Supporting Information

Synthesis and Structures of Mononuclear and Dinuclear Gallium Complexes with α-Diimine Ligands: Reduction of Metal or Ligand?

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Table of contents:

Experimental Section

Table S1. Crystallographic data and refinement details for compounds **2**−**7**.

Compound	**2**	**3**	**4**
Empirical formula	$C_{44}H_{72}Cl_2GaN_2NaO_4$	$C_{80}H_{128}Ga_2N_4NaO_6$	$C_{35}H_{48}Cl6Ga_2N_2$
Fw	856.65	1404.29	848.89
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*P*2(1)/*c*	*P*2(1)/n	*P*2(1)
a /Å	15.511(1)	13.817(1)	12.039(1)
b /Å	13.646(1)	17.598(1)	13.907(1)
c /Å	22.867(2)	32.893(3)	12.714(1)
α /°	90	90	90
β /°	95.466 (1)	94.644(1)	105.968(1)
γ /°	90	90	90
V /Å^3	4817.8(7)	7971.5(1)	2046.5(3)
Z	4	4	2
D_{calc}/g cm^{-3}	1.181	1.170	1.378
F (000)	1832	3028	872
μ /mm^{-1}	0.730	0.732	1.734
Reflns collected	23915	51542	13599
Independent reflns	8497	13968	7029
(R_{int})	0.0312	0.0594	0.0230
Observed reflns[$I>2\sigma(I)$]	6246	9424	6710
R_1;wR_2 [$I>2\sigma(I)$]	0.0444; 0.1362	0.1053; 0.1926	0.0262; 0.0281
R_1; wR_2 (all data)	0.0666; 0.1556	0.1472; 0.2123	0.0605; 0.0614
GOF (F^2)	1.057	1.123	1.007

Compound	**5**	**6**
Empirical formula	$C_{48}H_{64}Cl_2Ga_2N_4$	$C_{40}H_{48}Cl_2Ga_2N_4$
Fw	907.38	795.16
Crystal system	Monoclinic	Triclinic
Space group	*P*2(1)/*c*	*P*-1
a /Å	21.791(1)	8.3517(19)

b /Å	13.884(1)	11.301(3)
c /Å	15.558(1)	11.780(3)
α /°	90	116.796(3)
β /°	91.794(1)	92.365(4)
γ /°	90	93.472(4)
V /Å^3	4704.5(4)	987.7(4)
Z	4	1
D_{calc}/g cm^{-3}	1.267	1.337
F(000)	1864	412
μ /mm^{-1}	1.294	1.531
Reflns collected	23344	4927
Independent reflns	8294	3430
(R_{int})	0.0286	0.0228
Observed reflns[$I > 2\sigma(I)$]	6033	2621
R_1;wR_2 [$I > 2\sigma(I)$]	0.0429; 0.0911	0.0443; 0.0946
R_1; wR_2 (all data)	0.0653; 0.1006	0.0662; 0.1052
GOF (F^2)	1.067	1.006

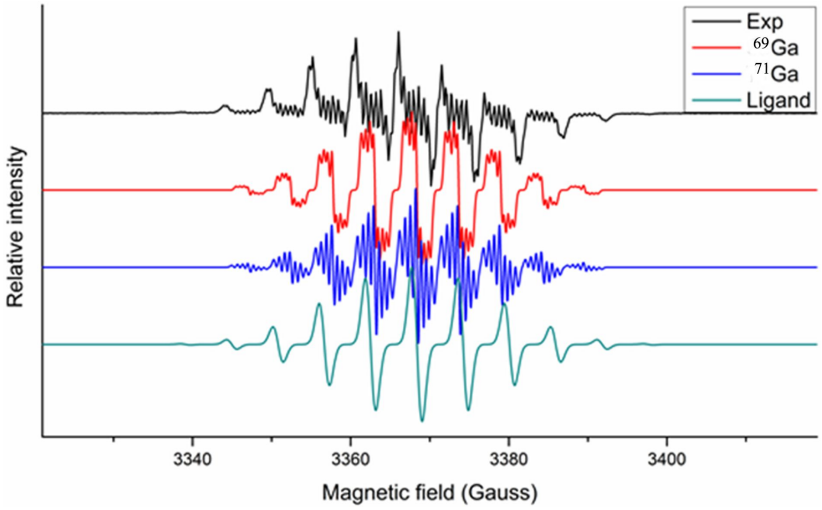

Fig. S1. EPR spectrum of complex **3**

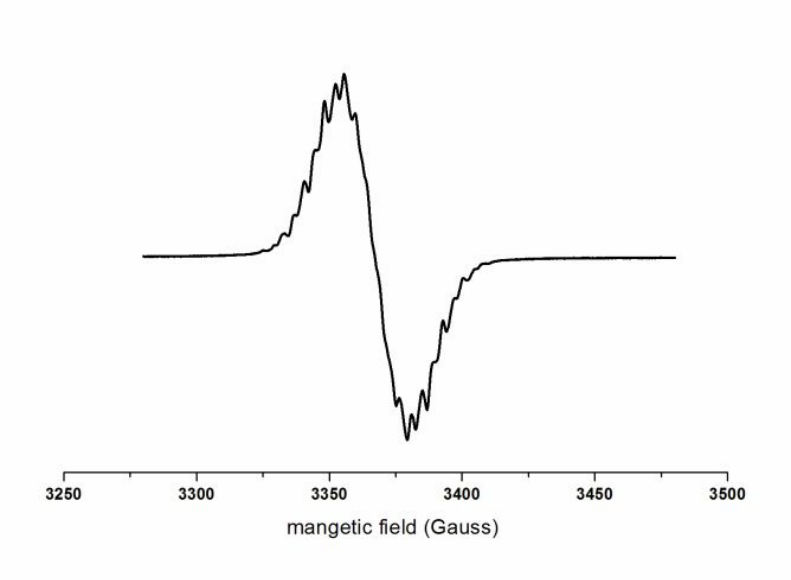

Fig. S2. The solid-state EPR spectrum of **5** recorded at room temperature

S2. DFT computations

The structure optimization and NBO bonding analysis for the compound [(L'Ga(μ_2-Cl)$_2$Na(H_2O)$_4$] (**2H**), [L'GaGaL'] $^-$ (**3H**) [LGaCl2][GaCl4] [($LGaCl_2$)•($GaCl_4$)] (**4H**) (L' = $(NArCH)_2$), [(L^{Et})ClGa–GaCl(L^{Et})] (**5H**) and [(L^{Me})ClGa–GaCl(L^{Me})] (**6H**) were carried out at the DFT (B3LYP) level with a 6-31g* basis set using the Gaussian 09 program.[1] The B3LYP method is a hybrid of the HF and DFT methods, incorporating Becke's three-parameter exchange functional (B3)[2] with the Lee, Yang, and Parr (LYP) correlation functional. Geometry optimizations gave bond distances that were in good agreement with the X-ray structures.Bonding analyses were performed by means of natural bond orbital (NBO) analysis and natural population analysis (NPA). Wiberg bond indices (WBI) were evaluated with Weinhold's natural bond orbital method.[3]

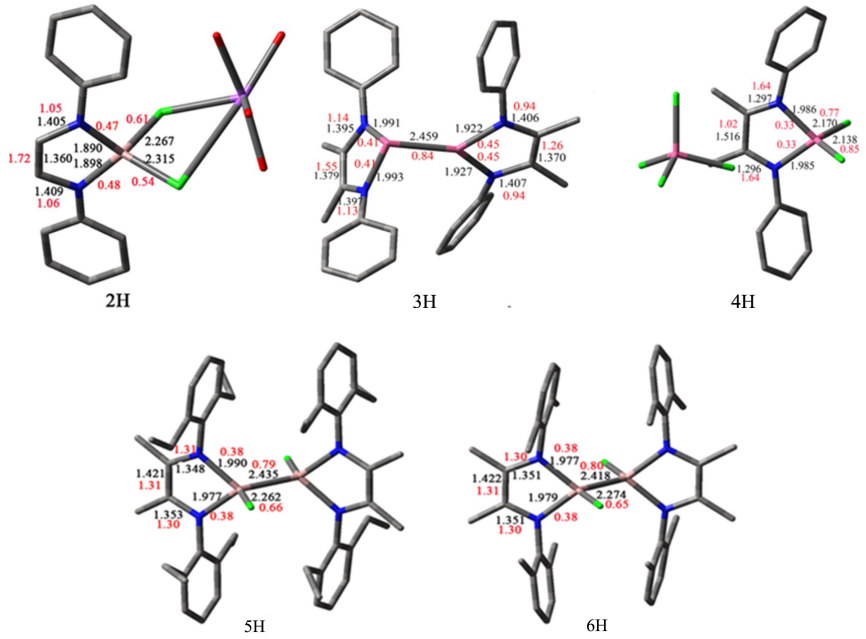

Fig. S3. Optimized structures of **2H–6H** and their selected bond lengths (black) and bond orders (red).

Table S2. Natural charges of the model compounds **1H−6H**.

	1H	**2H**	**3H**	**5H**	**6H**
Ga	1.415	1.561	0.533, 0.476	1.077	1.075
L	−0.461	−1.314	−1.010	−0.550	−0.546

Table S3. Cartesian coordinates of the optimized geometry for **2H**.

Ga	-0.54093100	0.32425000	0.24318900	C	-6.01626000	-0.78813100	-0.47467000
Na	1.89977700	-2.87049500	-0.56751200	H	-6.97675200	-1.28033200	-0.61769000
Cl	-0.12981500	-1.07768900	2.03931800	C	-5.84750900	0.56476500	-0.80123600
Cl	0.11169500	-1.00051300	-1.47589600	H	-6.68185400	1.13322700	-1.21264300
N	-2.25877400	1.09817500	0.09749400	C	-4.61593500	1.20528800	-0.62361500
N	0.26909000	2.04023400	0.25345000	C	1.60067200	2.40893100	0.12065100
O	3.58330100	-3.70756800	-1.89873200	C	2.00393600	3.60227500	-0.53022800
O	2.80761500	-2.32159300	1.66484400	C	3.35741100	3.93690000	-0.64152800
O	3.86164000	-1.26738200	-0.72224300	H	3.63180800	4.85862200	-1.15481400
O	0.17979300	-4.00361500	0.54274800	C	4.35884700	3.10467100	-0.11887800
C	-2.05952600	2.48835500	0.07810100	H	5.40982800	3.37468700	-0.20333100
C	-0.78764900	2.96537800	0.14441700	C	3.97153800	1.92222400	0.53328700
C	-3.50469100	0.50340300	-0.09685500	H	4.72969000	1.28281800	0.98867600
C	-3.68708700	-0.86185400	0.23070100	C	2.62053000	1.57837700	0.65242400
C	-4.91720500	-1.49410400	0.04088800	H	2.33002400	0.69521500	1.22131700
H	-5.02249100	-2.54536400	0.31025000	H	1.25312900	4.25157000	-0.97487600

H	-2.85675400	-1.41957500	0.66416600	H	3.72840000	-0.31544500	-0.87652800
H	-4.51257700	2.24609000	-0.92136700	H	3.90425700	-1.36431500	0.24699300
H	-0.21356600	-3.28355800	1.07427100	H	3.10301200	-2.94426500	2.34580700
H	-0.56999900	-4.47433200	0.15038800	H	2.03130100	-1.85747200	2.04479800
H	3.90026300	-4.19749800	-2.66874700	H	-0.57527400	4.02737300	0.22263600
H	4.09040900	-2.87391500	-1.84461000	H	-2.91694000	3.15315400	0.10059500

Table S4. Cartesian coordinates of the optimized geometry for **3H**

Ga	-0.46083500	1.25307900	1.01466900	C	4.65564000	-0.39592500	0.45948300
Ga	0.66126900	-0.81702300	0.30733400	C	-1.94247000	2.14163100	-1.21877000
N	0.44533300	-2.41632200	-0.74490400	C	-2.85948500	1.43875900	-0.46598600
N	2.44125200	-1.47990100	0.60198000	C	-2.28791400	2.72858900	-2.56895500
N	-0.63359400	2.18279000	-0.73705000	H	-1.39770700	2.79410100	-3.20099000
N	-2.38266500	0.83153600	0.69824900	H	-2.72141900	3.73899400	-2.51985800
C	1.60681200	-3.21016400	-0.74909900	H	-3.01502600	2.10134900	-3.09432000
C	2.66864500	-2.70968900	-0.04093700	C	-4.27834600	1.20392600	-0.93366200
C	1.56095000	-4.58586200	-1.36709000	H	-4.31762800	1.07941400	-2.02060300
H	2.32495700	-5.24200900	-0.94204600	H	-4.97376000	2.01990900	-0.68420600
H	1.70739800	-4.58883200	-2.45595700	H	-4.68503700	0.29090400	-0.48987100
H	0.58553600	-5.05407800	-1.18570900	C	0.35824200	3.03525400	-1.21386100
C	3.95847600	-3.44684300	0.21433300	C	1.70711800	2.61013100	-1.14532200
H	3.87230600	-4.50726900	-0.03508200	C	2.74905000	3.42818000	-1.56401700
H	4.24060000	-3.37507600	1.27306900	H	3.76892100	3.05493000	-1.49924300
H	4.80972600	-3.05396300	-0.35800500	C	2.49909800	4.71208400	-2.06069700
C	-0.63982100	-2.63738800	-1.60464700	H	3.31573300	5.34933200	-2.39122600
C	-0.48165300	-2.88641000	-2.98441300	C	1.17769700	5.16109500	-2.10933400
C	-1.58673200	-3.05759100	-3.81556000	H	0.95751400	6.16633200	-2.46571800
H	-1.43040600	-3.25158500	-4.87523800	C	0.12753900	4.35035500	-1.68150000
C	-2.88402200	-2.95314900	-3.30801000	C	-3.18988200	0.33308400	1.71355900
H	-3.74519700	-3.08127600	-3.95929000	C	-4.44352500	0.87527000	2.08606800
C	-3.05439800	-2.67284000	-1.94985500	C	-5.18137800	0.33689800	3.13850100
H	-4.05504600	-2.57886800	-1.53380700	H	-6.14203600	0.78292800	3.39180500
C	-1.95424900	-2.51625900	-1.11028000	C	-4.69660400	-0.74149400	3.88242800
C	3.46782100	-0.70197900	1.15686900	H	-5.27521700	-1.15590600	4.70426700
C	3.28099100	-0.10607800	2.42032700	C	-3.44290000	-1.26751100	3.55206300
C	4.25044600	0.72818200	2.97205800	H	-3.03517200	-2.10162400	4.12004900
H	4.07591900	1.17056900	3.95034700	C	-2.70393600	-0.74255800	2.49865500
C	5.43573400	0.99840100	2.28366100	H	-0.88310600	4.74338600	-1.68235700
H	6.19199800	1.64747200	2.71802700	H	1.92145500	1.61038300	-0.77856600
C	5.62857900	0.42703200	1.02351600	H	-1.73804400	-1.17167500	2.24633400
H	6.53547200	0.64215500	0.46131100	H	-4.82233800	1.74400700	1.55925000

H	-2.10084300	-2.32918600	-0.05083200	H	4.79457300	-0.79251300	-0.54174500
H	0.51991000	-2.91829300	-3.40167800	H	2.37710800	-0.34122700	2.97470900

Table S5. Cartesian coordinates of the optimized geometry for **4H**

Ga	-2.53547000	0.39879300	-0.35689000	C	-1.84822300	5.02828400	0.09704000
Cl	-4.46901100	0.78854000	0.54687200	H	-2.69241000	5.70673600	0.17436600
Cl	-2.35443900	0.38876600	-2.48721900	C	-2.02228100	3.68111900	0.40315500
N	-1.12909400	1.42845200	0.59449300	C	-2.05882900	-2.49017100	0.29309900
N	-1.68129300	-1.13747600	0.56613700	C	-1.10711900	-3.39100700	-0.20268900
C	-0.39564700	0.69561800	1.37339800	C	-1.51138300	-4.68067500	-0.54423100
C	-0.72753000	-0.78387600	1.36958100	H	-0.77855400	-5.38085500	-0.93343400
C	0.69470100	1.20892600	2.24982100	C	-2.84696700	-5.06307000	-0.40352200
H	0.60476700	2.28700600	2.39182700	H	-3.15444700	-6.06966800	-0.67081700
H	1.67571300	1.01501000	1.79549100	C	-3.79029000	-4.14797900	0.07014600
H	0.68233900	0.70629200	3.21988100	H	-4.83091500	-4.44006100	0.17375900
C	-0.00630700	-1.69772500	2.29860300	C	-3.40783400	-2.84870300	0.39759900
H	-0.39468500	-2.71354600	2.24070800	Ga	3.55209200	-0.46952500	-0.21652200
H	-0.12276900	-1.33056800	3.32585300	Cl	1.45404000	-0.64183600	-1.01020900
H	1.07183800	-1.71321400	2.08628400	Cl	3.81708800	1.66946800	0.32027500
C	-0.91956800	2.81827200	0.33765000	Cl	4.99211200	-1.16702800	-1.68119500
C	0.32867900	3.27525700	-0.10609300	Cl	3.59644500	-1.65552000	1.66229700
C	0.47848000	4.62290700	-0.42981900	H	-4.13285900	-2.13661800	0.77918200
H	1.44442100	4.97733600	-0.77590500	H	-0.07957700	-3.07018900	-0.34583900
C	-0.60193600	5.50051000	-0.32381900	H	-2.98408800	3.31304200	0.74644200
H	-0.47671400	6.54926600	-0.57632800	H	1.16169200	2.58914400	-0.22359800

Table S6. Cartesian coordinates of the optimized geometry for **5H**

Ga	0.77662400	-0.89609300	-0.32822000	C	5.80894900	0.27961900	-0.04936600
N	2.45923700	-1.18751800	0.63849200	H	6.66427800	0.09242900	-0.69450700
N	0.40163400	-2.73757300	0.25446900	C	5.83934700	1.33942300	0.85015200
Cl	1.11538600	-0.87474100	-2.55482200	H	6.71284100	1.98408100	0.90633600
C	3.48535300	-2.59538000	2.40917300	C	4.74932700	1.56730000	1.68712200
H	4.45697800	-2.75131600	1.92310600	H	4.77903300	2.39671200	2.38595300
H	3.26103800	-3.47609800	3.01073700	C	3.61598900	0.74786700	1.64666200
H	3.61347700	-1.74694900	3.09103100	C	4.72684300	-1.71583900	-1.13026200
C	2.40913500	-2.31199100	1.39730500	H	5.60021400	-2.34570600	-0.90819500
C	1.29430800	-3.16128200	1.18198700	H	3.84408000	-2.34777000	-1.00675000
C	1.06951400	-4.44068600	1.94358600	C	4.80116000	-1.25439700	-2.59535300
H	0.53880600	-5.16875400	1.32483600	H	3.90857500	-0.68049200	-2.85649800
H	0.45564500	-4.27700400	2.84074100	H	4.85440900	-2.11979000	-3.26603700
H	2.00975600	-4.89332800	2.26385000	H	5.68367400	-0.63148000	-2.78006400
C	3.59899900	-0.32050400	0.71883800	C	2.43582500	1.00805500	2.56780700
C	4.69533000	-0.56560200	-0.13770000	H	1.75222600	1.71671800	2.08305900

H	1.85119100	0.09264800	2.69088400
C	2.78747200	1.55931600	3.95619700
H	3.22605500	2.56145700	3.90610900
H	3.49619300	0.90837200	4.48236900
H	1.87775900	1.63273000	4.56122100
C	-0.74029900	-3.52881200	-0.09716900
C	-1.94699400	-3.41109300	0.62243300
C	-3.04779800	-4.16496400	0.19081600
H	-3.99352400	-4.06881300	0.71554300
C	-2.95247100	-5.02123800	-0.89896900
H	-3.81712100	-5.59953600	-1.21475500
C	-1.74401800	-5.14461400	-1.58499900
H	-1.67728900	-5.82715300	-2.42577100
C	-0.62114200	-4.40384800	-1.20645500
C	-2.08396400	-2.48690900	1.82000600
H	-1.10415000	-2.11278500	2.12496200
H	-2.65486700	-1.59828100	1.51952300
C	-2.76492600	-3.11998400	3.04364700
H	-3.79914800	-3.41572200	2.83860600
H	-2.78592000	-2.40209600	3.87065000
H	-2.22600700	-4.01327900	3.38147900
C	0.70512600	-4.52994800	-1.94042400
H	0.93509700	-3.57052100	-2.41999400
H	1.50582700	-4.67589800	-1.20343900
C	0.78908900	-5.64375400	-2.98834600
H	0.08276000	-5.48578400	-3.81125700
H	0.58675000	-6.63080900	-2.55581500
H	1.79418100	-5.66930300	-3.42267100
Ga	-0.77662400	0.89609300	0.32822000
Cl	-1.11538600	0.87474100	2.55482200
N	-2.45923700	1.18751800	-0.63849200
N	-0.40163400	2.73757300	-0.25446900
C	-3.48535300	2.59538000	-2.40917300
H	-4.45697800	2.75131600	-1.92310600
H	-3.26103800	3.47609800	-3.01073700
H	-3.61347700	1.74694900	-3.09103100
C	-2.40913500	2.31199100	-1.39730500
C	-1.29430800	3.16128200	-1.18198700
C	-1.06951400	4.44068600	-1.94358600
H	-0.53880600	5.16875400	-1.32483600
H	-0.45564500	4.27700400	-2.84074100
H	-2.00975600	4.89332800	-2.26385000
C	-3.59899900	0.32050400	-0.71883800
C	-4.69533000	0.56560200	0.13770000
C	-5.80894900	-0.27961900	0.04936600
H	-6.66427800	-0.09242900	0.69450700
C	-5.83934700	-1.33942300	-0.85015200
H	-6.71284100	-1.98408100	-0.90633600
C	-4.74932700	-1.56730000	-1.68712200
H	-4.77903300	-2.39671200	-2.38595300
C	-3.61598900	-0.74786700	-1.64666200
C	-4.72684300	1.71583900	1.13026200
H	-5.60021400	2.34570600	0.90819500
H	-3.84408000	2.34777000	1.00675000
C	-4.80116000	1.25439700	2.59535300
H	-3.90857500	0.68049200	2.85649800
H	-4.85440900	2.11979000	3.26603700
H	-5.68367400	0.63148000	2.78006400
C	-2.43582500	-1.00805500	-2.56780700
H	-1.75222600	-1.71671800	-2.08305900
H	-1.85119100	-0.09264800	-2.69088400
C	-2.78747200	-1.55931600	-3.95619700
H	-3.22605500	-2.56145700	-3.90610900
H	-3.49619300	-0.90837200	-4.48236900
H	-1.87775900	-1.63273000	-4.56122100
C	0.74029900	3.52881200	0.09716900
C	1.94699400	3.41109300	-0.62243300
C	3.04779800	4.16496400	-0.19081600
H	3.99352400	4.06881300	-0.71554300
C	2.95247100	5.02123800	0.89896900
H	3.81712100	5.59953600	1.21475500
C	1.74401800	5.14461400	1.58499900
H	1.67728900	5.82715300	2.42577100
C	0.62114200	4.40384800	1.20645500
C	2.08396400	2.48690900	-1.82000600
H	1.10415000	2.11278500	-2.12496200
H	2.65486700	1.59828100	-1.51952300
C	2.76492600	3.11998400	-3.04364700
H	3.79914800	3.41572200	-2.83860600
H	2.78592000	2.40209600	-3.87065000
H	2.22600700	4.01327900	-3.38147900
C	-0.70512600	4.52994800	1.94042400
H	-0.93509700	3.57052100	2.41999400
H	-1.50582700	4.67589800	1.20343900
C	-0.78908900	5.64375400	2.98834600
H	-0.08276000	5.48578400	3.81125700
H	-0.58675000	6.63080900	2.55581500
H	-1.79418100	5.66930300	3.42267100

Table S7. Cartesian coordinates of the optimized geometry for **6H**

Ga	0.03041200	1.16015100	0.38128200	H	-2.73755900	-0.08855500	-2.00582700
Cl	0.01393000	1.20759100	2.63743900	H	-1.90866800	1.34919200	-2.56976900
N	1.37412800	2.40773600	-0.30996700	H	-3.56224700	1.00391500	-3.11422900
N	-1.23507400	2.47987200	-0.32929100	C	-2.37495300	3.96130300	1.85234000
C	1.65757800	4.27324400	-1.93267800	H	-1.73062200	3.30891300	2.45149700
H	2.46069600	4.71761700	-1.33443100	H	-3.00345700	4.54253700	2.53436500
H	1.06987100	5.08007500	-2.37228600	H	-1.71329800	4.65823000	1.32500400
H	2.14374500	3.72977900	-2.75393100	Ga	-0.03041700	-1.16012500	-0.38124500
C	0.80829600	3.35538400	-1.09749500	Cl	-0.01392100	-1.20754800	-2.63740300
C	-0.60938700	3.39770300	-1.10715700	N	-1.37412800	-2.40773200	0.30997700
C	-1.37906600	4.37515600	-1.95749200	N	1.23507300	-2.47985000	0.32930900
H	-2.43248500	4.39165400	-1.67332800	C	-1.65757000	-4.27329700	1.93262400
H	-1.32883900	4.11402700	-3.02346900	H	-2.46065100	-4.71769600	1.33434800
H	-0.98705300	5.39205300	-1.85402000	H	-1.06984800	-5.08010900	2.37224700
C	2.79768800	2.32616900	-0.16953700	H	-2.14378400	-3.72985400	2.75386300
C	3.39706600	3.01394200	0.91066900	C	-0.80829100	-3.35540100	1.09747800
C	4.78458700	2.93442600	1.06305100	C	0.60939000	-3.39770900	1.10714600
H	5.25438900	3.46565100	1.88737200	C	1.37907100	-4.37518800	1.95745100
C	5.56475900	2.19451500	0.17567000	H	2.43248600	-4.39169100	1.67327000
H	6.64269400	2.14639900	0.30687400	H	1.32886400	-4.11408000	3.02343500
C	4.95903300	1.52618300	-0.88296800	H	0.98704600	-5.39207900	1.85396400
H	5.56274700	0.94694300	-1.57715500	C	-2.79768800	-2.32618800	0.16953100
C	3.57196400	1.57646900	-1.07675600	C	-3.39702100	-3.01389900	-0.91074000
C	2.57064900	3.83019100	1.87721600	C	-4.78454100	-2.93442400	-1.06314400
H	3.21996100	4.39120500	2.55669100	H	-5.25430800	-3.46560000	-1.88751700
H	1.91284200	3.19346600	2.47871000	C	-5.56475900	-2.19461400	-0.17571900
H	1.92290800	4.54642700	1.35853000	H	-6.64269300	-2.14652900	-0.30693900
C	2.95544800	0.81962600	-2.22976600	C	-4.95907900	-1.52634700	0.88298600
H	2.00166300	1.24127000	-2.55345400	H	-5.56282900	-0.94718800	1.57721000
H	2.75618200	-0.22415300	-1.96137700	C	-3.57201100	-1.57659300	1.07679600
H	3.63779400	0.80481400	-3.08658500	C	-2.57055200	-3.83003200	-1.87734100
C	-2.66022400	2.45648900	-0.18703800	H	-3.21982800	-4.39103000	-2.55686400
C	-3.46481100	1.73459500	-1.09110100	H	-1.91277300	-3.19322500	-2.47878100
C	-4.85140500	1.72658200	-0.88720700	H	-1.92277600	-4.54627100	-1.35870400
H	-5.47753700	1.16831700	-1.57867100	C	-2.95555600	-0.81983400	2.22989400
C	-5.42838700	2.41076200	0.17718600	H	-2.00175100	-1.24145600	2.55355200
H	-6.50622100	2.39517800	0.31666300	H	-2.75635000	0.22398600	1.96161800
C	-4.61931400	3.12743200	1.05778400	H	-3.63791600	-0.80515400	3.08670400
H	-5.06666600	3.67442800	1.88425300	C	2.66022300	-2.45645300	0.18704800
C	-3.23113600	3.16482100	0.89551200	C	3.46482000	-1.73460400	1.09113800
C	-2.88259800	0.96865200	-2.25581400	C	4.85141200	-1.72658500	0.88723200

H	5.47755300	-1.16835700	1.57871800	H	2.73758900	0.08849900	2.00597900
C	5.42838400	-2.41071300	-0.17720100	H	1.90869600	-1.34927700	2.56984700
H	6.50621600	-2.39512400	-0.31668700	H	3.56228400	-1.00403900	3.11430500
C	4.61930100	-3.12734000	-1.05782400	C	2.37493100	-3.96117500	-1.85239400
H	5.06664500	-3.67429800	-1.88432400	H	1.73059700	-3.30875700	-2.45151900
C	3.23112400	-3.16473700	-0.89553900	H	3.00342700	-4.54238200	-2.53445000
C	2.88262500	-0.96872300	2.25590100	H	1.71327700	-4.65812000	-1.32508300

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