240700	0.17184900
H	-4.65680100	-3.19923100	0.39924400
N	4.09281300	-0.63988800	2.68079900
N	-0.23791300	-2.23238000	1.14467600
C	2.96753000	-0.48709700	1.88583500
C	1.94049400	-1.42962300	1.91065200
H	2.01236900	-2.24782900	2.61045800
C	0.77058700	-1.27969700	1.13875800
C	0.59351000	-0.10333400	0.37058300

C	4.53859600	0.45464400	3.55547200
H	4.20176000	0.27385800	4.58591500
H	5.63126400	0.51989200	3.55857300
C	4.39781100	-1.95243900	3.23676200
H	4.27158800	-2.72441200	2.47498200
H	5.44288600	-1.95696100	3.55696800
H	3.77859200	-2.20341900	4.11254300
C	0.00443100	-3.53309500	1.77481700
H	-0.27648300	-3.53550100	2.83380100
H	-0.56500700	-4.29883000	1.25032000
H	1.05895200	-3.78762500	1.68044000
C	1.64806800	0.84700400	0.28557600
C	2.87687400	0.64192700	0.97572300
H	4.12778100	1.40763900	3.23003800
C	3.96386900	1.49556700	0.69822600
H	4.93468100	1.29003100	1.12941700

Structure 13

Neutral singlet

56

E(UB3LYP/6-31G(d,p)) = -1225.493738

C	-1.67127500	-0.83210300	-0.23437100
C	-2.90590500	-0.63933700	-0.92082800
H	-4.12041900	-1.38727300	-3.29886600
C	-3.99287100	-1.51921600	-0.65906300
H	-4.95108900	-1.32412700	-1.12419900
H	-5.38679400	-0.37974400	-4.02295500
C	-4.52292200	1.94105500	-3.06030400
H	-4.43850200	2.64904300	-2.23218100
H	-5.56023200	1.94326200	-3.41159000

N	-4.18630500	0.60229200	-2.60401000
N	0.25596000	2.19527100	-1.22006000
C	-2.99692300	0.46160000	-1.83494500
C	-1.94950200	1.36527500	-1.94068200
H	-2.03104400	2.16869300	-2.65963000
C	-0.76789700	1.23285600	-1.17455300
C	-0.60763000	0.10260900	-0.37138600
C	-4.34925300	-0.38832800	-3.67155400
H	-3.69191700	-0.18325300	-4.53465800
H	-3.89445800	2.30253100	-3.89523300
C	0.01455700	3.48149100	-1.85223700
H	0.33215100	3.50913400	-2.90400200
H	0.55687200	4.25805900	-1.30805600
H	-1.04717500	3.72332300	-1.80038600
C	1.51073500	1.95953300	-0.63667600
C	2.59779000	2.79752300	-0.86780000
H	2.52554000	3.61919400	-1.56843000
C	3.83091300	2.56005100	-0.22320600
H	4.66839900	3.21479700	-0.44748700
C	-1.51073500	-1.95953300	0.63667600
C	-2.59779000	-2.79752300	0.86780000
H	-2.52554000	-3.61919400	1.56843000
C	-3.83091300	-2.56005100	0.22320600
H	-4.66839900	-3.21479700	0.44748700
N	4.18630500	-0.60229200	2.60401000
N	-0.25596000	-2.19527100	1.22006000
C	2.99692300	-0.46160000	1.83494500
C	1.94950200	-1.36527500	1.94068200
H	2.03104400	-2.16869300	2.65963000
C	0.76789700	-1.23285600	1.17455300
C	0.60763000	-0.10260900	0.37138600

C	4.34925300	0.38832800	3.67155400
H	3.69191700	0.18325300	4.53465800
H	5.38679400	0.37974400	4.02295500
C	4.52292200	-1.94105500	3.06030400
H	4.43850200	-2.64904300	2.23218100
H	5.56023200	-1.94326200	3.41159000
H	3.89445800	-2.30253100	3.89523300
C	-0.01455700	-3.48149100	1.85223700
H	-0.33215100	-3.50913400	2.90400200
H	-0.55687200	-4.25805900	1.30805600
H	1.04717500	-3.72332300	1.80038600
C	1.67127500	0.83210300	0.23437100
C	2.90590500	0.63933700	0.92082800
H	4.12041900	1.38727300	3.29886600
C	3.99287100	1.51921600	0.65906300
H	4.95108900	1.32412700	1.12419900

Structure 10

Monocation

60

UB3LYP/6-31g(d,p) -1265.1828663

C	1.583586	-0.934991	-0.081014
C	3.007221	-0.788505	-0.100690
H	5.136326	-0.700189	1.630307
C	3.821765	-1.930349	-0.241648
H	4.890772	-1.799036	-0.354476
H	6.660663	0.003866	1.061075
C	5.519583	1.967766	-0.398521
H	5.093790	2.250115	-1.363800
H	6.597624	1.836284	-0.524698
N	4.949381	0.701941	0.049327
N	0.456010	2.589617	-0.221061

C	3.557395	0.548760	-0.034301
C	2.703868	1.634819	-0.096939
H	3.125104	2.625735	-0.017345
C	1.291060	1.484291	-0.155671
C	0.737084	0.202706	-0.088810
C	5.607786	0.213508	1.271111
H	5.557999	0.962097	2.076874
H	5.367536	2.793450	0.316378
C	1.001369	3.912767	-0.523126
H	1.226232	4.488721	0.382263
H	0.279187	4.466860	-1.123820
H	1.907165	3.809610	-1.117936
C	-0.926510	2.470031	0.003522
C	-1.729073	3.591858	0.201604
H	-1.298794	4.583312	0.241738
C	-3.109340	3.445967	0.406865
H	-3.704212	4.333604	0.597698
C	1.054816	-2.249422	-0.101058
C	1.878695	-3.357241	-0.181896
H	1.478175	-4.364267	-0.199923
C	3.270717	-3.195312	-0.274801
H	3.901395	-4.070085	-0.386117
N	-4.924249	-0.401200	0.212894
N	-0.444847	-2.489853	-0.059433
C	-3.521505	-0.275840	0.137251
C	-2.686410	-1.376889	0.068576
H	-3.140086	-2.359062	0.040488
C	-1.282994	-1.229981	0.000026
C	-0.686227	0.014622	-0.046725
C	-5.675231	0.062955	-0.962836
H	-5.654273	-0.678632	-1.777910
H	-6.718173	0.236687	-0.682555
C	-5.456761	-1.652244	0.733335
H	-4.943813	-1.921351	1.660073

H	-6.517705	-1.513811	0.958847
H	-5.381270	-2.496318	0.024145
C	-0.837646	-3.255438	-1.315893
H	-0.584648	-2.632698	-2.172119
H	-0.289055	-4.193946	-1.355528
H	-1.907561	-3.448360	-1.295085
C	-1.524405	1.171189	0.027855
C	-2.938581	1.045810	0.172529
H	-5.259356	0.996303	-1.341430
C	-3.715381	2.206864	0.386736
H	-4.775214	2.107015	0.579933
C	-0.751626	-3.325145	1.175259
H	-1.817746	-3.536149	1.208518
H	-0.187764	-4.254355	1.130753
H	-0.455907	-2.744257	2.047113

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