

Electronic supplementary information

Comparative study on the N-heterocyclic carbene adducts of I_h -C₆₀, D_{5h} -C₇₀ and



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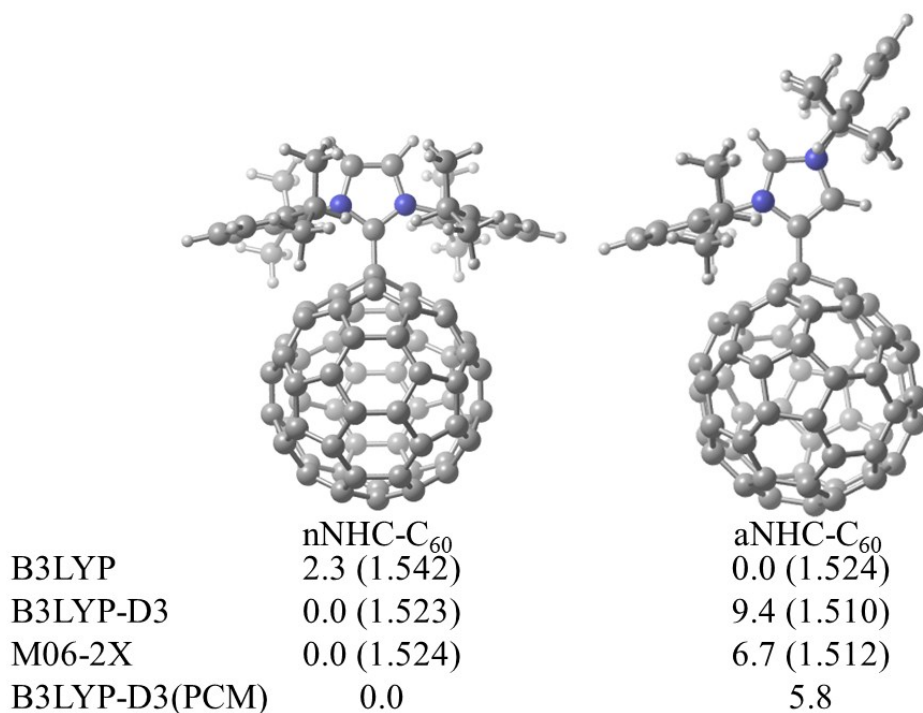


Fig. S1 Optimized geometries (B3LYP-D3/6-31G* level) of the two NHC-C₆₀ adducts with relative energies (kcal mol⁻¹) and R_{CC} distances (Å, in parentheses) obtained at different levels of theory.

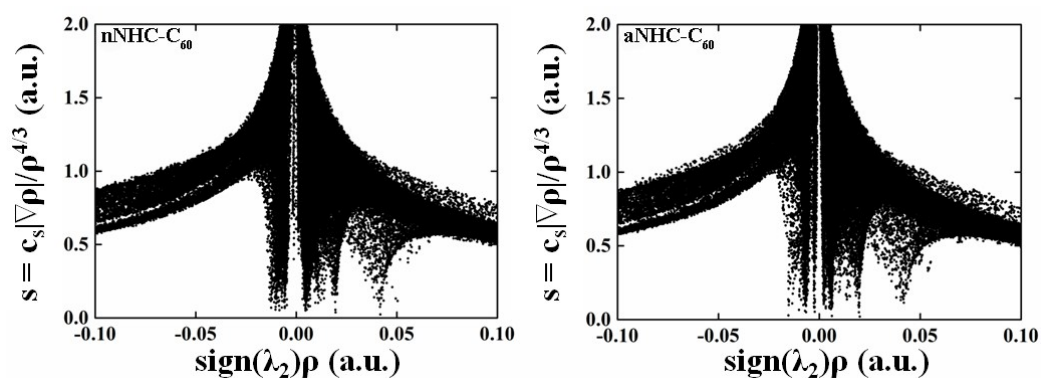


Fig. S2 Plots of the RDG versus $\text{sign}(\lambda_2)\rho$ value for the two NHC-C₆₀ adducts.

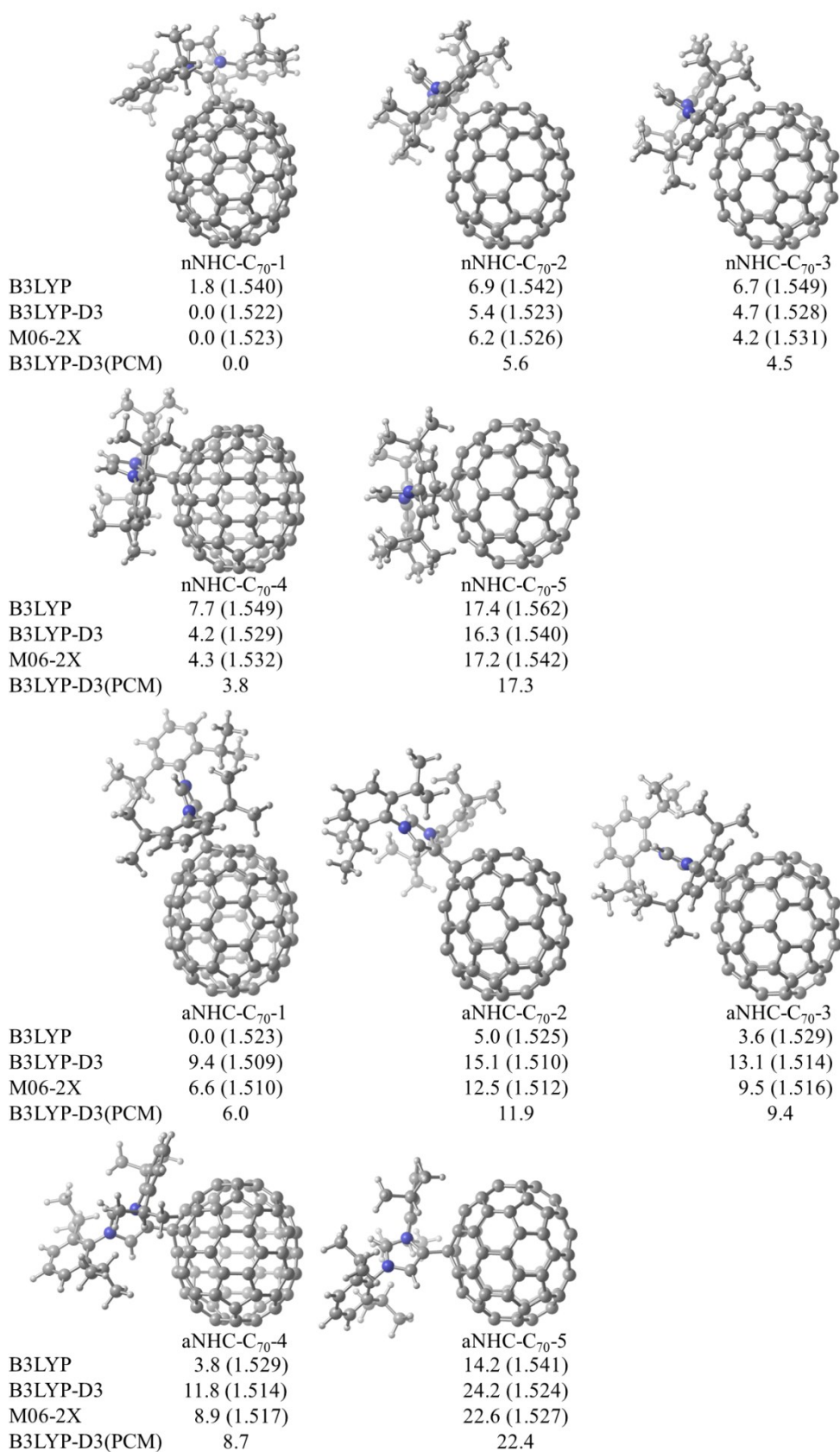


Fig. S3 Optimized geometries (B3LYP-D3/6-31G* level) of the ten NHC-C₇₀ adducts with relative energies (kcal mol⁻¹) and R_{CC} distances (Å, in parentheses) obtained at different levels of theory.

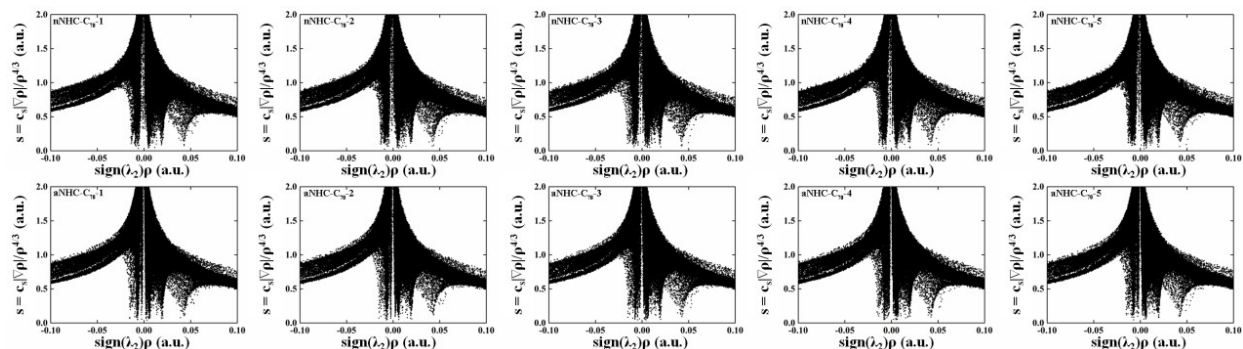


Fig. S4 Plots of the RDG versus $\text{sign}(\lambda_2)\rho$ value for the ten NHC- C_{70} adducts.

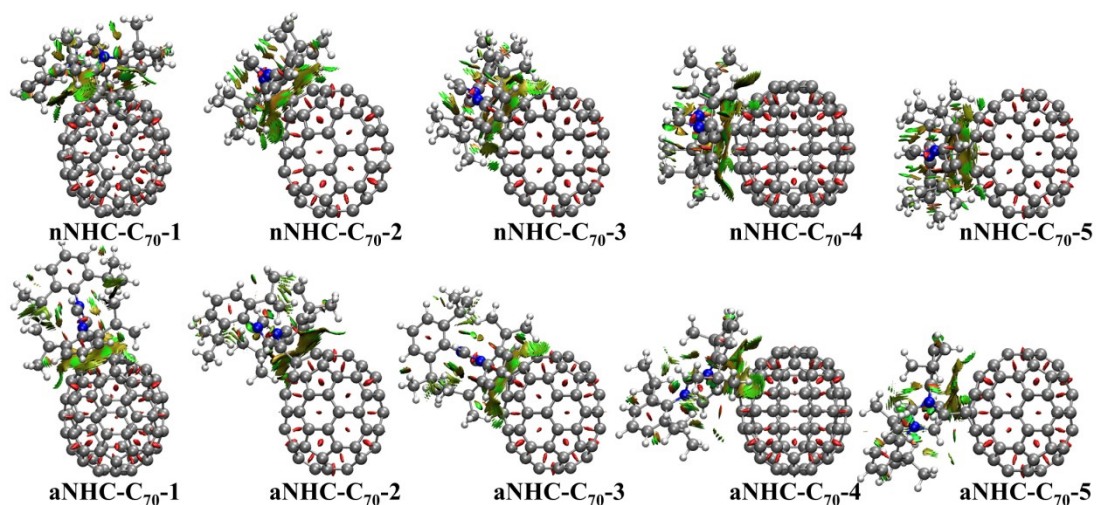
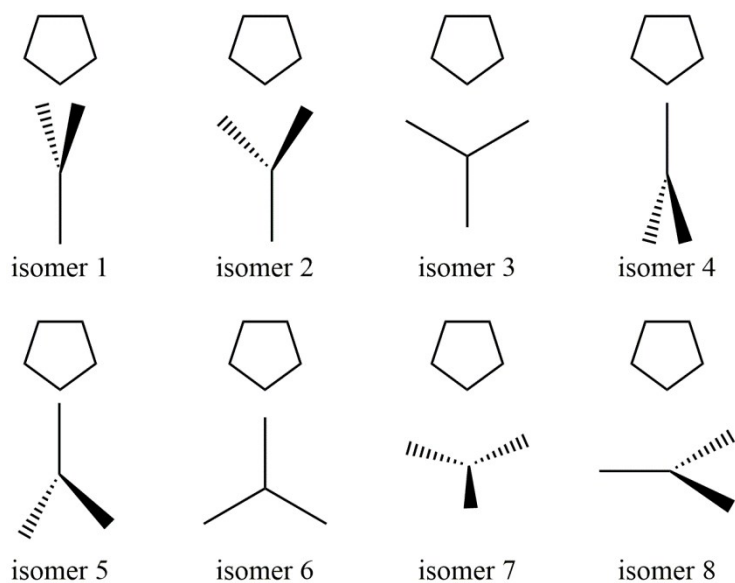


Fig. S5 RDG isosurfaces ($s = 0.5$ a.u.) for the ten NHC- C_{70} adducts colored on a blue-green-red scale according to the $\text{sign}(\lambda_2)\rho$ value (-0.04–0.02 a.u.).



Scheme S1. Schematic representation of the relative orientations of the Sc_3N unit with respect to the N-heterocyclic rings of the normal or abnormal NHC groups.

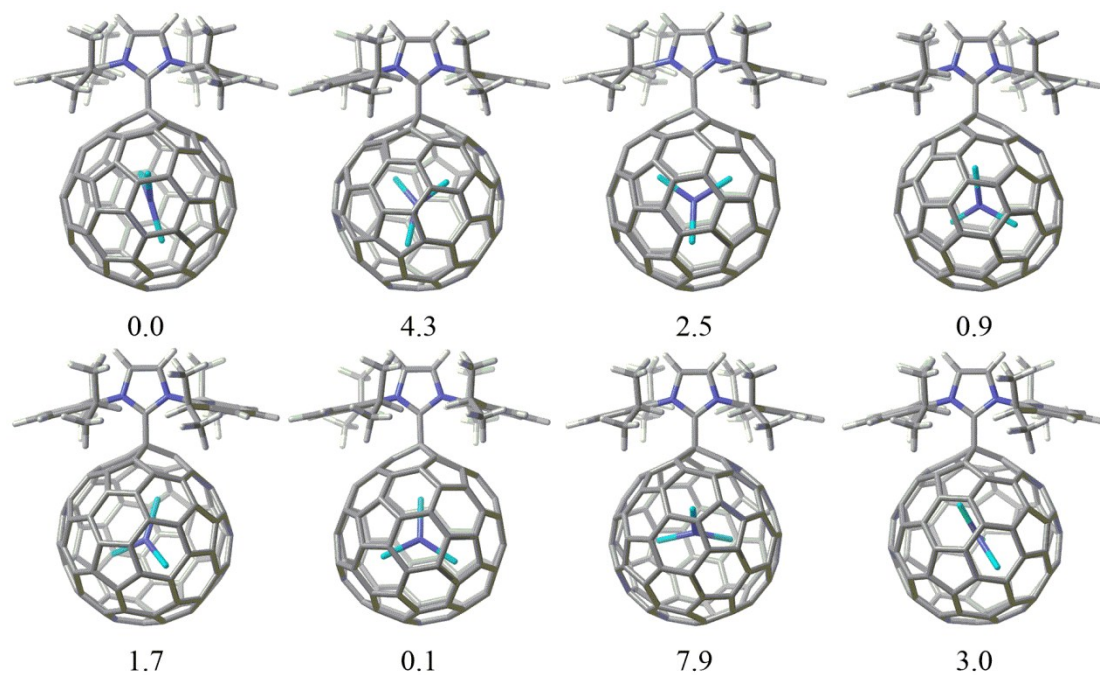


Fig. S6 Optimized geometries (with relative energies in kcal mol⁻¹) of different nNHC-Sc₃N@C₈₀-[6,6,6] adduct isomers (B3LYP-D3(PCM)/6-31G*~LanL2DZ level).

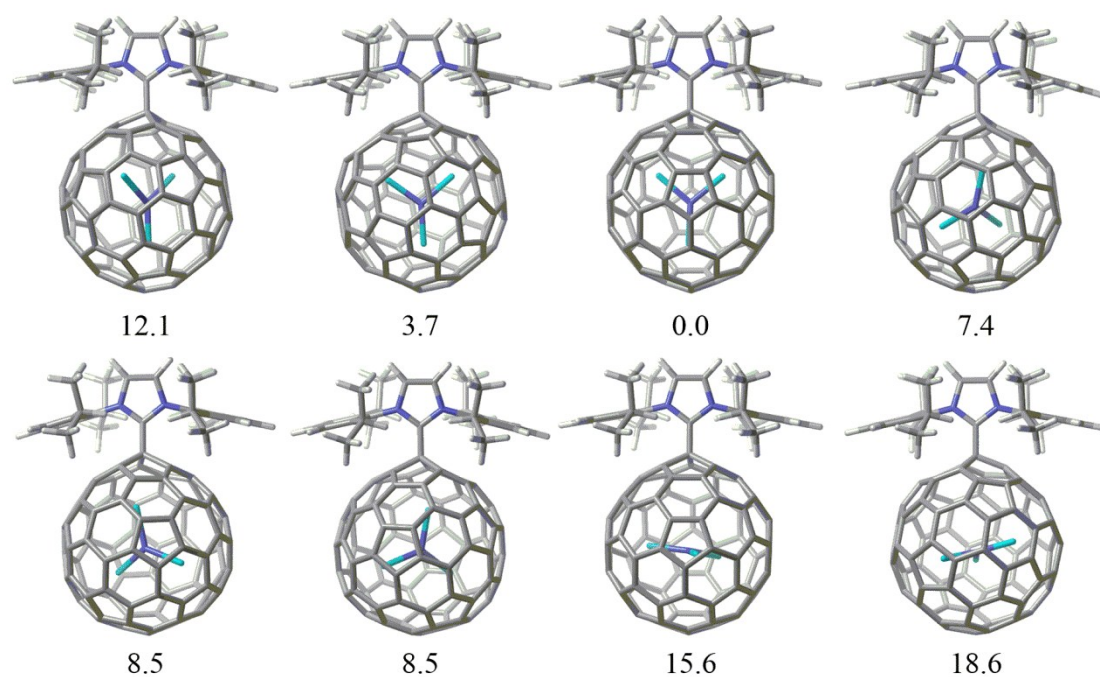


Fig. S7 Optimized geometries (with relative energies in kcal mol⁻¹) of different nNHC-Sc₃N@C₈₀-[5,6,6] adduct isomers (B3LYP-D3(PCM)/6-31G*~LanL2DZ level).

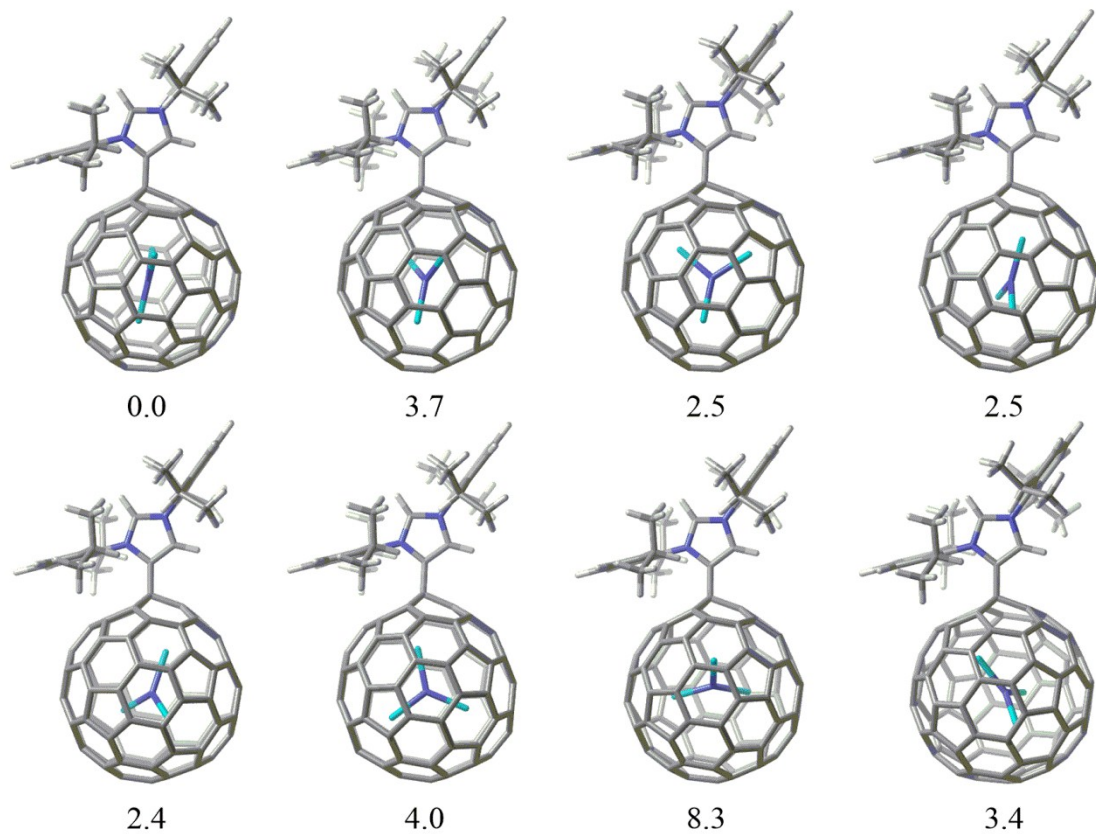


Fig. S8 Optimized geometries (with relative energies in kcal mol⁻¹) of different aNHC-Sc₃N@C₈₀-[6,6,6] adduct isomers (B3LYP-D3(PCM)/6-31G*~LanL2DZ level).

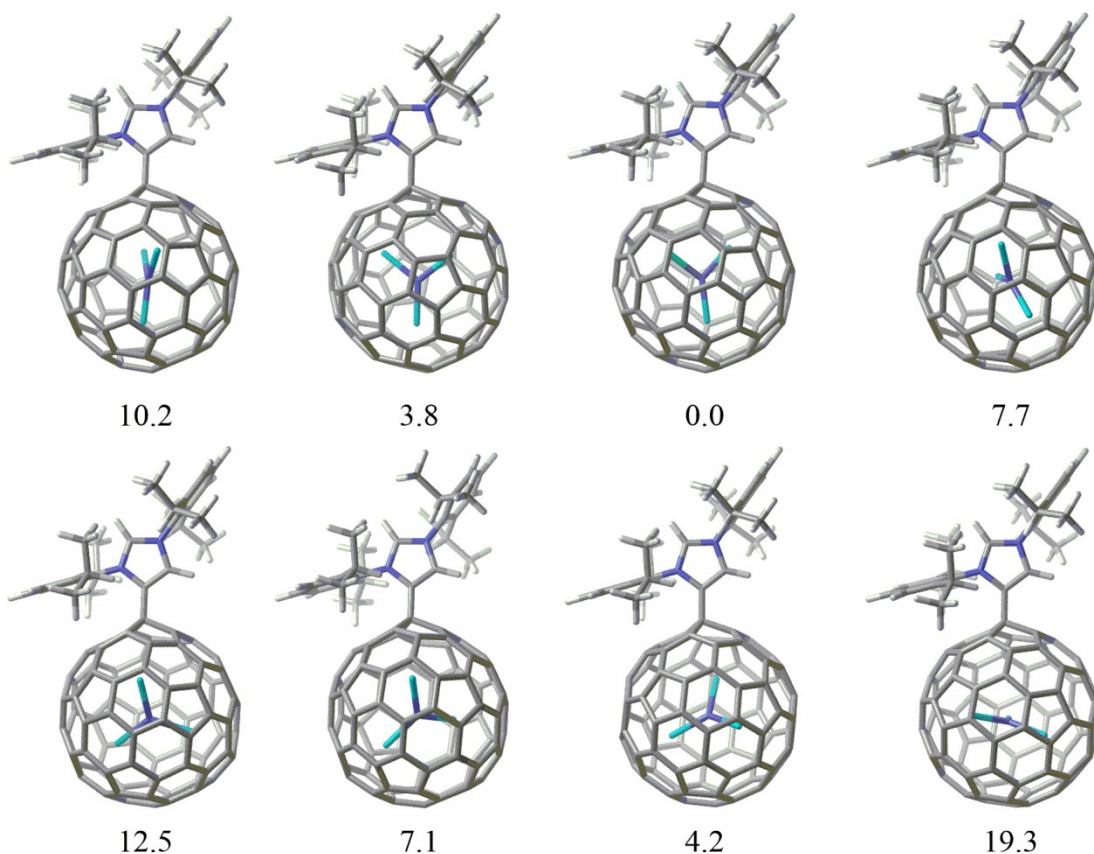


Fig. S9 Optimized geometries (with relative energies in kcal mol⁻¹) of different aNHC-Sc₃N@C₈₀-[5,6,6] adduct isomers (B3LYP-D3(PCM)/6-31G*~LanL2DZ level).

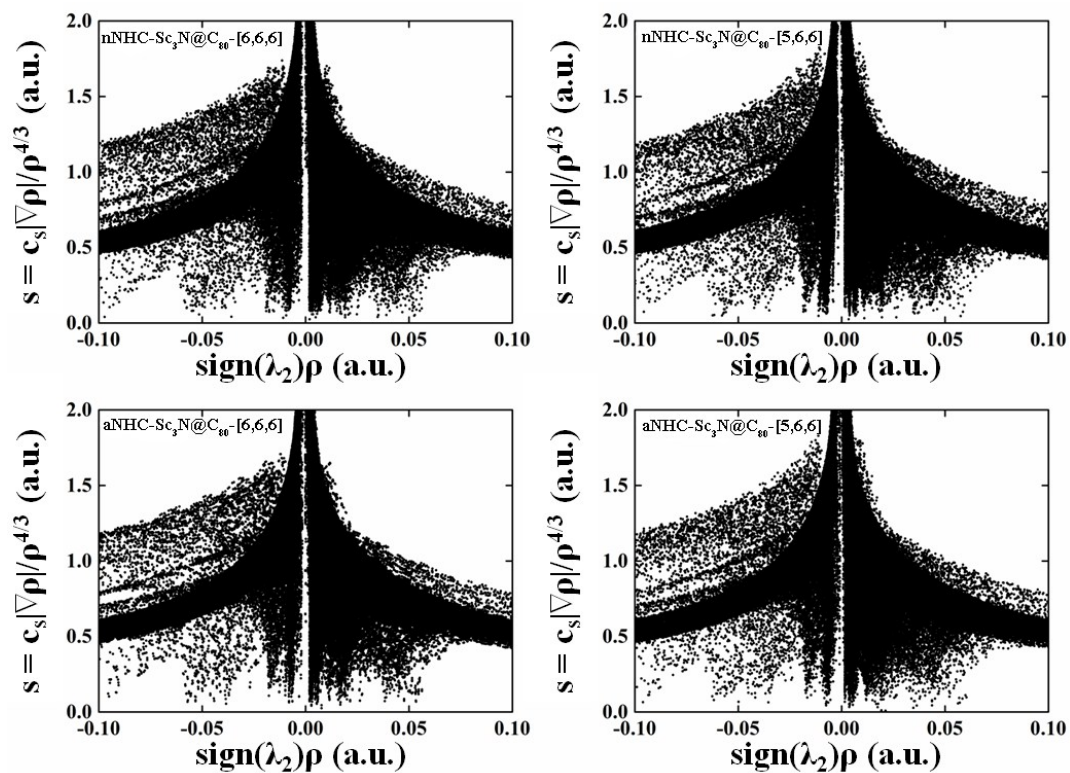


Fig. S10 Plots of the RDG versus $\text{sign}(\lambda_2)\rho$ value for the four NHC-Sc₃N@C₈₀ adducts.

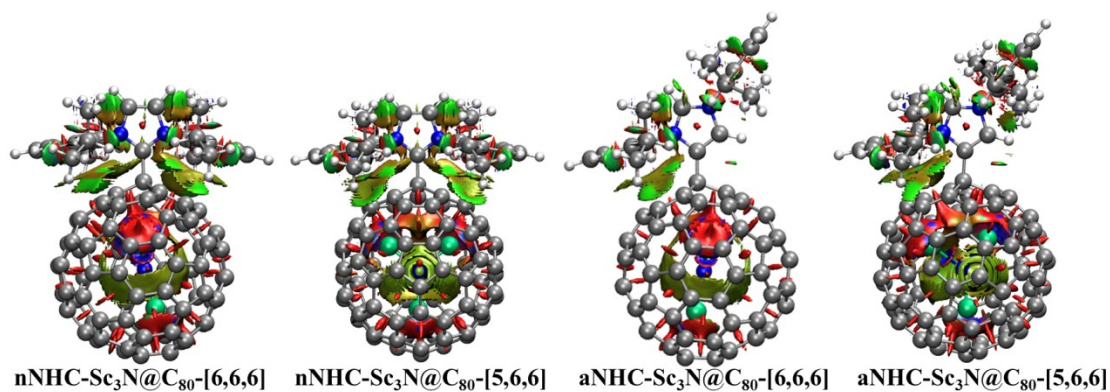


Fig. S11 RDG isosurfaces ($s = 0.5$ a.u.) for the four NHC-Sc₃N@C₈₀ adducts colored on a blue-green-red scale according to the $\text{sign}(\lambda_2)\rho$ value (-0.04–0.02 a.u.).

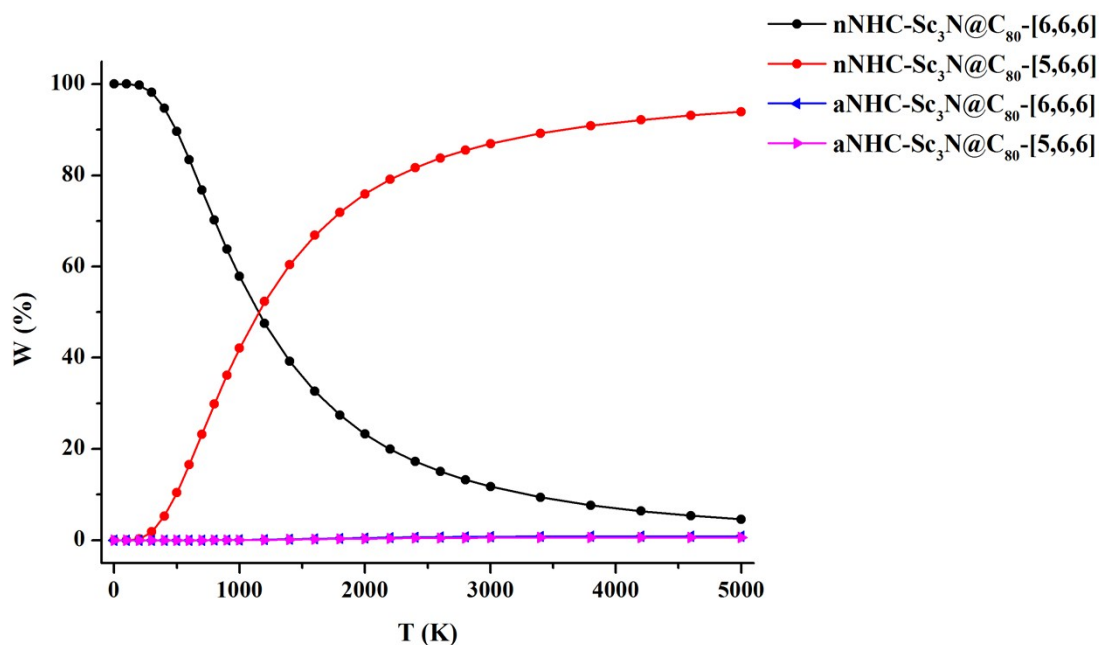


Fig. S12 Relative concentrations of four NHC-Sc₃N@C₈₀ isomers at different temperatures.

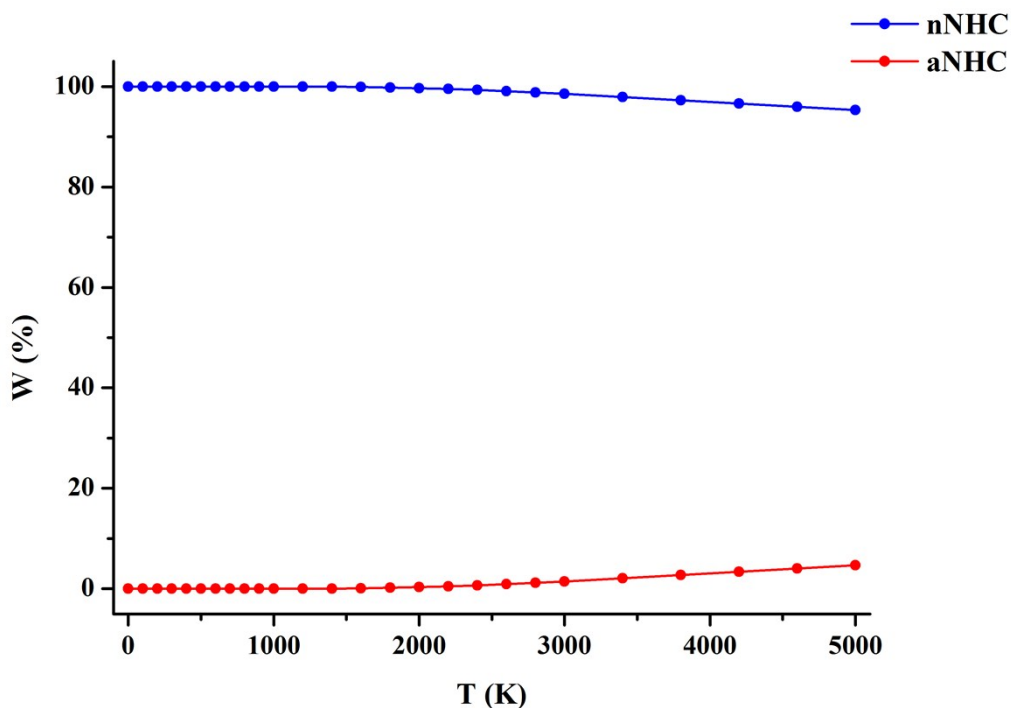


Fig. S13 Relative concentrations of the nNHC and aNHC isomers at different temperatures.

Cartesian coordinates of the NHC-C_{60/70} and the low-lying NHC-Sc₃N@C₈₀ adducts (B3LYP-D3/6-31G*~LanL2DZ level)

nNHC-C₆₀

N	3.99137100	1.08034300	0.17576600
C	3.64783300	2.48247400	0.03851700
C	5.31435900	0.66282300	0.25911300
H	6.11843500	1.37753500	0.29338800
C	3.16971800	0.00081800	0.15136000
C	3.49954000	3.24739600	1.20752800
C	1.64860900	0.00441700	0.08590400
C	3.53184200	3.00667700	-1.26085000
C	0.51421700	0.93743500	-2.03180800
C	1.15499600	-0.14881900	-1.35706400
C	3.21263400	4.60425400	1.04363800
H	3.07127400	5.22995500	1.91754100
C	3.23749800	4.37054800	-1.36190500
H	3.11666100	4.81685200	-2.34184300
C	-5.53784500	0.15079600	1.27729300
C	1.03683600	1.27746200	0.74396400
C	-5.76843500	0.00490900	-0.09258400
C	3.63433800	2.63662400	2.59477100

H	3.38798800	1.57187400	2.51734000
C	3.07790300	5.15813400	-0.22655400
H	2.83955100	6.21243000	-0.33204000
C	-5.45405500	1.08991100	-1.00818700
C	0.24074700	2.18239500	-1.44053700
C	3.73752500	2.15356000	-2.50751200
H	3.36261200	1.14797300	-2.28978700
C	-4.94280500	0.50535400	-2.23912600
C	0.45714600	2.29239300	0.00517900
C	2.95414700	2.66047700	-3.72714000
H	1.90770000	2.84787700	-3.47958200
H	2.98741200	1.90552900	-4.51940500
H	3.39045200	3.57979800	-4.13513300
C	-0.41716800	0.40134200	-3.02735300
C	2.66237100	3.25110400	3.61312100
H	2.94877000	4.27548800	3.87610700
H	2.67585400	2.66267200	4.53649500
H	1.63786100	3.26394600	3.23526000
C	-3.82633500	2.93451800	-1.24501200
C	-4.90127000	2.27524400	-0.52192300
C	-4.04749700	1.04784900	2.86202400
C	-0.54199600	1.71085200	2.59998000
C	0.48237900	0.94515700	2.02821800
C	-2.83181200	0.33392900	-3.50090600
C	-3.41332100	3.16580100	1.06448400
C	-0.61499300	3.08897200	0.56906500
C	-1.62458900	1.05890000	3.32900300
C	-1.59454300	1.08230200	-3.33775200
C	-2.89930300	3.47356400	-0.26542200
C	-4.65404800	2.42846900	0.90604700
C	-3.32726600	2.36762100	-2.42226800
C	-3.90679100	1.13015200	-2.93131600
C	5.08213300	2.75376100	3.10903000
H	5.79543400	2.24766400	2.45125500
H	5.16968000	2.30774900	4.10604100
H	5.38004200	3.80595600	3.18014300
C	-1.10479900	2.80806600	1.84873100
C	-4.96291300	1.38656100	1.78383100
C	-2.85797200	1.76229700	3.01758200
C	-1.00241600	2.85179200	-1.73828800
C	5.23271100	2.04717500	-2.86752300
H	5.36012400	1.42858100	-3.76308900
H	5.82584200	1.59724600	-2.06707600
H	5.64679100	3.03973200	-3.07878700

C	-1.52480200	3.43277600	-0.50411500
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N	3.97654500	-1.08983300	0.18675300
C	3.61652400	-2.48869000	0.05770300
C	5.30453500	-0.69031400	0.26724300
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C	3.43633800	-3.23978200	1.23046200
C	3.53333300	-3.02867600	-1.23733600
C	0.50655600	-1.35130000	-1.78664500
C	3.15408800	-4.59881200	1.07558400
H	2.99106500	-5.21356000	1.95372800
C	3.24420900	-4.39425100	-1.33085000
H	3.15259400	-4.85232200	-2.30876400
C	1.03127700	-1.09916500	0.99851100
C	3.54320900	-2.61374300	2.61259200
H	3.34014800	-1.54261700	2.51140200
C	3.05638300	-5.16867500	-0.19096200
H	2.82424400	-6.22500600	-0.28999200
C	-5.46033000	-1.25077700	-0.75776400
C	0.22836100	-2.44182300	-0.94799500
C	3.78258200	-2.19229500	-2.48612400
H	3.45911500	-1.16948300	-2.27008700
C	-4.94716600	-0.94258700	-2.08440200
C	0.44738300	-2.24469600	0.48958000
C	2.97001500	-2.66114200	-3.70148100
H	1.91341100	-2.78011200	-3.45437900
H	3.05026600	-1.91814500	-4.50179400
H	3.34621200	-3.61043000	-4.09999300
C	-0.42246200	-1.03181300	-2.87298200
C	2.50855800	-3.17476600	3.59926900
H	2.74752300	-4.20325500	3.89216500
H	2.50078800	-2.56940900	4.51146100
H	1.50203500	-3.16478700	3.17588000
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C	-4.05127800	-0.39897400	3.01674200
C	-0.54907800	-1.12159800	2.90397800
C	0.47982900	-0.50034500	2.18463000
C	-2.83612500	-1.05366600	-3.35303800
C	-3.42956400	-2.85206800	1.70723400
C	-0.63148800	-2.89616000	1.20808300
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C	-1.60304500	-1.75704100	-3.03442500

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C	-4.66582200	-2.15804200	1.39557600
C	-3.34203900	-2.81053600	-1.86933500
C	-3.91584300	-1.70586600	-2.62896800
C	4.96739900	-2.77539700	3.17684100
H	5.71867000	-2.30599400	2.53330300
H	5.03909600	-2.31584700	4.16898600
H	5.22551900	-3.83598000	3.27411000
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C	-2.86550800	-1.07117400	3.32110200
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C	5.28152000	-2.16615000	-2.84328800
H	5.44555900	-1.54975500	-3.73443100
H	5.89497900	-1.75440500	-2.03698900
H	5.64287400	-3.17816800	-3.05906400
C	-1.54361300	-3.45517700	0.23166400
C	-2.54988400	-2.32712000	2.65540900
C	-1.91741600	-2.85041800	-2.13452700
aNHC-C₆₀			
N	4.78450600	-0.65645300	0.01115000
C	5.99444200	-1.43995700	0.00973300
C	3.48825400	-1.15366000	0.03959100
H	3.28507500	-2.21083100	0.05876500
C	4.72802100	0.67735000	-0.01771700
C	6.56269400	-1.77678400	1.24836900
C	1.11939200	-0.08728400	0.00535300
C	6.51924200	-1.83905900	-1.22928700
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C	0.55367500	0.50944800	-1.28340000
C	7.72348900	-2.55633500	1.21810600
H	8.19611900	-2.84454600	2.15164600
C	7.68171900	-2.61648400	-1.20039800
H	8.12258900	-2.94992800	-2.13448400
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C	0.49617400	0.60322300	1.25358800
C	-6.27381400	-0.51672800	0.01171300
C	5.94607900	-1.34535900	2.57062900
H	5.10974400	-0.67160700	2.35978700
C	8.27570300	-2.97115900	0.00842700
H	9.17620100	-3.57825200	0.00803100
C	-6.06537900	0.90737400	-0.19542700
C	-0.46506300	2.46770800	-0.10502300
C	5.86155900	-1.46785900	-2.54987400

H	5.00860500	-0.81441800	-2.34169600
C	-5.59628500	1.09894000	-1.56011200
C	-0.16920000	1.81409200	1.17568500
C	6.82316900	-0.68474500	-3.45851700
H	7.19633400	0.21657700	-2.96059900
H	6.30888000	-0.37893700	-4.37569700
H	7.68816100	-1.29164200	-3.74763200
C	-1.12357900	1.74824300	-2.38094400
C	6.94698700	-0.56578400	3.43846900
H	7.79936800	-1.18854700	3.73095100
H	6.45893300	-0.21889500	4.35540500
H	7.33649200	0.30947700	2.90765200
C	-4.54653300	2.71083100	0.54701300
C	-5.54515900	1.69376900	0.83316400
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C	-3.55367600	1.77094600	-2.76662200
C	-4.01587500	1.71528900	2.61739800
C	-1.24940000	2.11317700	2.09961200
C	-2.00204500	-1.13570000	3.38532500
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C	-4.63303200	2.06730900	-1.83809300
C	5.37079600	-2.55724200	3.32437600
H	4.62318500	-3.08094800	2.71958100
H	4.89053800	-2.23363200	4.25390300
H	6.15833400	-3.27432000	3.58148000
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C	-1.75265900	3.10037900	0.02489400
C	5.30883200	-2.71723100	-3.25730100
H	4.79745500	-2.43350300	-4.18307300
H	4.59156100	-3.24656800	-2.62161800
H	6.11191600	-3.41678800	-3.51479500
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C	-3.06698400	0.96140600	3.31050400
C	-2.68015200	3.10903200	-1.03260900
N	3.44137500	1.05239500	-0.01178200
C	3.02708400	2.44240700	-0.02151800
C	2.62928000	-0.08838500	0.02454900

C	2.83958200	3.07927800	1.21607100
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C	-0.03847100	-0.32329200	-2.28152100
C	2.45673400	4.42280800	1.17911100
H	2.28600400	4.95440500	2.10819700
C	2.47622500	4.41597900	-1.24002700
H	2.31909100	4.94181800	-2.17474000
C	0.61350600	-1.54313800	0.20784200
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H	2.88356500	1.29383600	2.37644600
C	2.27544600	5.08120900	-0.03409100
H	1.96555200	6.12201800	-0.03938100
C	-5.94239400	-1.20647100	-1.22430600
C	-0.21540400	-1.71254800	-2.14219500
C	3.11221000	2.33961700	-2.57530700
H	2.90006800	1.27899700	-2.40631600
C	-5.51922100	-0.20897200	-2.19617600
C	0.07401300	-2.29219800	-0.82285100
C	4.58594500	2.48939800	-3.00088600
H	5.27988800	2.10939400	-2.24309800
H	4.77288200	1.93918300	-3.92990100
H	4.83290400	3.54289100	-3.17498700
C	-1.04523600	0.45389900	-3.01265400
C	4.56188400	2.50713400	2.96120100
H	4.80967500	3.56140100	3.12816900
H	4.74723600	1.96286300	3.89409900
H	5.25451200	2.12100900	2.20547900
C	-4.22844200	-2.75179700	-2.11073200
C	-5.30464200	-2.44709000	-1.18233000
C	-4.36856800	-2.37705600	2.39654200
C	-0.84724500	-2.68215600	1.84505300
C	0.10532600	-1.70224800	1.54348700
C	-3.47943000	0.51733500	-3.37513100
C	-3.70064000	-3.71796200	-0.02732500
C	-0.93407100	-3.29823100	-0.53370300
C	-1.93036000	-2.38512600	2.77673500
C	-2.19651500	-0.15881700	-3.50536100
C	-3.23023600	-3.52460800	-1.39370400
C	-4.98593800	-3.05516900	0.10314700
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C	2.16300000	2.82179000	3.66812800
H	1.11377500	2.78417500	3.36744900
H	2.29334300	2.16911100	4.53763200

H	2.39633200	3.84291900	3.99004200
C	-1.38226400	-3.49399000	0.77701200
C	-5.31116700	-2.39254800	1.28911300
C	-3.13609700	-3.02118700	2.27240100
C	-1.43541500	-2.31942700	-2.61284500
C	2.18770500	2.79391700	-3.71302400
H	2.31321900	2.12914100	-4.57397300
H	1.13917900	2.76209200	-3.40980900
H	2.42437300	3.81014900	-4.04859500
C	-1.87127200	-3.31490000	-1.63608300
C	-2.79593800	-3.71039500	1.03555900
C	-2.40605500	-1.58188000	-3.31422900
H	5.57628700	1.33990100	-0.03911600

nNHC-C₇₀-1

C	-3.79549700	0.03172200	-0.00798900
C	-5.91200600	0.78179900	0.03346800
H	-6.68660200	1.52926600	0.03616800
C	-5.95832800	-0.57053300	0.06709900
H	-6.78189000	-1.26203700	0.11054700
C	-4.15536100	2.53153500	0.05986000
C	-3.95642100	3.10195600	1.32877200
C	-3.59987600	4.45391200	1.36125200
H	-3.41994200	4.93311000	2.31662100
C	-3.45789500	5.18718800	0.18746600
H	-3.16928300	6.23295800	0.23752400
C	-3.67663700	4.59010600	-1.05093300
H	-3.55438100	5.17337700	-1.95665200
C	-4.03280300	3.24262300	-1.14487200
C	-4.16077500	2.31193500	2.61503600
H	-3.92304600	1.26522800	2.40216800
C	-3.22979800	2.75194400	3.75364700
H	-3.50597300	3.73747700	4.14544800
H	-2.18765900	2.78473600	3.42998000
H	-3.30571300	2.04006500	4.58222100
C	-5.62749700	2.39517300	3.08085600
H	-5.90255300	3.43293700	3.30130300
H	-5.76780500	1.80538000	3.99378900
H	-6.32472900	2.01575500	2.32837100
C	-4.29873600	2.59188100	-2.49423600
H	-4.14407200	1.51385800	-2.38167400
C	-3.33846500	3.06919600	-3.59310000
H	-3.53117100	4.11080800	-3.87339200
H	-3.47525800	2.45959400	-4.49221500

H	-2.29573700	2.98631100	-3.28023800
C	-5.76066200	2.82074000	-2.92304800
H	-6.47005500	2.41477500	-2.19443800
H	-5.95545100	2.33947200	-3.88793800
H	-5.96695800	3.89171300	-3.02931200
C	-4.31545800	-2.43017600	0.17066600
C	-4.09189100	-2.94312200	1.46045700
C	-3.78451900	-4.30446900	1.54730800
H	-3.58221100	-4.74331900	2.51704100
C	-3.71062100	-5.09903700	0.40724700
H	-3.45620300	-6.15069700	0.50027000
C	-3.95274600	-4.55648200	-0.85158200
H	-3.87990800	-5.18851900	-1.72913600
C	-4.26180000	-3.20250000	-1.00189800
C	-4.18822400	-2.07580800	2.71091500
H	-3.81787700	-1.07682600	2.45561800
C	-3.32312800	-2.58303700	3.87373500
H	-3.73595900	-3.49742200	4.31559200
H	-3.29570900	-1.82437900	4.66270300
H	-2.29720000	-2.77724800	3.55474100
C	-5.64993400	-1.94264100	3.18262100
H	-6.29566800	-1.49240500	2.42437800
H	-5.69998800	-1.31341600	4.07844700
H	-6.06032800	-2.92685000	3.43574400
C	-4.52612400	-2.60298000	-2.37619100
H	-4.25024200	-1.54287500	-2.33667700
C	-3.68378600	-3.24749100	-3.48683900
H	-2.62267600	-3.26503200	-3.22918000
H	-3.79881900	-2.67442800	-4.41286500
H	-4.00981600	-4.27225400	-3.69715400
C	-6.02213300	-2.69507000	-2.73479700
H	-6.34480800	-3.74197300	-2.76037100
H	-6.20382600	-2.25911800	-3.72340500
H	-6.65419200	-2.16737900	-2.01454600
C	-2.27526500	-0.00793200	-0.06359300
C	-0.02681800	2.65525900	-1.69991200
C	5.42086600	0.14497400	-2.25919000
C	1.24336400	-0.71852200	3.28202800
C	1.51438300	3.07656600	1.53342400
C	-0.28360000	0.70584600	-3.15773500
C	4.99840800	-2.73185500	-0.22691800
C	-0.29405300	-2.05899000	-2.49300800
C	2.00649600	0.55442000	-3.70686500
C	0.32903200	-3.03987100	-1.64688400

C	0.54309400	3.19155100	0.49363000
C	-1.07006200	2.13585100	-0.83862600
C	3.26994000	3.48798100	-0.19036200
C	-0.96331200	-0.67927600	2.05365600
C	5.41435100	-1.20528300	-1.93638600
C	5.88248900	-0.83086700	1.70125500
C	-0.71787700	2.49556200	0.53041400
C	0.51540400	-2.63225500	1.88619200
C	4.59888200	-2.85280600	1.09903400
C	0.96198300	3.31219000	-0.88126400
C	-1.27160700	0.20069200	-2.29466700
C	2.72075300	-3.42345900	-1.00854700
C	2.85833000	3.35720500	1.18413000
C	4.03883300	-2.97463800	-1.28794500
C	5.07530600	2.57516400	1.01555700
C	-1.27395600	-1.20771800	-1.95320200
C	5.05439700	-1.88786900	2.08304800
C	0.05762600	-0.04444800	2.88482400
C	-0.94899600	1.53830400	1.52057300
C	2.30302000	-3.55083600	0.39712500
C	3.25312600	-0.09814600	-3.49291200
C	3.71527800	-0.38281200	3.49396000
C	3.24669000	-1.52808100	-3.15178600
C	2.36063900	1.50554400	3.26366200
C	4.62727000	2.99537900	-0.29931400
C	4.29773300	-2.03828200	-2.34679700
C	5.87537600	1.12073600	-1.28885800
C	1.25787500	2.10948700	2.60547500
C	5.89362600	1.45307400	1.15527000
C	2.83030700	-2.48876800	2.58222900
C	6.30817500	0.70578700	-0.02463600
C	0.93013500	-3.36581100	0.71548700
C	5.63756500	0.50239500	2.22341300
C	6.30133500	-0.70237200	0.31217000
C	0.35344000	1.95542400	-2.84063300
C	-0.73975900	-1.98368700	1.60043600
C	-1.08902500	-2.27919900	0.21664700
C	0.75255800	-0.17260400	-3.67672600
C	-0.05472600	-3.14168400	-0.31342900
C	4.31034700	0.71197200	-3.00362600
C	-1.65251700	0.31609700	1.30096600
C	4.57466800	0.71816400	3.10542800
C	3.96861500	2.79023400	1.92823600
C	1.73697500	-3.12961700	-1.99092900

C	1.48970600	-2.06848200	2.76404900
C	-1.72805600	-1.36147900	-0.60031500
C	2.35348100	0.10795100	3.59718300
C	1.99349700	-2.19508500	-3.05004300
C	2.33561800	3.32067000	-1.24578600
C	5.02188900	2.28306400	-1.42583900
C	3.94727400	-1.65641100	2.99137600
C	5.86231200	-1.64072700	-0.62840600
C	0.74706000	-1.52079200	-3.35358000
C	-1.71777500	0.95403300	-1.15595700
C	3.23771800	-3.23073100	1.41609600
C	3.72656700	1.88383900	2.95217500
C	4.06249900	2.02845300	-2.48405700
C	0.06636900	1.33818100	2.55225600
C	2.74915400	2.56705400	-2.44067200
C	1.76109800	1.86855300	-3.18557100
N	-4.57168500	1.14393600	-0.00113000
N	-4.64442000	-1.02370600	0.05005000

nNHC-C₇₀-2

C	3.68625400	0.08506300	0.30202800
C	5.81126300	-0.52235400	0.70355700
H	6.61491200	-1.21501600	0.88504400
C	5.78380000	0.82764100	0.61110400
H	6.55841700	1.57056500	0.69053700
C	4.19264800	-2.38514800	0.45781500
C	3.86211600	-3.02930300	1.66178100
C	3.60203300	-4.39985900	1.59578600
H	3.32523900	-4.93454800	2.49739800
C	3.67241600	-5.08345800	0.38474500
H	3.45412200	-6.14687100	0.35337300
C	4.01334300	-4.41461600	-0.78586400
H	4.05617900	-4.96119800	-1.72075200
C	4.28659600	-3.04254300	-0.78012900
C	3.80165500	-2.28011700	2.98493800
H	3.58222800	-1.23032500	2.76421200
C	2.68479100	-2.78483800	3.90954400
H	2.91436400	-3.77632500	4.31567500
H	1.72654900	-2.84223000	3.38944400
H	2.57218700	-2.10324200	4.75888300
C	5.16128400	-2.34139500	3.70662800
H	5.43095400	-3.37970900	3.93029300
H	5.11652400	-1.79045300	4.65278400
H	5.96600400	-1.90910400	3.10342300

C	4.71258700	-2.32163800	-2.05270600
H	4.39065400	-1.27898700	-1.96854200
C	4.05363700	-2.88556500	-3.31950900
H	4.44489200	-3.87739800	-3.57300400
H	4.26771800	-2.22559800	-4.16660400
H	2.96962200	-2.95534400	-3.21078100
C	6.24559500	-2.35070100	-2.20765700
H	6.75806400	-1.88164900	-1.36284100
H	6.54365500	-1.81726800	-3.11734800
H	6.60381100	-3.38351800	-2.28632700
C	4.08685000	2.57364300	0.13134100
C	3.76735500	3.36111900	1.25065500
C	3.42523900	4.69342400	1.00839900
H	3.15341000	5.33482700	1.83878600
C	3.40162600	5.20066200	-0.28790800
H	3.11620200	6.23486100	-0.45635700
C	3.73232000	4.39209000	-1.37090000
H	3.69505800	4.80241900	-2.37293200
C	4.09015700	3.05220700	-1.19066900
C	3.78165200	2.79744200	2.66509800
H	3.56288500	1.72560000	2.59835600
C	2.71068800	3.42141300	3.57200000
H	2.95763000	4.45654400	3.83306100
H	2.64729300	2.85670600	4.50796800
H	1.72549600	3.40818000	3.10153700
C	5.17083000	2.96317900	3.31154800
H	5.95555800	2.45408100	2.74471100
H	5.16911800	2.55070800	4.32660400
H	5.43760800	4.02410700	3.37634200
C	4.46993700	2.16932600	-2.37447400
H	4.09654600	1.15928800	-2.17071600
C	3.83441200	2.61881200	-3.69807000
H	2.75868400	2.77300400	-3.59403600
H	3.99443400	1.84674200	-4.45766800
H	4.29071100	3.54301700	-4.07177800
C	6.00039800	2.09416900	-2.54604900
H	6.41328200	3.09175900	-2.73488400
H	6.25076900	1.45639300	-3.40126800
H	6.50229700	1.68158000	-1.66729200
C	1.89574400	-0.35845400	-1.42014200
C	-0.27765900	-3.33761500	-0.95762600
C	-5.85336900	-0.98370600	-0.94109700
C	-0.31173200	2.03148300	2.05148500
C	-0.78811800	-2.09432900	2.40119400

C	-0.64234400	-2.28739200	-3.13370700
C	-5.07417500	2.46377200	-0.68204200
C	-0.65309000	0.46813500	-3.84908900
C	-2.99250200	-2.24795000	-2.97868900
C	-1.06694600	1.77939100	-3.42146500
C	-0.17813000	-2.73671200	1.29397600
C	0.93716400	-2.58183300	-0.78088400
C	-2.92553900	-3.13341700	1.67527600
C	1.46341300	1.34164300	0.41992600
C	-5.85906900	0.35822500	-1.29048400
C	-5.20373400	1.73385100	2.06776300
C	0.97073700	-2.16789200	0.61818300
C	-0.20193500	3.02442900	-0.20454300
C	-4.31983400	3.15722600	0.25442600
C	-0.95006500	-3.45540900	0.32516800
C	0.51051500	-1.50601100	-2.96152900
C	-3.19515000	2.56811500	-2.33987100
C	-2.14838100	-2.42221500	2.64994700
C	-4.49609100	2.12652900	-1.97127200
C	-4.36750400	-1.65786400	2.81369500
C	0.50653600	-0.12042300	-3.32284900
C	-4.38677200	2.78944400	1.65638800
C	0.76313000	1.17950300	1.66330000
C	1.47433000	-0.95143500	1.01820400
C	-2.39314000	3.29108800	-1.34307700
C	-4.16413900	-1.48575100	-2.72806300
C	-2.57161600	2.01099600	3.12694200
C	-4.16996100	-0.06112500	-3.09859900
C	-1.20340100	0.13906600	3.39295000
C	-4.29517300	-2.66241000	1.76920500
C	-4.98160200	0.83278800	-2.34950800
C	-5.92162600	-1.36946300	0.45344400
C	-0.29799800	-0.77161300	2.78369300
C	-5.19333700	-0.54203200	2.65912600
C	-2.17296200	3.39429300	1.13607700
C	-5.98987100	-0.39428800	1.45391900
C	-0.97795900	3.17381000	-1.39927900
C	-4.70645100	0.77445400	3.04224900
C	-5.99663000	1.01096100	1.08851500
C	-1.04624200	-3.22562100	-2.11938700
C	0.95020100	2.20656400	-0.51971300
C	0.91798500	1.88590200	-1.94147600
C	-1.84565400	-1.67669700	-3.66273300
C	-0.30214600	2.44987500	-2.46300600

C	-4.96984400	-1.90732900	-1.63634600
C	2.18790800	0.02182900	0.03678500
C	-3.41965400	0.91518200	3.56254800
C	-3.02762400	-1.50448200	3.34689200
C	-2.51630300	1.78943800	-3.31341300
C	-0.80941700	2.99896000	1.07603200
C	1.30202200	0.58790800	-2.31584000
C	-1.20932800	1.52716300	3.03152100
C	-3.00311100	0.49098000	-3.69025700
C	-2.36414700	-3.54227300	0.43487800
C	-5.05217100	-2.51839700	0.61465300
C	-3.04630800	2.92562900	2.19366500
C	-5.93416900	1.37501900	-0.26074700
C	-1.85096700	-0.33244400	-4.01120700
C	1.30886600	-1.62836800	-1.73904200
C	-2.95413500	3.53467500	-0.05992200
C	-2.56216700	-0.24715500	3.71521800
C	-4.47475300	-2.84842600	-0.67667600
C	0.77180100	-0.20915500	2.02883800
C	-3.17015500	-3.40434700	-0.78656200
C	-2.49622900	-3.19394300	-2.01758100
N	4.51297000	-0.97182600	0.50180200
N	4.46718800	1.19245300	0.35482100

nNHC-C₇₀-3

C	3.57673200	0.16012200	-0.37326700
C	5.62867000	1.00726800	-0.72356300
H	6.37325200	1.78261000	-0.77961600
C	5.69727800	-0.33037800	-0.92072800
H	6.51433800	-0.97823600	-1.18772300
C	3.90847200	2.63000500	0.02227500
C	3.51416400	3.54073700	-0.97057100
C	3.14359700	4.81882700	-0.54320300
H	2.81336500	5.54958700	-1.27248200
C	3.17412800	5.16028200	0.80608000
H	2.86849700	6.15506400	1.11653600
C	3.59241600	4.23758000	1.76006600
H	3.61124300	4.51952600	2.80666900
C	3.97578300	2.94475700	1.39059300
C	3.50862200	3.17175800	-2.44648200
H	3.35324100	2.08999100	-2.51957800
C	2.37438000	3.84779500	-3.22900300
H	2.55641300	4.92116300	-3.35482100
H	1.41040600	3.71709300	-2.73509300

H	2.30431700	3.41004500	-4.22999700
C	4.86519500	3.50761800	-3.09649100
H	5.06888000	4.58190500	-3.02372700
H	4.85481200	3.23467200	-4.15745700
H	5.69619600	2.97703800	-2.62217500
C	4.48815100	1.95377000	2.42677500
H	4.30378200	0.94452500	2.04880100
C	3.76682800	2.05561400	3.77783400
H	4.03350400	2.97484200	4.31134400
H	4.06114000	1.21430000	4.41384600
H	2.68175600	2.02996900	3.65921800
C	6.00856900	2.11434600	2.61771600
H	6.55579500	1.97051400	1.68084500
H	6.37996700	1.37960100	3.34088900
H	6.24620900	3.11509800	2.99575200
C	4.21298500	-2.28511800	-0.68513700
C	3.89483500	-2.92290000	-1.89486200
C	3.80476700	-4.31629400	-1.86837100
H	3.54063600	-4.84910000	-2.77460100
C	4.02712800	-5.02817400	-0.69204900
H	3.94412800	-6.11094800	-0.69331100
C	4.33812600	-4.36045800	0.48807000
H	4.48841500	-4.92739400	1.39958000
C	4.44038900	-2.96633000	0.52321500
C	3.63916700	-2.13837000	-3.17351200
H	3.24249300	-1.15939500	-2.88337000
C	2.58936300	-2.79857100	-4.08040200
H	2.98786000	-3.69441700	-4.57042200
H	2.29187900	-2.09880600	-4.86784000
H	1.69464100	-3.07768900	-3.52003600
C	4.94428300	-1.91295500	-3.96091400
H	5.68510100	-1.35121700	-3.38396600
H	4.74058900	-1.35177400	-4.87973900
H	5.39335900	-2.87228400	-4.24203800
C	4.78147100	-2.23779400	1.81847800
H	4.31013600	-1.24960000	1.78016200
C	4.23333300	-2.93727300	3.07093600
H	3.16882400	-3.15913100	2.96955600
H	4.36315300	-2.28225700	3.93914800
H	4.77078100	-3.86849500	3.28316800
C	6.30257700	-2.03599900	1.96577500
H	6.81402500	-3.00487000	1.99258200
H	6.52584900	-1.50873500	2.90033800
H	6.72787700	-1.45272700	1.14486200

C	1.38464200	-0.53282800	2.34238500
C	-1.52487600	1.25077300	3.76046100
C	-5.98249700	-0.62328700	0.12643500
C	0.52606100	0.79632100	-2.05536200
C	-1.26327200	3.29172500	0.80037600
C	-1.70732100	-1.19433800	4.00615200
C	-4.10466700	-2.22509100	-2.43727500
C	-0.89288100	-3.31035200	2.28398700
C	-3.88977000	-1.32335600	3.13305000
C	-0.82849400	-3.68267500	0.89580900
C	-1.00615500	2.80957300	2.10740800
C	-0.11814600	1.09103500	3.44286700
C	-3.68632100	3.04088300	1.30020800
C	2.08153000	0.03227300	-0.08340500
C	-5.57621600	-1.65029500	-0.71819800
C	-4.18794800	0.45476000	-3.40519400
C	0.19478900	2.04634400	2.41075500
C	0.72082100	-1.59829400	-1.51709100
C	-3.06505400	-1.73891600	-3.22636800
C	-2.06434800	2.32007900	2.93871000
C	-0.35510700	-1.35146200	3.69037800
C	-2.46089400	-3.44558300	-0.99476500
C	-2.62324000	3.53422100	0.47030600
C	-3.79233500	-3.03972900	-1.27973400
C	-4.44586900	3.02046400	-0.93140600
C	0.07401400	-2.42983000	2.81025400
C	-3.11423700	-0.37680200	-3.72794500
C	1.24706400	1.08495800	-0.86545900
C	1.06432600	1.68148200	1.38872500
C	-1.37395500	-2.93329400	-1.84365700
C	-4.72479600	-1.65572900	2.03291600
C	-1.52475500	1.45782200	-3.34088700
C	-4.30599300	-2.74627600	1.13947700
C	-0.82815700	2.84061000	-1.59834400
C	-4.80932100	2.71333800	0.43810700
C	-4.70667400	-2.69605400	-0.22329300
C	-6.03913400	0.73762100	-0.36350900
C	-0.33701400	2.92049600	-0.27734100
C	-4.86820100	2.19242200	-1.97534800
C	-0.87813000	-0.90938900	-3.19694700
C	-5.68493500	1.02401100	-1.68514900
C	-0.08733600	-2.78052900	-1.26183400
C	-3.94526100	1.84125500	-3.04000500
C	-5.26976900	-0.04771500	-2.57170100

C	-2.30048700	0.13103000	4.02618000
C	1.54322600	-1.34159700	-0.39341300
C	1.17886500	-2.26335700	0.63097400
C	-2.69689400	-2.09153400	3.44360600
C	0.18523400	-3.18149500	0.08109300
C	-5.51178000	-0.60015900	1.49940400
C	1.73257300	0.41043900	1.38769500
C	-2.63602400	2.33052200	-3.01318300
C	-3.08317100	3.51577900	-0.90556500
C	-2.17672300	-3.76149100	0.36307600
C	0.27438200	-0.60218100	-2.43852300
C	1.15906700	-1.94512600	1.99527300
C	-0.41066000	1.78031400	-2.47292400
C	-3.09034200	-3.42362200	1.41853400
C	-3.41142700	2.29846600	2.47813100
C	-5.58455100	1.59620300	0.71573300
C	-1.75694400	0.13429000	-3.69047200
C	-5.21436500	-1.35941400	-2.09491400
C	-2.29784700	-3.11592700	2.59598700
C	0.45603100	-0.18450200	3.40149300
C	-1.69333300	-2.07721300	-2.92718000
C	-2.20155600	3.18235400	-1.92515700
C	-5.27117600	0.76790600	1.86461600
C	0.77500600	2.07945300	0.02469300
C	-4.23339400	1.11554800	2.77034100
C	-3.64829400	0.04377000	3.49787900
N	4.31589800	1.29939500	-0.38211100
N	4.42712700	-0.84571300	-0.69394900

nNHC-C₇₀-4

C	3.47059300	0.05709100	0.05479900
C	5.57807100	0.81673300	0.21580900
H	6.34322000	1.54579600	0.41783400
C	5.64064500	-0.46747300	-0.20620800
H	6.47204100	-1.10693300	-0.44749300
C	3.82434700	2.49592000	0.66777000
C	3.63211200	3.37558600	-0.41275400
C	3.28811000	4.69460700	-0.09510000
H	3.10920100	5.40335400	-0.89501100
C	3.14913100	5.10193500	1.22605800
H	2.86501300	6.12650400	1.44714600
C	3.36980100	4.20572200	2.26991400
H	3.25414600	4.54033400	3.29420400
C	3.72096900	2.87862100	2.01625900

C	3.83810300	2.95455700	-1.86415200
H	3.55782900	1.89985900	-1.95159400
C	2.96557200	3.73721800	-2.85700200
H	3.33334800	4.76098600	-2.99092000
H	1.92544000	3.78350500	-2.53309600
H	2.99976600	3.24979500	-3.83671500
C	5.31694900	3.09615200	-2.27796500
H	5.64049800	4.13867900	-2.18192300
H	5.44467300	2.79620600	-3.32431000
H	5.98456200	2.47871600	-1.67237400
C	3.99200100	1.90679200	3.15570500
H	3.74676600	0.89979400	2.80132100
C	3.12500900	2.17598700	4.39440200
H	3.43443300	3.09218100	4.90979200
H	3.23420200	1.35057800	5.10561800
H	2.06743800	2.26038500	4.13696100
C	5.48204200	1.92695500	3.55020000
H	6.13602000	1.64381700	2.72008700
H	5.66543800	1.22812600	4.37393200
H	5.77619600	2.92878000	3.88277600
C	4.03220900	-2.24258800	-0.83477300
C	3.82573700	-2.37433600	-2.21968600
C	3.56876300	-3.66418000	-2.69532200
H	3.38425600	-3.81409600	-3.75257900
C	3.53432300	-4.75474400	-1.83167900
H	3.32173900	-5.74483000	-2.22404000
C	3.76941800	-4.58776600	-0.46993100
H	3.73603200	-5.44748100	0.18974900
C	4.02671200	-3.32237700	0.06337600
C	3.93017000	-1.19006000	-3.17389500
H	3.57253700	-0.30104100	-2.64427200
C	3.06435000	-1.33789200	-4.43302900
H	3.46811700	-2.09658500	-5.11320100
H	3.04922200	-0.38833800	-4.97792200
H	2.03408700	-1.60174000	-4.18836300
C	5.39565500	-0.94855400	-3.58836800
H	6.04676600	-0.75486500	-2.73205100
H	5.45963000	-0.08355000	-4.25802400
H	5.78998500	-1.82102700	-4.12149800
C	4.30970500	-3.13880600	1.54725100
H	4.06047000	-2.10562100	1.81083500
C	3.45561800	-4.04846900	2.44223500
H	2.39612600	-3.98851000	2.18747600
H	3.57282600	-3.74932100	3.48879300

H	3.76765600	-5.09608100	2.36642300
C	5.80555100	-3.35915400	1.84476000
H	6.10484000	-4.37901400	1.57793100
H	6.00562900	-3.21482100	2.91224600
H	6.44415700	-2.66723800	1.28675300
C	0.27812400	-1.97638800	2.90615000
C	-2.21385400	0.56345200	3.89277100
C	-5.68716800	0.81851600	-1.03164600
C	1.29692000	0.04602500	-1.24132300
C	-0.42744700	2.65934600	1.56786200
C	-3.22200900	-1.65730700	3.59686000
C	-3.72347400	-1.05277500	-3.32068300
C	-2.60240000	-3.70260800	1.71650500
C	-4.96131600	-0.91108700	2.18894700
C	-2.22995000	-3.93644100	0.33177200
C	-0.74713600	1.98557800	2.77617000
C	-0.90031900	-0.05631100	3.90353700
C	-2.84304100	3.26749300	1.40897400
C	1.55150900	-1.38412700	0.86897500
C	-5.39471000	-0.18156100	-1.94922500
C	-2.66792200	1.56238100	-3.71060100
C	0.00308300	0.84053400	3.20813100
C	0.55762400	-2.34037200	-1.19435400
C	-2.40674800	-0.89133400	-3.73226600
C	-2.11670500	1.83308900	3.21655300
C	-1.95252900	-2.25766800	3.61041900
C	-3.06063600	-2.93915800	-1.81002600
C	-1.47495700	3.41447300	0.97461000
C	-4.04851800	-2.05514800	-2.32406000
C	-2.83454300	3.75238500	-0.89538000
C	-1.64176400	-3.30152400	2.64750400
C	-1.86950600	0.43960200	-3.93759600
C	1.94950500	-0.06681500	0.15443000
C	0.98136800	0.32407600	2.35149500
C	-1.66849900	-2.76497400	-2.24238500
C	-5.47108900	-0.79812200	0.86916300
C	0.01488800	1.51480300	-2.77879800
C	-5.15155100	-1.85651500	-0.09995900
C	0.60320700	2.40770700	-0.68571300
C	-3.68102300	3.44910400	0.24968800
C	-5.07627100	-1.51735300	-1.47741900
C	-5.16846000	2.16207700	-1.22461200
C	0.63645300	2.11691600	0.71098100
C	-3.17126400	3.26514700	-2.16246200

C	-0.19561900	-0.90654700	-2.97845600
C	-4.35491600	2.44791200	-2.32961500
C	-0.61803700	-3.13236700	-1.34776500
C	-2.12191800	2.71366000	-3.00993100
C	-4.04709600	1.39538600	-3.28487800
C	-3.35380600	-0.22929100	3.74577400
C	0.98596500	-2.44547900	0.19890700
C	0.08626200	-3.35019600	0.88445500
C	-4.20890700	-2.07472100	2.61608300
C	-0.91295800	-3.76741300	-0.07197900
C	-5.69301000	0.52028100	0.38686200
C	1.13970400	-1.11335700	2.21926800
C	-0.80254800	2.68764700	-2.55828200
C	-1.46491200	3.73725700	-0.43146200
C	-3.31236400	-3.48142900	-0.52094900
C	0.70079500	-1.10716400	-1.88937100
C	-0.26227200	-3.12351500	2.21980200
C	0.86977000	1.32000300	-1.62227200
C	-4.34161900	-2.94511600	0.32281600
C	-3.18501400	2.34418500	2.43488700
C	-4.82438700	2.67144800	0.08118100
C	-0.50087900	0.41844100	-3.45612900
C	-4.56403900	0.11009000	-3.10034600
C	-3.90847100	-3.07616500	1.70245300
C	-0.77227100	-1.43742100	3.77155600
C	-1.36867900	-1.72140000	-3.14860800
C	-0.45538600	3.19881200	-1.23840700
C	-5.14754900	1.65856700	1.07111400
C	1.33920200	0.97495700	1.14103800
C	-4.38446000	1.51093500	2.26135400
C	-4.42118100	0.22983800	2.87677900
N	4.23437700	1.13603600	0.36270600
N	4.33448800	-0.92302400	-0.31553100

nNHC-C₇₀-5

C	3.41807100	0.03393000	0.17267100
C	5.55891200	0.72183600	0.17478900
H	6.36220600	1.42648900	0.04773100
C	5.55087500	-0.58389700	0.52668600
H	6.34380900	-1.26667300	0.77774800
C	3.90735000	2.41387600	-0.55070200
C	3.85473700	2.58731400	-1.94568600
C	3.57836600	3.87653800	-2.41173000
H	3.50855800	4.05193000	-3.47909800

C	3.38859600	4.93380400	-1.52783100
H	3.16636000	5.92482700	-1.91259300
C	3.48809600	4.73211900	-0.15445400
H	3.34469500	5.56743900	0.52140900
C	3.75646600	3.46469000	0.37010100
C	4.15375100	1.45347600	-2.91802200
H	3.84361300	0.51740300	-2.44529500
C	3.38214700	1.56079700	-4.24048700
H	3.76729300	2.37295800	-4.86768400
H	2.31621100	1.72716400	-4.07509700
H	3.49684800	0.63081900	-4.80687400
C	5.66546500	1.36979000	-3.20836600
H	6.01867400	2.29561300	-3.67643300
H	5.87210000	0.54138000	-3.89560500
H	6.25439400	1.20516400	-2.30189800
C	3.91715100	3.25703200	1.86896900
H	3.64576700	2.22030400	2.09112900
C	2.99675300	4.15735900	2.70568600
H	3.33294100	5.20043400	2.69043000
H	3.00828200	3.82699700	3.74936900
H	1.96556700	4.12215600	2.35128000
C	5.38100900	3.48031300	2.29775500
H	6.07191200	2.79432700	1.79956400
H	5.48494900	3.33239100	3.37848300
H	5.69772400	4.50300800	2.06347600
C	3.90084100	-2.40548500	0.71504800
C	3.90395100	-3.24622400	-0.41336900
C	3.63685800	-4.60009500	-0.18812800
H	3.60733000	-5.28390300	-1.02823500
C	3.39004900	-5.08010500	1.09416600
H	3.17192500	-6.13364600	1.24231900
C	3.41862400	-4.22043400	2.18845800
H	3.21903200	-4.61046600	3.17969500
C	3.68112900	-2.85745000	2.02701100
C	4.20467900	-2.73371200	-1.81847200
H	3.82172000	-1.71013700	-1.89334100
C	3.52172700	-3.54944300	-2.92627300
H	3.99045400	-4.53261100	-3.04831100
H	3.62271500	-3.02076400	-3.87988900
H	2.45733600	-3.68873900	-2.73001100
C	5.72288700	-2.70051200	-2.08835800
H	6.26122300	-2.05466700	-1.39110500
H	5.91527700	-2.32908700	-3.10126100
H	6.14438700	-3.70917000	-2.01103800

C	3.73154900	-1.92019100	3.22668600
H	3.39496200	-0.93225900	2.89492600
C	2.80540300	-2.35417400	4.37305500
H	1.80075800	-2.58857600	4.01628500
H	2.72495700	-1.54409400	5.10446100
H	3.20191500	-3.23153700	4.89687000
C	5.17167300	-1.78213200	3.75987000
H	5.56154900	-2.75927300	4.06700600
H	5.18842900	-1.12059100	4.63313500
H	5.85455000	-1.36577300	3.01448500
C	-1.08219700	2.09984400	3.41676900
C	-3.64328500	3.37219600	1.08709400
C	-4.95262400	-1.59119500	-2.10124300
C	1.88191600	0.07780300	0.07392700
C	-1.00720400	3.10028500	-1.37754800
C	-4.54737900	1.70612700	2.65517700
C	-2.33263000	-3.74024000	-1.04883800
C	-3.35747000	-0.63010600	3.74828000
C	-5.57896300	0.39835400	0.99030300
C	-2.49052100	-1.74540900	3.41715400
C	-1.80398100	3.64621800	-0.32926300
C	-2.46762200	3.49621300	1.92751500
C	-3.14993900	2.48824800	-2.49890500
C	0.88405000	1.13696100	2.23397500
C	-4.36730300	-2.73356100	-1.57093700
C	-1.10125400	-2.44500700	-3.27032100
C	-1.33218100	3.64489600	1.03785900
C	0.71098800	-1.27823900	1.94837500
C	-0.95678000	-3.55639300	-1.07472800
C	-3.22749800	3.46995100	-0.30143900
C	-3.41520500	1.81710300	3.46529300
C	-2.38970100	-3.24396200	1.40855500
C	-1.72588300	2.66491200	-2.52860800
C	-3.06125800	-3.53191800	0.18968500
C	-2.25888400	0.86830600	-3.95698100
C	-2.80162500	0.62163900	4.02223900
C	-0.31872200	-2.89831300	-2.20163600
C	1.34511100	1.27462500	0.87743700
C	-0.12932500	3.02736300	1.35071500
C	-0.93713900	-3.05035100	1.37335700
C	-5.54697200	-0.77923100	0.19526400
C	1.04348100	-0.84579300	-2.20935700
C	-4.92595600	-1.98623300	0.75693200
C	0.74138800	1.40743400	-1.86873100

C	-3.48530100	1.37902100	-3.37454100
C	-4.31525600	-2.91322400	-0.13121200
C	-4.33893200	-0.92340900	-3.23218200
C	0.27621600	2.48141500	-1.05619800
C	-2.09242100	-0.50385400	-4.15578200
C	0.78723700	-2.25447400	-0.22973900
C	-3.15821900	-1.42200400	-3.78739600
C	-0.34297000	-2.18026900	2.32020400
C	-0.82500600	-1.13497400	-3.82775000
C	-2.54500400	-2.61832700	-3.23203800
C	-4.65895400	2.49593500	1.44223200
C	0.62282300	-0.10581600	2.81120700
C	-0.52378100	-0.27331000	3.67982400
C	-5.11098500	0.40253200	2.36334200
C	-1.11386000	-1.56594700	3.37811200
C	-5.50184800	-0.58491000	-1.21198700
C	0.00854200	2.25853100	2.55996000
C	0.21941800	-0.36257400	-3.31358500
C	-1.17395900	1.65927300	-3.40896400
C	-3.13847100	-2.54633700	2.39420500
C	1.23804600	-1.24821400	0.64486900
C	-1.35824900	0.80335100	4.00470200
C	1.43545600	0.26719700	-1.38618900
C	-4.39337300	-1.92813000	2.07381400
C	-3.90795800	2.76381900	-1.32960700
C	-4.50183900	0.50368300	-3.01943900
C	0.77601100	-2.10860000	-1.67871100
C	-3.14837700	-3.26408600	-2.15033100
C	-4.52600200	-0.73918200	2.89596800
C	-2.34962100	2.73261300	3.09066600
C	-0.26403300	-3.16111000	0.13164700
C	0.03019000	1.04621100	-3.08854700
C	-5.22749000	0.70506100	-1.77872300
C	0.65934900	2.37819900	0.31235500
C	-4.98221500	1.83490700	-0.95228200
C	-5.30445100	1.68841400	0.42395700
N	4.24078300	1.09321000	-0.04705300
N	4.22550700	-1.00415100	0.51193300

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C	-5.39092800	0.67783800	0.12555000
C	-4.16450100	-1.15726200	-0.02045800
H	-3.96772600	-2.21496900	-0.06406500
C	-3.30127200	-0.09587400	-0.03523500

C	-6.66566300	-1.43633200	0.13619800
C	-7.12964300	-1.84658200	1.39559900
C	-8.29216200	-2.62428600	1.41576900
H	-8.68733500	-2.96679900	2.36686700
C	-8.94405500	-2.96843400	0.23408900
H	-9.84320900	-3.57625000	0.27284500
C	-8.45145200	-2.54216000	-0.99719000
H	-8.96858500	-2.82168100	-1.90945800
C	-7.29372200	-1.76160000	-1.07640600
C	-6.41038700	-1.48542600	2.68660100
H	-5.56207600	-0.83848100	2.44195600
C	-7.32468400	-0.69716300	3.63871000
H	-8.18208100	-1.29767500	3.96156300
H	-7.71049900	0.20991500	3.16134000
H	-6.76903800	-0.40045800	4.53452000
C	-5.83788400	-2.74110400	3.36653600
H	-6.63480500	-3.43398800	3.65866800
H	-5.28335500	-2.46394300	4.26916600
H	-5.15457300	-3.27574100	2.69872200
C	-6.74013900	-1.31900800	-2.42268300
H	-5.90860500	-0.62984100	-2.24553000
C	-7.78859700	-0.55774000	-3.24944900
H	-8.64003100	-1.19587500	-3.50929600
H	-7.34325500	-0.20155100	-4.18437200
H	-8.17296700	0.30977400	-2.70238800
C	-6.17418100	-2.52105100	-3.19926700
H	-5.39211600	-3.03061300	-2.62672800
H	-5.73932500	-2.19006200	-4.14834200
H	-6.95863800	-3.25279100	-3.42231800
C	-3.67790700	2.43345100	0.07062700
C	-3.44669100	3.03888500	1.31583000
C	-3.04773100	4.37822000	1.29680200
H	-2.84361200	4.88627200	2.23236600
C	-2.88774700	5.06037900	0.09400500
H	-2.56244100	6.09642700	0.10282100
C	-3.12946200	4.42510300	-1.12092200
H	-2.98944600	4.96989700	-2.04736900
C	-3.53228300	3.08740400	-1.16362500
C	-3.65879100	2.28987100	2.62414000
H	-3.48868200	1.22648400	2.42726000
C	-5.10509000	2.47432700	3.12357600
H	-5.31071200	3.53066700	3.33057300
H	-5.26497900	1.90961700	4.04887100
H	-5.84538800	2.13262500	2.39186900

C	-2.66587100	2.69442500	3.72231800
H	-1.63454000	2.62832100	3.37019000
H	-2.77595000	2.02292400	4.58021200
H	-2.84873300	3.71370500	4.08124300
C	-3.84328900	2.38946700	-2.48150400
H	-3.62640600	1.32352100	-2.35261200
C	-5.33696900	2.53762100	-2.83328700
H	-5.99067100	2.12860500	-2.05534700
H	-5.56298200	2.01366400	-3.76886300
H	-5.59867600	3.59364000	-2.96373800
C	-2.97764500	2.87844700	-3.65053500
H	-3.23245100	3.90332500	-3.94284100
H	-3.14675600	2.23982100	-4.52371500
H	-1.91464300	2.84203700	-3.40232600
C	-1.79334900	-0.10106400	-0.09081000
C	0.52919100	2.04804000	-2.27677300
C	5.89633500	-0.69171300	-2.19304900
C	1.68351200	-0.12694700	3.36204800
C	2.07946300	3.15200200	0.78916300
C	0.21407900	-0.17640700	-3.24945700
C	5.37806900	-3.00945300	0.44230800
C	0.11310100	-2.71509400	-1.96781400
C	2.49877500	-0.52110300	-3.72699500
C	0.70347900	-3.48986700	-0.91044800
C	1.11289000	3.05451500	-0.25843800
C	-0.53322600	1.77380900	-1.32821100
C	3.84953000	3.10218200	-0.96738300
C	-0.52074200	-0.30565700	2.13989800
C	5.84616000	-1.93078500	-1.56838300
C	6.31950400	-0.74397100	1.89020100
C	-0.16886600	2.42639100	-0.07451400
C	0.89381000	-2.28752100	2.43537800
C	4.97148500	-2.80924900	1.75679700
C	1.53778400	2.84288600	-1.62111000
C	-0.79080000	-0.43961300	-2.30212500
C	3.08020800	-3.79039300	-0.17954200
C	3.43166100	3.30400200	0.39718100
C	4.41328200	-3.46012100	-0.54319700
C	5.62315600	2.43654100	0.43258000
C	-0.84002500	-1.73417100	-1.64887500
C	5.45601600	-1.65828900	2.49646500
C	0.52063000	0.47314700	2.81173100
C	-0.42845600	1.72695900	1.10706000
C	2.65540900	-3.57763100	1.21323700

C	3.72320600	-1.14412600	-3.35646800
C	4.16513800	0.17180700	3.51278000
C	3.67045200	-2.45620500	-2.69548300
C	2.87257200	1.99799600	2.84362600
C	5.18981000	2.55570700	-0.94767300
C	4.70379400	-2.80084500	-1.78633600
C	6.37993900	0.46671000	-1.46882100
C	1.79082300	2.46674900	2.05345400
C	6.40501400	1.35143400	0.83374600
C	3.21232800	-2.05795300	3.09919800
C	6.79748100	0.34018800	-0.13894000
C	1.28824800	-3.28270300	1.46770600
C	6.11634800	0.68039100	2.08914400
C	6.74467300	-0.95131800	0.51212700
C	0.88889500	1.09272900	-3.22305700
C	-0.34133100	-1.68737100	2.00227000
C	-0.70197900	-2.28668700	0.71930200
C	1.22230500	-1.18281100	-3.54219200
C	0.31219000	-3.27590500	0.40760700
C	4.80561100	-0.27723600	-3.05793800
C	-1.16000100	0.50787000	1.16168800
C	5.06015000	1.12662500	2.88890600
C	4.52267200	2.88982000	1.26161500
C	2.10838600	-3.69994900	-1.21191900
C	1.88603500	-1.56668000	3.16824200
C	-1.29470100	-1.55675000	-0.29866300
C	2.81961200	0.71556200	3.48926500
C	2.39697300	-3.04368800	-2.45557000
C	2.91192900	2.72496100	-1.96464700
C	5.56420800	1.59183000	-1.87690000
C	4.35550500	-1.18974400	3.31720800
C	6.27737400	-2.06715700	-0.19140400
C	1.17303900	-2.42018100	-2.91829200
C	-1.21658400	0.56844600	-1.37139800
C	3.59828700	-3.06112700	2.13963200
C	4.25047800	2.25175300	2.46488900
C	4.59911900	1.13042300	-2.85702500
C	0.57541700	1.74160900	2.16970700
C	3.30318700	1.70461000	-2.95033400
C	2.29423200	0.88527800	-3.52518200
N	-5.45504600	-0.65540100	0.08217600
N	-4.10444500	1.04741000	0.05730800
H	-6.23320300	1.34397900	0.20237500

aNHC-C₇₀-2

C	5.32961600	0.39210200	0.42732400
C	3.19124000	-0.12034700	0.03205800
C	3.97828600	-1.15687600	-0.39020800
H	3.70852700	-2.09054200	-0.85358200
C	3.74302900	2.13721500	1.10310900
C	3.46139800	2.20673200	2.47703100
C	3.16397500	3.47059900	2.99377100
H	2.92713300	3.57471000	4.04635500
C	3.14930100	4.59360900	2.17089600
H	2.90312900	5.56423700	2.59114600
C	3.43421700	4.48311400	0.81312300
H	3.40407700	5.36670800	0.18604700
C	3.73827800	3.24467800	0.24023400
C	3.51862100	0.97399400	3.36955700
H	3.25874800	0.10505200	2.75607300
C	4.94569900	0.76573900	3.91311600
H	5.24990000	1.61482400	4.53536900
H	5.68317600	0.66357400	3.10975300
H	4.99298200	-0.14033200	4.52767300
C	2.51058100	1.01355400	4.52618300
H	2.78128800	1.76667700	5.27465200
H	2.49383600	0.04283100	5.03244200
H	1.50141000	1.22885900	4.16771600
C	4.08547300	3.11561500	-1.23690500
H	3.80671300	2.10497300	-1.55324100
C	5.59851700	3.30740200	-1.45812600
H	5.91071600	4.31019800	-1.14510600
H	5.84704100	3.19052100	-2.51887000
H	6.19854400	2.58509400	-0.89406100
C	3.29823400	4.08444600	-2.13017800
H	2.22410500	4.01035500	-1.94858300
H	3.48219200	3.84290100	-3.18222700
H	3.60889500	5.12412900	-1.97573600
C	6.45926900	-1.60474400	-0.48065000
C	6.97106000	-2.48559300	0.48400500
C	8.08900900	-3.24244000	0.11730600
H	8.52222900	-3.93455000	0.83264800
C	8.64810700	-3.12303200	-1.15249300
H	9.51308300	-3.72352000	-1.41837900
C	8.10625600	-2.24213400	-2.08590100
H	8.55091800	-2.16503900	-3.07288700
C	6.99378000	-1.45555000	-1.77079700
C	6.35553300	-2.62463900	1.86800900

H	5.48151400	-1.96812700	1.92567400
C	7.34094800	-2.17522000	2.95983700
H	8.23115800	-2.81350100	2.97945900
H	6.86651000	-2.22865200	3.94541700
H	7.67283500	-1.14392800	2.79736300
C	5.85784600	-4.05861300	2.11521700
H	5.13515200	-4.36307800	1.35122800
H	5.36965900	-4.12591500	3.09319900
H	6.68442000	-4.77740400	2.10284500
C	6.38469100	-0.51295300	-2.79860900
H	5.63027700	0.10345600	-2.30010800
C	7.43085300	0.44467100	-3.39095800
H	7.93716300	1.01661000	-2.60621500
H	6.94601800	1.15333900	-4.07047700
H	8.19469500	-0.09276000	-3.96317800
C	5.66417800	-1.30915000	-3.90115800
H	6.36718200	-1.94889400	-4.44637800
H	5.19558600	-0.62754800	-4.61880100
H	4.88094700	-1.94933400	-3.48218300
C	1.30478800	1.14730700	-1.06068300
C	-0.74897400	-0.74927900	-3.49251100
C	-6.36043900	-0.12488500	-1.30241500
C	-0.67832800	-1.04609100	2.66005000
C	-1.04419500	-3.23149000	-0.87701700
C	-1.29340600	1.63442900	-3.51752300
C	-5.63476300	1.23640500	1.88696500
C	-1.41601200	3.50247200	-1.37124800
C	-3.62634400	1.34001500	-3.37910500
C	-1.82314000	3.67320200	-0.00124100
C	-0.50095100	-2.48766700	-1.95597500
C	0.46275100	-0.48262800	-2.76008800
C	-3.20751200	-3.20094400	-2.09975600
C	0.98640800	0.23409900	1.28765600
C	-6.41928500	0.78419100	-0.25695800
C	-5.55258900	-1.55112700	2.46234200
C	0.58819100	-1.54777300	-1.76727700
C	-0.75335700	1.42013400	2.53827100
C	-4.83031600	0.76593400	2.91582800
C	-1.32642400	-1.99609800	-3.01673600
C	-0.14645100	1.91674400	-2.76150300
C	-3.88355000	2.90146200	1.21615800
C	-2.37685800	-3.69681500	-1.03957500
C	-5.14505400	2.27969700	1.00283700
C	-4.59433300	-3.66558400	-0.25226600

C	-0.21003100	2.85476800	-1.68134900
C	-4.78828300	-0.65380000	3.21226800
C	0.38231700	-1.00043300	1.70974100
C	1.07579200	-1.31742900	-0.50026000
C	-3.02654800	2.39227300	2.29616100
C	-4.79360600	1.37011700	-2.57120700
C	-2.85718900	-2.17949800	3.14700100
C	-4.85635300	2.33542000	-1.46165700
C	-1.43542400	-3.15060100	1.57210300
C	-4.57611400	-3.17500900	-1.61755100
C	-5.63028100	2.00531600	-0.31662900
C	-6.32077200	-1.54646100	-1.02521800
C	-0.55821900	-2.94675700	0.47224500
C	-5.45269000	-3.09263500	0.68897100
C	-2.63048600	0.24270500	3.49230600
C	-6.33677900	-2.00990900	0.29464700
C	-1.61665100	2.49424100	2.14707700
C	-4.96743000	-2.81209300	2.03189700
C	-6.39812900	-1.05807100	1.38938200
C	-1.60308100	0.28112300	-3.89939000
C	0.39335400	1.42322400	1.64989600
C	0.26109700	2.54783300	0.72739000
C	-2.54488900	2.28991200	-3.18956400
C	-1.00403600	3.17157100	1.01634700
C	-5.51058500	0.14929900	-2.45129300
C	1.69389100	0.04039700	-0.08016500
C	-3.64937600	-3.11810100	2.37178000
C	-3.22276200	-3.97469500	0.10450200
C	-3.26079400	3.47331300	0.07620600
C	-1.26626600	0.22005900	3.09459400
C	0.63648300	2.32679000	-0.60662000
C	-1.49559300	-2.20960700	2.65345700
C	-3.74785300	3.19620200	-1.24742200
C	-2.72786100	-2.23508700	-3.02505200
C	-5.41800300	-2.13754400	-1.99365200
C	-3.41613900	-0.97386300	3.55578800
C	-6.44064900	0.31277100	1.11263900
C	-2.60497500	3.20179700	-2.14362600
C	0.74298000	0.82879900	-2.33599700
C	-3.49828600	1.31478500	3.09433300
C	-2.75935800	-3.70906100	1.38793000
C	-4.92785000	-1.08977700	-2.87226000
C	0.43816800	-1.94131000	0.62477300
C	-3.62222600	-1.14373200	-3.43461400

C	-3.04134700	0.09767000	-3.80295700
N	4.07195000	0.84126100	0.54168900
N	5.30120300	-0.81709900	-0.13924000
H	6.21603200	0.91813300	0.73793800

aNHC-C₇₀-3

C	5.22982800	0.22719200	-0.63041600
C	3.95550000	-0.60346900	0.97594800
H	3.71668400	-1.13896600	1.87856900
C	3.12732000	0.05740800	0.11139800
C	6.41998400	-1.11383900	1.06875500
C	6.69273400	-2.44175200	0.69882000
C	7.81293000	-3.03899700	1.28465000
H	8.06160000	-4.06536500	1.03628200
C	8.61318800	-2.33471600	2.18224700
H	9.47976300	-2.81838500	2.62333000
C	8.31137300	-1.01822200	2.51976500
H	8.94517100	-0.48309700	3.21954700
C	7.19567700	-0.37467800	1.97322200
C	5.79561700	-3.21281300	-0.25972300
H	5.16826400	-2.49392400	-0.79681900
C	6.59616500	-3.98547000	-1.31874400
H	7.18515100	-4.79488600	-0.87444500
H	7.28128400	-3.32611800	-1.86191800
H	5.91131100	-4.43948900	-2.04261400
C	4.85165000	-4.14898300	0.51800100
H	5.42147500	-4.88958200	1.09020000
H	4.19177600	-4.68399900	-0.17303600
H	4.22169500	-3.59270800	1.21926500
C	6.86575100	1.06438300	2.33902700
H	5.90036500	1.32036700	1.89096000
C	7.91525000	2.02817500	1.75813000
H	8.90586800	1.83688600	2.18540100
H	7.64481300	3.06600400	1.98001900
H	7.99613600	1.92284200	0.67052500
C	6.71949800	1.24552800	3.85858900
H	5.96094200	0.56980300	4.26631500
H	6.41951300	2.27347800	4.08745800
H	7.66255500	1.04968700	4.38046300
C	3.57719000	1.31746400	-2.07423100
C	3.30949100	0.59162800	-3.24579500
C	2.93841600	1.33221600	-4.37186800
H	2.70866900	0.81682400	-5.29746700
C	2.83658900	2.71953100	-4.31348400

H	2.53331700	3.27366500	-5.19681500
C	3.10681900	3.40237000	-3.13081300
H	3.00701900	4.48123200	-3.10065700
C	3.48309000	2.71380400	-1.97417800
C	3.43285700	-0.92469900	-3.29909600
H	3.25692100	-1.31071300	-2.28935500
C	4.85084400	-1.34269500	-3.73414600
H	5.07051200	-0.96779700	-4.73995800
H	4.93880000	-2.43473600	-3.75127500
H	5.62328000	-0.95517100	-3.06108500
C	2.38476100	-1.57711900	-4.21098600
H	1.37827800	-1.22272900	-3.98165700
H	2.40065100	-2.66308100	-4.07382900
H	2.58982000	-1.37821100	-5.26896800
C	3.80064800	3.44572300	-0.67841100
H	3.57980900	2.76595300	0.15053500
C	5.29714000	3.80736400	-0.61602200
H	5.93837400	2.92297300	-0.70180000
H	5.53228600	4.30107600	0.33355200
H	5.56499600	4.49044500	-1.42998800
C	2.93398200	4.69427200	-0.46502600
H	3.19806800	5.49544800	-1.16454200
H	3.08855200	5.08083000	0.54739300
H	1.87149900	4.46906100	-0.58293300
C	0.67334000	2.33526300	1.28099600
C	-2.36185400	3.80758300	-0.22719900
C	-6.40910100	-0.59846300	0.66531200
C	0.30171500	-1.71443800	-1.01491600
C	-1.77302300	1.42482000	-2.86848300
C	-2.58048200	3.47858500	2.20509200
C	-4.27259700	-3.24480800	1.71177100
C	-1.59431200	1.42127600	3.90902700
C	-4.65658100	2.37653700	2.07498700
C	-1.38284400	0.00058700	3.96598500
C	-1.66081100	2.61066000	-2.10015900
C	-0.92982200	3.61182000	-0.10199700
C	-4.23736600	1.59945800	-2.58053400
C	1.62177500	0.18722200	0.20839600
C	-5.91887600	-1.60413800	1.49082400
C	-4.23765100	-3.59094300	-1.11768400
C	-0.50202500	2.86191800	-1.25557200
C	0.43922200	-1.71801500	1.45260400
C	-3.15048500	-3.78999600	1.09234900
C	-2.80477700	3.19493300	-1.46772300

C	-1.20255000	3.27795400	2.32714600
C	-2.79995300	-1.94759900	3.26721900
C	-3.08828000	1.01665500	-3.21525100
C	-4.09134000	-2.27267700	2.77158100
C	-4.75009700	-0.64745200	-3.07650600
C	-0.68394900	2.22758000	3.19467600
C	-3.13881900	-3.97656600	-0.34782500
C	0.88476400	-0.42044500	-1.01148000
C	0.46818700	1.87832600	-1.10000100
C	-1.62460200	-2.54296500	2.61300500
C	-5.36975900	1.14919200	2.13090900
C	-1.59222200	-3.02655300	-2.00547500
C	-4.86262400	0.08342900	3.00844600
C	-1.08117800	-0.95666400	-2.94907200
C	-5.26169100	0.57301900	-2.48440000
C	-5.11377100	-1.26818900	2.64577400
C	-6.40634100	-0.77462000	-0.77130300
C	-0.73656000	0.39364200	-2.72167900
C	-5.06110600	-1.88859200	-2.51342000
C	-0.97559600	-3.34718600	0.35437200
C	-5.91025000	-1.95452300	-1.33390000
C	-0.40717300	-1.81212400	2.63218900
C	-4.02969700	-2.90195700	-2.38133300
C	-5.40612800	-3.00991000	-0.47401300
C	-3.16641000	3.73317700	0.90127800
C	1.13822300	-0.48449100	1.47685600
C	0.65804900	0.26833100	2.58915900
C	-3.50768000	2.63021800	2.92659500
C	-0.28357200	-0.57198500	3.32744900
C	-6.08915500	0.78623900	0.96100200
C	1.11900000	1.65475000	0.15919800
C	-2.72870200	-2.63001400	-2.81479300
C	-3.39611300	-0.36933700	-3.51467700
C	-2.66578900	-0.67346000	3.88505000
C	0.09317900	-2.42675300	0.25875400
C	0.48683000	1.66178600	2.57628900
C	-0.57675500	-1.99775500	-2.09617700
C	-3.68728200	0.32931500	3.76489500
C	-4.09422400	2.60245900	-1.58682800
C	-6.06701100	0.51093600	-1.35574200
C	-1.79115200	-3.68273400	-0.79800500
C	-5.40891300	-2.83567800	0.91213600
C	-3.02381000	1.62115400	3.74784400
C	-0.36101700	3.34459600	1.14915200

C	-1.82116800	-3.43367700	1.52835700
C	-2.41059200	-1.33996200	-3.39184900
C	-5.88363200	1.47149200	-0.28438500
C	0.33262700	0.61513400	-1.80288600
C	-4.94821400	2.53538500	-0.39236300
C	-4.44998100	3.06130100	0.83055600
N	5.25243000	-0.48936900	0.49730200
N	3.96126300	0.57166900	-0.89278000
H	6.08653500	0.47625700	-1.23356400

aNHC-C₇₀-4

C	-5.12029200	0.48387600	0.18103300
C	-3.69604300	-0.95285900	-0.70998000
H	-3.37436500	-1.87531800	-1.15935400
C	-2.96666800	0.13148700	-0.30637200
C	-6.07555700	-1.70784500	-0.45130800
C	-6.09513500	-2.68109300	0.56374300
C	-7.10058100	-3.64936200	0.48238500
H	-7.15350800	-4.42624800	1.23781100
C	-8.03481400	-3.62706200	-0.55134000
H	-8.80968500	-4.38694200	-0.59162700
C	-7.98378400	-2.64186200	-1.53448100
H	-8.71924900	-2.64025900	-2.33208000
C	-6.98895900	-1.65851800	-1.51340700
C	-5.06262700	-2.70337000	1.68411000
H	-4.54588800	-1.73869100	1.69555900
C	-5.70902900	-2.87591800	3.06724200
H	-6.18219500	-3.85759100	3.17701600
H	-6.46981400	-2.11012500	3.25138200
H	-4.94298200	-2.79323200	3.84533500
C	-3.99464100	-3.78471400	1.43253400
H	-4.43969000	-4.78574300	1.46278100
H	-3.21106800	-3.72776300	2.19474600
H	-3.51089300	-3.65913800	0.45946500
C	-6.92720100	-0.57121100	-2.57552400
H	-5.94836000	-0.08472000	-2.50549800
C	-7.99976200	0.50153500	-2.31212700
H	-9.00544400	0.07127700	-2.37604900
H	-7.92547100	1.30818600	-3.04921200
H	-7.89238500	0.94239500	-1.31444600
C	-7.04864300	-1.13584100	-3.99917100
H	-6.29498100	-1.90740400	-4.18567700
H	-6.90721800	-0.33447000	-4.73189600
H	-8.03541200	-1.57536700	-4.17961900

C	-3.65020300	2.32299900	0.84387700
C	-3.50492700	2.38554900	2.23882800
C	-3.28666200	3.65158800	2.78965800
H	-3.15379400	3.74971300	3.86108500
C	-3.21117900	4.78174000	1.98035300
H	-3.02852700	5.75338200	2.42961100
C	-3.35047500	4.67609500	0.59910000
H	-3.26994500	5.56414600	-0.01717000
C	-3.56963800	3.43592400	-0.00677100
C	-3.58187100	1.14547000	3.11824400
H	-3.31581400	0.28168700	2.50068800
C	-5.01069600	0.93879700	3.65563400
H	-5.31783200	1.78919700	4.27469200
H	-5.05863800	0.03449100	4.27200800
H	-5.74690400	0.83431300	2.85081600
C	-2.57673800	1.17812100	4.27924600
H	-1.57234500	1.42755800	3.93194900
H	-2.53753000	0.19520400	4.75956900
H	-2.86801600	1.90574300	5.04519100
C	-3.73893800	3.30406200	-1.51336800
H	-3.40624600	2.30183500	-1.80054700
C	-5.22332300	3.44030000	-1.90328900
H	-5.84814100	2.69083300	-1.40430900
H	-5.34784100	3.31640000	-2.98494700
H	-5.60729200	4.42893600	-1.62754500
C	-2.87377800	4.29531300	-2.30364000
H	-3.23362800	5.32473600	-2.19602400
H	-2.90899100	4.04667900	-3.36913100
H	-1.83045700	4.25894700	-1.98046200
C	0.49123600	3.46678300	-0.28855000
C	2.76258700	2.68465800	2.51621400
C	5.96743300	-1.88388600	0.22971700
C	-0.87065800	-0.99292400	-0.92411900
C	0.67207200	-0.23212900	2.89489400
C	3.96851500	3.55023400	0.55858600
C	4.09568100	-2.60052400	-2.69937900
C	3.46662900	3.14480600	-2.21348600
C	5.56181300	1.81097500	0.50990300
C	3.05600800	2.14970500	-3.18819700
C	1.11441000	1.11423900	3.00787500
C	1.51835500	3.15291300	1.93230700
C	3.00953800	-0.91436400	3.44727900
C	-0.92606700	1.56033200	-0.98442000
C	5.73302700	-2.08055900	-1.12443100

C	2.77186400	-4.24833000	-0.79225200
C	0.50042800	2.16894500	2.25030800
C	0.05937000	0.26584700	-2.86136300
C	2.75329000	-2.91269900	-2.86838000
C	2.51095900	1.43964000	3.19912200
C	2.76547200	4.00302300	-0.00810100
C	3.68797000	-0.25592400	-3.48319800
C	1.61444700	-1.23261000	3.25458500
C	4.56126100	-1.25425000	-2.97032400
C	2.84775400	-3.10061000	2.58772800
C	2.51433700	3.79446900	-1.42579700
C	2.07917500	-3.75602200	-1.89993500
C	-1.46004400	0.28393000	-0.29957400
C	-0.45113700	1.81957900	1.28808500
C	2.26805500	-0.58484200	-3.65773900
C	5.99707100	0.60047200	-0.08998700
C	0.15490600	-3.19925100	-0.47442700
C	5.73831000	0.39432700	-1.52232700
C	-0.44236700	-1.89152400	1.39342300
C	3.77116200	-2.05710300	3.00998300
C	5.56864200	-0.93293100	-1.99873400
C	5.31186900	-2.72633600	1.21541700
C	-0.38032400	-0.55967000	1.91627500
C	3.17524000	-3.92530000	1.50598200
C	0.58959600	-2.07650000	-2.59963800
C	4.42397700	-3.72894400	0.80090300
C	1.29936400	0.45961000	-3.53519500
C	2.14785700	-4.23684900	0.52115000
C	4.17901500	-3.92864100	-0.61863600
C	3.96700700	2.88859000	1.83948100
C	-0.30173900	1.53020400	-2.21389700
C	0.71772700	2.50993900	-2.53643600
C	4.94683100	2.86777100	-0.27040000
C	1.71162700	1.84291600	-3.34609400
C	6.06672900	-0.53779800	0.75845100
C	-0.47277500	2.49906700	0.00525200
C	0.85864900	-3.72632400	0.67265700
C	1.50815900	-2.58169600	2.75274200
C	4.04903200	1.09172700	-3.21375400
C	-0.22656000	-0.97365400	-2.21923400
C	1.10529800	3.46871200	-1.59335400
C	-0.62215700	-2.05088300	-0.05117800
C	5.05851400	1.41148100	-2.24554000
C	3.48665000	0.41171000	3.25748600

C	4.97810400	-1.88092700	2.33607600
C	0.74239300	-3.21795300	-1.73339300
C	4.82693800	-3.12425700	-1.55999300
C	4.70344800	2.67435700	-1.62358400
C	1.52048500	3.80249400	0.69792500
C	1.82814100	-1.88230300	-3.30492500
C	0.51704700	-2.87329200	1.80559800
C	5.44294000	-0.53406100	2.05133500
C	-0.92310700	0.49000700	1.14829700
C	4.75327800	0.61002900	2.53690300
C	4.94437400	1.81613500	1.80802400
N	-5.02530500	-0.72055900	-0.39096500
N	-3.89627100	1.02570100	0.24551400
H	-6.02621600	0.93961500	0.54284200

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C	-5.05713000	-0.64314300	0.19937000
C	-2.94331500	-0.10225700	-0.29577300
C	-3.77076800	0.90542100	-0.71057300
H	-3.53258100	1.84056600	-1.18560000
C	-3.43397800	-2.32986400	0.89317200
C	-3.27030600	-2.34545900	2.28822600
C	-2.94787900	-3.57602400	2.86809600
H	-2.79655800	-3.63602000	3.93994600
C	-2.80326400	-4.71882700	2.08669600
H	-2.54164600	-5.66200200	2.55718600
C	-2.98074500	-4.66323000	0.70702400
H	-2.85188700	-5.56150900	0.11461600
C	-3.29856800	-3.45991100	0.07128800
C	-3.47295400	-1.09921900	3.14129700
H	-3.27299400	-0.22568000	2.51202300
C	-4.92770200	-1.01507300	3.64382200
H	-5.16573600	-1.87747600	4.27653400
H	-5.65382500	-0.99755200	2.82430500
H	-5.07303700	-0.10665500	4.23860400
C	-2.50826100	-1.01388300	4.33286900
H	-2.74344800	-1.76290900	5.09747200
H	-2.59515700	-0.02943100	4.80383500
H	-1.47185400	-1.15325500	4.02097300
C	-3.52452500	-3.38367500	-1.43310200
H	-3.18975600	-2.39583300	-1.76696400
C	-5.02230200	-3.53065000	-1.76675900
H	-5.39660700	-4.50712600	-1.43872300
H	-5.17976300	-3.45283300	-2.84842900

H	-5.63511700	-2.76174700	-1.28504500
C	-2.70918400	-4.41547200	-2.22397700
H	-1.65017900	-4.37657400	-1.95860100
H	-2.79841500	-4.20780200	-3.29524500
H	-3.07470300	-5.43554400	-2.05821800
C	-6.21803100	1.42675900	-0.49451700
C	-6.39422700	2.38310500	0.52096400
C	-7.49050500	3.24094800	0.39045500
H	-7.66681500	4.00050700	1.14480000
C	-8.36086800	3.13203000	-0.69241300
H	-9.20819500	3.80685200	-0.77088500
C	-8.15367200	2.16802500	-1.67542900
H	-8.84122700	2.09777900	-2.51218000
C	-7.06403300	1.29324000	-1.60429200
C	-5.42895700	2.50623900	1.69307900
H	-4.82737900	1.59308900	1.74066200
C	-6.15965200	2.62781600	3.03914900
H	-6.71898400	3.56625700	3.11682300
H	-5.43159300	2.61334900	3.85701100
H	-6.86128800	1.80077200	3.18990900
C	-4.45398500	3.68010200	1.48377600
H	-3.87417200	3.56627400	0.56319700
H	-3.74227100	3.73360400	2.31404600
H	-4.99543500	4.63132900	1.43049300
C	-6.83130000	0.23717700	-2.67360700
H	-5.84463800	-0.20661200	-2.50540200
C	-7.87297500	-0.88993100	-2.55927600
H	-7.86062500	-1.34763900	-1.56368800
H	-7.67144600	-1.67477000	-3.29613700
H	-8.88482600	-0.50844600	-2.73619100
C	-6.81803900	0.84233600	-4.08630300
H	-7.79423500	1.25856300	-4.35777400
H	-6.57117000	0.07045700	-4.82281100
H	-6.07516400	1.64221300	-4.16742900
C	1.77117400	-3.75897400	-1.02715800
C	4.31807200	-1.83276200	-2.86855400
C	5.20582700	2.86020000	0.83301000
C	-1.41998700	-0.10345200	-0.34989700
C	1.58499500	0.43816900	-3.54371400
C	5.17641300	-2.72433500	-0.74260100
C	2.49555000	2.42278700	3.08236400
C	3.88540300	-3.06215100	1.76453700
C	6.06465400	-0.67130700	-0.00486100
C	2.93999100	-2.43383200	2.66907600

C	2.45038900	-0.68570700	-3.67906900
C	3.18285900	-2.73001600	-2.76626500
C	3.64344100	1.81283100	-3.23170400
C	-0.28714300	-2.43038100	-0.59680500
C	4.56964400	2.69918800	2.05728900
C	1.26743800	4.03239700	1.07696500
C	2.02632800	-2.00138800	-3.25255700
C	-0.27705800	-1.37367700	1.60279100
C	1.13216400	2.31412600	2.83846400
C	3.86010400	-0.57673500	-3.43507900
C	4.08297300	-3.58662800	-0.63550300
C	2.67281300	-0.05493100	3.42076800
C	2.23376700	1.70682100	-3.47487500
C	3.28034600	1.22560000	3.32504500
C	2.60472000	3.66965300	-2.22216200
C	3.41784800	-3.75751200	0.64640600
C	0.49385500	3.13055500	1.82031600
C	-0.80927200	-1.23081500	-1.19789300
C	0.79635900	-2.16417500	-2.62838800
C	1.23437400	-0.16232700	3.16073900
C	5.93109700	0.45999700	0.84484200
C	-0.72212600	2.39330000	-0.18395100
C	5.25689000	0.28882000	2.13875700
C	-0.27268200	1.35993500	-2.18869100
C	3.87917100	3.01822700	-2.45569200
C	4.55853700	1.39532600	2.69514500
C	4.59403200	3.67810500	-0.19654900
C	0.27804000	0.26464300	-2.91715400
C	2.34707600	4.29473700	-0.99991800
C	-0.50900600	1.00098800	1.81535100
C	3.36514900	4.29964900	0.03732400
C	0.73138900	-1.37432300	2.62464900
C	1.05545800	4.12018500	-0.35552600
C	2.69819000	4.12922700	1.31890400
C	5.29161900	-1.82923300	-1.87940200
C	-0.07867600	-2.55699300	0.77537400
C	1.08052300	-3.26253800	1.27164200
C	5.64825800	-1.99487000	0.41872700
C	1.57732500	-2.52995700	2.42394900
C	5.84724900	1.72358400	0.19953900
C	0.66089700	-3.06025100	-1.51015200
C	0.08209200	3.32790100	-0.96610000
C	1.59067200	2.83779200	-2.84140600
C	3.49904000	-1.17181400	3.12017000

C	-0.84571800	-0.17997600	1.12418700
C	1.98889500	-3.87829200	0.40117000
C	-0.99526900	1.22932700	-0.98070700
C	4.77693700	-1.00239500	2.49042800
C	4.45861600	0.65998100	-3.07357600
C	4.85153100	3.02245200	-1.46559100
C	-0.53773900	2.32585400	1.19945000
C	3.29978400	3.35234300	2.31136700
C	5.01232900	-2.15779800	1.64290000
C	3.06229100	-3.58829200	-1.67168800
C	0.50656100	1.01001900	2.83326900
C	0.36376500	2.67089000	-2.21586300
C	5.63207600	1.82470100	-1.21592800
C	-0.07484600	-1.01748300	-2.39592900
C	5.48628200	0.66417800	-2.02344700
C	5.84895000	-0.57042900	-1.42033800
N	-3.78748900	-1.07022300	0.26961900
N	-5.07282500	0.55722200	-0.38666700
H	-5.91853400	-1.17511500	0.56531800

nNHC-Sc₃N@C₈₀-[6,6,6]

C	-1.93880700	-0.86488100	-1.24604300
C	-1.35546400	-2.15110200	-1.06062300
C	-1.11423200	-2.74633800	0.21655500
C	-1.42345500	-1.92024100	1.34037700
C	-2.00024800	-0.62261700	1.23385100
C	-2.54651900	-0.06664600	-0.08668500
C	-1.90383800	1.27938000	-0.20802100
C	-1.42106500	1.84971500	-1.42272600
C	-1.21853800	1.09939500	-2.63133000
C	-1.52767100	-0.32553100	-2.52336300
C	-0.60731200	-1.31046500	-3.10643800
C	-0.52059600	-2.42172900	-2.18803600
C	0.63064000	-3.27184100	-2.05589000
C	0.84563900	-3.89593300	-0.79656900
C	-0.01469000	-3.62469300	0.33122500
C	0.78780600	-3.66628200	1.53250700
C	0.51548200	-2.80410200	2.63067700
C	-0.63988800	-1.95553000	2.53788000
C	-0.75560600	-0.68057200	3.20590000
C	-1.62750800	0.16410700	2.38355100
C	-1.32371700	1.58127400	2.22556100
C	-1.47103900	2.08092900	0.89046800
C	-0.70145100	3.17814700	0.34668000

C	-0.66823500	3.03732200	-1.06887900
C	0.48840900	3.39775100	-1.82380400
C	0.76704100	2.61835000	-2.99665800
C	-0.05858300	1.48839300	-3.38922300
C	0.82639200	0.49623600	-3.98400200
C	0.59128600	-0.91389300	-3.81974300
C	1.73884000	-1.76010700	-3.70907500
C	1.74961500	-2.94505500	-2.87108300
C	3.07993800	-3.12693200	-2.37288500
C	3.29672400	-3.64269400	-1.05912200
C	2.18465200	-4.08009400	-0.29496300
C	2.14805700	-3.93561900	1.14436900
C	3.22328800	-3.34676600	1.85986700
C	2.94928300	-2.58332900	3.03446300
C	1.59655000	-2.31344900	3.41532700
C	1.54998100	-0.98607800	4.00237500
C	0.40032700	-0.14344500	3.89647400
C	0.63304200	1.27553900	3.79131200
C	-0.21382500	2.12465700	2.96255700
C	0.63712700	3.15231100	2.38844000
C	0.41803600	3.68527900	1.07273200
C	1.53766100	4.12520900	0.32181600
C	1.57271300	3.98281100	-1.11841600
C	2.93072100	3.70576000	-1.50158400
C	3.22019700	2.84858900	-2.60313100
C	2.12292300	2.33927800	-3.37199300
C	2.16856800	1.03622500	-3.98099300
C	3.30483400	0.18907600	-3.81711600
C	3.07605500	-1.21801500	-3.72274900
C	3.90222200	-2.06036300	-2.89953000
C	4.97627400	-1.50524300	-2.13648200
C	5.30634000	-2.10629700	-0.86659500
C	4.41641100	-3.10552000	-0.33007700
C	4.37124200	-2.95427300	1.09080700
C	5.21673600	-1.84989600	1.45597600
C	4.85759300	-1.02542800	2.58565900
C	3.75275200	-1.43368000	3.38972400
C	2.89006800	-0.44813100	3.98374800
C	3.12128500	0.95069300	3.80591800
C	1.97933300	1.80538500	3.73662700
C	1.97101700	2.96118200	2.87897700
C	3.10783600	3.31728700	2.08333900
C	2.87423100	3.93830200	0.82044400
C	3.73570300	3.69138600	-0.30611600

C	4.84547300	2.80789600	-0.18787900
C	5.18691400	2.01772000	-1.32684700
C	4.39164500	2.03723500	-2.52310600
C	4.42948000	0.72944200	-3.12226300
C	5.23436300	-0.11080500	-2.28215900
C	5.71218700	0.68543700	-1.16926500
C	5.98201400	0.11163600	0.11337900
C	5.83193900	-1.32624800	0.24904300
C	5.65462700	0.92484800	1.24145200
C	5.13154100	0.36828700	2.47626300
C	4.28706200	1.35334000	3.08390800
C	4.27875200	2.51587100	2.22911400
C	5.12677300	2.25980400	1.10054000
C	-6.20535200	0.64972300	-0.34216100
C	-6.21350400	-0.70380800	-0.31236600
H	-7.01716200	-1.41820200	-0.35111000
C	-4.07664200	-0.03374200	-0.15130300
C	-4.52972400	-2.50679100	-0.01051000
C	-4.45004600	-2.99190700	1.30806700
C	-4.11082800	-4.33911100	1.46294100
H	-4.01742900	-4.75419900	2.45981300
C	-3.87810600	-5.15069400	0.35587600
H	-3.60082900	-6.19051200	0.50064900
C	-4.00180100	-4.64336000	-0.93435700
H	-3.82394400	-5.29274800	-1.78374300
C	-4.33848800	-3.30322600	-1.15178700
C	-4.78351900	-2.11948000	2.51237100
H	-4.53405800	-1.08367800	2.26146200
C	-3.98349900	-2.47766000	3.77243200
H	-2.91167600	-2.52242700	3.57229600
H	-4.29917200	-3.44041700	4.18967500
H	-4.15556100	-1.71827500	4.54233500
C	-6.29306300	-2.18390200	2.82166000
H	-6.53333700	-1.53061200	3.66803200
H	-6.58518800	-3.20614500	3.08710700
H	-6.90627100	-1.87008500	1.97195700
C	-4.55029000	-2.76316000	-2.55975400
H	-4.33743500	-1.68873300	-2.54626900
C	-6.01804200	-2.95998200	-2.99073400
H	-6.17274000	-2.56527100	-4.00102600
H	-6.72152000	-2.45508400	-2.32226000
H	-6.27251500	-4.02576400	-2.99919400
C	-3.62167200	-3.39867400	-3.60460000
H	-3.70839700	-2.85489000	-4.55090700

H	-3.89383700	-4.44152800	-3.80270200
H	-2.57748700	-3.36839100	-3.28956200
C	-4.55690500	2.46997200	-0.10492700
C	-4.36787000	3.22505400	-1.27501000
C	-4.15258500	4.59752200	-1.11165300
H	-3.98110700	5.21636900	-1.98442300
C	-4.14034500	5.17744500	0.15276600
H	-3.96458700	6.24409900	0.25478100
C	-4.33828500	4.39832800	1.28905000
H	-4.31044300	4.86530600	2.26646500
C	-4.55189700	3.02021200	1.19143000
C	-4.41099900	2.60059200	-2.66391700
H	-4.04501800	1.57151100	-2.57966000
C	-3.51180200	3.32668600	-3.67759700
H	-3.94717200	4.28571700	-3.98078700
H	-3.40870600	2.71505900	-4.57945500
H	-2.51339700	3.51380100	-3.27769400
C	-5.85352000	2.55169000	-3.20722600
H	-6.27595200	3.56133500	-3.26219700
H	-6.51451800	1.94238800	-2.58469600
H	-5.86085300	2.12533900	-4.21653400
C	-4.77601700	2.17530700	2.44162000
H	-4.35626700	1.18047600	2.25548600
C	-6.27802100	2.00999900	2.75074100
H	-6.73983300	2.98861500	2.92354600
H	-6.41041100	1.40768500	3.65663400
H	-6.82245600	1.51625400	1.94246700
C	-4.06943400	2.73469800	3.68639600
H	-4.57174800	3.63348800	4.06151500
H	-3.02403100	2.97851000	3.48840900
H	-4.09727700	1.98764500	4.48644000
N	1.75662100	-0.09884200	0.00882300
N	-4.89456300	-1.11537000	-0.19030300
N	-4.88036700	1.05679800	-0.23480800
Sc	0.48577600	0.33971100	1.51238000
Sc	0.47828700	0.01985100	-1.53473400
Sc	3.67144800	-0.62228700	-0.01031900
H	-6.99976900	1.37237500	-0.41198200

nNHC-Sc₃N@C₈₀-[5,6,6]

C	1.50744200	-1.22428600	-1.79498200
C	0.58103900	-1.21258100	-2.88953100
C	0.09937700	-0.00179800	-3.46805500
C	0.58470200	1.20992500	-2.89248600

C	1.51614800	1.22595800	-1.79996800
C	1.94516000	0.00082100	-1.21076000
C	2.57771000	0.00005700	0.16122200
C	1.99290400	-1.19271700	0.95210000
C	1.51123700	-2.38746500	0.36438100
C	1.37565000	-2.47543000	-1.08764600
C	0.26848800	-3.21481100	-1.72053200
C	-0.20370400	-2.40525000	-2.82977000
C	-1.57149500	-2.37344400	-3.29165200
C	-2.03183700	-1.17692900	-3.91783100
C	-1.19684700	-0.00297900	-4.02273300
C	-2.03141600	1.16953600	-3.91802800
C	-1.56956200	2.36748700	-3.29567100
C	-0.20141500	2.40077600	-2.83303900
C	0.27159600	3.21269800	-1.72527200
C	1.38684000	2.48089000	-1.09420500
C	1.52001000	2.39322000	0.36060500
C	1.99143700	1.19354700	0.94879500
C	1.54403800	0.71788300	2.22790700
C	1.54406900	-0.71598400	2.22879700
C	0.55812000	-1.44319900	2.96937700
C	0.10623300	-2.68387000	2.41978800
C	0.56148400	-3.14444900	1.12926600
C	-0.52352600	-3.88296900	0.51077400
C	-0.72477000	-3.89783000	-0.91776000
C	-2.08610300	-3.88931800	-1.37344800
C	-2.49985500	-3.17437400	-2.56971200
C	-3.84945700	-2.72581800	-2.37742400
C	-4.27509000	-1.47422000	-2.91105900
C	-3.38543200	-0.72784100	-3.73063100
C	-3.38626600	0.71873200	-3.73202100
C	-4.27755400	1.46547500	-2.91593600
C	-3.84766300	2.71667300	-2.38385100
C	-2.49856600	3.16955800	-2.57617800
C	-2.08604900	3.88465200	-1.38045900
C	-0.72468600	3.89058300	-0.92212400
C	-0.52258300	3.87999300	0.50598800
C	0.56497500	3.14586100	1.12552900
C	0.10795500	2.68435100	2.41627800
C	0.55823600	1.44424100	2.96797100
C	-0.34204900	0.72009800	3.79379400
C	-0.34225900	-0.71957100	3.79412200
C	-1.69888000	-1.16646900	3.98433300
C	-2.17661600	-2.35367900	3.35743800

C	-1.24006800	-3.13639400	2.60727900
C	-1.63851100	-3.86212900	1.43118400
C	-2.98615900	-3.82871200	0.96304000
C	-3.19446300	-3.87825700	-0.45121000
C	-4.28226400	-3.16680000	-1.07125200
C	-5.17092000	-2.38070900	-0.27903100
C	-5.71061200	-1.17019200	-0.85575300
C	-5.21225000	-0.71898000	-2.12739800
C	-5.22269700	0.71291900	-2.13308900
C	-5.74115200	1.16860300	-0.86767600
C	-5.17483600	2.36456400	-0.28736400
C	-4.27845500	3.15146500	-1.07530500
C	-3.19273400	3.86737900	-0.45664400
C	-2.98387000	3.82094300	0.95714500
C	-1.63738300	3.86008100	1.42656600
C	-1.23934000	3.13430200	2.60242300
C	-2.17514400	2.35020600	3.35301700
C	-1.69873200	1.16523800	3.98295200
C	-2.53427200	-0.00133800	4.11132400
C	-3.86458100	-0.00349200	3.59942200
C	-4.36518200	-1.22284100	3.05076000
C	-3.53912400	-2.39119100	2.93905200
C	-3.93735800	-3.12408600	1.76082000
C	-5.00723800	-2.40205400	1.13611600
C	-5.27652200	-1.21808700	1.93213200
C	-5.77509900	-0.00755600	1.35739600
C	-6.07481000	-0.00484800	-0.06477200
C	-5.27539900	1.20480700	1.93107400
C	-4.99789300	2.37894900	1.12702300
C	-3.93061200	3.10864000	1.75165400
C	-3.53731000	2.38250800	2.93177100
C	-4.36551000	1.21480900	3.04895900
C	6.25514900	0.67087100	0.24255100
C	6.25257600	-0.68280500	0.23831800
H	7.05021900	-1.40497700	0.26586000
C	4.11198100	-0.00161300	0.15944800
C	4.59392700	-2.49490800	0.03892500
C	4.50276000	-3.02393500	-1.26072400
C	4.25162000	-4.39674200	-1.36376500
H	4.15554400	-4.84834800	-2.34411900
C	4.10141500	-5.18629600	-0.22838100
H	3.89493600	-6.24725300	-0.33403500
C	4.20733600	-4.62635700	1.04261200
H	4.07634400	-5.25388100	1.91671200

C	4.46220500	-3.26248200	1.20810100
C	4.69947600	-2.16997600	-2.50842800
H	4.34876700	-1.15713000	-2.28230600
C	3.89231000	-2.66550600	-3.71823900
H	2.84693400	-2.84782900	-3.46317200
H	4.31380600	-3.58895900	-4.13111700
H	3.92438300	-1.91191500	-4.51199400
C	6.19098300	-2.08177100	-2.88992900
H	6.31515000	-1.46339600	-3.78603500
H	6.58820900	-3.07957400	-3.10749100
H	6.79944800	-1.64192900	-2.09527700
C	4.59560800	-2.65209400	2.59564900
H	4.33762700	-1.59044400	2.52300300
C	6.04744200	-2.75983500	3.10162800
H	6.13484500	-2.31713200	4.09999500
H	6.75433000	-2.24490200	2.44328200
H	6.35454000	-3.80975000	3.16751000
C	3.63349100	-3.27743900	3.61672100
H	3.63555100	-2.68281000	4.53587900
H	3.93699700	-4.29555100	3.88543300
H	2.60963000	-3.31208900	3.23971600
C	4.60367400	2.49031900	0.05135900
C	4.47074200	3.25278300	1.22368900
C	4.22171300	4.61839100	1.06374500
H	4.09021400	5.24232700	1.94032900
C	4.12224000	5.18468500	-0.20495700
H	3.92029900	6.24694200	-0.30626900
C	4.27300200	4.39986300	-1.34356300
H	4.18191800	4.85642400	-2.32210700
C	4.51860200	3.02566500	-1.24612300
C	4.59629000	2.63497700	2.60869800
H	4.33080000	1.57563300	2.53035000
C	3.63614400	3.26243900	3.63033300
H	3.94782600	4.27610800	3.90647100
H	3.62969700	2.66203300	4.54569200
H	2.61386000	3.30864700	3.25015100
C	6.04753100	2.72921400	3.11907800
H	6.36272600	3.77637200	3.19039100
H	6.75210700	2.21139400	2.46053600
H	6.12856600	2.28150500	4.11574700
C	4.71595100	2.17679300	-2.49717600
H	4.36381400	1.16337400	-2.27588300
C	6.20793700	2.08859800	-2.87690100
H	6.60629100	3.08678500	-3.09061000

H	6.33289200	1.47305800	-3.77484000
H	6.81496800	1.64575700	-2.08282100
C	3.91118400	2.67839900	-3.70615100
H	4.33379600	3.60366100	-4.11379200
H	2.86540400	2.85990100	-3.45213400
H	3.94461600	1.92859800	-4.50344300
N	-1.84591000	0.01358900	-0.28917500
N	4.92720900	-1.08848800	0.17408200
N	4.93128100	1.08201900	0.18063900
Sc	-0.54274000	1.53139500	-0.42988700
Sc	-0.58024200	-1.54880900	-0.42963800
Sc	-3.79818000	0.09890600	-0.05266100
H	7.05552200	1.38983100	0.27448500

aNHC-Sc₃N@C₈₀-[6,6,6]

C	1.55394200	0.71775000	-1.24342200
C	0.93086100	1.99733000	-1.20749100
C	0.62789500	2.69939000	0.00126700
C	0.93113400	1.99619200	1.20926200
C	1.55401200	0.71647100	1.24362800
C	2.15297500	0.06115800	-0.00025000
C	1.57464700	-1.32203600	-0.00094700
C	1.16480400	-2.03482100	-1.16746400
C	0.96089500	-1.40729600	-2.44640200
C	1.19622600	0.03604100	-2.46314200
C	0.26399900	0.92212700	-3.17138500
C	0.11661300	2.12026700	-2.37752200
C	-1.07293100	2.92500100	-2.35538000
C	-1.34764900	3.66098100	-1.16897300
C	-0.51001400	3.53681400	0.00177200
C	-1.34751100	3.65976500	1.17276800
C	-1.07264700	2.92248500	2.35835000
C	0.11693700	2.11785300	2.37949100
C	0.26415400	0.91871300	3.17183300
C	1.19620100	0.03339300	2.46250200
C	0.96115000	-1.40990800	2.44450600
C	1.16486300	-2.03603300	1.16486700
C	0.44292800	-3.20975100	0.70988100
C	0.44286800	-3.20901000	-0.71365100
C	-0.68133600	-3.68047100	-1.45690000
C	-0.95764300	-3.02626100	-2.70481600
C	-0.16077100	-1.91405400	-3.19472500
C	-1.06632100	-1.02109500	-3.90816400
C	-0.89262700	0.40851800	-3.87766200

C	-2.07550200	1.21188600	-3.87672600
C	-2.15589800	2.47078700	-3.15852800
C	-3.50631900	2.64574100	-2.71674800
C	-3.77814500	3.27840100	-1.46613800
C	-2.70579100	3.83423500	-0.72160200
C	-2.70568400	3.83345600	0.72578700
C	-3.77793500	3.27677700	1.46988300
C	-3.50602000	2.64282000	2.71979800
C	-2.15552900	2.46738300	3.16113700
C	-2.07506000	1.20776000	3.87804600
C	-0.89220400	0.40440900	3.87793600
C	-1.06580300	-1.02527100	3.90711200
C	-0.16030700	-1.91749800	3.19263700
C	-0.95733400	-3.02901600	2.70143500
C	-0.68117000	-3.68198000	1.45279700
C	-1.76283800	-4.23640000	0.72148500
C	-1.76292400	-4.23563600	-0.72597800
C	-3.11900600	-4.05372300	-1.16891800
C	-3.41101700	-3.32082900	-2.35623200
C	-2.31155000	-2.84211400	-3.14025700
C	-2.38888300	-1.60980000	-3.87833700
C	-3.56322600	-0.79934300	-3.83214400
C	-3.39178700	0.61836600	-3.87444400
C	-4.27349800	1.50327000	-3.16148800
C	-5.34064000	0.97677800	-2.37201800
C	-5.71641500	1.67874900	-1.16799500
C	-4.89281100	2.76856200	-0.71338100
C	-4.89258100	2.76768500	0.71670200
C	-5.71580700	1.67718900	1.17020800
C	-5.34034700	0.97416800	2.37373500
C	-4.27319700	1.49994600	3.16357200
C	-3.39137600	0.61428700	3.87545200
C	-3.56281500	-0.80337800	3.83160300
C	-2.38841100	-1.61385900	3.87666600
C	-2.31118700	-2.84537200	3.13725500
C	-3.41077400	-3.32332200	2.35294500
C	-3.11888000	-4.05497300	1.16482500
C	-3.95735800	-3.95641700	-0.00192700
C	-5.10318300	-3.11140000	-0.00137300
C	-5.44207000	-2.45087900	-1.22104300
C	-4.61498700	-2.55636200	-2.38960500
C	-4.68982600	-1.31710400	-3.12109700
C	-5.55121000	-0.43247600	-2.39250600
C	-6.02258600	-1.13177900	-1.21184100

C	-6.34897900	-0.44694700	0.00016400
C	-6.26066700	1.00244500	0.00085900
C	-6.02249600	-1.13304500	1.21139600
C	-5.55115500	-0.43506500	2.39290800
C	-4.68958900	-1.32045200	3.12029800
C	-4.61475700	-2.55894600	2.38738800
C	-5.44193200	-2.45217000	1.21904000
C	3.66467300	-0.00261000	-0.00035200
C	4.45909000	-1.11632200	-0.00108800
H	4.19726800	-2.16104000	-0.00177100
C	5.80157700	0.64232000	0.00013200
H	6.68772000	1.25353700	0.00061500
C	6.94191400	-1.54877500	-0.00094900
C	7.46277900	-1.95053400	1.23910900
C	8.57546800	-2.79783100	1.20905000
H	9.01229000	-3.13594900	2.14322500
C	9.12452800	-3.21570600	-0.00137500
H	9.98666800	-3.87599700	-0.00154300
C	8.57599000	-2.79652800	-1.21158500
H	9.01321400	-3.13364200	-2.14593400
C	7.46330800	-1.94920100	-1.24121200
C	6.84899800	-1.51430300	2.56129600
H	6.04414900	-0.80223400	2.35286000
C	7.87537100	-0.79223500	3.44991000
H	8.30364000	0.07674400	2.93872700
H	8.69983700	-1.45567000	3.73271600
H	7.39677000	-0.44442800	4.37152600
C	6.21553400	-2.71215400	3.29102200
H	5.73748200	-2.38155400	4.21926200
H	6.97011800	-3.46395500	3.54742100
H	5.45473400	-3.19712100	2.67038200
C	6.85010100	-1.51157100	-2.56320000
H	6.04471900	-0.80023500	-2.35432700
C	6.21776900	-2.70878500	-3.29494400
H	5.74015300	-2.37718900	-4.22305300
H	5.45682200	-3.19499700	-2.67545800
H	6.97291000	-3.45984600	-3.55186900
C	7.87664800	-0.78772600	-3.45016800
H	7.39847700	-0.43896000	-4.37164500
H	8.70169300	-1.45031200	-3.73328000
H	8.30406500	0.08081900	-2.93752900
C	4.18612000	2.49785100	0.00140000
C	4.02794300	3.13652700	-1.23975600
C	3.68181400	4.49067500	-1.20744500

H	3.53350100	5.02549800	-2.13827000
C	3.50521100	5.15506300	0.00368600
H	3.22093700	6.20300100	0.00458400
C	3.68246100	4.48876800	1.21366800
H	3.53465200	5.02210500	2.14542900
C	4.02855800	3.13455800	1.24363300
C	4.26836300	2.40498200	-2.55421100
H	4.00587300	1.35188800	-2.40541200
C	5.75706700	2.48008100	-2.94971500
H	6.06073500	3.52120000	-3.10649000
H	5.93197400	1.93090500	-3.88153500
H	6.41522400	2.05583200	-2.18412100
C	3.39750800	2.92129600	-3.70804500
H	3.70703900	3.92163700	-4.03136800
H	2.34257000	2.95745500	-3.42918500
H	3.49835700	2.25400000	-4.57004800
C	4.26946600	2.40094200	2.55683000
H	4.00746500	1.34796700	2.40633000
C	3.39843900	2.91494500	3.71156900
H	3.70760100	3.91484600	4.03659500
H	3.49956100	2.24621500	4.57242800
H	2.34349000	2.95119500	3.43277400
C	5.75817500	2.47612000	2.95229200
H	6.06129800	3.51711800	3.11092300
H	6.41647300	2.05364000	2.18583300
H	5.93349800	1.92534500	3.88308700
N	-2.13452700	-0.08226900	-0.00026800
N	5.78021100	-0.69344700	-0.00070000
N	4.53801300	1.09116200	0.00027700
Sc	-0.85085900	-0.31977900	1.53373700
Sc	-0.85014700	-0.31692300	-1.53381300
Sc	-4.06409900	0.37387400	-0.00144100

aNHC-Sc₃N@C₈₀-[5,6,6]

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C	0.25623100	-0.67305800	-3.00965300
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C	0.09795600	1.70606500	-2.55118500
C	1.02977100	1.56943800	-1.47141000
C	1.53311900	0.28323400	-1.12042400
C	2.18068600	0.06292100	0.22150000
C	1.66190600	-1.27557700	0.77163500
C	1.30334900	-2.38981900	-0.02719200
C	1.16193600	-2.20869600	-1.47919400

C	0.07051300	-2.86935500	-2.22559900
C	-0.46248300	-1.89728100	-3.16326800
C	-1.83520200	-1.86263600	-3.61015700
C	-2.37644900	-0.60147400	-4.00103300
C	-1.61509700	0.61839000	-3.88645700
C	-2.51762300	1.69981300	-3.56555200
C	-2.12317000	2.78691000	-2.72912100
C	-0.75440700	2.81806500	-2.27098700
C	-0.31776500	3.43439000	-1.03006500
C	0.83696300	2.65736100	-0.54605700
C	1.00228800	2.30980400	0.86588500
C	1.56981300	1.06253300	1.22719100
C	1.15711900	0.33071800	2.39314500
C	1.22645700	-1.07641200	2.12258900
C	0.30395800	-1.99108900	2.71810500
C	-0.07370100	-3.13302900	1.94189400
C	0.39727800	-3.32508900	0.58827600
C	-0.65568800	-3.99078700	-0.15626700
C	-0.87522400	-3.74027300	-1.55985600
C	-2.23833400	-3.73628800	-2.01073700
C	-2.70570900	-2.83880100	-3.05164000
C	-4.07767300	-2.51272300	-2.77948400
C	-4.58951700	-1.21437400	-3.07160100
C	-3.75369800	-0.27641900	-3.73431800
C	-3.83913800	1.14207800	-3.46378800
C	-4.76281100	1.66846300	-2.52035000
C	-4.40722200	2.82345800	-1.76379000
C	-3.08937000	3.38200800	-1.87071100
C	-2.70442400	3.88633400	-0.56270400
C	-1.34069900	3.89348400	-0.11399900
C	-1.12142500	3.62496100	1.28693100
C	0.01415300	2.85323500	1.75836600
C	-0.39539000	2.13763100	2.94400800
C	0.13809100	0.84751100	3.25725300
C	-0.71187900	-0.07299700	3.92760100
C	-0.62713100	-1.48678400	3.66360200
C	-1.95249800	-2.04032300	3.76604600
C	-2.36325600	-3.11353200	2.92420200
C	-1.39166900	-3.68554700	2.04002900
C	-1.75957500	-4.20484200	0.75088700
C	-3.11137000	-4.16281900	0.29700900
C	-3.33358700	-3.96031600	-1.10069400
C	-4.46742000	-3.20925600	-1.57506000
C	-5.40181600	-2.63816600	-0.65525600

C	-6.04624400	-1.39264900	-1.00341900
C	-5.57007400	-0.67929400	-2.16223200
C	-5.64260800	0.72457900	-1.88978700
C	-6.14859000	0.90116400	-0.55560000
C	-5.67983400	2.01662700	0.23507500
C	-4.84943000	2.98799300	-0.39828000
C	-3.79877300	3.63787000	0.34223700
C	-3.57064600	3.33938800	1.72275200
C	-2.22150400	3.36544800	2.18741000
C	-1.76564600	2.46185500	3.20975000
C	-2.64540000	1.49828600	3.80069800
C	-2.09052000	0.24699600	4.19687800
C	-2.85431000	-0.96983000	4.10564000
C	-4.18782200	-0.95405200	3.60387000
C	-4.62151700	-2.07828500	2.83758500
C	-3.72585000	-3.15049000	2.50420300
C	-4.08946800	-3.66826900	1.21000300
C	-5.20510500	-2.90080700	0.73226500
C	-5.54305400	-1.91610300	1.74104700
C	-6.11967800	-0.65085700	1.40283100
C	-6.43452400	-0.40936700	0.00512800
C	-5.68987400	0.46056500	2.19260200
C	-5.50099900	1.78544500	1.62926000
C	-4.46898500	2.44291700	2.37626500
C	-4.01267700	1.52989300	3.39765700
C	-4.76684300	0.31334600	3.29175900
C	4.49796100	-1.06091900	0.46840400
C	3.69401600	0.01257400	0.19442100
C	5.82436300	0.60817900	-0.11747600
C	4.20872800	2.38448500	-0.61508500
C	4.04500200	2.58932900	-1.99524600
C	3.71084900	3.88498200	-2.40051000
H	3.56097400	4.09363300	-3.45370600
C	3.54956300	4.90537300	-1.46671400
H	3.27574900	5.90127600	-1.80204600
C	3.72823400	4.66238100	-0.10660400
H	3.59026200	5.46958400	0.60335000
C	4.06443800	3.38699600	0.35702900
C	4.26667200	1.47066800	-3.00600500
H	4.05943400	0.51785600	-2.50587300
C	5.73362700	1.45512100	-3.48133000
H	6.44077400	1.33446600	-2.65398100
H	5.98036800	2.39308100	-3.99107800
H	5.89820300	0.63171600	-4.18500100

C	3.33083200	1.54841700	-4.22095700
H	3.44230400	0.64388500	-4.82776000
H	3.57256400	2.40317200	-4.86236600
H	2.28484500	1.63009900	-3.92093600
C	4.30260100	3.10519100	1.83508800
H	4.01582200	2.06540100	2.02601800
C	3.45208000	3.97804200	2.76829000
H	3.56345900	3.62659200	3.79916200
H	2.39246400	3.93095200	2.50700400
H	3.77057200	5.02638600	2.74529900
C	5.79695900	3.26441100	2.18015900
H	5.97029000	3.03486500	3.23739000
H	6.12706600	4.29312200	1.99669800
H	6.43456500	2.60118600	1.58587400
C	6.97024700	-1.52792100	0.36287200
C	7.67664000	-1.56149600	1.57396000
C	8.78318900	-2.41622800	1.63328600
H	9.36421300	-2.47339800	2.54820000
C	9.14261400	-3.19718100	0.53777800
H	10.00127000	-3.85840200	0.60715200
C	8.41036000	-3.14008400	-0.64697900
H	8.70411700	-3.75827600	-1.48867000
C	7.30145100	-2.29657800	-0.76636500
C	7.28164700	-0.71025400	2.77124300
H	6.34874600	-0.18955700	2.53216800
C	8.34827000	0.36150100	3.05642500
H	9.30712300	-0.09623300	3.32388600
H	8.03439100	1.00013900	3.88897900
H	8.51647400	1.00033000	2.18220200
C	7.00947000	-1.57568400	4.01294700
H	7.91325000	-2.09875700	4.34381500
H	6.23954800	-2.32728300	3.81055300
H	6.66468800	-0.94828100	4.84155800
C	6.47898700	-2.24923800	-2.04696200
H	5.83943000	-1.36108700	-2.01456200
C	5.55018200	-3.47456200	-2.14041900
H	6.13126500	-4.40300600	-2.16954700
H	4.94143300	-3.42221100	-3.04933600
H	4.86964700	-3.52883400	-1.28465600
C	7.35746100	-2.11995400	-3.30098600
H	7.97258800	-3.01166300	-3.46191700
H	8.02567500	-1.25491500	-3.23360900
H	6.72441800	-1.99590400	-4.18596500
N	-2.21641900	-0.13595000	-0.21974100

N	4.55994300	1.04990900	-0.17300300
N	5.81328600	-0.67115500	0.26776700
Sc	-1.05564900	1.51026000	-0.08050900
Sc	-0.79551000	-1.49568700	-0.62631500
Sc	-4.15319000	-0.39955400	-0.00738000
H	4.24359500	-2.05959100	0.77928600
H	6.70192300	1.18419600	-0.35596100