

Electronic Supplementary Information

Graphane versus Graphene: A Computational Investigation of the Interaction of Nucleobases, Aminoacids, Heterocycles, Small Molecules (CO₂, H₂O, NH₃, CH₄, H₂), Metal Ions and Onium Ions

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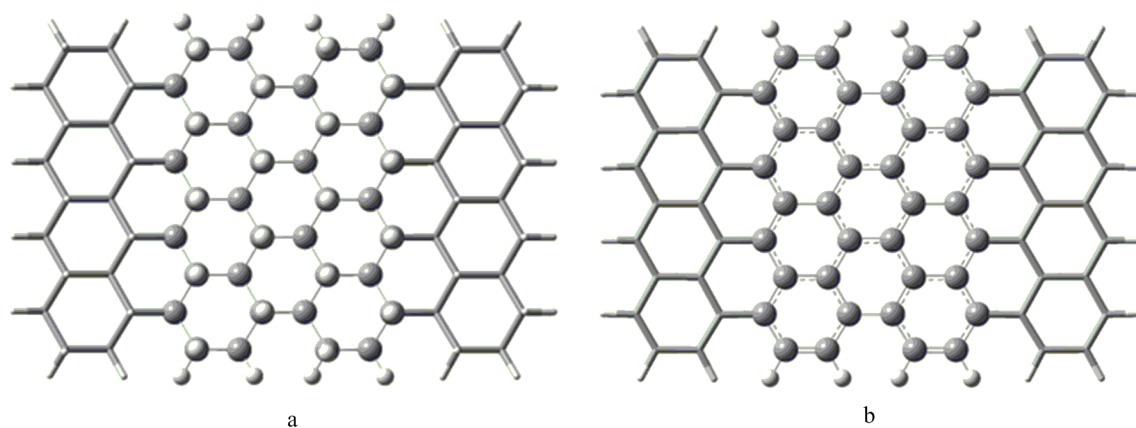


Fig. S1: The atoms shown by the ball-and-stick model were considered for the higher layer and the rest of the atoms shown by the tube model were considered for the lower layer in the ONIOM calculation for (a) graphane and (b) graphene.

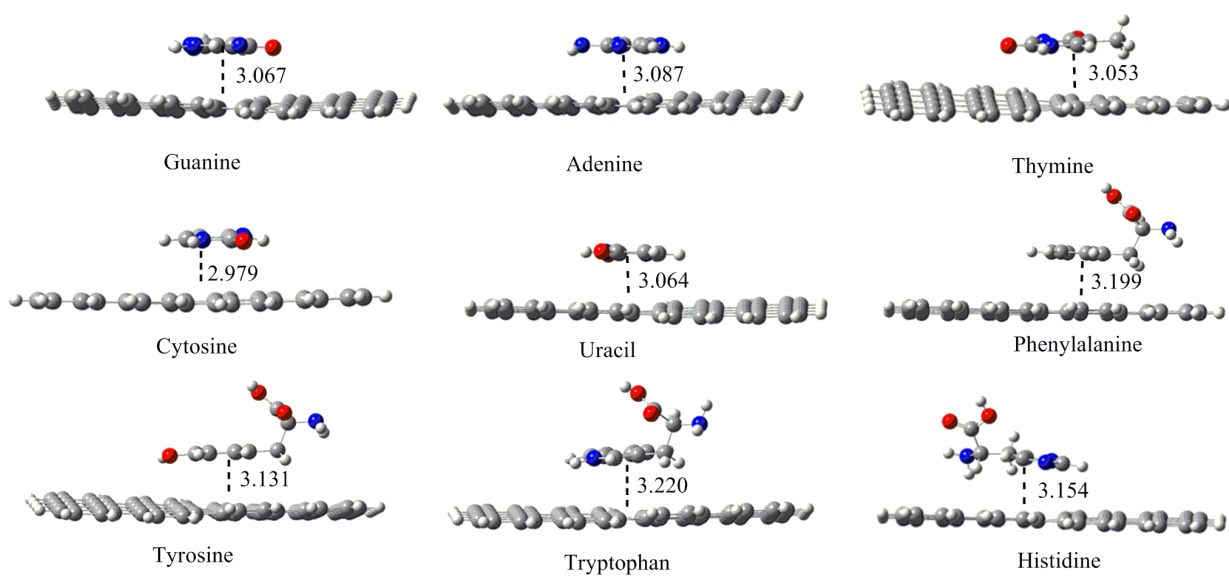


Fig. S2: Optimized structures and distances (\AA) of the complexes of graphene with nucleobases and aminoacids.

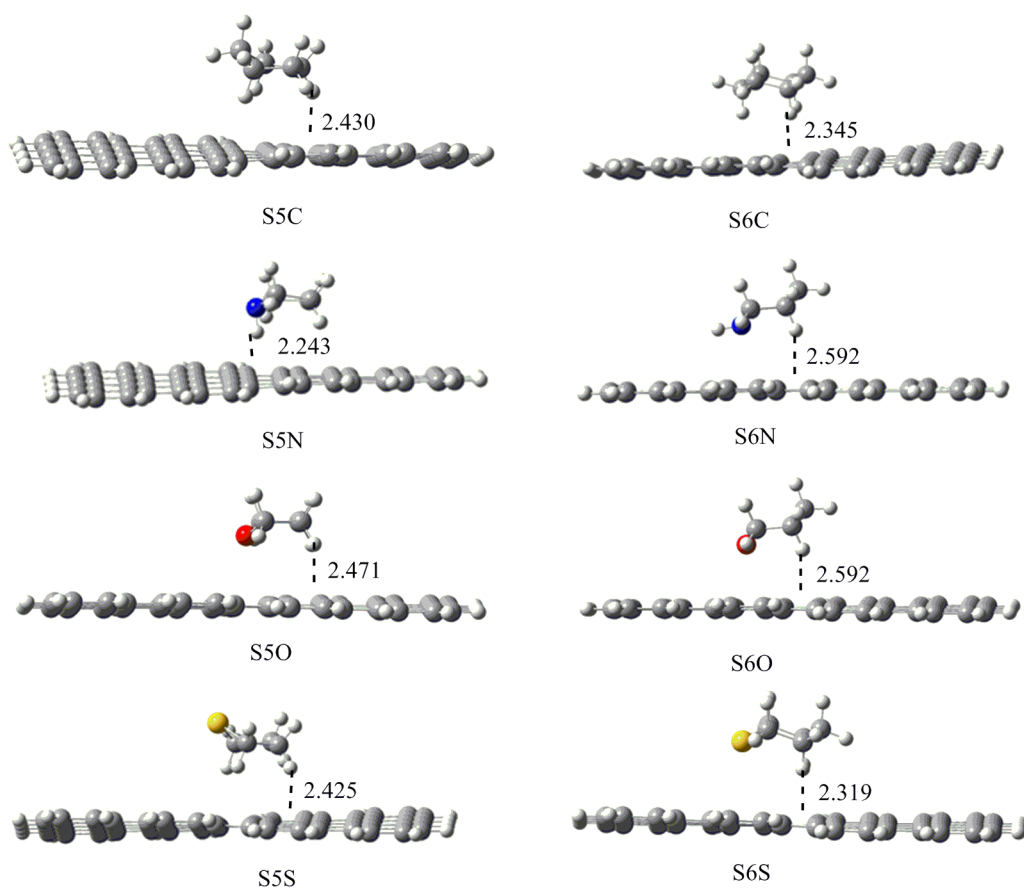


Fig. S3: Optimized structures and distances (Å) of the complexes of graphene with various saturated heterocyclic compounds.

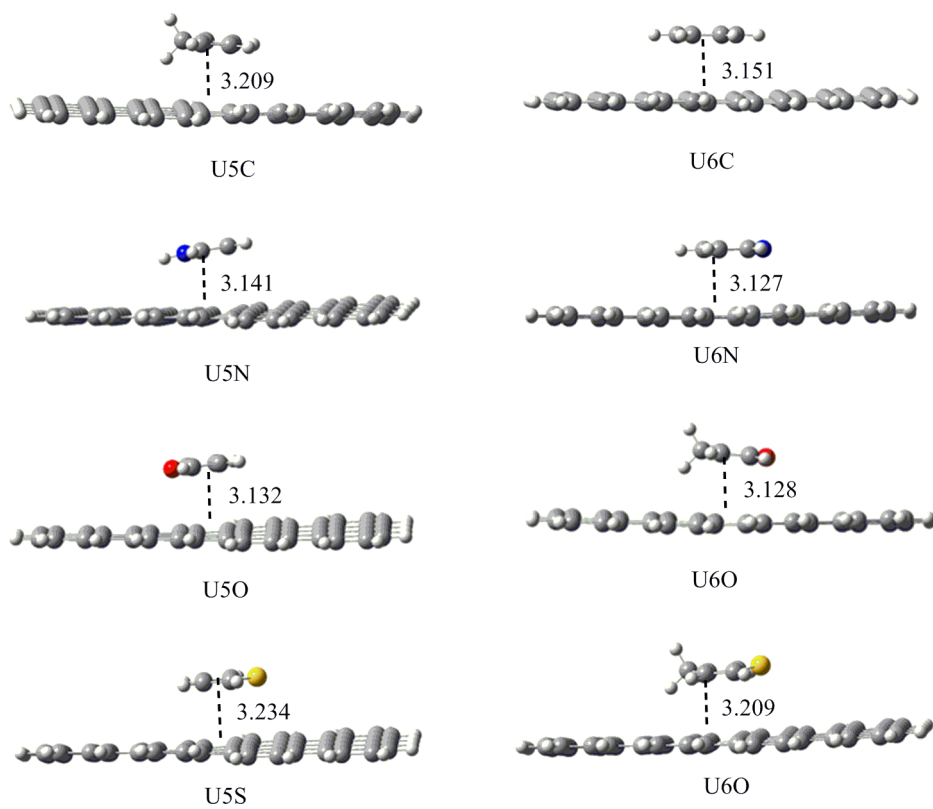


Fig. S4: Optimized structures and distances (\AA) of the complexes of graphene with various unsaturated heterocyclic compounds.

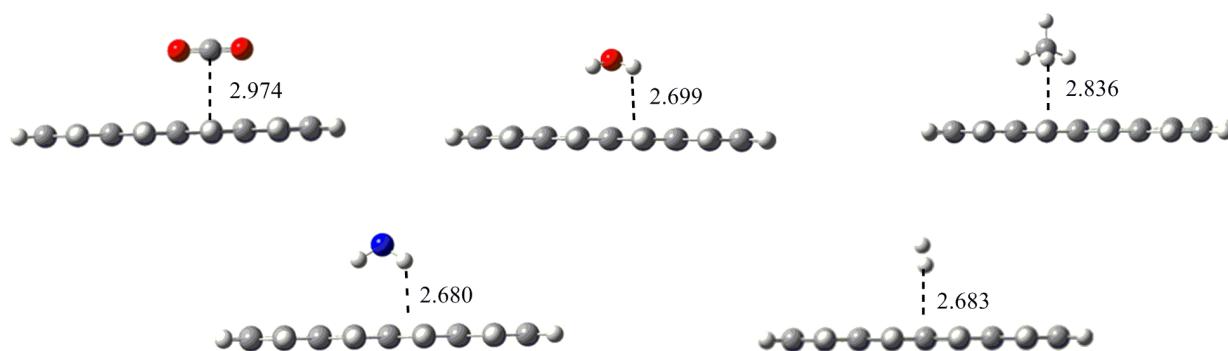


Fig. S5: Optimized structures and distances (\AA) of the complexes of graphene with small molecules.

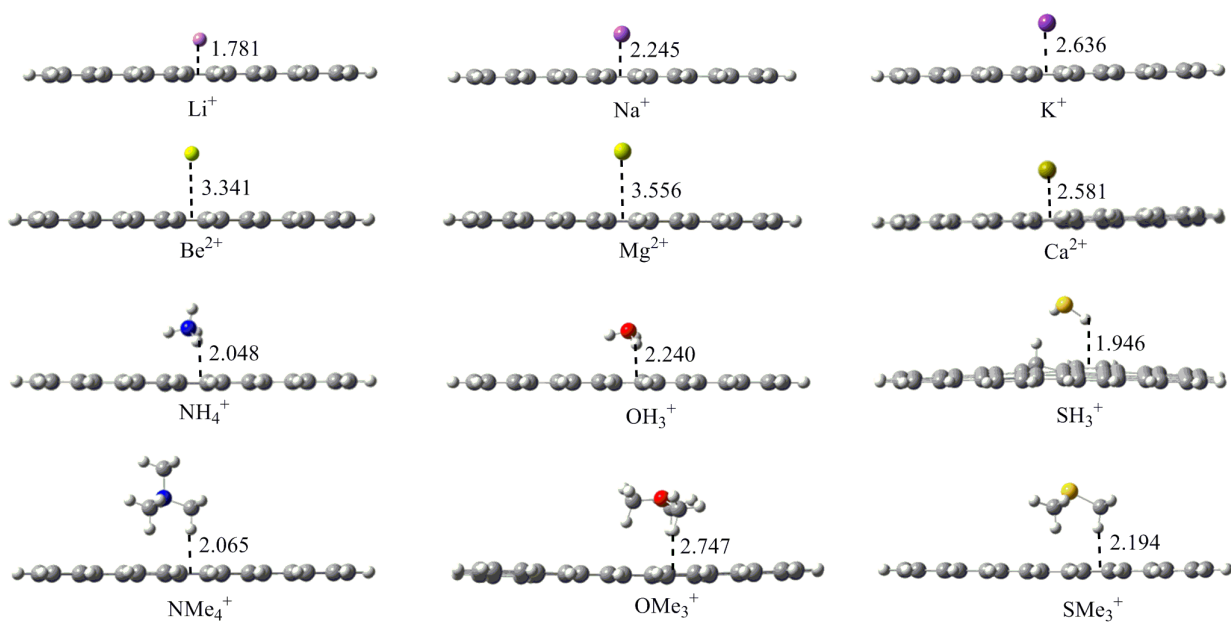


Fig. S6: Optimized structures and distances (Å) of the complexes of graphene with cations.

Table S1 Binding energy (kcal/mol), charge transfer (amu) and HOMO-LUMO energy gap (eV) of graphene complexes with biomolecules

Biomolecules	Binding energy	Charge transfer	HOMO-LUMO energy gap
Nucleobases			
G	21.21	-0.014	0.76
A	19.14	-0.007	0.78
T	18.62	-0.004	0.76
C	18.08	-0.007	0.76
U	16.38	-0.001	0.76
Aminoacids			
PHE	15.98	0.006	0.76
TYR	19.23	-0.001	0.76
TRP	20.38	-0.002	0.75
HIS	17.80	-0.006	0.77

Table S2 Binding energy (kcal/mol), charge transfer (amu) and HOMO-LUMO energy gap (eV) of graphene complexes with heterocyclic compounds

Heterocycles	Binding energy	Charge transfer	HOMO-LUMO energy gap
Unsaturated			
U5C	10.40	0.003	0.78
U5N	10.69	-0.005	0.76
U5O	9.42	-0.002	0.78
U5S	10.32	-0.003	0.77
U6C	11.24	0.004	0.77
U6N	11.13	0.005	0.76
U6O	12.58	-0.001	0.77
U6S	14.14	-0.005	0.77
Saturated			
S5C	8.38	0.002	0.79
S5N	9.00	-0.001	0.78
S5O	10.66	-0.007	0.77
S5S	9.09	0.001	0.77
S6C	8.13	0.004	0.78
S6N	10.96	-0.008	0.77
S6O	11.13	-0.005	0.77
S6S	8.83	-0.002	0.76

Table S3 Binding energy (kcal/mol), charge transfer (amu) and HOMO-LUMO energy gap (eV) of graphene complexes with small molecules

Small molecules	Binding energy	Charge transfer	HOMO-LUMO energy gap
CO ₂	4.57	-0.001	0.78
H ₂ O	4.69	-0.005	0.77
CH ₄	3.49	0.000	0.78
NH ₃	3.78	-0.004	0.77
H ₂	1.55	0.001	0.78

Table S4 Binding energy (kcal/mol), charge transfer (amu) and HOMO-LUMO energy gap (eV) of graphene complexes with cations

Cations	Binding energy	Charge transfer	HOMO-LUMO energy gap
Metal ions			
Li ⁺	55.30	0.063	0.69
Na ⁺	40.14	0.021	0.69
K ⁺	33.18	0.022	0.69
Be ²⁺	355.89	2.006	2.66
Mg ²⁺	253.35	2.002	1.59
Ca ²⁺	151.55	1.046	0.92
Onium ions			
NH ₄ ⁺	33.08	0.016	0.69
NMe ₄ ⁺	25.62	0.015	0.69
OH ₃ ⁺	44.20	0.044	0.70
OMe ₃ ⁺	28.50	0.017	0.69
SMe ₃ ⁺	27.59	0.017	0.68

XYZ coordinates (in Å) of graphane complexes optimized at ONIOM (M06-2X/6-31G*/PM6) level.

Graphane-His

C	5.20203500	-1.04925300	-0.84130500
C	5.90776700	-2.35227100	-0.39580100
C	3.72181400	-1.06646000	-0.40853500
C	8.11163700	-1.10609300	-0.25294300
C	7.39429900	-2.33694700	-0.83371500
C	5.19669200	-3.58881100	-0.99694600
C	3.00943800	-2.29157800	-1.00023900
C	8.10645500	-3.62716800	-0.38296000
C	5.91130100	-4.87316100	-0.52422100
C	3.70654800	-3.60621700	-0.60133300
C	1.52907700	-2.31000300	-0.58331000
C	7.39013100	-4.86743600	-0.92939300
H	5.82377500	-4.97105200	0.57398000
C	2.97733800	-4.79745000	-1.23671800
C	0.81233900	-0.99905400	-0.94592900
C	0.78027100	-3.52455300	-1.15515100
H	7.88605000	-5.78366400	-0.55816100
C	1.51306000	-4.82630400	-0.81960300
H	3.03867600	-4.71571100	-2.33080100
C	-0.65799000	-1.02263000	-0.49398900
C	-0.67400100	-3.54252900	-0.66277800
H	1.02065400	-5.67392200	-1.30446600
C	-1.40423500	-2.24755700	-1.04889700
C	-1.43508600	-4.78023600	-1.14451900
C	-2.87203600	-2.26826500	-0.58774800
C	-2.88873600	-4.77789600	-0.68977800
H	-1.38617300	-4.82771100	-2.24446000
C	-3.57337300	-0.95629500	-0.96481200
C	-3.60438300	-3.50145100	-1.15074100
H	-3.39645900	-5.67124900	-1.07485300
C	-5.04144600	-0.98218700	-0.49219700
C	-5.08427200	-3.51406800	-0.71716800
C	-5.78277100	-2.19075500	-1.11202200
C	-5.83499200	-4.70315100	-1.35462300
C	-7.25939600	-2.21602300	-0.64274200
H	-5.34425200	-5.65418900	-1.07121300
C	-7.30483800	-4.73158800	-0.91954000
C	-8.00637200	-3.41251700	-1.26363100
C	-7.96290500	-0.89973100	-1.01667100
H	-7.82632300	-5.57547200	-1.40795000
C	-7.93946400	4.12817500	-0.56189900
C	-7.94077400	1.61324800	-0.78087900
C	-7.21283000	5.35039500	0.01095100
C	-7.21337400	2.82547000	-0.17374900
C	-7.22702500	0.30377900	-0.40211300

C	-5.74539500	5.37582300	-0.43261400
H	-7.72059100	6.27769800	-0.31352200
C	-5.73796000	2.86006900	-0.64611300
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C	-2.79106200	5.28871500	0.17897700
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H	5.89408600	0.10440000	0.87373000
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H	5.27000800	-3.53478000	-2.11015100
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H	7.43604900	-2.28170700	-1.94855900
H	7.47269400	2.79929000	-1.63398700
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H	-0.04651200	1.88239700	3.54752400
C	-0.32437800	-0.12594900	3.44592000
H	-1.07810900	-0.20196000	2.63750300
C	0.55617600	-1.37928000	3.40728800
C	-1.13151000	0.04291000	4.72678200
H	1.31735000	-1.20905200	2.63195800
H	1.09675600	-1.45620600	4.35845600
C	-0.17822000	-2.64800700	3.10397400
O	-1.58414900	1.10207400	5.08423400
N	0.48607000	-3.83332800	2.87419000
C	-1.50621800	-2.98074900	3.00005000
H	1.48871500	-3.95618800	2.85856100
C	-0.45035000	-4.80009800	2.65511000
N	-1.66524500	-4.31755300	2.72267800
H	-2.36060000	-2.33175300	3.13601100
H	-0.18415100	-5.82670000	2.44323000
H	0.87517200	1.15114500	2.40076400
O	-1.31276900	-1.09415000	5.41217600
H	-1.86046100	-0.87024900	6.18575400

Graphane-Phe

C	-4.98270300	1.66819200	-0.83017600
C	-5.72109300	2.84632900	-0.15076900
C	-3.52285800	1.58976200	-0.33684100
C	-7.91664900	1.59960300	-0.37177400
C	-7.18534000	2.92393400	-0.65199000

C	-4.99323200	4.18169600	-0.43790700
C	-2.79640200	2.91572700	-0.60714900
C	-7.93103800	4.09235100	0.02166700
C	-5.74504800	5.33841500	0.25508600
C	-3.52791100	4.10898600	0.03741100
C	-1.34030200	2.83643800	-0.11704300
C	-7.20099700	5.41865400	-0.21873100
H	-5.71388000	5.20350400	1.35260300
C	-2.77897500	5.41158200	-0.27329700
C	-0.59505400	1.64386200	-0.74081400
C	-0.57833400	4.15043500	-0.35592700
H	-7.72412400	6.23826600	0.30813700
C	-1.34149700	5.34412800	0.22467500
H	-2.77831000	5.57924000	-1.35945200
C	0.85393700	1.55985900	-0.23166100
C	0.85199300	4.05792300	0.19564700
H	-0.83388400	6.27910700	-0.02981900
C	1.61125400	2.88163800	-0.44110200
C	1.62527000	5.36910400	0.02621300
C	3.05895900	2.79271600	0.07246000
C	3.05632200	5.26693800	0.53649800
H	1.63241000	5.64249800	-1.04057700
C	3.78891700	1.60801000	-0.57760300
C	3.80572000	4.12122900	-0.15653300
H	3.57332400	6.22239500	0.38414000
C	5.23630600	1.51939600	-0.05051200
C	5.26346200	4.03280800	0.33869900
C	5.99200600	2.84106100	-0.32788700
C	6.02976200	5.33883500	0.03697800
C	7.44661400	2.75252400	0.19893200
H	5.51810600	6.19745200	0.51211000
C	7.47836600	5.26210500	0.53315800
C	8.20768200	4.06265500	-0.08284300
C	8.17911200	1.56546200	-0.45006200
H	8.01233000	6.19764800	0.28257400
C	8.18897300	-3.41884200	-1.24140400
C	8.17283000	-0.92781600	-0.83558900
C	7.45103000	-4.74431900	-1.02161900
C	7.43257900	-2.25162500	-0.57785700
C	7.42929000	0.24917800	-0.18048600
C	6.00510200	-4.65826600	-1.52412500
H	7.98251700	-5.56279700	-1.54207700
C	5.97962300	-2.16772300	-1.10998700
C	5.97869800	0.33609700	-0.71488800
C	5.24241700	-3.50208200	-0.84205700
H	5.99667500	-4.51853900	-2.62166900
C	5.22937300	-0.98973500	-0.44348800
C	3.78743200	-3.42531800	-1.34750100
C	3.78272800	-0.90465700	-0.97333800
C	3.02856900	-4.72539500	-1.04987900

C	3.04563500	-2.22830600	-0.72098700
C	3.04369100	0.28455600	-0.33822700
C	1.59948600	-4.65240100	-1.57074300
H	3.54239800	-5.58871200	-1.49016200
C	1.59694800	-2.14614200	-1.23410500
C	1.60078400	0.37076300	-0.85710600
C	0.83477000	-3.45940300	-0.99146800
H	1.61002700	-4.57129000	-2.66882700
C	0.84720800	-0.94854200	-0.62588000
C	-0.60337500	-3.37424400	-1.52204700
C	-0.60297100	-0.86678700	-1.13080500
C	-1.36935300	-4.68333300	-1.30808100
C	-1.35188800	-2.18840500	-0.89006500
C	-1.34266300	0.32304500	-0.49821800
C	-2.81183300	-4.59541200	-1.78658400
H	-0.87246700	-5.50613500	-1.83047500
C	-2.81229300	-2.11242800	-1.36831100
C	-2.79594400	0.40161600	-0.98760600
C	-3.54772200	-3.43916500	-1.09717600
H	-2.82260500	-4.43543400	-2.87388600
C	-3.52922500	-0.92172700	-0.71469000
C	-5.01703200	-3.36388100	-1.55891500
C	-4.99051200	-0.84490300	-1.20398700
C	-5.77120600	-4.66805700	-1.22117700
C	-5.73426800	-2.16560700	-0.89202000
C	-5.72087500	0.34181000	-0.53234200
C	-7.23074800	-4.60313700	-1.68600000
H	-5.26731600	-5.53194700	-1.69497700
C	-7.20093800	-2.08878400	-1.38629300
C	-7.18371400	0.41965200	-1.03377500
C	-7.95062900	-3.39778000	-1.07041200
H	-7.27277600	-4.54430900	-2.79051500
C	-7.92328400	-0.89639000	-0.73552500
H	8.31728500	4.21086300	-1.17375400
H	8.28090700	1.72978100	-1.53899600
H	9.20319500	-0.98898100	-0.44023700
H	9.21408400	-3.48483300	-0.83327900
H	-8.03537500	-3.53180900	0.02456900
H	-8.96228100	-0.83691300	-1.10774900
H	-7.99881400	1.43324200	0.71843100
H	-8.96427300	4.15404900	-0.36601200
H	0.79789500	-1.10779400	0.46715300
H	0.80463100	1.37822300	0.85738300
H	-1.36902600	0.15329300	0.59353900
H	1.64933000	0.54246200	-1.94918500
H	-0.56917600	-0.69774600	-2.22369500
H	-0.55721100	1.81229400	-1.83372400
H	1.64494900	-1.98824400	-2.32831500
H	2.99770900	-2.39231700	0.37079000
H	3.81175100	-0.73773200	-2.07002200

H	2.98817700	0.11199800	0.75144100
H	3.81643200	1.78564000	-1.67273700
H	3.01053200	2.61107200	1.16046700
H	1.66040700	3.07168800	-1.53015900
H	0.77665200	3.85128500	1.27927000
H	-0.50616300	4.29793200	-1.44872200
H	-1.37362900	2.66582200	0.97561600
H	0.77396800	-3.60506800	0.10205300
H	-0.54936600	-3.18916800	-2.61012000
H	-1.37531200	-2.35517500	0.20419600
H	-2.79422200	-1.94819400	-2.45985200
H	-3.52412300	-1.08513600	0.38282500
H	-2.77118600	0.56676700	-2.07888900
H	-3.52143800	1.42037300	0.75991200
H	-2.77041300	3.08104000	-1.69833000
H	5.20686200	1.34945800	1.05211300
H	6.02330600	3.01186400	-1.42964600
H	5.25806800	3.87462900	1.44394400
H	3.80812900	4.31752500	-1.24745200
H	6.01531500	5.54058100	-1.05075000
H	7.49559800	5.18790100	1.63744900
H	9.23464200	3.99700000	0.32046800
H	7.41577200	2.59301700	1.30393000
H	9.21018900	1.49873100	-0.05757500
H	6.01541400	0.50847800	-1.81644800
H	7.39462100	0.07866100	0.92297100
H	8.27688300	-0.75472500	-1.92296400
H	7.39845100	-2.43392300	0.52349500
H	6.01473700	-1.99353800	-2.21115000
H	5.19867300	-1.16331800	0.65845200
H	8.30407000	-3.22930900	-2.32534800
H	7.46237300	-5.00904000	0.05312200
H	5.48776900	-5.61824800	-1.33601900
H	5.23160600	-3.68861400	0.25853900
H	3.79592400	-3.27316400	-2.44527700
H	-3.52293900	-3.61542800	-0.00249700
H	-5.03810600	-3.22107000	-2.66612600
H	-8.98646600	-3.34113700	-1.45165400
H	-7.75545400	-5.53693200	-1.41051100
H	-5.73157700	-4.85417400	-0.13118100
H	-3.32173100	-5.54948800	-1.60463200
H	-1.35229600	-4.93326400	-0.23489400
H	1.08631800	-5.58731700	-1.32842500
H	3.00807000	-4.89357400	0.03689500
H	-8.00250700	-1.04948200	0.35686200
H	-8.95469400	1.65576600	-0.74722600
H	-8.02359100	3.90735100	1.10846500
H	-7.23390700	5.67791200	-1.29439200
H	-5.23394100	6.29873500	0.05192500
H	-3.28705100	6.27346300	0.17675000

H	-1.33578500	5.26906200	1.32372000
H	1.11772800	6.18099100	0.55546700
H	3.04157900	5.08746900	1.62074800
H	-5.73963400	-2.32212300	0.21223000
H	-4.99045300	-0.68632100	-2.30870200
H	-5.73158600	0.17780900	0.57090400
H	-4.97944100	1.83649100	-1.93344500
H	-5.73205700	2.67535200	0.95118400
H	-5.00426900	4.36442600	-1.53939500
H	-3.51359200	3.95377700	1.13559900
H	-7.17465900	0.58083800	-2.13910200
H	-7.17485400	3.10072400	-1.75470900
H	-7.19589900	-1.94307800	-2.49357400
N	1.24140900	-4.62914500	4.05754700
H	0.61516200	-5.30543100	3.62251100
C	0.53025600	-3.36510700	4.17895500
H	1.11418100	-2.67269400	4.79320000
C	0.19000500	-2.69618100	2.82552100
C	-0.77829600	-3.65897600	4.88725600
H	1.13637400	-2.49656800	2.30554700
H	-0.36659600	-3.43079000	2.22883700
C	-0.61128400	-1.42700900	2.96590800
O	-1.53821100	-4.52901900	4.53530600
C	0.02194600	-0.19705900	3.16166700
C	-2.00906400	-1.46835900	2.95097800
H	1.10974300	-0.15101400	3.16345500
C	-0.72176500	0.96757200	3.33312100
C	-2.75653700	-0.30592300	3.12306700
H	-2.51003600	-2.42285200	2.79750200
H	-0.21394200	1.91823900	3.47114000
C	-2.11404300	0.91575800	3.31411400
H	-3.84169000	-0.35213800	3.09381500
H	-2.69538400	1.82549200	3.43650000
H	2.04117800	-4.51465800	3.43865900
O	-1.02936300	-2.82831300	5.90550500
H	-1.90910900	-3.06439500	6.25059600

Graphane-Trp

C	-5.05765700	1.79164100	-0.73153600
C	-5.80508500	2.90575900	0.03978400
C	-3.58932300	1.70461200	-0.26476500
C	-7.98307800	1.63905200	-0.23684000
C	-7.27820000	2.99269200	-0.43289700
C	-5.10413300	4.27063200	-0.16301200
C	-2.88841900	3.05831000	-0.45099600
C	-8.03242500	4.09709100	0.33302300
C	-5.86392400	5.36194700	0.62141500
C	-3.63043200	4.19075700	0.28475200
C	-1.42484200	2.97045900	0.01541000
C	-7.32842400	5.44981400	0.17642400

H	-5.81250400	5.15041400	1.70603500
C	-2.90857300	5.52501000	0.05539200
C	-0.66869600	1.83626500	-0.69770200
C	-0.68871700	4.31146100	-0.14279600
H	-7.85639600	6.22080200	0.76786600
C	-1.46345200	5.44877900	0.52939200
H	-2.92555100	5.76716500	-1.01648500
C	0.78738600	1.74205800	-0.21130800
C	0.75137800	4.20705000	0.38070200
H	-0.97551500	6.40827900	0.33474100
C	1.51923300	3.08819700	-0.34372500
C	1.50063800	5.53962500	0.28543200
C	2.97688100	2.99169700	0.13938200
C	2.94129600	5.42981400	0.76621800
H	1.48687500	5.88079200	-0.76168800
C	3.71449600	1.86579100	-0.60088600
C	3.69783100	4.34525900	-0.01229100
H	3.43972900	6.40224500	0.66870800
C	5.17283600	1.76791700	-0.10638300
C	5.16488400	4.24867000	0.45360300
C	5.90133600	3.11853700	-0.30545400
C	5.90503400	5.58549900	0.23231100
C	7.36650800	3.01919900	0.18911900
H	5.38767300	6.39992400	0.77416200
C	7.36276200	5.49908900	0.69949700
C	8.10104500	4.35910200	-0.01149000
C	8.10631400	1.89379600	-0.55472400
H	7.87721700	6.45910500	0.50816300
C	8.18249200	-3.02793600	-1.67695500
C	8.13319500	-0.56774700	-1.11129200
C	7.47355100	-4.37836500	-1.52156300
C	7.42171000	-1.91902600	-0.92421100
C	7.38415100	0.54868900	-0.36286400
C	6.01412400	-4.28947500	-1.98294000
H	8.00613700	-5.15349800	-2.10315100
C	5.95582600	-1.82915000	-1.41849000
C	5.92186900	0.64518800	-0.86242200
C	5.24862900	-3.19076900	-1.21427400
H	5.97521300	-4.08487200	-3.06942600
C	5.20050400	-0.70868500	-0.66454500
C	3.78051500	-3.11399400	-1.67929900
C	3.74283100	-0.61602000	-1.16142300
C	3.04948200	-4.43857100	-1.42217600
C	3.03314900	-1.96492500	-0.97609500
C	2.99649200	0.51634600	-0.43671100
C	1.61203100	-4.36954400	-1.92090700
H	3.57069600	-5.27493000	-1.90425600
C	1.57603900	-1.87858900	-1.46294600
C	1.54364400	0.60971500	-0.92477700
C	0.83333400	-3.21354200	-1.28734100

H	1.60682000	-4.24715500	-3.01553900
C	0.81528700	-0.73501500	-0.77101800
C	-0.60369600	-3.11538900	-1.81883800
C	-0.64014600	-0.64146900	-1.25979900
C	-1.34839800	-4.44777700	-1.69518400
C	-1.36797500	-1.98703400	-1.10534600
C	-1.39099900	0.48909100	-0.53869500
C	-2.79535700	-4.35050000	-2.15785900
H	-0.84133700	-5.22471900	-2.27506500
C	-2.83234500	-1.90219800	-1.56725600
C	-2.85167800	0.57730200	-1.00540100
C	-3.54133000	-3.25731000	-1.38248700
H	-2.81798700	-4.11310500	-3.23058600
C	-3.55983500	-0.77450700	-0.82120000
C	-5.01983900	-3.17661900	-1.81299500
C	-5.03016500	-0.68871700	-1.28123600
C	-5.74724300	-4.51476000	-1.56080500
C	-5.74713500	-2.04116100	-1.05338700
C	-5.76936600	0.43489100	-0.51733800
C	-7.21415600	-4.44165400	-2.00095200
H	-5.23590200	-5.33194900	-2.10505900
C	-7.22178800	-1.95479100	-1.52199600
C	-7.24078600	0.52229500	-0.99143400
C	-7.94585100	-3.29583800	-1.29264200
H	-7.27178300	-4.30452300	-3.09803500
C	-7.95444800	-0.82448400	-0.77865200
H	8.18919000	4.58550700	-1.09079900
H	8.18294300	2.13463200	-1.63132300
H	9.17335000	-0.63530300	-0.74411600
H	9.21829200	-3.09910600	-1.29822900
H	-8.01732900	-3.50903500	-0.20969500
H	-8.99911800	-0.75618900	-1.13348100
H	-8.04553600	1.39507600	0.83988600
H	-9.07260300	4.16785300	-0.03386500
H	0.77944500	-0.97078100	0.30916700
H	0.75459400	1.48685900	0.86351500
H	-1.39893700	0.24437600	0.53871700
H	1.57108900	0.85335800	-2.00397600
H	-0.61693500	-0.39532100	-2.33835500
H	-0.64676400	2.07988900	-1.77683000
H	1.60585600	-1.65524200	-2.54661100
H	3.00830000	-2.19115800	0.10399800
H	3.74700400	-0.37939300	-2.24574400
H	2.96406700	0.27164700	0.63956300
H	3.71866200	2.11660100	-1.68200500
H	2.95074000	2.73716300	1.21322600
H	1.54695300	3.35021600	-1.41855800
H	0.69630100	3.92846900	1.44914200
H	-0.63602200	4.53482000	-1.22375100
H	-1.43990100	2.72520800	1.09431600

H	0.76416300	-3.40914300	-0.20291800
H	-0.55026600	-2.85719800	-2.89216600
H	-1.37995100	-2.22900600	-0.02715400
H	-2.83193900	-1.66112400	-2.64442000
H	-3.53351100	-1.01852200	0.26132200
H	-2.84300600	0.81854200	-2.08261000
H	-3.56848300	1.46116600	0.81713700
H	-2.87923300	3.29944100	-1.52816900
H	5.16628500	1.52241600	0.98240700
H	5.90975300	3.36464700	-1.39321700
H	5.17999200	4.01380500	1.54501200
H	3.67965300	4.61342800	-1.08769500
H	5.86937900	5.86197600	-0.83833700
H	7.39927100	5.34659000	1.79525300
H	9.13564300	4.28307900	0.36970300
H	7.35814800	2.78131500	1.28034700
H	9.14592800	1.81880200	-0.18739500
H	5.93305100	0.89051000	-1.95048600
H	7.37425700	0.30211300	0.72670900
H	8.20770200	-0.32186800	-2.18686300
H	7.41487400	-2.17197300	0.16379000
H	5.96192400	-1.58825400	-2.50732100
H	5.19307300	-0.95410600	0.42454100
H	8.26629200	-2.76985800	-2.74942600
H	7.51529800	-4.70675200	-0.46518400
H	5.51747500	-5.26800000	-1.83943700
H	5.26741800	-3.44259900	-0.12622000
H	3.75823600	-2.90997000	-2.76875300
H	-3.49113100	-3.50806200	-0.30229200
H	-5.06058200	-2.95519500	-2.90702000
H	-8.98672000	-3.22943100	-1.65901000
H	-7.72008200	-5.40166900	-1.78775700
H	-5.68920400	-4.78069400	-0.48923400
H	-3.28973300	-5.32317800	-2.04153100
H	-1.31928100	-4.76812900	-0.64093800
H	1.11715400	-5.32185800	-1.70803400
H	3.04925700	-4.64720800	-0.34240300
H	-8.01736900	-1.05560100	0.30073000
H	-9.02754800	1.70357500	-0.59263000
H	-8.10408900	3.83432900	1.40526500
H	-7.38296300	5.78385300	-0.87753000
H	-5.37186600	6.34304400	0.47944500
H	-3.42526000	6.34465500	0.56996000
H	-1.44127100	5.29715000	1.62023100
H	0.98886300	6.30751300	0.87320300
H	2.94731600	5.17953500	1.83637000
H	-5.73536700	-2.27423900	0.03633900
H	-5.04988000	-0.45245600	-2.37192700
H	-5.76022800	0.19485500	0.57166600
H	-5.07344200	2.03710500	-1.82006000

H	-5.79535800	2.65793400	1.12706500
H	-5.13548700	4.53037100	-1.24846400
H	-3.59636800	3.96014700	1.36917100
H	-7.25078900	0.76230300	-2.08243900
H	-7.28823600	3.24738500	-1.52028700
H	-7.23399700	-1.72973700	-2.61602000
N	2.87852500	-4.41437900	3.83602000
H	2.75064300	-5.37070800	3.50477000
C	1.56488400	-3.79510300	3.92466100
H	1.64367100	-2.83951700	4.45167800
C	1.03196700	-3.55758900	2.49900700
C	0.55012600	-4.67145500	4.64530300
H	1.75022800	-2.90684600	1.98605200
H	1.03996100	-4.52387300	1.97785000
C	-0.34562500	-2.97535800	2.47422500
O	0.41329200	-5.85196700	4.42672300
C	-1.51984000	-3.64409900	2.25467500
C	-0.70591900	-1.61289600	2.76945400
H	-1.67955400	-4.68669000	2.01234700
N	-2.58612300	-2.78177700	2.39117400
C	-2.11684200	-1.52793500	2.70592600
C	0.03374000	-0.45784300	3.07255500
H	-3.55111000	-3.01614700	2.21552000
C	-2.80428100	-0.33332900	2.94625100
C	-0.64096300	0.72791700	3.30780100
H	1.12009200	-0.49520200	3.11426300
H	-3.88828400	-0.28369200	2.88795100
C	-2.04832700	0.78693500	3.24828100
H	-0.08185100	1.62983500	3.53882700
H	-2.54999400	1.73249400	3.43377500
H	3.29252700	-4.48943600	4.76284900
O	-0.19880800	-4.00035300	5.53305200
H	-0.84207600	-4.63512000	5.89604100

Graphane-Tyr

C	-4.91205900	1.62884200	-0.95554400
C	-5.66252400	2.81085000	-0.29614900
C	-3.46171400	1.55264100	-0.43414400
C	-7.85474900	1.56637200	-0.55328900
C	-7.11599400	2.88793200	-0.82726400
C	-4.92661800	4.14426600	-0.57158600
C	-2.73019300	2.87697600	-0.70010300
C	-7.87384800	4.06064000	-0.17478500
C	-5.69179500	5.30358800	0.10217400
C	-3.47296600	4.06738200	-0.06248200
C	-1.28077600	2.79677100	-0.19022900
C	-7.13653300	5.38470300	-0.40480800
H	-5.68618800	5.16887700	1.20042100
C	-2.71726800	5.37221700	-0.34594200
C	-0.52743100	1.60161100	-0.79909700

C	-0.51667500	4.11158300	-0.41438500
H	-7.66981700	6.20732900	0.10690000
C	-1.28745700	5.29724500	0.17198100
H	-2.69758700	5.55387700	-1.42963700
C	0.91684900	1.52139100	-0.27590300
C	0.91154700	4.01977100	0.14216000
H	-0.77602000	6.23653200	-0.05704200
C	1.67469700	2.84221200	-0.48794000
C	1.68369400	5.33189400	-0.02711400
C	3.12034400	2.75824400	0.03235700
C	3.11477400	5.23370100	0.48365500
H	1.69091600	5.60322100	-1.09432000
C	3.85373200	1.56765100	-0.60284400
C	3.86598600	4.08600400	-0.20417300
H	3.63009600	6.18940000	0.32737500
C	5.29889300	1.48694800	-0.06850000
C	5.32392800	4.00429600	0.29122800
C	6.05408600	2.80555100	-0.36095900
C	6.08830900	5.30765200	-0.02676800
C	7.50822100	2.72553900	0.16847900
H	5.57555700	6.17144400	0.43764100
C	7.53722000	5.23923700	0.46970100
C	8.26789700	4.03263200	-0.13058900
C	8.24242500	1.53004600	-0.46276700
H	8.06988900	6.17206400	0.20642200
C	8.25848200	-3.46856700	-1.16458600
C	8.23926000	-0.96995300	-0.80647800
C	7.52083800	-4.78998900	-0.92056700
C	7.49946600	-2.28938500	-0.52575400
C	7.49348300	0.21748700	-0.17328100
C	6.07621500	-4.71507000	-1.42854700
H	8.05430800	-5.61821600	-1.42328100
C	6.04805500	-2.21681500	-1.06357100
C	6.04424500	0.29443000	-0.71269300
C	5.31051300	-3.54614500	-0.77205900
H	6.07081100	-4.59736100	-2.52872100
C	5.29469400	-1.02717600	-0.42194600
C	3.85753300	-3.48038900	-1.28487900
C	3.85091700	-0.95215100	-0.96097100
C	3.09665900	-4.77319000	-0.96174800
C	3.11208300	-2.27073600	-0.68810900
C	3.10782800	0.24713800	-0.35036700
C	1.67125800	-4.71293200	-1.49466600
H	3.61324700	-5.64683600	-1.37782700
C	1.66809500	-2.19859900	-1.21559100
C	1.66891100	0.32543900	-0.88138100
C	0.90125500	-3.50536800	-0.95368600
H	1.69062100	-4.66076400	-2.59441800
C	0.91263100	-0.99020400	-0.63739700
C	-0.52804200	-3.42852700	-1.50925300

C	-0.53111600	-0.91474700	-1.16209800
C	-1.29901900	-4.73326600	-1.28807400
C	-1.28552400	-2.23120600	-0.91086100
C	-1.27866100	0.28310200	-0.55502600
C	-2.73237200	-4.65075100	-1.79408400
H	-0.79386000	-5.56422200	-1.78930100
C	-2.73734300	-2.16092900	-1.41503500
C	-2.72526600	0.35896900	-1.06468500
C	-3.47903400	-3.48277700	-1.13699700
H	-2.72267300	-4.50811600	-2.88381800
C	-3.46428600	-0.96099500	-0.78998500
C	-4.93900500	-3.41284800	-1.62795500
C	-4.91633500	-0.88873300	-1.30632800
C	-5.70129800	-4.71137100	-1.28672400
C	-5.66742400	-2.20477200	-0.99178500
C	-5.65734600	0.30566400	-0.66067800
C	-7.15095900	-4.65148300	-1.78211000
H	-5.18911800	-5.58263700	-1.73743600
C	-7.12397400	-2.13286800	-1.51570600
C	-7.11024000	0.38015700	-1.19072800
C	-7.88156100	-3.43697500	-1.19801600
H	-7.17046700	-4.60797300	-2.88793900
C	-7.85735800	-0.93202700	-0.89361000
H	8.37741800	4.16657000	-1.22335000
H	8.34434200	1.67805400	-1.55400300
H	9.26914000	-1.02310100	-0.40875600
H	9.28262700	-3.52575900	-0.75273200
H	-7.98903600	-3.55606400	-0.10325600
H	-8.88849700	-0.87534600	-1.28736600
H	-7.95900300	1.40827200	0.53647000
H	-8.89855200	4.12224000	-0.58422400
H	0.85012600	-1.13304800	0.45757900
H	0.85799500	1.34816100	0.81355200
H	-1.32034500	0.12367500	0.53718000
H	1.72573500	0.48240200	-1.97525400
H	-0.48287800	-0.76182500	-2.25679800
H	-0.47928800	1.76410300	-1.89242000
H	1.72643200	-2.06270900	-2.31221800
H	3.05459200	-2.41251600	0.40623100
H	3.88588300	-0.80463900	-2.06025700
H	3.04431400	0.09085200	0.74121300
H	3.88546200	1.73315200	-1.69970500
H	3.06739800	2.58576900	1.12179200
H	1.72804000	3.02874800	-1.57731200
H	0.83286300	3.81460700	1.22662600
H	-0.43954100	4.26863500	-1.50525300
H	-1.33411600	2.62713900	0.90198300
H	0.82196800	-3.62517300	0.14207200
H	-0.45497800	-3.26178700	-2.59918500
H	-1.32796400	-2.37736900	0.18587300

H	-2.70047200	-2.01232500	-2.50834400
H	-3.47968100	-1.11067300	0.30921300
H	-2.68488600	0.51429200	-2.15702000
H	-3.48179200	1.39890500	0.66427700
H	-2.68772700	3.04161500	-1.79090500
H	5.26511500	1.33229900	1.03628100
H	6.08629600	2.96321500	-1.46464600
H	5.31939300	3.85932400	1.39827900
H	3.86766600	4.27651100	-1.29604900
H	6.07336300	5.49581800	-1.11697700
H	7.55515300	5.17982500	1.57486800
H	9.29493700	3.97345700	0.27355100
H	7.47643900	2.58142600	1.27559900
H	9.27347200	1.47028700	-0.06910200
H	6.08362400	0.44941800	-1.81672300
H	7.45623100	0.06537100	0.93280600
H	8.34459500	-0.81627700	-1.89662100
H	7.46231800	-2.45066900	0.57879000
H	6.08632000	-2.06381000	-2.16777900
H	5.25838400	-1.18143600	0.68271400
H	8.37609800	-3.30017000	-2.25173600
H	7.52950800	-5.03334200	0.15923400
H	5.55895200	-5.67146000	-1.22276300
H	5.29546000	-3.71088800	0.33193500
H	3.87099900	-3.35229900	-2.38569700
H	-3.47496900	-3.64165800	-0.03935000
H	-4.93859000	-3.28546600	-2.73724800
H	-8.90923800	-3.38428700	-1.60123700
H	-7.68236800	-5.58079900	-1.50432500
H	-5.68424500	-4.88144800	-0.19346600
H	-3.24728900	-5.60105200	-1.60651100
H	-1.30116400	-4.96694600	-0.21110600
H	1.15547200	-5.64098300	-1.23217100
H	3.06897100	-4.91512800	0.12846000
H	-7.95883600	-1.07265000	0.19873800
H	-8.88476600	1.62108800	-0.95016100
H	-7.98908600	3.88018700	0.91078100
H	-7.14488600	5.63921400	-1.48199800
H	-5.17549500	6.26299000	-0.09026400
H	-3.23061200	6.22986000	0.10614100
H	-1.29812900	5.20489400	1.27104800
H	1.17478100	6.14436300	0.49993900
H	3.10072400	5.05883100	1.56873700
H	-5.69487700	-2.34634100	0.11425800
H	-4.89659500	-0.74283600	-2.41252000
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H	-4.88885200	1.78960600	-2.05946400
H	-5.69528100	2.64353100	0.80667000
H	-4.91270800	4.32440600	-1.67329600
H	-3.48492800	3.89667200	1.03291600

H	-7.08010800	0.53095900	-2.29702100
H	-7.08346100	3.05834200	-1.93043100
H	-7.09720200	-2.00092600	-2.62433800
N	0.84701100	-4.75155900	4.19039600
H	0.18817400	-5.38461900	3.73857900
C	0.23525300	-3.43201600	4.25613900
H	0.84594100	-2.77522900	4.88334100
C	0.00976300	-2.76625500	2.87747200
C	-1.12185400	-3.60668200	4.91057000
H	0.99127700	-2.65860800	2.39689700
H	-0.57851700	-3.46560400	2.26835700
C	-0.68321100	-1.42985900	2.95227300
O	-1.93677900	-4.41445400	4.53319000
C	0.04439100	-0.24875900	3.09835100
C	-2.08041200	-1.34301900	2.91736500
H	1.13202000	-0.28803200	3.12135600
C	-0.59199700	0.98602000	3.18867700
C	-2.73097200	-0.11923000	3.00684300
H	-2.66593700	-2.25444400	2.80596400
H	-0.00748900	1.89950300	3.28246200
C	-1.98316300	1.05213700	3.13346500
H	-3.81307600	-0.04670900	2.95636000
H	1.67977100	-4.71461200	3.60637000
O	-1.34630000	-2.74735000	5.91116800
H	-2.25584000	-2.90787400	6.22053400
O	-2.66515400	2.23116700	3.17856300
H	-2.03444600	2.96611100	3.17503500

Graphane-G

C	-5.21668500	1.37342700	-0.62309200
C	-5.93040500	2.61827300	-0.04416400
C	-3.73050300	1.36301700	-0.20967300
C	-8.11710700	1.33755400	0.01413500
C	-7.42297100	2.62594600	-0.46073200
C	-5.24052600	3.91470100	-0.53310400
C	-3.03731300	2.65173700	-0.67436700
C	-8.14288300	3.86003000	0.11695000
C	-5.96481600	5.14097700	0.06301600
C	-3.74820500	3.91175800	-0.14508100
C	-1.55679000	2.64268800	-0.25701300
C	-7.44843500	5.15382500	-0.32343400
H	-5.86371300	5.13944500	1.16453900
C	-3.03565500	5.16671700	-0.66516000
C	-0.82460500	1.38794300	-0.76269500
C	-0.82114800	3.92141600	-0.68922800
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C	-1.57400000	5.17618100	-0.23740600
H	-3.09260000	5.18686200	-1.76236600
C	0.64238600	1.37344400	-0.30082800
C	0.62857300	3.90562500	-0.18202600

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C	1.38149400	2.66469700	-0.68907300
C	1.38337700	5.19039300	-0.53240800
C	2.83908300	2.64664300	-0.19522200
C	2.82402300	5.16067700	-0.03899300
H	1.36849500	5.32664600	-1.62518400
C	3.56688900	1.39847800	-0.71645900
C	3.57116600	3.94164300	-0.59637800
H	3.33092800	6.09323100	-0.31685500
C	5.02060200	1.38089100	-0.20135800
C	5.03503100	3.92175800	-0.11229400
C	5.76466600	2.66375100	-0.64227000
C	5.78978800	5.18758500	-0.57289300
C	7.22448400	2.64567900	-0.12292900
H	5.27724900	6.09307900	-0.19663300
C	7.24320500	5.17700100	-0.08437600
C	7.97502200	3.91782100	-0.56325700
C	7.95882600	1.39416300	-0.63441600
H	7.76910000	6.07993000	-0.44568000
C	7.99187200	-3.65027000	-0.80992900
C	7.96456400	-1.12791100	-0.71598200
C	7.26464400	-4.94180500	-0.41836000
C	7.23499900	-2.41310800	-0.28817400
C	7.21954900	0.11610300	-0.20074100
C	5.81276700	-4.92564400	-0.91128200
H	7.79566000	-5.81618100	-0.83784100
C	5.77595500	-2.40255500	-0.80984400
C	5.76338100	0.13005100	-0.72652200
C	5.05142400	-3.69702200	-0.36812900
H	5.79200900	-4.92121900	-2.01738500
C	5.02565600	-1.15559900	-0.28438300
C	3.58937400	-3.69070900	-0.85714500
C	3.57361200	-1.14282400	-0.80298100
C	2.84492900	-4.94621500	-0.38301100
C	2.85074700	-2.42826900	-0.37336300
C	2.83739700	0.11036800	-0.30304300
C	1.40535500	-4.94932500	-0.88011200
H	3.35719600	-5.85746100	-0.71612400
C	1.39233200	-2.42034400	-0.86506000
C	1.38367100	0.12366900	-0.79986600
C	0.64324100	-3.69514900	-0.44510700
H	1.39578800	-5.01028100	-1.97953300
C	0.64667400	-1.16146300	-0.39296900
C	-0.80597900	-3.68234000	-0.95436700
C	-0.82008000	-1.15024500	-0.85688700
C	-1.55169800	-4.96652900	-0.58052800
C	-1.54692100	-2.43829600	-0.43702900
C	-1.54737500	0.10053500	-0.33835400
C	-3.01305700	-4.93704600	-1.00787700
H	-1.06572500	-5.83422000	-1.03684200

C	-3.02695100	-2.42612900	-0.85536600
C	-3.02445400	0.11177600	-0.75586600
C	-3.73052400	-3.72110900	-0.40791500
H	-3.06958900	-4.88583100	-2.10418200
C	-3.72445700	-1.17727900	-0.29672500
C	-5.22368200	-3.70600200	-0.79301300
C	-5.21090800	-1.16435000	-0.71008900
C	-5.94186300	-4.97294900	-0.28031000
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C	-7.42571500	-4.96646900	-0.66638200
H	-5.45401800	-5.87734900	-0.69132000
C	-7.41176800	-2.43495200	-0.63245200
C	-7.40841300	0.09576400	-0.55462100
C	-8.12582900	-3.70856900	-0.13938300
H	-7.52902200	-5.02226400	-1.76717200
C	-8.11145200	-1.18482000	-0.07123000
H	8.07365300	3.93767800	-1.66481900
H	8.04742500	1.42765800	-1.73600500
H	8.99902400	-1.13457400	-0.32742400
H	9.02128600	-3.65950100	-0.40795200
H	-8.14825400	-3.72730200	0.96643100
H	-9.17127700	-1.17353300	-0.38461100
H	-8.12989500	1.29632000	1.11908300
H	-9.19882300	3.86812500	-0.20961900
H	0.63108400	-1.18734600	0.71139100
H	0.63597800	1.32215200	0.80163100
H	-1.52299200	0.05364000	0.76662800
H	1.40600000	0.16250600	-1.90584300
H	-0.82444800	-1.10705100	-1.96212600
H	-0.83099500	1.42614700	-1.86798100
H	1.41840500	-2.40031900	-1.97128700
H	2.83362700	-2.44546700	0.72966500
H	3.58630500	-1.11308200	-1.91316000
H	2.81524900	0.07546400	0.79856400
H	3.57800400	1.44635700	-1.82603400
H	2.81059800	2.58838100	0.90615000
H	1.40590600	2.72049800	-1.79441600
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H	-0.79091700	3.92702500	-1.79354300
H	-1.53294400	2.61192300	0.85069700
H	0.59342000	-3.69875400	0.65926200
H	-0.77553100	-3.61755600	-2.05717000
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H	-3.06488000	-2.38004500	-1.95749300
H	-3.65713900	-1.22037200	0.81085200
H	-3.05957500	0.15128000	-1.85808900
H	-3.66880700	1.32597800	0.89955300
H	-3.06977300	2.68069000	-1.77696800
H	5.00166900	1.34188400	0.91577800

H	5.78399400	2.70310700	-1.75642800
H	5.04191600	3.89220300	1.00443800
H	3.55972000	4.00481500	-1.70346100
H	5.76472600	5.25918300	-1.67644300
H	7.26902000	5.22981700	1.02112300
H	9.00547900	3.90488800	-0.16419800
H	7.20331500	2.61615700	0.99367100
H	8.99374400	1.37999500	-0.24734000
H	5.78696300	0.16673900	-1.84082300
H	7.19450700	0.07976000	0.91598800
H	8.05451900	-1.08879600	-1.81728700
H	7.21217300	-2.45649400	0.82797200
H	5.79719800	-2.36604400	-1.92414800
H	5.00384500	-1.19058800	0.83378600
H	8.09372800	-3.59614800	-1.91009400
H	7.28798200	-5.06813200	0.68113500
H	5.30341800	-5.85713500	-0.60049400
H	5.05687800	-3.74188900	0.74795200
H	3.58012500	-3.68198000	-1.96568600
H	-3.64532100	-3.77993800	0.69696800
H	-5.30614800	-3.68053000	-1.90631200
H	-9.18185900	-3.69935100	-0.46559800
H	-7.92297900	-5.87025700	-0.26791600
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H	-3.50685200	-5.87119400	-0.71196900
H	-1.48938300	-5.10157400	0.51111100
H	0.90323900	-5.84879300	-0.51095500
H	2.84727100	-4.97215700	0.71715000
H	-8.12370100	-1.21862500	1.03398300
H	-9.17683600	1.34293200	-0.29980500
H	-8.16568200	3.80404200	1.22153600
H	-7.55197500	5.28387800	-1.41788900
H	-5.48095000	6.07335100	-0.28565100
H	-3.53273300	6.07738600	-0.30862300
H	-1.51411600	5.25134700	0.86039500
H	0.87843000	6.05928200	-0.09932600
H	2.82784300	5.11526500	1.05908200
H	-5.86052100	-2.48567400	0.89600400
H	-5.27220900	-1.12776000	-1.82403700
H	-5.86354500	0.04624900	0.97957900
H	-5.27770000	1.41265100	-1.73705400
H	-5.87330800	2.58010400	1.06875800
H	-5.32159700	3.96398000	-1.64571400
H	-3.66626900	3.90075300	0.96125300
H	-7.46473000	0.13338000	-1.66974100
H	-7.48083800	2.67336200	-1.57518500
H	-7.47022600	-2.40702800	-1.74752600
H	0.33192300	3.08695600	3.36446800
C	0.43779700	2.01184100	3.31346700
N	-0.66169900	1.18065200	3.27370100

N	1.56643100	1.35959100	3.28189100
C	-0.18755100	-0.09680500	3.21413700
H	-1.63678100	1.44632300	3.26330000
C	1.19470000	0.03570200	3.22032900
N	-0.94394900	-1.22536100	3.17212300
C	2.00096500	-1.15623000	3.13257700
C	-0.21569800	-2.30735500	3.11960100
N	1.15376800	-2.30619700	3.10456200
O	3.20271000	-1.29733100	3.05771300
N	-0.82766200	-3.53168800	3.01525200
H	1.65580600	-3.17623800	2.96066400
H	-0.36459300	-4.32555400	3.43660700
H	-1.82452600	-3.48976500	3.18528100

Graphane-A

C	-5.15439300	1.33008500	-0.66953800
C	-5.87624200	2.58935200	-0.13336800
C	-3.67903200	1.32145700	-0.21816600
C	-8.07123000	1.32124800	-0.10991200
C	-7.35708300	2.59678200	-0.58977900
C	-5.16632800	3.87305700	-0.62719000
C	-2.96821700	2.59745700	-0.69124900
C	-8.08543700	3.84470500	-0.05388200
C	-5.89975500	5.11301600	-0.07194400
C	-3.68487000	3.86909500	-0.19838700
C	-1.49720600	2.58758700	-0.24015500
C	-7.37232100	5.12687000	-0.49842700
H	-5.82795400	5.12913000	1.03202200
C	-2.95430500	5.11262000	-0.72154900
C	-0.76503300	1.32180800	-0.71777800
C	-0.75032800	3.85500000	-0.68735000
H	-7.88074700	6.00982300	-0.06837000
C	-1.50141400	5.12074500	-0.26475200
H	-2.98831700	5.11802300	-1.82004500
C	0.69827200	1.30748300	-0.24307200
C	0.69422700	3.84123600	-0.16557600
H	-1.00716200	6.00850200	-0.67073300
C	1.44316800	2.58927900	-0.65101100
C	1.45714500	5.11865900	-0.52603500
C	2.90300100	2.57332100	-0.16430500
C	2.89863800	5.08727300	-0.03502600
H	1.44295200	5.24691400	-1.61954700
C	3.62265500	1.31107500	-0.66218900
C	3.63882000	3.86026800	-0.58336700
H	3.41039800	6.01457600	-0.32051000
C	5.08272400	1.29721600	-0.16262300
C	5.10768500	3.84036100	-0.11322100
C	5.82539600	2.57090400	-0.63208700
C	5.86146500	5.09543200	-0.60375300
C	7.29315000	2.55437800	-0.13553700

H	5.35775400	6.00946100	-0.23591200
C	7.32173100	5.08651900	-0.13673400
C	8.04114400	3.81690400	-0.60629500
C	8.01379300	1.29286100	-0.64169600
H	7.84560700	5.98116700	-0.52198800
C	8.02350400	-3.75491700	-0.75031500
C	8.00775300	-1.23064000	-0.69229800
C	7.30041800	-5.03678100	-0.32084900
C	7.28232900	-2.50710200	-0.23206000
C	7.27781200	0.02303200	-0.17952100
C	5.83771400	-5.02379400	-0.78031500
H	7.81852300	-5.92016500	-0.73804100
C	5.81339100	-2.49985800	-0.72527900
C	5.81294500	0.03554700	-0.68056600
C	5.09207600	-3.78237100	-0.24480700
H	5.79074500	-5.04280100	-1.88544400
C	5.07705000	-1.24064000	-0.20944100
C	3.62006500	-3.78105700	-0.70503500
C	3.61669600	-1.23297500	-0.70748600
C	2.87805600	-5.01897300	-0.18413800
C	2.89349600	-2.50451000	-0.24084100
C	2.88995500	0.03285400	-0.22520700
C	1.43325300	-5.03114000	-0.66629600
H	3.38310300	-5.94104500	-0.49787700
C	1.43142100	-2.50127500	-0.72205500
C	1.43387500	0.04391600	-0.71452700
C	0.67782700	-3.76141600	-0.26506500
H	1.41163200	-5.12962500	-1.76315500
C	0.69314300	-1.22854900	-0.27587600
C	-0.76746200	-3.75600500	-0.78557900
C	-0.77048800	-1.22071000	-0.74979600
C	-1.52438100	-5.02441300	-0.38187600
C	-1.50859800	-2.49602300	-0.30892300
C	-1.49868000	0.04673500	-0.27489900
C	-2.97759700	-5.00297000	-0.83694100
H	-1.03511200	-5.90803500	-0.80228300
C	-2.97995700	-2.48744500	-0.75880900
C	-2.96705100	0.05620900	-0.72367800
C	-3.70242300	-3.76575000	-0.29238100
H	-3.01372700	-4.98858900	-1.93529300
C	-3.68525000	-1.21975200	-0.25662600
C	-5.18446200	-3.75364100	-0.71877200
C	-5.16162000	-1.21003000	-0.70337300
C	-5.92311500	-5.00273100	-0.19202400
C	-5.88871200	-2.47840700	-0.19624100
C	-5.87623500	0.05527100	-0.17310200
C	-7.39548900	-5.00035100	-0.61934100
H	-5.42861800	-5.92047600	-0.56399100
C	-7.36956200	-2.46849700	-0.65279600
C	-7.35446100	0.06461900	-0.63400500

C	-8.10356500	-3.72552000	-0.14664400
H	-7.46880600	-5.08661000	-1.72050700
C	-8.07785700	-1.20150800	-0.14263600
H	8.12392400	3.81947700	-1.70960400
H	8.08498900	1.31111900	-1.74517700
H	9.05022700	-1.23642200	-0.32549700
H	9.06181400	-3.76189600	-0.37180800
H	-8.15757900	-3.71486200	0.95828200
H	-9.12789300	-1.19245600	-0.48778200
H	-8.11512300	1.30210800	0.99493500
H	-9.13228400	3.85219000	-0.40832100
H	0.67637600	-1.23135200	0.82807400
H	0.67720700	1.27756000	0.86069000
H	-1.49420800	0.03735700	0.83085700
H	1.45430500	0.05875900	-1.82092600
H	-0.76414400	-1.20598400	-1.85598400
H	-0.75832900	1.33716200	-1.82388300
H	1.45094800	-2.50812700	-1.82892300
H	2.87761800	-2.49759600	0.86230700
H	3.61612200	-1.22404700	-1.81766700
H	2.86276300	0.00604100	0.87810900
H	3.62533700	1.34001100	-1.77158800
H	2.87474700	2.53976200	0.94042200
H	1.46949700	2.62658400	-1.75657000
H	0.64147100	3.78193800	0.93720000
H	-0.70659000	3.84332600	-1.79147500
H	-1.49385900	2.57095200	0.86603600
H	0.62519800	-3.73259200	0.83769700
H	-0.72854800	-3.72208700	-1.88965900
H	-1.50241600	-2.51609500	0.79713900
H	-2.99075400	-2.47332100	-1.86236400
H	-3.64822500	-1.23444900	0.85321800
H	-2.97711700	0.07290100	-1.82701000
H	-3.64326900	1.30822300	0.89237400
H	-2.97762200	2.60680700	-1.79502000
H	5.08103900	1.27390100	0.95278200
H	5.82884000	2.59290800	-1.74733500
H	5.12866000	3.83109900	1.00252400
H	3.61808300	3.90913700	-1.69034400
H	5.82105900	5.15006500	-1.70818400
H	7.36605700	5.15926000	0.96677400
H	9.07787400	3.80620200	-0.22324500
H	7.29135100	2.54108400	0.98113400
H	9.05543800	1.27971700	-0.27252800
H	5.81856600	0.05604800	-1.79581600
H	7.27366400	0.00013800	0.93739300
H	8.07573500	-1.20773200	-1.79580400
H	7.28198900	-2.53521100	0.88462400
H	5.81289900	-2.48491600	-1.84036300
H	5.07311000	-1.26113300	0.90731000

H	8.10057800	-3.71981500	-1.85334000
H	7.34874800	-5.14625500	0.77965300
H	5.33145300	-5.94661600	-0.43849800
H	5.11836200	-3.80838800	0.87137600
H	3.59086400	-3.79943600	-1.81330200
H	-3.64817900	-3.79387900	0.81567400
H	-5.23627600	-3.75813500	-1.83421100
H	-9.14991800	-3.72046100	-0.50281500
H	-7.90798300	-5.89065800	-0.20962200
H	-5.85170300	-5.04571700	0.91106200
H	-3.48084900	-5.92424000	-0.51832600
H	-1.48191200	-5.12740400	0.71381500
H	0.93240700	-5.91492900	-0.26016000
H	2.89103900	-5.01188900	0.91521300
H	-8.12400900	-1.20933000	0.96221400
H	-9.12183100	1.32595800	-0.45324200
H	-8.13742300	3.80884300	1.05067000
H	-7.44586200	5.23796800	-1.59730200
H	-5.40144000	6.03691700	-0.42236200
H	-3.45305100	6.03093200	-0.38771900
H	-1.46235000	5.20849300	0.83253400
H	0.95642500	5.99307400	-0.09992100
H	2.90444000	5.05270400	1.06427100
H	-5.86238700	-2.48685200	0.91837700
H	-5.19692600	-1.19982200	-1.81904500
H	-5.85290200	0.04118500	0.94172900
H	-5.18688300	1.34773800	-1.78519300
H	-5.84825900	2.57224900	0.98144900
H	-5.21744100	3.90291200	-1.74209900
H	-3.63138600	3.87439200	0.90878200
H	-7.38069500	0.07913200	-1.75071600
H	-7.38506700	2.62398400	-1.70599500
H	-7.39740200	-2.46909300	-1.76935200
H	0.74344100	3.11446100	3.40289100
C	0.64170100	2.03758900	3.37577600
N	-0.49177900	1.38912100	3.34249100
N	1.74406700	1.21535700	3.37103200
C	-0.11147700	0.06276500	3.31429600
C	1.27496400	-0.07384900	3.32827000
H	2.71551100	1.49229000	3.37262300
C	-0.84597400	-1.14012900	3.26949900
N	1.96940100	-1.21700500	3.30134600
N	-0.18280000	-2.30172500	3.23242700
N	-2.19676800	-1.14966800	3.28050700
C	1.15908400	-2.26965800	3.25566600
H	-2.66771700	-2.02280800	3.09145800
H	-2.69595000	-0.28409100	3.13423200
H	1.64489400	-3.24299000	3.22240100

Graphane-T

C	-5.17868500	1.43450400	-0.59278900
C	-5.91989000	2.66407000	-0.01521800
C	-3.70720000	1.42290500	-0.12891300
C	-8.09992500	1.37382400	-0.05971400
C	-7.39522700	2.67267700	-0.48850700
C	-5.21725600	3.97383700	-0.44676600
C	-3.00614500	2.72684000	-0.53592500
C	-8.14411100	3.89315000	0.08154000
C	-5.97310200	5.18374100	0.14338400
C	-3.74374100	3.96508200	0.00884700
C	-1.54122100	2.70966700	-0.06611200
C	-7.43881500	5.19789100	-0.30600000
H	-5.91871600	5.15799800	1.24818900
C	-3.01779900	5.24170500	-0.43430300
C	-0.79106600	1.48093500	-0.60814700
C	-0.80258400	4.00756500	-0.43047500
H	-7.96348600	6.05951200	0.14700600
C	-1.57407200	5.23951600	0.05046800
H	-3.03167100	5.30561800	-1.53151900
C	0.66996900	1.45799800	-0.12517600
C	0.63527700	3.97838500	0.11004500
H	-1.08203900	6.15353000	-0.29561700
C	1.40149300	2.76973100	-0.45259400
C	1.38473400	5.28523500	-0.16312800
C	2.86149400	2.73978300	0.03282500
C	2.82686200	5.23851100	0.32508700
H	1.36822000	5.48796800	-1.24548100
C	3.59483600	1.52156900	-0.54657000
C	3.58079500	4.05988300	-0.30455600
H	3.32724000	6.18858000	0.10062400
C	5.05751900	1.49214700	-0.05519000
C	5.05155800	4.02632700	0.15929200
C	5.78224800	2.80275600	-0.44470600
C	5.78871300	5.31990000	-0.24918000
C	7.25278100	2.77124200	0.04267800
H	5.27590100	6.20081400	0.18207400
C	7.25125000	5.29738700	0.20997000
C	7.98326700	4.07099600	-0.34684600
C	7.98546800	1.55505800	-0.55000200
H	7.76257000	6.22221200	-0.11649000
C	8.05400500	-3.47073800	-1.01485200
C	8.00920700	-0.95826400	-0.77284100
C	7.35074100	-4.79020700	-0.67633000
C	7.30371300	-2.27342300	-0.39955000
C	7.26845800	0.24802900	-0.16965500
C	5.88301700	-4.76079300	-1.11839000
H	7.87426000	-5.63273200	-1.16575500
C	5.82967600	-2.24922700	-0.87712500
C	5.79947800	0.27612100	-0.65801100

C	5.12941600	-3.57200000	-0.48370600
H	5.82395300	-4.69749700	-2.22149500
C	5.08332500	-1.03826500	-0.26798500
C	3.65082500	-3.55833600	-0.92354100
C	3.61772400	-1.01618000	-0.75152600
C	2.93590800	-4.83876700	-0.47434400
C	2.91412000	-2.32513100	-0.36591800
C	2.87914400	0.20897900	-0.18927600
C	1.47730600	-4.83851800	-0.91302800
H	3.44134200	-5.72888400	-0.86909400
C	1.44557100	-2.31035500	-0.82740300
C	1.41985400	0.23216400	-0.66881700
C	0.71535500	-3.60185600	-0.42756900
H	1.42480600	-4.87798600	-2.01236400
C	0.69612400	-1.07321800	-0.30578600
C	-0.74119300	-3.59462500	-0.91496700
C	-0.77023900	-1.05926000	-0.77223000
C	-1.47473900	-4.88098800	-0.52526200
C	-1.48999300	-2.36126800	-0.38389800
C	-1.51203600	0.17594200	-0.23773300
C	-2.93265100	-4.86811300	-0.96547400
H	-0.98105200	-5.75050700	-0.96938300
C	-2.96527500	-2.35434800	-0.81999200
C	-2.97954900	0.18866100	-0.68771100
C	-3.66867600	-3.65439600	-0.38356400
H	-2.98031300	-4.83059200	-2.06313300
C	-3.68172400	-1.11289800	-0.26863500
C	-5.15141700	-3.64744300	-0.80835800
C	-5.15774200	-1.10411100	-0.71725100
C	-5.87570200	-4.91832200	-0.31468000
C	-5.87077700	-2.39578000	-0.25044900
C	-5.88894500	0.13448200	-0.14767600
C	-7.34754900	-4.92230200	-0.74399900
H	-5.36988100	-5.82060800	-0.70784500
C	-7.35071800	-2.38990300	-0.70998400
C	-7.36441900	0.14241100	-0.61708000
C	-8.07114200	-3.66855600	-0.23925400
H	-7.41847900	-4.98047900	-1.84703600
C	-8.07569300	-1.14600300	-0.16724200
H	8.05947100	4.14832500	-1.44794700
H	8.04958000	1.64810500	-1.65026900
H	9.05464400	-0.97626100	-0.41459900
H	9.09617500	-3.49283200	-0.64738700
H	-8.12588600	-3.68772700	0.86564100
H	-9.12409800	-1.13875100	-0.51672900
H	-8.15396500	1.31720200	1.04352800
H	-9.18597700	3.90259300	-0.28694000
H	0.68569600	-1.14452600	0.79758800
H	0.64017800	1.36874800	0.97575600
H	-1.51379000	0.11448100	0.86490600

H	1.43621700	0.31186600	-1.77217800
H	-0.76750600	-0.99467500	-1.87644500
H	-0.77734400	1.55708600	-1.71179600
H	1.45026100	-2.25631300	-1.93270900
H	2.90654800	-2.40204300	0.73690900
H	3.60773100	-0.93651100	-1.85818400
H	2.85634700	0.11761000	0.91230300
H	3.59100400	1.61786400	-1.65186300
H	2.83902200	2.63673400	1.13319600
H	1.42733200	2.87632100	-1.55371100
H	0.57379100	3.84646900	1.20544100
H	-0.74322400	4.05943800	-1.53294700
H	-1.54975600	2.62685000	1.03602200
H	0.68412400	-3.63251500	0.67630000
H	-0.72665100	-3.52708700	-2.01814300
H	-1.48267800	-2.43354200	0.71898900
H	-2.98681000	-2.30361100	-1.92246500
H	-3.64689600	-1.16988700	0.84071000
H	-2.99028700	0.24897000	-1.78961600
H	-3.67875400	1.35731200	0.97872300
H	-3.00231600	2.78968000	-1.63818200
H	5.06236700	1.39952000	1.05634700
H	5.77903700	2.89770400	-1.55614300
H	5.07577500	3.94381400	1.27217500
H	3.55526700	4.17975500	-1.40610400
H	5.74156500	5.44886700	-1.34709500
H	7.30004500	5.29671100	1.31573600
H	9.02226600	4.04771000	0.02942300
H	7.25734900	2.68440800	1.15601600
H	9.02969900	1.53086800	-0.18860800
H	5.79664100	0.36994200	-1.76978600
H	7.27461800	0.14982900	0.94288100
H	8.06942300	-0.85701600	-1.87261000
H	7.31639200	-2.38279300	0.71172300
H	5.81812400	-2.15500600	-1.98854600
H	5.09416300	-1.13450000	0.84314500
H	8.12055700	-3.35307300	-2.11303100
H	7.41383700	-4.98361700	0.41158400
H	5.39121900	-5.71319700	-0.84286500
H	5.17193000	-3.68086000	0.62643200
H	3.60535500	-3.50116600	-2.02942800
H	-3.60743000	-3.71062300	0.72174600
H	-5.20440500	-3.62213700	-1.92331600
H	-9.11689900	-3.66594800	-0.59661900
H	-7.84987200	-5.82871300	-0.35793500
H	-5.80440100	-4.98705800	0.78742500
H	-3.41985400	-5.80269600	-0.66129200
H	-1.41722800	-4.99785900	0.56795200
H	0.99757000	-5.74873500	-0.54205700
H	2.98586300	-4.91211000	0.62138700

H	-8.12568600	-1.18662900	0.93689000
H	-9.14692400	1.37857600	-0.41340200
H	-8.21036200	3.81662800	1.18329200
H	-7.49622100	5.34712500	-1.40125400
H	-5.47990600	6.12562100	-0.16340800
H	-3.53250000	6.13595600	-0.06152200
H	-1.55570700	5.26466600	1.15117500
H	0.87394700	6.12225800	0.32182800
H	2.83448000	5.13070600	1.41900500
H	-5.84519000	-2.43679500	0.86393500
H	-5.19223100	-1.05868500	-1.83189100
H	-5.87086100	0.08079800	0.96652400
H	-5.20286600	1.49340700	-1.70694000
H	-5.90448800	2.60160800	1.09845800
H	-5.24921900	4.04709000	-1.56020900
H	-3.71027700	3.91291600	1.11536900
H	-7.38454600	0.19030700	-1.73281900
H	-7.41100000	2.73788100	-1.60323800
H	-7.37637600	-2.36040300	-1.82606800
O	-0.76829200	1.04243700	3.15200400
C	-0.19324200	-0.02492600	3.20200700
N	-0.83183000	-1.24890100	3.13942800
N	1.18040200	-0.14245800	3.30859100
C	-0.25405100	-2.52481100	3.15739500
H	-1.84115300	-1.21252200	3.03824200
C	1.84451800	-1.34862000	3.35961700
H	1.68513000	0.73361800	3.32038600
C	1.20624100	-2.53333300	3.30346500
O	-0.94629200	-3.51763100	3.04205400
H	2.92439900	-1.27644500	3.44382100
C	1.88463800	-3.86595400	3.37622800
H	1.59441300	-4.39927400	4.28711800
H	1.58398100	-4.49364100	2.53179700
H	2.97216800	-3.75426000	3.36351900

Graphane-C

C	-5.14231900	1.40242600	-0.58358700
C	-5.87277100	2.64701600	-0.02488400
C	-3.66946500	1.38798300	-0.12588500
C	-8.06108600	1.37014700	-0.03798200
C	-7.35032400	2.65691500	-0.49167200
C	-5.16460300	3.94449900	-0.48395600
C	-2.96178800	2.68039700	-0.55882700
C	-8.08846300	3.89194200	0.06067000
C	-5.90889600	5.16988400	0.08885700
C	-3.68837100	3.93584000	-0.03941700
C	-1.49516000	2.66463500	-0.09569400
C	-7.37706700	5.18527900	-0.35275700
H	-5.84954700	5.16362300	1.19353100
C	-2.95584800	5.19731500	-0.51447400

C	-0.75221100	1.41469400	-0.59760000
C	-0.74678000	3.94928800	-0.48605200
H	-7.89401400	6.05787400	0.08806600
C	-1.51007600	5.19783500	-0.03556700
H	-2.97371600	5.23538500	-1.61253400
C	0.70828900	1.39423700	-0.11309200
C	0.69160800	3.92312400	0.05319800
H	-1.01303000	6.09939700	-0.40557300
C	1.44962200	2.69261600	-0.47165100
C	1.45025800	5.21722800	-0.25386900
C	2.90903100	2.66664900	0.01526300
C	2.89180700	5.17334000	0.23588100
H	1.43513800	5.38927700	-1.34132700
C	3.63421000	1.42757100	-0.53019100
C	3.63723300	3.97167500	-0.35965800
H	3.39833200	6.11328700	-0.01536600
C	5.09406700	1.40298400	-0.03049300
C	5.10707800	3.94239400	0.10634200
C	5.83031200	2.69531000	-0.45738200
C	5.85384800	5.21727200	-0.34178100
C	7.29860100	2.66910400	0.03716100
H	5.34655300	6.11530600	0.05933800
C	7.31516300	5.19938400	0.12168000
C	8.03981200	3.95008200	-0.39230300
C	8.02475800	1.42830300	-0.51068400
H	7.83395200	6.10924300	-0.23377000
C	8.05938700	-3.61244200	-0.78800300
C	8.03136900	-1.09217100	-0.64231200
C	7.34269300	-4.91261900	-0.40581100
C	7.31270600	-2.38719700	-0.22580100
C	7.29568900	0.14067700	-0.08901200
C	5.87988200	-4.88976200	-0.86408400
H	7.86465200	-5.77732600	-0.85672200
C	5.84344300	-2.37004700	-0.71790600
C	5.83048900	0.16261600	-0.58884500
C	5.12811700	-3.67226900	-0.28413000
H	5.83274900	-4.86895900	-1.96942100
C	5.10083900	-1.13234200	-0.16047700
C	3.65632100	-3.66235400	-0.74654900
C	3.64024100	-1.11455700	-0.65969200
C	2.91901700	-4.92165400	-0.27365600
C	2.92143300	-2.40547800	-0.24237600
C	2.90698800	0.13153400	-0.13822700
C	1.47460700	-4.92191700	-0.75661400
H	3.43027300	-5.82868800	-0.61923400
C	1.45854200	-2.39413800	-0.72201600
C	1.45054200	0.15038000	-0.62646900
C	0.71287300	-3.67259400	-0.30645500
H	1.45494500	-4.97839800	-1.85631000
C	0.71341200	-1.14005500	-0.23660800

C	-0.73672800	-3.66018800	-0.81545700
C	-0.74899800	-1.12644900	-0.71582700
C	-1.48356700	-4.93744000	-0.42038800
C	-1.48127800	-2.41481900	-0.30573300
C	-1.48373300	0.12247300	-0.20354800
C	-2.93767300	-4.91609300	-0.87264400
H	-0.99334600	-5.81446600	-0.85447500
C	-2.95289900	-2.40272100	-0.75368500
C	-2.95000500	0.13792800	-0.65748500
C	-3.66631100	-3.69227800	-0.30298800
H	-2.97758800	-4.88557600	-1.97111700
C	-3.66140600	-1.15150400	-0.21440300
C	-5.14888500	-3.68011300	-0.72965700
C	-5.13669800	-1.13700600	-0.66691300
C	-5.88116800	-4.94061700	-0.22127200
C	-5.85854900	-2.41767200	-0.18368900
C	-5.85910700	0.11433000	-0.11456900
C	-7.35447900	-4.93901300	-0.64527200
H	-5.38228100	-5.85019700	-0.60629000
C	-7.33973900	-2.40698400	-0.63835500
C	-7.33607000	0.12517800	-0.57902700
C	-8.06721500	-3.67506300	-0.15023700
H	-7.42980400	-5.00773500	-1.74730000
C	-8.05396800	-1.15155100	-0.10759000
H	8.12018300	3.99064200	-1.49506300
H	8.09451900	1.48310700	-1.61312700
H	9.07407100	-1.10490400	-0.27597800
H	9.09797000	-3.62817900	-0.41024000
H	-8.11518000	-3.68220800	0.95521200
H	-9.10432500	-1.14213800	-0.45067500
H	-8.11037800	1.33095500	1.06621600
H	-9.13202000	3.90150900	-0.30342000
H	0.68973800	-1.18037400	0.86699000
H	0.68527900	1.32294300	0.99153900
H	-1.48666000	0.06173000	0.89922300
H	1.47093100	0.20632600	-1.73132600
H	-0.73810900	-1.07955400	-1.82136400
H	-0.73379100	1.46630200	-1.70215100
H	1.47960400	-2.36411200	-1.82816000
H	2.89946100	-2.44331300	0.86225900
H	3.64186600	-1.06886200	-1.76832600
H	2.87620300	0.07501100	0.96398300
H	3.63622100	1.49520400	-1.63775500
H	2.88640100	2.59285600	1.11754800
H	1.47628100	2.76843100	-1.57504100
H	0.63125000	3.82592200	1.15412100
H	-0.68692000	3.97319100	-1.58882000
H	-1.51019300	2.61730600	1.01122700
H	0.66162900	-3.68959500	0.79595300
H	-0.70663400	-3.60602600	-1.91965600

H	-1.48563400	-2.46380300	0.79632600
H	-2.97109100	-2.36476700	-1.85728900
H	-3.62138100	-1.19435900	0.89364400
H	-2.95812200	0.17947100	-1.76037400
H	-3.64237000	1.34471800	0.98448100
H	-2.95955800	2.71932400	-1.66162700
H	5.09169100	1.34564300	1.08378900
H	5.83222900	2.75584200	-1.57117200
H	5.12981300	3.89441100	1.22141900
H	3.61315700	4.06083800	-1.46412000
H	5.81056000	5.31073600	-1.44346500
H	7.36135300	5.23477100	1.22700600
H	9.07742800	3.93164000	-0.01191300
H	7.29778600	2.61947500	1.15287400
H	9.06712600	1.40859400	-0.14367100
H	5.83592300	0.21964900	-1.70301100
H	7.29306000	0.08260300	1.02644000
H	8.10007800	-1.03202900	-1.74456400
H	7.31445800	-2.45427300	0.88888600
H	5.84324400	-2.31630400	-1.83212300
H	5.09968600	-1.18877400	0.95349800
H	8.13674700	-3.53739600	-1.88921200
H	7.39331000	-5.06409900	0.68936400
H	5.37779700	-5.82721000	-0.55724900
H	5.15480300	-3.74040600	0.82939600
H	3.62954900	-3.63992700	-1.85427200
H	-3.60553100	-3.73602500	0.80214600
H	-5.20170100	-3.66656700	-1.84449400
H	-9.11471400	-3.66909900	-0.50181400
H	-7.86145400	-5.83785000	-0.24791700
H	-5.80595500	-4.99814400	0.88145900
H	-3.43454300	-5.84480200	-0.56550000
H	-1.43562600	-5.04326300	0.67361600
H	0.97763700	-5.82204400	-0.38486500
H	2.93067900	-4.95717900	0.82604300
H	-8.09679800	-1.17799500	0.99734400
H	-9.10982200	1.37555800	-0.38663700
H	-8.15101300	3.83456500	1.16375600
H	-7.43975800	5.31610400	-1.45014400
H	-5.41201300	6.10304700	-0.23790800
H	-3.46355800	6.10321600	-0.16115300
H	-1.48782800	5.25300100	1.06459700
H	0.94455700	6.07091000	0.20705000
H	2.89904900	5.09699000	1.33253600
H	-5.82804400	-2.44663200	0.93138000
H	-5.16927700	-1.10686400	-1.78192900
H	-5.83709800	0.07655600	1.00029900
H	-5.17052800	1.44172400	-1.69868700
H	-5.85395200	2.60409500	1.08940500
H	-5.20415700	3.99751800	-1.59853700

H	-3.64874100	3.90952400	1.06867600
H	-7.35985200	0.15592100	-1.69532000
H	-7.37076300	2.70297100	-1.60735900
H	-7.36915300	-2.39056500	-1.75454800
H	-0.45701400	1.89488300	3.28095300
N	-0.92123700	1.00809900	3.40838500
C	-0.21099300	-0.14721500	3.34414900
H	-1.89648800	0.95233800	3.14493800
C	1.21959600	-0.08742600	3.50238900
N	-0.88798400	-1.25808700	3.15117900
C	1.87098100	-1.27371300	3.44751300
H	1.74371100	0.84786000	3.64905200
C	-0.23480700	-2.46147900	3.11273300
N	1.17413500	-2.41917300	3.26546700
H	2.94860400	-1.36610100	3.53554100
O	-0.76314500	-3.54255500	2.93083800
H	1.63742000	-3.31692200	3.20282500

Graphane-U

C	-5.13998400	1.40633900	-0.59247400
C	-5.87280000	2.65195300	-0.03918200
C	-3.67017200	1.39184700	-0.12349000
C	-8.06324200	1.37824600	-0.06773900
C	-7.34695800	2.66405100	-0.51611400
C	-5.15896000	3.94823700	-0.49273600
C	-2.95744100	2.68192100	-0.55426600
C	-8.08725900	3.89978600	0.03183400
C	-5.90601900	5.17409300	0.07535500
C	-3.68599400	3.93653200	-0.03543400
C	-1.49369100	2.66265400	-0.08077500
C	-7.37099200	5.19218800	-0.37635700
H	-5.85344800	5.16686300	1.18054000
C	-2.94914700	5.19816100	-0.50326800
C	-0.75211500	1.41643700	-0.59385600
C	-0.74362500	3.94661500	-0.47108000
H	-7.88946200	6.06538900	0.06137700
C	-1.50584900	5.19441700	-0.01691100
H	-2.96130900	5.23989400	-1.60154300
C	0.70742100	1.39246500	-0.10646600
C	0.69335200	3.91767000	0.07188800
H	-1.00632900	6.09717700	-0.38128500
C	1.45052900	2.69043800	-0.46189300
C	1.45366500	5.21213800	-0.22930800
C	2.90950600	2.65991400	0.02640300
C	2.89506000	5.16477800	0.26091600
H	1.43944300	5.39109200	-1.31584900
C	3.63387400	1.42244100	-0.52252700
C	3.63976100	3.96596400	-0.34085300
H	3.40331400	6.10529400	0.01503600
C	5.09532600	1.39344400	-0.02748000

C	5.10991500	3.93193600	0.12469100
C	5.83116800	2.68806500	-0.44837800
C	5.85738900	5.20920700	-0.31516200
C	7.30095500	2.65707600	0.04123700
H	5.35136800	6.10456300	0.09383100
C	7.31953300	5.18656100	0.14516700
C	8.04196400	3.94079200	-0.38030200
C	8.02422000	1.42024900	-0.51938900
H	7.83828800	6.09883000	-0.20416600
C	8.05284900	-3.61766900	-0.84452500
C	8.02778100	-1.09874800	-0.67483100
C	7.33874200	-4.92090300	-0.46786700
C	7.31122100	-2.39715600	-0.26550400
C	7.29626000	0.12945600	-0.10575300
C	5.87188500	-4.89342700	-0.91282100
H	7.85629300	-5.78177500	-0.93099000
C	5.83833900	-2.37526200	-0.74659700
C	5.82842800	0.15640000	-0.59751300
C	5.12633200	-3.68027900	-0.31592300
H	5.81474400	-4.86365000	-2.01742800
C	5.10047300	-1.14123600	-0.17471800
C	3.64959200	-3.66809700	-0.76180000
C	3.63690900	-1.12025100	-0.66467800
C	2.91816600	-4.92658400	-0.27733200
C	2.92118900	-2.41212500	-0.24600300
C	2.90668600	0.12467400	-0.13547000
C	1.46749800	-4.92749200	-0.74080800
H	3.42307300	-5.83429400	-0.63031100
C	1.45440300	-2.39872800	-0.71336800
C	1.44873300	0.14795600	-0.61886600
C	0.71106100	-3.67555700	-0.28789700
H	1.43229300	-4.98809600	-1.83989800
C	0.71273000	-1.14245200	-0.22717200
C	-0.74103000	-3.66535200	-0.78903800
C	-0.75089600	-1.12718500	-0.70192400
C	-1.48990500	-4.93766900	-0.38253200
C	-1.48383000	-2.41477900	-0.29039500
C	-1.48505700	0.12540200	-0.19816900
C	-2.94324500	-4.92004900	-0.83716300
H	-0.99946100	-5.81939700	-0.80574400
C	-2.95577300	-2.40408500	-0.73763700
C	-2.95047700	0.14098000	-0.65483100
C	-3.67340400	-3.69009700	-0.28311300
H	-2.98052900	-4.90114800	-1.93571000
C	-3.66542000	-1.14670400	-0.21445600
C	-5.15290100	-3.67835700	-0.71885100
C	-5.13888300	-1.13412300	-0.67130100
C	-5.89075800	-4.93514100	-0.20950200
C	-5.86514900	-2.41171100	-0.18637200
C	-5.86241300	0.12017500	-0.12696400

C	-7.35992600	-4.93394500	-0.64772700
H	-5.38998600	-5.84771100	-0.58514800
C	-7.34246200	-2.40142600	-0.65400400
C	-7.33594200	0.13196600	-0.60234800
C	-8.07598700	-3.66649400	-0.16707900
H	-7.42475800	-5.00900200	-1.75012200
C	-8.05970100	-1.14309300	-0.13478100
H	8.11929800	3.98990100	-1.48295100
H	8.08979700	1.48424900	-1.62162700
H	9.07281200	-1.11527100	-0.31533600
H	9.09443500	-3.63709000	-0.47528200
H	-8.13700000	-3.66769100	0.93765300
H	-9.10646300	-1.13305800	-0.48909800
H	-8.12095700	1.34038300	1.03611300
H	-9.12836000	3.91115400	-0.33876600
H	0.69517100	-1.18439100	0.87750700
H	0.67361500	1.32954100	0.99642200
H	-1.49228100	0.08780900	0.90570100
H	1.46868600	0.20114000	-1.72368000
H	-0.74117800	-1.08649700	-1.80718400
H	-0.73429400	1.46822600	-1.69876200
H	1.46469000	-2.37167500	-1.81968600
H	2.90946100	-2.45590400	0.85727600
H	3.63140700	-1.06869500	-1.77296300
H	2.88036700	0.06149300	0.96814600
H	3.63299000	1.49234100	-1.62976200
H	2.88466900	2.58339400	1.12896400
H	1.47921400	2.77138100	-1.56505100
H	0.62916100	3.81100500	1.16997100
H	-0.68235400	3.97482300	-1.57426900
H	-1.50615000	2.60431400	1.02297500
H	0.67345700	-3.68784100	0.81620800
H	-0.71529700	-3.61963400	-1.89320000
H	-1.48525300	-2.46280800	0.81366400
H	-2.96882000	-2.37371200	-1.84097500
H	-3.63716500	-1.18246200	0.89598000
H	-2.95555500	0.17982100	-1.75770000
H	-3.64597800	1.34833700	0.98535500
H	-2.95068500	2.72285100	-1.65748500
H	5.09751400	1.32905100	1.08602900
H	5.82972000	2.75563000	-1.56182800
H	5.13306200	3.87681300	1.23927500
H	3.61583800	4.06052800	-1.44488200
H	5.81169000	5.31142000	-1.41597700
H	7.36804400	5.21338500	1.25061900
H	9.08058500	3.91868800	-0.00291500
H	7.30392600	2.59859100	1.15643700
H	9.06801700	1.39696000	-0.15666800
H	5.82828600	0.22130800	-1.71134100
H	7.29985600	0.06100600	1.00903100

H	8.08953100	-1.02861300	-1.77691400
H	7.32103900	-2.47474500	0.84849800
H	5.82962300	-2.31364900	-1.86032100
H	5.10662100	-1.20704400	0.93867000
H	8.12135000	-3.53296300	-1.94560100
H	7.39881200	-5.08221400	0.62548300
H	5.37190700	-5.83295400	-0.60880300
H	5.16438700	-3.75682400	0.79702000
H	3.60973000	-3.64566400	-1.86923000
H	-3.62106600	-3.72685500	0.82348300
H	-5.19795500	-3.67106100	-1.83439500
H	-9.11967000	-3.66109100	-0.53040300
H	-7.87199000	-5.83005900	-0.25055200
H	-5.82664100	-4.98703300	0.89397100
H	-3.44156400	-5.84493800	-0.52153400
H	-1.44397600	-5.03514000	0.71288900
H	0.97520100	-5.82600500	-0.35876800
H	2.94476700	-4.96019900	0.82157900
H	-8.11490500	-1.16543800	0.96961700
H	-9.10916100	1.38539500	-0.42460600
H	-8.15615600	3.84234100	1.13458700
H	-7.42577700	5.32351600	-1.47404200
H	-5.40493800	6.10663800	-0.24674200
H	-3.45714200	6.10381400	-0.14933200
H	-1.48835800	5.24233000	1.08305900
H	0.94914900	6.06364500	0.23668800
H	2.90122600	5.08216700	1.35705400
H	-5.84589600	-2.43396600	0.92867600
H	-5.16709500	-1.10777800	-1.78673300
H	-5.84915100	0.08619300	0.98807600
H	-5.16011800	1.44554000	-1.70758400
H	-5.86048700	2.60950600	1.07547800
H	-5.18925400	4.00211000	-1.60733500
H	-3.65414800	3.90626700	1.07197000
H	-7.35138700	0.16188700	-1.71878800
H	-7.35966300	2.71080800	-1.63182200
H	-7.36200900	-2.38951900	-1.77053900
O	-0.76366900	1.07448700	3.19195800
C	-0.18503700	0.01146300	3.26179100
N	-0.81331800	-1.21700400	3.21454000
N	1.19385500	-0.08865200	3.38178400
C	-0.22672400	-2.49409800	3.24072400
H	-1.82225500	-1.18811500	3.10649100
C	1.86682000	-1.28402700	3.44114100
H	1.68679400	0.79444000	3.38444500
C	1.22629000	-2.46622100	3.38740600
O	-0.91568000	-3.48726400	3.12962100
H	2.94529800	-1.20397200	3.52352500
H	1.75371500	-3.40919100	3.42447800

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C	-5.05666600	1.42700800	-0.62664800
C	-5.78610700	2.66985100	-0.06300000
C	-3.59129500	1.39843000	-0.14422300
C	-7.98432300	1.40884400	-0.12552200
C	-7.25763400	2.69745300	-0.54793600
C	-5.06382800	3.96728700	-0.49951400
C	-2.86879500	2.68680400	-0.56452400
C	-7.99335500	3.92886200	0.01553100
C	-5.80455900	5.19013700	0.08341000
C	-3.59038000	3.94499300	-0.04457900
C	-1.40442500	2.66031500	-0.09265300
C	-7.26849600	5.22316200	-0.37098500
H	-5.75448300	5.16838700	1.18840400
C	-2.84797700	5.20266800	-0.51481400
C	-0.66795400	1.40603900	-0.59272300
C	-0.64750200	3.93808000	-0.49177500
H	-7.78305500	6.09257100	0.07885700
C	-1.40140100	5.19146600	-0.03864000
H	-2.86723300	5.24549700	-1.61285500
C	0.78951700	1.37635800	-0.10065400
C	0.79276200	3.90704500	0.04183000
H	-0.89955900	6.08994300	-0.40953000
C	1.54261800	2.66553500	-0.46898800
C	1.56177000	5.18911500	-0.28934300
C	2.99703300	2.63268000	0.03312200
C	2.99915800	5.14417500	0.21223900
H	1.55477300	5.33846200	-1.38039400
C	3.71875500	1.38146100	-0.48854800
C	3.74143900	3.92566700	-0.35209100
H	3.51512800	6.07492400	-0.05404100
C	5.17157100	1.34901200	0.03017700
C	5.20260400	3.89045800	0.14015900
C	5.92538800	2.63152200	-0.39643500
C	5.96815500	5.15433300	-0.30748300
C	7.38386100	2.59863400	0.12599200
H	5.46026800	6.06066500	0.07369500
C	7.41958000	5.12987400	0.18578500
C	8.14404600	3.86957300	-0.30080500
C	8.11075600	1.34772400	-0.39726100
H	7.95284100	6.03193700	-0.16768800
C	8.11072900	-3.69093500	-0.66629100
C	8.09967500	-1.17171000	-0.51854500
C	7.37446800	-4.98592300	-0.30467000
C	7.36113100	-2.46077400	-0.11857900
C	7.36243700	0.06838600	0.01650100
C	5.92364500	-4.94973400	-0.79911800
H	7.90045600	-5.85415300	-0.74345300
C	5.90290800	-2.43017800	-0.64189100
C	5.90685500	0.10007700	-0.51038500

C	5.16800000	-3.72896100	-0.23124400
H	5.90402100	-4.92290500	-1.90496800
C	5.16006400	-1.18870400	-0.09255300
C	3.70755700	-3.70209400	-0.72658500
C	3.70702900	-1.15806100	-0.61103600
C	2.95362200	-4.96588200	-0.29220400
C	2.97353400	-2.44772800	-0.21390300
C	2.97698600	0.09310000	-0.09581100
C	1.51581300	-4.94406300	-0.79416200
H	3.46038300	-5.86828700	-0.65585800
C	1.51844500	-2.41805400	-0.71512500
C	1.52688600	0.12406700	-0.60144200
C	0.75964500	-3.69758600	-0.32673300
H	1.50750700	-4.97477500	-1.89498200
C	0.77800700	-1.16356900	-0.22259600
C	-0.68598900	-3.66581900	-0.84518200
C	-0.68026100	-1.13298900	-0.71251000
C	-1.44987300	-4.94469200	-0.48988900
C	-1.42871600	-2.42112300	-0.33109900
C	-1.41228000	0.11902400	-0.20367200
C	-2.89700000	-4.90462600	-0.96211500
H	-0.95811600	-5.81662400	-0.93095600
C	-2.89361300	-2.39212200	-0.80123700
C	-2.87310600	0.14776600	-0.67680100
C	-3.62719600	-3.68304700	-0.38961400
H	-2.91739400	-4.85751500	-2.05998400
C	-3.60391500	-1.14057800	-0.26551300
C	-5.09986800	-3.65220000	-0.84644400
C	-5.06967900	-1.11039300	-0.74642600
C	-5.85278500	-4.91532200	-0.37596700
C	-5.81099900	-2.39234300	-0.29683300
C	-5.79186000	0.13857900	-0.18836300
C	-7.31579000	-4.89396600	-0.83396200
H	-5.35333500	-5.82241300	-0.76638000
C	-7.28213700	-2.36237900	-0.78248100
C	-7.26045500	0.16840600	-0.67784800
C	-8.02989000	-3.63311200	-0.33365600
H	-7.36598200	-4.94290900	-1.93866600
C	-7.99701000	-1.11101700	-0.24369700
H	8.24676300	3.89837100	-1.40200800
H	8.20444600	1.39451900	-1.49824800
H	9.13327300	-1.19282900	-0.12774900
H	9.13970300	-3.71602200	-0.26363100
H	-8.10579400	-3.65880800	0.76979200
H	-9.04011500	-1.08677100	-0.60814700
H	-8.04919500	1.35214800	0.97705000
H	-9.03295100	3.95153400	-0.35899000
H	0.75226400	-1.21583900	0.88191300
H	0.76122300	1.32254200	1.00305200
H	-1.42731300	0.06806200	0.90210100

H	1.56155700	0.17702900	-1.70615100
H	-0.65863300	-1.07765300	-1.81705700
H	-0.64529200	1.45498900	-1.69740700
H	1.55264700	-2.37402400	-1.82035100
H	2.93737100	-2.49942800	0.88871200
H	3.72448900	-1.10570600	-1.71955000
H	2.93634000	0.03974600	1.00650700
H	3.73603200	1.43696600	-1.59689800
H	2.96167500	2.57466400	1.13486900
H	1.57811100	2.72995700	-1.57312200
H	0.73606800	3.82574500	1.14245300
H	-0.59420900	3.95867900	-1.59526000
H	-1.41982100	2.61629300	1.01348100
H	0.71482600	-3.73068900	0.77660300
H	-0.64479000	-3.59226300	-1.94706500
H	-1.44707800	-2.47971500	0.77458400
H	-2.88561100	-2.33949300	-1.90377100
H	-3.59494000	-1.19512300	0.84315000
H	-2.86073000	0.20076200	-1.77910400
H	-3.57961700	1.34704700	0.96501200
H	-2.85882100	2.73149300	-1.66735600
H	5.15316500	1.29902800	1.14497600
H	5.94834400	2.68013300	-1.51049300
H	5.20435500	3.85421400	1.25614200
H	3.73674200	3.99716100	-1.45826600
H	5.94735000	5.23553500	-1.41064700
H	7.44308300	5.17557800	1.29150900
H	9.17340600	3.84648600	0.10095700
H	7.36118300	2.55890600	1.24190400
H	9.14456200	1.32187300	-0.00731600
H	5.93317100	0.15382600	-1.62437500
H	7.33800500	0.01483900	1.13198400
H	8.19411400	-1.11285100	-1.61889800
H	7.33777400	-2.52883000	0.99592500
H	5.92679000	-2.37007100	-1.75540800
H	5.14184500	-1.24656400	1.02182500
H	8.21478300	-3.61359100	-1.76503300
H	7.39580000	-5.13865400	0.79145300
H	5.40771900	-5.88453600	-0.50838100
H	5.16766200	-3.80176000	0.88289500
H	3.70532000	-3.65954800	-1.83427100
H	-3.59510500	-3.74553900	0.71720700
H	-5.12862000	-3.62002000	-1.96219000
H	-9.06873700	-3.61255200	-0.71036700
H	-7.83922100	-5.79561100	-0.46508900
H	-5.80505700	-4.99274400	0.72660900
H	-3.40615800	-5.83403600	-0.67864100
H	-1.42144400	-5.08258400	0.60279300
H	1.00780200	-5.84912700	-0.44914500
H	2.95105100	-5.02768900	0.80514700

H	-8.06355700	-1.15598700	0.85933000
H	-9.02801500	1.42840400	-0.48856700
H	-8.06729100	3.85551400	1.11696400
H	-7.32013700	5.37174300	-1.46667400
H	-5.29722200	6.12381300	-0.22566100
H	-3.34894200	6.11065400	-0.15700100
H	-1.37546800	5.24457500	1.06110000
H	1.06102400	6.05646400	0.15089300
H	2.99600500	5.08988000	1.30996800
H	-5.80618000	-2.43712000	0.81766000
H	-5.08063500	-1.06260500	-1.86132900
H	-5.78965800	0.08612900	0.92597900
H	-5.06573100	1.48219600	-1.74141400
H	-5.78032300	2.61470300	1.05093300
H	-5.09429700	4.03482000	-1.61360800
H	-3.55738100	3.91486400	1.06306500
H	-7.26464400	0.22062500	-1.79366300
H	-7.26349500	2.76231900	-1.66290800
H	-7.28765300	-2.32517600	-1.89867200
C	0.20792500	-0.11336200	3.77878000
C	-1.20797200	-0.00723900	4.34981300
C	-2.07027200	-1.19152900	3.90495200
C	-1.42096000	-2.52525300	4.28267000
C	-0.00652200	-2.62848600	3.70775900
C	0.86299000	-1.44721900	4.14631600
H	-3.07476600	-1.11739300	4.33660900
H	-1.15526500	0.00773300	5.44773900
H	-1.67156100	0.93700900	4.04022300
H	0.15230700	-0.03647500	2.68372100
H	0.82528000	0.72510500	4.12165300
H	-1.37296100	-2.60598800	5.37800800
H	-2.03636100	-3.36101900	3.92917700
H	0.45953900	-3.57662900	3.99962700
H	-0.07173800	-2.63236900	2.61024000
H	1.00846400	-1.49083600	5.23513100
H	1.85778000	-1.51914700	3.68990700
H	-2.19202600	-1.15325700	2.81190700

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C	-5.14353100	1.39229600	-0.54369000
C	-5.87320900	2.62986700	0.03114000
C	-3.67052800	1.37366500	-0.08456300
C	-8.06263600	1.35277300	0.00326700
C	-7.35211700	2.64651900	-0.43113400
C	-5.16665300	3.93235100	-0.41619300
C	-2.96331400	2.66794500	-0.51203300
C	-8.08808100	3.87315100	0.14238600
C	-5.90779300	5.15049000	0.17597800
C	-3.68711100	3.92009800	0.01893400
C	-1.49385500	2.65028800	-0.05624800

C	-7.37851600	5.17218100	-0.25658900
H	-5.84102800	5.13092000	1.28006200
C	-2.95893200	5.18365900	-0.45743300
C	-0.75396800	1.40181600	-0.56611700
C	-0.74942700	3.93464000	-0.45670800
H	-7.89266600	6.03852500	0.19951800
C	-1.50790000	5.18201400	0.00553000
H	-2.98881200	5.22718700	-1.55518900
C	0.70752900	1.38062800	-0.08555100
C	0.69576100	3.91098200	0.06462700
H	-1.01540100	6.08465300	-0.36803300
C	1.44724900	2.67587200	-0.45930900
C	1.45169700	5.20051600	-0.26781200
C	2.91087800	2.65221800	0.01572200
C	2.89810400	5.16158900	0.20816900
H	1.42593000	5.35887000	-1.35734200
C	3.63051200	1.40787300	-0.52517200
C	3.63696300	3.95220200	-0.37997500
H	3.40285700	6.09802600	-0.05989800
C	5.09493800	1.38596600	-0.03912100
C	5.11067700	3.92644700	0.07440500
C	5.82858400	2.67378900	-0.48365200
C	5.85497400	5.19671100	-0.39086000
C	7.30072400	2.65089200	-0.00058100
H	5.35122300	6.09840000	0.00638500
C	7.31983200	5.18180000	0.06152400
C	8.03963200	3.92748200	-0.44721900
C	8.02207100	1.40470100	-0.54281500
H	7.83650400	6.08817500	-0.30521300
C	8.05073000	-3.63899400	-0.77116700
C	8.02560400	-1.11704200	-0.65167700
C	7.33487500	-4.93405300	-0.37020000
C	7.30802200	-2.40712300	-0.21798600
C	7.29465000	0.12153900	-0.10451600
C	5.86992900	-4.91510200	-0.82210200
H	7.85416700	-5.80458800	-0.81228300
C	5.83607500	-2.39324000	-0.70195400
C	5.82594400	0.14063400	-0.59391700
C	5.12189600	-3.69067600	-0.25180800
H	5.81777400	-4.90581900	-1.92720500
C	5.09834600	-1.15014700	-0.15005000
C	3.64843600	-3.68290200	-0.70770900
C	3.63461100	-1.13400400	-0.63872800
C	2.91099400	-4.93606700	-0.21792700
C	2.91799400	-2.42184500	-0.20900500
C	2.90614300	0.11513600	-0.11761000
C	1.46822400	-4.94220300	-0.70607800
H	3.42088000	-5.84825200	-0.55193900
C	1.45559000	-2.40864900	-0.68838400
C	1.44677500	0.13368200	-0.59672600

C	0.70479700	-3.68612300	-0.27763800
H	1.45190000	-5.01294300	-1.80506100
C	0.71004100	-1.15512500	-0.20150800
C	-0.73475600	-3.66855400	-0.81391400
C	-0.74844400	-1.13655000	-0.69160800
C	-1.48997000	-4.95555300	-0.47033900
C	-1.48499400	-2.42897000	-0.30096500
C	-1.48421900	0.10911400	-0.17237300
C	-2.93983300	-4.91967700	-0.93511600
H	-0.99305900	-5.81924000	-0.92242200
C	-2.95360400	-2.41009600	-0.75753000
C	-2.95024900	0.12909100	-0.62785100
C	-3.67241700	-3.70816000	-0.34422900
H	-2.96680900	-4.85942800	-2.03216500
C	-3.66529100	-1.16516400	-0.20848400
C	-5.15283900	-3.68584600	-0.77611400
C	-5.13924900	-1.14469800	-0.66494400
C	-5.88865500	-4.95671500	-0.29947300
C	-5.86376400	-2.43361200	-0.20844000
C	-5.86197500	0.09819500	-0.09418100
C	-7.35976900	-4.94363600	-0.73112900
H	-5.38942100	-5.85773200	-0.70417500
C	-7.34305300	-2.41248300	-0.66935600
C	-7.33833900	0.11760400	-0.56032000
C	-8.07393400	-3.69014400	-0.21254800
H	-7.42910700	-4.98769400	-1.83503600
C	-8.05810000	-1.16772700	-0.11556000
H	8.11076900	3.95808200	-1.55084200
H	8.08324800	1.44966900	-1.64609500
H	9.07051000	-1.12744000	-0.29208800
H	9.09125000	-3.65133900	-0.39897400
H	-8.13007500	-3.72090500	0.89184700
H	-9.10740900	-1.15060800	-0.46213300
H	-8.10965800	1.29608900	1.10663700
H	-9.13336400	3.88795400	-0.21632600
H	0.66920800	-1.19626100	0.90174200
H	0.68546500	1.31989600	1.01919600
H	-1.47619400	0.04585900	0.93059600
H	1.46394000	0.18722500	-1.70215100
H	-0.73347100	-1.08132800	-1.79699300
H	-0.73968700	1.45560600	-1.67083600
H	1.47828100	-2.38003900	-1.79476800
H	2.90388300	-2.45175600	0.89470000
H	3.62775800	-1.09323800	-1.74787400
H	2.88877800	0.06354100	0.98528700
H	3.62249300	1.46572100	-1.63355100
H	2.89791500	2.58912700	1.11798100
H	1.46462700	2.74335500	-1.56375900
H	0.64973500	3.82413700	1.16542600
H	-0.70481600	3.95912900	-1.56047900

H	-1.49924400	2.60360300	1.05002900
H	0.64265700	-3.69062000	0.82642200
H	-0.68096000	-3.59448400	-1.91526400
H	-1.48377900	-2.47682300	0.80290700
H	-2.96067200	-2.35171900	-1.85982100
H	-3.63674200	-1.22163300	0.90086200
H	-2.95533800	0.18253000	-1.73023700
H	-3.64172500	1.32256400	1.02453700
H	-2.96675600	2.71421400	-1.61477500
H	5.10191400	1.33718700	1.07583600
H	5.82139400	2.72409400	-1.59782800
H	5.14167800	3.88802900	1.18973400
H	3.60421500	4.02940000	-1.48535200
H	5.80296500	5.28013400	-1.49285600
H	7.37390100	5.22582600	1.16620900
H	9.08006700	3.91143100	-0.07486100
H	7.30824000	2.61102300	1.11552800
H	9.06681600	1.38719500	-0.18299100
H	5.82287800	0.18926900	-1.70832600
H	7.29924500	0.07333500	1.01151300
H	8.08615000	-1.06709200	-1.75476900
H	7.31514400	-2.46239100	0.89747700
H	5.82900800	-2.34913600	-1.81635300
H	5.10335800	-1.19767900	0.96503700
H	8.12140300	-3.57591000	-1.87343300
H	7.38942700	-5.07108300	0.72679400
H	5.36853000	-5.84829500	-0.50207900
H	5.15243800	-3.74617500	0.86277300
H	3.61655600	-3.67132400	-1.81579700
H	-3.62224900	-3.77917100	0.76163700
H	-5.20024800	-3.64828500	-1.89101100
H	-9.11937300	-3.67543200	-0.57082800
H	-7.87023800	-5.85066100	-0.35747500
H	-5.82065600	-5.04011900	0.80145700
H	-3.44212100	-5.85540000	-0.65982600
H	-1.45745900	-5.10688300	0.62075700
H	0.96852400	-5.83792100	-0.32515600
H	2.92032700	-4.95469700	0.88132200
H	-8.10533800	-1.21507400	0.98822600
H	-9.11198400	1.36452900	-0.34339200
H	-8.14459600	3.80056100	1.24483300
H	-7.44739600	5.31866000	-1.35163400
H	-5.41188400	6.08731400	-0.14211300
H	-3.46292500	6.08782400	-0.09409300
H	-1.47279700	5.23352200	1.10516800
H	0.95213600	6.06080100	0.18759300
H	2.91566800	5.09819800	1.30530200
H	-5.83994500	-2.48329500	0.90532800
H	-5.16760700	-1.09439700	-1.77959800
H	-5.84166600	0.04520700	1.01968900

H	-5.17018100	1.44734000	-1.65818400
H	-5.85002700	2.57501300	1.14475500
H	-5.21260100	3.99882700	-1.52977800
H	-3.63956800	3.88846800	1.12617300
H	-7.36030000	0.17016100	-1.67596400
H	-7.37546100	2.71037800	-1.54595100
H	-7.36714400	-2.37195500	-1.78524400
C	0.93928600	-0.05475200	3.94560400
C	-0.58050600	-0.12848100	3.82376800
C	-0.52004300	-2.55326000	3.71374500
C	1.00165100	-2.56256600	3.83318800
C	1.48395300	-1.32760200	4.59744900
H	-1.02073200	-0.12643000	4.83947100
H	-0.96456100	0.75182500	3.29421700
H	1.36668000	0.05180500	2.93964700
H	1.22386900	0.83174600	4.52262400
H	-0.95803500	-2.66966800	4.72359800
H	-0.86055900	-3.39950800	3.10513000
H	1.33024500	-3.48207500	4.32968500
H	1.43201000	-2.55790000	2.82285900
H	1.12347300	-1.38303100	5.63460200
H	2.57797300	-1.30225000	4.64012800
N	-0.95306500	-1.31891200	3.06448000
H	-1.96140700	-1.33790100	2.92823300

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C	-5.00188300	1.43903900	-0.64076500
C	-5.73214400	2.68366600	-0.08203200
C	-3.54138400	1.40283600	-0.14327900
C	-7.93501000	1.43205200	-0.17074400
C	-7.19844700	2.71859300	-0.58217800
C	-5.00045600	3.97939200	-0.50764800
C	-2.81052500	2.68965400	-0.55473600
C	-7.93517900	3.95159900	-0.02325500
C	-5.74211900	5.20374100	0.07113700
C	-3.53151400	3.94974500	-0.03874000
C	-1.34987000	2.65728200	-0.07200600
C	-7.20110400	5.24402700	-0.39852700
H	-5.70385000	5.17822300	1.17644300
C	-2.78036700	5.20646900	-0.49802400
C	-0.61552100	1.39908500	-0.56508100
C	-0.58593100	3.93293100	-0.46477700
H	-7.71686500	6.11429700	0.04806200
C	-1.33726600	5.18778700	-0.01177800
H	-2.79114100	5.25376000	-1.59600100
C	0.83868500	1.36614800	-0.06375700
C	0.85300800	3.89696200	0.07206400
H	-0.82948800	6.08600000	-0.37523700
C	1.59816800	2.65103200	-0.43478600
C	1.62676000	5.17580800	-0.26157100

C	3.05371400	2.61522300	0.06351200
C	3.06583500	5.12638300	0.23451700
H	1.61681400	5.32444600	-1.35268400
C	3.76892000	1.35857300	-0.45377500
C	3.80067000	3.90390500	-0.33085900
H	3.58421900	6.05474500	-0.03555800
C	5.22393100	1.32487700	0.05896800
C	5.26527800	3.86649500	0.15094100
C	5.97976900	2.60126900	-0.38199300
C	6.03161900	5.12450300	-0.31180500
C	7.44182000	2.56735500	0.13018700
H	5.52971900	6.03523600	0.06682900
C	7.48699400	5.09875300	0.16957600
C	8.20307800	3.83205300	-0.31293800
C	8.16038900	1.30926200	-0.38732100
H	8.02040200	5.99606700	-0.19558600
C	8.14066900	-3.73293900	-0.59824300
C	8.13956300	-1.21174500	-0.48201800
C	7.40222200	-5.02035400	-0.21453700
C	7.39904200	-2.49315200	-0.06156200
C	7.41040500	0.03680900	0.04427500
C	5.94830300	-4.98548600	-0.69987600
H	7.92219800	-5.89619500	-0.64528300
C	5.93780200	-2.46389200	-0.57637900
C	5.95179400	0.06841500	-0.47403100
C	5.20041700	-3.75432100	-0.14421100
H	5.92161600	-4.97368800	-1.80588500
C	5.20229100	-1.21300500	-0.03888600
C	3.73748800	-3.72910400	-0.63251700
C	3.74756500	-1.18285300	-0.55299600
C	2.97962900	-4.98168600	-0.17325900
C	3.00978300	-2.46421000	-0.13761100
C	3.02334400	0.07614400	-0.04940700
C	1.54205800	-4.96463500	-0.67616400
H	3.48320600	-5.89302900	-0.51875200
C	1.55524500	-2.43554100	-0.64023400
C	1.57312300	0.10841300	-0.55451700
C	0.78793200	-3.70603900	-0.23845300
H	1.53507600	-5.01947000	-1.77602900
C	0.81562400	-1.17224900	-0.16941500
C	-0.65091400	-3.67443400	-0.77519000
C	-0.63661000	-1.13977000	-0.67649000
C	-1.42611800	-4.94502300	-0.41545100
C	-1.39440600	-2.42022000	-0.28778700
C	-1.36780400	0.11663800	-0.17840200
C	-2.86255000	-4.90492700	-0.91905200
H	-0.92931700	-5.82669000	-0.83111500
C	-2.85211300	-2.38869700	-0.78025500
C	-2.82329300	0.14936700	-0.66827600
C	-3.59818600	-3.67415700	-0.37461800

H	-2.85826200	-4.86900800	-2.01753200
C	-3.56417500	-1.13329600	-0.25491600
C	-5.06193800	-3.63970500	-0.85955800
C	-5.02238900	-1.09836600	-0.75981700
C	-5.82817000	-4.90029100	-0.40372900
C	-5.77620200	-2.37679800	-0.32100300
C	-5.74712600	0.15330300	-0.21129400
C	-7.28367100	-4.87143600	-0.88477600
H	-5.32686300	-5.80879400	-0.78806700
C	-7.24009000	-2.34031000	-0.82711600
C	-7.20971500	0.18984800	-0.71763400
C	-7.99975700	-3.60879900	-0.39184600
H	-7.31631000	-4.91636300	-1.99028600
C	-7.95700600	-1.08723400	-0.29488700
H	8.29673000	3.85173400	-1.41515900
H	8.24552000	1.34553500	-1.48939400
H	9.17593300	-1.23213100	-0.09869700
H	9.17231500	-3.75645800	-0.20246600
H	-8.09101400	-3.63633300	0.71034800
H	-8.99540700	-1.05813700	-0.67168500
H	-8.01153900	1.37289700	0.93095100
H	-8.97059200	3.97934600	-0.40870600
H	0.77298100	-1.21085200	0.93591000
H	0.80289100	1.31652000	1.04091100
H	-1.39648000	0.05577700	0.92400100
H	1.60902200	0.15403800	-1.65942000
H	-0.60169800	-1.09405600	-1.78138700
H	-0.58363000	1.44818300	-1.66962400
H	1.59279500	-2.40730000	-1.74580200
H	2.97479200	-2.49977600	0.96544400
H	3.76162800	-1.14365400	-1.66206900
H	2.98457000	0.03305000	1.05313300
H	3.78172800	1.40705200	-1.56248700
H	3.02223400	2.56328900	1.16571100
H	1.63235100	2.71157900	-1.53913400
H	0.79447700	3.81858400	1.17291300
H	-0.52888200	3.95563600	-1.56801700
H	-1.37408600	2.61394300	1.03443600
H	0.72924800	-3.71987700	0.86520200
H	-0.59308600	-3.61718200	-1.87735000
H	-1.42813700	-2.45285100	0.81701800
H	-2.82736600	-2.34225100	-1.88321300
H	-3.56153300	-1.17910400	0.85215500
H	-2.80051700	0.20100000	-1.77101300
H	-3.54232800	1.34801700	0.96572800
H	-2.79071600	2.73640200	-1.65739600
H	5.21042600	1.28446000	1.17415000
H	5.99490200	2.64186400	-1.49652000
H	5.27524300	3.83824500	1.26702500
H	3.78853000	3.97183800	-1.43720000

H	6.00202600	5.19787500	-1.41535200
H	7.51988000	5.15317500	1.27463300
H	9.23562700	3.80849300	0.08044000
H	7.42709400	2.53727800	1.24651700
H	9.19711400	1.28325400	-0.00532100
H	5.97148500	0.11113800	-1.58862900
H	7.39267500	-0.00495900	1.16037800
H	8.22598200	-1.16588900	-1.58364100
H	7.38228300	-2.54713700	1.05381300
H	5.95512700	-2.41840800	-1.69071600
H	5.18780500	-1.25798000	1.07607000
H	8.23729500	-3.67033400	-1.69860900
H	7.43033500	-5.15855000	0.88331800
H	5.43067200	-5.91424500	-0.39324400
H	5.20579500	-3.81202000	0.97068500
H	3.73019800	-3.70537900	-1.74074200
H	-3.59055100	-3.72782600	0.73317300
H	-5.06997400	-3.60664000	-1.97541000
H	-9.03294500	-3.58294600	-0.78320000
H	-7.81678000	-5.77181400	-0.52719700
H	-5.79859200	-4.97938900	0.69925600
H	-3.38148700	-5.82972900	-0.63764000
H	-1.42184000	-5.06508500	0.68021300
H	1.02995700	-5.86024100	-0.31272700
H	2.97738400	-5.02151100	0.92516100
H	-8.03607100	-1.13390200	0.80726700
H	-8.97448200	1.45648500	-0.54503800
H	-8.02090500	3.87538000	1.07708100
H	-7.24041000	5.39539500	-1.49434200
H	-5.22785100	6.13616500	-0.22987600
H	-3.28037800	6.11518900	-0.14046900
H	-1.31869300	5.23617500	1.08843000
H	1.13053400	6.04543500	0.17937700
H	3.06731900	5.07398200	1.33238900
H	-5.78641500	-2.42037700	0.79368000
H	-5.01604500	-1.05053100	-1.87443000
H	-5.75658900	0.10022000	0.90329200
H	-4.99929700	1.49563900	-1.75532500
H	-5.73814500	2.62530600	1.03170700
H	-5.01966900	4.04982600	-1.62181400
H	-3.50942700	3.91652500	1.06925900
H	-7.20074700	0.24434900	-1.83323000
H	-7.19227800	2.78613900	-1.69694800
H	-7.22985600	-2.30036700	-1.94309500
C	-0.26223300	-0.07403300	3.93659800
C	-1.76680700	0.02286300	3.70784800
C	-2.01723400	-2.31065800	3.58350700
C	-0.52873500	-2.55865400	3.80335000
C	0.07942100	-1.40688100	4.60725800
H	-2.29394200	0.05314000	4.67697300

H	-2.03067600	0.92478400	3.14667300
H	0.24311600	-0.01030100	2.96383500
H	0.07686600	0.77402000	4.54189100
H	-2.54974100	-2.33126500	4.54985000
H	-2.45955700	-3.07183900	2.93301500
H	-0.38221900	-3.51868300	4.31065400
H	-0.03737100	-2.62340300	2.82338800
H	-0.33757200	-1.41675400	5.62433500
H	1.16314200	-1.52831700	4.70382900
O	-2.24625700	-1.06856400	2.94438800

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C	-5.01304200	1.46728700	-0.69402800
C	-5.74198500	2.70683100	-0.12244700
C	-3.55117800	1.42805800	-0.20164000
C	-7.94394600	1.45448300	-0.21173700
C	-7.21010200	2.74451000	-0.61694100
C	-5.01240000	4.00636300	-0.54004400
C	-2.82164300	2.71864800	-0.60328400
C	-7.94553200	3.97282800	-0.04620700
C	-5.75308300	5.22559400	0.05061900
C	-3.54227300	3.97398600	-0.07518700
C	-1.36012800	2.68258000	-0.12320100
C	-7.21354500	5.26850700	-0.41418200
H	-5.71149900	5.19130900	1.15562900
C	-2.79266000	5.23442000	-0.52668600
C	-0.62609400	1.42966000	-0.63017000
C	-0.59717000	3.96167100	-0.50672100
H	-7.72841600	6.13501300	0.04075100
C	-1.34861100	5.21271900	-0.04338800
H	-2.80585700	5.29008600	-1.62423700
C	0.82986200	1.39238300	-0.13406700
C	0.84151100	3.92138500	0.03014200
H	-0.84184700	6.11366300	-0.40139000
C	1.58880800	2.68189500	-0.48916200
C	1.61570500	5.20375700	-0.28800600
C	3.04123700	2.64034200	0.01806300
C	3.05158000	5.15014100	0.21688200
H	1.61193100	5.36218900	-1.37776000
C	3.76103400	1.39018500	-0.50863300
C	3.79150400	3.93360100	-0.35473100
H	3.57138400	6.08121700	-0.04069200
C	5.21129000	1.34966100	0.01685000
C	5.25092700	3.89020500	0.14208100
C	5.97133500	2.63195900	-0.39922400
C	6.02222100	5.15399900	-0.29584700
C	7.42765800	2.59122500	0.12864100
H	5.51596900	6.05992500	0.08851400
C	7.47185900	5.12200700	0.20218800
C	8.19372500	3.86180700	-0.28855300

C	8.15220200	1.34053100	-0.39831500
H	8.00935100	6.02407400	-0.14490500
C	8.13627000	-3.69675400	-0.69120300
C	8.13311600	-1.17828900	-0.53160800
C	7.39381500	-4.99091700	-0.33946500
C	7.38837300	-2.46667600	-0.14106000
C	7.39784900	0.06176700	0.00613900
C	5.94555600	-4.94725100	-0.84075700
H	7.91890700	-5.85875400	-0.78018800
C	5.93274600	-2.42851600	-0.67101200
C	5.94469400	0.10106300	-0.52692300
C	5.19115100	-3.72675400	-0.27067900
H	5.93153300	-4.91483300	-1.94659200
C	5.19144600	-1.18722700	-0.11918900
C	3.73361100	-3.69191800	-0.77423900
C	3.74115300	-1.14891900	-0.64509100
C	2.97240400	-4.95584200	-0.35317800
C	3.00069200	-2.43797500	-0.25880300
C	3.01269100	0.10208000	-0.12761000
C	1.53838800	-4.92527100	-0.86536200
H	3.47880200	-5.85766000	-0.71881500
C	1.54861900	-2.40008800	-0.76837000
C	1.56525300	0.14125800	-0.64026500
C	0.78301300	-3.67988000	-0.39388000
H	1.53806500	-4.94731500	-1.96635200
C	0.80902500	-1.14573600	-0.27398400
C	-0.65980600	-3.63920900	-0.91875500
C	-0.64623900	-1.10749200	-0.77205200
C	-1.42983400	-4.91737900	-0.57410000
C	-1.40091800	-2.39513300	-0.40132500
C	-1.37740600	0.14205100	-0.25611800
C	-2.87335400	-4.87012100	-1.05613000
H	-0.93815400	-5.78987900	-1.01443300
C	-2.86180200	-2.35772600	-0.88387900
C	-2.83392100	0.18017900	-0.74176100
C	-3.60315200	-3.64796500	-0.48425500
H	-2.88502000	-4.81865600	-2.15398400
C	-3.57181800	-1.10815900	-0.34258500
C	-5.07167300	-3.61004700	-0.95394700
C	-5.03336300	-1.06917800	-0.83625600
C	-5.83269100	-4.87381400	-0.49818200
C	-5.78263400	-2.35157400	-0.40121000
C	-5.75541100	0.17735200	-0.27254000
C	-7.29188400	-4.84416600	-0.96786100
H	-5.33326800	-5.78002700	-0.89019300
C	-7.25013900	-2.31308900	-0.89676200
C	-7.22067500	0.21665100	-0.77094900
C	-8.00539700	-3.58474100	-0.46306800
H	-7.33322800	-4.88391700	-2.07322700
C	-7.96441900	-1.06382100	-0.35226000

H	8.30052000	3.89620200	-1.38922400
H	8.25013300	1.39263900	-1.49872500
H	9.16498900	-1.20484100	-0.13660200
H	9.16328800	-3.72739900	-0.28392600
H	-8.08840400	-3.61837100	0.63973500
H	-9.00518500	-1.03304500	-0.72233400
H	-8.01542900	1.38716900	0.88994200
H	-8.98235200	4.00283100	-0.42773300
H	0.77578200	-1.20272000	0.83034600
H	0.79898200	1.33149000	0.96927000
H	-1.40636700	0.07373800	0.84793800
H	1.60543200	0.20184500	-1.74429700
H	-0.61733900	-1.04449900	-1.87627300
H	-0.59846700	1.48872500	-1.73433800
H	1.58980200	-2.34941900	-1.87301300
H	2.95791500	-2.49527900	0.84361700
H	3.76464600	-1.09105500	-1.75314000
H	2.96607100	0.04297400	0.97435000
H	3.78366000	1.45266600	-1.61643500
H	3.00118300	2.57496800	1.11937000
H	1.62807400	2.75563000	-1.59250500
H	0.78201200	3.83076100	1.13005800
H	-0.54054200	3.99310600	-1.60975500
H	-1.38187800	2.62863500	0.98269000
H	0.73205000	-3.72190300	0.70898400
H	-0.61247900	-3.56080200	-2.02012500
H	-1.42992400	-2.45378900	0.70359000
H	-2.84486500	-2.29956800	-1.98639100
H	-3.56638100	-1.17039700	0.76422000
H	-2.81333500	0.24375400	-1.84371000
H	-3.54784400	1.36407600	0.90690800
H	-2.80393300	2.77502600	-1.70551600
H	5.18757600	1.29378300	1.13117800
H	5.99874600	2.68704200	-1.51289800
H	5.24889700	3.84765600	1.25780000
H	3.79058400	4.01364100	-1.46027600
H	6.00545200	5.24144800	-1.39862400
H	7.49186300	5.16201700	1.30816800
H	9.22158600	3.83305800	0.11668900
H	7.40058700	2.54577700	1.24421400
H	9.18450800	1.30913000	-0.00482900
H	5.97613300	0.16049500	-1.64052200
H	7.36847000	0.00301300	1.12120000
H	8.23254200	-1.11448900	-1.63128400
H	7.35971300	-2.53992800	0.97294500
H	5.96222800	-2.36290100	-1.78413700
H	5.16752500	-1.25057400	0.99464200
H	8.24583300	-3.61442100	-1.78907500
H	7.40947900	-5.14925100	0.75590400
H	5.42501300	-5.88177600	-0.55748100

H	5.18450100	-3.80523300	0.84292300
H	3.73816700	-3.64233600	-1.88158000
H	-3.58091700	-3.71422600	0.62252900
H	-5.09084100	-3.57013800	-2.06951500
H	-9.04150800	-3.55774000	-0.84649700
H	-7.82125000	-5.74677400	-0.61022900
H	-5.79438000	-4.95771300	0.60436300
H	-3.38766000	-5.79922400	-0.78057600
H	-1.40985400	-5.05898600	0.51853700
H	1.02462900	-5.83122600	-0.53147500
H	2.96181400	-5.02466200	0.74384000
H	-8.03676000	-1.11779900	0.75017200
H	-8.98521800	1.48097000	-0.58088400
H	-8.02743600	3.88822200	1.05386800
H	-7.25652800	5.42820400	-1.50864700
H	-5.24040800	6.16076100	-0.24449100
H	-3.29223900	6.14012100	-0.16110800
H	-1.32802700	5.25324700	1.05708400
H	1.11662300	6.06910000	0.15802200
H	3.04535300	5.08740000	1.31420700
H	-5.78488300	-2.40344000	0.71339100
H	-5.03545600	-1.01261900	-1.95049700
H	-5.75969800	0.11430500	0.84167400
H	-5.01451200	1.53322800	-1.80809400
H	-5.74401000	2.63940500	0.99090100
H	-5.03486700	4.08565100	-1.65353100
H	-3.51721600	3.93208900	1.03233300
H	-7.21783200	0.27864500	-1.88615500
H	-7.20827800	2.82015800	-1.73118500
H	-7.24797900	-2.26681100	-2.01252300
C	0.12278000	-0.04509200	3.69573900
C	-1.29705200	0.04117300	4.24782400
C	-1.30339600	-2.70078500	4.17578800
C	0.11704500	-2.59407600	3.62834100
C	0.84166600	-1.33281400	4.10400000
H	-1.28671700	0.02977100	5.34447400
H	-1.78655500	0.96607600	3.92888000
H	0.07706300	0.01392500	2.60183700
H	0.69444800	0.82458500	4.04361900
H	-1.29222900	-2.74616200	5.27151100
H	-1.79754200	-3.60567300	3.81031100
H	0.68390900	-3.48287900	3.93231400
H	0.07209900	-2.59699500	2.53244200
H	0.93782100	-1.36248300	5.19889000
H	1.86008900	-1.32413400	3.69827200
S	-2.36259700	-1.31289900	3.65203200

Graphane-S5C

C	-5.12015100	1.47277600	-0.47959100
C	-5.85074100	2.70318800	0.10931600

C	-3.65075500	1.44398700	-0.01031500
C	-8.04174400	1.43118800	0.05258700
C	-7.32664100	2.72904700	-0.36180000
C	-5.13776400	4.01050200	-0.31321100
C	-2.93662300	2.74333000	-0.41045000
C	-8.06383000	3.94966700	0.22267400
C	-5.88142300	5.22169000	0.28978500
C	-3.66239600	3.98799400	0.13567600
C	-1.47113200	2.71457700	0.05823100
C	-7.34859900	5.25216000	-0.15413400
H	-5.82367500	5.18658600	1.39407600
C	-2.92659100	5.25784100	-0.31149100
C	-0.72979000	1.47473100	-0.47019300
C	-0.72022600	4.00370100	-0.31350900
H	-7.86452700	6.11366100	0.30915400
C	-1.47987700	5.24418000	0.16476900
H	-2.94633300	5.32123100	-1.40852600
C	0.72957100	1.43844600	0.01706000
C	0.72041400	3.96635700	0.21950000
H	-0.98180100	6.15211100	-0.18783600
C	1.47337500	2.74079000	-0.32455700
C	1.48187900	5.26051900	-0.08104200
C	2.93429700	2.70380000	0.15760700
C	2.92412900	5.20842300	0.40573900
H	1.46492000	5.44102600	-1.16731000
C	3.65543600	1.47195800	-0.40938400
C	3.66567900	4.01109300	-0.20310700
H	3.43270900	6.14951800	0.16255700
C	5.11559900	1.43374200	0.08775400
C	5.13495200	3.97122500	0.26416800
C	5.85596600	2.73093000	-0.31691900
C	5.88632900	5.25057200	-0.16308800
C	7.32278300	2.69277200	0.18123700
H	5.38016800	6.14373600	0.25013500
C	7.34614100	5.22164700	0.30464300
C	8.06907300	3.97825200	-0.22591300
C	8.04768100	1.45893400	-0.38392900
H	7.86855400	6.13538100	-0.03477500
C	8.06931800	-3.57486000	-0.75703700
C	8.04770100	-1.05824100	-0.56113100
C	7.34484000	-4.87999200	-0.40798500
C	7.32172000	-2.35894800	-0.17591800
C	7.31260700	0.16623100	0.01156000
C	5.88684000	-4.84273000	-0.88072000
H	7.86873800	-5.73751900	-0.86971400
C	5.85621500	-2.32613500	-0.67821900
C	5.84946400	0.20226100	-0.49349500
C	5.13327200	-3.63595100	-0.28111200
H	5.85113500	-4.79699100	-1.98556400
C	5.11484400	-1.09946400	-0.09502500

C	3.66650800	-3.60808300	-0.75701800
C	3.65584800	-1.06459600	-0.59590700
C	2.92161500	-4.87978600	-0.33036900
C	2.93292800	-2.36536600	-0.21727600
C	2.92621100	0.16972200	-0.04128200
C	1.48206900	-4.86035500	-0.82747800
H	3.43151300	-5.77684600	-0.70277500
C	1.47379600	-2.33247900	-0.70557800
C	1.46916400	0.20520900	-0.52587700
C	0.72131100	-3.62318600	-0.34436400
H	1.47097300	-4.88045800	-1.92858400
C	0.73117200	-1.09557500	-0.17353600
C	-0.72334000	-3.58433100	-0.86523000
C	-0.73125300	-1.05943300	-0.65165500
C	-1.47746200	-4.88255100	-0.56210000
C	-1.47013400	-2.36276300	-0.30358200
C	-1.46682300	0.17641500	-0.10819700
C	-2.93161600	-4.82899600	-1.01128800
H	-0.98561900	-5.72836600	-1.05170400
C	-2.93951100	-2.32695600	-0.75685600
C	-2.93035400	0.20709100	-0.57128100
C	-3.65830300	-3.63547100	-0.37707700
H	-2.96890700	-4.73508200	-2.10571700
C	-3.64895800	-1.09398200	-0.17831300
C	-5.14059800	-3.60006800	-0.80084500
C	-5.12054100	-1.06172700	-0.64049100
C	-5.87669000	-4.87788400	-0.34330600
C	-5.84789200	-2.35730100	-0.20828600
C	-5.84298200	0.17333500	-0.05276400
C	-7.34902200	-4.85568500	-0.77046500
H	-5.37981200	-5.77291000	-0.76378200
C	-7.32720500	-2.32580700	-0.66875200
C	-7.31758100	0.20193800	-0.52372100
C	-8.05980100	-3.60908900	-0.23089600
H	-7.42179000	-4.88311000	-1.87465700
C	-8.04008700	-1.08801300	-0.09710900
H	8.15311800	4.03539700	-1.32757800
H	8.12296000	1.53241800	-1.48483500
H	9.08749200	-1.08196600	-0.18734000
H	9.10426800	-3.60190100	-0.37015100
H	-8.11400100	-3.65710700	0.87305800
H	-9.08941700	-1.06407700	-0.44317400
H	-8.09372300	1.36031500	1.15500000
H	-9.10658400	3.97156800	-0.14300300
H	0.71588300	-1.17803300	0.92958600
H	0.70684400	1.34844100	1.11990000
H	-1.47630500	0.10264200	0.99497100
H	1.48889100	0.28892500	-1.62901700
H	-0.71681800	-0.97449600	-1.75443000
H	-0.70903900	1.54919800	-1.57346100

H	1.49895700	-2.25944700	-1.80948500
H	2.90797000	-2.43524300	0.88491300
H	3.65910600	-0.98699900	-1.70304000
H	2.90295300	0.08792400	1.05949500
H	3.65618300	1.55837500	-1.51588100
H	2.91576300	2.61521300	1.25766300
H	1.49655700	2.83107900	-1.42729100
H	0.66563600	3.85762300	1.31774100
H	-0.66622600	4.04812900	-1.41626600
H	-1.48521400	2.64737800	1.16269300
H	0.67084300	-3.67324900	0.75804900
H	-0.68167200	-3.46807700	-1.96334300
H	-1.47636800	-2.45935700	0.79947400
H	-2.94459000	-2.24121700	-1.85736000
H	-3.62148300	-1.17473600	0.92886800
H	-2.92739000	0.28051500	-1.67245300
H	-3.63065900	1.37310600	1.09718500
H	-2.93023200	2.80864800	-1.51226000
H	5.11332100	1.35591700	1.20116100
H	5.86087500	2.80882700	-1.42953000
H	5.15525800	3.90600700	1.37860200
H	3.64276800	4.11299400	-1.30669600
H	5.84632400	5.36032700	-1.26326100
H	7.38830000	5.23942000	1.41061600
H	9.10515100	3.95091800	0.15791400
H	7.31818900	2.62538500	1.29606400
H	9.08787500	1.42957100	-0.01166900
H	5.85920900	0.28239000	-1.60610200
H	7.30463200	0.08769500	1.12585400
H	8.12417600	-0.97618700	-1.66134800
H	7.31430300	-2.44830900	0.93734900
H	5.86400100	-2.24523600	-1.79059200
H	5.11002800	-1.18098700	1.01811700
H	8.15659200	-3.47712000	-1.85559200
H	7.38286400	-5.05204500	0.68481700
H	5.37947200	-5.78497000	-0.59889200
H	5.14812500	-3.72848800	0.83142200
H	3.64982200	-3.55035800	-1.86393400
H	-3.60149200	-3.73920700	0.72565600
H	-5.19338000	-3.54239700	-1.91472800
H	-9.10589600	-3.58679400	-0.58685500
H	-7.85988300	-5.76742600	-0.40885300
H	-5.80584800	-4.97929200	0.75609000
H	-3.43265400	-5.77209800	-0.76035000
H	-1.43415700	-5.07620100	0.52154900
H	0.97832300	-5.77067500	-0.48970700
H	2.92357300	-4.95042200	0.76691400
H	-8.08729500	-1.15092100	1.00598300
H	-9.08958000	1.44956700	-0.29833700
H	-8.12824600	3.86269600	1.32370500

H	-7.40865300	5.41292200	-1.24767400
H	-5.38143200	6.16196700	-0.01115300
H	-3.43148300	6.15664400	0.06350900
H	-1.45469700	5.27536000	1.26537700
H	0.98040700	6.11234900	0.38782900
H	2.93254000	5.12082500	1.50127400
H	-5.82358700	-2.42806200	0.90446000
H	-5.14468600	-0.99285300	-1.75433600
H	-5.82655300	0.10292100	1.06040700
H	-5.13993900	1.54442400	-1.59318300
H	-5.83489300	2.63133600	1.22225500
H	-5.17351700	4.09316900	-1.42602700
H	-3.62542300	3.93664100	1.24242700
H	-7.33585500	0.26851100	-1.63868200
H	-7.34325200	2.80691300	-1.47581200
H	-7.35131400	-2.26871400	-1.78395000
C	0.95712100	-1.61746600	3.87584400
C	-0.53865300	-1.32210500	3.68599900
C	-1.22266100	-2.59390700	4.19333300
C	-0.34180300	-3.70675800	3.61167400
C	1.10014900	-3.15040300	3.67979600
H	1.58769400	-1.04441400	3.18747500
H	1.25911800	-1.33923000	4.89138500
H	-0.76181000	-1.19896000	2.61863000
H	-0.86470500	-0.41217500	4.19874400
H	-1.19126300	-2.62026600	5.28999600
H	-2.27062300	-2.67363500	3.88682600
H	-0.45250800	-4.66071000	4.13468500
H	-0.62857900	-3.87784500	2.56607900
H	1.65194100	-3.59594800	4.51276800
H	1.65957200	-3.39138300	2.76947100

Graphane-S5N

C	-5.11445200	1.37780700	-0.51900500
C	-5.84686000	2.62339800	0.03467200
C	-3.64604500	1.36025700	-0.04506800
C	-8.03931200	1.35179700	-0.00269000
C	-7.32060400	2.63871600	-0.44387900
C	-5.13194500	3.91933600	-0.41829000
C	-2.93137500	2.64871300	-0.47809100
C	-8.05970800	3.87345600	0.10784100
C	-5.87657500	5.14547700	0.15262400
C	-3.65741800	3.90750200	0.03374700
C	-1.46622400	2.63173100	-0.00828400
C	-7.34219600	5.16626200	-0.29703800
H	-5.82254200	5.13716200	1.25752900
C	-2.92091100	5.16539700	-0.44503000
C	-0.72583800	1.37639500	-0.50013000
C	-0.71557000	3.91079400	-0.41410400
H	-7.85922500	6.03881000	0.14369800

C	-1.47447600	5.16358900	0.03220300
H	-2.93947800	5.20035600	-1.54334500
C	0.73307500	1.35705700	-0.01097800
C	0.72635500	3.88809400	0.11627000
H	-0.97614500	6.06230100	-0.34312100
C	1.47714400	2.64705500	-0.39451900
C	1.48653700	5.17370900	-0.22193500
C	2.93997200	2.62442200	0.08247200
C	2.93191100	5.13454600	0.25703600
H	1.46350400	5.32574800	-1.31242400
C	3.65710100	1.37422700	-0.44789400
C	3.66879100	3.91993700	-0.32261100
H	3.43917100	6.06822300	-0.01586400
C	5.12164700	1.35358900	0.03786500
C	5.14244500	3.89461200	0.13190000
C	5.85756600	2.63643500	-0.41719300
C	5.88902900	5.16004300	-0.34271200
C	7.33002100	2.61423000	0.06491500
H	5.38722700	6.06550000	0.04845800
C	7.35409800	5.14542300	0.10896300
C	8.07106800	3.88611700	-0.39139100
C	8.04825400	1.36262100	-0.46891400
H	7.87234700	6.04817800	-0.26445900
C	8.06642800	-3.68310800	-0.65578400
C	8.04653900	-1.16008600	-0.55785900
C	7.34924700	-4.97323000	-0.24146600
C	7.32757100	-2.44503100	-0.11143800
C	7.31904600	0.08436100	-0.01950400
C	5.88291400	-4.95543000	-0.68894500
H	7.86548500	-5.84854900	-0.67770100
C	5.85444000	-2.43276500	-0.59190800
C	5.84965600	0.10215800	-0.50691500
C	5.13902400	-3.72443200	-0.12738200
H	5.82734500	-4.95598300	-1.79393000
C	5.12027100	-1.18314800	-0.05022500
C	3.66395500	-3.71858000	-0.57814800
C	3.65579500	-1.16917500	-0.53667800
C	2.92595700	-4.96479200	-0.07187200
C	2.93731700	-2.45062200	-0.09124400
C	2.93051000	0.08659700	-0.02789100
C	1.48162700	-4.97420500	-0.55523900
H	3.43324500	-5.88148100	-0.39738700
C	1.47389800	-2.44038300	-0.56773800
C	1.47079600	0.10309600	-0.50598700
C	0.72050900	-3.71141300	-0.14227900
H	1.46186600	-5.05962200	-1.65308100
C	0.72864100	-1.17944000	-0.09932500
C	-0.71803100	-3.69769200	-0.68179600
C	-0.72688400	-1.16376600	-0.59776400
C	-1.47811400	-4.97703300	-0.32093000

C	-1.46821900	-2.44879200	-0.19203800
C	-1.46252300	0.08989700	-0.09839100
C	-2.92369100	-4.94596600	-0.79928900
H	-0.97986500	-5.85019000	-0.75299200
C	-2.93244900	-2.43299200	-0.66303900
C	-2.92407500	0.10811600	-0.56816800
C	-3.65884900	-3.72263500	-0.23669200
H	-2.94014100	-4.90518200	-1.89747200
C	-3.64571700	-1.17888400	-0.13721900
C	-5.13422500	-3.70334900	-0.68597000
C	-5.11517400	-1.16088800	-0.60881200
C	-5.87876100	-4.96588600	-0.20078200
C	-5.84807100	-2.44181100	-0.14319000
C	-5.84074600	0.09084100	-0.06149400
C	-7.34476500	-4.95496300	-0.64957000
H	-5.37730400	-5.87349200	-0.58751700
C	-7.32212100	-2.42317600	-0.62067600
C	-7.31204300	0.10817900	-0.54350800
C	-8.06151100	-3.69300300	-0.15567000
H	-7.40141000	-5.01322300	-1.75352300
C	-8.04006800	-1.16971900	-0.09074900
H	8.14145500	3.90874500	-1.49525400
H	8.10779900	1.39901800	-1.57260100
H	9.09227500	-1.16936200	-0.20063100
H	9.10796500	-3.69417500	-0.28634900
H	-8.13021400	-3.70916300	0.94830900
H	-9.08538000	-1.15439700	-0.44917800
H	-8.09880900	1.30802700	1.10066800
H	-9.10080200	3.88699300	-0.26289100
H	0.68114700	-1.20704900	1.00477000
H	0.70702900	1.30725400	1.09462400
H	-1.46746600	0.03385400	1.00425000
H	1.48842100	0.14331100	-1.61181500
H	-0.70319200	-1.12390900	-1.70369600
H	-0.70307800	1.41972800	-1.60522100
H	1.49558800	-2.42495100	-1.67426900
H	2.92691300	-2.46842700	1.01283900
H	3.64698500	-1.14067000	-1.64613000
H	2.91585900	0.04625500	1.07534900
H	3.64862500	1.42210600	-1.55670500
H	2.92626700	2.57048100	1.18515500
H	1.49679300	2.70426000	-1.49946800
H	0.67393500	3.80974700	1.21744200
H	-0.66333000	3.92602300	-1.51771800
H	-1.48201400	2.59535400	1.09829000
H	0.65783300	-3.70244300	0.96191800
H	-0.65943500	-3.64219700	-1.78409300
H	-1.47877100	-2.47474900	0.91224800
H	-2.92968100	-2.39123600	-1.76626000
H	-3.62510500	-1.22026800	0.97225000

H	-2.92011100	0.14833600	-1.67126700
H	-3.62847400	1.32026600	1.06458300
H	-2.92370500	2.68440500	-1.58121300
H	5.12911400	1.31405500	1.15317400
H	5.84960300	2.67824200	-1.53171700
H	5.17355800	3.86433400	1.24746600
H	3.63619200	3.98939700	-1.42850300
H	5.83656300	5.23587200	-1.44523500
H	7.40892100	5.19717600	1.21326400
H	9.11176700	3.87070800	-0.01970800
H	7.33836300	2.58241500	1.18128300
H	9.09354200	1.34591100	-0.11061700
H	5.84503800	0.14085400	-1.62170700
H	7.32524400	0.04506200	1.09687500
H	8.10465100	-1.11960300	-1.66147100
H	7.33736900	-2.49067900	1.00444800
H	5.84471800	-2.39935300	-1.70666800
H	5.12734200	-1.22043800	1.06521400
H	8.13426500	-3.62984600	-1.75875000
H	7.40703400	-5.10098900	0.85646500
H	5.38069400	-5.88475100	-0.35904800
H	5.17343700	-3.76974000	0.98753200
H	3.62814100	-3.71921500	-1.68615300
H	-3.62141500	-3.77546200	0.87053100
H	-5.16876500	-3.68071900	-1.80170500
H	-9.10272900	-3.68038900	-0.52605600
H	-7.86185400	-5.85574700	-0.27004000
H	-5.82355500	-5.03445400	0.90186600
H	-3.43060300	-5.87569500	-0.51224600
H	-1.45548700	-5.10806900	0.77299100
H	0.98130100	-5.86380700	-0.16110300
H	2.93942400	-4.97134800	1.02740300
H	-8.09952700	-1.20303800	1.01295500
H	-9.08463400	1.36211600	-0.36128800
H	-8.12892000	3.81295600	1.21028500
H	-7.39809200	5.30091800	-1.39432200
H	-5.37468900	6.07769600	-0.16948900
H	-3.42614900	6.07372100	-0.09395700
H	-1.44971100	5.22287300	1.13173500
H	0.98780100	6.03776500	0.22723200
H	2.94756000	5.07774900	1.35456100
H	-5.83638100	-2.47653100	0.97134600
H	-5.13197300	-1.12495600	-1.72421400
H	-5.83218000	0.05147600	1.05311300
H	-5.12995300	1.42009100	-1.63420400
H	-5.83595500	2.58012000	1.14899600
H	-5.16507400	3.97420500	-1.53294500
H	-3.62262800	3.88544200	1.14170000
H	-7.32195600	0.14711900	-1.65985400
H	-7.33159700	2.69005600	-1.55951100

H	-7.33373200	-2.39692100	-1.73716700
C	-0.51198400	-0.11430600	3.80399400
C	-0.52309100	-2.43327100	3.77875400
C	0.96751100	-2.05776900	3.79487000
C	0.97510400	-0.50792800	3.82868900
H	-0.70356000	0.80152800	3.23349800
H	-0.87566900	0.04220000	4.83417100
H	-0.87860700	-2.60189900	4.81009400
H	-0.73221900	-3.33631500	3.19486800
H	1.48486700	-2.50060300	4.64916800
H	1.45676200	-2.42247800	2.88642000
H	1.47913500	-0.11007900	4.71259200
H	1.48765300	-0.10766000	2.94857200
N	-1.14221000	-1.26412900	3.15852100
H	-2.15327900	-1.26000100	3.27251700

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C	-5.11791700	1.37477000	-0.51909400
C	-5.85356200	2.62181500	0.02707900
C	-3.65246200	1.35836000	-0.03624400
C	-8.04545100	1.35021900	-0.01892400
C	-7.32431600	2.63563300	-0.46052400
C	-5.13568400	3.91675400	-0.42401700
C	-2.93550400	2.64622500	-0.46779700
C	-8.06688800	3.87209000	0.08268300
C	-5.88427700	5.14432000	0.13857300
C	-3.66451300	3.90552500	0.03881700
C	-1.47250700	2.63003400	0.00891600
C	-7.34678400	5.16372300	-0.32124900
H	-5.83803000	5.13854700	1.24390000
C	-2.92492200	5.16366900	-0.43470800
C	-0.73094600	1.37429900	-0.48006500
C	-0.72062100	3.90902700	-0.39468200
H	-7.86683400	6.03750300	0.11337400
C	-1.48103500	5.16130000	0.05021000
H	-2.93725200	5.19980000	-1.53308600
C	0.72906100	1.35584600	0.00654000
C	0.72066600	3.88611600	0.13731600
H	-0.98071600	6.06052600	-0.32123000
C	1.47166300	2.64666700	-0.37694500
C	1.48008500	5.17324900	-0.19698000
C	2.93596900	2.62381600	0.09528000
C	2.92668200	5.13288000	0.27817600
H	1.45449200	5.32999900	-1.28673300
C	3.65174600	1.37551000	-0.44120400
C	3.66230000	3.92104700	-0.30876400
H	3.43273000	6.06788800	0.00773500
C	5.11863200	1.35460900	0.03719300
C	5.13808300	3.89519300	0.13863900
C	5.85121800	2.63923300	-0.41814400

C	5.88135700	5.16266300	-0.33566100
C	7.32631900	2.61650000	0.05576900
H	5.38117800	6.06647100	0.06140500
C	7.34891000	5.14744000	0.10781400
C	8.06389300	3.89028800	-0.40071500
C	8.04228400	1.36695800	-0.48591000
H	7.86450800	6.05176900	-0.26551300
C	8.06231700	-3.67869300	-0.68484800
C	8.04154200	-1.15570700	-0.58166100
C	7.34908400	-4.97001400	-0.26743100
C	7.32652500	-2.44208100	-0.13314800
C	7.31670200	0.08697400	-0.03574500
C	5.87944500	-4.95258400	-0.70397600
H	7.86269300	-5.84423300	-0.70899100
C	5.85016700	-2.43015700	-0.60372200
C	5.84447400	0.10496100	-0.51450500
C	5.13907100	-3.72278100	-0.13519900
H	5.81577200	-4.95169000	-1.80856200
C	5.11869900	-1.18167000	-0.05594500
C	3.66050800	-3.71825000	-0.57409500
C	3.65153500	-1.16821000	-0.53392300
C	2.92736400	-4.96365900	-0.05878000
C	2.93671900	-2.44992800	-0.08372000
C	2.92810500	0.08654600	-0.02012500
C	1.47912500	-4.97537200	-0.53010000
H	3.43252700	-5.88078300	-0.38619700
C	1.46999300	-2.44149800	-0.54985100
C	1.46609200	0.10258200	-0.49086200
C	0.71999600	-3.71161100	-0.11617100
H	1.45035400	-5.06460300	-1.62737000
C	0.72570200	-1.17998500	-0.08120500
C	-0.72184200	-3.70082100	-0.64728300
C	-0.73171100	-1.16601900	-0.57461400
C	-1.48113500	-4.97779500	-0.27674400
C	-1.47276400	-2.44943600	-0.16446100
C	-1.46880300	0.08803300	-0.07878300
C	-2.92562800	-4.95087900	-0.75876600
H	-0.98163000	-5.85424500	-0.70056200
C	-2.93620400	-2.43615500	-0.63860500
C	-2.92870400	0.10471900	-0.55380400
C	-3.66339300	-3.72395700	-0.20723800
H	-2.93857700	-4.91889900	-1.85733100
C	-3.65132400	-1.18047200	-0.11780900
C	-5.13619700	-3.70750300	-0.66496500
C	-5.11767400	-1.16456600	-0.59903200
C	-5.88307600	-4.96772200	-0.17725800
C	-5.85292500	-2.44349300	-0.13165100
C	-5.84644000	0.08927200	-0.06083500
C	-7.34681700	-4.95914600	-0.63354200
H	-5.37981300	-5.87738500	-0.55630800

C	-7.32450600	-2.42724300	-0.61656800
C	-7.31508200	0.10447900	-0.55071800
C	-8.06597400	-3.69493700	-0.14897000
H	-7.39794400	-5.02247200	-1.73744900
C	-8.04515700	-1.17149700	-0.09579900
H	8.12799000	3.91656800	-1.50490600
H	8.09544000	1.40657000	-1.58982200
H	9.08967700	-1.16497600	-0.23141000
H	9.10653300	-3.68964400	-0.32301700
H	-8.13910600	-3.70572000	0.95489900
H	-9.08884100	-1.15795600	-0.45874500
H	-8.11086700	1.31036700	1.08435600
H	-9.10558200	3.88446500	-0.29463000
H	0.68342900	-1.20608700	1.02359000
H	0.70735400	1.30524700	1.11236900
H	-1.48467600	0.03386200	1.02344900
H	1.47833400	0.14205100	-1.59662900
H	-0.70971400	-1.12931800	-1.68039600
H	-0.70824600	1.41621900	-1.58514100
H	1.48402600	-2.42856500	-1.65637500
H	2.93480200	-2.46710000	1.02049600
H	3.63585200	-1.13947300	-1.64320000
H	2.91949900	0.04438100	1.08325300
H	3.63755800	1.42556000	-1.54980200
H	2.92638100	2.56689300	1.19794600
H	1.48809600	2.70531700	-1.48182900
H	0.66779900	3.80471100	1.23828600
H	-0.66630100	3.92472600	-1.49819800
H	-1.49333300	2.59473500	1.11549500
H	0.66676900	-3.69919900	0.98871000
H	-0.66755700	-3.65199500	-1.75005600
H	-1.49102900	-2.47013700	0.93936000
H	-2.92975500	-2.40001300	-1.74209200
H	-3.63331900	-1.21716500	0.99084400
H	-2.92014600	0.14162900	-1.65706400
H	-3.64141500	1.31940000	1.07300000
H	-2.92172300	2.68085300	-1.57094200
H	5.13194800	1.31234600	1.15233500
H	5.83718600	2.68443000	-1.53248700
H	5.17476800	3.86147500	1.25390900
H	3.62447400	3.99407300	-1.41424100
H	5.82279800	5.24239600	-1.43763100
H	7.40992200	5.19567200	1.21196900
H	9.10672800	3.87444800	-0.03507100
H	7.34094000	2.58131700	1.17197200
H	9.08973000	1.35002400	-0.13386600
H	5.83336900	0.14596100	-1.62917800
H	7.32957800	0.04475200	1.08048200
H	8.09249900	-1.11279700	-1.68554500
H	7.34391400	-2.48993100	0.98257000

H	5.83293600	-2.39581800	-1.71836100
H	5.13250500	-1.22068900	1.05938100
H	8.12222100	-3.62361700	-1.78821400
H	7.41522100	-5.09970800	0.82982100
H	5.38033900	-5.88275600	-0.37176700
H	5.18253400	-3.76933900	0.97936400
H	3.61545300	-3.72110600	-1.68168800
H	-3.63198400	-3.76886400	0.90004900
H	-5.16492500	-3.69032700	-1.78087300
H	-9.10555000	-3.68417700	-0.52372900
H	-7.86568000	-5.85810700	-0.25222100
H	-5.83366500	-5.02990300	0.92620200
H	-3.43235900	-5.87889700	-0.46599700
H	-1.46103500	-5.10001100	0.81830100
H	0.98232900	-5.86371800	-0.12892000
H	2.95026700	-4.96764600	1.04041800
H	-8.10908800	-1.19987900	1.00793400
H	-9.08874100	1.35906100	-0.38324800
H	-8.14302200	3.81471400	1.18490000
H	-7.39515700	5.29499800	-1.41929100
H	-5.38045200	6.07582100	-0.18232100
H	-3.43183900	6.07178900	-0.08558800
H	-1.46178200	5.21873200	1.14994700
H	0.98176800	6.03501500	0.25694300
H	2.94553300	5.07151700	1.37540800
H	-5.84622100	-2.47287300	0.98339500
H	-5.12804900	-1.13340900	-1.71453800
H	-5.84321200	0.05383900	1.05427000
H	-5.12733100	1.41353600	-1.63437400
H	-5.84953800	2.58073700	1.14166900
H	-5.16086200	3.96894400	-1.53897400
H	-3.63782900	3.88345700	1.14691100
H	-7.31931100	0.13851000	-1.66719100
H	-7.32865300	2.68312000	-1.57631500
H	-7.33077900	-2.40619600	-1.73314800
C	-0.48826200	-0.14224100	3.68982300
O	-1.09142500	-1.25883400	3.06103000
C	-0.48477800	-2.39684700	3.64585500
C	1.00647000	-2.04461400	3.77634200
C	1.00324600	-0.49769400	3.82010300
H	-0.68442000	0.73860900	3.07152100
H	-0.93975100	0.01531100	4.68132500
H	-0.92837700	-2.58853400	4.63511800
H	-0.68636000	-3.25531100	2.99878700
H	1.45338700	-2.49188300	4.66730500
H	1.56204200	-2.40561000	2.90543000
H	1.43404300	-0.10123700	4.74251900
H	1.57179800	-0.08461900	2.98124800

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C	-5.10117200	1.45569500	-0.54238700
C	-5.82677600	2.68853100	0.04752300
C	-3.62935400	1.42641300	-0.08011500
C	-8.01970100	1.41849600	0.00814400
C	-7.30616000	2.71504900	-0.41264200
C	-5.11654200	3.99393400	-0.38524800
C	-2.91717600	2.72284800	-0.49350700
C	-8.03752800	3.93721800	0.17607100
C	-5.85343000	5.20737700	0.22183100
C	-3.63687300	3.97249900	0.04902600
C	-1.44839400	2.69685400	-0.03567600
C	-7.32454600	5.23858300	-0.20895900
H	-5.78599200	5.17398900	1.32564300
C	-2.90481800	5.23771900	-0.41729600
C	-0.71178600	1.45060800	-0.55554800
C	-0.69885900	3.98143300	-0.42662000
H	-7.83551900	6.10112600	0.25776200
C	-1.45340000	5.22800500	0.04435300
H	-2.93560000	5.29069700	-1.51463600
C	0.74825900	1.42040500	-0.07135800
C	0.74502800	3.95000400	0.09767400
H	-0.95835300	6.13172600	-0.32323000
C	1.49587500	2.71570500	-0.42902700
C	1.50845100	5.23732300	-0.22591000
C	2.95381500	2.68254800	0.06285200
C	2.94937000	5.19199600	0.26576900
H	1.49402100	5.39712000	-1.31538600
C	3.67566500	1.43860800	-0.47579500
C	3.69153100	3.98134900	-0.31553700
H	3.46084200	6.12685400	0.00527400
C	5.13251800	1.40543300	0.03169200
C	5.15678900	3.94591500	0.16471600
C	5.87904200	2.69408800	-0.38914200
C	5.91497900	5.21597800	-0.27783600
C	7.34195700	2.66079400	0.12075000
H	5.40770400	6.11733500	0.11581800
C	7.37067700	5.19144100	0.20265300
C	8.09468200	3.93770100	-0.30128800
C	8.06824000	1.41666500	-0.41946100
H	7.89821400	6.09817200	-0.14756200
C	8.08035500	-3.62060300	-0.72765100
C	8.06336200	-1.10213700	-0.56179000
C	7.35090600	-4.92022300	-0.36863300
C	7.33189500	-2.39633800	-0.16543200
C	7.32719400	0.13157200	-0.01066100
C	5.89590700	-4.88500800	-0.85063000
H	7.87569200	-5.78381900	-0.81802000
C	5.86958100	-2.36636100	-0.67719800
C	5.86752200	0.16372700	-0.52594500

C	5.14154600	-3.66991600	-0.26908200
H	5.86713500	-4.85134000	-1.95617100
C	5.12739300	-1.13069100	-0.11418500
C	3.67754000	-3.64486200	-0.75370300
C	3.67140200	-1.09938200	-0.62432000
C	2.92674300	-4.90877100	-0.31423100
C	2.94392000	-2.39384900	-0.23365500
C	2.94019200	0.14390500	-0.09209300
C	1.49148400	-4.89299600	-0.82358200
H	3.43801100	-5.81230100	-0.66861000
C	1.48695700	-2.36376400	-0.72972100
C	1.48708100	0.17615400	-0.58902300
C	0.72781500	-3.64930300	-0.36183700
H	1.49014300	-4.92513900	-1.92434600
C	0.74055200	-1.11690500	-0.22547400
C	-0.71073300	-3.61137100	-0.89905200
C	-0.71633300	-1.08378700	-0.71770000
C	-1.46978300	-4.90499100	-0.58904000
C	-1.45767500	-2.38190500	-0.35673300
C	-1.44821600	0.15586600	-0.17901000
C	-2.92104100	-4.85179100	-1.04685500
H	-0.97680000	-5.75749000	-1.06612300
C	-2.92578600	-2.34741000	-0.81358400
C	-2.91291200	0.18641300	-0.63890300
C	-3.64690200	-3.65173100	-0.42451600
H	-2.95155400	-4.76549700	-2.14212300
C	-3.63240700	-1.11144800	-0.23729500
C	-5.12854000	-3.61721700	-0.85063900
C	-5.10492100	-1.07864300	-0.69761800
C	-5.86637600	-4.89314000	-0.39052900
C	-5.83337600	-2.37200900	-0.26042600
C	-5.82359200	0.15824000	-0.10917400
C	-7.33896900	-4.86921000	-0.81676300
H	-5.37124600	-5.78967900	-0.80947700
C	-7.31377000	-2.33927600	-0.71679900
C	-7.30049500	0.18829900	-0.57253100
C	-8.04712100	-3.62138400	-0.27658800
H	-7.41250600	-4.89641200	-1.92085200
C	-8.02293000	-1.10053300	-0.14246600
H	8.18781700	3.97657000	-1.40305700
H	8.15262300	1.47336000	-1.52076100
H	9.10042900	-1.12327400	-0.18027700
H	9.11281700	-3.64543300	-0.33396800
H	-8.09845800	-3.66843400	0.82760200
H	-9.07372200	-1.07536000	-0.48355400
H	-8.06303300	1.34828900	1.11103100
H	-9.08335200	3.95922400	-0.18053600
H	0.70177700	-1.17954900	0.87898000
H	0.72447800	1.35326300	1.03285200
H	-1.45175500	0.07867700	0.92413600

H	1.51684000	0.24308000	-1.69297800
H	-0.69465600	-1.00702600	-1.82121200
H	-0.69370900	1.51532900	-1.65955900
H	1.52146900	-2.30635600	-1.83424200
H	2.91782800	-2.45183000	0.86877100
H	3.68182000	-1.03667000	-1.73226000
H	2.90685800	0.07768200	1.01022900
H	3.68475500	1.50505200	-1.58358000
H	2.92678700	2.61432500	1.16434600
H	1.52429300	2.79117300	-1.53260000
H	0.69523700	3.85853800	1.19789400
H	-0.65274000	4.01366300	-1.53013000
H	-1.45494700	2.64070800	1.06965200
H	0.66318600	-3.69022200	0.74129900
H	-0.65581700	-3.50936000	-1.99799600
H	-1.46659500	-2.45389600	0.74651200
H	-2.93208900	-2.26823400	-1.91488400
H	-3.60015500	-1.18754200	0.86891100
H	-2.91328800	0.25623500	-1.74071100
H	-3.60283500	1.36056400	1.02741400
H	-2.91876300	2.78064900	-1.59583300
H	5.12294000	1.34540100	1.14595300
H	5.89265700	2.75298400	-1.50290100
H	5.16768000	3.89976500	1.28020300
H	3.67792700	4.06317600	-1.42089100
H	5.88443800	5.30722500	-1.38001900
H	7.40371800	5.22763100	1.30845600
H	9.12758000	3.91425400	0.09129200
H	7.32883100	2.61129100	1.23638800
H	9.10539300	1.39066100	-0.03850400
H	5.88513100	0.22772000	-1.63959700
H	7.31181500	0.06863200	1.10445300
H	8.14812700	-1.03444300	-1.66244700
H	7.31757400	-2.47238800	0.94867600
H	5.88460000	-2.29906000	-1.79047900
H	5.11612400	-1.19724600	0.99968600
H	8.17498600	-3.53559800	-1.82671300
H	7.38220400	-5.08058400	0.72609200
H	5.38457200	-5.82298400	-0.56188900
H	5.15018800	-3.74976700	0.84437400
H	3.66708100	-3.60161300	-1.86124600
H	-3.59216300	-3.74531500	0.67917300
H	-5.18037700	-3.56192500	-1.96452300
H	-9.09394800	-3.59793400	-0.63002200
H	-7.85085300	-5.78005500	-0.45455900
H	-5.79520100	-4.99193600	0.70914500
H	-3.42526500	-5.79235800	-0.79236800
H	-1.43469200	-5.08765000	0.49732700
H	0.98297300	-5.79885200	-0.48093200
H	2.91921700	-4.96205000	0.78408000

H	-8.06454200	-1.16311900	0.96096700
H	-9.07004800	1.43752700	-0.33480400
H	-8.09232600	3.85185200	1.27776800
H	-7.39418700	5.39766900	-1.30213400
H	-5.35500200	6.14640700	-0.08524500
H	-3.40527900	6.14054700	-0.04584800
H	-1.41745500	5.27154400	1.14428100
H	1.00778100	6.09882100	0.22570200
H	2.95386000	5.12690800	1.36295400
H	-5.80581100	-2.43939100	0.85274400
H	-5.13154000	-1.01181300	-1.81125700
H	-5.80087200	0.08978100	1.00425700
H	-5.12640800	1.52462800	-1.65597300
H	-5.80242400	2.62008900	1.16057300
H	-5.16315900	4.07340400	-1.49788500
H	-3.58890100	3.93086200	1.15574100
H	-7.32452000	0.25502500	-1.68730600
H	-7.33092000	2.79167400	-1.52656200
H	-7.34113300	-2.28212900	-1.83182100
C	0.03635500	-0.48166600	3.88473900
C	-0.52142700	-3.08888700	3.57624200
C	0.96428100	-2.72296300	3.60463700
C	1.08842000	-1.44469700	4.43297700
H	0.38035500	-0.01177700	2.95737500
H	-0.22921200	0.30313500	4.59573700
H	-0.80907400	-3.64768300	4.47042300
H	-0.78558600	-3.68240900	2.69601200
H	1.56357100	-3.54405300	4.01092800
H	1.31330700	-2.52704300	2.58357300
H	0.87567400	-1.66179900	5.48587300
H	2.09110800	-1.00959500	4.37011000
S	-1.44941100	-1.50199600	3.54042400

Graphane-U6C

C	5.16401000	-1.18097200	-0.56694100
C	5.88718600	-2.46476000	-0.09420800
C	3.69161900	-1.19214100	-0.10568300
C	8.08416900	-1.20207700	-0.02545400
C	7.36526900	-2.45320200	-0.55941100
C	5.17248000	-3.72350500	-0.64233200
C	2.97659000	-2.44270700	-0.63783300
C	8.09476100	-3.72555100	-0.08599700
C	5.90675600	-4.98872300	-0.14856600
C	3.69291400	-3.73693100	-0.20727300
C	1.50647500	-2.45289200	-0.18438500
C	7.37677100	-4.98508000	-0.58416800
H	5.84160300	-5.05526400	0.95378600
C	2.95794200	-4.95541800	-0.78076300
C	0.77435100	-1.16321100	-0.59119000
C	0.75649000	-3.69626900	-0.69037500

H	7.88631300	-5.88749100	-0.19811200
C	1.50585400	-4.97972000	-0.32203100
H	2.98914000	-4.91360300	-1.87855400
C	-0.68898100	-1.17302700	-0.11547100
C	-0.69059500	-3.70549200	-0.17481500
H	1.00936800	-5.84925700	-0.76291500
C	-1.43294600	-2.42842600	-0.60110800
C	-1.45243900	-4.96014700	-0.61014300
C	-2.89801600	-2.43498800	-0.12984700
C	-2.89887800	-4.95066500	-0.13316300
H	-1.42776300	-5.03107800	-1.70897500
C	-3.60977300	-1.14808300	-0.57148000
C	-3.63025600	-3.69572300	-0.62714300
H	-3.40852500	-5.86164800	-0.47090100
C	-5.07520100	-1.15671500	-0.08721900
C	-5.10474000	-3.69801100	-0.17420600
C	-5.81499400	-2.40147100	-0.63270700
C	-5.85488800	-4.92363100	-0.73902800
C	-7.28776700	-2.40870000	-0.15103300
H	-5.35631600	-5.85653500	-0.41377500
C	-7.32026300	-4.93663500	-0.28831000
C	-8.03273100	-3.64227800	-0.69727800
C	-8.00150100	-1.11995800	-0.59482300
H	-7.84119100	-5.80847600	-0.72601300
C	-8.00294000	3.92568200	-0.43561400
C	-7.99149400	1.40223200	-0.50759400
C	-7.28102300	5.18308700	0.06231200
C	-7.26807100	2.65156200	0.02442700
C	-7.26821000	0.12114000	-0.05664800
C	-5.81521300	5.18994200	-0.38715400
H	-7.79467400	6.08713000	-0.31442100
C	-5.79487900	2.66628100	-0.45589700
C	-5.79844300	0.13234800	-0.54322100
C	-5.07529400	3.92236800	0.09212100
H	-5.76069400	5.26262200	-1.48978600
C	-5.06554300	1.38068800	0.00206900
C	-3.60024100	3.94045200	-0.35812700
C	-3.59975600	1.39422100	-0.48037300
C	-2.86021300	5.15291700	0.22218800
C	-2.87892900	2.64198900	0.05093000
C	-2.88016100	0.10361800	-0.05779000
C	-1.41177800	5.18380600	-0.24814500
H	-3.36126600	6.08834600	-0.05606000
C	-1.41336400	2.65722700	-0.41816100
C	-1.41879500	0.11391800	-0.53068500
C	-0.66067500	3.89505900	0.09764400
H	-1.38127600	5.33313500	-1.33880500
C	-0.67968700	1.36385700	-0.02725900
C	0.78605900	3.91013900	-0.41933400
C	0.78492800	1.37636700	-0.49921500

C	1.54669700	5.16089100	0.02990600
C	1.52699000	2.62895800	-0.00289300
C	1.51232100	0.08716700	-0.08714400
C	2.99718200	5.15489900	-0.43469400
H	1.05565600	6.06057200	-0.35258000
C	2.99634300	2.63824700	-0.45982600
C	2.97862700	0.09765100	-0.54268400
C	3.72394000	3.89536200	0.05425500
H	3.02540800	5.18646000	-1.53289800
C	3.70227200	1.34827600	-0.01743600
C	5.20196300	3.89924200	-0.38615700
C	5.17379300	1.35764300	-0.48125500
C	5.94758500	5.12326400	0.18790300
C	5.90761100	2.60121300	0.07517800
C	5.89086400	0.06838900	-0.01589500
C	7.41661200	5.13661300	-0.25072700
H	5.45232700	6.05711000	-0.13978700
C	7.38496400	2.60884500	-0.39233000
C	7.36585500	0.07821900	-0.48665200
C	8.12527000	3.84151000	0.16225600
H	7.48155400	5.26898100	-1.34778400
C	8.09429900	1.31968600	0.05731200
H	-8.10280600	-3.58563500	-1.79995500
H	-8.06123300	-1.07820500	-1.69833800
H	-9.03691200	1.39062200	-0.14933200
H	-9.04407900	3.91577300	-0.06485000
H	8.18603200	3.78316100	1.26537700
H	9.14256300	1.32456500	-0.29282000
H	8.13413600	-1.23370100	1.07886600
H	9.13932000	-3.71821100	-0.44713600
H	-0.66841900	1.31090300	1.07691600
H	-0.67631600	-1.20424100	0.98871800
H	1.50968500	0.04494200	1.01775600
H	-1.42854100	0.15386400	-1.63689400
H	0.77736300	1.41541100	-1.60465400
H	0.76644600	-1.12130000	-1.69685300
H	-1.42617900	2.71468100	-1.52327200
H	-2.87011100	2.58933300	1.15408900
H	-3.58876200	1.44217600	-1.58924200
H	-2.86302900	0.06119100	1.04478500
H	-3.60034300	-1.11600300	-1.68108200
H	-2.88410300	-2.45838900	0.97355500
H	-1.44619500	-2.40528700	-1.70789900
H	-0.64752700	-3.70292400	0.92893700
H	0.71887000	-3.63425800	-1.79318700
H	1.50633600	-2.49531800	0.92097600
H	-0.61835100	3.81737600	1.19947500
H	0.74419600	3.92205500	-1.52342300
H	1.53185200	2.59506800	1.10384600
H	2.99815800	2.67092100	-1.56304900

H	3.67721700	1.31154200	1.09199700
H	2.98196000	0.13609500	-1.64564500
H	3.66436400	-1.23339700	1.00382500
H	2.98325300	-2.39967600	-1.74079600
H	-5.08378500	-1.19604200	1.02801000
H	-5.80626000	-2.36394600	-1.74738100
H	-5.13754400	-3.74749700	0.94058000
H	-3.59607900	-3.68756900	-1.73523200
H	-5.80172800	-4.92020400	-1.84412100
H	-7.37626600	-5.06754600	0.80935600
H	-9.07356700	-3.65005200	-0.32565300
H	-7.29697400	-2.45647500	0.96473400
H	-9.04678400	-1.12503700	-0.23603400
H	-5.79317500	0.17148000	-1.65803600
H	-7.27531000	0.08253100	1.05971500
H	-8.05094300	1.43742800	-1.61135200
H	-7.27794000	2.62218700	1.14085500
H	-5.78531400	2.70628600	-1.57046700
H	-5.07556400	1.34215600	1.11735000
H	-8.07234000	3.94596500	-1.53959800
H	-7.33735200	5.23824300	1.16639000
H	-5.31005600	6.09422900	0.00241800
H	-5.10961200	3.89472400	1.20770800
H	-3.56388200	4.00798500	-1.46397400
H	3.68004400	3.87692900	1.16191500
H	5.24419700	3.95159600	-1.50065900
H	9.16923400	3.84968400	-0.20057400
H	7.93414200	6.00776100	0.19232400
H	5.88522700	5.11753500	1.29244900
H	3.50339100	6.06199300	-0.08196000
H	1.51257700	5.22377700	1.12898800
H	-0.91169400	6.04642500	0.20218900
H	-2.88234600	5.09938500	1.31982000
H	8.14491800	1.27808400	1.16127900
H	9.13267600	-1.19206300	-0.37475300
H	8.15389400	-3.74025800	1.01864600
H	7.44336100	-5.04587400	-1.68741700
H	5.40488200	-5.89486200	-0.53815700
H	3.45625800	-5.88796300	-0.48807800
H	1.46702000	-5.11289100	0.77113400
H	-0.95859000	-5.85747100	-0.22537300
H	-2.91627100	-4.97021100	0.96617900
H	5.88824700	2.56056500	1.18956500
H	5.19764400	1.39771600	-1.59641700
H	5.87376800	0.03093400	1.09880900
H	5.18937200	-1.14650200	-1.68228600
H	5.86623200	-2.49858800	1.02034500
H	5.21799700	-3.70228900	-1.75775600
H	3.64486200	-3.79223300	0.89924000
H	7.38474600	0.11483800	-1.60297600

H	7.38651900	-2.42884600	-1.67581900
H	7.40471100	2.65764800	-1.50796100
C	-1.24726100	-2.49440300	3.54274100
C	0.14531600	-2.44097300	3.51967600
C	0.79547600	-1.20855900	3.53498000
C	0.05334500	-0.02933600	3.57342500
C	-1.33909700	-0.08255500	3.59645600
H	1.88114800	-1.16641100	3.50877000
H	-1.75477000	-3.45499800	3.52359000
H	0.72415100	-3.35987900	3.48196300
H	0.56080100	0.93174400	3.57640000
H	-1.91769600	0.83692100	3.61808600
C	-1.98923000	-1.31511500	3.58117500
H	-3.07476600	-1.35672500	3.59214700

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C	5.15588400	-1.16928800	-0.57346000
C	5.87349800	-2.45492100	-0.09750000
C	3.67839700	-1.18321600	-0.12902900
C	8.06845300	-1.19110400	0.00787200
C	7.35804500	-2.44036300	-0.54153600
C	5.16751200	-3.71070900	-0.66338200
C	2.96985000	-2.43077200	-0.67638100
C	8.08117200	-3.71463300	-0.06362700
C	5.89505500	-4.97862200	-0.16640100
C	3.68181400	-3.72866100	-0.25024400
C	1.49543800	-2.44649300	-0.23745900
C	7.37154300	-4.97182700	-0.57946400
H	5.81322700	-5.05201100	0.93441000
C	2.95553600	-4.94005800	-0.84946200
C	0.76464100	-1.15357300	-0.63650100
C	0.74959000	-3.68444900	-0.76325300
H	7.87567500	-5.87605900	-0.19059800
C	1.49834600	-4.97227300	-0.40818500
H	3.00035900	-4.88294500	-1.94607100
C	-0.69751300	-1.16738300	-0.15949300
C	-0.69656400	-3.70243500	-0.24636700
H	1.00739200	-5.83522200	-0.86780700
C	-1.44405400	-2.42020100	-0.64794400
C	-1.46195800	-4.94919500	-0.69657600
C	-2.90189300	-2.43221600	-0.15436400
C	-2.89901300	-4.95073900	-0.19184800
H	-1.45737900	-4.99635100	-1.79690500
C	-3.62272400	-1.14408300	-0.57773500
C	-3.64201200	-3.68916800	-0.65032700
H	-3.41412700	-5.85658500	-0.53492900
C	-5.07958700	-1.15648200	-0.06922400
C	-5.10593000	-3.69776300	-0.16497700
C	-5.82771600	-2.40089600	-0.60422100
C	-5.86605300	-4.92304500	-0.71696200

C	-7.29033700	-2.41183200	-0.09276900
H	-5.35951400	-5.85616000	-0.40522800
C	-7.32123100	-4.93956800	-0.23438600
C	-8.04451700	-3.64575800	-0.62552700
C	-8.01523400	-1.12395600	-0.52070100
H	-7.85007700	-5.81159800	-0.66195800
C	-8.02169000	3.92078100	-0.37226900
C	-8.00753300	1.39758800	-0.43592200
C	-7.29262800	5.18141400	0.10659400
C	-7.27613500	2.64952700	0.07865600
C	-7.27338700	0.11835800	0.00278300
C	-5.83568300	5.18864400	-0.37086300
H	-7.81492500	6.08304300	-0.26389500
C	-5.81202600	2.66475100	-0.42873900
C	-5.81292800	0.13174500	-0.51115600
C	-5.08489900	3.92447000	0.10044100
H	-5.80233500	5.25594900	-1.47466700
C	-5.07280900	1.38170500	0.02075700
C	-3.61823200	3.94243100	-0.37629200
C	-3.61478700	1.39620300	-0.48410100
C	-2.87159000	5.16158100	0.18127600
C	-2.88818600	2.64785700	0.03021500
C	-2.88702300	0.10690700	-0.07070700
C	-1.42881300	5.18932300	-0.30646900
H	-3.37739200	6.09330200	-0.10072400
C	-1.42848000	2.66327800	-0.45736100
C	-1.43206600	0.12067000	-0.56315100
C	-0.67389400	3.90489800	0.04622800
H	-1.41030700	5.32626700	-1.39899100
C	-0.69026000	1.37241100	-0.06766100
C	0.77247800	3.91767300	-0.47174500
C	0.77301100	1.38496900	-0.54217500
C	1.53060100	5.17240800	-0.02876000
C	1.51243100	2.63895900	-0.04551500
C	1.49889000	0.09621600	-0.12563500
C	2.98524900	5.16245300	-0.48001600
H	1.04260400	6.06829200	-0.42392500
C	2.98544800	2.64709000	-0.48962700
C	2.96910000	0.10775200	-0.56812500
C	3.70648000	3.90685200	0.02687900
H	3.02420100	5.18441100	-1.57810600
C	3.68691600	1.35865200	-0.03588600
C	5.19052300	3.90944800	-0.39246100
C	5.16356600	1.36816200	-0.48286000
C	5.92737600	5.13494000	0.18982500
C	5.88974900	2.61250700	0.08166600
C	5.87514900	0.07877700	-0.00971400
C	7.40289600	5.14769500	-0.22643900
H	5.43681400	6.06783700	-0.14754900
C	7.37355000	2.61992900	-0.36484400

C	7.35635400	0.09004500	-0.46038700
C	8.10540900	3.85330900	0.19923100
H	7.48449100	5.27837400	-1.32259500
C	8.07650700	1.33104200	0.09544200
H	-8.13807600	-3.58708600	-1.72633300
H	-8.09791300	-1.08171600	-1.62270300
H	-9.04549900	1.38486800	-0.05661500
H	-9.05551400	3.91062000	0.01838600
H	8.14942600	3.79653200	1.30321600
H	9.12997300	1.33626800	-0.23869100
H	8.10158500	-1.22635200	1.11267800
H	9.13109300	-3.70483300	-0.40876500
H	-0.67085900	1.32324300	1.03572400
H	-0.67839800	-1.20534100	0.94453900
H	1.48511500	0.05694600	0.98024700
H	-1.45590100	0.16149500	-1.66902600
H	0.76726300	1.42137600	-1.64760900
H	0.75777700	-1.10532500	-1.74170600
H	-1.45368300	2.71631800	-1.56241800
H	-2.86432000	2.60189300	1.13351100
H	-3.62103800	1.44052900	-1.59316700
H	-2.85720000	0.05879300	1.03152900
H	-3.63108900	-1.10702300	-1.68721000
H	-2.87321800	-2.45845900	0.94884400
H	-1.47300800	-2.38479600	-1.75403000
H	-0.64661300	-3.71841200	0.85619600
H	0.71497800	-3.60695100	-1.86507200
H	1.48367900	-2.50524300	0.86806600
H	-0.62853100	3.83583200	1.14852400
H	0.73192200	3.92231900	-1.57589000
H	1.50866700	2.60851700	1.06131300
H	2.99821600	2.67564300	-1.59287000
H	3.64879300	1.32355500	1.07327500
H	2.98118100	0.14808000	-1.67091100
H	3.63960800	-1.23022000	0.98008000
H	2.98655400	-2.37872200	-1.77880200
H	-5.06847900	-1.19768400	1.04640500
H	-5.84170500	-2.35954200	-1.71869300
H	-5.11425900	-3.75027600	0.95021300
H	-3.63238600	-3.66616900	-1.75869400
H	-5.83705800	-4.91623000	-1.82292000
H	-7.35291000	-5.07211600	0.86409800
H	-9.07713100	-3.65609700	-0.23174700
H	-7.27656700	-2.46091600	1.02295100
H	-9.05277000	-1.13109700	-0.14011700
H	-5.82845200	0.17115500	-1.62585900
H	-7.25921700	0.08050400	1.11916000
H	-8.08920600	1.43030200	-1.53833800
H	-7.26535300	2.62379300	1.19516600
H	-5.82306200	2.70014900	-1.54347200

H	-5.06550000	1.34461100	1.13622000
H	-8.11217200	3.93644500	-1.47480100
H	-7.32791200	5.24094700	1.21133100
H	-5.32499400	6.09568200	0.00468200
H	-5.09912900	3.90175900	1.21661600
H	-3.60140500	4.00106800	-1.48308900
H	3.64696000	3.89516600	1.13393400
H	5.24873700	3.95943200	-1.50633900
H	9.15472800	3.86109200	-0.14776500
H	7.91356300	6.01959500	0.22303400
H	5.84835200	5.13184700	1.29332100
H	3.48811100	6.07253200	-0.13020400
H	1.48728000	5.24599100	1.06934000
H	-0.92513900	6.05753500	0.12880400
H	-2.87981100	5.12011900	1.27962000
H	8.11032600	1.28901600	1.19999800
H	9.12216100	-1.17951400	-0.32534500
H	8.12344600	-3.73511100	1.04168300
H	7.45501900	-5.02661700	-1.68188900
H	5.39947800	-5.88249000	-0.56915500
H	3.45134400	-5.87603000	-0.56357400
H	1.44768300	-5.12241500	0.68227700
H	-0.96039100	-5.85374700	-0.33997000
H	-2.89497500	-4.98973000	0.90721300
H	5.85457900	2.57394500	1.19572000
H	5.20027500	1.40823700	-1.59772400
H	5.84294100	0.03922600	1.10453800
H	5.19410600	-1.13058100	-1.68834300
H	5.83666500	-2.49508300	1.01639700
H	5.22942100	-3.68268100	-1.77788400
H	3.61745100	-3.79671300	0.85477700
H	7.39040900	0.12875800	-1.57632300
H	7.39517300	-2.41103000	-1.65744200
H	7.40914300	2.66799900	-1.48013900
C	-1.14984500	-2.43004700	3.36616000
C	0.17244300	-2.51117600	3.49322700
C	1.05025500	-1.29649800	3.64635400
C	0.19069000	-0.06053200	3.58619900
C	-1.13252600	-0.11213200	3.45402400
H	1.60651900	-1.33656800	4.59398000
H	-1.80633700	-3.28578900	3.25550500
H	0.62294800	-3.49883800	3.48458500
H	0.65568100	0.91806000	3.65460100
H	-1.77565000	0.75954600	3.40925100
O	-1.86625200	-1.26332500	3.34617100
H	1.81724000	-1.27184800	2.85640700

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C	5.19083000	-1.16496000	-0.60919700
C	5.90152900	-2.45603700	-0.13770600

C	3.71065200	-1.17700800	-0.17428100
C	8.10023300	-1.20019900	-0.01375300
C	7.38828600	-2.44353800	-0.57445900
C	5.19424200	-3.70590000	-0.71497700
C	3.00117200	-2.41851700	-0.73379300
C	8.10491400	-3.72319100	-0.10123600
C	5.91497700	-4.97919700	-0.22198100
C	3.70612200	-3.72131600	-0.31072900
C	1.52382500	-2.43150200	-0.30460000
C	7.39345100	-4.97479700	-0.62795200
H	5.82764100	-5.05910400	0.87790700
C	2.97946400	-4.92718800	-0.92042300
C	0.79911900	-1.13416100	-0.69927100
C	0.77769300	-3.66410200	-0.84235300
H	7.89273900	-5.88309000	-0.24223400
C	1.51932700	-4.95638600	-0.48890500
H	3.03135100	-4.86478000	-2.01640200
C	-0.66703800	-1.14653700	-0.23315200
C	-0.67347200	-3.68020000	-0.33982500
H	1.02840300	-5.81520000	-0.95600600
C	-1.41299600	-2.39279600	-0.73874400
C	-1.43843300	-4.92099300	-0.80717800
C	-2.87432800	-2.40461400	-0.25687700
C	-2.88029900	-4.92238800	-0.31657100
H	-1.42306900	-4.95892300	-1.90776400
C	-3.58790600	-1.10996400	-0.67307500
C	-3.61532100	-3.65422000	-0.76977900
H	-3.39455600	-5.82349700	-0.67316100
C	-5.04790200	-1.12177100	-0.17410300
C	-5.08215500	-3.66202300	-0.29348700
C	-5.79698500	-2.35875300	-0.72490800
C	-5.84326900	-4.87977800	-0.86055400
C	-7.26241900	-2.36942100	-0.22156000
H	-5.34149400	-5.81729900	-0.55448100
C	-7.30094000	-4.89571800	-0.38549800
C	-8.01791000	-3.59612500	-0.76904400
C	-7.98085100	-1.07546700	-0.64207100
H	-7.83049100	-5.76228600	-0.82305700
C	-7.97138000	3.96782600	-0.44901500
C	-7.96510400	1.44522100	-0.53549300
C	-7.24088900	5.22160800	0.04543900
C	-7.23244300	2.69003100	-0.00568500
C	-7.23759500	0.15974900	-0.10392200
C	-5.78118100	5.22834700	-0.42361700
H	-7.75811800	6.12831500	-0.31964100
C	-5.76548300	2.70505700	-0.50480700
C	-5.77428100	0.17259200	-0.60968600
C	-5.03744100	3.95737900	0.04056400
H	-5.74129600	5.30540700	-1.52654000
C	-5.03310500	1.41550600	-0.06304000

C	-3.56756600	3.97516200	-0.42608600
C	-3.57226200	1.42978100	-0.55945300
C	-2.82058800	5.18568900	0.14973200
C	-2.84490000	2.67392400	-0.02804600
C	-2.85137700	0.13496300	-0.15206300
C	-1.37424700	5.21338600	-0.32727700
H	-3.32097600	6.12219600	-0.12596900
C	-1.38160000	2.68882400	-0.50457800
C	-1.39323600	0.14702900	-0.63380100
C	-0.62629100	3.92261500	0.01683500
H	-1.34743200	5.36187300	-1.41812000
C	-0.65089900	1.39164900	-0.12168100
C	0.82329800	3.93574400	-0.49185400
C	0.81615100	1.40353500	-0.58448400
C	1.58289700	5.18386000	-0.03307400
C	1.55664500	2.65096800	-0.07301600
C	1.53528500	0.10874300	-0.17506800
C	3.03980900	5.17338800	-0.47682400
H	1.09973900	6.08483200	-0.42249400
C	3.03213300	2.65806800	-0.50862100
C	3.00819600	0.11918500	-0.60840100
C	3.75441600	3.91108900	0.02253200
H	3.08461600	5.20524200	-1.57444000
C	3.72677700	1.36364300	-0.06193600
C	5.24043400	3.91237200	-0.38950000
C	5.20601200	1.37189100	-0.50002000
C	5.97831800	5.13090200	0.20585300
C	5.93325400	2.60953200	0.07775200
C	5.91102700	0.07678100	-0.03280000
C	7.45571100	5.14227100	-0.20367100
H	5.49221600	6.06799400	-0.12645300
C	7.41913900	2.61571400	-0.36183600
C	7.39444600	0.08651100	-0.47627700
C	8.15226500	3.84241200	0.21500900
H	7.54269600	5.28136300	-1.29839300
C	8.11596700	1.32115100	0.09176700
H	-8.10549600	-3.52749000	-1.86972400
H	-8.05756900	-1.02340900	-1.74404400
H	-9.00516300	1.43257600	-0.16200500
H	-9.00732600	3.95743100	-0.06402500
H	8.19136100	3.77703400	1.31869200
H	9.17085900	1.32556400	-0.23798700
H	8.12892500	-1.24295200	1.09089400
H	9.15639300	-3.71481100	-0.44181200
H	-0.64215800	1.33155500	0.98126100
H	-0.66093300	-1.19321400	0.87144200
H	1.51698600	0.05785700	0.93039600
H	-1.40758700	0.19682600	-1.73953700
H	0.81872900	1.44937400	-1.68956600
H	0.80013300	-1.07803100	-1.80412900

H	-1.39803800	2.75277900	-1.60922800
H	-2.82923600	2.61647500	1.07494800
H	-3.57153700	1.48487800	-1.66809700
H	-2.82824500	0.08052200	0.95015800
H	-3.58948400	-1.06362100	-1.78241900
H	-2.85288500	-2.44358900	0.84627700
H	-1.43168700	-2.34879800	-1.84479900
H	-0.63624200	-3.70397800	0.76320800
H	0.75335600	-3.58020800	-1.94396000
H	1.50654600	-2.49462600	0.80079400
H	-0.58850700	3.84170300	1.11876800
H	0.78951100	3.95047700	-1.59612300
H	1.54689500	2.61204000	1.03373900
H	3.05102500	2.69596700	-1.61147200
H	3.68191500	1.31947400	1.04684900
H	3.02735100	0.16789500	-1.71068300
H	3.66479600	-1.23130500	0.93441800
H	3.02513000	-2.35983000	-1.83568300
H	-5.04345500	-1.17272300	0.94141200
H	-5.80455000	-2.30713000	-1.83896600
H	-5.09693100	-3.72412900	0.82132500
H	-3.59834200	-3.62193200	-1.87786200
H	-5.80851200	-4.86303700	-1.96618700
H	-7.33841300	-5.03739700	0.71170200
H	-9.05252200	-3.60643700	-0.38057800
H	-7.25467300	-2.42825400	0.89380000
H	-9.02029300	-1.08245000	-0.26678300
H	-5.78333500	0.22131900	-1.72403400
H	-7.22950000	0.11214400	1.01219400
H	-8.04039400	1.48786500	-1.63798400
H	-7.22783700	2.65403400	1.11062500
H	-5.77004500	2.75091600	-1.61915400
H	-5.03180200	1.36806100	1.05225500
H	-8.05576100	3.99382300	-1.55180200
H	-7.28221900	5.27100400	1.15048600
H	-5.26972000	6.13020400	-0.03689900
H	-5.05904600	3.92411200	1.15642600
H	-3.54283500	4.04549400	-1.53204100
H	3.68929600	3.88981300	1.12913700
H	5.30423700	3.97099200	-1.50268800
H	9.20312900	3.84962700	-0.12739400
H	7.96705800	6.00906000	0.25488400
H	5.89422400	5.11955500	1.30890600
H	3.54361800	6.07863300	-0.11608700
H	1.53397600	5.24742300	1.06541600
H	-0.87059000	6.07501900	0.12085100
H	-2.83697400	5.13262700	1.24749200
H	8.14519800	1.27090800	1.19609800
H	9.15536900	-1.18979600	-0.34263900
H	8.14248800	-3.75065500	1.00407100

H	7.48204000	-5.02330400	-1.73030200
H	5.41849600	-5.87901500	-0.63271400
H	3.47023900	-5.86623200	-0.63606400
H	1.46102900	-5.11275500	0.60047700
H	-0.94332000	-5.83020600	-0.45331400
H	-2.88705200	-4.97169900	0.78207800
H	5.89281300	2.56250400	1.19126900
H	5.24918000	1.42034600	-1.61439200
H	5.87346800	0.02931500	1.08091300
H	5.23601800	-1.11882900	-1.72360500
H	5.85928800	-2.50310900	0.97566600
H	5.26250000	-3.67127500	-1.82900000
H	3.63492700	-3.79504400	0.79368900
H	7.43398800	0.13307300	-1.59175200
H	7.43090900	-2.40723900	-1.68999200
H	7.46004800	2.67228300	-1.47657200
C	-1.12797000	-2.61686300	3.41876700
C	0.20133100	-2.53998900	3.35981300
C	1.01501100	-1.29836900	3.61713600
C	0.22531900	-0.02690700	3.44619200
C	-1.10241400	0.07046100	3.50953000
H	1.44221000	-1.33769000	4.63207300
H	-1.64985400	-3.55170300	3.23586000
H	0.74946400	-3.44695900	3.11133100
H	0.78993000	0.88512100	3.25994600
H	-1.60608200	1.02552500	3.39019000
H	1.88057100	-1.28371300	2.94049300
S	-2.22079200	-1.27172900	3.73580900

Graphane-U6N

C	5.16233100	-1.18039500	-0.56717000
C	5.88582300	-2.46423600	-0.09505600
C	3.69002400	-1.19192000	-0.10609500
C	8.08254900	-1.20109700	-0.02660300
C	7.36371100	-2.45210900	-0.56088200
C	5.17110400	-3.72292800	-0.64335300
C	2.97495500	-2.44275400	-0.63762000
C	8.09369300	-3.72454000	-0.08854500
C	5.90589900	-4.98823400	-0.15066900
C	3.69180200	-3.73690200	-0.20766800
C	1.50498300	-2.45317200	-0.18360300
C	7.37569300	-4.98392300	-0.58698900
H	5.84137300	-5.05571200	0.95161600
C	2.95644200	-4.95547400	-0.78043400
C	0.77223900	-1.16366400	-0.58985900
C	0.75437100	-3.69706400	-0.68747500
H	7.88568300	-5.88647700	-0.20176100
C	1.50483500	-4.98013800	-0.32013000
H	2.98648700	-4.91357600	-1.87820100
C	-0.69096300	-1.17329100	-0.11399300

C	-0.69207800	-3.70619800	-0.16992900
H	1.00783500	-5.84967300	-0.76023500
C	-1.43613800	-2.42965000	-0.59520100
C	-1.45475300	-4.96155200	-0.60165400
C	-2.90054100	-2.43467100	-0.12176200
C	-2.90004700	-4.95073100	-0.12127600
H	-1.43247100	-5.03355600	-1.70043900
C	-3.61223900	-1.14940000	-0.56839400
C	-3.63229400	-3.69669600	-0.61659800
H	-3.41010100	-5.86258800	-0.45599000
C	-5.07684600	-1.15759200	-0.08385600
C	-5.10610700	-3.69836700	-0.16297500
C	-5.81679300	-2.40357500	-0.62602500
C	-5.85628400	-4.92655000	-0.72221800
C	-7.28899000	-2.40973900	-0.14270300
H	-5.35754100	-5.85793500	-0.39324100
C	-7.32128700	-4.93783700	-0.27000300
C	-8.03435000	-3.64532300	-0.68389700
C	-8.00347300	-1.12235700	-0.58932600
H	-7.84257000	-5.81175300	-0.70280300
C	-8.00600400	3.92367600	-0.42988700
C	-7.99403700	1.40018900	-0.50339100
C	-7.28381800	5.18092000	0.06804500
C	-7.27037400	2.64939100	0.02859900
C	-7.26989300	0.11936500	-0.05293300
C	-5.81853800	5.18841100	-0.38327900
H	-7.79818000	6.08512300	-0.30716600
C	-5.79759200	2.66456000	-0.45296700
C	-5.80064800	0.13058300	-0.54103500
C	-5.07792400	3.92073600	0.09478000
H	-5.76557700	5.26114200	-1.48595000
C	-5.06789900	1.37905500	0.00444300
C	-3.60345300	3.93905700	-0.35676300
C	-3.60242000	1.39241800	-0.47751200
C	-2.86313900	5.15225500	0.22182400
C	-2.88163500	2.64092700	0.05261600
C	-2.88310300	0.10213300	-0.05340000
C	-1.41508100	5.18325900	-0.24967700
H	-3.36451400	6.08732400	-0.05701000
C	-1.41647400	2.65679100	-0.41765400
C	-1.42218200	0.11328800	-0.52772400
C	-0.66349600	3.89498900	0.09682500
H	-1.38540400	5.33136500	-1.34052300
C	-0.68208500	1.36379100	-0.02699400
C	0.78319200	3.91003700	-0.42032500
C	0.78250200	1.37624900	-0.49896500
C	1.54373200	5.16102200	0.02841800
C	1.52454900	2.62918200	-0.00351100
C	1.51040500	0.08714400	-0.08715100
C	2.99439200	5.15511100	-0.43561600

H	1.05257900	6.06030900	-0.35470500
C	2.99397000	2.63855400	-0.46016800
C	2.97672400	0.09783900	-0.54261200
C	3.72120000	3.89588000	0.05398200
H	3.02312500	5.18635700	-1.53379200
C	3.70011600	1.34878300	-0.01765000
C	5.19945600	3.89988100	-0.38548900
C	5.17170300	1.35826500	-0.48094400
C	5.94455200	5.12388200	0.18925300
C	5.90515600	2.60188600	0.07588400
C	5.88895900	0.06900600	-0.01586300
C	7.41378700	5.13761300	-0.24862000
H	5.44931500	6.05773200	-0.13861400
C	7.38260300	2.60993000	-0.39132200
C	7.36389200	0.07932400	-0.48684200
C	8.12252800	3.84245900	0.16402700
H	7.47930900	5.27066700	-1.34557400
C	8.09211800	1.32064800	0.05768000
H	-8.10509400	-3.59290300	-1.78662800
H	-8.06318400	-1.08264200	-1.69277700
H	-9.03903000	1.38812700	-0.14400300
H	-9.04665100	3.91317900	-0.05777500
H	8.18319200	3.78372300	1.26711200
H	9.14035200	1.32591200	-0.29269600
H	8.13339600	-1.23326500	1.07762900
H	9.13803300	-3.71680700	-0.45048400
H	-0.66956800	1.31371400	1.07749900
H	-0.67722500	-1.20311900	0.99016400
H	1.50934000	0.04565000	1.01825800
H	-1.43243100	0.15260200	-1.63386500
H	0.77468700	1.41455900	-1.60430200
H	0.76365800	-1.12218400	-1.69531600
H	-1.42996200	2.71340500	-1.52275200
H	-2.87255200	2.58872100	1.15571700
H	-3.59065600	1.43992800	-1.58654700
H	-2.87149800	0.05509800	1.04871500
H	-3.60116900	-1.11890800	-1.67827800
H	-2.89189000	-2.44976800	0.98148400
H	-1.45057200	-2.40804700	-1.70192700
H	-0.64690100	-3.70438800	0.93401000
H	0.71487600	-3.63533300	-1.79011400
H	1.50684800	-2.49587800	0.92215300
H	-0.62100100	3.81844400	1.19877800
H	0.74130000	3.92141400	-1.52438100
H	1.52956500	2.59608500	1.10338600
H	2.99602100	2.67113300	-1.56334200
H	3.67491300	1.31228100	1.09188800
H	2.97965400	0.13629700	-1.64547400
H	3.66311900	-1.23314700	1.00359300
H	2.98078200	-2.39971300	-1.74048600

H	-5.08280100	-1.19499400	1.03271700
H	-5.80884800	-2.36952000	-1.74064100
H	-5.13797400	-3.74214300	0.95248700
H	-3.59832300	-3.69101200	-1.72487100
H	-5.80428100	-4.92743700	-1.82728300
H	-7.37568800	-5.06306900	0.82850500
H	-9.07478500	-3.65172600	-0.31122300
H	-7.29618600	-2.45378300	0.97346800
H	-9.04849000	-1.12701100	-0.22992700
H	-5.79604000	0.16928300	-1.65568600
H	-7.27503700	0.08100800	1.06368900
H	-8.05426100	1.43539000	-1.60700600
H	-7.27904300	2.61902800	1.14510000
H	-5.78899500	2.70462000	-1.56748900
H	-5.07771500	1.33878600	1.12014000
H	-8.07671900	3.94445900	-1.53372100
H	-7.33865400	5.23485600	1.17228000
H	-5.31330700	6.09271200	0.00594600
H	-5.11139800	3.89233300	1.21044000
H	-3.56797400	4.00579000	-1.46272200
H	3.67663300	3.87765400	1.16166200
H	5.24234500	3.95255100	-1.49998600
H	9.16659000	3.85101600	-0.19862700
H	7.93097100	6.00867200	0.19509500
H	5.88161100	5.11812400	1.29374200
H	3.50035700	6.06232300	-0.08292800
H	1.50913700	5.22462900	1.12745600
H	-0.91483300	6.04646200	0.19938800
H	-2.88452800	5.09986500	1.31948500
H	8.14313500	1.27860000	1.16158400
H	9.13089300	-1.19070900	-0.37656900
H	8.15381600	-3.73987000	1.01600600
H	7.44181000	-5.04420400	-1.69032100
H	5.40418200	-5.89428300	-0.54079300
H	3.45530100	-5.88787600	-0.48838700
H	1.46742100	-5.11365600	0.77314100
H	-0.95964000	-5.85830100	-0.21702100
H	-2.91561000	-4.96778600	0.97806500
H	5.88564700	2.56116600	1.19023100
H	5.19586400	1.39866400	-1.59613900
H	5.87220900	0.03135900	1.09877200
H	5.18770300	-1.14553900	-1.68256900
H	5.86554200	-2.49848700	1.01943500
H	5.21610400	-3.70119900	-1.75883800
H	3.64451600	-3.79223500	0.89897100
H	7.38260200	0.11661900	-1.60318000
H	7.38449000	-2.42715300	-1.67731900
H	7.40257800	2.65937400	-1.50694900
C	-1.29020200	-2.39430000	3.47202500
C	0.10159400	-2.45226900	3.51998800

C	0.81222600	-1.25737000	3.57232400
C	0.10130900	-0.06145700	3.57885500
C	-1.29039000	-0.11729800	3.52774600
N	-1.98584500	-1.25523000	3.47231300
H	1.89860300	-1.25780800	3.59906200
H	-1.87579100	-3.31068300	3.42199000
H	0.60980400	-3.41152200	3.50500200
H	0.60908100	0.89769300	3.61162300
H	-1.87609800	0.80035000	3.52131100

Graphane-U5C

C	-5.19165700	1.32187900	-0.43063800
C	-5.92544000	2.56292000	0.13139000
C	-3.72029000	1.31293400	0.03383500
C	-8.11226300	1.27998000	0.10663300
C	-7.40368800	2.57281300	-0.33343000
C	-5.22228900	3.86324200	-0.32737300
C	-3.01627700	2.60217200	-0.41433600
C	-8.14296400	3.80116800	0.23212300
C	-5.96527300	5.08378600	0.25757400
C	-3.74108400	3.85996700	0.10233400
C	-1.54309900	2.59598400	0.03076800
C	-7.43637300	5.09961300	-0.17408900
H	-5.89765300	5.07144300	1.36175600
C	-3.01983200	5.11895800	-0.39646200
C	-0.80481800	1.33955700	-0.46120600
C	-0.80832600	3.87438300	-0.40552700
H	-7.95219500	5.96716700	0.27791400
C	-1.56348900	5.12647900	0.04946600
H	-3.06157600	5.14934500	-1.49428800
C	0.66389700	1.33428100	-0.00369400
C	0.64729700	3.86595900	0.08605100
H	-1.07822900	6.02534500	-0.34210900
C	1.39245000	2.62112500	-0.42393600
C	1.39195200	5.14908900	-0.29343300
C	2.86410300	2.61389100	0.02653500
C	2.84834100	5.12710300	0.15252200
H	1.34295700	5.27967600	-1.38583300
C	3.57931300	1.35550900	-0.48705600
C	3.57976900	3.90415000	-0.41698900
H	3.34389700	6.05732600	-0.15183100
C	5.04978800	1.35258100	-0.01907800
C	5.06127600	3.89529700	0.01189300
C	5.77388400	2.62653300	-0.51582000
C	5.79437200	5.15092800	-0.50776800
C	7.25271700	2.62327700	-0.05282700
H	5.29430900	6.06434300	-0.13327300
C	7.26618300	5.15481600	-0.07815800
C	7.98167100	3.88520500	-0.55408100
C	7.97006800	1.36035500	-0.56047100

H	7.77462900	6.04905800	-0.48410400
C	8.01049600	-3.68856900	-0.60455400
C	7.97977400	-1.16392600	-0.57705300
C	7.30175900	-4.96973300	-0.14996800
C	7.27027100	-2.43901700	-0.08906000
C	7.25182600	0.09212600	-0.06705200
C	5.83268100	-4.97052200	-0.58863500
H	7.81920300	-5.85467900	-0.56481300
C	5.79350600	-2.44574700	-0.55811800
C	5.77746400	0.09060500	-0.53946800
C	5.08681400	-3.72808800	-0.05580100
H	5.77048300	-5.00120100	-1.69283500
C	5.05833000	-1.18557300	-0.04270000
C	3.60959600	-3.73938000	-0.49913000
C	3.58989200	-1.18934300	-0.51713500
C	2.87858100	-4.97549200	0.04136400
C	2.88076900	-2.46384700	-0.03717000
C	2.86373500	0.07474700	-0.02966200
C	1.43328100	-5.00301100	-0.43856400
H	3.38831800	-5.89869000	-0.26107700
C	1.41630600	-2.46857700	-0.50816100
C	1.39945100	0.07651400	-0.49267800
C	0.66841700	-3.73321300	-0.05535400
H	1.41223300	-5.11601900	-1.53393700
C	0.67241500	-1.20308800	-0.05047600
C	-0.76833400	-3.73476000	-0.60057900
C	-0.79136300	-1.20040000	-0.52507700
C	-1.52469200	-5.01731900	-0.24439000
C	-1.52789300	-2.48820500	-0.11940700
C	-1.52940100	0.05387400	-0.03156000
C	-2.96812800	-4.99130900	-0.73096700
H	-1.01930200	-5.88614100	-0.67664900
C	-2.99271700	-2.47858400	-0.58830200
C	-2.99569200	0.06156300	-0.48845300
C	-3.71257600	-3.77389100	-0.16732600
H	-2.97910400	-4.94687200	-1.82902100
C	-3.71105000	-1.22895700	-0.05771400
C	-5.18692000	-3.75823100	-0.61959300
C	-5.18034800	-1.21599100	-0.52814900
C	-5.92619800	-5.02723000	-0.14364600
C	-5.90622200	-2.50309400	-0.06849300
C	-5.90928600	0.03024400	0.02717000
C	-7.39255100	-5.01865500	-0.59126300
H	-5.42171900	-5.93008900	-0.53743500
C	-7.38126000	-2.48734900	-0.54272400
C	-7.38304000	0.04333800	-0.44731300
C	-8.11400500	-3.76392100	-0.08615900
H	-7.45020100	-5.06826800	-1.69558900
C	-8.10275500	-1.24118400	-0.00051300
H	8.03662100	3.87789100	-1.65901300

H	8.01645900	1.36631000	-1.66534900
H	9.02856900	-1.15903800	-0.22872600
H	9.05461400	-3.68526600	-0.24226400
H	-8.18071500	-3.78899400	1.01786400
H	-9.14981900	-1.22822400	-0.35406600
H	-8.16255200	1.22975300	1.21023700
H	-9.18807000	3.81134500	-0.12729700
H	0.66748200	-1.20851400	1.05490900
H	0.66298600	1.29939800	1.10016000
H	-1.52414200	0.02390000	1.07528900
H	1.40145700	0.09632300	-1.59948800
H	-0.78118400	-1.16493800	-1.63059500
H	-0.80943900	1.36693700	-1.56701800
H	1.42982600	-2.47027700	-1.61504200
H	2.86838700	-2.45525100	1.06578200
H	3.57301800	-1.18553300	-1.62721400
H	2.85428300	0.05935400	1.07373200
H	3.55690000	1.37999100	-1.59656400
H	2.86891400	2.58330000	1.13049300
H	1.39060400	2.66339400	-1.52987300
H	0.62472500	3.80444800	1.18940700
H	-0.78545800	3.87936000	-1.51027700
H	-1.53682400	2.57171200	1.13760400
H	0.60659300	-3.69696600	1.04832300
H	-0.70568400	-3.67887700	-1.70232600
H	-1.55005200	-2.52858500	0.98617000
H	-2.98791300	-2.43270700	-1.69097500
H	-3.69101200	-1.27313800	1.05154500
H	-2.99438100	0.10100600	-1.59134700
H	-3.69533900	1.27949700	1.14314200
H	-3.02589800	2.63302600	-1.51761100
H	5.07051100	1.34163100	1.09685100
H	5.75085700	2.64048800	-1.63077200
H	5.11147800	3.89395800	1.12730500
H	3.52702300	3.95133500	-1.52324100
H	5.72492400	5.19695700	-1.61097700
H	7.33729500	5.23737600	1.02338100
H	9.02749900	3.88422700	-0.19671500
H	7.27570900	2.62264200	1.06384800
H	9.01958200	1.35793200	-0.21428200
H	5.76126900	0.10072800	-1.65476100
H	7.26969800	0.08465500	1.04988800
H	8.02834300	-1.15384900	-1.68181000
H	7.28901400	-2.45356400	1.02754700
H	5.77526700	-2.44080000	-1.67326900
H	5.07439600	-1.19372700	1.07325500
H	8.07049400	-3.66533100	-1.70900500
H	7.36685900	-5.06661600	0.95074900
H	5.33682900	-5.89277300	-0.23051900
H	5.12710800	-3.74381200	1.05973600

H	3.56856700	-3.76824400	-1.60673400
H	-3.67864000	-3.82991200	0.93954800
H	-5.22030300	-3.72834300	-1.73513500
H	-9.15606600	-3.75307700	-0.45437000
H	-7.90552700	-5.92472200	-0.21855300
H	-5.87034400	-5.10398100	0.95858500
H	-3.47194500	-5.92424900	-0.44959000
H	-1.50701600	-5.15171700	0.84876000
H	0.93619200	-5.88417300	-0.02146800
H	2.89414400	-4.95266800	1.14050700
H	-8.15734500	-1.28273900	1.10325400
H	-9.16062600	1.28710400	-0.24316200
H	-8.20010300	3.73506700	1.33499300
H	-7.50638900	5.24034400	-1.26980600
H	-5.47160700	6.01965400	-0.06674900
H	-3.52207000	6.02626800	-0.03860500
H	-1.51477200	5.19242400	1.14775500
H	0.89940400	6.01928800	0.15048400
H	2.88910800	5.09428300	1.25040200
H	-5.89263300	-2.54422800	1.04598500
H	-5.19918600	-1.17424000	-1.64337900
H	-5.89494400	-0.01270000	1.14170900
H	-5.21491400	1.36726700	-1.54568500
H	-5.90379200	2.51836900	1.24555800
H	-5.27193000	3.92104400	-1.44139800
H	-3.68856500	3.84430500	1.20957800
H	-7.39910900	0.09041500	-1.56331200
H	-7.42536400	2.63041900	-1.44864300
H	-7.39581200	-2.45216000	-1.65893200
C	-0.09449000	-1.54131100	3.74501300
H	-0.70941500	-1.88784700	2.90094800
H	-0.63012700	-1.83469600	4.65833400
C	1.29279300	-2.11515300	3.69351300
H	1.51088600	-3.17642700	3.71734000
C	2.18507400	-1.11079400	3.61692400
H	3.26368600	-1.21267200	3.56366900
C	0.14459600	-0.05967100	3.68086700
H	-0.64549800	0.68242400	3.69234100
C	1.46815400	0.17282600	3.60860700
H	1.94699200	1.14446500	3.54699100

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C	-5.17953000	1.33526400	-0.43565400
C	-5.90978500	2.58166000	0.11905500
C	-3.70514600	1.32926300	0.01937300
C	-8.09574800	1.29867900	0.12636700
C	-7.39107000	2.58597300	-0.33577100
C	-5.20901500	3.87714800	-0.35668500
C	-3.00295900	2.61600100	-0.43831100
C	-8.12706900	3.82124100	0.21886700

C	-5.94995900	5.10434400	0.21681100
C	-3.72703700	3.87732000	0.07023500
C	-1.53081800	2.61120500	0.00927400
C	-7.42308400	5.11444300	-0.20800200
H	-5.87728200	5.10507100	1.32077700
C	-3.00520800	5.13214600	-0.43788800
C	-0.79118600	1.35434900	-0.47985500
C	-0.79283600	3.88849500	-0.42468100
H	-7.93690900	5.98771900	0.23506700
C	-1.55122700	5.14400400	0.01551100
H	-3.04196200	5.15175500	-1.53613600
C	0.67399800	1.34722100	-0.01075100
C	0.65607400	3.88019700	0.08629200
H	-1.06363200	6.03963100	-0.38087400
C	1.40790500	2.63611700	-0.41535800
C	1.40673800	5.16371100	-0.27904400
C	2.87281300	2.62672200	0.05679300
C	2.85471400	5.14032400	0.19332500
H	1.37701500	5.29618000	-1.37188300
C	3.59608600	1.37269500	-0.45582400
C	3.59633100	3.91941800	-0.36683600
H	3.35623200	6.07131400	-0.09859500
C	5.05925200	1.36425000	0.03557100
C	5.06939900	3.90713800	0.09065800
C	5.79171900	2.64334300	-0.43555100
C	5.81226300	5.16734300	-0.40314200
C	7.26206600	2.63501400	0.05356900
H	5.30524300	6.07735900	-0.02948300
C	7.27563200	5.16683200	0.05418000
C	7.99994400	3.90203600	-0.42100200
C	7.98834500	1.37799100	-0.45595400
H	7.79155200	6.06504300	-0.33338300
C	8.02955800	-3.66741600	-0.58767700
C	7.99836900	-1.14465100	-0.51039700
C	7.31330000	-4.95794500	-0.17355300
C	7.28092200	-2.42854600	-0.05871700
C	7.26179900	0.10317800	0.00729300
C	5.85184700	-4.94832500	-0.63666700
H	7.83750600	-5.83359800	-0.59987400
C	5.81182200	-2.42545500	-0.55145400
C	5.79520200	0.10884200	-0.48891200
C	5.09719000	-3.71799000	-0.08850900
H	5.80804200	-4.95419700	-1.74226500
C	5.06854800	-1.17506600	-0.02352000
C	3.62689200	-3.71887100	-0.55569000
C	3.60617600	-1.17056500	-0.51830200
C	2.88999100	-4.97065400	-0.06217100
C	2.89038500	-2.45453700	-0.07417800
C	2.87332600	0.08701800	-0.02385400
C	1.44790600	-4.98121600	-0.55236800

H	3.40278600	-5.88335100	-0.39014200
C	1.42833300	-2.44926200	-0.55427400
C	1.41361600	0.09268900	-0.50209300
C	0.68343000	-3.72472900	-0.12775800
H	1.43323700	-5.05645000	-1.65103700
C	0.68381000	-1.19091700	-0.07716400
C	-0.76088000	-3.71558500	-0.65027000
C	-0.77909800	-1.18427000	-0.55425500
C	-1.50957200	-5.00157800	-0.28890200
C	-1.50967600	-2.47283200	-0.14093700
C	-1.51541700	0.06795000	-0.05291300
C	-2.96319500	-4.97404400	-0.74251500
H	-1.01424300	-5.86761200	-0.73834000
C	-2.98125500	-2.46318100	-0.58964500
C	-2.98385200	0.07556400	-0.50168800
C	-3.69513700	-3.75849500	-0.15866500
H	-2.99888400	-4.92545900	-1.83993300
C	-3.69446300	-1.21241400	-0.05563500
C	-5.17749000	-3.74486800	-0.58438100
C	-5.16888000	-1.20289900	-0.51081900
C	-5.90798900	-5.01023200	-0.08521400
C	-5.88871400	-2.48610500	-0.03174800
C	-5.89279500	0.04792800	0.04067800
C	-7.38129500	-5.00708700	-0.50955700
H	-5.40862700	-5.91621400	-0.47822500
C	-7.37012600	-2.47543900	-0.48607600
C	-7.37122400	0.05548600	-0.41896600
C	-8.09562200	-3.74757400	-0.00596000
H	-7.45630000	-5.06787700	-1.61223300
C	-8.08523700	-1.22375700	0.05169300
H	8.07555200	3.90615700	-1.52479800
H	8.05554500	1.39814200	-1.55972900
H	9.04082500	-1.14607200	-0.14320700
H	9.06740500	-3.67235500	-0.20759700
H	-8.14520500	-3.76166100	1.09917600
H	-9.13678300	-1.21496800	-0.28810800
H	-8.13576200	1.26186400	1.23094600
H	-9.17437200	3.82672600	-0.13407900
H	0.66661300	-1.21312900	1.02696300
H	0.66026200	1.30331800	1.09313900
H	-1.50391600	0.03098100	1.05200300
H	1.42812800	0.12320000	-1.60851900
H	-0.77246300	-1.14685900	-1.66020900
H	-0.78814600	1.38360700	-1.58572000
H	1.44966400	-2.43095500	-1.66092200
H	2.86505700	-2.47311200	1.02984200
H	3.60578600	-1.14872000	-1.62781700
H	2.84768500	0.05909200	1.07943400
H	3.59197300	1.40736900	-1.56502800
H	2.86072100	2.58909200	1.16074600

H	1.42260800	2.68166700	-1.52099900
H	0.61732000	3.81724100	1.18907400
H	-0.75645600	3.88865300	-1.52905400
H	-1.52823200	2.58720700	1.11603000
H	0.63106000	-3.71648000	0.97529000
H	-0.71965900	-3.64960200	-1.75274200
H	-1.50184500	-2.51280800	0.96444600
H	-2.99118300	-2.41973400	-1.69267500
H	-3.66150400	-1.25052900	1.05332700
H	-2.99203000	0.10826000	-1.60492400
H	-3.67309400	1.30114600	1.12862800
H	-3.01237800	2.63951100	-1.54177600
H	5.06316500	1.34149900	1.15100700
H	5.78867000	2.66806400	-1.55067200
H	5.09815800	3.89589700	1.20666700
H	3.56512300	3.97130500	-1.47362500
H	5.76345900	5.22419800	-1.50699300
H	7.32619100	5.23881900	1.15756400
H	9.03902100	3.89745000	-0.04436900
H	7.26561100	2.62222500	1.17029100
H	9.03140700	1.37112200	-0.09060500
H	5.79758500	0.13469200	-1.60429400
H	7.26223600	0.07917400	1.12393500
H	8.06754600	-1.11522600	-1.61387800
H	7.28245100	-2.46552000	1.05733400
H	5.81198000	-2.39758700	-1.66664100
H	5.07116700	-1.20253300	1.09131800
H	8.10894700	-3.62061000	-1.69027800
H	7.36057100	-5.08022800	0.92545000
H	5.35021600	-5.87856400	-0.30829800
H	5.12020300	-3.75938800	1.02648800
H	3.60369300	-3.71666800	-1.66384400
H	-3.64004700	-3.81820800	0.94706100
H	-5.23036900	-3.72381100	-1.69939700
H	-9.14311800	-3.74060300	-0.35825200
H	-7.88761900	-5.90949800	-0.11943900
H	-5.83449900	-5.07635600	1.01671400
H	-3.46048500	-5.90830800	-0.45345200
H	-1.46775700	-5.14297500	0.80271400
H	0.95012900	-5.87673200	-0.16865000
H	2.89681000	-4.98510200	1.03758800
H	-8.12494000	-1.25292100	1.15651100
H	-9.14718200	1.30137700	-0.21390300
H	-8.17718700	3.76890100	1.32282900
H	-7.49839500	5.24052900	-1.30511400
H	-5.45812300	6.03634600	-0.12096900
H	-3.50920600	6.04278000	-0.09104100
H	-1.50911200	5.21936500	1.11349900
H	0.90651300	6.03316500	0.15764400
H	2.87510500	5.10388100	1.29172000

H	-5.85924900	-2.51896800	1.08272500
H	-5.19942100	-1.17105700	-1.62604700
H	-5.86696100	0.01494700	1.15543900
H	-5.21039100	1.36951300	-1.55078900
H	-5.88070200	2.54790500	1.23351200
H	-5.26149200	3.92249600	-1.47101300
H	-3.67296700	3.86977700	1.17752900
H	-7.39862400	0.08842300	-1.53521300
H	-7.42046200	2.62905000	-1.45140600
H	-7.39963800	-2.45232100	-1.60230200
C	1.20557500	-0.09069100	3.51634000
C	-0.13873000	-0.36436700	3.61623000
C	-0.28448100	-1.77980300	3.61221400
C	0.97657500	-2.32102300	3.51082400
N	1.87061900	-1.28559900	3.45534100
H	2.86893800	-1.38756700	3.35664600
H	1.74066900	0.84720500	3.48505600
H	-0.92841400	0.37039600	3.68901500
H	-1.20772900	-2.33755400	3.68216100
H	1.31097000	-3.34749000	3.47746100

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C	-5.15396300	1.35806400	-0.45585200
C	-5.88618500	2.60482500	0.09547800
C	-3.68256600	1.34878700	0.00821400
C	-8.07426000	1.32574100	0.08406800
C	-7.36369100	2.61214200	-0.37146100
C	-5.17911900	3.89997200	-0.37175100
C	-2.97477300	2.63601500	-0.43916100
C	-8.10230400	3.84807900	0.17808700
C	-5.92312600	5.12745400	0.19701000
C	-3.70110500	3.89640900	0.06860900
C	-1.50597000	2.62697600	0.01955300
C	-7.39234600	5.14052100	-0.24097500
H	-5.86032600	5.12669100	1.30155400
C	-2.97260200	5.15247900	-0.42659400
C	-0.76462800	1.37152300	-0.47061800
C	-0.76257600	3.90534800	-0.40122000
H	-7.90866800	6.01421900	0.19843300
C	-1.52268500	5.15943200	0.03968000
H	-2.99965200	5.17789400	-1.52497800
C	0.69885200	1.35828300	0.00477300
C	0.68228300	3.89104000	0.12077600
H	-1.03005300	6.05625600	-0.34738400
C	1.43619700	2.64998300	-0.38535700
C	1.43691600	5.17662500	-0.22901900
C	2.89864900	2.63461100	0.09338300
C	2.88225100	5.14679000	0.25070400
H	1.41308700	5.31872300	-1.32081400
C	3.62096500	1.38376600	-0.42843200

C	3.62476700	3.92999100	-0.31720200
H	3.38613000	6.07992100	-0.03012000
C	5.08345400	1.36933600	0.06332800
C	5.09573100	3.91156400	0.14599200
C	5.81803200	2.65289700	-0.39223700
C	5.84164300	5.17681400	-0.33007300
C	7.28716000	2.63732100	0.10032100
H	5.33442400	6.08286600	0.05257800
C	7.30328500	5.16897600	0.13274800
C	8.02779000	3.90948800	-0.35599800
C	8.01348400	1.38626000	-0.42361300
H	7.82164100	6.07150400	-0.24105300
C	8.04891400	-3.65748900	-0.61515600
C	8.02048900	-1.13550100	-0.51037800
C	7.33141100	-4.95143400	-0.21386900
C	7.30125600	-2.42347800	-0.07349300
C	7.28454300	0.10653200	0.02205400
C	5.86978800	-4.93563500	-0.67651000
H	7.85466300	-5.82336300	-0.64860100
C	5.83233900	-2.41351200	-0.56679400
C	5.81862900	0.11972900	-0.47599300
C	5.11696800	-3.70977700	-0.11571700
H	5.82574400	-4.93013200	-1.78201800
C	5.09022600	-1.16832400	-0.02542400
C	3.64614300	-3.70481600	-0.58002500
C	3.62825000	-1.15666500	-0.51933400
C	2.90993900	-4.96043200	-0.09487500
C	2.91194600	-2.44371800	-0.08617300
C	2.89645600	0.09476800	-0.00775800
C	1.46600900	-4.96619000	-0.57933400
H	3.42055600	-5.87066000	-0.43304400
C	1.44905800	-2.43550000	-0.56425400
C	1.43888100	0.10667300	-0.49236000
C	0.70475700	-3.71241800	-0.14087300
H	1.44635500	-5.03194300	-1.67854500
C	0.70499500	-1.17913000	-0.08129100
C	-0.74293400	-3.70077600	-0.65438400
C	-0.75782700	-1.16788200	-0.55787600
C	-1.49330000	-4.98306000	-0.28365700
C	-1.49051400	-2.45610600	-0.14761200
C	-1.49421100	0.08441400	-0.05604600
C	-2.94627900	-4.95765600	-0.73938700
H	-0.99886100	-5.85362900	-0.72478900
C	-2.96120300	-2.44500500	-0.59964000
C	-2.96026900	0.09540300	-0.51214300
C	-3.67882000	-3.73755400	-0.16615800
H	-2.97968300	-4.91733700	-1.83716600
C	-3.67464200	-1.19220800	-0.07067000
C	-5.15888600	-3.72330100	-0.59957400
C	-5.14709100	-1.18073600	-0.53182900

C	-5.89406200	-4.98613600	-0.10100300
C	-5.87150000	-2.46207500	-0.05445500
C	-5.87233800	0.07147400	0.01482800
C	-7.36467900	-4.98218200	-0.53454900
H	-5.39373800	-5.89404700	-0.48840700
C	-7.35000800	-2.45033100	-0.51825900
C	-7.34756300	0.08118200	-0.45515300
C	-8.08047100	-3.72013900	-0.03953200
H	-7.43289600	-5.04652700	-1.63749400
C	-8.06697100	-1.19642000	0.01173600
H	8.10687600	3.92725400	-1.45936500
H	8.08300900	1.42017900	-1.52682100
H	9.06262600	-1.14224600	-0.14253400
H	9.08662700	-3.66714400	-0.23492800
H	-8.13791100	-3.73108800	1.06525000
H	-9.11582900	-1.18653500	-0.33648400
H	-8.12427300	1.28881000	1.18822500
H	-9.14643200	3.85586200	-0.18426100
H	0.68800400	-1.21190800	1.02274200
H	0.68535300	1.30738900	1.10931300
H	-1.49136900	0.04365200	1.04879800
H	1.45580500	0.14586000	-1.59826200
H	-0.74952400	-1.12815700	-1.66353900
H	-0.75364100	1.40704900	-1.57603800
H	1.46711500	-2.41142600	-1.67076600
H	2.89245700	-2.46785600	1.01722000
H	3.62585200	-1.12227900	-1.62880500
H	2.87113500	0.05239600	1.09470400
H	3.61740800	1.42808000	-1.53756700
H	2.88318200	2.58685600	1.19608200
H	1.45535400	2.70288800	-1.49053100
H	0.63566200	3.82005600	1.22285700
H	-0.71742400	3.91162700	-1.50519900
H	-1.51253800	2.59767100	1.12642600
H	0.66273000	-3.71180800	0.96264400
H	-0.70742600	-3.63925800	-1.75730200
H	-1.48765000	-2.49684100	0.95806800
H	-2.96833400	-2.40455700	-1.70271300
H	-3.64710300	-1.23010800	1.03884800
H	-2.96339900	0.12987600	-1.61522900
H	-3.65785600	1.31653500	1.11771600
H	-2.97544200	2.66378000	-1.54250100
H	5.08594300	1.33220200	1.17888200
H	5.81776900	2.68975600	-1.50696500
H	5.12018200	3.88676300	1.26199400
H	3.59786000	3.99186500	-1.42368500
H	5.79721900	5.24655500	-1.43333100
H	7.34954800	5.22621000	1.23721500
H	9.06557200	3.89893800	0.02400300
H	7.28760700	2.60990200	1.21686400

H	9.05556500	1.37360700	-0.05576900
H	5.82215800	0.15867300	-1.59083300
H	7.28267900	0.06815700	1.13848300
H	8.08981500	-1.09322000	-1.61331400
H	7.30150900	-2.47226700	1.04229000
H	5.83246300	-2.37444900	-1.68145700
H	5.09129900	-1.20772100	1.09000100
H	8.12819500	-3.59946700	-1.71714200
H	7.37836100	-5.08399100	0.88402400
H	5.36738400	-5.86844200	-0.35704900
H	5.14147900	-3.76084700	0.99917600
H	3.62031300	-3.69370500	-1.68819900
H	-3.62951400	-3.79145100	0.94026300
H	-5.20573100	-3.70540000	-1.71498700
H	-9.12552500	-3.71272400	-0.39916200
H	-7.87474800	-5.88268400	-0.14479000
H	-5.82744500	-5.04929900	1.00149600
H	-3.44499900	-5.88926400	-0.44441900
H	-1.45234600	-5.11515400	0.80952000
H	0.96948200	-5.86466800	-0.20093200
H	2.92108500	-4.98442000	1.00451900
H	-8.11578400	-1.22380400	1.11622100
H	-9.12273500	1.33034300	-0.26543900
H	-8.16255600	3.79465000	1.28148200
H	-7.45767500	5.26809100	-1.33858200
H	-5.42693700	6.05921600	-0.13516400
H	-3.47820300	6.06205900	-0.07946400
H	-1.48989600	5.22874700	1.13841200
H	0.93524100	6.04277500	0.21266200
H	2.89716400	5.10000900	1.34870900
H	-5.84935200	-2.49257000	1.06019500
H	-5.17261500	-1.15020300	-1.64728900
H	-5.85471400	0.03820700	1.12966800
H	-5.17776500	1.39358500	-1.57116800
H	-5.86647900	2.56897200	1.21003000
H	-5.22144700	3.94741600	-1.48645900
H	-3.65725600	3.88347100	1.17635600
H	-7.36706700	0.11322400	-1.57160500
H	-7.38388100	2.65613900	-1.48728500
H	-7.37231700	-2.43003100	-1.63473100
C	0.19098500	-0.27773900	3.54367500
C	-0.75956000	-1.24642600	3.59062800
C	-0.05265500	-2.49311600	3.56601700
C	1.26566200	-2.17344600	3.50546600
O	1.42814200	-0.82816700	3.49215400
H	0.15464100	0.80085100	3.54375300
H	-1.82871600	-1.09620300	3.63469400
H	-0.47248300	-3.48841900	3.58714400
H	2.17222900	-2.75794300	3.47356200

Graphane-U5S

C	-5.17375600	1.36270500	-0.50497500
C	-5.91202000	2.60428300	0.05014000
C	-3.70499800	1.35310500	-0.03254400
C	-8.09796600	1.32179900	0.01250500
C	-7.38593000	2.61261000	-0.42805100
C	-5.20380100	3.90433400	-0.40146500
C	-2.99744500	2.64517800	-0.46622100
C	-8.13100000	3.84307800	0.12514800
C	-5.95426600	5.12582800	0.17161900
C	-3.72899100	3.89934900	0.04956600
C	-1.53032600	2.63465600	-0.00218600
C	-7.41997700	5.13999200	-0.27791000
H	-5.90010500	5.11602300	1.27657600
C	-2.99975300	5.16217200	-0.42705400
C	-0.78561500	1.38505200	-0.50211000
C	-0.78847300	3.91885100	-0.40725700
H	-7.94127100	6.00930000	0.16433900
C	-1.55218700	5.16596700	0.04652800
H	-3.02109200	5.20059000	-1.52519300
C	0.67840400	1.37141700	-0.02819600
C	0.65619100	3.90088800	0.11540200
H	-1.05932800	6.06854900	-0.32663100
C	1.41093700	2.66816300	-0.40955400
C	1.40697200	5.19372900	-0.21559800
C	2.87657800	2.65017400	0.05894900
C	2.85510400	5.15867000	0.25549700
H	1.37747900	5.35502500	-1.30458200
C	3.59693700	1.40800500	-0.48569300
C	3.59578400	3.95331300	-0.33857300
H	3.35552700	6.09759400	-0.01180100
C	5.06559600	1.39144500	-0.01255000
C	5.07213500	3.93171000	0.10715400
C	5.79042800	2.68333200	-0.45992300
C	5.80870200	5.20633500	-0.35830500
C	7.26670000	2.66410800	0.01048000
H	5.30473600	6.10471600	0.04615400
C	7.27675900	5.19470600	0.08357600
C	7.99722100	3.94540800	-0.43628200
C	7.98776700	1.42325100	-0.54421100
H	7.78754400	6.10467600	-0.28259700
C	8.03193200	-3.61935300	-0.79800100
C	7.99909700	-1.09785900	-0.66659000
C	7.32735500	-4.91888500	-0.39145300
C	7.29235300	-2.39263400	-0.22937200
C	7.26989800	0.13521000	-0.10476500
C	5.85537600	-4.90411200	-0.82014200
H	7.84310600	-5.78554400	-0.84517300
C	5.81379000	-2.38310800	-0.69308100
C	5.79585400	0.15044900	-0.57794800

C	5.11213900	-3.68414100	-0.23413300
H	5.78566300	-4.89179800	-1.92421200
C	5.07844900	-1.14412400	-0.12890400
C	3.63056600	-3.68340200	-0.66268300
C	3.60887100	-1.13398700	-0.59963200
C	2.90934500	-4.93637100	-0.14864400
C	2.90381900	-2.42329500	-0.15613200
C	2.88078900	0.11270300	-0.07150500
C	1.45564800	-4.95194600	-0.60253100
H	3.41462400	-5.84886400	-0.48887100
C	1.43408300	-2.41893200	-0.61200900
C	1.41787700	0.12484800	-0.53899200
C	0.69636200	-3.69386700	-0.17168500
H	1.41401800	-5.03494500	-1.70001900
C	0.69053200	-1.16373200	-0.12544500
C	-0.75235700	-3.69035400	-0.68351700
C	-0.77362900	-1.15587500	-0.59852100
C	-1.50135100	-4.97116200	-0.30600100
C	-1.50495300	-2.44480600	-0.18777500
C	-1.51317700	0.09413200	-0.09600600
C	-2.95081800	-4.95256100	-0.77364600
H	-1.00168000	-5.84450400	-0.73542800
C	-2.97306800	-2.43795900	-0.64789200
C	-2.97788200	0.10399400	-0.55673800
C	-3.69137400	-3.73045800	-0.21521900
H	-2.97491400	-4.92022200	-1.87192700
C	-3.69205900	-1.18637900	-0.12320300
C	-5.16709500	-3.71978300	-0.66344200
C	-5.16171100	-1.17658200	-0.59314400
C	-5.90496400	-4.98445200	-0.17384000
C	-5.88735200	-2.46038600	-0.12403300
C	-5.89307200	0.07217700	-0.04657700
C	-7.37099700	-4.98237400	-0.62267900
H	-5.39929300	-5.89108900	-0.55725500
C	-7.36159900	-2.45033800	-0.60121700
C	-7.36460300	0.08169500	-0.52809000
C	-8.09425300	-3.72269900	-0.13266600
H	-7.42760400	-5.04466400	-1.72642000
C	-8.08579400	-1.19947300	-0.07376200
H	8.05983200	3.98114300	-1.54027500
H	8.03837600	1.47341500	-1.64781200
H	9.04849000	-1.10552800	-0.32014200
H	9.07781200	-3.62884500	-0.44096200
H	-8.16321600	-3.73600600	0.97143000
H	-9.13116600	-1.19010700	-0.43240200
H	-8.15772300	1.27763300	1.11593700
H	-9.17219500	3.85199500	-0.24552600
H	0.67808200	-1.19442200	0.97911400
H	0.66704100	1.31028500	1.07537100
H	-1.51482300	0.05025300	1.00884200

H	1.42422600	0.16866800	-1.64495900
H	-0.76665500	-1.11601600	-1.70421800
H	-0.77621600	1.42855000	-1.60734600
H	1.43581300	-2.40077600	-1.71886400
H	2.90398500	-2.45041900	0.94666500
H	3.58840900	-1.09481100	-1.70880800
H	2.86769100	0.05936400	1.03141800
H	3.57951300	1.46511000	-1.59403200
H	2.86887700	2.58679700	1.16153900
H	1.42384800	2.73433200	-1.51416900
H	0.61000800	3.81302800	1.21630000
H	-0.74178500	3.93801200	-1.51104500
H	-1.54046100	2.59454600	1.10440500
H	0.66021200	-3.68085700	0.93314200
H	-0.71457100	-3.63745400	-1.78678900
H	-1.50872200	-2.48131500	0.91749000
H	-2.97479400	-2.39922400	-1.75101400
H	-3.67205300	-1.22589600	0.98659200
H	-2.97699000	0.14351400	-1.65963300
H	-3.68665800	1.31310000	1.07694700
H	-2.99353900	2.68257400	-1.56927700
H	5.08303600	1.33951600	1.10203900
H	5.77377200	2.73651800	-1.57389000
H	5.11026800	3.88972000	1.22209000
H	3.55645500	4.03209200	-1.44358500
H	5.74864700	5.29404800	-1.45957400
H	7.33871900	5.23387500	1.18804200
H	9.04061300	3.93162400	-0.07205200
H	7.28404700	2.61894000	1.12627800
H	9.03600200	1.40831200	-0.19442400
H	5.78054700	0.20160600	-1.69215600
H	7.28706500	0.08124800	1.01089200
H	8.04567200	-1.04292000	-1.77010900
H	7.31485300	-2.45281500	0.88570900
H	5.79093300	-2.33745300	-1.80713800
H	5.09714200	-1.19471800	0.98598100
H	8.08639400	-3.55190900	-1.90091000
H	7.39961100	-5.06027800	0.70401400
H	5.36261400	-5.84014400	-0.49492900
H	5.16258500	-3.74174100	0.87987300
H	3.57734600	-3.67979000	-1.77009400
H	-3.65317400	-3.77831100	0.89200600
H	-5.20272300	-3.70084900	-1.77926900
H	-9.13556400	-3.71659400	-0.50310200
H	-7.88341900	-5.88462500	-0.24008800
H	-5.84965600	-5.04890900	0.92917100
H	-3.44978800	-5.88321800	-0.47623500
H	-1.46854300	-5.09333800	0.78864900
H	0.96848200	-5.84548600	-0.20061700
H	2.94492100	-4.94770300	0.95007300

H	-8.14563900	-1.23130400	1.03008500
H	-9.14331500	1.32692800	-0.34627200
H	-8.20005300	3.78089200	1.22757700
H	-7.47680000	5.27626000	-1.37495200
H	-5.45716300	6.06117700	-0.14888700
H	-3.50868900	6.06675900	-0.07187600
H	-1.52467500	5.22107000	1.14622200
H	0.90568000	6.05095600	0.24363600
H	2.87685300	5.09255100	1.35244300
H	-5.87555900	-2.49211100	0.99074100
H	-5.18044600	-1.14252800	-1.70861100
H	-5.88421200	0.03363400	1.06822300
H	-5.19104200	1.40533600	-1.62014600
H	-5.90074400	2.55994500	1.16452300
H	-5.23802500	3.96074400	-1.51604300
H	-3.69303500	3.87479500	1.15738600
H	-7.37539400	0.11987800	-1.64443700
H	-7.39765000	2.66493100	-1.54362000
H	-7.37386300	-2.42679800	-1.71775600
C	1.24625900	-0.27673100	3.65932700
C	-0.08870600	-0.01988700	3.54296700
C	-0.87214500	-1.21371000	3.49149200
C	-0.10891300	-2.34161800	3.57016900
S	1.56644400	-1.96853700	3.71102600
H	2.06065500	0.43255200	3.71710400
H	-0.50213800	0.98105300	3.48862900
H	-1.95204300	-1.22876500	3.39436200
H	-0.43611000	-3.37247500	3.55221900

Graphane-CH₄

C	5.11756900	-1.26989800	-0.35189100
C	5.85145000	-2.53456800	0.15469000
C	3.65106600	-1.27123400	0.12765700
C	8.04328200	-1.26150500	0.15901200
C	7.32439200	-2.53219700	-0.32653700
C	5.13625100	-3.81337700	-0.34416400
C	2.93540400	-2.54184100	-0.35388200
C	8.06443700	-3.78555600	0.18000400
C	5.88165600	-5.05900700	0.18176700
C	3.66203400	-3.81925100	0.10887800
C	1.47004400	-2.54343800	0.11596800
C	7.34681600	-5.06336800	-0.26975700
H	5.82877800	-5.09021100	1.28642100
C	2.92597100	-5.05762200	-0.41899300
C	0.72954400	-1.27062800	-0.32820000
C	0.72047200	-3.80545200	-0.34219800
H	7.86446700	-5.95082700	0.13946800
C	1.47895200	-5.07463300	0.05616300
H	2.94554200	-5.04985500	-1.51782300
C	-0.73179900	-1.26970800	0.15374800

C	-0.72291400	-3.80400800	0.18438000
H	0.98142800	-5.95780200	-0.35532800
C	-1.47365500	-2.54499500	-0.28025900
C	-1.48166400	-5.07534800	-0.20647000
C	-2.93659300	-2.54120500	0.19729600
C	-2.92752100	-5.05673400	0.27226600
H	-1.45735400	-5.18282500	-1.30223100
C	-3.65514600	-1.27198500	-0.28366500
C	-3.66560700	-3.82021500	-0.25732400
H	-3.43359300	-5.97878200	-0.03941200
C	-5.11845400	-1.26968900	0.20566300
C	-5.13780000	-3.81303800	0.20233500
C	-5.85531500	-2.53495700	-0.29508900
C	-5.88573500	-5.05939400	-0.31830700
C	-7.32577200	-2.53191000	0.19365800
H	-5.38209600	-5.97923000	0.03515800
C	-7.34878300	-5.06309800	0.14002700
C	-8.06842700	-3.78574600	-0.30783700
C	-8.04697300	-1.26158000	-0.28934700
H	-7.86839300	-5.95098500	-0.26577500
C	-8.06844000	3.78591500	-0.30789800
C	-8.04697900	1.26175000	-0.28936300
C	-7.34880100	5.06327600	0.13994500
C	-7.32578200	2.53209000	0.19362100
C	-7.31605500	0.00008900	0.20221900
C	-5.88575500	5.05956800	-0.31839400
H	-7.86841700	5.95115700	-0.26586400
C	-5.85532300	2.53513400	-0.29511800
C	-5.84865500	0.00009100	-0.29164400
C	-5.13781700	3.81322900	0.20228400
H	-5.83803400	5.09230400	-1.42324400
C	-5.11846200	1.26987600	0.20566100
C	-3.66561200	3.82040300	-0.25734400
C	-3.65514900	1.27217600	-0.28364700
C	-2.92754900	5.05694100	0.27223900
C	-2.93661300	2.54140000	0.19732400
C	-2.92823800	0.00009100	0.18200800
C	-1.48165600	5.07553900	-0.20639300
H	-3.43359600	5.97897800	-0.03951500
C	-1.47364800	2.54519200	-0.28016000
C	-1.46954200	0.00011000	-0.29901400
C	-0.72295500	3.80420000	0.18455700
H	-1.45725500	5.18299300	-1.30215300
C	-0.73181600	1.26989100	0.15388500
C	0.72049400	3.80566600	-0.34183200
C	0.72954100	1.27084800	-0.32800800
C	1.47890800	5.07480700	0.05678100
C	1.47002600	2.54361600	0.11630100
C	1.46583900	0.00007000	0.12443700
C	2.92598300	5.05788900	-0.41820600

H	0.98141700	5.95802100	-0.35465700
C	2.93540200	2.54208000	-0.35349500
C	2.92779600	0.00011900	-0.34582700
C	3.66202400	3.81942400	0.10947300
H	2.94568400	5.05036900	-1.51703600
C	3.65106000	1.27139900	0.12786100
C	5.13624200	3.81361700	-0.34358400
C	5.11756100	1.27013900	-0.35169400
C	5.88166100	5.05916300	0.18251700
C	5.85145000	2.53473500	0.15506800
C	5.84485800	0.00008200	0.14926100
C	7.34680400	5.06359900	-0.26906200
H	5.37965000	5.97954300	-0.17185300
C	7.32438200	2.53242900	-0.32619300
C	7.31494500	0.00012000	-0.33656900
C	8.06445300	3.78572200	0.18046500
H	7.40180800	5.15969800	-1.37044300
C	8.04327600	1.26167500	0.15919500
H	-8.14423300	-3.76582500	-1.41140100
H	-8.11314600	-1.25747200	-1.39327600
H	-9.09022300	1.25875900	0.07544200
H	-9.10735200	3.78540100	0.06916300
H	8.13503300	3.76434100	1.28435200
H	9.08824000	1.25902500	-0.20066100
H	8.10424200	-1.25678900	1.26325200
H	9.10515300	-3.78561000	-0.19205200
H	-0.71271400	1.26105000	1.25929200
H	-0.71255100	-1.26082700	1.25913200
H	1.47634900	-0.00003300	1.23031700
H	-1.48665100	0.00017000	-1.40533900
H	0.71349300	1.26859600	-1.43387100
H	0.71349900	-1.26823200	-1.43406300
H	-1.49264100	2.56063900	-1.38648400
H	-2.92241400	2.53112700	1.30101700
H	-3.64935500	1.27811700	-1.39350400
H	-2.90890900	0.00007100	1.28591700
H	-3.64936500	-1.27792500	-1.39352100
H	-2.92235100	-2.53091200	1.30099000
H	-1.49271200	-2.56043400	-1.38658300
H	-0.67350600	-3.76875800	1.28782700
H	0.67175300	-3.77661900	-1.44573200
H	1.48422900	-2.55116200	1.22294500
H	-0.67368700	3.76896200	1.28800700
H	0.67192500	3.77694700	-1.44537600
H	1.48414700	2.55126900	1.22327900
H	2.92736500	2.53566600	-1.45717500
H	3.63770000	1.27422200	1.23780700
H	2.91863800	0.00021400	-1.44936400
H	3.63770300	-1.27422500	1.23760200
H	2.92733100	-2.53526200	-1.45756000

H	-5.12351600	-1.27118600	1.32174800
H	-5.85203100	-2.53413400	-1.41042700
H	-5.16529400	-3.82599600	1.31844200
H	-3.63608600	-3.84563400	-1.36519000
H	-5.83801200	-5.09216200	-1.42315600
H	-7.39871700	-5.15776300	1.24177100
H	-9.10733700	-3.78522800	0.06923200
H	-7.32946000	-2.54261400	1.31047000
H	-9.09021800	-1.25858700	0.07545700
H	-5.84900700	0.00008700	-1.40718500
H	-7.31759200	0.00009500	1.31930300
H	-8.11315400	1.25762300	-1.39329200
H	-7.32947400	2.54281100	1.31043400
H	-5.85203100	2.53428600	-1.41045600
H	-5.12353800	1.27138000	1.32174600
H	-8.14423900	3.76597300	-1.41146300
H	-7.39873000	5.15795400	1.24168900
H	-5.38212000	5.97941800	0.03504100
H	-5.16532700	3.82621000	1.31839200
H	-3.63606200	3.84579800	-1.36520900
H	3.62755600	3.84046200	1.21732300
H	5.16878400	3.82848400	-1.45952900
H	9.10514000	3.78583100	-0.19167600
H	7.86446600	5.95099700	0.14028300
H	5.82882600	5.09019000	1.28717800
H	3.43118700	5.97880300	-0.10181700
H	1.45200400	5.17725700	1.15298200
H	-0.98303600	5.95675100	0.20798100
H	-2.94412100	5.04565100	1.37109300
H	8.10422200	1.25681000	1.26343500
H	9.08824200	-1.25880000	-0.20085800
H	8.13492500	-3.76432900	1.28390000
H	7.40186300	-5.15929100	-1.37115000
H	5.37965400	-5.97932600	-0.17277100
H	3.43122800	-5.97859500	-0.10286400
H	1.45219000	-5.17722800	1.15235500
H	-0.98302100	-5.95655700	0.20787900
H	-2.94402100	-5.04539300	1.37112100
H	5.84249600	2.53193900	1.27037600
H	5.12980600	1.27270900	-1.46773900
H	5.83914900	-0.00000300	1.26481100
H	5.12981800	-1.27230500	-1.46793600
H	5.84247500	-2.53194500	1.27000000
H	5.16880900	-3.82808600	-1.46010900
H	3.62755500	-3.84047400	1.21672400
H	7.32258100	0.00019900	-1.45361200
H	7.33377700	-2.54397300	-1.44329600
H	7.33374200	2.54432600	-1.44295100
H	0.11132000	-0.00426700	4.95310900
C	0.07002600	-0.00512500	3.86248500

H	0.57373800	0.88399400	3.47648600
H	-0.97216500	-0.00173800	3.53530500
H	0.56734200	-0.89855500	3.47813000

Graphane-NH₃

C	-5.11928900	1.26998300	-0.34516100
C	-5.85170300	2.53481000	0.16319200
C	-3.65180000	1.27164300	0.13043700
C	-8.04335700	1.26167600	0.17360100
C	-7.32593800	2.53233300	-0.31407300
C	-5.13792400	3.81356500	-0.33787500
C	-2.93732100	2.54201900	-0.35344200
C	-8.06446100	3.78566900	0.19457700
C	-5.88174000	5.05911300	0.19038400
C	-3.66257100	3.81979600	0.11090100
C	-1.47067800	2.54374800	0.11202000
C	-7.34814000	5.06350800	-0.25705300
H	-5.82595500	5.09016500	1.29498400
C	-2.92778600	5.05758100	-0.41999700
C	-0.73092800	1.27105200	-0.33375900
C	-0.72173300	3.80582700	-0.34702000
H	-7.86461100	5.95089100	0.15401500
C	-1.47974400	5.07513400	0.05186700
H	-2.95010300	5.04889400	-1.51874300
C	0.73083900	1.27016000	0.14671800
C	0.72201700	3.80468000	0.17843900
H	-0.98308100	5.95773200	-0.36169400
C	1.47327400	2.54557800	-0.28501400
C	1.48102800	5.07538700	-0.21376200
C	2.93515100	2.54175100	0.19572500
C	2.92597500	5.05774600	0.26766000
H	1.45825500	5.18067800	-1.30973100
C	3.65531900	1.27240300	-0.28256600
C	3.66562700	3.82049700	-0.25798000
H	3.43247200	5.97906600	-0.04514800
C	5.11672800	1.26987000	0.21147400
C	5.13598900	3.81339400	0.20693700
C	5.85536500	2.53503800	-0.28706400
C	5.88589800	5.05938500	-0.31160900
C	7.32381100	2.53211900	0.20771500
H	5.38104800	5.97957800	0.03931000
C	7.34696800	5.06327400	0.15296800
C	8.06852700	3.78574400	-0.29111600
C	8.04695100	1.26170500	-0.27201600
H	7.86833400	5.95101500	-0.25100000
C	8.06853900	-3.78544800	-0.29396200
C	8.04694500	-1.26142600	-0.27297900
C	7.34708600	-5.06334700	0.14924400
C	7.32388700	-2.53219900	0.20591700
C	7.31406300	-0.00004300	0.21624900

C	5.88588600	-5.05909300	-0.31492100
H	7.86834200	-5.95074100	-0.25563400
C	5.85535600	-2.53480200	-0.28861900
C	5.84861200	0.00011400	-0.28342700
C	5.13614000	-3.81347600	0.20477900
H	5.84259000	-5.09043700	-1.41998200
C	5.11677200	-1.26994200	0.21076600
C	3.66559700	-3.82037700	-0.25954300
C	3.65530800	-1.27225400	-0.28311200
C	2.92616900	-5.05778100	0.26606800
C	2.93524800	-2.54179000	0.19482900
C	2.92680900	-0.00001800	0.18037900
C	1.48103000	-5.07529400	-0.21477600
H	3.43255500	-5.97901900	-0.04716600
C	1.47322000	-2.54551800	-0.28548900
C	1.46930800	0.00002400	-0.30420500
C	0.72217700	-3.80470100	0.17812400
H	1.45783200	-5.18018200	-1.31077400
C	0.73089800	-1.27016300	0.14664800
C	-0.72186100	-3.80586200	-0.34651300
C	-0.73096400	-1.27105500	-0.33353100
C	-1.47972400	-5.07502200	0.05313700
C	-1.47061800	-2.54368300	0.11259200
C	-1.46614700	0.00003700	0.11990000
C	-2.92790700	-5.05765000	-0.41829400
H	-0.98319800	-5.95781600	-0.36015900
C	-2.93737400	-2.54206900	-0.35255300
C	-2.92967400	-0.00002500	-0.34450200
C	-3.66253200	-3.81968100	0.11241100
H	-2.95054800	-5.04931900	-1.51703500
C	-3.65178300	-1.27151500	0.13095200
C	-5.13800400	-3.81364500	-0.33595200
C	-5.11930800	-1.27005800	-0.34452700
C	-5.88170200	-5.05886800	0.19325600
C	-5.85168400	-2.53461900	0.16454200
C	-5.84516800	0.00009400	0.15823100
C	-7.34817500	-5.06359000	-0.25393100
H	-5.38084400	-5.97962000	-0.16181200
C	-7.32596800	-2.53240600	-0.31258000
C	-7.31652800	-0.00004500	-0.32374000
C	-8.06446900	-3.78543600	0.19685300
H	-7.40674900	-5.16082200	-1.35501200
C	-8.04332700	-1.26145900	0.17443300
H	8.14961300	3.76536800	-1.39428800
H	8.11855400	1.25762400	-1.37560500
H	9.08857400	-1.25867600	0.09669700
H	9.10581900	-3.78542400	0.08780300
H	-8.13214200	-3.76349200	1.30097300
H	-9.08939500	-1.25891100	-0.18237100
H	-8.10156400	1.25716200	1.27806800

H	-9.10628100	3.78578800	-0.17451600
H	0.70995900	-1.26033900	1.25220700
H	0.70967000	1.26000800	1.25227200
H	-1.47035200	0.00025700	1.22630900
H	1.48906300	0.00004300	-1.41031100
H	-0.71671900	-1.26904100	-1.43924700
H	-0.71649000	1.26881600	-1.43946800
H	1.49381400	-2.56058200	-1.39168900
H	2.91896900	-2.53317800	1.29856100
H	3.65262700	-1.27726900	-1.39288900
H	2.90551800	-0.00025700	1.28476000
H	3.65276700	1.27782900	-1.39234200
H	2.91858300	2.53269500	1.29944800
H	1.49423000	2.56074800	-1.39120900
H	0.67325700	3.77102500	1.28203200
H	-0.67426700	3.77633600	-1.45052500
H	-1.48256300	2.55186000	1.21949800
H	0.67406100	-3.77125000	1.28175300
H	-0.67503100	-3.77664400	-1.45005400
H	-1.48224000	-2.55165800	1.22007500
H	-2.93251800	-2.53552200	-1.45618300
H	-3.63552800	-1.27449700	1.24090200
H	-2.92356700	-0.00024200	-1.44798800
H	-3.63564800	1.27503400	1.24038900
H	-2.93225600	2.53504100	-1.45706900
H	5.11859800	1.27156200	1.32768300
H	5.85675600	2.53372100	-1.40240900
H	5.15959700	3.82709100	1.32325000
H	3.63976600	3.84426300	-1.36593600
H	5.84290800	5.09156200	-1.41665800
H	7.39227800	5.15864200	1.25491100
H	9.10575600	3.78545000	0.09078300
H	7.32299600	2.54317400	1.32460000
H	9.08854400	1.25872300	0.09775900
H	5.85354100	0.00042900	-1.39896800
H	7.31126700	-0.00046600	1.33340400
H	8.11844200	-1.25655900	-1.37657200
H	7.32325600	-2.54408500	1.32279600
H	5.85655900	-2.53284600	-1.40396400
H	5.11875800	-1.27231200	1.32697600
H	8.14948000	-3.76423700	-1.39712800
H	7.39271300	-5.15965800	1.25109000
H	5.38110900	-5.97954000	0.03543900
H	5.16019900	-3.82794000	1.32107500
H	3.63927400	-3.84383700	-1.36749300
H	-3.62441200	-3.84109800	1.22009200
H	-5.17436500	-3.82911000	-1.45179300
H	-9.10628000	-3.78578900	-0.17228000
H	-7.86456500	-5.95066800	0.15790900
H	-5.82573200	-5.08919100	1.29786600

H	-3.43226100	-5.97866400	-0.10118100
H	-1.45012000	-5.17831200	1.14915000
H	0.98179100	-5.95716900	0.19716400
H	2.94109700	-5.04928500	1.36491100
H	-8.10138900	-1.25629300	1.27890500
H	-9.08938000	1.25893000	-0.18333900
H	-8.13209200	3.76443200	1.29871400
H	-7.40652100	5.15989500	-1.35822000
H	-5.38085300	5.97964700	-0.16520600
H	-3.43223200	5.97869700	-0.10333200
H	-1.45046100	5.17893900	1.14784000
H	0.98160500	5.95710200	0.19830600
H	2.94046500	5.04898100	1.36650700
H	-5.83980400	-2.53171800	1.27990600
H	-5.13492300	-1.27291600	-1.46058100
H	-5.83681900	0.00037700	1.27384300
H	-5.13482500	1.27225500	-1.46121500
H	-5.83993400	2.53247800	1.27855900
H	-5.17397200	3.82836200	-1.45373400
H	-3.62477100	3.84157600	1.21858700
H	-7.32731300	-0.00040900	-1.44077100
H	-7.33852600	2.54412500	-1.43081100
H	-7.33866600	-2.54483800	-1.42931000
H	0.90954200	-0.00036600	3.35537500
N	-0.02203500	-0.00138600	3.76643600
H	-0.49864300	-0.81628700	3.38484200
H	-0.50097600	0.81157800	3.38364400

Graphane-CO₂

C	-5.04443400	1.32825700	-0.45257400
C	-5.77808900	2.58549100	0.07246600
C	-3.58147000	1.31700100	0.03743800
C	-7.97338000	1.31856200	0.04003800
C	-7.24818700	2.59614400	-0.41722400
C	-5.05671400	3.87117400	-0.39908300
C	-2.85931300	2.59345100	-0.41876500
C	-7.98771100	3.84175300	0.10878400
C	-5.80163400	5.10889500	0.14594500
C	-3.58499700	3.86488900	0.06199200
C	-1.39679200	2.58388700	0.05990500
C	-7.26434300	5.12578000	-0.31324200
H	-5.75473400	5.11904100	1.25131800
C	-2.84292900	5.11003700	-0.44109000
C	-0.65554700	1.31674600	-0.39910300
C	-0.64095400	3.85064200	-0.37488000
H	-7.78179000	6.00680000	0.10992200
C	-1.39801000	5.11515500	0.04062100
H	-2.85763700	5.12147300	-1.53997900
C	0.80052800	1.30398700	0.09876800
C	0.80012000	3.83841300	0.15825800

H	-0.89640500	6.00369600	-0.35387500
C	1.55011100	2.58185700	-0.31437800
C	1.56533400	5.11075100	-0.21692300
C	3.00941500	2.56844900	0.17410900
C	3.00792200	5.08343400	0.27112100
H	1.54825000	5.22754000	-1.31183400
C	3.72792900	1.30112200	-0.31214100
C	3.74597900	3.84910200	-0.26360100
H	3.51905000	6.00639400	-0.02938000
C	5.18661300	1.29005500	0.19058400
C	5.21438300	3.83331900	0.20773000
C	5.93201200	2.55680300	-0.29351600
C	5.97053100	5.08120200	-0.29719300
C	7.39800800	2.54532500	0.20834000
H	5.46679400	5.99998300	0.05887200
C	7.42962500	5.07680600	0.17361800
C	8.14901400	3.80040200	-0.27738500
C	8.11949000	1.27615600	-0.27724700
H	7.95549800	5.96591700	-0.22131800
C	8.12515100	-3.77126400	-0.33015900
C	8.11150700	-1.24719600	-0.29486500
C	7.39688400	-5.04914900	0.10199400
C	7.38141000	-2.51845000	0.17219500
C	7.37991300	0.01339300	0.19839200
C	5.93868300	-5.03781800	-0.37145300
H	7.91788500	-5.93606600	-0.30412300
C	5.91603800	-2.51341800	-0.33150400
C	5.91739200	0.02173300	-0.30959900
C	5.18912500	-3.79255800	0.14942800
H	5.90234500	-5.06339300	-1.47690300
C	5.17820600	-1.24937400	0.17083200
C	3.72210000	-3.79171500	-0.32661000
C	3.72012600	-1.24314700	-0.33370100
C	2.97333300	-5.02908600	0.18575700
C	2.99213300	-2.51376400	0.12913400
C	2.99282900	0.02733800	0.13584100
C	1.53410600	-5.04009100	-0.31291000
H	3.48062300	-5.95091700	-0.12461600
C	1.53550400	-2.50875400	-0.36702500
C	1.53901100	0.03651400	-0.35961900
C	0.77338200	-3.76910600	0.07497700
H	1.52501800	-5.14110000	-1.40959800
C	0.79202100	-1.23575300	0.07085200
C	-0.65965100	-3.76091400	-0.47970100
C	-0.66202700	-1.22672400	-0.43334900
C	-1.42811900	-5.03333000	-0.11192900
C	-1.41315600	-2.50302200	-0.01722100
C	-1.40007700	0.04095500	0.02358000
C	-2.86805900	-5.00396400	-0.60749900
H	-0.92713700	-5.91147700	-0.53001300

C	-2.87238600	-2.48962700	-0.50397600
C	-2.85884400	0.05243400	-0.45566000
C	-3.60712600	-3.77215000	-0.06905500
H	-2.87232900	-4.97752200	-1.70618900
C	-3.58882500	-1.22481800	-0.00888200
C	-5.07675400	-3.75447000	-0.53591400
C	-5.05161800	-1.21125400	-0.49856700
C	-5.83004900	-5.00749800	-0.03980300
C	-5.79275100	-2.48278400	-0.02035000
C	-5.77875200	0.05154700	0.02050500
C	-7.29116200	-4.99917500	-0.50418700
H	-5.32744800	-5.92249600	-0.40716800
C	-7.26171700	-2.46739200	-0.51326800
C	-7.24540700	0.06468100	-0.47523400
C	-8.00917200	-3.72802700	-0.03660200
H	-7.33680700	-5.07418800	-1.60762600
C	-7.98072800	-1.20409300	-0.00905700
H	8.23441200	3.78835800	-1.38036100
H	8.19586800	1.27979500	-1.38051500
H	9.15111300	-1.25022800	0.08016100
H	9.16019000	-3.77661900	0.05737000
H	-8.08916000	-3.72728200	1.06685100
H	-9.02300900	-1.19156200	-0.37638900
H	-8.04037000	1.29310300	1.14372000
H	-9.02647300	3.85156600	-0.26849600
H	0.75598100	-1.24100900	1.17588100
H	0.76957900	1.28419900	1.20455300
H	-1.42319300	0.03250200	1.12949100
H	1.56724700	0.04890600	-1.46557100
H	-0.63012500	-1.20904400	-1.53854800
H	-0.62740300	1.33209100	-1.50438600
H	1.56925300	-2.51274300	-1.47314900
H	2.96408200	-2.51218100	1.23237800
H	3.72599900	-1.23961000	-1.44359100
H	2.96287800	0.01754700	1.23891600
H	3.73232700	1.31728800	-1.42188300
H	2.98678900	2.54874800	1.27746300
H	1.57748800	2.60897700	-1.42023500
H	0.74543900	3.79314000	1.26100400
H	-0.58719900	3.83918200	-1.47849800
H	-1.41842500	2.57358400	1.16646500
H	0.70234500	-3.74110000	1.17736700
H	-0.59060700	-3.71768500	-1.58170600
H	-1.43988800	-2.52830100	1.08872700
H	-2.85292900	-2.46517100	-1.60717800
H	-3.58473900	-1.24318000	1.10151900
H	-2.84133300	0.07140500	-1.55886700
H	-3.57446000	1.29747200	1.14699400
H	-2.84488000	2.60595800	-1.52240200
H	5.18135200	1.28280900	1.30667900

H	5.93870600	2.56478400	-1.40880200
H	5.23289500	3.83762000	1.32411300
H	3.72529100	3.88429100	-1.37137100
H	5.93236100	5.12238400	-1.40212300
H	7.47044400	5.16333100	1.27639200
H	9.18459900	3.79372200	0.10868400
H	7.39168800	2.54794900	1.32520100
H	9.15929300	1.26705700	0.09714700
H	5.92853000	0.03028600	-1.42503900
H	7.37063300	0.00555200	1.31542300
H	8.18850400	-1.23564300	-1.39803100
H	7.37364400	-2.53667900	1.28890000
H	5.92416400	-2.50468400	-1.44677300
H	5.17158400	-1.25916600	1.28691000
H	8.21216000	-3.74429900	-1.43273500
H	7.43501900	-5.15097300	1.20356700
H	5.42849000	-5.95824500	-0.02904500
H	5.20415100	-3.81312400	1.26567100
H	3.70510400	-3.80911000	-1.43494200
H	-3.58380100	-3.81081200	1.03885900
H	-5.09887600	-3.74888100	-1.65220200
H	-9.04670900	-3.71820000	-0.41739300
H	-7.81477000	-5.89273000	-0.11631200
H	-5.78716700	-5.05960800	1.06446000
H	-3.38075800	-5.92829400	-0.31402500
H	-1.41721800	-5.15301500	0.98276300
H	1.02691900	-5.92217800	0.08908700
H	2.97486600	-5.02409800	1.28471300
H	-8.04977100	-1.21997300	1.09464800
H	-9.01627700	1.32562200	-0.32558600
H	-8.06389300	3.80001800	1.21175800
H	-7.31327000	5.24243100	-1.41288400
H	-5.29526900	6.03430000	-0.18844500
H	-3.34696800	6.02688500	-0.11132200
H	-1.37595500	5.19930800	1.13846000
H	1.06693500	5.99005200	0.20168400
H	3.01692200	5.06299600	1.36994300
H	-5.79326800	-2.49970600	1.09485900
H	-5.05592900	-1.19351200	-1.61457100
H	-5.78029600	0.03169800	1.13612000
H	-5.04911900	1.35123500	-1.56839300
H	-5.77531700	2.56240500	1.18773400
H	-5.08330300	3.90651800	-1.51469000
H	-3.55647000	3.86650800	1.17007200
H	-7.24555700	0.08631500	-1.59208600
H	-7.25113100	2.62906200	-1.53358500
H	-7.26224200	-2.45788400	-1.63008400
O	-2.54412500	-0.18421200	3.54857500
C	-1.64198600	-0.91812000	3.53557000
O	-0.73923600	-1.65203200	3.52588100

Graphane-H₂O

C	-5.10402500	1.30210800	-0.34276300
C	-5.83799800	2.56345200	0.17199800
C	-3.63922900	1.29765300	0.14171100
C	-8.03100300	1.29291800	0.16059400
C	-7.30954300	2.56648500	-0.31339600
C	-5.11990000	3.84560800	-0.31396300
C	-2.92085400	2.57167100	-0.32715000
C	-8.04969200	3.81661700	0.20090200
C	-5.86577600	5.08767400	0.21969800
C	-3.64743800	3.84595000	0.14460200
C	-1.45705600	2.56820800	0.14760600
C	-7.32945400	5.09718300	-0.23659700
H	-5.81671200	5.10943900	1.32481000
C	-2.90821600	5.08832000	-0.36941300
C	-0.71767600	1.29780100	-0.30522200
C	-0.70473400	3.83298600	-0.29848200
H	-7.84750000	5.98187800	0.17812200
C	-1.46250900	5.09934600	0.10992700
H	-2.92462100	5.09122200	-1.46832300
C	0.74370100	1.29137500	0.17694800
C	0.73797100	3.82586800	0.23011500
H	-0.96289100	5.98577100	-0.29187400
C	1.48795500	2.56995000	-0.24383800
C	1.49890300	5.09919100	-0.15018100
C	2.95121000	2.56021200	0.23266100
C	2.94466400	5.07487200	0.32851200
H	1.47468300	5.21584600	-1.24496100
C	3.66850100	1.29459800	-0.25963400
C	3.68136500	3.84226400	-0.21183500
H	3.45185800	5.99882400	0.02467100
C	5.13147600	1.28618000	0.22997700
C	5.15373100	3.82946200	0.24695000
C	5.86972000	2.55456500	-0.26081300
C	5.90281500	5.07897300	-0.26429500
C	7.34022400	2.54597800	0.22771000
H	5.40047000	5.99664000	0.09676400
C	7.36608200	5.07741200	0.19331700
C	8.08407800	3.80269700	-0.26454300
C	8.05979900	1.27841200	-0.26486800
H	7.88653100	5.96776400	-0.20614900
C	8.07527900	-3.76906800	-0.31929700
C	8.05675500	-1.24499300	-0.28342800
C	7.35439500	-5.04853700	0.12033400
C	7.33419100	-2.51782800	0.19070200
C	7.32745900	0.01397600	0.21721500
C	5.89120900	-5.04035400	-0.33748300
H	7.87293700	-5.93428900	-0.29168900
C	5.86378300	-2.51606300	-0.29825200

C	5.86022000	0.01939300	-0.27704600
C	5.14487700	-3.79647300	0.19126300
H	5.84328400	-5.06625800	-1.44254300
C	5.12830000	-1.25321800	0.21049100
C	3.67276000	-3.79990300	-0.26809300
C	3.66578200	-1.25025900	-0.28042900
C	2.93271700	-5.03698700	0.25755400
C	2.94504600	-2.52175000	0.19134700
C	2.93999400	0.01908600	0.19458400
C	1.48689400	-5.05282000	-0.22127900
H	3.43748200	-5.95864600	-0.05690500
C	1.48296800	-2.52182800	-0.28859000
C	1.48169200	0.02563600	-0.28736400
C	0.72854600	-3.78114000	0.16896500
H	1.46225000	-5.15853600	-1.31705200
C	0.74072300	-1.24799800	0.14720500
C	-0.71429600	-3.77841900	-0.35909300
C	-0.72134100	-1.24344000	-0.33335000
C	-1.47421600	-5.04894300	0.03205600
C	-1.46331500	-2.51811000	0.10355800
C	-1.45604500	0.02357300	0.13325700
C	-2.91960000	-5.02772300	-0.44770600
H	-0.97625900	-5.93107700	-0.38129400
C	-2.92717900	-2.51187100	-0.37006300
C	-2.91653900	0.02940200	-0.34128000
C	-3.65563800	-3.79124700	0.08467000
H	-2.93520100	-5.01456800	-1.54658500
C	-3.64174000	-1.24461300	0.12273300
C	-5.12838600	-3.78145000	-0.37274000
C	-5.10661200	-1.23788700	-0.36178100
C	-5.87628800	-5.02983200	0.14303600
C	-5.84333900	-2.50537800	0.13356600
C	-5.83396800	0.02906600	0.14679300
C	-7.34039400	-5.02952200	-0.31198700
H	-5.37457800	-5.94845400	-0.21596700
C	-7.31510800	-2.49799800	-0.35094100
C	-7.30278500	0.03425100	-0.34265300
C	-8.05751200	-3.75409700	0.14529600
H	-7.39310800	-5.11766600	-1.41407000
C	-8.03359000	-1.23006200	0.14231900
H	8.15968100	3.79119100	-1.36825000
H	8.12632400	1.28261400	-1.36879300
H	9.10008500	-1.24582400	0.08138000
H	9.11434800	-3.77222100	0.05755300
H	-8.12971800	-3.74047100	1.24928600
H	-9.07790300	-1.22358700	-0.21916800
H	-8.09439100	1.27974000	1.26472500
H	-9.08939100	3.82067300	-0.17393900
H	0.71720500	-1.24928300	1.25303300
H	0.72527700	1.27499900	1.28439200

H	-1.47353100	0.00206300	1.23817500
H	1.49898400	0.03822100	-1.39318800
H	-0.70363800	-1.23109900	-1.43907600
H	-0.69806600	1.30546400	-1.41087400
H	1.50318300	-2.53285100	-1.39453700
H	2.92965700	-2.51787100	1.29543000
H	3.66064900	-1.24828400	-1.39012600
H	2.92072800	0.01005800	1.29838200
H	3.66276000	1.31026300	-1.36928100
H	2.93837600	2.54125000	1.33625000
H	1.50645100	2.59368000	-1.34987700
H	0.68756100	3.78265800	1.33317900
H	-0.65410900	3.81395900	-1.40212700
H	-1.47525600	2.56692700	1.25411200
H	0.67754500	-3.75118000	1.27430500
H	-0.66200300	-3.74552800	-1.46231700
H	-1.48397400	-2.52186500	1.20880600
H	-2.91824600	-2.49778400	-1.47390200
H	-3.62774700	-1.25685300	1.23185700
H	-2.90474000	0.03861900	-1.44495200
H	-3.62920700	1.29002900	1.25122100
H	-2.90910300	2.57486500	-1.43084700
H	5.13674900	1.27918100	1.34605700
H	5.86640600	2.56272800	-1.37614600
H	5.18193900	3.83382100	1.36313900
H	3.65110200	3.87677000	-1.31938600
H	5.85458200	5.12074800	-1.36882500
H	7.41683200	5.16397800	1.29568800
H	9.12317200	3.79819700	0.11216100
H	7.34419100	2.54841900	1.34459800
H	9.10307200	1.27146800	0.10000400
H	5.86103000	0.02796200	-1.39257200
H	7.32888600	0.00582100	1.33430300
H	8.12322800	-1.23311500	-1.38730100
H	7.33788800	-2.53621300	1.30745200
H	5.86078100	-2.50823100	-1.41358800
H	5.13284900	-1.26247500	1.32655400
H	8.15118600	-3.74198400	-1.42271900
H	7.40486900	-5.15088900	1.22136400
H	5.38684500	-5.96199600	0.01031500
H	5.17304500	-3.81660300	1.30726300
H	3.64272800	-3.82088000	-1.37591400
H	-3.62387000	-3.81716400	1.19215800
H	-5.15818000	-3.78849200	-1.48875000
H	-9.09758600	-3.75038000	-0.22839800
H	-7.85988500	-5.91918700	0.09009000
H	-5.82620900	-5.06786500	1.24774800
H	-3.42638400	-5.94992700	-0.13784100
H	-1.45181400	-5.15562700	1.12802300
H	0.98611800	-5.93325600	0.19165200

H	2.94980500	-5.02955000	1.35650900
H	-8.09616900	-1.23328100	1.24659200
H	-9.07511400	1.29403000	-0.20159700
H	-8.12328000	3.78661200	1.30443800
H	-7.38092600	5.20184700	-1.33731500
H	-5.36183900	6.01045400	-0.12538600
H	-3.41304300	6.00691400	-0.04589900
H	-1.43866200	5.19133900	1.20709200
H	1.00111300	5.97730500	0.27148200
H	2.96129100	5.05420100	1.42721900
H	-5.83652600	-2.51068000	1.24914000
H	-5.11568300	-1.23204200	-1.47776100
H	-5.83062300	0.02045000	1.26255800
H	-5.11318600	1.31329600	-1.45869300
H	-5.83224900	2.55135000	1.28739700
H	-5.14859700	3.86952700	-1.42981500
H	-3.61708300	3.85687400	1.25261200
H	-7.30786200	0.04234900	-1.45963500
H	-7.31590600	2.58685100	-1.43001700
H	-7.32221500	-2.50180900	-1.46772300
H	-0.25843000	-2.04086400	3.11677200
O	-0.76193800	-1.28455600	3.44807600
H	-0.26604000	-0.51735700	3.13057000

Graphane-H₂

C	5.11795500	-1.26986600	-0.29291100
C	5.85305800	-2.53456200	0.21186700
C	3.65268600	-1.27149400	0.19044100
C	8.04486400	-1.26142800	0.21129100
C	7.32493100	-2.53216100	-0.27259700
C	5.13687400	-3.81335000	-0.28561500
C	2.93596300	-2.54176200	-0.29062000
C	8.06611800	-3.78547600	0.23237100
C	5.88335000	-5.05894200	0.23888400
C	3.66343700	-3.81949800	0.17002700
C	1.47124400	-2.54410600	0.18154700
C	7.34757300	-5.06334900	-0.21576000
H	5.83281800	-5.09001700	1.34364300
C	2.92680800	-5.05756800	-0.35782500
C	0.73051800	-1.27051900	-0.25990600
C	0.72163900	-3.80516800	-0.27949600
H	7.86607900	-5.95074600	0.19251300
C	1.47993800	-5.07478800	0.11779400
H	2.94585400	-5.04943900	-1.45667000
C	-0.73124800	-1.27035000	0.22097400
C	-0.72245200	-3.80496100	0.24525200
H	0.98235700	-5.95763100	-0.29432000
C	-1.47254300	-2.54473500	-0.21720200
C	-1.48088100	-5.07501200	-0.15040900
C	-2.93647100	-2.54172000	0.25739600

C	-2.92734700	-5.05752400	0.32651100
H	-1.45516700	-5.17927300	-1.24645000
C	-3.65394700	-1.27165400	-0.22308400
C	-3.66469800	-3.81977600	-0.20118600
H	-3.43300900	-5.97881600	0.01196100
C	-5.11827100	-1.26983300	0.26314200
C	-5.13743100	-3.81332300	0.25672100
C	-5.85432600	-2.53464200	-0.24000700
C	-5.88479000	-5.05904300	-0.26622200
C	-7.32539700	-2.53207100	0.24688400
H	-5.38151700	-5.97931600	0.08661900
C	-7.34828400	-5.06327900	0.19074800
C	-8.06749100	-3.78547700	-0.25651500
C	-8.04605600	-1.26142600	-0.23613600
H	-7.86748000	-5.95074200	-0.21651000
C	-8.06746600	3.78581200	-0.25568000
C	-8.04605300	1.26175700	-0.23584300
C	-7.34827500	5.06350600	0.19191800
C	-7.32539200	2.53229000	0.24746500
C	-7.31574500	0.00010700	0.25674500
C	-5.88476800	5.05937800	-0.26501300
H	-7.86745800	5.95107000	-0.21513300
C	-5.85431300	2.53496800	-0.23939700
C	-5.84762200	0.00016400	-0.23495400
C	-5.13742300	3.81353100	0.25765000
H	-5.83596600	5.09103900	-1.36983300
C	-5.11827000	1.27003600	0.26346100
C	-3.66469200	3.82009200	-0.20024700
C	-3.65394400	1.27196300	-0.22275000
C	-2.92733800	5.05771500	0.32772800
C	-2.93648100	2.54192200	0.25804400
C	-2.92834900	0.00009300	0.24584400
C	-1.48088700	5.07532700	-0.14923200
H	-3.43300400	5.97907800	0.01339900
C	-1.47256100	2.54505900	-0.21656400
C	-1.46839600	0.00012500	-0.23129200
C	-0.72241700	3.80518800	0.24606700
H	-1.45520600	5.17987000	-1.24524600
C	-0.73124400	1.27053600	0.22116100
C	0.72160900	3.80549400	-0.27886700
C	0.73053900	1.27081500	-0.25960600
C	1.47995300	5.07505600	0.11849700
C	1.47128800	2.54437600	0.18187400
C	1.46717000	0.00010300	0.19284400
C	2.92675300	5.05791800	-0.35734800
H	0.98229900	5.95794400	-0.29343100
C	2.93595100	2.54207300	-0.29046000
C	2.92829400	0.00014800	-0.28057400
C	3.66349300	3.81977300	0.17016800
H	2.94563900	5.05001900	-1.45619700

C	3.65270400	1.27177100	0.19046700
C	5.13683600	3.81362000	-0.28582100
C	5.11794400	1.27013300	-0.29297900
C	5.88344200	5.05925400	0.23838800
C	5.85310500	2.53486600	0.21162600
C	5.84643100	0.00015000	0.20644500
C	7.34757000	5.06360300	-0.21654900
H	5.38065100	5.97958400	-0.11499000
C	7.32491000	2.53238700	-0.27303800
C	7.31536800	0.00011300	-0.28281000
C	8.06621700	3.78577900	0.23154700
H	7.40005400	5.15954300	-1.31804500
C	8.04487600	1.26174200	0.21104400
H	-8.14224200	-3.76449000	-1.36013600
H	-8.11105400	-1.25675900	-1.34014300
H	-9.08966900	1.25888300	0.12787200
H	-9.10676300	3.78559900	0.12032600
H	8.13943700	3.76466200	1.33526800
H	9.08902600	1.25897000	-0.15113400
H	8.10821100	-1.25662000	1.31539500
H	9.10602800	-3.78550900	-0.14192900
H	-0.71435900	1.26582500	1.32715500
H	-0.71423700	-1.26585700	1.32681800
H	1.48091700	-0.00012200	1.29918200
H	-1.48288200	0.00031400	-1.33758500
H	0.71383800	1.26661500	-1.36537600
H	0.71394200	-1.26615500	-1.36568500
H	-1.48945900	2.55758300	-1.32291900
H	-2.92478100	2.53361200	1.36167800
H	-3.64587800	1.27673800	-1.33261100
H	-2.91230300	-0.00007300	1.34941100
H	-3.64588500	-1.27613200	-1.33294700
H	-2.92474900	-2.53364900	1.36102500
H	-1.48941000	-2.55706600	-1.32356500
H	-0.67476100	-3.77309800	1.34874200
H	0.67410800	-3.77471000	-1.38305100
H	1.48617500	-2.55382400	1.28809700
H	-0.67460000	3.77312500	1.34955400
H	0.67392800	3.77519600	-1.38241700
H	1.48643600	2.55402000	1.28843600
H	2.92602400	2.53480300	-1.39412600
H	3.64246700	1.27560400	1.30030700
H	2.91572200	0.00015800	-1.38405000
H	3.64236500	-1.27539000	1.30027800
H	2.92618600	-2.53443800	-1.39429000
H	-5.12559000	-1.27201000	1.37921900
H	-5.84962000	-2.53250400	-1.35534600
H	-5.16623000	-3.82761600	1.37279200
H	-3.63376800	-3.84269500	-1.30907100
H	-5.83601800	-5.09044400	-1.37105100

H	-7.39924000	-5.15906900	1.29233000
H	-9.10676900	-3.78535000	0.11954500
H	-7.33048400	-2.54359600	1.36367900
H	-9.08967400	-1.25863400	0.12757300
H	-5.84632300	0.00030300	-1.35050100
H	-7.31893000	-0.00002300	1.37381100
H	-8.11105600	1.25734200	-1.33985000
H	-7.33050000	2.54357500	1.36426300
H	-5.84958500	2.53309900	-1.35473600
H	-5.12560300	1.27194500	1.37953800
H	-8.14215900	3.76508200	-1.35930900
H	-7.39925900	5.15902200	1.29352300
H	-5.38150200	5.97956400	0.08806100
H	-5.16623500	3.82756200	1.37372200
H	-3.63376400	3.84325700	-1.30812600
H	3.63110900	3.84170800	1.27802500
H	5.16711100	3.82816800	-1.40184500
H	9.10601800	3.78575800	-0.14307000
H	7.86616000	5.95103400	0.19155300
H	5.83313600	5.09045600	1.34315400
H	3.43213800	5.97898000	-0.04169000
H	1.45350500	5.17827100	1.21461100
H	-0.98290200	5.95769200	0.26339800
H	-2.94526100	5.04876000	1.42657700
H	8.10825600	1.25712700	1.31514800
H	9.08902700	-1.25871400	-0.15085700
H	8.13900600	-3.76420700	1.33611300
H	7.40027000	-5.15937600	-1.31723900
H	5.38060700	-5.97930000	-0.11448700
H	3.43216900	-5.97868700	-0.04228600
H	1.45332800	-5.17813900	1.21389200
H	-0.98291500	-5.95748900	0.26200900
H	-2.94528900	-5.04881300	1.42536100
H	5.84670900	2.53245500	1.32695700
H	5.12734100	1.27239500	-1.40904300
H	5.84328600	0.00017900	1.32199400
H	5.12743100	-1.27223100	-1.40897300
H	5.84650700	-2.53208400	1.32719500
H	5.16740200	-3.82800400	-1.40163000
H	3.63077900	-3.84156500	1.27787200
H	7.32041100	0.00000500	-1.39986500
H	7.33185900	-2.54398400	-1.38937800
H	7.33168900	2.54396200	-1.38982200
H	0.06245100	0.01949500	3.58909800
H	0.17341200	-0.09192000	4.31037200

Graphane-Be²⁺

C	-5.14336000	1.27605100	-0.27663500
C	-5.87681000	2.54051500	0.23373500
C	-3.68459300	1.28858500	0.20485800

C	-8.06440200	1.26133500	0.20000200
C	-7.34523900	2.53824700	-0.26519600
C	-5.15765100	3.82439400	-0.24937000
C	-2.96158200	2.55877900	-0.27878400
C	-8.08921400	3.78443100	0.24819600
C	-5.90626700	5.06150100	0.29092700
C	-3.68652600	3.83653700	0.20213100
C	-1.49063100	2.58091000	0.18587500
C	-7.36771600	5.06843100	-0.17200200
H	-5.86621200	5.08232700	1.39699100
C	-2.94611500	5.07530800	-0.32119300
C	-0.75858000	1.31844300	-0.28151200
C	-0.72786000	3.83710200	-0.28257400
H	-7.89115900	5.94894900	0.25185600
C	-1.49298700	5.09599000	0.14020500
H	-2.98130700	5.08708100	-1.41814000
C	0.76190900	1.32596800	0.17715600
C	0.72713200	3.84504400	0.22736900
H	-1.00235500	5.97906200	-0.27405200
C	1.50425500	2.60211200	-0.24127300
C	1.49491300	5.10221700	-0.19707700
C	2.96311500	2.56334500	0.24542800
C	2.94487100	5.08244100	0.27693300
H	1.45763100	5.18955300	-1.29266500
C	3.68304500	1.28550000	-0.22677600
C	3.69323200	3.84052500	-0.23027300
H	3.44795800	5.99251600	-0.06198300
C	5.13376700	1.27565100	0.27987900
C	5.15587200	3.82720800	0.24601100
C	5.87778900	2.53899900	-0.22123500
C	5.91465400	5.06097500	-0.28779600
C	7.33869800	2.53739400	0.29932600
H	5.41406800	5.99338600	0.03828400
C	7.36830800	5.06790600	0.19847300
C	8.09291600	3.78087500	-0.20606000
C	8.06395700	1.25996300	-0.15348600
H	7.89992500	5.94565600	-0.22114900
C	8.09288300	-3.78089500	-0.20635900
C	8.06394600	-1.25998700	-0.15358700
C	7.36826700	-5.06795500	0.19806800
C	7.33868100	-2.53744800	0.29913100
C	7.32512400	-0.00002800	0.32494800
C	5.91460100	-5.06096800	-0.28816400
H	7.89986600	-5.94566900	-0.22165000
C	5.87776700	-2.53900200	-0.22141400
C	5.86718000	-0.00000200	-0.20155200
C	5.15584300	-3.82723200	0.24575100
H	5.89265200	-5.07591900	-1.39512800
C	5.13375800	-1.27568500	0.27979600
C	3.69318700	-3.84050600	-0.23049300

C	3.68303500	-1.28549600	-0.22685400
C	2.94485100	-5.08246100	0.27664900
C	2.96308400	-2.56334600	0.24531400
C	2.96465300	-0.00001100	0.24491900
C	1.49487900	-5.10219000	-0.19730100
H	3.44792400	-5.99250600	-0.06237100
C	1.50421500	-2.60207700	-0.24129800
C	1.52191000	-0.00000500	-0.25766000
C	0.72712100	-3.84504600	0.22727900
H	1.45755500	-5.18943500	-1.29289500
C	0.76178100	-1.32592600	0.17733100
C	-0.72790900	-3.83710500	-0.28256500
C	-0.75857200	-1.31845500	-0.28146700
C	-1.49298900	-5.09600200	0.14026500
C	-1.49065000	-2.58091900	0.18594700
C	-1.52659700	-0.00005200	0.15664900
C	-2.94618700	-5.07533900	-0.32092500
H	-1.00242400	-5.97905300	-0.27411800
C	-2.96160900	-2.55879200	-0.27865700
C	-2.99193400	-0.00000700	-0.28237400
C	-3.68654600	-3.83651600	0.20235600
H	-2.98154700	-5.08726900	-1.41786300
C	-3.68461000	-1.28856900	0.20492800
C	-5.15768900	-3.82439300	-0.24909400
C	-5.14338000	-1.27605400	-0.27654500
C	-5.90629800	-5.06145400	0.29132100
C	-5.87682800	-2.54047400	0.23393100
C	-5.86809300	0.00002000	0.21699600
C	-7.36776700	-5.06841000	-0.17154200
H	-5.40987900	-5.99148700	-0.04818200
C	-7.34526700	-2.53823500	-0.26496800
C	-7.33375700	0.00000600	-0.28818100
C	-8.08923800	-3.78436400	0.24856500
H	-7.42134800	-5.19375500	-1.27073700
C	-8.06441200	-1.26127200	0.20011900
H	8.20877700	3.74271400	-1.30651600
H	8.17497900	1.24933800	-1.25480600
H	9.09941000	-1.25906700	0.24214500
H	9.12374300	-3.78745400	0.19963600
H	-8.18858300	-3.74986200	1.35054800
H	-9.10536500	-1.26070000	-0.18120200
H	-8.15992800	1.25207200	1.30250700
H	-9.12599300	3.79217700	-0.14256400
H	0.78432200	-1.38573600	1.32853600
H	0.78446000	1.38560300	1.32843200
H	-1.60509400	-0.00015700	1.30764500
H	1.48121800	-0.00014000	-1.35446500
H	-0.71954900	-1.26617400	-1.37710800
H	-0.71959400	1.26602200	-1.37714600
H	1.50729200	-2.58675000	-1.34436800

H	2.94757800	-2.57340400	1.34806900
H	3.68392500	-1.27889100	-1.33401900
H	2.93820700	-0.00006200	1.34872200
H	3.68394300	1.27894500	-1.33394300
H	2.94753400	2.57335000	1.34818300
H	1.50745400	2.58694500	-1.34434700
H	0.70116800	3.82386200	1.33162900
H	-0.70004100	3.81128600	-1.38548200
H	-1.49282500	2.58126500	1.29343800
H	0.70121700	-3.82395100	1.33154100
H	-0.70017700	-3.81128100	-1.38547400
H	-1.49278000	-2.58130000	1.29350800
H	-2.95994300	-2.56208000	-1.38044900
H	-3.66875100	-1.28063700	1.31365400
H	-2.96456800	-0.00004600	-1.38203900
H	-3.66874800	1.28071400	1.31358200
H	-2.95987800	2.56200100	-1.38057500
H	5.13590900	1.28734800	1.39688700
H	5.90496100	2.52646900	-1.33697300
H	5.17735900	3.86368700	1.36290500
H	3.67036600	3.83992700	-1.33685000
H	5.89273500	5.07600300	-1.39476100
H	7.40516200	5.19757700	1.29766800
H	9.12377500	3.78738900	0.19993900
H	7.32288500	2.56533000	1.41633500
H	9.09941900	1.25900600	0.24225100
H	5.90033200	0.00003400	-1.31751800
H	7.30658300	-0.00007300	1.44246900
H	8.17496200	-1.24927900	-1.25490700
H	7.32288100	-2.56547000	1.41613900
H	5.90492900	-2.52639200	-1.33715200
H	5.13591300	-1.28745900	1.39680200
H	8.20874200	-3.74264300	-1.30681300
H	7.40514700	-5.19773000	1.29725000
H	5.41401500	-5.99339800	0.03786500
H	5.17735500	-3.86379400	1.36264300
H	3.67029000	-3.83983300	-1.33706900
H	-3.64597300	-3.84166900	1.30893700
H	-5.19623500	-3.85638500	-1.36603000
H	-9.12603100	-3.79213500	-0.14215500
H	-7.89120000	-5.94888100	0.25242700
H	-5.86619300	-5.08220600	1.39738500
H	-3.44564400	-5.98795400	0.01680800
H	-1.44863400	-5.18951900	1.23544700
H	1.00085000	-5.98674500	0.20930400
H	2.97006900	-5.10261700	1.37388500
H	-8.15992800	-1.25190900	1.30262400
H	-9.10535300	1.26073900	-0.18132800
H	-8.18860000	3.75002900	1.35017900
H	-7.42124600	5.19366900	-1.27121200

H	-5.40982300	5.99150600	-0.04861600
H	-3.44562000	5.98797100	0.01633700
H	-1.44879600	5.18943800	1.23539900
H	1.00087200	5.98674100	0.20958500
H	2.97003600	5.10250200	1.37417300
H	-5.88750100	-2.53164300	1.34959100
H	-5.16253600	-1.28676800	-1.39434300
H	-5.88555200	0.00006300	1.33277900
H	-5.16250300	1.28668200	-1.39443200
H	-5.88750800	2.53176500	1.34939400
H	-5.19616200	3.85629800	-1.36630900
H	-3.64599100	3.84175200	1.30871200
H	-7.33111700	-0.00004500	-1.40612000
H	-7.34572400	2.56389500	-1.38259600
H	-7.34577600	-2.56399500	-1.38236600
Be	-0.00566300	0.00012500	0.91120100

Graphane-Ca²⁺

C	-5.17612600	1.26906400	-0.28452500
C	-5.88489800	2.54177200	0.23960100
C	-3.69302600	1.28227200	0.12337800
C	-8.06925800	1.26247200	0.36616200
C	-7.38137800	2.53052900	-0.16573100
C	-5.20274000	3.81416500	-0.32104700
C	-3.00677300	2.54261800	-0.42830400
C	-8.09444800	3.78732200	0.36615100
C	-5.91712200	5.06652800	0.23052800
C	-3.70679700	3.83587000	0.03780200
C	-1.52503600	2.56668900	-0.02387500
C	-7.40611100	5.06115400	-0.13447700
H	-5.80360200	5.11845000	1.32985600
C	-2.99906600	5.05111700	-0.57718300
C	-0.79757100	1.27691500	-0.43995100
C	-0.78024500	3.80974400	-0.54857000
H	-7.90262400	5.95199800	0.29781800
C	-1.53014700	5.09310600	-0.17400800
H	-3.07701600	5.00503600	-1.67105300
C	0.65806600	1.32567000	0.04578600
C	0.67412000	3.83862600	-0.04487500
H	-1.05474400	5.95386300	-0.65039000
C	1.43781800	2.56036800	-0.43361100
C	1.45039300	5.07748700	-0.49760100
C	2.88172500	2.55935300	0.10134500
C	2.87440100	5.08500100	0.04687000
H	1.46646000	5.11101600	-1.59630500
C	3.62911800	1.28036300	-0.30310400
C	3.64067600	3.82285500	-0.37041000
H	3.39885700	5.97838300	-0.30451900
C	5.07184000	1.27837000	0.23222200
C	5.08419100	3.82559400	0.16552300

C	5.82705700	2.53624400	-0.26293000
C	5.85930000	5.05501000	-0.35501600
C	7.27290800	2.54080700	0.29731200
H	5.34726100	5.98993800	-0.05426100
C	7.29804000	5.06977800	0.17290800
C	8.03771300	3.78136200	-0.19892000
C	8.01137900	1.26016900	-0.12543300
H	7.83919300	5.94485800	-0.24105300
C	8.03765000	-3.78157700	-0.19673200
C	8.01136000	-1.26034200	-0.12469100
C	7.29785700	-5.06975600	0.17567500
C	7.27280800	-2.54072300	0.29869500
C	7.26175500	0.00005500	0.33672300
C	5.85923700	-5.05523100	-0.35258200
H	7.83907000	-5.94509500	-0.23765500
C	5.82703800	-2.53640000	-0.26174900
C	5.81683700	-0.00006500	-0.22447600
C	5.08403400	-3.82553200	0.16713900
H	5.86935800	-5.06128500	-1.46028900
C	5.07179300	-1.27828800	0.23275000
C	3.64068200	-3.82294300	-0.36923500
C	3.62912500	-1.28042600	-0.30271700
C	2.87420500	-5.08495600	0.04808200
C	2.88161700	-2.55928800	0.10191800
C	2.91225400	0.00002800	0.17469400
C	1.45045000	-5.07749900	-0.49705500
H	3.39879700	-5.97845400	-0.30280300
C	1.43786500	-2.56038700	-0.43346000
C	1.42180100	-0.00000300	-0.24667600
C	0.67403000	-3.83856600	-0.04481000
H	1.46705000	-5.11115700	-1.59574700
C	0.65803700	-1.32558100	0.04552800
C	-0.78016000	-3.80969000	-0.54896500
C	-0.79755700	-1.27681400	-0.44032000
C	-1.53019500	-5.09303100	-0.17463400
C	-1.52506000	-2.56662900	-0.02443800
C	-1.50768900	-0.00001500	0.03970500
C	-2.99897300	-5.05100400	-0.57828600
H	-1.05464400	-5.95380700	-0.65082600
C	-3.00675000	-2.54250900	-0.42900000
C	-2.99146900	0.00004400	-0.36119700
C	-3.70687800	-3.83586000	0.03669400
H	-3.07657500	-5.00472200	-1.67217400
C	-3.69305200	-1.28231800	0.12298600
C	-5.20271700	-3.81402000	-0.32259400
C	-5.17612300	-1.26893700	-0.28502800
C	-5.91727200	-5.06662800	0.22819000
C	-5.88498100	-2.54186100	0.23846900
C	-5.87627200	-0.00004700	0.25618300
C	-7.40617100	-5.06102500	-0.13717700

H	-5.44398600	-5.98451700	-0.17137100
C	-7.38139400	-2.53038900	-0.16708200
C	-7.36841700	0.00007000	-0.16113400
C	-8.09459200	-3.78745100	0.36399000
H	-7.53031500	-5.15318400	-1.23395000
C	-8.06931300	-1.26260700	0.36542400
H	8.18277000	3.73349000	-1.29590800
H	8.15372700	1.24398200	-1.22364600
H	9.03576900	-1.26285600	0.29861000
H	9.05743900	-3.79521600	0.23572300
H	-8.11748700	-3.78019200	1.47017200
H	-9.13326600	-1.25693000	0.05733000
H	-8.08391400	1.26500500	1.47191500
H	-9.15449100	3.78313800	0.04582100
H	0.53279500	-1.58162500	1.14280800
H	0.53323500	1.58191000	1.14306800
H	-1.48155300	-0.00017800	1.16661200
H	1.47617200	0.00057200	-1.34621200
H	-0.76876200	-1.24174000	-1.54152300
H	-0.76882100	1.24207500	-1.54116800
H	1.48665200	-2.50617200	-1.53374700
H	2.82150200	-2.60203800	1.21385900
H	3.64860700	-1.23248900	-1.40680300
H	3.06384800	0.00026500	1.29903000
H	3.64848700	1.23215400	-1.40718100
H	2.82194000	2.60244400	1.21326800
H	1.48623800	2.50601800	-1.53390600
H	0.63360500	3.86742400	1.06255200
H	-0.75717700	3.73785000	-1.64921500
H	-1.50432100	2.61353800	1.08590400
H	0.63314800	-3.86721200	1.06261600
H	-0.75677600	-3.73780300	-1.64960600
H	-1.50447500	-2.61349500	1.08534800
H	-3.05237400	-2.50624900	-1.52946800
H	-3.62382600	-1.31029600	1.23097300
H	-3.01018400	0.00019600	-1.46321900
H	-3.62371700	1.30993400	1.23137100
H	-3.05247200	2.50665700	-1.52877800
H	5.05397000	1.30336500	1.34703900
H	5.88485500	2.51044000	-1.37793300
H	5.06241300	3.87732600	1.28014400
H	3.66631200	3.77912500	-1.47573500
H	5.86916600	5.06049100	-1.46272600
H	7.30390800	5.21142400	1.27077100
H	9.05757800	3.79519600	0.23334900
H	7.22809600	2.57922700	1.41256600
H	9.03582000	1.26287900	0.29778600
H	5.87876900	-0.00030200	-1.34028200
H	7.21829800	0.00037900	1.45266500
H	8.15379400	-1.24475900	-1.22290100

H	7.22785200	-2.57850900	1.41396300
H	5.88500000	-2.51108400	-1.37675800
H	5.05382300	-1.30276600	1.34757600
H	8.18290200	-3.73430800	-1.29371900
H	7.30347100	-5.21076500	1.27362300
H	5.34711000	-5.98999400	-0.05146200
H	5.06193300	-3.87672000	1.28177800
H	3.66666700	-3.77949400	-1.47456500
H	-3.60164500	-3.89061900	1.13884000
H	-5.30876400	-3.81291200	-1.43539100
H	-9.15456800	-3.78308200	0.04344100
H	-7.90281000	-5.95209900	0.29449700
H	-5.80402000	-5.11909300	1.32752200
H	-3.48705100	-5.98073000	-0.26949500
H	-1.45123300	-5.24647100	0.91283600
H	0.93773400	-5.98046400	-0.16022900
H	2.84480100	-5.15273700	1.14442500
H	-8.08406800	-1.26572800	1.47117300
H	-9.13324000	1.25696900	0.05816700
H	-8.11711500	3.77947600	1.47233500
H	-7.53052300	5.15393000	-1.23116700
H	-5.44389800	5.98459400	-0.16869900
H	-3.48704500	5.98078900	-0.26807400
H	-1.45080600	5.24656700	0.91342900
H	0.93785800	5.98050800	-0.16063000
H	2.84551900	5.15311700	1.14320600
H	-5.82373800	-2.56034700	1.35155800
H	-5.24605800	-1.26178600	-1.40079400
H	-5.82307600	-0.00026500	1.36965800
H	-5.24615900	1.26241100	-1.40028600
H	-5.82349200	2.55980200	1.35268700
H	-5.30911100	3.81358000	-1.43381600
H	-3.60123100	3.89044600	1.13992600
H	-7.43007800	0.00039800	-1.27763400
H	-7.45027300	2.53330200	-1.28140800
H	-7.45012400	-2.53253500	-1.28277000
Ca	1.17436000	-0.00014000	2.43703500

Graphane-K⁺

C	-5.12311100	1.27141500	-0.38954300
C	-5.85306000	2.53490200	0.12638700
C	-3.65344000	1.27276600	0.07157300
C	-8.04484100	1.26134200	0.13019500
C	-7.32769700	2.53416400	-0.35102800
C	-5.14039400	3.81625500	-0.36994700
C	-2.94129000	2.54630800	-0.40660000
C	-8.06590200	3.78469600	0.16315700
C	-5.88250500	5.05880100	0.16695900
C	-3.66414000	3.82180600	0.07044100
C	-1.47122300	2.54791500	0.04784600

C	-7.34919900	5.06496800	-0.27917500
H	-5.82685000	5.08662600	1.27140300
C	-2.93146000	5.06251700	-0.45602500
C	-0.73293300	1.27621100	-0.40194200
C	-0.72336500	3.81180700	-0.40874700
H	-7.86617400	5.94994200	0.13851100
C	-1.47975100	5.07758900	0.00406000
H	-2.96393000	5.06498600	-1.55381100
C	0.73466800	1.27519100	0.06054100
C	0.72502800	3.80964500	0.10345100
H	-0.98657800	5.96110900	-0.40916300
C	1.47894900	2.55271400	-0.36145300
C	1.48442400	5.07878500	-0.29338100
C	2.93794300	2.54574500	0.12785400
C	2.92874100	5.06300900	0.18984600
H	1.46047100	5.17924000	-1.38894100
C	3.66311900	1.27403800	-0.33705900
C	3.67282000	3.82380700	-0.32507600
H	3.43499500	5.98045500	-0.13012400
C	5.11745600	1.27147600	0.17307000
C	5.13757200	3.81715200	0.15371600
C	5.86176000	2.53481300	-0.32300200
C	5.89316600	5.05776600	-0.36898400
C	7.32438100	2.53430800	0.18964600
H	5.38677800	5.98334500	-0.03446200
C	7.34879300	5.06553900	0.11174100
C	8.07480100	3.78355500	-0.30991900
C	8.05192900	1.26095700	-0.27384000
H	7.87538100	5.94841700	-0.29889700
C	8.07486000	-3.78324900	-0.31020100
C	8.05194900	-1.26066000	-0.27392700
C	7.34883500	-5.06527600	0.11128700
C	7.32438400	-2.53405600	0.18941100
C	7.31397700	0.00012500	0.20726500
C	5.89325100	-5.05749000	-0.36956300
H	7.87547300	-5.94811400	-0.29937600
C	5.86179800	-2.53452300	-0.32333400
C	5.85456100	0.00014500	-0.31069200
C	5.13758100	-3.81693100	0.15315100
H	5.86464600	-5.07953200	-1.47589400
C	5.11745100	-1.27126200	0.17287600
C	3.67289300	-3.82352600	-0.32585400
C	3.66312900	-1.27373900	-0.33730700
C	2.92880800	-5.06287800	0.18870700
C	2.93795400	-2.54556800	0.12727600
C	2.93085800	0.00010300	0.11985200
C	1.48443400	-5.07851500	-0.29435000
H	3.43500500	-5.98021900	-0.13165300
C	1.47897900	-2.55248100	-0.36209600
C	1.47623800	0.00017900	-0.37155600

C	0.72509000	-3.80943100	0.10277400
H	1.46033200	-5.17877000	-1.38992500
C	0.73476200	-1.27499700	0.06006600
C	-0.72339600	-3.81155400	-0.40914900
C	-0.73294900	-1.27594000	-0.40211000
C	-1.47969600	-5.07738100	0.00369400
C	-1.47119300	-2.54768800	0.04761300
C	-1.46972800	0.00011100	0.03467600
C	-2.93152100	-5.06231100	-0.45602700
H	-0.98663300	-5.96082900	-0.40981300
C	-2.94130700	-2.54607700	-0.40668700
C	-2.93785200	0.00012300	-0.41255400
C	-3.66411600	-3.82156100	0.07045200
H	-2.96425500	-5.06493600	-1.55380400
C	-3.65343000	-1.27252800	0.07153500
C	-5.14040600	-3.81602200	-0.36982200
C	-5.12312300	-1.27118900	-0.38949600
C	-5.88246800	-5.05857200	0.16713700
C	-5.85303700	-2.53465600	0.12654000
C	-5.84643400	0.00012400	0.11467800
C	-7.34922900	-5.06473400	-0.27877900
H	-5.38456800	-5.98216400	-0.18615200
C	-7.32770800	-2.53394800	-0.35077800
C	-7.31836800	0.00010600	-0.36724500
C	-8.06586100	-3.78443400	0.16358400
H	-7.41063500	-5.17190100	-1.37921400
C	-8.04482400	-1.26108100	0.13035300
H	8.17462100	3.75399200	-1.41183100
H	8.14391700	1.25325800	-1.37646100
H	9.08916900	-1.25917900	0.11072800
H	9.10763000	-3.78700200	0.08587700
H	-8.14142400	-3.75780500	1.26698600
H	-9.08989200	-1.25965900	-0.23324300
H	-8.11378800	1.25446500	1.23386600
H	-9.10710200	3.78797400	-0.21085500
H	0.73200500	-1.29732900	1.17478700
H	0.73148800	1.29734100	1.17529000
H	-1.50862800	0.00008500	1.14967400
H	1.50110500	0.00044800	-1.47534600
H	-0.72081800	-1.27573300	-1.50570100
H	-0.72064900	1.27611100	-1.50553200
H	1.50212100	-2.56605400	-1.46671000
H	2.91399200	-2.54496000	1.23272400
H	3.67180700	-1.27316300	-1.44573200
H	2.90511200	0.00002200	1.22805700
H	3.67175400	1.27371100	-1.44548400
H	2.91405200	2.54490200	1.23329500
H	1.50206500	2.56632200	-1.46607100
H	0.68516100	3.77863600	1.20952600
H	-0.68655900	3.78680000	-1.51186600

H	-1.47919500	2.55613500	1.15949100
H	0.68542200	-3.77856200	1.20887200
H	-0.68677700	-3.78646800	-1.51227000
H	-1.47910300	-2.55602800	1.15928600
H	-2.94261800	-2.54658500	-1.50934100
H	-3.62921600	-1.26919700	1.18338800
H	-2.93977100	0.00015400	-1.51454100
H	-3.62928000	1.26939200	1.18342100
H	-2.94251400	2.54680100	-1.50925700
H	5.11131700	1.27795600	1.28869700
H	5.87892900	2.52746100	-1.43869500
H	5.15337800	3.84176300	1.26981900
H	3.65578200	3.84063600	-1.43236500
H	5.86446500	5.07988500	-1.47530900
H	7.38530800	5.17753200	1.21231200
H	9.10760400	3.78728600	0.08606800
H	7.31204600	2.55363600	1.30623900
H	9.08916600	1.25944300	0.11076700
H	5.87628900	0.00022800	-1.42663800
H	7.29957200	0.00008700	1.32414500
H	8.14398900	-1.25285600	-1.37654300
H	7.31197700	-2.55346800	1.30600100
H	5.87904200	-2.52700200	-1.43902400
H	5.11127600	-1.27788000	1.28850000
H	8.17478000	-3.75358500	-1.41210100
H	7.38525600	-5.17736000	1.21185300
H	5.38686600	-5.98310600	-0.03514500
H	5.15322700	-3.84164800	1.26925200
H	3.65601700	-3.84009400	-1.43314700
H	-3.61941800	-3.83478200	1.17862900
H	-5.18330100	-3.83766400	-1.48613900
H	-9.10711600	-3.78772000	-0.21027800
H	-7.86615300	-5.94967700	0.13904700
H	-5.82665400	-5.08644600	1.27157100
H	-3.43241300	-5.97924800	-0.12603500
H	-1.43962000	-5.17628700	1.10013400
H	0.98419300	-5.96020900	0.11447500
H	2.94346500	-5.06578300	1.28778200
H	-8.11371700	-1.25409000	1.23402800
H	-9.08988900	1.25989100	-0.23345900
H	-8.14162000	3.75812800	1.26655000
H	-7.41043300	5.17205900	-1.37962900
H	-5.38453800	5.98240200	-0.18620900
H	-3.43243400	5.97949300	-0.12627000
H	-1.43998900	5.17631500	1.10052700
H	0.98413800	5.96041200	0.11553800
H	2.94326300	5.06550500	1.28892300
H	-5.84318800	-2.52805600	1.24144100
H	-5.14971400	-1.27715000	-1.50626300
H	-5.84068200	0.00015000	1.22976700

H	-5.14964300	1.27730800	-1.50630800
H	-5.84329100	2.52833500	1.24129300
H	-5.18321200	3.83789600	-1.48626700
H	-3.61952600	3.83508200	1.17861700
H	-7.32995000	0.00003800	-1.48474800
H	-7.34094300	2.55176000	-1.46815700
H	-7.34101900	-2.55166200	-1.46790600
K	-0.04309100	-0.00335200	3.26073600

Graphane-Li⁺

C	-5.12186300	1.27212400	-0.28633800
C	-5.86514700	2.53550800	0.21094700
C	-3.66723800	1.27614800	0.21696000
C	-8.05528600	1.26087000	0.15478400
C	-7.32668400	2.53462300	-0.30557300
C	-5.14072500	3.81765100	-0.26579500
C	-2.94133300	2.54825800	-0.24670200
C	-8.07834600	3.78371400	0.19187400
C	-5.89644600	5.05853000	0.25581000
C	-3.67536600	3.82659400	0.20879400
C	-1.47973800	2.56155500	0.23890600
C	-7.35109900	5.06539500	-0.22804900
H	-5.86981700	5.08296200	1.36169800
C	-2.93424900	5.06539800	-0.31219200
C	-0.73857700	1.28014300	-0.17115400
C	-0.72943900	3.81215900	-0.25362100
H	-7.87902600	5.94884200	0.17978200
C	-1.48345800	5.08172300	0.15229600
H	-2.96165400	5.06959800	-1.41010500
C	0.74376400	1.29408800	0.26879700
C	0.72986700	3.82267800	0.22824300
H	-0.99006100	5.96206000	-0.26657300
C	1.47826700	2.55559800	-0.21933100
C	1.48412600	5.07620900	-0.22426600
C	2.94510700	2.55437900	0.24703600
C	2.93534600	5.07378200	0.23883300
H	1.44260600	5.13972800	-1.32199900
C	3.66228200	1.27161400	-0.20223400
C	3.67470800	3.82053900	-0.24856200
H	3.43611700	5.98040000	-0.11742700
C	5.12453000	1.27418100	0.28067400
C	5.14156300	3.82146200	0.22175200
C	5.86255900	2.53184800	-0.23953200
C	5.89482100	5.05367200	-0.32319000
C	7.32830800	2.53721500	0.26474100
H	5.39082200	5.98487300	-0.00050300
C	7.35166400	5.06770400	0.15357100
C	8.07634700	3.78040200	-0.25293600
C	8.05370400	1.25968500	-0.19016700
H	7.87732300	5.94520600	-0.27005000

C	8.07635500	-3.78038900	-0.25301500
C	8.05370500	-1.25967400	-0.19019600
C	7.35167300	-5.06770400	0.15345100
C	7.32831200	-2.53721500	0.26468600
C	7.31872100	0.00000000	0.29842400
C	5.89482700	-5.05366100	-0.32330100
H	7.87733000	-5.94519100	-0.27020500
C	5.86256300	-2.53184000	-0.23958700
C	5.85480700	0.00000400	-0.20737100
C	5.14157000	-3.82146300	0.22166800
H	5.86306200	-5.05937700	-1.42969500
C	5.12453300	-1.27418600	0.28064400
C	3.67471500	-3.82053400	-0.24864300
C	3.66228500	-1.27161200	-0.20226400
C	2.93536500	-5.07379100	0.23873300
C	2.94511100	-2.55438600	0.24697900
C	2.94566600	-0.00000600	0.29292300
C	1.48413800	-5.07621200	-0.22434700
H	3.43613700	-5.98039500	-0.11756000
C	1.47826800	-2.55560400	-0.21938300
C	1.47756400	-0.00000400	-0.14959000
C	0.72987800	-3.82269300	0.22819500
H	1.44260400	-5.13971200	-1.32208000
C	0.74375900	-1.29410300	0.26877300
C	-0.72944700	-3.81216800	-0.25361600
C	-0.73857900	-1.28014400	-0.17115600
C	-1.48347900	-5.08172000	0.15232300
C	-1.47973400	-2.56155900	0.23892800
C	-1.49029000	0.00000500	0.25632000
C	-2.93426100	-5.06538500	-0.31219400
H	-0.99008900	-5.96207800	-0.26650400
C	-2.94134100	-2.54826100	-0.24665600
C	-2.94189500	-0.00000700	-0.24744600
C	-3.67536800	-3.82659600	0.20884500
H	-2.96163800	-5.06951400	-1.41010700
C	-3.66723700	-1.27614300	0.21699800
C	-5.14073900	-3.81765500	-0.26569500
C	-5.12186500	-1.27213000	-0.28629400
C	-5.89644600	-5.05851300	0.25598400
C	-5.86514800	-2.53549900	0.21102600
C	-5.85770300	0.00000600	0.19783800
C	-7.35110700	-5.06540900	-0.22784300
H	-5.39065500	-5.98395500	-0.08078000
C	-7.32668700	-2.53462600	-0.30548400
C	-7.31611700	-0.00000400	-0.32387600
C	-8.07836000	-3.78370100	0.19198900
H	-7.38488200	-5.17709200	-1.32898300
C	-8.05528000	-1.26085900	0.15485000
H	8.17458700	3.73680600	-1.35454900
H	8.14634000	1.24528400	-1.29278800

H	9.09146600	-1.26089100	0.19416900
H	9.11024500	-3.78962400	0.14088900
H	-8.18380500	-3.75451800	1.29311000
H	-9.09059300	-1.25949300	-0.23633000
H	-8.15469800	1.25303000	1.25642300
H	-9.10962200	3.78762600	-0.20916100
H	0.81339600	-1.43869000	1.38116200
H	0.81339700	1.43863200	1.38119300
H	-1.65581900	0.00000800	1.36900500
H	1.46495000	0.00000700	-1.25284800
H	-0.71627700	-1.25085100	-1.27353600
H	-0.71624600	1.25082600	-1.27353300
H	1.47320800	-2.52646000	-1.32330800
H	2.93892000	-2.58127800	1.35137800
H	3.64910200	-1.24724000	-1.31033900
H	2.96727600	-0.00001900	1.39994800
H	3.64910000	1.24727000	-1.31030900
H	2.93891700	2.58125100	1.35143600
H	1.47321900	2.52646400	-1.32325700
H	0.71722100	3.82447800	1.33448800
H	-0.71463700	3.76639700	-1.35669200
H	-1.50337900	2.60460200	1.34811800
H	0.71727500	-3.82450300	1.33444100
H	-0.71468400	-3.76640500	-1.35668700
H	-1.50335000	-2.60460300	1.34814100
H	-2.91560600	-2.54531900	-1.34902700
H	-3.67433500	-1.27314900	1.32798500
H	-2.89746500	-0.00002500	-1.34799600
H	-3.67434600	1.27317400	1.32794800
H	-2.91558800	2.54531200	-1.34907300
H	5.13965700	1.29037100	1.39651800
H	5.87363700	2.50808500	-1.35511200
H	5.16420800	3.86358300	1.33766000
H	3.64931600	3.80597400	-1.35564600
H	5.86306300	5.05940900	-1.42958400
H	7.39148000	5.19497400	1.25256000
H	9.11024100	3.78962800	0.14095700
H	7.32255900	2.56862700	1.38125100
H	9.09146400	1.26089600	0.19420300
H	5.86847600	0.00001800	-1.32366300
H	7.31392500	-0.00001300	1.41547200
H	8.14633600	-1.24524900	-1.29281800
H	7.32256200	-2.56864900	1.38119500
H	5.87364200	-2.50805400	-1.35516700
H	5.13965800	-1.29039900	1.39648800
H	8.17460700	-3.73676400	-1.35462600
H	7.39149500	-5.19501300	1.25243400
H	5.39083000	-5.98486700	-0.00062900
H	5.16421600	-3.86361100	1.33757500
H	3.64932200	-3.80595000	-1.35572600

H	-3.65453700	-3.84496300	1.31673500
H	-5.15814000	-3.84154800	-1.38280900
H	-9.10961700	-3.78763000	-0.20910000
H	-7.87902400	-5.94882400	0.18007400
H	-5.86979300	-5.08289400	1.36187300
H	-3.43575000	-5.98217500	0.01621900
H	-1.44339600	-5.18546200	1.24760200
H	0.99136100	-5.97095500	0.16344600
H	2.96533200	-5.11088500	1.33633200
H	-8.15465700	-1.25297900	1.25649200
H	-9.09058900	1.25949300	-0.23642600
H	-8.18373900	3.75458200	1.29300300
H	-7.38484700	5.17698400	-1.32919900
H	-5.39065800	5.98396100	-0.08098800
H	-3.43572100	5.98217400	0.01628700
H	-1.44334600	5.18550500	1.24757000
H	0.99133100	5.97094100	0.16353500
H	2.96529800	5.11084500	1.33643400
H	-5.88559800	-2.52827200	1.32610100
H	-5.11858800	-1.27897800	-1.40339700
H	-5.88341200	0.00002600	1.31303800
H	-5.11858700	1.27894100	-1.40343900
H	-5.88560800	2.52830500	1.32602300
H	-5.15808700	3.84150100	-1.38291200
H	-3.65457500	3.84493600	1.31668500
H	-7.29826000	-0.00003200	-1.44128200
H	-7.31092400	2.55445600	-1.42262600
H	-7.31093500	-2.55448100	-1.42253700
Li	-0.00007300	-0.00002900	2.06954200

Graphane-Mg²⁺

C	5.13482000	-1.27529000	-0.31183800
C	5.87616700	-2.53707500	0.19373300
C	3.68084900	-1.28187000	0.18516400
C	8.06478000	-1.26051800	0.12038900
C	7.33662500	-2.53805400	-0.32839000
C	5.15090800	-3.82311500	-0.27195100
C	2.95289700	-2.55669000	-0.27103800
C	8.08941300	-3.78245800	0.17685900
C	5.90760700	-5.05827800	0.26155700
C	3.68603500	-3.83322700	0.19948900
C	1.48660100	-2.57676300	0.20629100
C	7.36099500	-5.06810100	-0.22592400
H	5.88574600	-5.07400900	1.36795600
C	2.94518000	-5.07495900	-0.31636500
C	0.74905000	-1.29727100	-0.20956200
C	0.73564700	-3.82587400	-0.29684800
H	7.89133000	-5.94712600	0.19179200
C	1.48819800	-5.09005300	0.13121600
H	2.98733200	-5.09522000	-1.41292100

C	-0.75489300	-1.31677700	0.19555400
C	-0.73481500	-3.84170700	0.15634300
H	1.00120500	-5.97227600	-0.28863000
C	-1.49211400	-2.57970100	-0.29218900
C	-1.49029300	-5.08510000	-0.32463200
C	-2.95450400	-2.56671000	0.18733100
C	-2.94321500	-5.08804400	0.13759500
H	-1.44246200	-5.12761100	-1.42233200
C	-3.67558800	-1.27558200	-0.23714800
C	-3.69076800	-3.82746400	-0.32100400
H	-3.44280100	-5.98410700	-0.24185100
C	-5.12865400	-1.27781300	0.26532200
C	-5.14771900	-3.82897700	0.17411200
C	-5.87523900	-2.53169600	-0.25532300
C	-5.91294500	-5.05104300	-0.37691800
C	-7.33091900	-2.54093800	0.27956000
H	-5.40723700	-5.99035300	-0.08060400
C	-7.35931000	-5.07023600	0.13009300
C	-8.09049600	-3.77622700	-0.23849400
C	-8.06320700	-1.25837800	-0.14697700
H	-7.89593000	-5.93987300	-0.29969300
C	-8.09051400	3.77625600	-0.23784900
C	-8.06321300	1.25839000	-0.14676100
C	-7.35930900	5.07020500	0.13091100
C	-7.33092000	2.54088100	0.27997400
C	-7.31939100	-0.00003200	0.32927300
C	-5.91296600	5.05108900	-0.37616300
H	-7.89594400	5.93991200	-0.29871600
C	-5.87525600	2.53172300	-0.25495300
C	-5.86490200	0.00001200	-0.20605800
C	-5.14772000	3.82894000	0.17464400
H	-5.90670900	5.04015800	-1.48349700
C	-5.12865500	1.27777100	0.26549700
C	-3.69080400	3.82749200	-0.32056100
C	-3.67559800	1.27561500	-0.23699900
C	-2.94323800	5.08802100	0.13812800
C	-2.95449000	2.56669300	0.18759700
C	-2.95818700	-0.00000500	0.26064700
C	-1.49037200	5.08515300	-0.32427600
H	-3.44290000	5.98412800	-0.24111500
C	-1.49214200	2.57973700	-0.29201800
C	-1.49545300	0.00001500	-0.19008800
C	-0.73478600	3.84173100	0.15646200
H	-1.44267400	5.12780400	-1.42197800
C	-0.75484800	1.31679900	0.19561600
C	0.73561900	3.82590200	-0.29695600
C	0.74903300	1.29730800	-0.20960200
C	1.48826600	5.09010600	0.13087800
C	1.48663800	2.57680600	0.20614900
C	1.51020100	0.00002600	0.19274500

C	2.94521300	5.07494100	-0.31681600
H	1.00129700	5.97228600	-0.28907200
C	2.95288900	2.55668000	-0.27128500
C	2.97004300	-0.00000300	-0.29226700
C	3.68608000	3.83324400	0.19908100
H	2.98727600	5.09511500	-1.41337800
C	3.68086000	1.28190500	0.18501400
C	5.15091000	3.82307100	-0.27247900
C	5.13482400	1.27524800	-0.31201500
C	5.90764300	5.05831800	0.26077400
C	5.87618900	2.53709800	0.19335400
C	5.86783200	0.00001300	0.16985600
C	7.36100700	5.06805100	-0.22678700
H	5.40514700	5.98934300	-0.06670900
C	7.33662900	2.53799200	-0.32882200
C	7.32564900	-0.00003400	-0.35721900
C	8.08943700	3.78247800	0.17619100
H	7.39529100	5.19673000	-1.32645300
C	8.06479200	1.26052800	0.12015300
H	-8.22084000	-3.71702800	-1.33654300
H	-8.19106300	-1.23750400	-1.24661200
H	-9.09224500	1.26212300	0.26484700
H	-9.11560900	3.79167500	0.18175900
H	8.20741600	3.74398200	1.27604400
H	9.09835200	1.26108800	-0.28048200
H	8.18001000	-1.24867700	1.22078600
H	9.11909800	-3.79150400	-0.23195900
H	-0.87604900	1.55400400	1.32263300
H	-0.87620000	-1.55403600	1.32255300
H	1.76557200	0.00008800	1.32398300
H	-1.47564700	0.00005800	-1.29082100
H	0.72683800	1.25854000	-1.30964500
H	0.72690400	-1.25855600	-1.30960600
H	-1.48173200	2.53263300	-1.39410100
H	-2.93735100	2.61385300	1.29175500
H	-3.67535500	1.23509500	-1.34338500
H	-2.97570700	-0.00007100	1.37141600
H	-3.67532100	-1.23494000	-1.34353000
H	-2.93741700	-2.61399700	1.29148500
H	-1.48160900	-2.53257200	-1.39426900
H	-0.74595900	-3.85572700	1.26326800
H	0.74580300	-3.78173600	-1.39936600
H	1.50109200	-2.62085200	1.31896200
H	-0.74575200	3.85567700	1.26339000
H	0.74560800	3.78168900	-1.39947400
H	1.50122000	2.62093700	1.31881100
H	2.93081700	2.56442900	-1.37282100
H	3.68390300	1.26684700	1.29642400
H	2.92248300	-0.00007300	-1.39151400
H	3.68386600	-1.26669700	1.29657200

H	2.93088200	-2.56454400	-1.37257400
H	-5.13379800	-1.30335400	1.38111800
H	-5.91277400	-2.49470900	-1.37044500
H	-5.15482000	-3.89041400	1.28972800
H	-3.68070200	-3.79087200	-1.42685100
H	-5.90664400	-5.03993900	-1.48425000
H	-7.38017100	-5.22180000	1.22673100
H	-9.11561000	-3.79171100	0.18106400
H	-7.30402200	-2.58639200	1.39542600
H	-9.09224400	-1.26217800	0.26461600
H	-5.90576800	0.00008900	-1.32237100
H	-7.29446400	-0.00012800	1.44610100
H	-8.19108600	1.23769600	-1.24639800
H	-7.30399000	2.58614800	1.39584700
H	-5.91282300	2.49489500	-1.37007800
H	-5.13378000	1.30315200	1.38129700
H	-8.22090900	3.71723300	-1.33590100
H	-7.38012500	5.22159800	1.22757400
H	-5.40724000	5.99035000	-0.07972300
H	-5.15475500	3.89020900	1.29026700
H	-3.68080700	3.79101400	-1.42641200
H	3.66065400	3.83986900	1.30655200
H	5.17268400	3.85882800	-1.38998000
H	9.11911000	3.79145100	-0.23265700
H	7.89136400	5.94715000	0.19074200
H	5.88584000	5.07424200	1.36717100
H	3.44135200	5.98605300	0.03040900
H	1.43180600	5.18539000	1.22575000
H	-0.99955700	5.98532800	0.05028100
H	-2.97508100	5.15422600	1.23377700
H	8.18005300	1.24887600	1.22055000
H	9.09834900	-1.26114700	-0.28022200
H	8.20735700	-3.74377500	1.27670700
H	7.39534100	-5.19698000	-1.32556500
H	5.40512500	-5.98935900	-0.06578700
H	3.44126000	-5.98605700	0.03098100
H	1.43165600	-5.18516700	1.22609800
H	-0.99947100	-5.98530400	0.04986500
H	-2.97519700	-5.15441300	1.23322900
H	5.90388500	2.52289000	1.30828200
H	5.13952900	1.28837900	-1.42994500
H	5.90228500	0.00008700	1.28495500
H	5.13955200	-1.28858900	-1.42976500
H	5.90381600	-2.52270700	1.30865900
H	5.17277200	-3.85904900	-1.38944700
H	3.66051600	-3.83976800	1.30695900
H	7.30574900	-0.00013900	-1.47493600
H	7.31859200	-2.56743600	-1.44559000
H	7.31855500	2.56718500	-1.44602500
Mg	-0.01532000	-0.00009300	1.83391600

Graphane-Na⁺

C	-5.12377300	1.27177400	-0.33219700
C	-5.85650700	2.53477300	0.18116400
C	-3.65733100	1.27321300	0.13744800
C	-8.04802000	1.26109600	0.17049700
C	-7.32828800	2.53446200	-0.30517100
C	-5.14091700	3.81682500	-0.30899900
C	-2.94163900	2.54734800	-0.33415700
C	-8.06946600	3.78419000	0.20642300
C	-5.88634300	5.05845800	0.22543100
C	-3.66744000	3.82266300	0.14022600
C	-1.47381100	2.55133100	0.12895500
C	-7.35027400	5.06516000	-0.22959700
H	-5.83759100	5.08457900	1.33034100
C	-2.93255900	5.06384400	-0.38245200
C	-0.73461400	1.27768300	-0.31238900
C	-0.72523900	3.81249200	-0.33509200
H	-7.86984900	5.94938300	0.18675700
C	-1.48098900	5.07843500	0.07854900
H	-2.96411900	5.06940100	-1.48023100
C	0.73681300	1.27906900	0.14046500
C	0.72626100	3.81285000	0.16841100
H	-0.98780200	5.96159500	-0.33508800
C	1.47916000	2.55447200	-0.29447800
C	1.48428800	5.07872500	-0.24157300
C	2.93969900	2.54807400	0.19037100
C	2.93063300	5.06596200	0.23582700
H	1.45488000	5.17124600	-1.33766000
C	3.66307700	1.27354000	-0.26996900
C	3.67346500	3.82342900	-0.27294400
H	3.43531100	5.98078500	-0.09354100
C	5.11901100	1.27217400	0.23403900
C	5.13852700	3.81833800	0.20411900
C	5.86196100	2.53404000	-0.26828600
C	5.89380900	5.05673900	-0.32417100
C	7.32520100	2.53501900	0.24283400
H	5.38798900	5.98386400	0.00705300
C	7.34950800	5.06608600	0.15621300
C	8.07528400	3.78263700	-0.26111400
C	8.05227500	1.26054700	-0.21813900
H	7.87612800	5.94752800	-0.25764500
C	8.07530200	-3.78249100	-0.26175700
C	8.05227900	-1.26040700	-0.21836200
C	7.34956200	-5.06601100	0.15541500
C	7.32522600	-2.53495900	0.24241600
C	7.31494500	0.00002700	0.26464700
C	5.89383700	-5.05661100	-0.32489000
H	7.87617000	-5.94738600	-0.25860200
C	5.86197200	-2.53391700	-0.26866300

C	5.85451900	0.00006300	-0.25061800
C	5.13857200	-3.81828400	0.20360100
H	5.86484600	-5.07428500	-1.43127000
C	5.11902300	-1.27212600	0.23385000
C	3.67348500	-3.82334600	-0.27337800
C	3.66308700	-1.27342800	-0.27015300
C	2.93070100	-5.06590600	0.23540700
C	2.93973000	-2.54802400	0.19003900
C	2.93445900	0.00002000	0.19612500
C	1.48430400	-5.07867500	-0.24183600
H	3.43535800	-5.98071000	-0.09404400
C	1.47918100	-2.55441700	-0.29477500
C	1.47682100	0.00005200	-0.28458300
C	0.72631900	-3.81278900	0.16819700
H	1.45476500	-5.17122900	-1.33791600
C	0.73685300	-1.27904300	0.14025600
C	-0.72525300	-3.81242300	-0.33510100
C	-0.73463400	-1.27760500	-0.31236000
C	-1.48095300	-5.07837200	0.07861500
C	-1.47378100	-2.55126400	0.12903900
C	-1.47583400	0.00006400	0.11512300
C	-2.93259200	-5.06379300	-0.38216900
H	-0.98783100	-5.96151900	-0.33512200
C	-2.94164900	-2.54729700	-0.33395200
C	-2.94064800	0.00002700	-0.34481300
C	-3.66741800	-3.82258900	0.14053700
H	-2.96431000	-5.06941100	-1.47994300
C	-3.65731800	-1.27312200	0.13757900
C	-5.14092100	-3.81678100	-0.30859700
C	-5.12376700	-1.27173400	-0.33204200
C	-5.88631700	-5.05836000	0.22600100
C	-5.85649200	-2.53468000	0.18146200
C	-5.84970500	0.00004900	0.16750200
C	-7.35027100	-5.06512200	-0.22895400
H	-5.38662500	-5.98283000	-0.12243900
C	-7.32828100	-2.53442600	-0.30484800
C	-7.31880600	0.00001500	-0.32309900
C	-8.06945500	-3.78409300	0.20689900
H	-7.40526100	-5.17459900	-1.32947500
C	-8.04801000	-1.26100400	0.17067300
H	8.17541000	3.74943100	-1.36290000
H	8.14508100	1.25111100	-1.32070800
H	9.08952000	-1.25964200	0.16666700
H	9.10820500	-3.78768400	0.13426300
H	-8.15200800	-3.75581100	1.30985200
H	-9.09094900	-1.25985100	-0.19926400
H	-8.12417600	1.25349900	1.27381400
H	-9.10853800	3.78805800	-0.17364700
H	0.75788600	-1.33787900	1.25807500
H	0.75764000	1.33772400	1.25830900

H	-1.56134700	0.00023300	1.23211400
H	1.49449000	0.00013200	-1.38822400
H	-0.72050500	-1.27309000	-1.41567100
H	-0.72016800	1.27325500	-1.41569700
H	1.49552300	-2.55871100	-1.39932000
H	2.91949500	-2.55461700	1.29525100
H	3.66697300	-1.26646700	-1.37857900
H	2.92010200	-0.00005300	1.30465100
H	3.66697300	1.26672800	-1.37839700
H	2.91945900	2.55456400	1.29557800
H	1.49556600	2.55877800	-1.39902600
H	0.69440100	3.78881900	1.27467500
H	-0.69509100	3.78375900	-1.43833800
H	-1.48653800	2.56763800	1.24063700
H	0.69459700	-3.78873500	1.27447200
H	-0.69524800	-3.78365300	-1.43834800
H	-1.48642300	-2.56760300	1.24074100
H	-2.93522600	-2.54965000	-1.43655600
H	-3.64002800	-1.26707200	1.24935900
H	-2.93221100	-0.00003100	-1.44647600
H	-3.64006900	1.26726200	1.24922700
H	-2.93516100	2.54962900	-1.43676100
H	5.11877900	1.28146000	1.34980500
H	5.87809000	2.52231000	-1.38395200
H	5.15585800	3.84755500	1.32025800
H	3.65452900	3.83262100	-1.38025800
H	5.86487700	5.07455600	-1.43055100
H	7.38645200	5.18218800	1.25640300
H	9.10816600	3.78778300	0.13496000
H	7.31411800	2.55748200	1.35944100
H	9.08950800	1.25972900	0.16690900
H	5.87464700	0.00014800	-1.36665600
H	7.30274900	-0.00007000	1.38160900
H	8.14506500	-1.25078600	-1.32093100
H	7.31417400	-2.55760500	1.35902000
H	5.87806500	-2.52203900	-1.38432800
H	5.11879900	-1.28157200	1.34961400
H	8.17537300	-3.74911900	-1.36354200
H	7.38656500	-5.18227800	1.25558600
H	5.38804100	-5.98378200	0.00624200
H	5.15596100	-3.84764800	1.31973600
H	3.65447800	-3.83249300	-1.38069100
H	-3.62888900	-3.83477900	1.24861400
H	-5.17744200	-3.84035000	-1.42514500
H	-9.10852400	-3.78800800	-0.17318500
H	-7.86982300	-5.94928400	0.18756200
H	-5.83751000	-5.08436400	1.33091100
H	-3.43345900	-5.97987300	-0.05024800
H	-1.44045500	-5.17668100	1.17479200
H	0.98613400	-5.96285700	0.16365400

H	2.94987600	-5.07701100	1.33409000
H	-8.12414800	-1.25326400	1.27398900
H	-9.09095300	1.25989300	-0.19945600
H	-8.15200200	3.75604900	1.30938200
H	-7.40521000	5.17446500	-1.33013800
H	-5.38663500	5.98289300	-0.12308000
H	-3.43347600	5.97994200	-0.05065300
H	-1.44066000	5.17671000	1.17473300
H	0.98606600	5.96291900	0.16382900
H	2.94969700	5.07702200	1.33451300
H	-5.85370900	-2.52647200	1.29652100
H	-5.14460400	-1.27875900	-1.44894100
H	-5.85104100	0.00011900	1.28278100
H	-5.14460100	1.27867600	-1.44909400
H	-5.85374800	2.52668100	1.29622500
H	-5.17737600	3.84028000	-1.42555000
H	-3.62898400	3.83489400	1.24830400
H	-7.32410900	-0.00006000	-1.44064100
H	-7.33503100	2.55349100	-1.42232300
H	-7.33504100	-2.55358300	-1.42200000
Na	-0.04339500	-0.00178300	2.74535300

Graphane-NH₄⁺

C	5.11248300	-1.25572200	-0.33828200
C	5.84369200	-2.51109200	0.19486200
C	3.64325100	-1.24977700	0.12167400
C	8.03582100	-1.23603300	0.16617400
C	7.31712800	-2.51774000	-0.28747900
C	5.13224200	-3.80047700	-0.28215800
C	2.93310200	-2.53091900	-0.33907500
C	8.05697600	-3.75850500	0.24730400
C	5.87391100	-5.03408800	0.27555400
C	3.65487700	-3.80209800	0.15195000
C	1.46083800	-2.53165200	0.10673400
C	7.34060900	-5.04696900	-0.17073400
H	5.81906000	-5.04452700	1.38013200
C	2.92451700	-5.04881700	-0.36390900
C	0.72025100	-1.25690900	-0.33287700
C	0.71434400	-3.79841300	-0.34265700
H	7.85850400	-5.92395600	0.26278400
C	1.46917400	-5.06003300	0.08515900
H	2.96491800	-5.06462700	-1.46106000
C	-0.75301400	-1.25984400	0.11772400
C	-0.74059800	-3.79288700	0.15028800
H	0.97891400	-5.94673100	-0.32383000
C	-1.48861700	-2.53543100	-0.32326600
C	-1.49228600	-5.06377400	-0.25688700
C	-2.95347300	-2.53306800	0.14778700
C	-2.94629400	-5.04866100	0.19660100
H	-1.44659600	-5.16477900	-1.35159500

C	-3.67211800	-1.25390200	-0.30851800
C	-3.68063100	-3.80709600	-0.32781400
H	-3.44469700	-5.96549600	-0.13706600
C	-5.13084900	-1.26140200	0.18809200
C	-5.15376800	-3.80595000	0.12336700
C	-5.86942200	-2.51427000	-0.34127000
C	-5.90041800	-5.03583600	-0.43651800
C	-7.33900100	-2.52328200	0.15137800
H	-5.40019300	-5.96826900	-0.11235900
C	-7.36400800	-5.05226200	0.01952500
C	-8.08238600	-3.76083900	-0.38625300
C	-8.05965400	-1.23904700	-0.29204600
H	-7.88427000	-5.92553800	-0.41885000
C	-8.08121400	3.80585400	-0.18531600
C	-8.05971900	1.28270600	-0.22371300
C	-7.35730400	5.07365500	0.28069900
C	-7.33562400	2.54174200	0.28286100
C	-7.32712700	0.00873000	0.22981300
C	-5.89839100	5.07955900	-0.18994900
H	-7.88047700	5.96924800	-0.10593500
C	-5.86928500	2.55598600	-0.21833300
C	-5.86282300	0.02099500	-0.27372800
C	-5.14656800	3.82326500	0.29947900
H	-5.86192300	5.13591600	-1.29477100
C	-5.12926900	1.27909700	0.24819000
C	-3.68010400	3.84108500	-0.17389700
C	-3.67209500	1.29432000	-0.25300800
C	-2.93414600	5.06554900	0.37167400
C	-2.94750300	2.55196400	0.24982700
C	-2.94308400	0.01046200	0.17936500
C	-1.49561700	5.09518700	-0.12760500
H	-3.44388500	5.99191800	0.08419000
C	-1.48949000	2.56725800	-0.24143200
C	-1.48698700	0.01996200	-0.30757200
C	-0.72893200	3.81835100	0.22887500
H	-1.48590700	5.22359800	-1.22064400
C	-0.74085000	1.28224400	0.15328000
C	0.70407800	3.82849800	-0.32639100
C	0.71702000	1.29462400	-0.33991000
C	1.47047600	5.09346500	0.06963400
C	1.46342600	2.56338600	0.10517500
C	1.46284900	0.02313200	0.08899600
C	2.90953200	5.07918300	-0.42944100
H	0.96568600	5.97741900	-0.32860000
C	2.92409200	2.56329400	-0.37910800
C	2.92540900	0.01712000	-0.37381500
C	3.65510900	3.84015400	0.08200300
H	2.91329300	5.07861500	-1.52775600
C	3.64495600	1.29363400	0.09547100
C	5.12305500	3.83214100	-0.38602900

C	5.11064300	1.28726300	-0.37640300
C	5.87278300	5.08234500	0.12105300
C	5.84439700	2.55788800	0.11625300
C	5.83767400	0.02377900	0.14204700
C	7.33302700	5.08181700	-0.34543600
H	5.36969500	6.00038700	-0.23978700
C	7.31346300	2.55062300	-0.37750300
C	7.30625900	0.01577100	-0.35034700
C	8.05664000	3.80943300	0.10808400
H	7.37910400	5.17122500	-1.44822000
C	8.03633000	1.28602300	0.11737700
H	-8.16536200	-3.70760700	-1.48865500
H	-8.13658300	-1.20449000	-1.39523400
H	-9.10068000	1.27148700	0.15044000
H	-9.11712400	3.79886800	0.20231000
H	8.14602900	3.80065300	1.21075100
H	9.07742100	1.27920800	-0.25790500
H	8.11275900	-1.20835300	1.26889600
H	9.09743500	-3.76781000	-0.12950100
H	-0.71484100	1.26511800	1.26959400
H	-0.78186600	-1.27944800	1.22921700
H	1.51554800	0.05346900	1.19937100
H	-1.50542500	0.03664000	-1.41164100
H	0.68581800	1.29785300	-1.44338800
H	0.71128200	-1.26467300	-1.43624100
H	-1.51956600	2.59491600	-1.34620500
H	-2.92557400	2.52146500	1.35356500
H	-3.67388700	1.32285400	-1.36135100
H	-2.91988600	-0.01211000	1.28460400
H	-3.66927000	-1.23764400	-1.41691400
H	-2.94285900	-2.54437600	1.25282800
H	-1.49601000	-2.54627000	-1.42793300
H	-0.71650400	-3.76136800	1.25810500
H	0.69105600	-3.77614800	-1.44572600
H	1.48304500	-2.56638800	1.22630900
H	-0.65919600	3.76796900	1.33140800
H	0.63436500	3.80976100	-1.42821600
H	1.49210000	2.56186100	1.21389100
H	2.90692200	2.55913800	-1.48159900
H	3.62964100	1.29567300	1.20740200
H	2.92126200	0.00494800	-1.47543700
H	3.61862700	-1.23330700	1.23518000
H	2.93151100	-2.54351600	-1.44115200
H	-5.13534600	-1.29101000	1.30348800
H	-5.87129900	-2.48648600	-1.45669200
H	-5.19067400	-3.85122900	1.23841100
H	-3.64213000	-3.81803600	-1.43453800
H	-5.85379700	-5.03552700	-1.54249000
H	-7.41917300	-5.18789400	1.11665300
H	-9.12128200	-3.77188600	-0.00650400

H	-7.34181900	-2.56765000	1.26741100
H	-9.10206500	-1.24571800	0.07829300
H	-5.87338200	0.04779800	-1.38939400
H	-7.32363100	-0.02096700	1.34649200
H	-8.14056500	1.30612400	-1.32690700
H	-7.33191100	2.52825700	1.39963900
H	-5.87809500	2.58002300	-1.33386500
H	-5.12998800	1.25639000	1.36372600
H	-8.17192900	3.80950600	-1.28835000
H	-7.40115400	5.15147500	1.38398100
H	-5.39369800	5.99389700	0.17676800
H	-5.16662500	3.81531000	1.41571000
H	-3.66005300	3.88546800	-1.28063800
H	3.63176100	3.85423200	1.19060900
H	5.14584000	3.83921600	-1.50297300
H	9.09319900	3.80796400	-0.27876700
H	7.85508700	5.97388000	0.05054300
H	5.83215600	5.12814300	1.22557900
H	3.41856600	5.99711600	-0.11500500
H	1.46045900	5.18975300	1.16666600
H	-0.99023100	5.96668200	0.29713400
H	-2.93713900	5.03422100	1.47014800
H	8.11812900	1.29871100	1.22009200
H	9.07882500	-1.24082300	-0.20412600
H	8.13666100	-3.71226900	1.34968900
H	7.40192300	-5.17478000	-1.26911300
H	5.37697200	-5.96374100	-0.06325500
H	3.42353400	-5.96142300	-0.01983100
H	1.42028700	-5.15074000	1.18229300
H	-0.99964800	-5.94494200	0.16252600
H	-2.98347700	-5.05549600	1.29504000
H	5.84766200	2.56534600	1.23121800
H	5.12922500	1.27799000	-1.49332800
H	5.84086500	0.04142000	1.25672900
H	5.13758900	-1.27880800	-1.45545000
H	5.83834500	-2.48816400	1.30916100
H	5.17888200	-3.83953500	-1.39828900
H	3.60668200	-3.80395500	1.26067300
H	7.30992300	-0.00509100	-1.46781200
H	7.32643300	-2.55628400	-1.40431900
H	7.31456200	2.55020100	-1.49484100
H	-0.04273000	-1.26310200	3.97420400
N	0.57561300	-0.80646200	3.29346300
H	0.06284100	-0.06851600	2.78608500
H	0.89509000	-1.49273600	2.58639600
H	1.38905400	-0.39834400	3.76957800
Graphane-NMe ₄ ⁺			
C	-5.10807700	1.27071500	-0.61971100
C	-5.83264800	2.53709100	-0.10383800

C	-3.63380500	1.27358300	-0.17283600
C	-8.02386600	1.26244400	-0.06594800
C	-7.31313700	2.53303900	-0.56258200
C	-5.12654000	3.81453400	-0.61981100
C	-2.92583600	2.54370300	-0.66627100
C	-8.04487600	3.78689900	-0.04732400
C	-5.86189000	5.06197700	-0.08495700
C	-3.64512200	3.82354600	-0.19715200
C	-1.45620500	2.54863200	-0.21288500
C	-7.33480500	5.06371600	-0.51021600
H	-5.79039900	5.10129800	1.01795600
C	-2.91544900	5.05772500	-0.74280900
C	-0.71492800	1.27363800	-0.65082900
C	-0.70477000	3.80897700	-0.67179300
H	-7.84634300	5.95213700	-0.09347700
C	-1.46407100	5.08030600	-0.28135900
H	-2.94745900	5.04229500	-1.84048800
C	0.74634600	1.27258000	-0.16822100
C	0.73502800	3.80763500	-0.13463900
H	-0.96983600	5.95827500	-0.70582300
C	1.49333700	2.54917600	-0.58807500
C	1.49910800	5.07830700	-0.51677800
C	2.94860300	2.54383300	-0.08783000
C	2.93762900	5.06033000	-0.01646000
H	1.48975400	5.18315300	-1.61222900
C	3.67716500	1.27449900	-0.55451300
C	3.68592900	3.82347200	-0.53084200
H	3.44790500	5.98012000	-0.32402600
C	5.12883700	1.27124600	-0.03516800
C	5.14877700	3.81633800	-0.04509900
C	5.87528100	2.53593100	-0.52385800
C	5.90589700	5.05911200	-0.56043800
C	7.33620700	2.53404800	-0.00673900
H	5.39815500	5.98312700	-0.22389200
C	7.36049400	5.06540400	-0.07650900
C	8.08766300	3.78485800	-0.50088700
C	8.06514700	1.26167300	-0.47108100
H	7.88780200	5.94955700	-0.48335800
C	8.08761800	-3.78398400	-0.50135000
C	8.06513500	-1.26080700	-0.47121700
C	7.36032900	-5.06456400	-0.07728600
C	7.33611200	-2.53322800	-0.00713900
C	7.32579100	0.00041100	0.00694200
C	5.90585400	-5.05816500	-0.56157900
H	7.88771500	-5.94868600	-0.48410200
C	5.87526000	-2.53497800	-0.52446500
C	5.86843700	0.00047600	-0.51641700
C	5.14862400	-3.81549100	-0.04616100
H	5.88001400	-5.08424800	-1.66795400
C	5.12878800	-1.27040500	-0.03553000

C	3.68591100	-3.82242800	-0.53231900
C	3.67715800	-1.27344500	-0.55499200
C	2.93743800	-5.05951600	-0.01875200
C	2.94850100	-2.54296500	-0.08893600
C	2.94201200	0.00044100	-0.10479200
C	1.49905300	-5.07720600	-0.51947300
H	3.44777000	-5.97917200	-0.32661700
C	1.49331700	-2.54804400	-0.58944900
C	1.48976400	0.00056900	-0.60513800
C	0.73491500	-3.80672200	-0.13682100
H	1.48999300	-5.18142900	-1.61498400
C	0.74630600	-1.27167200	-0.16898500
C	-0.70480100	-3.80775400	-0.67420200
C	-0.71496500	-1.27237300	-0.65165700
C	-1.46411700	-5.07931300	-0.28452300
C	-1.45625800	-2.54766100	-0.21463900
C	-1.45205400	0.00052900	-0.20644900
C	-2.91553900	-5.05642500	-0.74581800
H	-0.96991600	-5.95701600	-0.70958100
C	-2.92591200	-2.54244800	-0.66792000
C	-2.91921400	0.00064400	-0.65628300
C	-3.64510700	-3.82254300	-0.19935600
H	-2.94766400	-5.04035300	-1.84348200
C	-3.63379200	-1.27260100	-0.17363200
C	-5.12662900	-3.81334200	-0.62160300
C	-5.10811100	-1.26950200	-0.62033900
C	-5.86183800	-5.06098200	-0.08699400
C	-5.83262200	-2.53610600	-0.10494300
C	-5.82616900	0.00048900	-0.10573900
C	-7.33484600	-5.06259500	-0.51193100
H	-5.36889300	-5.98058100	-0.45758400
C	-7.31318200	-2.53188800	-0.56346700
C	-7.30351300	0.00057900	-0.57060400
C	-8.04483000	-3.78592600	-0.04849400
H	-7.41144800	-5.15953500	-1.61245000
C	-8.02384900	-1.26145800	-0.06633400
H	8.18886200	3.75868100	-1.60280000
H	8.15826900	1.25559600	-1.57363200
H	9.10167500	-1.25880300	-0.08529200
H	9.11968000	-3.78664900	-0.10383900
H	-8.10472300	-3.76823700	1.05582200
H	-9.07380100	-1.25853900	-0.41542300
H	-8.07700200	1.25914100	1.03827300
H	-9.09112500	3.78695000	-0.40691900
H	0.72480200	-1.27257500	0.94171100
H	0.72495900	1.27276400	0.94250000
H	-1.46895100	0.00032200	0.90405700
H	1.52168000	0.00088600	-1.70948800
H	-0.69449200	-1.26777300	-1.75584600
H	-0.69448800	1.26980300	-1.75502300

H	1.52780500	-2.56077400	-1.69416200
H	2.91542900	-2.53579100	1.01615700
H	3.69265700	-1.27785100	-1.66344800
H	2.91080900	0.00024300	1.00145400
H	3.69257200	1.27934600	-1.66296900
H	2.91573500	2.53621100	1.01725200
H	1.52762100	2.56247500	-1.69279000
H	0.67484600	3.77403000	0.97046300
H	-0.65028900	3.77449600	-1.77392100
H	-1.46998400	2.56846200	0.89661800
H	0.67452300	-3.77371900	0.96830200
H	-0.65018800	-3.77268000	-1.77630000
H	-1.47010600	-2.56829900	0.89483100
H	-2.93198600	-2.53175900	-1.77050700
H	-3.59692100	-1.27693800	0.93829200
H	-2.92438600	0.00097500	-1.75857300
H	-3.59701800	1.27716500	0.93908700
H	-2.93176100	2.53363000	-1.76887000
H	5.11563000	1.27550000	1.08006400
H	5.89587800	2.53251200	-1.63956200
H	5.15951200	3.83683600	1.07078600
H	3.67518500	3.84527000	-1.63819400
H	5.87976900	5.08545200	-1.66679900
H	7.39456300	5.17364000	1.02436500
H	9.11979400	3.78743800	-0.10355400
H	7.32055500	2.55052200	1.10970700
H	9.10171900	1.25958000	-0.08524200
H	5.89387700	0.00062800	-1.63226400
H	7.30732100	0.00034600	1.12362400
H	8.15835000	-1.25455700	-1.57375900
H	7.32030500	-2.54986000	1.10930300
H	5.89601900	-2.53126800	-1.64016300
H	5.11549800	-1.27493500	1.07970000
H	8.18900800	-3.75764300	-1.60324000
H	7.39413100	-5.17292200	1.02358400
H	5.39802400	-5.98225100	-0.22537300
H	5.15907400	-3.83623500	1.06971600
H	3.67549000	-3.84370300	-1.63968200
H	-3.58838900	-3.84860500	0.90844800
H	-5.18279000	-3.82464500	-1.73746300
H	-9.09114000	-3.78585300	-0.40791700
H	-7.84628700	-5.95114900	-0.09535500
H	-5.79011700	-5.10065100	1.01589100
H	-3.41768300	-5.97854200	-0.43153800
H	-1.42777900	-5.19536500	0.81056500
H	0.99332100	-5.95818200	-0.11484900
H	2.93839000	-5.05451300	1.08055700
H	-8.07690100	-1.25853600	1.03789200
H	-9.07379100	1.25966700	-0.41512000
H	-8.10495100	3.76884800	1.05697900

H	-7.41116500	5.16099300	-1.61072200
H	-5.36888400	5.98170700	-0.45514600
H	-3.41759800	5.97967200	-0.42804100
H	-1.42782600	5.19565300	0.81380200
H	0.99350300	5.95906400	-0.11152000
H	2.93888700	5.05478500	1.08284200
H	-5.80849800	-2.53866500	1.00936200
H	-5.14419200	-1.27035100	-1.73705200
H	-5.80691800	0.00021900	1.00863200
H	-5.14403900	1.27204800	-1.73642500
H	-5.80867700	2.53913800	1.01047300
H	-5.18238000	3.82626000	-1.73568600
H	-3.58868500	3.84901900	0.91067100
H	-7.32744700	0.00075000	-1.68808300
H	-7.34002600	2.54403600	-1.67966700
H	-7.34023700	-2.54254000	-1.68055100
N	-0.20229000	-0.00623900	4.22735600
C	-0.86519300	1.22125100	3.67846200
H	-0.37498600	2.10143400	4.09740700
H	-0.76413600	1.21557000	2.59172100
H	-1.92040700	1.20519000	3.95628700
C	1.24229600	-0.01035600	3.82652200
H	1.71365900	-0.91031600	4.22440300
H	1.30318800	-0.00449800	2.73611100
H	1.72154100	0.88091700	4.23445400
C	-0.87433000	-1.22557800	3.67151400
H	-0.39111200	-2.11185600	4.08568700
H	-1.92950500	-1.20299400	3.94910500
H	-0.77300400	-1.21482700	2.58486000
C	-0.31046300	-0.01019700	5.71992000
H	0.18196700	0.88139600	6.11035900
H	-1.36602700	-0.00714400	5.99506900
H	0.17536600	-0.90769100	6.10508300

Graphane-OH₃⁺

C	-5.10743400	1.30624100	-0.32699600
C	-5.82835000	2.57076000	0.19896200
C	-3.63321100	1.30837500	0.11613500
C	-8.02009700	1.29776600	0.23581300
C	-7.30989500	2.57078800	-0.25591000
C	-5.12027200	3.85016300	-0.30954800
C	-2.92015600	2.57887300	-0.36717500
C	-8.03835000	3.82200100	0.26948500
C	-5.85370200	5.09442500	0.23463300
C	-3.63898100	3.85548500	0.11429900
C	-1.45017100	2.57816300	0.08807700
C	-7.32760200	5.10075000	-0.18676300
H	-5.77924800	5.12781900	1.33792100
C	-2.90688600	5.09200000	-0.42235400
C	-0.70824500	1.30905700	-0.36443900

C	-0.69676100	3.84017400	-0.36338600
H	-7.83659000	5.98696800	0.23874700
C	-1.45528000	5.10841500	0.03910000
H	-2.94038100	5.08637100	-1.52015100
C	0.74955900	1.29636300	0.12855500
C	0.74346400	3.83353500	0.17364800
H	-0.96029500	5.98834300	-0.37964800
C	1.49960500	2.57498000	-0.28420000
C	1.50999700	5.10176000	-0.21246500
C	2.95639000	2.56419600	0.21145100
C	2.94905200	5.08101200	0.28595200
H	1.49837000	5.20588400	-1.30814000
C	3.68252300	1.29757600	-0.26623600
C	3.69469300	3.84403900	-0.23160900
H	3.45983100	5.99991500	-0.02278500
C	5.13393000	1.28695000	0.25125700
C	5.15710900	3.83199500	0.25424400
C	5.88242800	2.55319700	-0.23057900
C	5.91672300	5.07638900	-0.25307900
C	7.34226400	2.54617900	0.28947700
H	5.41018000	5.99918200	0.08932300
C	7.37036900	5.07751500	0.23395800
C	8.09673600	3.79844700	-0.19614800
C	8.07038900	1.27511300	-0.17985700
H	7.89991300	5.96354300	-0.16582700
C	8.08543100	-3.76990100	-0.24089300
C	8.06633600	-1.24710900	-0.19470500
C	7.35533300	-5.05218200	0.17247900
C	7.33425400	-2.52130500	0.25891700
C	7.32795000	0.01242500	0.28917500
C	5.90244300	-5.04113400	-0.31697900
H	7.88331000	-5.93460200	-0.23748200
C	5.87470000	-2.51754500	-0.26242100
C	5.87163500	0.01810700	-0.23747400
C	5.14617600	-3.80098100	0.20559300
H	5.88124600	-5.05929900	-1.42351800
C	5.13001300	-1.25498400	0.23459500
C	3.68486700	-3.80339800	-0.28156000
C	3.67956900	-1.25082400	-0.28462900
C	2.93372800	-5.04124400	0.22757900
C	2.95159500	-2.52492900	0.17285900
C	2.94703800	0.02096200	0.17816700
C	1.49469000	-5.05551700	-0.27121800
H	3.43936400	-5.96045600	-0.08751100
C	1.49655000	-2.52521600	-0.32647800
C	1.49548800	0.03095700	-0.32315400
C	0.73335900	-3.78418000	0.11601300
H	1.48305200	-5.15425500	-1.36708800
C	0.75824600	-1.24698600	0.10282000
C	-0.70321800	-3.78507900	-0.42885400

C	-0.71345100	-1.23902400	-0.35366700
C	-1.46947400	-5.05876200	-0.05996500
C	-1.46173700	-2.52895200	0.02600200
C	-1.45454800	0.04032800	0.07211100
C	-2.92236500	-5.02455900	-0.51731300
H	-0.97563400	-5.92657600	-0.50335800
C	-2.93509100	-2.51135000	-0.40655900
C	-2.92079100	0.03662500	-0.37713500
C	-3.65117200	-3.79891600	0.04877600
H	-2.95907600	-4.99436100	-1.61408700
C	-3.63488200	-1.24022200	0.09753200
C	-5.13387900	-3.77985900	-0.36261700
C	-5.11052000	-1.23484300	-0.33829100
C	-5.86767700	-5.03067700	0.16604200
C	-5.83371500	-2.50515900	0.16955300
C	-5.82457700	0.03423300	0.18410700
C	-7.34264300	-5.02557500	-0.25228200
H	-5.37964300	-5.94927700	-0.21389700
C	-7.31616300	-2.49458500	-0.28475200
C	-7.30336300	0.03783800	-0.27738700
C	-8.04749400	-3.75103700	0.22370900
H	-7.42600200	-5.11616500	-1.35286700
C	-8.02227000	-1.22635800	0.22290700
H	8.20130900	3.77858600	-1.29764600
H	8.16805500	1.27538800	-1.28186700
H	9.10139500	-1.24916200	0.19600500
H	9.11600200	-3.77638300	0.16140000
H	-8.10557400	-3.74173300	1.32837800
H	-9.07415200	-1.22001800	-0.12198800
H	-8.07172700	1.28962700	1.34037500
H	-9.08578400	3.82631000	-0.08720700
H	0.79024100	-1.25267500	1.22050900
H	0.72088900	1.28336400	1.24035700
H	-1.48479100	0.08194100	1.18258100
H	1.52239500	0.03678100	-1.42715000
H	-0.69245600	-1.23086800	-1.45637100
H	-0.68542100	1.31045300	-1.46815100
H	1.52705400	-2.52556300	-1.43074100
H	2.92108500	-2.52798100	1.27702200
H	3.69421100	-1.24728400	-1.39311600
H	2.91221400	0.01537200	1.28250200
H	3.69607600	1.30915800	-1.37487600
H	2.92961600	2.55245000	1.31498000
H	1.53081300	2.59126000	-1.38931300
H	0.68573000	3.80059500	1.27705300
H	-0.64393900	3.81469900	-1.46603600
H	-1.45677600	2.58091000	1.19636600
H	0.66988000	-3.76160100	1.22259800
H	-0.64614100	-3.72792500	-1.52904500
H	-1.51347800	-2.64413000	1.15430700

H	-2.93659900	-2.48784700	-1.50785800
H	-3.59368300	-1.25430900	1.21301800
H	-2.92656500	0.04252700	-1.47854700
H	-3.59543100	1.30262700	1.22773400
H	-2.92733400	2.57861500	-1.46975600
H	5.12134100	1.28551700	1.36732500
H	5.90501700	2.55590400	-1.34611900
H	5.16686200	3.84642400	1.37080500
H	3.68318100	3.86742000	-1.33913300
H	5.89248000	5.11014200	-1.35902700
H	7.40183800	5.17911300	1.33571800
H	9.12765900	3.79734400	0.20485800
H	7.32398700	2.55693300	1.40626700
H	9.10551100	1.26948700	0.21041000
H	5.89994900	0.02577100	-1.35315700
H	7.30683100	0.00628200	1.40602800
H	8.16487400	-1.23363300	-1.29659100
H	7.31509700	-2.54474900	1.37552300
H	5.89876600	-2.50566400	-1.37791600
H	5.11682900	-1.26594100	1.35057600
H	8.19230000	-3.73650900	-1.34190900
H	7.38529600	-5.16741200	1.27292600
H	5.39374900	-5.96742500	0.01165200
H	5.15614200	-3.82903800	1.32190700
H	3.67360200	-3.81781500	-1.38890700
H	-3.58845700	-3.83878800	1.15655000
H	-5.19903400	-3.78178700	-1.47854500
H	-9.09567800	-3.74621800	-0.13199500
H	-7.85415700	-5.91625400	0.16109900
H	-5.79288100	-5.07998000	1.26856100
H	-3.42509100	-5.94869600	-0.21294100
H	-1.42780100	-5.19792500	1.03226800
H	0.98673900	-5.93568900	0.13179200
H	2.93737300	-5.04338200	1.32633700
H	-8.07350200	-1.22920400	1.32743800
H	-9.07134500	1.29855500	-0.11036600
H	-8.09598400	3.79749000	1.37401500
H	-7.40770300	5.20739600	-1.28596900
H	-5.36065400	6.01652200	-0.13032700
H	-3.40727600	6.01126200	-0.09833200
H	-1.41746600	5.21452200	1.13444000
H	1.00728000	5.98326200	0.19412400
H	2.95214800	5.07466200	1.38468900
H	-5.80850800	-2.51779300	1.28373200
H	-5.15319800	-1.22805600	-1.45577100
H	-5.80500600	0.03025200	1.29867300
H	-5.14811500	1.31507800	-1.44361600
H	-5.80195700	2.56644200	1.31371300
H	-5.17637300	3.87036200	-1.42518300
H	-3.58196500	3.87065400	1.22150000

H	-7.33093600	0.04425100	-1.39478700
H	-7.34053200	2.58911400	-1.37280800
H	-7.34706300	-2.49749100	-1.40199300
H	-0.09992200	-0.76490400	2.75015700
H	-1.14731300	-1.87212400	2.25092100
H	-1.62261700	-0.69262600	3.26737000
O	-0.87763700	-1.30098800	3.05492900

Graphane-OMe₃⁺

C	5.02174700	-1.26874200	-0.60012200
C	5.75544800	-2.53557100	-0.09824600
C	3.55462400	-1.27398900	-0.13183900
C	7.94707200	-1.26021000	-0.10277300
C	7.22710300	-2.53112400	-0.58494500
C	5.03979000	-3.81274500	-0.60168700
C	2.83708500	-2.54347000	-0.61037100
C	7.96851800	-3.78478500	-0.08370700
C	5.78483500	-5.06027000	-0.08104600
C	3.56594400	-3.82240100	-0.15342700
C	1.37611300	-2.54743900	-0.12914600
C	7.24978700	-5.06163000	-0.53269800
H	5.73280400	-5.10236500	1.02268900
C	2.82652300	-5.05765200	-0.68255700
C	0.62614200	-1.27194600	-0.55010000
C	0.61736100	-3.80789800	-0.57538500
H	7.76897600	-5.95006600	-0.12501400
C	1.38328300	-5.07853700	-0.19595500
H	2.83978400	-5.04503900	-1.78053600
C	-0.82887500	-1.27017800	-0.04794000
C	-0.81524700	-3.80587700	-0.01917500
H	0.88184300	-5.95675500	-0.61072300
C	-1.57809600	-2.54697200	-0.46407900
C	-1.58247000	-5.07717100	-0.39363900
C	-3.02967600	-2.54272000	0.04657000
C	-3.01729100	-5.05854400	0.11706600
H	-1.58129400	-5.18299300	-1.48910800
C	-3.76057500	-1.27251000	-0.41473800
C	-3.76911400	-3.82202900	-0.39328000
H	-3.52901200	-5.97892900	-0.18629000
C	-5.20885700	-1.27028200	0.11320100
C	-5.22849600	-3.81533500	0.10210300
C	-5.95829200	-2.53479000	-0.37131500
C	-5.98906400	-5.05826400	-0.40778600
C	-7.41545700	-2.53322000	0.15635200
H	-5.47881300	-5.98210700	-0.07478400
C	-7.43988000	-5.06454400	0.08754800
C	-8.17047200	-3.78427200	-0.33183000
C	-8.14806600	-1.26102200	-0.30275100
H	-7.97030100	-5.94906400	-0.31406600
C	-8.17105400	3.78481100	-0.33037300

C	-8.14827100	1.26154500	-0.30224200
C	-7.44086900	5.06504700	0.08984200
C	-7.41601800	2.53368400	0.15760000
C	-7.40543200	0.00022400	0.17035200
C	-5.98979000	5.05921500	-0.40472100
H	-7.97122900	5.94962400	-0.31172900
C	-5.95867200	2.53578900	-0.36956500
C	-5.95170900	0.00051500	-0.36294600
C	-5.22929300	3.81615100	0.10497500
H	-5.97169400	5.08578200	-1.51111600
C	-5.20915000	1.27107900	0.11428000
C	-3.76962300	3.82341800	-0.38955100
C	-3.76075200	1.27408700	-0.41331800
C	-3.01826100	5.05964800	0.12211700
C	-3.03017100	2.54387900	0.04963000
C	-3.02251600	0.00060300	0.03343300
C	-1.58337700	5.07902800	-0.38835900
H	-3.53014900	5.98018300	-0.18051500
C	-1.57842600	2.54884700	-0.46053700
C	-1.57552000	0.00110600	-0.48097600
C	-0.81585600	3.80762900	-0.01482600
H	-1.58211400	5.18576600	-1.48374700
C	-0.82878800	1.27175000	-0.04588100
C	0.61653600	3.81032800	-0.57158900
C	0.62582900	1.27444600	-0.54897700
C	1.38244000	5.08078000	-0.19156100
C	1.37561600	2.54955800	-0.12677600
C	1.37019600	0.00121000	-0.11765100
C	2.82535800	5.06049800	-0.67912900
H	0.88057800	5.95923300	-0.60532200
C	2.83646800	2.54630800	-0.60836300
C	2.82967900	0.00144800	-0.59274100
C	3.56533600	3.82511500	-0.15107700
H	2.83791800	5.04849600	-1.77712800
C	3.55441900	1.27665200	-0.13089500
C	5.03890500	3.81586600	-0.60032400
C	5.02144400	1.27190500	-0.59953300
C	5.78401900	5.06346500	-0.07997300
C	5.75502800	2.53871500	-0.09746300
C	5.74822000	0.00155800	-0.09847400
C	7.24877500	5.06507000	-0.53226000
H	5.28444900	5.98296600	-0.44280600
C	7.22654300	2.53461600	-0.58457900
C	7.21668300	0.00175600	-0.59198500
C	7.96786800	3.78836600	-0.08345300
H	7.30502300	5.16355400	-1.63400500
C	7.94684800	1.26379000	-0.10265700
H	-8.28012400	-3.75832400	-1.43282800
H	-8.24908500	-1.25473200	-1.40447600
H	-9.18188700	1.25925700	0.09141000

H	-9.20013100	3.78699500	0.07480300
H	8.05101300	3.77075700	1.01924500
H	8.98917900	1.26105800	-0.47516000
H	8.02600900	-1.25755500	0.99962600
H	9.00758100	-3.78513500	-0.46436200
H	-0.79955400	1.26250600	1.06364000
H	-0.80100300	-1.26257700	1.06139200
H	1.39827500	0.00135300	0.99576500
H	-1.61555400	0.00207200	-1.58531600
H	0.59013300	1.26848600	-1.65269800
H	0.59093800	-1.26498400	-1.65383300
H	-1.62100500	2.56184300	-1.56512400
H	-2.99151100	2.53628700	1.15346400
H	-3.78280300	1.27970400	-1.52195500
H	-2.97755700	0.00000700	1.13731200
H	-3.78285500	-1.27683800	-1.52337100
H	-2.99049200	-2.53614500	1.15042400
H	-1.62076300	-2.55910200	-1.56865300
H	-0.74193600	-3.77288600	1.08503200
H	0.54744200	-3.77330200	-1.67657600
H	1.41233900	-2.57066100	0.98054200
H	-0.74224700	3.77391500	1.08927000
H	0.54614200	3.77663200	-1.67278800
H	1.41169500	2.57111500	0.98294300
H	2.82190500	2.53654200	-1.71056900
H	3.53949800	1.29267200	0.98328500
H	2.81234700	0.00192800	-1.69445600
H	3.53933500	-1.29056500	0.98218900
H	2.82284500	-2.53313500	-1.71256700
H	-5.18819800	-1.27452500	1.22874200
H	-5.98670800	-2.53078200	-1.48670300
H	-5.23153700	-3.83537900	1.21830800
H	-3.76535400	-3.84413800	-1.50079300
H	-5.97156400	-5.08429100	-1.51420400
H	-7.46489800	-5.17144000	1.18891000
H	-9.19937900	-3.78680000	0.07378100
H	-7.39134600	-2.54927200	1.27279900
H	-9.18162100	-1.25914000	0.09106600
H	-5.98446400	0.00097000	-1.47845400
H	-7.37889200	-0.00000600	1.28704100
H	-8.24911400	1.25577700	-1.40398600
H	-7.39229500	2.54930100	1.27405900
H	-5.98671900	2.53254700	-1.48497000
H	-5.18874800	1.27454900	1.22982800
H	-8.28023300	3.75930300	-1.43142900
H	-7.46647500	5.17153800	1.19122900
H	-5.47983300	5.98296800	-0.07100600
H	-5.23296900	3.83560100	1.22118800
H	-3.76526000	3.84640700	-1.49705500
H	3.52914900	3.84827800	0.95814600

H	5.07418000	3.82761000	-1.71725400
H	9.00685600	3.78891600	-0.46428900
H	7.76798300	5.95361700	-0.12485000
H	5.73244500	5.10551000	1.02379200
H	3.33341700	5.98110600	-0.37042100
H	1.36486300	5.19442800	0.90425100
H	-1.07523300	5.95934700	0.01499100
H	-3.01200900	5.05199200	1.22119500
H	8.02584800	1.26103300	0.99974500
H	8.98943300	-1.25719500	-0.47520800
H	8.05148700	-3.76718300	1.01899800
H	7.30652100	-5.16018300	-1.63441600
H	5.28556600	-5.97983500	-0.44413200
H	3.33457400	-5.97833300	-0.37405100
H	1.36500700	-5.19308000	0.89976600
H	-1.07408100	-5.95770300	0.00893200
H	-3.01083200	-5.05191000	1.21615600
H	5.75336200	2.54212600	1.01667000
H	5.03915500	1.27297800	-1.71714900
H	5.75218500	0.00134700	1.01524200
H	5.03973500	-1.26941600	-1.71773100
H	5.75350500	-2.53926700	1.01587000
H	5.07576300	-3.82430700	-1.71860700
H	3.52905900	-3.84613200	0.95580200
H	7.21822400	0.00182400	-1.70998100
H	7.23265900	-2.54266800	-1.70252000
H	7.23179000	2.54625500	-1.70215100
O	1.49301600	-0.01929000	4.16314900
C	0.80802300	1.22922600	3.79959100
H	-0.18571400	1.16993300	4.23938300
H	1.38717200	2.03460800	4.24756100
H	0.77179700	1.30480500	2.71013600
C	0.76054200	-1.23191600	3.77040500
H	1.28777400	-2.06626000	4.22913900
H	-0.24156600	-1.12876000	4.18202000
H	0.75190400	-1.29839000	2.67993800
C	2.91248200	-0.04079900	3.78383200
H	3.36921300	0.82280100	4.26356700
H	3.32006200	-0.96937800	4.17848300
H	2.98433100	0.00788200	2.69438700

Graphane-SH₃⁺

C	-5.10210800	1.29518100	-0.43756600
C	-5.83181700	2.56394100	0.06569400
C	-3.63200400	1.29825800	0.02011900
C	-8.02433400	1.29298100	0.07640400
C	-7.30416600	2.55907700	-0.41844500
C	-5.11354100	3.84011300	-0.43588600
C	-2.91461600	2.57120500	-0.44978700
C	-8.04387600	3.81627100	0.07654200

C	-5.85962500	5.08846700	0.08105300
C	-3.64291300	3.84527600	0.02302000
C	-1.45213200	2.56732400	0.02792300
C	-7.32269600	5.09020200	-0.37639700
H	-5.81220500	5.12985300	1.18543900
C	-2.89969900	5.08704400	-0.48476600
C	-0.70602800	1.30253300	-0.42936000
C	-0.69319700	3.83637300	-0.39279100
H	-7.84206300	5.98089600	0.02620700
C	-1.45959700	5.09894700	0.01086600
H	-2.90677800	5.09184200	-1.58299300
C	0.74951100	1.28692800	0.07060700
C	0.73847900	3.82295300	0.16550400
H	-0.95557800	5.98480600	-0.38391600
C	1.50149400	2.57453700	-0.30764000
C	1.50680900	5.10128100	-0.18199800
C	2.95555600	2.55614000	0.19493200
C	2.94227200	5.06967400	0.32580200
H	1.50316700	5.23347600	-1.27458000
C	3.68350000	1.29969500	-0.30591500
C	3.69170900	3.84671300	-0.21843700
H	3.45391800	5.99673200	0.04412700
C	5.13644500	1.28294700	0.20729500
C	5.15428300	3.82694700	0.26646600
C	5.88064200	2.56098300	-0.24938200
C	5.91034100	5.08448100	-0.21324000
C	7.34290100	2.54482900	0.26356900
H	5.40290700	5.99798700	0.15163800
C	7.36527300	5.07683600	0.26952700
C	8.09269700	3.81025200	-0.19427100
C	8.07066600	1.28731600	-0.24140400
H	7.89185500	5.97344600	-0.11005800
C	8.09340500	-3.75579300	-0.41749600
C	8.07052500	-1.23419500	-0.31728800
C	7.37178900	-5.04794000	-0.01975900
C	7.34632000	-2.51935100	0.11761800
C	7.33424900	0.01218600	0.20258500
C	5.91147100	-5.03005900	-0.48605900
H	7.89489200	-5.92040200	-0.45629100
C	5.88042100	-2.50883700	-0.38576800
C	5.87388600	0.02616000	-0.31225900
C	5.16114300	-3.80118800	0.07119500
H	5.87248800	-5.02742400	-1.59229500
C	5.13798900	-1.25703600	0.14075400
C	3.69109300	-3.80113700	-0.39005900
C	3.68317400	-1.24861000	-0.36728800
C	2.95363800	-5.04366200	0.12748000
C	2.96072600	-2.52762200	0.08240800
C	2.95024300	0.01499600	0.11647000
C	1.50208200	-5.05744100	-0.33365100

H	3.45368400	-5.95974100	-0.20586100
C	1.49943500	-2.52994900	-0.39984300
C	1.49901500	0.02531400	-0.38525400
C	0.74941300	-3.78670100	0.07214200
H	1.46160300	-5.15684400	-1.42876000
C	0.75891600	-1.25391100	0.03092400
C	-0.70441700	-3.79310100	-0.42368600
C	-0.70887800	-1.25163000	-0.43645400
C	-1.45974500	-5.05181100	0.01167600
C	-1.44911900	-2.52194100	0.01493200
C	-1.45122500	0.02692400	-0.01262200
C	-2.91559800	-5.04228700	-0.43481500
H	-0.97046400	-5.94066300	-0.39367800
C	-2.92387800	-2.52456400	-0.42115100
C	-2.91722000	0.02414500	-0.46255100
C	-3.64318600	-3.79349800	0.07901300
H	-2.95887300	-5.06187200	-1.53181000
C	-3.63090400	-1.24241800	0.04005400
C	-5.12281200	-3.79302900	-0.34750200
C	-5.10435600	-1.24833400	-0.40600900
C	-5.86138800	-5.02639800	0.21476000
C	-5.83166500	-2.50357200	0.13278400
C	-5.82558800	0.03033000	0.08240400
C	-7.33047800	-5.03953000	-0.22340200
H	-5.36615500	-5.95612200	-0.12653300
C	-7.30816000	-2.51025300	-0.34010300
C	-7.29767200	0.02383700	-0.39966000
C	-8.04471600	-3.75122900	0.19874100
H	-7.39783700	-5.16729700	-1.32144100
C	-8.02413600	-1.22889700	0.11897700
H	8.19289500	3.81727700	-1.29646300
H	8.15996900	1.31404600	-1.34386200
H	9.11016900	-1.24205900	0.06064700
H	9.12947500	-3.76793100	-0.03022100
H	-8.11816200	-3.70522800	1.30155800
H	-9.06915200	-1.23324400	-0.24569700
H	-8.09995300	1.30202200	1.17956900
H	-9.08274400	3.81660500	-0.30421500
H	0.76476400	-1.27155800	1.14264700
H	0.71509100	1.26489400	1.18902100
H	-1.49296800	0.04155200	1.09557500
H	1.52840800	0.04526800	-1.48907800
H	-0.69459200	-1.26424700	-1.53969100
H	-0.66990200	1.31773200	-1.53247500
H	1.51529700	-2.54377700	-1.50454100
H	2.94171000	-2.54002000	1.18708300
H	3.68915300	-1.23064800	-1.47570000
H	2.91586900	-0.01082800	1.22144500
H	3.69455700	1.33177800	-1.41409500
H	2.92462000	2.52194100	1.29841900

H	1.53953600	2.60883800	-1.41197900
H	0.66559800	3.76739400	1.26781500
H	-0.62175400	3.82510300	-1.49451000
H	-1.47785400	2.55509300	1.13764700
H	0.72262800	-3.75477300	1.17940700
H	-0.67978100	-3.77820100	-1.52706000
H	-1.46000200	-2.53593500	1.13621900
H	-2.92960100	-2.54089500	-1.52328500
H	-3.59656700	-1.22325000	1.15381100
H	-2.92623900	0.01499600	-1.56405600
H	-3.60638000	1.29242000	1.13296100
H	-2.90282700	2.57378300	-1.55224100
H	5.12800000	1.25671200	1.32273800
H	5.89850100	2.58831200	-1.36472300
H	5.16564200	3.81553900	1.38279000
H	3.68034900	3.89495500	-1.32510100
H	5.88321200	5.14370000	-1.31819800
H	7.40001800	5.15128700	1.37336700
H	9.12525400	3.80168500	0.20220800
H	7.33018400	2.52751800	1.38023300
H	9.10870500	1.27460500	0.14071200
H	5.89307700	0.05575500	-1.42772100
H	7.32203800	-0.02092700	1.31911800
H	8.15538000	-1.19683000	-1.41978400
H	7.34084400	-2.56648000	1.23355400
H	5.89036200	-2.47884100	-1.50106000
H	5.13355400	-1.28943900	1.25613900
H	8.18422100	-3.70010100	-1.51913300
H	7.41902100	-5.18594000	1.07747000
H	5.40863100	-5.96297800	-0.16730600
H	5.19015500	-3.84872000	1.18643800
H	3.66031700	-3.81029400	-1.49710900
H	-3.58899700	-3.79060200	1.18751100
H	-5.17520400	-3.83285400	-1.46332700
H	-9.08726300	-3.76073100	-0.17224500
H	-7.84581200	-5.91666800	0.21287600
H	-5.80017500	-5.03668200	1.31899900
H	-3.41421100	-5.95334200	-0.08610100
H	-1.40910300	-5.13697300	1.10906700
H	1.00742100	-5.93906000	0.08230000
H	2.98481300	-5.05302700	1.22596600
H	-8.09519600	-1.20285700	1.22212200
H	-9.06762400	1.28768200	-0.29290500
H	-8.12689100	3.80324200	1.17963500
H	-7.37560300	5.18399600	-1.47854500
H	-5.35853800	6.00783800	-0.27928800
H	-3.40801700	6.00323800	-0.16429900
H	-1.44732700	5.19004600	1.10838100
H	0.99905400	5.97121100	0.24304300
H	2.93849100	5.03539600	1.42418500

H	-5.81916400	-2.48006100	1.24698600
H	-5.13952200	-1.27067400	-1.52293200
H	-5.82128200	0.04497600	1.19705400
H	-5.13054900	1.28995400	-1.55444000
H	-5.82787500	2.56661000	1.18057400
H	-5.14337400	3.85189700	-1.55265800
H	-3.61294100	3.85274200	1.13171800
H	-7.30911900	0.00563800	-1.51711300
H	-7.31250300	2.56278700	-1.53577300
H	-7.32456200	-2.54827500	-1.45687300
H	0.03876500	0.17335500	2.66228000
H	-0.94014400	-1.54812800	2.57815600
H	-1.73969900	0.00131900	3.54793700
S	-0.56470400	-0.66502500	3.55047400

Graphane-SMe₃⁺

C	5.10893100	-1.26998900	-0.59707600
C	5.83278700	-2.53689800	-0.08146000
C	3.63420600	-1.27354500	-0.15200000
C	8.02377900	-1.26199600	-0.03885000
C	7.31407800	-2.53230700	-0.53763600
C	5.12770500	-3.81385700	-0.60018800
C	2.92700400	-2.54296200	-0.64854100
C	8.04491000	-3.78653300	-0.02203900
C	5.86208000	-5.06180700	-0.06517900
C	3.64554300	-3.82356700	-0.18044900
C	1.45717900	-2.54913900	-0.19634900
C	7.33585600	-5.06300300	-0.48743600
H	5.78842800	-5.10237800	1.03756000
C	2.91639800	-5.05667700	-0.72928200
C	0.71550000	-1.27281600	-0.62996200
C	0.70502200	-3.80853200	-0.65643200
H	7.84662900	-5.95173100	-0.07033300
C	1.46472500	-5.08048100	-0.26871100
H	2.94929400	-5.03897400	-1.82686400
C	-0.74558700	-1.27244800	-0.14676100
C	-0.73381800	-3.80747600	-0.11636800
H	0.97063200	-5.95752400	-0.69517600
C	-1.49272200	-2.54860900	-0.56763300
C	-1.49856400	-5.07812300	-0.49724800
C	-2.94809400	-2.54332700	-0.06778100
C	-2.93670300	-5.05970300	0.00419500
H	-1.49015100	-5.18338000	-1.59263700
C	-3.67652200	-1.27417300	-0.53536400
C	-3.68512000	-3.82316300	-0.51074100
H	-3.44718500	-5.97957700	-0.30253300
C	-5.12854300	-1.27079400	-0.01720900
C	-5.14828900	-3.81586100	-0.02613300
C	-5.87446800	-2.53567500	-0.50612900
C	-5.90493700	-5.05885700	-0.54163800

C	-7.33589900	-2.53356100	0.00957200
H	-5.39756200	-5.98275800	-0.20420000
C	-7.35998800	-5.06490000	-0.05907900
C	-8.08680800	-3.78459400	-0.48477500
C	-8.06430100	-1.26131000	-0.45597600
H	-7.88690800	-5.94928700	-0.46597100
C	-8.08680700	3.78461000	-0.48526100
C	-8.06429300	1.26132900	-0.45615800
C	-7.36002000	5.06498400	-0.05970600
C	-7.33591700	2.53363700	0.00927400
C	-7.32555500	0.00003900	0.02270100
C	-5.90491600	5.05887100	-0.54210100
H	-7.88689400	5.94929900	-0.46681600
C	-5.87445700	2.53570400	-0.50634400
C	-5.86766300	0.00001400	-0.49918000
C	-5.14832900	3.81592900	-0.02637300
H	-5.87767700	5.08560100	-1.64843200
C	-5.12855700	1.27085500	-0.01729400
C	-3.68509400	3.82321800	-0.51078200
C	-3.67651600	1.27421900	-0.53539000
C	-2.93674100	5.05972200	0.00432600
C	-2.94812300	2.54337000	-0.06775400
C	-2.94211300	0.00002200	-0.08503700
C	-1.49853200	5.07820200	-0.49691100
H	-3.44718900	5.97962300	-0.30238000
C	-1.49271900	2.54866900	-0.56750700
C	-1.48895500	0.00003300	-0.58276000
C	-0.73383000	3.80749700	-0.11611700
H	-1.48994200	5.18364300	-1.59228100
C	-0.74560600	1.27248400	-0.14666800
C	0.70502300	3.80858400	-0.65615800
C	0.71550400	1.27288600	-0.62982200
C	1.46470200	5.08053800	-0.26840500
C	1.45717600	2.54918000	-0.19612600
C	1.45260800	0.00001500	-0.18424900
C	2.91638700	5.05674900	-0.72894500
H	0.97060500	5.95756400	-0.69490400
C	2.92700000	2.54303300	-0.64833300
C	2.91979600	0.00003800	-0.63386000
C	3.64553200	3.82361400	-0.18016800
H	2.94929500	5.03909700	-1.82652800
C	3.63420500	1.27358100	-0.15189100
C	5.12769600	3.81393300	-0.59990500
C	5.10892400	1.27006300	-0.59696800
C	5.86207200	5.06184300	-0.06481200
C	5.83278400	2.53693900	-0.08127300
C	5.82625300	0.00001900	-0.08149600
C	7.33584300	5.06308300	-0.48708000
H	5.36989300	5.98126700	-0.43689700
C	7.31406500	2.53237900	-0.53747500

C	7.30428900	0.00003700	-0.54422900
C	8.04491800	3.78657200	-0.02183300
H	7.41452200	5.15965400	-1.58748600
C	8.02377400	1.26203900	-0.03877100
H	-8.18706300	-3.75893400	-1.58678000
H	-8.15624000	-1.25548700	-1.55862300
H	-9.10135200	1.25921900	-0.07154100
H	-9.11933200	3.78712600	-0.08886800
H	8.10306200	3.76941900	1.08259600
H	9.07438900	1.25903300	-0.38596100
H	8.07498600	-1.25932600	1.06547000
H	9.09187200	-3.78620700	-0.37963000
H	-0.72357300	1.27400200	0.96454000
H	-0.72350800	-1.27400700	0.96445100
H	1.46844800	-0.00008600	0.92711800
H	-1.51962200	0.00008100	-1.68710500
H	0.69415300	1.26649400	-1.73393400
H	0.69414400	-1.26633100	-1.73407000
H	-1.52701900	2.56049100	-1.67219200
H	-2.91588000	2.53541900	1.03752000
H	-3.69082200	1.27927100	-1.64380700
H	-2.91408500	0.00004500	1.02129100
H	-3.69087700	-1.27921300	-1.64378100
H	-2.91575600	-2.53536200	1.03749200
H	-1.52708000	-2.56036300	-1.67231700
H	-0.67124900	-3.77444900	0.98883600
H	0.64861400	-3.77234800	-1.75835200
H	1.47182100	-2.57331500	0.91288600
H	-0.67127700	3.77438000	0.98908400
H	0.64861800	3.77243600	-1.75807900
H	1.47184000	2.57328300	0.91311100
H	2.93424600	2.53103400	-1.75085100
H	3.59643500	1.27913400	0.96016100
H	2.92434600	0.00008100	-1.73611400
H	3.59644500	-1.27919800	0.96005400
H	2.93427200	-2.53089000	-1.75105800
H	-5.11633000	-1.27485100	1.09805500
H	-5.89405600	-2.53273200	-1.62185700
H	-5.16003200	-3.83593800	1.08974200
H	-3.67362200	-3.84510100	-1.61806400
H	-5.87782000	-5.08571100	-1.64796900
H	-7.39515300	-5.17263300	1.04182400
H	-9.11932200	-3.78706600	-0.08836000
H	-7.32138100	-2.54959700	1.12605500
H	-9.10134400	-1.25916200	-0.07131500
H	-5.89198300	-0.00002700	-1.61504600
H	-7.30824800	0.00011900	1.13942500
H	-8.15617900	1.25537400	-1.55880800
H	-7.32146200	2.54981000	1.12575600
H	-5.89397300	2.53269200	-1.62207100

H	-5.11638300	1.27501200	1.09797200
H	-8.18703100	3.75880800	-1.58726300
H	-7.39531200	5.17291300	1.04117300
H	-5.39756600	5.98280400	-0.20471100
H	-5.16022500	3.83610900	1.08949800
H	-3.67344100	3.84518900	-1.61810200
H	3.58710100	3.85084500	0.92762200
H	5.18578100	3.82456600	-1.71568600
H	9.09185600	3.78627500	-0.37950100
H	7.84661600	5.95176800	-0.06988200
H	5.78842800	5.10233700	1.03793000
H	3.41839300	5.97918300	-0.41562600
H	1.42799800	5.19843100	0.82652000
H	-0.99254800	5.95865600	-0.09152400
H	-2.93761400	5.05355300	1.10361700
H	8.07497900	1.25929700	1.06554900
H	9.07439300	-1.25896100	-0.38604200
H	8.10297500	-3.76946500	1.08239600
H	7.41454200	-5.15944600	-1.58785200
H	5.36991000	-5.98120500	-0.43733300
H	3.41840600	-5.97912500	-0.41600600
H	1.42806200	-5.19835800	0.82621900
H	-0.99252900	-5.95865200	-0.09209100
H	-2.93743300	-5.05362700	1.10348600
H	5.80704000	2.54025300	1.03298800
H	5.14626700	1.27063100	-1.71367700
H	5.80547500	-0.00003300	1.03282200
H	5.14628000	-1.27048000	-1.71377900
H	5.80703100	-2.54029400	1.03280200
H	5.18579500	-3.82441400	-1.71596800
H	3.58711900	-3.85086000	0.92734000
H	7.32984900	0.00006800	-1.66169500
H	7.34294300	-2.54249100	-1.65469000
H	7.34290700	2.54261600	-1.65453100
C	0.98488300	1.40252300	3.65694100
H	0.51655000	2.31306100	4.03580000
H	2.04930600	1.40549200	3.90146300
H	0.83425200	1.30363000	2.57940600
C	-1.43901700	-0.00046900	3.81181400
H	-1.95057500	-0.89335200	4.17670700
H	-1.95053100	0.89261500	4.17627200
H	-1.38383100	-0.00077100	2.71997600
C	0.98502700	-1.40287100	3.65635400
H	2.04907600	-1.40706900	3.90245800
H	0.51531000	-2.31350500	4.03327600
H	0.83606900	-1.30242900	2.57873100
S	0.22913800	-0.00040800	4.51032700

XYZ coordinates (in Å) of graphene complexes optimized at ONIOM (M06-2X/6-31G*/PM6) level.

Graphene-Trp

C	-5.14530200	1.37095200	-0.38809400
C	-5.89707200	2.54071900	-0.12146000
C	-3.69567200	1.42959000	-0.47679900
C	-7.97594200	1.24121000	-0.22719800
C	-7.32938200	2.46280800	-0.04234800
C	-5.24986100	3.81114700	0.07067100
C	-3.04201300	2.68663100	-0.30381200
C	-8.07163200	3.66955300	0.23080700
C	-6.00318700	4.93897600	0.32950200
C	-3.77974000	3.85963000	-0.02012800
C	-1.61494000	2.75608000	-0.39668600
C	-7.42431600	4.85878200	0.40869000
H	-5.53561000	5.90881600	0.47593200
C	-3.09957300	5.06162900	0.18779400
C	-0.85172700	1.55634200	-0.62940800
C	-0.95828300	3.98928500	-0.20600400
H	-7.98001800	5.77294200	0.61435000
C	-1.72172100	5.12394200	0.10185300
H	-3.65894000	5.96381500	0.42755500
C	0.56872100	1.60945000	-0.65662000
C	0.49903200	4.05282200	-0.29970800
H	-1.24081100	6.07338000	0.29593600
C	1.24364300	2.86713600	-0.48393900
C	1.18797700	5.26999400	-0.20723000
C	2.67534200	2.92678600	-0.50653400
C	2.56892700	5.33560700	-0.23897100
H	0.63421400	6.19797700	-0.11483900
C	3.41821400	1.71662000	-0.65962700
C	3.32944800	4.17358700	-0.37290700
H	3.05321100	6.30444500	-0.15600500
C	4.87132800	1.77259300	-0.65193200
C	4.79997700	4.23989400	-0.38060800
C	5.54190900	3.00993100	-0.51487800
C	5.48524700	5.43178300	-0.25738000
C	6.97820200	3.05349700	-0.50738600
H	4.94379500	6.37810000	-0.15576100
C	6.91277000	5.47591600	-0.25605500
C	7.64104100	4.32749500	-0.37501100
C	7.70807400	1.86924700	-0.62527400
H	7.40115000	6.44673900	-0.15630100
C	7.90328100	-3.04024400	-1.10176600
C	7.79555300	-0.58180300	-0.86831300
C	7.25824100	-4.23679200	-1.22426700
C	7.15213900	-1.81290700	-0.99736900
C	7.05745700	0.62077700	-0.75795900
C	5.83109800	-4.29070500	-1.25191200
H	7.81358000	-5.17302400	-1.30239100
C	5.71585600	-1.86769400	-1.02483200

C	5.62031900	0.57175100	-0.77799500
C	5.06354500	-3.14730300	-1.15716200
H	5.35775300	-5.27333700	-1.35104000
C	4.95890100	-0.67811800	-0.92061900
C	3.59278300	-3.18315700	-1.18778000
C	3.50626700	-0.72125300	-0.95366600
C	2.91736400	-4.40105800	-1.27848800
C	2.85202700	-1.98163200	-1.10807300
C	2.76856200	0.47438400	-0.81748400
C	1.53566600	-4.43467900	-1.31970900
H	3.46930100	-5.33596300	-1.31128600
C	1.41980800	-2.02304600	-1.14914500
C	1.31424400	0.42379000	-0.83191600
C	0.76239500	-3.26515400	-1.28544900
H	1.04891200	-5.40268200	-1.36617000
C	0.65644100	-0.81207100	-1.01126700
C	-0.69693700	-3.31318500	-1.35222600
C	-0.76437100	-0.86679800	-0.99718100
C	-1.38164400	-4.51653800	-1.57293600
C	-1.43947700	-2.12838300	-1.17031700
C	-1.51215500	0.31660300	-0.79803500
C	-2.76251900	-4.57142200	-1.55613800
H	-0.83681000	-5.43004000	-1.77011300
C	-2.87075200	-2.18432900	-1.13532400
C	-2.96487400	0.25313900	-0.72521400
C	-3.52546900	-3.42483000	-1.32242800
H	-3.25905600	-5.52499500	-1.72482200
C	-3.61147600	-0.98851200	-0.89023900
C	-4.99639000	-3.50316400	-1.27355600
C	-5.06111900	-1.05862400	-0.82738300
C	-5.67084000	-4.69293000	-1.46248800
C	-5.72929200	-2.29292000	-1.01167800
C	-5.80743300	0.12494400	-0.56868400
C	-7.09459000	-4.73682800	-1.39894400
H	-5.13836100	-5.61796900	-1.66526500
C	-7.16405000	-2.34065900	-0.94347200
C	-7.24831800	0.06116700	-0.49269800
C	-7.82176800	-3.60895300	-1.14712300
H	-7.58659900	-5.69593500	-1.55663000
C	-7.89249400	-1.18108100	-0.68442000
H	8.73172800	4.34693300	-0.37267300
H	8.80119500	1.90183300	-0.61456400
H	8.88825200	-0.53901700	-0.84930100
H	8.99252800	-2.98504300	-1.07857400
H	-8.90729600	-3.63462800	-1.09633700
H	-8.97615500	-1.22261700	-0.63083600
H	-9.05890100	1.18793000	-0.16982100
H	-9.15491200	3.60067300	0.28859100
N	3.60931400	-3.32608400	3.40599800
H	3.49209600	-4.23875700	2.96501900

C	2.28367500	-2.73141000	3.53191200
H	2.34143600	-1.82659400	4.14452900
C	1.76174500	-2.37257900	2.12867500
C	1.27807200	-3.68688100	4.15608100
H	2.48637000	-1.68587000	1.67807800
H	1.76490000	-3.29210600	1.52825300
C	0.39253700	-1.77045400	2.14262400
O	1.15762000	-4.84130100	3.81665600
C	-0.80039900	-2.41531500	1.95243600
C	0.06944400	-0.39098700	2.39914300
H	-0.98783300	-3.45466800	1.71133700
N	-1.84441700	-1.52817400	2.08798500
C	-1.34010700	-0.27554300	2.35123300
C	0.84088900	0.76110800	2.61987900
H	-2.80572800	-1.72278700	1.84296200
C	-1.99546000	0.94701800	2.52712800
C	0.19812800	1.97664700	2.78167000
H	1.92601400	0.70009500	2.64335500
H	-3.07932500	1.02069900	2.46653200
C	-1.20823900	2.06557400	2.73972300
H	0.78068900	2.87996800	2.93454100
H	-1.68555600	3.03594100	2.84969200
H	3.99093900	-3.51201700	4.33178300
O	0.52352500	-3.12326500	5.10945400
H	-0.12411200	-3.79543300	5.38851300

Graphene-Tyr

C	-5.47562000	1.25073600	-0.03551000
C	-6.24404400	2.40070800	0.25737100
C	-4.03202800	1.34502900	-0.18653900
C	-8.29341100	1.05733900	0.24240600
C	-7.66997900	2.29634700	0.40060100
C	-5.61393900	3.68894400	0.41592700
C	-3.40025200	2.61840800	-0.04209800
C	-8.43332500	3.48168500	0.70506900
C	-6.39229200	4.79112600	0.70644300
C	-4.15354400	3.77852300	0.25497400
C	-1.97920900	2.71521800	-0.20460400
C	-7.80911400	4.68654200	0.85298400
H	-5.93650500	5.77876300	0.83113400
C	-3.49991400	5.00222300	0.39912500
C	-1.20267100	1.53746400	-0.48533600
C	-1.34403700	3.97145800	-0.07215700
H	-8.37426000	5.59118300	1.08383100
C	-2.12874100	5.08961000	0.24086600
H	-4.06113900	5.90054600	0.64005500
C	0.21302200	1.63197700	-0.61277800
C	0.10456400	4.07612900	-0.24548300
H	-1.66048400	6.05844100	0.37604500
C	0.86411200	2.90899600	-0.48030200

C	0.76317500	5.30986700	-0.17830400
C	2.29023100	2.99770800	-0.59148300
C	2.13778900	5.40098900	-0.29933900
H	0.20461500	6.22464900	-0.03437500
C	3.05192300	1.80874500	-0.78870000
C	2.92009400	4.26216100	-0.49267900
H	2.61231500	6.37813500	-0.23623200
C	4.50123300	1.90249400	-0.84733200
C	4.38631700	4.37139600	-0.58953500
C	5.14521300	3.15856600	-0.74910600
C	5.03525500	5.58762000	-0.51991300
C	6.57879000	3.23000100	-0.81061600
H	4.48277100	6.51662200	-0.40514000
C	6.45779600	5.65712700	-0.59587600
C	7.20943700	4.52549100	-0.73204200
C	7.33300400	2.06444600	-0.93954200
H	6.92824600	6.63823200	-0.53970100
C	7.61725600	-2.85056600	-1.32819900
C	7.46864700	-0.38999700	-1.13702400
C	6.99433300	-4.06280600	-1.40701100
C	6.84736300	-1.63468300	-1.22202600
C	6.71383100	0.79853000	-1.02495400
C	5.57137000	-4.15835200	-1.38623000
H	7.57010500	-4.98449400	-1.48727900
C	5.41365600	-1.72828900	-1.19979000
C	5.27314800	0.71590200	-0.98967100
C	4.79200800	-3.02391100	-1.28631000
H	5.12391500	-5.14710500	-1.45145300
C	4.63525800	-0.55153200	-1.09616800
C	3.32018600	-3.08764800	-1.26167500
C	3.18323800	-0.62470000	-1.08065100
C	2.66741300	-4.32112500	-1.29358500
C	2.55421600	-1.89966100	-1.17848200
C	2.42810200	0.55255200	-0.91858900
C	1.28661100	-4.39641500	-1.27626700
H	3.24983900	-5.23956800	-1.32439800
C	1.12499300	-1.98270300	-1.15244900
C	0.97735700	0.46658600	-0.85220400
C	0.49442300	-3.24250100	-1.23083700
H	0.82855900	-5.37640900	-1.27135400
C	0.33978200	-0.79110900	-0.97141100
C	-0.96455400	-3.32087800	-1.21447900
C	-1.07683300	-0.87995700	-0.86483000
C	-1.63641200	-4.53414400	-1.41794400
C	-1.72764500	-2.15572900	-0.98389800
C	-1.83820100	0.28170500	-0.61390500
C	-3.01362500	-4.63165900	-1.33547800
H	-1.07166500	-5.42830000	-1.65955000
C	-3.15360000	-2.25163100	-0.88445500
C	-3.28270200	0.18330500	-0.46731000

C	-3.78666200	-3.50546700	-1.05041900
H	-3.48489200	-5.59742900	-1.49385000
C	-3.91016500	-1.07482400	-0.61078300
C	-5.25009200	-3.61296000	-0.93414100
C	-5.35520300	-1.17389600	-0.48133300
C	-5.91613400	-4.81186200	-1.08881600
C	-6.00499800	-2.41884700	-0.64020400
C	-6.11590000	-0.00849300	-0.19106700
C	-7.33676400	-4.89863400	-0.96437800
H	-5.36489100	-5.73147100	-1.31110500
C	-7.43413500	-2.50656000	-0.51036100
C	-7.54401300	-0.10459800	-0.05427400
C	-8.07661300	-3.78691100	-0.68328100
H	-7.80960400	-5.87316800	-1.09800000
C	-8.17489400	-1.36094300	-0.21988100
H	8.29452500	4.56954900	-0.78638200
H	8.41698800	2.12219500	-0.97907900
H	8.55248400	-0.32254700	-1.16218900
H	8.70137200	-2.76909200	-1.34524600
H	-9.16160400	-3.83989100	-0.58355000
H	-9.26157500	-1.42757300	-0.11738800
H	-9.37890600	0.97840800	0.34841800
H	-9.51483900	3.38849300	0.81281600
N	5.64519000	-1.51509600	3.52319700
H	5.88837600	-2.38054700	3.04091500
C	4.19228100	-1.40287000	3.53649600
H	3.89915400	-0.55642600	4.16442500
C	3.55220300	-1.25267700	2.13717800
C	3.65290600	-2.67533400	4.15945500
H	3.93253700	-0.31975900	1.69611700
H	3.92665400	-2.07671000	1.51259500
C	2.04546700	-1.25050600	2.14686700
O	3.98628600	-3.78382500	3.81557300
C	1.32494500	-0.06825400	2.31701300
C	1.32911200	-2.44655300	2.02335000
H	1.85952400	0.87812900	2.39250200
C	-0.06716700	-0.06735000	2.34854100
C	-0.05995200	-2.46330700	2.04651800
H	1.87451200	-3.37731400	1.87115200
H	-0.61207100	0.86856800	2.45264600
C	-0.75934400	-1.26737900	2.20309600
H	-0.61782200	-3.38424700	1.91287300
H	6.03624000	-0.75132400	2.97311600
O	2.72300400	-2.45225100	5.09992900
H	2.39528500	-3.32498800	5.37891200
O	-2.12340300	-1.32692300	2.16142000
H	-2.47717000	-0.42647600	2.17956500

Graphene-Phe

C	-5.58339200	1.17131200	-0.09188800
C	-6.35096500	2.34949400	0.05067300
C	-4.13603100	1.24233300	-0.22001700
C	-8.40659500	1.02067100	0.15993000
C	-7.78046800	2.26751900	0.17538600
C	-5.71691600	3.64543000	0.07234400
C	-3.49879200	2.51856400	-0.18633000
C	-8.54369500	3.48386000	0.31474200
C	-6.49508500	4.77710000	0.20787600
C	-4.25141000	3.70894600	-0.04866000
C	-2.07131800	2.58822800	-0.29624400
C	-7.91611600	4.69568900	0.32883200
H	-6.03617700	5.77094400	0.22619200
C	-3.59433800	4.93869500	-0.03758900
C	-1.30051800	1.38851600	-0.47606800
C	-1.42742200	3.84517100	-0.23895800
H	-8.48101200	5.62364300	0.43268300
C	-2.21566100	4.99869800	-0.13462400
H	-4.15788200	5.86376800	0.04531100
C	0.11511900	1.46523400	-0.61171500
C	0.03188700	3.91694400	-0.29935600
H	-1.74568300	5.97628200	-0.13888800
C	0.77936700	2.73821300	-0.51137500
C	0.71095600	5.13127900	-0.14099800
C	2.20794300	2.80792900	-0.60434500
C	2.08864500	5.20300500	-0.23365400
H	0.16638300	6.04160200	0.06965400
C	2.95517800	1.61254100	-0.81880700
C	2.85400400	4.06151200	-0.47559500
H	2.57927700	6.16652000	-0.11137500
C	4.40321700	1.69467100	-0.91351500
C	4.32036700	4.15631600	-0.58367200
C	5.06217600	2.94182300	-0.79999100
C	4.98441200	5.36233500	-0.48325500
C	6.49401100	3.00248800	-0.90208000
H	4.44485700	6.29210400	-0.32228700
C	6.40526900	5.42030500	-0.59055300
C	7.14060300	4.28757600	-0.79171600
C	7.23189900	1.83591500	-1.09843600
H	6.88793800	6.39356400	-0.50723400
C	7.45806200	-3.06635300	-1.64608200
C	7.33770200	-0.61070900	-1.38376100
C	6.82423000	-4.27412600	-1.70648500
C	6.70408100	-1.84973100	-1.46385300
C	6.59833000	0.57854700	-1.20171700
C	5.40607500	-4.36427700	-1.58487800
H	7.38785500	-5.19622800	-1.84600500
C	5.27394000	-1.93619700	-1.35671700
C	5.15982200	0.50524300	-1.10673700

C	4.64199800	-3.22833700	-1.41012700
H	4.94990300	-5.35002500	-1.63176700
C	4.50869300	-0.75653600	-1.19987700
C	3.17710100	-3.28750500	-1.26437600
C	3.05899900	-0.82202300	-1.10685700
C	2.52296400	-4.51975900	-1.22629200
C	2.42149100	-2.09707600	-1.13959700
C	2.31802300	0.36065400	-0.92715900
C	1.14965300	-4.59254000	-1.08857100
H	3.09898600	-5.44001900	-1.29802200
C	0.99700500	-2.17630000	-1.00843600
C	0.86965100	0.28435500	-0.80630500
C	0.36320500	-3.43700900	-0.99320100
H	0.69527300	-5.57296400	-1.04555500
C	0.22346000	-0.97289900	-0.84848700
C	-1.09175500	-3.51230300	-0.86345600
C	-1.19076600	-1.04877500	-0.69604100
C	-1.76865800	-4.73842400	-0.89656300
C	-1.84674900	-2.32728100	-0.70693200
C	-1.94443700	0.13221100	-0.52061000
C	-3.14233800	-4.82331100	-0.75692100
H	-1.21414500	-5.65890700	-1.04246200
C	-3.27083100	-2.40862400	-0.56051400
C	-3.38928400	0.05467500	-0.37514400
C	-3.90878200	-3.67161900	-0.58320200
H	-3.61612500	-5.80046000	-0.78911100
C	-4.02246900	-1.20629600	-0.39962200
C	-5.37025000	-3.76317800	-0.43295800
C	-5.46842200	-1.28806700	-0.26133500
C	-6.03765200	-4.97108400	-0.43774300
C	-6.12172100	-2.54112900	-0.27760100
C	-6.22753000	-0.09559300	-0.11176300
C	-7.45753000	-5.04015600	-0.29594600
H	-5.48875600	-5.91143400	-0.55201300
C	-7.55071900	-2.61037000	-0.13901900
C	-7.65733000	-0.17114900	0.01932200
C	-8.19523700	-3.90106600	-0.15221200
H	-7.93178900	-6.02299300	-0.30655800
C	-8.29063300	-1.43626000	0.00461500
H	8.22421500	4.32312400	-0.87424800
H	8.31413600	1.88636100	-1.17711500
H	8.41902500	-0.54884400	-1.46669000
H	8.53905200	-2.98938900	-1.73461100
H	-9.28004600	-3.93959000	-0.04462200
H	-9.37793000	-1.48814000	0.10767400
H	-9.49384400	0.95739800	0.25706800
H	-9.62789300	3.40758400	0.40736000
N	6.05590500	-1.05802700	3.26795800
H	6.17766400	-1.98808400	2.86711200
C	4.62657700	-0.82116400	3.41938600

H	4.46783000	0.10919700	3.97276300
C	3.84745100	-0.76794100	2.08480600
C	4.06404200	-1.96956500	4.23306800
H	4.24768800	0.07321000	1.49766400
H	4.08000700	-1.68705900	1.52893500
C	2.35796900	-0.62327400	2.24873700
O	4.28878500	-3.13236200	3.99797600
C	1.77686700	0.63489700	2.43134200
C	1.53270500	-1.75137700	2.24671400
H	2.40906300	1.52177700	2.41245100
C	0.40121200	0.76441400	2.59438400
C	0.15623300	-1.62580800	2.41647800
H	1.97824900	-2.73302100	2.09113600
H	-0.03786800	1.75160900	2.70728100
C	-0.41391200	-0.36644800	2.58466600
H	-0.47287700	-2.51067400	2.39022200
H	-1.48883500	-0.26395500	2.69487900
H	6.43553700	-0.39475900	2.59328600
O	3.24059500	-1.56890200	5.21331800
H	2.88031500	-2.37584900	5.62027000

Graphene-His

C	5.43322300	-1.14258400	-0.27802400
C	6.15537800	-2.35726300	-0.28851600
C	3.98238800	-1.14417600	-0.38455400
C	8.26426700	-1.12918000	-0.07102500
C	7.58928700	-2.34419100	-0.18631900
C	5.47014100	-3.62233400	-0.40011500
C	3.29419500	-2.38927700	-0.48561600
C	8.30547200	-3.59677500	-0.20420900
C	6.20451500	-4.79059000	-0.41186600
C	4.00141800	-3.61608700	-0.49318100
C	1.86346200	-2.39262800	-0.57333200
C	7.62987700	-4.77717900	-0.31450500
H	5.70656100	-5.76186000	-0.49556600
C	3.29365900	-4.81235400	-0.58987800
C	1.13854800	-1.15133600	-0.58769700
C	1.16939800	-3.62125700	-0.63866400
H	8.15856200	-5.73177100	-0.32959600
C	1.91167400	-4.80844500	-0.65930600
H	3.81938900	-5.76284200	-0.60655700
C	-0.28460600	-1.16071700	-0.66740500
C	-0.29151600	-3.63053000	-0.68305100
H	1.40394300	-5.76324600	-0.73533500
C	-0.99593300	-2.40788300	-0.71958500
C	-1.01503600	-4.82762000	-0.68039200
C	-2.42711000	-2.41318000	-0.76799300
C	-2.39674800	-4.83676400	-0.72968100
H	-0.50393500	-5.77866000	-0.61987100
C	-3.13095800	-1.17399600	-0.79622000

C	-3.12166600	-3.64631600	-0.78134600
H	-2.92153100	-5.78973400	-0.72419400
C	-4.58390200	-1.18780900	-0.86872700
C	-4.59331200	-3.67195200	-0.84172000
C	-5.29057200	-2.41186700	-0.88943300
C	-5.30487100	-4.85379900	-0.85730600
C	-6.72545000	-2.40657700	-0.96100000
H	-4.80031600	-5.81650000	-0.81990300
C	-6.73014300	-4.84528400	-0.92329800
C	-7.42246800	-3.67002400	-0.97489400
C	-7.41827300	-1.19763500	-1.01490400
H	-7.24995600	-5.80286200	-0.93189900
C	-7.45152900	3.73984600	-1.09024000
C	-7.42751300	1.26812400	-1.05352100
C	-6.77019900	4.92131400	-1.05720000
C	-6.74524800	2.48169200	-1.02852800
C	-6.73452100	0.03699200	-0.99741500
C	-5.34617300	4.94342900	-0.95641400
H	-7.29646200	5.87421200	-1.10471900
C	-5.31094900	2.50106100	-0.93509100
C	-5.29453700	0.04426100	-0.91619100
C	-4.62663700	3.76871900	-0.89407100
H	-4.85126300	5.91138500	-0.92879600
C	-4.59528000	1.28318700	-0.88941700
C	-3.15785400	3.75790800	-0.77715800
C	-3.14363800	1.28220200	-0.79182200
C	-2.44582400	4.95494600	-0.70706400
C	-2.45413700	2.52890200	-0.73387400
C	-2.44739400	0.05603200	-0.75669600
C	-1.06768600	4.95911300	-0.58731300
H	-2.97763100	5.90306700	-0.74636000
C	-1.02506900	2.53740600	-0.61417700
C	-0.99521900	0.06372700	-0.67472900
C	-0.33506400	3.76772000	-0.52981100
H	-0.56554200	5.91597100	-0.54389700
C	-0.30041500	1.29390000	-0.59350000
C	1.12085900	3.76920500	-0.38493700
C	1.12148300	1.29873600	-0.48987100
C	1.84271900	4.96134600	-0.24420100
C	1.82909700	2.54516900	-0.38248400
C	1.83117900	0.07520700	-0.49396400
C	3.22065300	4.97529700	-0.12406900
H	1.32019500	5.91098000	-0.22177600
C	3.25827300	2.55294900	-0.26140300
C	3.28132800	0.08183700	-0.38046000
C	3.94528100	3.78402300	-0.13733700
H	3.73057700	5.92860000	-0.01872900
C	3.96355700	1.31217000	-0.26942100
C	5.41187600	3.80202900	-0.01680700
C	5.41345300	1.32251200	-0.15206900

C	6.12690900	4.97621600	0.10529500
C	6.11618200	2.54287600	-0.03076300
C	6.12690000	0.09296100	-0.16268700
C	7.55067100	4.97423700	0.21862300
H	5.61422500	5.94328500	0.11756100
C	7.54875000	2.54139500	0.08129600
C	7.56056400	0.09872900	-0.05459700
C	8.24432800	3.79879000	0.20708500
H	8.06418200	5.93245900	0.31332500
C	8.24366100	1.33112000	0.06625500
H	-8.50864200	-3.65414200	-1.02620000
H	-8.50361800	-1.19712600	-1.07069400
H	-8.51238200	1.25598700	-1.11875000
H	-8.53640900	3.71296600	-1.16374200
H	9.33171500	3.78319300	0.29199400
H	9.33379900	1.32955800	0.14917900
H	9.35450000	-1.11822800	0.00857000
H	9.39312700	-3.57254300	-0.12754400
N	-4.33028600	1.66372000	2.45124100
H	-5.33019300	1.48266000	2.52025100
C	-3.61005300	0.40899100	2.63611900
H	-3.76000900	-0.32412400	1.81859700
C	-2.11414800	0.71996000	2.73712000
C	-4.21236400	-0.23439700	3.87668300
H	-1.89567000	1.43088900	1.92655300
H	-1.94056200	1.25859800	3.67657500
C	-1.18671700	-0.44740000	2.61283000
O	-5.38020400	-0.16249200	4.16797200
N	0.17781100	-0.25124200	2.55994500
C	-1.33521100	-1.80789400	2.52741900
H	0.64566000	0.64360100	2.55304700
C	0.76908700	-1.47396600	2.45168400
N	-0.11486600	-2.43848000	2.42770000
H	-2.25870100	-2.37229200	2.54399800
H	1.84185500	-1.59146200	2.38157500
H	-4.14331100	2.02453500	1.51760000
O	-3.32773700	-0.91821900	4.62229800
H	-3.83386600	-1.30665400	5.35687600

Graphene-G

C	4.94019700	-1.08817100	-0.55098500
C	5.66274400	-2.30487500	-0.62314600
C	3.48784300	-1.09067300	-0.59269800
C	7.77631200	-1.06820500	-0.45368600
C	7.09876500	-2.28013000	-0.58018200
C	4.98315300	-3.56607000	-0.74299400
C	2.80089900	-2.33709400	-0.68251600
C	7.81104900	-3.53181400	-0.66948900
C	5.70853600	-4.73868200	-0.82610700
C	3.50890100	-3.55934200	-0.75900500

C	1.36813200	-2.35179200	-0.67617600
C	7.13299500	-4.71114900	-0.79118500
H	5.21637600	-5.70146400	-0.92489700
C	2.79695300	-4.75734600	-0.85597800
C	0.63706700	-1.11239900	-0.62304000
C	0.67890300	-3.58246900	-0.70792000
H	7.66719100	-5.65765900	-0.86381500
C	1.41494800	-4.76873000	-0.83317400
H	3.33552200	-5.69908200	-0.95003900
C	-0.78508500	-1.12254800	-0.59209900
C	-0.77917100	-3.59247100	-0.58992200
H	0.90937700	-5.72131400	-0.92797600
C	-1.49238800	-2.37435100	-0.55563200
C	-1.49685100	-4.79418000	-0.47794600
C	-2.92120800	-2.39231300	-0.45103600
C	-2.87455500	-4.81718500	-0.38006100
H	-0.96562600	-5.73942100	-0.45834900
C	-3.62941500	-1.15174300	-0.41233200
C	-3.60382200	-3.62529800	-0.37429300
H	-3.38260500	-5.77398600	-0.29974100
C	-5.08064900	-1.17034600	-0.33251400
C	-5.07195900	-3.65213100	-0.27354400
C	-5.78136100	-2.39622900	-0.25900900
C	-5.78513000	-4.83123700	-0.19379200
C	-7.21592100	-2.40275400	-0.17127500
H	-5.26810300	-5.79674000	-0.20064300
C	-7.21033300	-4.83814800	-0.10027400
C	-7.90852500	-3.66520900	-0.08960300
C	-7.91478500	-1.19445400	-0.16539500
H	-7.72110700	-5.80044400	-0.03769300
C	-7.98772500	3.73880000	-0.33164000
C	-7.94122800	1.26875000	-0.24677800
C	-7.31354100	4.92355300	-0.40061900
C	-7.26788300	2.48875100	-0.32175000
C	-7.23447600	0.04308600	-0.24442600
C	-5.88634000	4.94208700	-0.45857100
H	-7.84490100	5.87674000	-0.40956700
C	-5.83200600	2.50788500	-0.38669700
C	-5.79818200	0.05586600	-0.32089600
C	-5.14777900	3.77609300	-0.45171800
H	-5.38845000	5.91664500	-0.50642900
C	-5.10589400	1.29469200	-0.38741100
C	-3.67636200	3.77635300	-0.49363800
C	-3.65327200	1.30210800	-0.44334000
C	-2.97123500	4.97991000	-0.54855400
C	-2.96737100	2.55476500	-0.48346500
C	-2.94996200	0.08160000	-0.46652700
C	-1.58936400	4.98128100	-0.54965400
H	-3.50058800	5.92760800	-0.58549900
C	-1.53559800	2.56317900	-0.50015300

C	-1.49746700	0.09555100	-0.53777500
C	-0.84618600	3.79363500	-0.49316000
H	-1.07861800	5.93611000	-0.60438600
C	-0.80590300	1.32440400	-0.53925500
C	0.61442200	3.80892800	-0.41965300
C	0.61631000	1.33861400	-0.54785500
C	1.32847300	5.00488600	-0.26142100
C	1.32613400	2.59115300	-0.46926000
C	1.33283500	0.11974600	-0.58347600
C	2.70942000	5.01460800	-0.18925800
H	0.80560900	5.94845900	-0.17354400
C	2.75746000	2.59726400	-0.39340700
C	2.78742700	0.12890200	-0.54166900
C	3.44325900	3.82818600	-0.25987400
H	3.22872800	5.96369300	-0.06816200
C	3.46692900	1.35817800	-0.43247800
C	4.91502000	3.85374900	-0.17820900
C	4.91784600	1.37485000	-0.36822500
C	5.61774200	5.03541400	-0.04704400
C	5.61687400	2.60018800	-0.23891500
C	5.63446600	0.14755200	-0.43157500
C	7.04114600	5.02565200	0.02546300
H	5.10860200	5.99355700	-0.00172000
C	7.05241200	2.59340500	-0.17269700
C	7.07847600	0.15646100	-0.37489500
C	7.74052200	3.85414100	-0.03454700
H	7.55686900	5.97964700	0.12843500
C	7.75249100	1.38979600	-0.24119500
H	-8.99720000	-3.65609200	-0.01872500
H	-9.00668200	-1.19887900	-0.09856400
H	-9.03352900	1.25375100	-0.18889900
H	-9.07720800	3.71038800	-0.28230400
H	8.82597200	3.83963300	0.01752000
H	8.83688300	1.39117100	-0.19455400
H	8.86099900	-1.05584600	-0.41726900
H	8.89707200	-3.50372500	-0.64032600
C	1.23672500	0.05617400	2.55954900
C	1.32439100	-2.15066300	2.44890500
C	-0.92184100	-1.06150800	2.50332000
C	-0.14948700	0.15117800	2.58746700
N	-0.04858900	-2.18704800	2.45121100
N	2.02069100	-1.04992600	2.51496300
N	-0.55381100	1.46924500	2.62273100
N	1.67959700	1.34448500	2.58379600
C	0.56039900	2.14761400	2.61339600
H	0.64279800	3.22647100	2.61910300
H	2.64397700	1.63252300	2.47395700
O	-2.12375000	-1.23413900	2.43935400
H	-0.52394300	-3.06302800	2.26190700
N	1.96398700	-3.35093000	2.30966700

H	2.97132500	-3.28622800	2.38415200
H	1.54820800	-4.17383500	2.72012400

Graphene-A

C	4.95668200	-1.19544900	-0.51713700
C	5.66746100	-2.41526500	-0.57696400
C	3.50123900	-1.18630600	-0.52629800
C	7.79487800	-1.19673800	-0.50714800
C	7.10391800	-2.40565100	-0.57948000
C	4.97184800	-3.67684400	-0.63215300
C	2.80178400	-2.42481900	-0.56305700
C	7.80530200	-3.66494100	-0.65648400
C	5.68805300	-4.85359000	-0.70419200
C	3.49951200	-3.65763700	-0.60388600
C	1.36920900	-2.42554100	-0.53805800
C	7.11546700	-4.84086700	-0.71833300
H	5.18531000	-5.81767700	-0.74982200
C	2.77773500	-4.84985600	-0.61600700
C	0.65241400	-1.18202500	-0.51284400
C	0.66686400	-3.65254300	-0.52091500
H	7.63745100	-5.79543300	-0.77771500
C	1.39369100	-4.84598700	-0.57551700
H	3.30336300	-5.80143800	-0.65514200
C	-0.77385800	-1.17801000	-0.48618400
C	-0.79276900	-3.64801600	-0.43943300
H	0.88354800	-5.79957000	-0.59123800
C	-1.49336400	-2.41847400	-0.44176500
C	-1.52583300	-4.83512800	-0.34247100
C	-2.92587000	-2.41819700	-0.37868600
C	-2.90974500	-4.84220600	-0.28076300
H	-1.01105800	-5.78856600	-0.30296600
C	-3.62256900	-1.17475600	-0.38669400
C	-3.62698200	-3.64882800	-0.30657200
H	-3.42905700	-5.79399400	-0.20839400
C	-5.07751600	-1.17671900	-0.33667000
C	-5.09784900	-3.65879700	-0.25184500
C	-5.79240800	-2.39295600	-0.27540200
C	-5.82451400	-4.82910800	-0.18432500
C	-7.22896400	-2.38201200	-0.23346400
H	-5.32096600	-5.79961500	-0.16444400
C	-7.25277900	-4.81710000	-0.13896100
C	-7.93753200	-3.63733500	-0.16378600
C	-7.91424300	-1.16747500	-0.26103200
H	-7.77596800	-5.77288400	-0.08513300
C	-7.92647900	3.76613700	-0.44122900
C	-7.91056700	1.29595300	-0.35302100
C	-7.23799800	4.94303700	-0.48950200
C	-7.22151600	2.50722500	-0.40698100
C	-7.21759800	0.06242600	-0.32291800
C	-5.80902200	4.94819100	-0.50335000

H	-7.75857000	5.90132900	-0.51673400
C	-5.78436900	2.51157800	-0.42774800
C	-5.78086900	0.05921000	-0.35550400
C	-5.08548200	3.77422400	-0.47241100
H	-5.30206000	5.91666900	-0.53800400
C	-5.07309500	1.29207900	-0.40416500
C	-3.61366800	3.75770900	-0.47570400
C	-3.61757000	1.28428000	-0.42723500
C	-2.89362000	4.95029400	-0.51435000
C	-2.91716000	2.52457200	-0.44979800
C	-2.92572100	0.05290100	-0.42459200
C	-1.50941800	4.93642300	-0.49476600
H	-3.41171800	5.90423600	-0.56066900
C	-1.48412700	2.51664900	-0.44179900
C	-1.47332600	0.04954000	-0.46292900
C	-0.78072600	3.74319300	-0.42933300
H	-0.98803700	5.88619800	-0.54419200
C	-0.76816800	1.27386500	-0.46534500
C	0.67894000	3.74144000	-0.35548600
C	0.65668900	1.27226200	-0.47574300
C	1.40504000	4.92772100	-0.19841600
C	1.37782900	2.51433000	-0.41473200
C	1.35984500	0.04378500	-0.50194700
C	2.78904900	4.92684900	-0.15552300
H	0.89262400	5.87477500	-0.09419000
C	2.81111900	2.50835900	-0.36714400
C	2.81346800	0.04010100	-0.48571100
C	3.51015800	3.73747600	-0.25168900
H	3.31574100	5.87185200	-0.04093700
C	3.50667200	1.26736300	-0.41176800
C	4.98236100	3.75175000	-0.21787900
C	4.96062800	1.27223400	-0.38184000
C	5.70117400	4.92535300	-0.12561000
C	5.67351900	2.48856800	-0.28950000
C	5.66508100	0.03673600	-0.44504900
C	7.12860500	4.90757300	-0.10165700
H	5.20173100	5.89043000	-0.07368000
C	7.11067600	2.47358800	-0.26919900
C	7.10571900	0.03417900	-0.43214100
C	7.81497100	3.73044900	-0.17116700
H	7.65309600	5.85979000	-0.02828400
C	7.79792100	1.26423800	-0.34316500
H	-9.02698000	-3.61458000	-0.13133100
H	-9.00605000	-1.15865400	-0.23383800
H	-9.00265700	1.29181800	-0.33321200
H	-9.01657900	3.74842300	-0.42754600
H	8.90244300	3.70696400	-0.15575000
H	8.88500700	1.25538600	-0.33208400
H	8.88208800	-1.19241300	-0.50557200
H	8.89294400	-3.64533600	-0.66289800

C	1.39933900	-0.06756000	2.65117200
C	1.23209800	-2.25899400	2.57567000
C	-0.74241800	-1.08500300	2.67058200
C	0.01612300	0.10075100	2.69849800
H	1.69526200	-3.24259900	2.50880900
N	-0.11218600	-2.26160600	2.60414700
N	2.06469600	-1.22594000	2.59663600
N	-2.09938400	-1.06499500	2.71302400
H	-2.57254000	-1.91743400	2.44949900
H	-2.56043200	-0.18872100	2.51529100
N	-0.33139900	1.43879300	2.71775300
N	1.90038700	1.20887400	2.64458400
C	0.81911100	2.05679500	2.67513100
H	0.95033000	3.13135900	2.65320300
H	2.87205900	1.45989000	2.51506300

Graphene-T

C	-4.85860900	1.58024500	-0.30066700
C	-5.54385600	2.80679900	-0.13404300
C	-3.40597000	1.54471200	-0.33097200
C	-7.69501900	1.63165000	-0.24533000
C	-6.98080700	2.81991600	-0.10673200
C	-4.82606600	4.04658800	0.00623200
C	-2.68204400	2.76593700	-0.20324900
C	-7.65562500	4.08406200	0.06763000
C	-5.51637900	5.23042400	0.17042000
C	-3.35353700	4.00171500	-0.03298700
C	-1.24899900	2.74255900	-0.24201000
C	-6.94243100	5.24033500	0.20075400
H	-4.99568600	6.17806000	0.27711900
C	-2.60589200	5.17071400	0.10864100
C	-0.55603200	1.48766600	-0.37957100
C	-0.52230100	3.94889400	-0.13002800
H	-7.44664200	6.19704500	0.33209300
C	-1.22289400	5.14462400	0.06630900
H	-3.11377900	6.12141500	0.25861700
C	0.86872100	1.45392700	-0.35721700
C	0.93878700	3.92011100	-0.20414200
H	-0.69096600	6.07667400	0.20301800
C	1.61412300	2.68209600	-0.27390000
C	1.69699100	5.09938200	-0.21113600
C	3.04658600	2.65465700	-0.27610100
C	3.07931600	5.08029200	-0.22653100
H	1.19752900	6.06190700	-0.21407100
C	3.71656000	1.39282600	-0.30481200
C	3.77076700	3.86802600	-0.24204000
H	3.62032600	6.02214000	-0.22489900
C	5.16950900	1.36583800	-0.26344700
C	5.24240500	3.84786500	-0.22712400
C	5.91078300	2.56943000	-0.22573200

C	5.99575300	5.00428700	-0.20526000
C	7.34653000	2.52984500	-0.18582700
H	5.51049400	5.98598400	-0.20896200
C	7.42301600	4.96516500	-0.17500600
C	8.08244200	3.76991500	-0.16245800
C	8.00523300	1.29882800	-0.16833900
H	7.96723100	5.91099700	-0.15994200
C	7.91109700	-3.63679600	-0.17602200
C	7.94842900	-1.16540100	-0.17251900
C	7.19746000	-4.79943800	-0.21459900
C	7.23417000	-2.36307600	-0.20869700
C	7.28298700	0.08361400	-0.19849100
C	5.77118600	-4.77200400	-0.29167900
H	7.69610800	-5.76989100	-0.18807000
C	5.79837900	-2.33609500	-0.27912900
C	5.84629900	0.11665000	-0.25471500
C	5.07273500	-3.58204700	-0.32695500
H	5.24183700	-5.73030700	-0.32286000
C	5.11301000	-1.09998500	-0.30196700
C	3.60451500	-3.53373300	-0.41652400
C	3.66116200	-1.06143100	-0.36984100
C	2.85904600	-4.71359800	-0.45946700
C	2.93684400	-2.28902600	-0.44880900
C	2.99769200	0.18286200	-0.36990800
C	1.48071000	-4.66984600	-0.55379600
H	3.35394700	-5.67938700	-0.41178000
C	1.50847300	-2.25006900	-0.55204100
C	1.54514500	0.21654600	-0.43007100
C	0.77914500	-3.45678800	-0.62429900
H	0.93751700	-5.60805800	-0.56160800
C	0.81732100	-0.98818100	-0.53971900
C	-0.67890400	-3.42412200	-0.73624900
C	-0.60566200	-0.95718700	-0.58404300
C	-1.43098900	-4.59552700	-0.87143800
C	-1.35184500	-2.18311900	-0.68280000
C	-1.28616200	0.28182100	-0.49675100
C	-2.81244800	-4.56436600	-0.91011800
H	-0.94261100	-5.55771000	-0.94461800
C	-2.78360100	-2.14708400	-0.71754000
C	-2.74139600	0.31142300	-0.48719600
C	-3.50790700	-3.35813100	-0.82718600
H	-3.36113300	-5.49934000	-1.00147500
C	-3.45605900	-0.89443100	-0.60896000
C	-4.98156000	-3.34361100	-0.84974600
C	-4.91006300	-0.87314100	-0.59065800
C	-5.72166900	-4.50033000	-0.98648900
C	-5.64732900	-2.07432800	-0.71421800
C	-5.58994700	0.36692400	-0.43506200
C	-7.14705800	-4.45399000	-0.99013900
H	-5.24027800	-5.46940500	-1.09046600

C	-7.08332700	-2.03187400	-0.70553600
C	-7.03326000	0.39463800	-0.41250500
C	-7.81129900	-3.26907200	-0.85265200
H	-7.69114500	-5.39108500	-1.10336300
C	-7.74697200	-0.81492700	-0.55442400
H	9.17216800	3.72604300	-0.13510600
H	9.09792200	1.26853300	-0.13073000
H	9.04083800	-1.18510500	-0.12229300
H	9.00048600	-3.64354300	-0.11886500
H	-8.89748900	-3.22575000	-0.85122000
H	-8.83253700	-0.78774900	-0.54591700
H	-8.78070600	1.64630600	-0.22753900
H	-8.74255900	4.08339400	0.08785900
C	-1.53641000	-0.32616000	2.57633800
C	0.72012200	-1.23324000	2.48659900
C	-1.29322600	-2.72614700	2.48035000
C	-2.13965700	-1.52967500	2.56724200
N	0.08634900	-2.45989900	2.46224300
N	-0.16329700	-0.17634200	2.55144600
O	-1.69560000	-3.87000400	2.41892400
H	0.69687800	-3.26474700	2.37851200
C	-3.62196900	-1.72877800	2.62688900
H	-3.94548100	-2.43178600	1.85181500
H	-3.92615800	-2.15088400	3.59036700
H	-4.15021200	-0.78132300	2.47587600
O	1.92773300	-1.09686800	2.44142400
H	0.25679300	0.74140500	2.49828200
H	-2.10072700	0.60250800	2.59289100

Graphene-C

C	-5.13086700	-1.14026900	-0.28892200
C	-5.82861300	-2.37141100	-0.29313700
C	-3.67935000	-1.11388300	-0.35603400
C	-7.96614700	-1.17345400	-0.16273900
C	-7.26453300	-2.37559500	-0.23079400
C	-5.12431700	-3.62431600	-0.36249600
C	-2.96790000	-2.34725300	-0.42943700
C	-7.95138500	-3.64485100	-0.24062400
C	-5.82558900	-4.81328100	-0.37033700
C	-3.65245200	-3.58698200	-0.42302600
C	-1.53493600	-2.33213400	-0.49673900
C	-7.25025200	-4.81431500	-0.30896500
H	-5.31484400	-5.77040800	-0.42618300
C	-2.91704400	-4.77215500	-0.46166300
C	-0.82865500	-1.07684400	-0.49119900
C	-0.81966900	-3.55014200	-0.54657900
H	-7.76402300	-5.77492100	-0.31874300
C	-1.53492500	-4.75497400	-0.51405800
H	-3.43555600	-5.72907700	-0.44515500
C	0.59443500	-1.05984500	-0.50812300

C	0.64195600	-3.52779700	-0.60194700
H	-1.01421000	-5.70294100	-0.52798000
C	1.32787300	-2.29815400	-0.56515100
C	1.38984100	-4.71312800	-0.66687300
C	2.76020000	-2.28777900	-0.54921500
C	2.76831000	-4.71013400	-0.65934400
H	0.88356800	-5.66983100	-0.72186400
C	3.44472600	-1.03792200	-0.47622300
C	3.47011800	-3.50641700	-0.58070100
H	3.29859900	-5.65671100	-0.69517500
C	4.89694800	-1.02636900	-0.45553000
C	4.94068200	-3.50542900	-0.54212100
C	5.62479400	-2.23872600	-0.48234700
C	5.67887600	-4.67274100	-0.54324800
C	7.06337900	-2.21902000	-0.44833700
H	5.17841900	-5.64762100	-0.56845200
C	7.10698300	-4.65490500	-0.50770300
C	7.78280600	-3.47025600	-0.46403300
C	7.73708400	-1.00094000	-0.39257200
H	7.63727700	-5.60902500	-0.51233400
C	7.70775400	3.93163800	-0.21181800
C	7.71136500	1.46104500	-0.30716500
C	7.00971300	5.10521200	-0.17181600
C	7.01177100	2.67145600	-0.26930800
C	7.02921600	0.22698500	-0.36516600
C	5.58292300	5.09811000	-0.18325300
H	7.52411300	6.06686100	-0.12969700
C	5.57645600	2.66421000	-0.28604300
C	5.59068300	0.21290100	-0.39110300
C	4.86705800	3.91808300	-0.23538600
H	5.06534500	6.06265400	-0.14869800
C	4.87325100	1.43702800	-0.34921000
C	3.39560900	3.89087600	-0.24052200
C	3.42013400	1.41655100	-0.37100200
C	2.66658000	5.07932600	-0.16797300
C	2.70920000	2.65746300	-0.30818500
C	2.73932200	0.18562100	-0.43924600
C	1.28511900	5.05597300	-0.16475300
H	3.17808100	6.03580700	-0.11070900
C	1.27512700	2.63974200	-0.31135400
C	1.28362700	0.17108500	-0.45383500
C	0.56121600	3.85665100	-0.23494000
H	0.76003100	6.00211800	-0.10149400
C	0.56868500	1.38664600	-0.37499700
C	-0.90231300	3.84436800	-0.22469200
C	-0.85595100	1.37336900	-0.35904600
C	-1.64467600	5.02972300	-0.16144400
C	-1.58865800	2.61033400	-0.27178700
C	-1.54807300	0.14024700	-0.40723700
C	-3.02737700	5.01352600	-0.13221600

H	-1.14798200	5.99016900	-0.13508500
C	-3.02141000	2.58972600	-0.23609600
C	-3.00257400	0.12220200	-0.34669000
C	-3.73394100	3.81138800	-0.16300800
H	-3.56818000	5.95653000	-0.08133900
C	-3.70536200	1.33942700	-0.26593600
C	-5.20693500	3.81204200	-0.11568000
C	-5.15833700	1.32895200	-0.20586100
C	-5.93459600	4.98316700	-0.05079700
C	-5.88337600	2.54224800	-0.13305700
C	-5.84976800	0.08599700	-0.21671500
C	-7.35942000	4.94932800	0.00212500
H	-5.44481200	5.95299600	-0.03874900
C	-7.31871500	2.51070100	-0.07619900
C	-7.29251200	0.06756200	-0.15453800
C	-8.03405600	3.76254700	-0.00837600
H	-7.89431700	5.89699500	0.05182500
C	-7.99364800	1.29136600	-0.08619500
H	8.87315800	-3.44178800	-0.43604700
H	8.83080300	-0.98368400	-0.36652700
H	8.80526300	1.46748300	-0.29040300
H	8.79874600	3.92310600	-0.20128000
H	-9.11984800	3.72796400	0.03279500
H	-9.07842300	1.27194000	-0.04221500
H	-9.05087500	-1.18110200	-0.11665800
H	-9.03731000	-3.63747600	-0.19391400
H	-0.38596300	-3.30817400	2.38556300
N	0.04218600	-2.39993600	2.51705500
C	1.45760000	-2.39536300	2.49412800
C	-0.70884500	-1.27691700	2.61272500
N	2.06587700	-1.16896100	2.57909700
O	2.03955300	-3.45751600	2.36932500
C	-0.10432000	-0.06954500	2.71746000
H	-1.78790300	-1.40488500	2.57625900
C	1.33232900	-0.08159700	2.68063000
H	-0.67360400	0.84959100	2.77969300
N	1.99233300	1.10666700	2.75855400
H	2.97344800	1.07417500	2.51742000
H	1.49829900	1.95511400	2.52235000

Graphene-U

C	-4.87344000	1.43802300	-0.39902600
C	-5.57636600	2.66547500	-0.38807800
C	-3.41981600	1.41954700	-0.40348700
C	-7.71219700	1.46451500	-0.37800200
C	-7.01343500	2.67303200	-0.38413200
C	-4.86636200	3.92058300	-0.38102900
C	-2.70946400	2.65802300	-0.37549400
C	-7.70881500	3.93644100	-0.38264300
C	-5.58214200	5.10123000	-0.37851700

C	-3.39493800	3.89263000	-0.36551800
C	-1.27773800	2.63892200	-0.34529300
C	-7.01015000	5.10930100	-0.38162800
H	-5.06439700	6.06649200	-0.37200700
C	-2.66554500	5.08293000	-0.34534100
C	-0.57099900	1.38664000	-0.39093100
C	-0.56447300	3.85427800	-0.28210000
H	-7.52319500	6.07262100	-0.38058200
C	-1.28501800	5.05718900	-0.30517100
H	-3.17570400	6.04169000	-0.35595900
C	0.85217800	1.37273900	-0.35731300
C	0.89574300	3.84007900	-0.19105200
H	-0.75663700	6.00368800	-0.29675100
C	1.58453700	2.60760500	-0.24067600
C	1.63416500	5.01989300	-0.03945200
C	3.01610900	2.58494700	-0.16536200
C	3.01530100	5.00186200	0.03558000
H	1.13351200	5.97592200	0.03576900
C	3.70168700	1.33606000	-0.22093500
C	3.72539100	3.80284000	-0.03008900
H	3.55198200	5.94141000	0.15230200
C	5.15367700	1.32446600	-0.14871400
C	5.19691700	3.80137700	0.05144800
C	5.87569000	2.53401800	-0.01386400
C	5.92182200	4.96818300	0.18660800
C	7.31051500	2.50118100	0.05749800
H	5.43055100	5.93592700	0.23747900
C	7.34555000	4.93247100	0.26128500
C	8.02255600	3.74852700	0.19963400
C	7.98764000	1.28480900	-0.01039500
H	7.87809200	5.87679100	0.36817800
C	7.95669600	-3.63512200	-0.44679600
C	7.96567200	-1.17224600	-0.22555600
C	7.25811400	-4.80079300	-0.57733800
C	7.26666200	-2.37047300	-0.36005500
C	7.28958400	0.06516200	-0.14881300
C	5.83283900	-4.80055900	-0.62640400
H	7.77420200	-5.75772300	-0.64622500
C	5.83059800	-2.36682000	-0.41486600
C	5.84700800	0.08369500	-0.21316300
C	5.12838800	-3.61631400	-0.54591800
H	5.32391900	-5.75488200	-0.72943200
C	5.13078800	-1.13900400	-0.34337900
C	3.65551600	-3.58136700	-0.58206300
C	3.67842500	-1.11350200	-0.39724200
C	2.92200900	-4.76334000	-0.69044300
C	2.96851200	-2.34529900	-0.50871000
C	3.00074500	0.12052200	-0.34278400
C	1.53868400	-4.74812900	-0.69617300
H	3.44237800	-5.71601900	-0.76900900

C	1.53542700	-2.33194300	-0.53417200
C	1.54579800	0.13814700	-0.40361000
C	0.82207200	-3.54922700	-0.59408700
H	1.01858000	-5.69187400	-0.79249500
C	0.82804900	-1.07873800	-0.49490500
C	-0.63900500	-3.53175700	-0.53391500
C	-0.59581400	-1.06139700	-0.50354500
C	-1.38289000	-4.71830400	-0.45795600
C	-1.32763400	-2.30120900	-0.51956200
C	-1.28502600	0.17060200	-0.46064200
C	-2.76266300	-4.71605600	-0.41640300
H	-0.87228500	-5.67352800	-0.41392000
C	-2.75969700	-2.29119100	-0.46981100
C	-2.74043100	0.18488900	-0.44104400
C	-3.46805100	-3.51263700	-0.42815800
H	-3.28995900	-5.66300100	-0.35285600
C	-3.44499700	-1.03786000	-0.44525500
C	-4.93916100	-3.51010600	-0.38736000
C	-4.89781500	-1.02822900	-0.41010400
C	-5.67722400	-4.67651800	-0.34611100
C	-5.62421800	-2.24180800	-0.38803000
C	-5.59111800	0.21207200	-0.39801100
C	-7.10497800	-4.65669300	-0.31731500
H	-5.17722000	-5.65149500	-0.33261300
C	-7.06142700	-2.22097400	-0.36021700
C	-7.02940900	0.22610300	-0.38048200
C	-7.78086200	-3.47077400	-0.32668000
H	-7.63598300	-5.60987600	-0.28644400
C	-7.73613500	-0.99967700	-0.36180600
H	9.10763000	3.71315000	0.25447200
H	9.07207400	1.26490500	0.04092700
H	9.05055500	-1.18002300	-0.18113800
H	9.04295400	-3.62727500	-0.40709200
H	-8.87126100	-3.44147700	-0.30631400
H	-8.82993300	-0.98324200	-0.34549000
H	-8.80611700	1.46990500	-0.36975600
H	-8.79976900	3.92846100	-0.38174900
C	0.69936100	-1.31403900	2.59023700
C	-1.29612100	0.07362600	2.59945400
C	-1.45362300	-2.43070500	2.62013400
C	0.00394000	-2.46635700	2.61813900
N	-1.97987100	-1.12679000	2.63527000
N	0.07960500	-0.08759400	2.60112200
O	-2.19968000	-3.38916500	2.59456300
H	-2.98988700	-1.05153000	2.60400000
O	-1.83973700	1.15703800	2.55970200
H	0.61237400	0.76815000	2.50822100
H	1.78441400	-1.28281800	2.53743300
H	0.49531500	-3.42946700	2.59082600

Graphene-S6C

C	-4.94251400	1.40936900	-0.39080000
C	-5.64852200	2.63156900	-0.38330000
C	-3.48643800	1.39518100	-0.37563600
C	-7.78033300	1.42388400	-0.41500300
C	-7.08573600	2.63291200	-0.40129400
C	-4.94442900	3.89246200	-0.35694600
C	-2.78132100	2.63182300	-0.33000800
C	-7.78504500	3.89565800	-0.40309200
C	-5.66236900	5.06973700	-0.35951600
C	-3.47299900	3.86885400	-0.32268100
C	-1.34823700	2.61901800	-0.28822800
C	-7.09149900	5.07014700	-0.38439100
H	-5.15196200	6.03639800	-0.34147400
C	-2.74790500	5.05751400	-0.28748800
C	-0.63737400	1.37411600	-0.32461800
C	-0.63844800	3.84252400	-0.22278900
H	-7.60762500	6.03104500	-0.38663200
C	-1.36352300	5.03857400	-0.24140200
H	-3.26226900	6.01477400	-0.29609800
C	0.79016000	1.36534700	-0.29845300
C	0.82215800	3.83178100	-0.14370900
H	-0.84176400	5.98884200	-0.22565400
C	1.51565100	2.59968400	-0.20199900
C	1.55696100	5.01281000	-0.00468600
C	2.94846700	2.58573000	-0.15316000
C	2.94109700	5.00363700	0.04648600
H	1.05333900	5.96690900	0.07575300
C	3.63870400	1.34416300	-0.22626000
C	3.65455800	3.81011800	-0.03328300
H	3.47211200	5.94711000	0.15264800
C	5.09361300	1.34050200	-0.19358600
C	5.12654400	3.81603800	0.01302600
C	5.81255600	2.55081500	-0.07595000
C	5.85092600	4.98350100	0.13409400
C	7.24897700	2.52857500	-0.04402900
H	5.35524600	5.94981700	0.20388100
C	7.27802100	4.95832000	0.17063900
C	7.95910100	3.77915800	0.08422700
C	7.93091000	1.31680100	-0.13669100
H	7.80635500	5.90618900	0.26846100
C	7.91817900	-3.60097300	-0.58768900
C	7.91717700	-1.13915800	-0.36039900
C	7.22401500	-4.76998800	-0.70267600
C	7.22167200	-2.34083800	-0.47968800
C	7.23296500	0.09371400	-0.25978800
C	5.79625900	-4.77502200	-0.71642600
H	7.74208700	-5.72490200	-0.78568900
C	5.78481600	-2.34288500	-0.49698000
C	5.79282200	0.10384800	-0.28380400

C	5.08452900	-3.59791200	-0.61588500
H	5.28986200	-5.73392700	-0.80779200
C	5.07965400	-1.12274100	-0.39877300
C	3.61199100	-3.57150600	-0.62047200
C	3.62457400	-1.10592700	-0.41249600
C	2.88427700	-4.75300700	-0.73958400
C	2.92020400	-2.33745500	-0.51325100
C	2.94069700	0.12408400	-0.33004800
C	1.49883400	-4.74297400	-0.72549400
H	3.40480300	-5.70226900	-0.84584700
C	1.48694200	-2.33104900	-0.50792700
C	1.48816500	0.13456700	-0.35594900
C	0.77859200	-3.55379900	-0.58428400
H	0.98204800	-5.68681500	-0.83845800
C	0.77569200	-1.08657400	-0.43361400
C	-0.68227500	-3.54636900	-0.51199300
C	-0.65198000	-1.07656400	-0.44481400
C	-1.41944500	-4.73335600	-0.45025600
C	-1.37795900	-2.31337800	-0.47769900
C	-1.34802800	0.15338400	-0.39271900
C	-2.80487900	-4.73549800	-0.41649700
H	-0.90606300	-5.68792100	-0.41655400
C	-2.81115800	-2.30889900	-0.44908100
C	-2.80018500	0.16224700	-0.40370000
C	-3.51668200	-3.53830900	-0.43104900
H	-3.33004100	-5.68601400	-0.37588800
C	-3.50144600	-1.06331000	-0.42805100
C	-4.98856700	-3.54398000	-0.41885300
C	-4.95741900	-1.06058600	-0.41815000
C	-5.72048000	-4.71261200	-0.41410900
C	-5.67768400	-2.27454500	-0.41846100
C	-5.65578600	0.17867900	-0.40897000
C	-7.14970800	-4.69581200	-0.41048400
H	-5.22146100	-5.68536400	-0.41397000
C	-7.11490600	-2.25870200	-0.41683800
C	-7.09265000	0.18713500	-0.41489600
C	-7.82925900	-3.51301700	-0.41304700
H	-7.67729600	-5.65046700	-0.40656100
C	-7.79500200	-1.04137500	-0.41882700
H	9.04625400	3.74973500	0.10961400
H	9.01789100	1.30226400	-0.11509100
H	9.00435700	-1.14009100	-0.34439100
H	9.00587200	-3.58684300	-0.57489100
H	-8.91903500	-3.48639500	-0.41170400
H	-8.88682900	-1.02836200	-0.42189700
H	-8.87219200	1.42390500	-0.42522300
H	-8.87493700	3.88208400	-0.41984500
C	0.15489600	-0.11314800	3.28582400
C	-1.31533500	-0.08898100	3.71020400
C	-2.09436000	-1.22937300	3.05029900

C	-1.45838000	-2.59035300	3.34535400
C	0.01982100	-2.61016800	2.94811300
C	0.79911300	-1.46551900	3.59909000
H	-3.14121100	-1.21883600	3.37641000
H	-1.37594100	-0.19195500	4.80369900
H	-1.76849200	0.87598500	3.45462100
H	0.21788100	0.06925700	2.20382400
H	0.70937700	0.69686800	3.77382800
H	-1.54710000	-2.80512000	4.42051100
H	-1.99985200	-3.38267800	2.81387700
H	0.47318600	-3.57594000	3.20153900
H	0.09592400	-2.50430300	1.85964400
H	0.82229100	-1.61114600	4.68897100
H	1.84023300	-1.47710200	3.25299900
H	-2.09918500	-1.06864300	1.96554200

Graphene-S6N

C	-4.90641300	1.39983400	-0.37490000
C	-5.60963700	2.62580500	-0.33075700
C	-3.45217700	1.37947000	-0.35061000
C	-7.74455700	1.42167200	-0.42656500
C	-7.04612900	2.62608100	-0.35942100
C	-4.90754200	3.88153200	-0.25676200
C	-2.74505300	2.61378500	-0.27809300
C	-7.73927700	3.89139400	-0.31493600
C	-5.61576600	5.06519400	-0.21470600
C	-3.43516800	3.85078000	-0.22850300
C	-1.31164400	2.60416100	-0.25351500
C	-7.04232200	5.06289500	-0.24493700
H	-5.10692400	6.02492200	-0.15874500
C	-2.70619100	5.03630100	-0.15165900
C	-0.60309700	1.35352900	-0.30124800
C	-0.60213600	3.82459800	-0.18168100
H	-7.55881200	6.02155400	-0.21088300
C	-1.32266100	5.02274700	-0.12774700
H	-3.22739500	5.99053800	-0.10900100
C	0.82493500	1.34135300	-0.27589100
C	0.86089400	3.81028300	-0.16552500
H	-0.80824000	5.97199700	-0.06437600
C	1.55317300	2.57572700	-0.20967400
C	1.60566600	4.99329200	-0.11002700
C	2.98683600	2.56634900	-0.18954100
C	2.99050100	4.99055200	-0.09020400
H	1.09962100	5.95197100	-0.08190200
C	3.67438800	1.31914400	-0.23505800
C	3.69697700	3.79101500	-0.12760100
H	3.51916100	5.93900300	-0.04521300
C	5.13061700	1.31188900	-0.21880700
C	5.16879600	3.79210100	-0.10514500
C	5.85456800	2.52225300	-0.15492400

C	5.90372100	4.95715500	-0.03919700
C	7.29167100	2.50263900	-0.13863100
H	5.40651400	5.93040400	0.00041400
C	7.33266600	4.93657200	-0.02077300
C	8.00927100	3.75301100	-0.06928200
C	7.96876400	1.28465300	-0.18999700
H	7.86246300	5.88860700	0.03236600
C	7.94836300	-3.64541200	-0.43342000
C	7.94844100	-1.17686400	-0.31110500
C	7.25236900	-4.81708200	-0.49538800
C	7.25134100	-2.38291400	-0.37530900
C	7.26316800	0.05993800	-0.25643100
C	5.82321100	-4.81297400	-0.50263600
H	7.76657300	-5.77803600	-0.54047200
C	5.81404100	-2.37773700	-0.38453700
C	5.82620600	0.07237000	-0.26898600
C	5.10735400	-3.63541400	-0.44884600
H	5.31002600	-5.77742100	-0.55257800
C	5.11023300	-1.15498800	-0.33193900
C	3.63562000	-3.60899600	-0.45383900
C	3.65416000	-1.13710500	-0.34209000
C	2.90875000	-4.79554900	-0.51943600
C	2.94620000	-2.37238800	-0.39921900
C	2.97007400	0.09726500	-0.29537500
C	1.52408600	-4.77403500	-0.51938800
H	3.42148800	-5.75210400	-0.57557400
C	1.51247100	-2.35649600	-0.40349500
C	1.51785100	0.11019100	-0.31455300
C	0.79969500	-3.57907400	-0.44785200
H	1.00061300	-5.72141100	-0.58710500
C	0.80326400	-1.10933500	-0.36990600
C	-0.66297400	-3.56804600	-0.43031900
C	-0.62264600	-1.09825400	-0.39379800
C	-1.40260700	-4.75782200	-0.40396600
C	-1.35127700	-2.33559800	-0.43749200
C	-1.31691200	0.13529500	-0.37080800
C	-2.78503100	-4.74754300	-0.43030400
H	-0.90210800	-5.71557500	-0.35715100
C	-2.78433500	-2.32061800	-0.46029800
C	-2.77082800	0.14722300	-0.39662300
C	-3.49389900	-3.54602600	-0.47319100
H	-3.32331200	-5.69313500	-0.41695700
C	-3.47161600	-1.07358400	-0.45369300
C	-4.96609900	-3.55214600	-0.51908100
C	-4.92596900	-1.06876100	-0.47150900
C	-5.69253900	-4.72455400	-0.56842600
C	-5.64859200	-2.28352200	-0.51182400
C	-5.62266100	0.17181600	-0.43860700
C	-7.11843000	-4.69748000	-0.60944000
H	-5.19867500	-5.69350200	-0.57934900

C	-7.08480600	-2.25915700	-0.54443700
C	-7.06408500	0.18392500	-0.46447400
C	-7.79727200	-3.51327900	-0.59699000
H	-7.64964600	-5.64778400	-0.65075300
C	-7.76402400	-1.04214000	-0.52250300
H	9.09899700	3.72317300	-0.05685600
H	9.06078200	1.26850900	-0.17922300
H	9.04060900	-1.17960700	-0.30290400
H	9.03851100	-3.63438200	-0.42674200
H	-8.88391900	-3.48310100	-0.62687900
H	-8.85027300	-1.02645800	-0.54881300
H	-8.83105300	1.42495700	-0.44951300
H	-8.82650500	3.87981200	-0.33902100
C	-0.20836800	0.09445100	3.24129600
C	-1.73059500	0.06617600	3.12321000
C	-1.74887900	-2.36289900	3.07481300
C	-0.22714300	-2.41887500	3.18982300
C	0.29465300	-1.18046200	3.92313000
H	-2.16998300	0.11812100	4.13942600
H	-2.08822800	0.94002900	2.56373300
H	0.21815900	0.16209100	2.23333100
H	0.10608400	0.98457900	3.79708200
H	-2.18773900	-2.44769500	4.08912500
H	-2.11938500	-3.20853800	2.48188000
H	0.07482600	-3.33546300	3.70852800
H	0.19701500	-2.45150500	2.17881500
H	-0.07013200	-1.19945500	4.96079400
H	1.38868300	-1.18952100	3.96822500
N	-2.13600600	-1.13155500	2.40193400
H	-3.13754500	-1.12043200	2.22623000

Graphene-S6O

C	-4.90269300	1.40375400	-0.37362500
C	-5.60648800	2.62802300	-0.34653700
C	-3.44724400	1.38414800	-0.35067700
C	-7.74084600	1.42709700	-0.42132500
C	-7.04349800	2.63441200	-0.37336900
C	-4.89945000	3.88548800	-0.29080100
C	-2.73914600	2.62264000	-0.28919500
C	-7.74048100	3.89765600	-0.34841300
C	-5.61565900	5.06409100	-0.26816700
C	-3.42794100	3.85851800	-0.25927900
C	-1.30571900	2.60656200	-0.25847900
C	-7.04437000	5.07000700	-0.29771200
H	-5.10142000	6.02925800	-0.22674100
C	-2.70157100	5.04689000	-0.20194400
C	-0.59782300	1.35695400	-0.29901600
C	-0.59364100	3.82690700	-0.19188300
H	-7.55823800	6.03224200	-0.27849000
C	-1.31840600	5.02475500	-0.17029800

H	-3.21437000	6.00463700	-0.18227700
C	0.82849600	1.34623800	-0.27407200
C	0.86916400	3.81575300	-0.15084100
H	-0.79554600	5.97365500	-0.12959600
C	1.55863800	2.58295700	-0.19823300
C	1.60894400	5.00039900	-0.06348300
C	2.99195000	2.56554600	-0.16739200
C	2.99231800	4.98766400	-0.03267600
H	1.10995400	5.95891400	-0.01493300
C	3.67919500	1.31914700	-0.21992200
C	3.70205200	3.78894600	-0.08532000
H	3.52960400	5.93168500	0.03473700
C	5.13334200	1.31287500	-0.19655600
C	5.17511400	3.79310600	-0.05394000
C	5.85614600	2.52613600	-0.11478900
C	5.90116700	4.96396200	0.02974600
C	7.29257800	2.49949600	-0.09217300
H	5.40817900	5.93156400	0.07725400
C	7.32708200	4.93467500	0.05504100
C	8.00540900	3.75150000	-0.00390300
C	7.97126100	1.28373500	-0.15489200
H	7.85934100	5.88278300	0.12208700
C	7.94218300	-3.64548000	-0.45973100
C	7.95017600	-1.17764500	-0.30678200
C	7.24358700	-4.81575200	-0.53696200
C	7.25079400	-2.38052500	-0.38752700
C	7.27165100	0.05947900	-0.23942900
C	5.81721300	-4.81877200	-0.54627200
H	7.75975500	-5.77343100	-0.59290600
C	5.81391300	-2.38058900	-0.40011900
C	5.82891700	0.07302500	-0.25726100
C	5.11109000	-3.63469400	-0.47934300
H	5.30778400	-5.77691500	-0.60785300
C	5.11222500	-1.15393000	-0.33600000
C	3.63800000	-3.60329300	-0.48298600
C	3.65841100	-1.13296300	-0.34826000
C	2.90670000	-4.78786700	-0.56171700
C	2.94985000	-2.36652000	-0.41544100
C	2.97840800	0.09964200	-0.29341700
C	1.52286000	-4.77487300	-0.55517600
H	3.42757700	-5.74083200	-0.63256800
C	1.51625000	-2.35687300	-0.41499300
C	1.52346200	0.11378100	-0.31538000
C	0.80499800	-3.57713500	-0.46349500
H	1.00482200	-5.72103800	-0.63764600
C	0.80615500	-1.10619200	-0.37352800
C	-0.65780000	-3.56112000	-0.42419300
C	-0.61836200	-1.09167700	-0.39732100
C	-1.40158400	-4.74764700	-0.37207000
C	-1.34856500	-2.32816800	-0.42685400

C	-1.31072000	0.13852400	-0.36340100
C	-2.78504200	-4.74605900	-0.38244700
H	-0.89236300	-5.70341600	-0.31570300
C	-2.78159100	-2.31976500	-0.43892600
C	-2.76453800	0.15174800	-0.38787500
C	-3.49072600	-3.54330300	-0.43286800
H	-3.31473900	-5.69415500	-0.34932700
C	-3.46768300	-1.07084700	-0.42432300
C	-4.96226300	-3.54521800	-0.46562000
C	-4.92351300	-1.06322900	-0.43949300
C	-5.69787400	-4.71148500	-0.49974700
C	-5.64824000	-2.27490300	-0.46570800
C	-5.61895900	0.17668700	-0.41972400
C	-7.12661700	-4.69225900	-0.53141800
H	-5.19976100	-5.68593800	-0.50384100
C	-7.08548200	-2.25594800	-0.49204900
C	-7.05611400	0.18945500	-0.44234300
C	-7.80321600	-3.50758400	-0.52711000
H	-7.65620500	-5.64571400	-0.55879700
C	-7.76203300	-1.03660600	-0.48188500
H	9.09202400	3.72019800	0.01372400
H	9.05718500	1.26749400	-0.13964400
H	9.03623300	-1.18157400	-0.29575700
H	9.02926800	-3.63430400	-0.45138100
H	-8.89314900	-3.47843300	-0.54975600
H	-8.85466000	-1.02043600	-0.50240500
H	-8.83360000	1.43093100	-0.44150700
H	-8.83075100	3.88760700	-0.37085800
C	-0.25611600	0.05695000	3.17662300
C	-1.77144200	-0.00411200	3.02296200
C	-1.77490100	-2.36220500	2.94040800
C	-0.25961700	-2.43834200	3.09361500
C	0.25097800	-1.21529900	3.85786400
H	-2.24771700	0.01090000	4.01978300
H	-2.15043400	0.84821400	2.44881800
H	0.20052700	0.14476300	2.18318400
H	0.02236900	0.95126600	3.74587500
H	-2.25266400	-2.44592000	3.93304300
H	-2.15346000	-3.17164200	2.30690700
H	0.01315200	-3.36889500	3.60489400
H	0.20214800	-2.46323500	2.09865700
H	-0.12183300	-1.24917600	4.89192700
H	1.34518800	-1.21863900	3.90991200
O	-2.18630500	-1.15939200	2.32028100

Graphene-S6S

C	-4.90041000	1.43589400	-0.44362200
C	-5.60375700	2.66123800	-0.42842000
C	-3.44556600	1.41684600	-0.42504300
C	-7.73864000	1.45927700	-0.46858700

C	-7.04081400	2.66749800	-0.44687000
C	-4.89570200	3.91855100	-0.39419500
C	-2.73679900	2.65542400	-0.37331800
C	-7.73726500	3.93097300	-0.44034100
C	-5.61183300	5.09780700	-0.38943000
C	-3.42425700	3.89164100	-0.36032400
C	-1.30395200	2.63839700	-0.33213800
C	-7.04035700	5.10394100	-0.41415800
H	-5.09668700	6.06336100	-0.36545800
C	-2.69648800	5.08062200	-0.31986300
C	-0.59606700	1.38828200	-0.37306400
C	-0.59143900	3.85728500	-0.26225200
H	-7.55403400	6.06657700	-0.41013600
C	-1.31407000	5.05721000	-0.27451600
H	-3.20806500	6.03908500	-0.32400700
C	0.82936400	1.37672100	-0.34440700
C	0.86974400	3.84367900	-0.18330100
H	-0.78846000	6.00536100	-0.25367900
C	1.55934900	2.61176100	-0.24063600
C	1.60753200	5.02466000	-0.04365400
C	2.99179600	2.59236900	-0.18480400
C	2.99002400	5.00990100	0.01304600
H	1.10686100	5.98052400	0.03256400
C	3.67917400	1.34644000	-0.25380200
C	3.70074900	3.81255900	-0.06122400
H	3.52595200	5.95100700	0.11988600
C	5.13257400	1.33837100	-0.20946200
C	5.17318800	3.81444900	-0.00467400
C	5.85439600	2.54891700	-0.08599100
C	5.89818200	4.98237200	0.12015900
C	7.29029000	2.52009800	-0.04163900
H	5.40509900	5.94883200	0.18336500
C	7.32331900	4.95076300	0.16818100
C	8.00202200	3.76880500	0.09028000
C	7.96926600	1.30571300	-0.12580800
H	7.85509700	5.89626300	0.26791300
C	7.94247900	-3.61288800	-0.57417700
C	7.94938900	-1.15068000	-0.34694600
C	7.24460900	-4.77966700	-0.69770200
C	7.25079300	-2.35003300	-0.47364400
C	7.27092000	0.08476700	-0.25439700
C	5.81861600	-4.78153500	-0.72782200
H	7.76134000	-5.73550700	-0.77553500
C	5.81419100	-2.34891400	-0.50650500
C	5.82826300	0.09990800	-0.29256000
C	5.11231400	-3.59931400	-0.63431000
H	5.30990000	-5.73676400	-0.82641100
C	5.11234400	-1.12383600	-0.41511100
C	3.63927800	-3.56698500	-0.65504800
C	3.65893200	-1.10164700	-0.44291600

C	2.90807000	-4.74748500	-0.78235300
C	2.95086500	-2.33277800	-0.55354900
C	2.97901500	0.12973500	-0.36501200
C	1.52409900	-4.73448000	-0.78076400
H	3.42906100	-5.69747900	-0.88452700
C	1.51757700	-2.32275100	-0.56125400
C	1.52428900	0.14496700	-0.40118300
C	0.80642100	-3.54086400	-0.64567800
H	1.00574700	-5.67669400	-0.89886100
C	0.80770000	-1.07311700	-0.48723700
C	-0.65567600	-3.52771300	-0.58370400
C	-0.61702000	-1.05870700	-0.50139900
C	-1.39745600	-4.71587100	-0.53607600
C	-1.34726200	-2.29603600	-0.54409500
C	-1.30942100	0.17083900	-0.44432200
C	-2.78047100	-4.71505600	-0.50734000
H	-0.88552300	-5.67156800	-0.51031900
C	-2.78012900	-2.28835400	-0.52382600
C	-2.76357000	0.18399800	-0.46020400
C	-3.48813100	-3.51237800	-0.51555500
H	-3.30858300	-5.66398500	-0.47640000
C	-3.46695100	-1.03862600	-0.49152000
C	-4.96000500	-3.51373000	-0.50729100
C	-4.92185600	-1.03129800	-0.48920300
C	-5.69652400	-4.68034900	-0.51150700
C	-5.64639700	-2.24403400	-0.49816200
C	-5.61691300	0.20865800	-0.47078900
C	-7.12533500	-4.66160700	-0.50925200
H	-5.19802400	-5.65491400	-0.51717100
C	-7.08385400	-2.22512100	-0.49775800
C	-7.05448400	0.22128500	-0.47768100
C	-7.80200900	-3.47673100	-0.50349800
H	-7.65543300	-5.61529500	-0.51227500
C	-7.76032100	-1.00534300	-0.49023800
H	9.08812400	3.73613900	0.12472000
H	9.05469500	1.28825900	-0.09418200
H	9.03504800	-1.15596400	-0.31985900
H	9.02927600	-3.60291100	-0.54950600
H	-8.89233200	-3.44806700	-0.50198600
H	-8.85346500	-0.98977000	-0.49213000
H	-8.83183400	1.46331000	-0.47788900
H	-8.82777800	3.92131500	-0.45682900
C	0.16715900	0.00223400	3.14010000
C	-1.27584600	0.07351500	3.63119700
C	-1.33154300	-2.65756600	3.31655400
C	0.12159000	-2.53389000	2.86800900
C	0.84053800	-1.32937100	3.47799400
H	-1.31676000	-0.03166700	4.72266000
H	-1.73172900	1.03274400	3.36970900
H	0.18252700	0.15521900	2.05523200

H	0.73692300	0.82602900	3.58909400
H	-1.39026200	-2.81127100	4.40142500
H	-1.81701800	-3.50856000	2.82918700
H	0.65563100	-3.45533000	3.13408300
H	0.14823300	-2.45289500	1.77778500
H	0.88553200	-1.44557000	4.57094500
H	1.87707700	-1.31109900	3.11900500
S	-2.33419400	-1.20040000	2.86995500

Graphene-S5C

C	-5.07910800	1.34744800	-0.11871200
C	-5.79789000	2.55485100	0.02359700
C	-3.62400700	1.35179100	-0.14490100
C	-7.91604400	1.32272100	-0.07490200
C	-7.23443300	2.53164700	0.05151700
C	-5.11172400	3.81805000	0.14198900
C	-2.93400100	2.59191300	-0.05210800
C	-7.94478300	3.77858700	0.21116800
C	-5.83656800	4.98155900	0.29268400
C	-3.63979300	3.81433600	0.09020200
C	-1.50152500	2.60707200	-0.10760000
C	-7.26387200	4.95504900	0.32881000
H	-5.34128900	5.94613500	0.38640000
C	-2.92577200	5.00620500	0.18607600
C	-0.77592800	1.37411700	-0.21180700
C	-0.80802800	3.83923700	-0.04546200
H	-7.79229500	5.90002600	0.45131900
C	-1.54157800	5.01699800	0.12198300
H	-3.45575200	5.94753000	0.31371500
C	0.65162600	1.38365300	-0.24289900
C	0.65097000	3.85193700	-0.15093100
H	-1.03641000	5.96912900	0.21697300
C	1.36139400	2.62874600	-0.21865400
C	1.37350500	5.04846600	-0.19686000
C	2.79368800	2.64231800	-0.27802700
C	2.75763000	5.06824700	-0.26343600
H	0.84956600	5.99779400	-0.18989200
C	3.49919800	1.40604700	-0.31571400
C	3.48405500	3.88030700	-0.29310100
H	3.27041000	6.02595700	-0.29300500
C	4.95522900	1.42022000	-0.33840700
C	4.95515500	3.90377300	-0.34504000
C	5.66003900	2.64266800	-0.35563200
C	5.67232000	5.08087200	-0.37676600
C	7.09714000	2.64378400	-0.38319100
H	5.16193500	6.04755000	-0.37230600
C	7.10135100	5.08101000	-0.41460400
C	7.79547200	3.90680000	-0.41549000
C	7.79217900	1.43495900	-0.37637500
H	7.61681500	6.04187500	-0.44069700

C	7.84176500	-3.50198200	-0.26741300
C	7.80752400	-1.03071100	-0.32724100
C	7.16214900	-4.68433300	-0.24056800
C	7.12761300	-2.24778100	-0.29904700
C	7.10535800	0.19792200	-0.34790600
C	5.73272600	-4.70176300	-0.24794900
H	7.68970100	-5.63862500	-0.21461800
C	5.69033700	-2.26423300	-0.30128800
C	5.66868800	0.18930400	-0.33771200
C	5.00081700	-3.53378700	-0.27936600
H	5.23418800	-5.67440600	-0.22938600
C	4.97084500	-1.05038100	-0.32325000
C	3.52888100	-3.52858300	-0.30135700
C	3.51485700	-1.05347500	-0.33265200
C	2.81509400	-4.72452700	-0.27738500
C	2.82456000	-2.29844900	-0.33898200
C	2.81369100	0.17266500	-0.32433800
C	1.42936300	-4.72198000	-0.33256000
H	3.33849600	-5.67488700	-0.21574800
C	1.39168100	-2.30261800	-0.37959700
C	1.36245900	0.16323800	-0.30933100
C	0.69558500	-3.53530300	-0.42331600
H	0.91265500	-5.67476000	-0.29244200
C	0.66676700	-1.06668800	-0.35651800
C	-0.76217800	-3.54088600	-0.53947300
C	-0.76112000	-1.07672000	-0.35878600
C	-1.47856600	-4.72603300	-0.72347200
C	-1.47163000	-2.31878000	-0.46107400
C	-1.47359200	0.14373600	-0.27738800
C	-2.86415400	-4.73490400	-0.76658100
H	-0.95747600	-5.66628100	-0.84836400
C	-2.90410900	-2.32427100	-0.49220500
C	-2.92578400	0.13334300	-0.26503400
C	-3.59402700	-3.55607000	-0.63553000
H	-3.38229600	-5.68137400	-0.90398500
C	-3.60904900	-1.09468500	-0.37756900
C	-5.06660600	-3.58063800	-0.65412500
C	-5.06424600	-1.11092700	-0.37894900
C	-5.77787300	-4.75378500	-0.79414000
C	-5.76811400	-2.32810100	-0.51288500
C	-5.77780500	0.11314100	-0.24105400
C	-7.20591900	-4.74789700	-0.79733500
H	-5.27105600	-5.71060500	-0.90414500
C	-7.20510900	-2.32548600	-0.50983900
C	-7.21778500	0.10283300	-0.22656000
C	-7.90084900	-3.58199300	-0.65875800
H	-7.72332500	-5.69992200	-0.91200500
C	-7.90128100	-1.12698000	-0.36487800
H	8.88516100	3.89339600	-0.44074700
H	8.88387100	1.43519800	-0.39226900

H	8.89923700	-1.01768900	-0.33170700
H	8.93148600	-3.47530300	-0.26474500
H	-8.98867000	-3.56756400	-0.65743700
H	-8.98865900	-1.12794000	-0.35787700
H	-9.00320200	1.30786200	-0.05790500
H	-9.03200900	3.74850500	0.23479300
C	1.79280300	-1.19630700	3.10277600
C	0.44235700	-0.45845900	3.27086300
C	-0.53052600	-1.52675400	3.78672400
C	-0.07401400	-2.78566100	3.04600500
C	1.45791900	-2.71121000	3.12778900
H	2.28560000	-0.90793200	2.17015700
H	2.48175000	-0.94135900	3.91421200
H	0.08866100	-0.09347400	2.29918500
H	0.51289600	0.40976700	3.93246600
H	-0.40364000	-1.66525700	4.86852100
H	-1.57960400	-1.27311100	3.60242800
H	-0.48301400	-3.71230900	3.46061800
H	-0.39939400	-2.71993200	2.00145800
H	1.79261400	-3.15135400	4.07449800
H	1.95062300	-3.26719700	2.32360000

Graphene-S5N

C	-5.10690500	1.35961000	-0.10206000
C	-5.83450600	2.56299300	0.03568000
C	-3.65215900	1.37303600	-0.12437400
C	-7.94463400	1.32157100	-0.06355500
C	-7.27127600	2.53743600	0.05938200
C	-5.15177800	3.82909200	0.15452300
C	-2.96826400	2.62130100	-0.02598000
C	-7.99255800	3.77779600	0.21081900
C	-5.89097800	4.98525900	0.29790300
C	-3.68047600	3.83634700	0.11342500
C	-1.53566200	2.63842000	-0.07243400
C	-7.31915600	4.95895000	0.32751200
H	-5.39539000	5.95655100	0.39233100
C	-2.97635800	5.03502800	0.21574600
C	-0.80288800	1.40768500	-0.18286300
C	-0.84751200	3.87140100	0.00158100
H	-7.85183800	5.90403100	0.44444700
C	-1.59356100	5.04530600	0.16304100
H	-3.50555700	5.97568200	0.33929700
C	0.62282900	1.42775800	-0.21174500
C	0.61307800	3.89619200	-0.08352600
H	-1.08758700	5.99953400	0.25945300
C	1.32766400	2.67974500	-0.16553700
C	1.32618900	5.09977800	-0.09106300
C	2.76012400	2.69560500	-0.21608000
C	2.70914300	5.11958400	-0.14387200
H	0.80497700	6.04714500	-0.06325800

C	3.47260200	1.46405900	-0.28093100
C	3.44437300	3.93618000	-0.19742400
H	3.22585400	6.07718200	-0.14382400
C	4.92669300	1.48900400	-0.30571900
C	4.91676300	3.97292900	-0.23890000
C	5.62401600	2.71898000	-0.28626400
C	5.61912200	5.16061300	-0.22823300
C	7.06062000	2.72357500	-0.31335300
H	5.10694600	6.11898100	-0.19389500
C	7.04560500	5.16272300	-0.26109100
C	7.74781400	3.99297200	-0.30094300
C	7.76396800	1.52075400	-0.34930600
H	7.55819300	6.12398400	-0.25233200
C	7.83522700	-3.41768200	-0.42385600
C	7.79310900	-0.94545300	-0.39028000
C	7.16059600	-4.60413700	-0.43386800
C	7.11845700	-2.16475400	-0.40104900
C	7.08951800	0.27958600	-0.36233500
C	5.73414100	-4.63653200	-0.42316900
H	7.69572700	-5.55292800	-0.45114200
C	5.68175700	-2.19469900	-0.38935900
C	5.64728100	0.26248800	-0.34524600
C	5.00420900	-3.46570800	-0.40153100
H	5.24456400	-5.60705900	-0.43460300
C	4.95591200	-0.98141000	-0.36553400
C	3.53103700	-3.46428600	-0.39500200
C	3.50194400	-0.99043700	-0.36131500
C	2.82296700	-4.66590000	-0.37640400
C	2.81875600	-2.23889600	-0.38959500
C	2.79710000	0.22963500	-0.31640000
C	1.43862500	-4.68002600	-0.38842400
H	3.36264300	-5.61029800	-0.34913900
C	1.38503700	-2.25779500	-0.40073800
C	1.34242600	0.21179000	-0.29423100
C	0.69819800	-3.49282700	-0.43694400
H	0.93715400	-5.63802400	-0.35419300
C	0.65090000	-1.02206500	-0.35578300
C	-0.76338400	-3.50310000	-0.51762000
C	-0.77486800	-1.03736400	-0.35092200
C	-1.48151500	-4.69578700	-0.67102100
C	-1.47996000	-2.28616200	-0.44560200
C	-1.49155400	0.17664500	-0.25867200
C	-2.86436000	-4.71929100	-0.70541500
H	-0.95118600	-5.63548500	-0.77947400
C	-2.91276200	-2.30505000	-0.46593500
C	-2.94529700	0.15840100	-0.24520800
C	-3.59605100	-3.53781100	-0.59010300
H	-3.37233600	-5.67230600	-0.82199100
C	-3.62429500	-1.07422200	-0.35344500
C	-5.06758100	-3.56621700	-0.60452000

C	-5.07888400	-1.09591100	-0.35190200
C	-5.78095300	-4.74063100	-0.73009200
C	-5.77887900	-2.31704800	-0.47477500
C	-5.79844500	0.12329100	-0.22042700
C	-7.20973900	-4.74942400	-0.73335000
H	-5.26347700	-5.70009100	-0.82926200
C	-7.21630600	-2.32666400	-0.47154000
C	-7.23586500	0.10567500	-0.20696700
C	-7.90962100	-3.58485200	-0.60697100
H	-7.72113700	-5.70774600	-0.83696900
C	-7.91691500	-1.12802600	-0.33618200
H	8.83489200	3.98541100	-0.32437500
H	8.85017000	1.52802500	-0.36724400
H	8.87922100	-0.92640300	-0.40255200
H	8.92201300	-3.38403300	-0.43284700
H	-9.00029300	-3.57778100	-0.60506500
H	-9.01004100	-1.13509000	-0.32875000
H	-9.03747400	1.30177300	-0.04883100
H	-9.08250200	3.74395300	0.22996400
C	1.85815000	-1.36904300	3.07743200
C	0.33981900	-1.05888700	3.13901200
C	0.48252600	-3.34788800	3.39934800
C	1.93609400	-2.91333500	3.12525900
H	2.30738800	-0.98488300	2.15595600
H	2.39421500	-0.90431900	3.91060000
H	0.03179800	-0.26680900	2.44916000
H	0.06092800	-0.74293400	4.15145600
H	0.29747800	-3.39991900	4.47987900
H	0.23122800	-4.32143300	2.96809300
H	2.63528200	-3.27804400	3.88393300
H	2.27008800	-3.30966500	2.15975300
N	-0.37868700	-2.30336100	2.83806100
H	-0.37202300	-2.42270800	1.82693300

Graphene-S5O

C	-5.10854400	1.37737800	-0.16160500
C	-5.83833500	2.58555300	-0.11004900
C	-3.65287000	1.39066900	-0.16816500
C	-7.94657300	1.33810300	-0.14559300
C	-7.27534800	2.56029300	-0.10389200
C	-5.15808900	3.85795500	-0.06262900
C	-2.97125500	2.64236700	-0.11191100
C	-7.99914500	3.80761700	-0.05354700
C	-5.89924800	5.02036900	-0.01528300
C	-3.68612100	3.86320400	-0.06345800
C	-1.53760100	2.65708900	-0.10481000
C	-7.32800200	4.99479400	-0.01129900
H	-5.40545800	5.99638000	0.02099800
C	-2.98504900	5.06696100	-0.02124600
C	-0.80307500	1.42489400	-0.17402900

C	-0.85144700	3.89210100	-0.03833400
H	-7.86231600	5.94529400	0.02674600
C	-1.60119200	5.07440100	-0.01216100
H	-3.51787200	6.01351200	0.00417800
C	0.62242200	1.44505800	-0.18341900
C	0.61112900	3.91151400	-0.00592900
H	-1.09746200	6.03435100	0.01119200
C	1.32663800	2.69618800	-0.09586600
C	1.32536200	5.10856000	0.11663600
C	2.76012500	2.71071800	-0.09224500
C	2.70891100	5.12617300	0.12519700
H	0.80575600	6.05209100	0.21512700
C	3.47344800	1.48208200	-0.19585200
C	3.44427000	3.94674800	0.01552500
H	3.22596900	6.07897000	0.22063500
C	4.92761700	1.50808800	-0.20242300
C	4.91723400	3.98314700	0.01802300
C	5.62475800	2.73447100	-0.09736000
C	5.61897600	5.16680200	0.12480400
C	7.06154800	2.73989500	-0.10522400
H	5.10592600	6.12102200	0.21361500
C	7.04547000	5.16921000	0.12005100
C	7.74833300	4.00429600	0.00872700
C	7.76558500	1.54248500	-0.22056600
H	7.55798200	6.12655600	0.20701000
C	7.83972300	-3.37518500	-0.67055200
C	7.79617700	-0.91298400	-0.44718600
C	7.16567600	-4.55873600	-0.76256200
C	7.12234400	-2.12899700	-0.54553100
C	7.09178700	0.30568300	-0.32797500
C	5.74008500	-4.59471900	-0.73344400
H	7.70151400	-5.50224500	-0.85972300
C	5.68588200	-2.16176700	-0.52297100
C	5.64905100	0.28685000	-0.31444900
C	5.00972500	-3.42952500	-0.61456800
H	5.25081400	-5.56224800	-0.80901900
C	4.95837500	-0.95368000	-0.41250200
C	3.53714700	-3.43226300	-0.57225000
C	3.50469200	-0.96556200	-0.39360800
C	2.83180500	-4.63473600	-0.62489800
C	2.82163400	-2.21334400	-0.47141700
C	2.79841800	0.24985900	-0.28979800
C	1.44894400	-4.65371100	-0.57726200
H	3.37276600	-5.57572200	-0.70514000
C	1.38825900	-2.23764600	-0.42948800
C	1.34277600	0.22919300	-0.27154500
C	0.70407800	-3.47192100	-0.47655000
H	0.95332200	-5.61384700	-0.63249600
C	0.65225200	-1.00522400	-0.34130300
C	-0.75754800	-3.48994900	-0.42605200

C	-0.77286600	-1.02236300	-0.32555300
C	-1.47440000	-4.69073200	-0.42265900
C	-1.47500400	-2.27345000	-0.36703600
C	-1.49000900	0.19097600	-0.24342400
C	-2.85886100	-4.72165400	-0.39478100
H	-0.94578600	-5.63758500	-0.44126600
C	-2.90656500	-2.29703100	-0.33761100
C	-2.94394600	0.17261300	-0.22955100
C	-3.59033100	-3.53732300	-0.35991800
H	-3.36564900	-5.68271400	-0.39937700
C	-3.62091900	-1.06514600	-0.27588700
C	-5.06206700	-3.57036700	-0.34351400
C	-5.07661300	-1.08912500	-0.25878900
C	-5.77324400	-4.75167200	-0.37604000
C	-5.77509000	-2.31593000	-0.29436900
C	-5.79815600	0.13493200	-0.20559300
C	-7.20247600	-4.76354500	-0.36336000
H	-5.25459900	-5.71466100	-0.41289600
C	-7.21266500	-2.32815900	-0.28161600
C	-7.23533400	0.11626900	-0.19525600
C	-7.90411500	-3.59454700	-0.31817900
H	-7.71181400	-5.72799700	-0.39089800
C	-7.91503900	-1.12454900	-0.23407400
H	8.83554700	3.99713800	0.00287400
H	8.85173200	1.55069800	-0.22909600
H	8.88200700	-0.89203200	-0.46236900
H	8.92610000	-3.33914900	-0.69026900
H	-8.99455500	-3.58891900	-0.30838400
H	-9.00792200	-1.13229700	-0.22565700
H	-9.03933600	1.31758900	-0.13971000
H	-9.08917200	3.77359700	-0.05025600
C	1.83504800	-1.58980500	2.99284300
C	0.32591200	-1.29364400	2.98698800
C	0.41795900	-3.54789600	2.90069800
C	1.89816600	-3.13366400	2.91513900
H	2.32808400	-1.13820200	2.12694300
H	2.31881500	-1.19475100	3.89017100
H	0.04778500	-0.41584800	2.39736500
H	-0.04922800	-1.16079300	4.01415000
H	0.06848200	-3.78377200	3.91884900
H	0.20211900	-4.39846900	2.24834800
H	2.43456200	-3.57604700	3.75892800
H	2.39920200	-3.45430800	1.99729700
O	-0.28636400	-2.42820400	2.39930400

Graphene-S5S

C	-5.06831900	1.30440900	-0.35852500
C	-5.78617600	2.52118300	-0.39120100
C	-3.61374400	1.30405400	-0.36294700
C	-7.90609500	1.29323400	-0.33993500

C	-7.22329800	2.50925000	-0.38938600
C	-5.09305700	3.78669200	-0.42650200
C	-2.91952800	2.55075600	-0.37256000
C	-7.93501100	3.76327200	-0.43713300
C	-5.82366400	4.95638100	-0.47231400
C	-3.62130700	3.77894700	-0.40405000
C	-1.48654300	2.55164100	-0.34052600
C	-7.25223500	4.94415900	-0.47983400
H	-5.32036600	5.92793400	-0.50255800
C	-2.90637100	4.97625000	-0.41658600
C	-0.76443500	1.31013800	-0.35301400
C	-0.78771500	3.77969700	-0.30740300
H	-7.77784800	5.89966100	-0.51821600
C	-1.52333200	4.97006100	-0.37101200
H	-3.42821400	5.92799900	-0.46097800
C	0.66114900	1.31523700	-0.33852200
C	0.67242200	3.78390100	-0.21371800
H	-1.00685600	5.92339200	-0.39467400
C	1.37664300	2.55948200	-0.25781500
C	1.39531100	4.97323100	-0.07151100
C	2.80942100	2.55747800	-0.20832000
C	2.77847800	4.97499300	-0.01485800
H	0.88172700	5.92181700	0.00982600
C	3.51119100	1.31992700	-0.28386400
C	3.50414000	3.78684400	-0.09149300
H	3.30254600	5.92244400	0.09259500
C	4.96522900	1.33017800	-0.26823400
C	4.97683300	3.80542300	-0.04702700
C	5.67303900	2.54854800	-0.14933500
C	5.68951800	4.97993600	0.08156000
C	7.10982100	2.53767500	-0.13125500
H	5.18596200	5.93992800	0.16287400
C	7.11606700	4.96572500	0.10897700
C	7.80803100	3.79382500	0.00484200
C	7.80238700	1.33343200	-0.24433200
H	7.63718800	5.91671300	0.21353800
C	7.82827200	-3.58053500	-0.75251900
C	7.80914400	-1.12070500	-0.49796900
C	7.14260600	-4.75550400	-0.86356500
C	7.12325300	-2.32817100	-0.61661700
C	7.11712700	0.10466900	-0.37276300
C	5.71605400	-4.77707300	-0.84201100
H	7.66896400	-5.70348700	-0.96924800
C	5.68642900	-2.34634400	-0.60479500
C	5.67459800	0.10115700	-0.37618700
C	4.99700600	-3.60654000	-0.71256100
H	5.21769100	-5.73919600	-0.92927800
C	4.97210600	-1.13149600	-0.48869400
C	3.52420700	-3.59578300	-0.66948100
C	3.51825700	-1.12860800	-0.47810400

C	2.80449400	-4.78833400	-0.73791700
C	2.82332600	-2.36997100	-0.55612700
C	2.82499200	0.09419600	-0.38301500
C	1.42203400	-4.79399100	-0.67005200
H	3.33320600	-5.73334300	-0.84413700
C	1.39088900	-2.37913100	-0.49903400
C	1.36992000	0.09068600	-0.38237200
C	0.69382200	-3.60759200	-0.52710200
H	0.91237300	-5.74541400	-0.74274200
C	0.66817300	-1.13737600	-0.42263000
C	-0.76507500	-3.61106100	-0.41070900
C	-0.75704300	-1.14036000	-0.39640100
C	-1.49114000	-4.80542700	-0.31825400
C	-1.47129100	-2.38706400	-0.38016800
C	-1.46335900	0.08238900	-0.37158700
C	-2.87291500	-4.82026800	-0.24913600
H	-0.96719800	-5.75455000	-0.28940000
C	-2.90319300	-2.39537500	-0.31903800
C	-2.91696600	0.07774600	-0.35273700
C	-3.59583500	-3.62770000	-0.26154300
H	-3.38719300	-5.77475000	-0.18222800
C	-3.60526500	-1.15365100	-0.31991800
C	-5.06670000	-3.64473000	-0.20958000
C	-5.05950000	-1.16289800	-0.29017300
C	-5.78851600	-4.81883800	-0.14204200
C	-5.76859000	-2.38389100	-0.23533400
C	-5.76943600	0.06855100	-0.31628700
C	-7.21675000	-4.81586100	-0.10341000
H	-5.27823400	-5.78697800	-0.11679300
C	-7.20568300	-2.38109500	-0.20391900
C	-7.20697800	0.06405500	-0.29885600
C	-7.90797100	-3.63967600	-0.13541600
H	-7.73499700	-5.77460800	-0.04863700
C	-7.89714000	-1.16992800	-0.23928800
H	8.89507600	3.77453500	0.02163400
H	8.88867400	1.32976900	-0.23514700
H	8.89541300	-1.11154000	-0.50202400
H	8.91525600	-3.55579200	-0.76453900
H	-8.99825800	-3.62356600	-0.10879800
H	-8.99022400	-1.16735900	-0.21974800
H	-8.99928200	1.28397500	-0.33225100
H	-9.02548600	3.74023500	-0.43838300
C	1.54557600	0.21573100	3.15108500
C	0.02770200	0.41317100	3.11925600
C	0.54768700	-2.10221800	3.05581200
C	1.85461000	-1.28920900	2.96526000
H	2.03211700	0.82548600	2.37969400
H	1.92538100	0.55201700	4.12039400
H	-0.34681500	0.46971900	2.09403400
H	-0.29341700	1.30816900	3.65640900

H	0.67295700	-3.03774300	3.60473700
H	0.16274800	-2.34187900	2.06043100
H	2.55197400	-1.62033400	3.74023600
H	2.34062200	-1.47731000	2.00212700
S	-0.67601500	-1.06296200	3.92647600

Graphene-U5C

C	-4.98588500	1.36060600	-0.15711000
C	-5.69415700	2.58097000	-0.06727800
C	-3.53142100	1.35011100	-0.17961300
C	-7.82372300	1.36454900	-0.11768100
C	-7.13082900	2.57174600	-0.04644000
C	-4.99771300	3.84011300	0.00292800
C	-2.82974500	2.58749200	-0.11888700
C	-7.82940800	3.83143000	0.04855800
C	-5.71076800	5.01801900	0.09238900
C	-3.52500300	3.81906500	-0.02667800
C	-1.39642500	2.58719400	-0.15135500
C	-7.13750700	5.00600000	0.11546000
H	-5.20660000	5.98003400	0.14636100
C	-2.80057800	5.00798500	0.04156500
C	-0.68125700	1.34261600	-0.22481500
C	-0.69239600	3.81212200	-0.10243400
H	-7.65829400	5.96021900	0.18724400
C	-1.41694300	5.00381900	0.00757000
H	-3.32530300	5.95751000	0.12531000
C	0.74424500	1.33698700	-0.23475300
C	0.76936300	3.80700600	-0.15960900
H	-0.90514700	5.95416400	0.07749800
C	1.46706000	2.57667000	-0.19985400
C	1.50725100	4.99638800	-0.18005200
C	2.90069600	2.57569400	-0.21603300
C	2.89147400	5.00185100	-0.20341800
H	0.99416400	5.95171600	-0.18348800
C	3.59375200	1.33008800	-0.23030600
C	3.60435300	3.80460200	-0.21162800
H	3.41515700	5.95383000	-0.21448400
C	5.04948500	1.32963100	-0.21341100
C	5.07633500	3.81262700	-0.21795000
C	5.76805900	2.54522200	-0.20916300
C	5.80695200	4.98246900	-0.22574500
C	7.20528200	2.53251700	-0.19559600
H	5.30513000	5.95461400	-0.23514800
C	7.23601600	4.96920700	-0.22017500
C	7.91774100	3.78755100	-0.20340200
C	7.88726900	1.31604500	-0.17391200
H	7.76191700	5.92504100	-0.22802700
C	7.88606300	-3.62011000	-0.10001500
C	7.87672600	-1.14868700	-0.13963700
C	7.19456000	-4.79611900	-0.10080600

C	7.18452300	-2.35940800	-0.13841900
C	7.18694500	0.08654800	-0.17039500
C	5.76597100	-4.79792200	-0.14293900
H	7.71203600	-5.75609500	-0.07055200
C	5.74757600	-2.36061500	-0.17606100
C	5.75004200	0.09228300	-0.19751900
C	5.04555000	-3.62241100	-0.18123000
H	5.25623500	-5.76598300	-0.14486800
C	5.03934800	-1.13939900	-0.20634700
C	3.57455300	-3.60279500	-0.23339400
C	3.58408400	-1.12825000	-0.24800300
C	2.85169400	-4.79357000	-0.23274300
C	2.88156200	-2.36750300	-0.27662900
C	2.89526000	0.10423900	-0.25667100
C	1.46779500	-4.77684400	-0.29646300
H	3.36572300	-5.74931400	-0.17800200
C	1.44941000	-2.35731800	-0.33978400
C	1.44232400	0.10934000	-0.28084000
C	0.74280900	-3.58308100	-0.37332000
H	0.94476600	-5.72658700	-0.27091600
C	0.73610800	-1.11270700	-0.33698700
C	-0.71645900	-3.57861400	-0.45346400
C	-0.68878500	-1.10983300	-0.33291600
C	-1.44722100	-4.76502100	-0.57458900
C	-1.41248900	-2.34991900	-0.39745700
C	-1.39008300	0.11871500	-0.27606800
C	-2.83166600	-4.76219300	-0.58644800
H	-0.93993700	-5.71576100	-0.66978700
C	-2.84562800	-2.34294400	-0.40647100
C	-2.84450300	0.12333200	-0.26240300
C	-3.54882300	-3.57092800	-0.48907000
H	-3.36269500	-5.70785300	-0.67453800
C	-3.53965300	-1.10188000	-0.32568800
C	-5.02184900	-3.58463000	-0.48373800
C	-4.99389800	-1.10554900	-0.31622400
C	-5.74263700	-4.75878300	-0.55989000
C	-5.71002200	-2.32234700	-0.39141400
C	-5.69602200	0.12934300	-0.22739500
C	-7.16939200	-4.73963900	-0.54818700
H	-5.24473100	-5.72286400	-0.63088500
C	-7.14683600	-2.30602000	-0.37788700
C	-7.13792500	0.13276100	-0.21036600
C	-7.85366800	-3.56202300	-0.45989300
H	-7.69652700	-5.69098400	-0.61140600
C	-7.83177800	-1.09573500	-0.28684100
H	9.00788400	3.76331900	-0.19595300
H	8.97976900	1.30534000	-0.15903800
H	8.96910300	-1.14671900	-0.11542400
H	8.97597100	-3.60456300	-0.06993600
H	-8.94079000	-3.53800600	-0.44986700

H	-8.91823100	-1.08672300	-0.27526800
H	-8.91020800	1.36090700	-0.10340900
H	-8.91660000	3.81276900	0.06444100
C	-1.55282600	-1.29607000	2.97739500
H	-2.28499100	-1.16879600	2.16504200
H	-2.13852400	-1.29471800	3.90885900
C	-0.75018200	-2.55659000	2.83389100
H	-1.18846300	-3.54623600	2.76706400
C	0.55853700	-2.24775100	2.79405200
H	1.38114500	-2.94727300	2.69415400
C	-0.50423500	-0.22103200	2.98454100
H	-0.72602600	0.83779600	3.05612100
C	0.71204800	-0.78761200	2.88764000
H	1.66318500	-0.26740900	2.86441200

Graphene-U5N

C	-5.07751100	1.30925600	-0.17430100
C	-5.79965900	2.52394200	-0.16268700
C	-3.62285500	1.31313900	-0.20401100
C	-7.91522300	1.28933500	-0.10554700
C	-7.23653400	2.50815700	-0.13147900
C	-5.11112200	3.79197100	-0.18219000
C	-2.93297200	2.56244200	-0.20618100
C	-7.95242800	3.76073100	-0.12675200
C	-5.84542500	4.96024600	-0.17724800
C	-3.63931600	3.78812600	-0.20037900
C	-1.49946300	2.56729800	-0.21066800
C	-7.27374900	4.94443100	-0.15049400
H	-5.34485300	5.93385200	-0.19275700
C	-2.93012000	4.98864700	-0.21582700
C	-0.77290600	1.32742200	-0.24766200
C	-0.80560500	3.79826800	-0.18907900
H	-7.80221000	5.89919300	-0.14827400
C	-1.54695200	4.98684400	-0.21276100
H	-3.45650900	5.93885000	-0.22924200
C	0.65070600	1.33746400	-0.26155400
C	0.65639800	3.80830500	-0.14227200
H	-1.03583600	5.94283200	-0.23507000
C	1.36329300	2.58648700	-0.19230500
C	1.37791800	5.00348900	-0.03576700
C	2.79614800	2.59073100	-0.15882100
C	2.76054700	5.01116000	-0.00414400
H	0.86294900	5.95208400	0.03632900
C	3.50111800	1.35233500	-0.21086600
C	3.48821500	3.82262700	-0.06931600
H	3.28415600	5.96163500	0.07805400
C	4.95477100	1.36622100	-0.17634300
C	4.96123900	3.84732600	-0.03438300
C	5.65979600	2.59004300	-0.08909900
C	5.67021600	5.02873100	0.04884900

C	7.09615600	2.58293300	-0.05604400
H	5.16378300	5.98943100	0.09000000
C	7.09595800	5.01883500	0.08220700
C	7.79093000	3.84474700	0.03246700
C	7.79198200	1.37612000	-0.10877500
H	7.61506700	5.97432200	0.14828600
C	7.83366600	-3.55378000	-0.40010900
C	7.80628900	-1.08574400	-0.25237500
C	7.15193200	-4.73360400	-0.48382900
C	7.12463700	-2.29817100	-0.33843100
C	7.11087000	0.14240500	-0.19640800
C	5.72618400	-4.75654100	-0.50940400
H	7.68197200	-5.68413800	-0.53279200
C	5.68791200	-2.31832100	-0.36638000
C	5.66752600	0.13606500	-0.22812900
C	5.00378800	-3.58173300	-0.45193600
H	5.23080500	-5.72136000	-0.57702000
C	4.96896300	-1.10082600	-0.31396500
C	3.53036300	-3.57048600	-0.46922600
C	3.51570900	-1.09997800	-0.33832100
C	2.81641900	-4.76771400	-0.53793200
C	2.82354500	-2.34488600	-0.41638300
C	2.81725600	0.12449300	-0.29513600
C	1.43353000	-4.77399200	-0.53399800
H	3.35199900	-5.71357200	-0.59304900
C	1.39044800	-2.35505500	-0.42051700
C	1.36202000	0.11627000	-0.31749900
C	0.69795600	-3.58462900	-0.45647500
H	0.93040600	-5.72992500	-0.59122600
C	0.66376600	-1.11418300	-0.36000600
C	-0.76213900	-3.59144700	-0.38470300
C	-0.75861200	-1.12128500	-0.33191500
C	-1.48780100	-4.78888300	-0.34702300
C	-1.46948500	-2.36953200	-0.32866800
C	-1.46751700	0.09819200	-0.27165200
C	-2.86925200	-4.80905500	-0.27833500
H	-0.96594400	-5.73903300	-0.36449100
C	-2.90157200	-2.38313600	-0.26286000
C	-2.92178600	0.08954800	-0.23217300
C	-3.59243500	-3.61771400	-0.23993400
H	-3.38244100	-5.76618300	-0.25244800
C	-3.60718600	-1.14393600	-0.22139000
C	-5.06281000	-3.64065600	-0.17576800
C	-5.06137800	-1.15818600	-0.17494300
C	-5.78112300	-4.81837300	-0.14193400
C	-5.76762700	-2.38181900	-0.15092900
C	-5.77489000	0.07103400	-0.15467600
C	-7.20883700	-4.82123200	-0.08718200
H	-5.26784700	-5.78543000	-0.15697300
C	-7.20428500	-2.38460300	-0.10150600

C	-7.21207900	0.06184900	-0.11503400
C	-7.90304300	-3.64656300	-0.06893900
H	-7.72405100	-5.78287500	-0.06129100
C	-7.89888800	-1.17496300	-0.08617700
H	8.87768700	3.82850600	0.05707000
H	8.87773400	1.37522300	-0.08458600
H	8.89198000	-1.07472800	-0.23015000
H	8.92026300	-3.52779500	-0.37965300
H	-8.99303900	-3.63430900	-0.02906200
H	-8.99177700	-1.17593900	-0.05128400
H	-9.00823100	1.27643400	-0.07785900
H	-9.04265500	3.73431800	-0.10408000
C	0.92186700	-0.18016200	2.83227200
C	-0.33611400	-0.70879100	3.00052900
C	-0.21449500	-2.12487900	2.91270800
C	1.11396100	-2.40698900	2.69573300
N	1.79347200	-1.22063800	2.65503400
H	2.77235500	-1.12265000	2.42365400
H	1.26865700	0.84344100	2.80807600
H	-1.24189500	-0.14359500	3.16545800
H	-1.00824500	-2.85285500	2.99835400
H	1.62860100	-3.34615800	2.54714300

Graphene-U5O

C	-5.07084400	1.31734900	-0.18536600
C	-5.78971800	2.53413800	-0.17544700
C	-3.61612800	1.31766500	-0.20824200
C	-7.90843400	1.29924800	-0.13314600
C	-7.22631600	2.51437600	-0.15345900
C	-5.10378700	3.80156900	-0.18773000
C	-2.92519700	2.56150400	-0.20210100
C	-7.93619200	3.77147600	-0.15259000
C	-5.82766900	4.97600000	-0.18685200
C	-3.63092200	3.79122300	-0.19524700
C	-1.49154900	2.57108100	-0.19890300
C	-7.25472300	4.95370300	-0.17037700
H	-5.33175600	5.94414900	-0.19792100
C	-2.91697400	4.98787800	-0.19961300
C	-0.76613100	1.33144300	-0.23566800
C	-0.79781800	3.80299900	-0.17119200
H	-7.78358000	5.90622800	-0.17134800
C	-1.53260500	4.99305600	-0.18984000
H	-3.45009300	5.93627800	-0.21007800
C	0.66030800	1.33754900	-0.24139900
C	0.66408900	3.80627900	-0.12279600
H	-1.02839300	5.94992700	-0.20424400
C	1.37228000	2.58143400	-0.17268900
C	1.39163000	4.99682500	-0.01627200
C	2.80583700	2.59034100	-0.14123800
C	2.77589800	5.01176100	0.01404000

H	0.87115300	5.94548000	0.05419800
C	3.50930100	1.35189100	-0.19775400
C	3.49897300	3.82285200	-0.05370300
H	3.29121200	5.96500400	0.09528000
C	4.96503900	1.36349800	-0.17202300
C	4.97048200	3.84252700	-0.02651500
C	5.67282100	2.58238900	-0.08923300
C	5.69014600	5.01624800	0.05430200
C	7.10995100	2.58117000	-0.06652000
H	5.18018600	5.98260000	0.10217000
C	7.11909400	5.01399600	0.07809900
C	7.81107600	3.83973700	0.01978700
C	7.80308500	1.37261400	-0.12822600
H	7.63643600	5.97213600	0.14352500
C	7.84795000	-3.55438500	-0.42433600
C	7.81550300	-1.08746600	-0.27605600
C	7.16750800	-4.73420500	-0.50192600
C	7.13439400	-2.30159900	-0.35660800
C	7.11387600	0.13971400	-0.21191500
C	5.73843500	-4.74831000	-0.51536900
H	7.69426700	-5.68797700	-0.55461200
C	5.69718200	-2.31469600	-0.37277900
C	5.67693100	0.13372300	-0.23215800
C	5.00720800	-3.58073200	-0.45200600
H	5.23804100	-5.71880000	-0.57766700
C	4.97711400	-1.10183300	-0.31216000
C	3.53539000	-3.57316400	-0.45957600
C	3.52095900	-1.10254400	-0.32862000
C	2.82467700	-4.76920800	-0.52789700
C	2.82946900	-2.34561600	-0.40096700
C	2.82114800	0.12225000	-0.27642600
C	1.43912100	-4.76626300	-0.52078300
H	3.34993100	-5.71863800	-0.58810300
C	1.39613100	-2.34905000	-0.40001500
C	1.36908100	0.11549400	-0.29466000
C	0.70005500	-3.58170900	-0.43792700
H	0.92875900	-5.72109400	-0.58211400
C	0.67176700	-1.11255400	-0.34630300
C	-0.76034900	-3.59257400	-0.36830400
C	-0.75418000	-1.12148400	-0.32567600
C	-1.48127000	-4.79023800	-0.32120000
C	-1.46642100	-2.36809300	-0.32746800
C	-1.46522900	0.10114300	-0.26996700
C	-2.86456200	-4.80027200	-0.26120300
H	-0.96707100	-5.74188800	-0.32366700
C	-2.89881900	-2.37402300	-0.26533300
C	-2.91882900	0.09353600	-0.23624600
C	-3.59103200	-3.61144000	-0.23875600
H	-3.38647200	-5.75448700	-0.22930200
C	-3.60311000	-1.13828700	-0.22957000

C	-5.06274900	-3.63805000	-0.18412600
C	-5.05725700	-1.15380800	-0.18763900
C	-5.77307300	-4.82039700	-0.15493900
C	-5.76254200	-2.37833000	-0.16563800
C	-5.77030500	0.07792800	-0.17067800
C	-7.19964500	-4.81378400	-0.10925700
H	-5.26665000	-5.78302600	-0.16741600
C	-7.19887500	-2.37432200	-0.12458300
C	-7.21116800	0.07000200	-0.13878600
C	-7.89423600	-3.63916600	-0.09557300
H	-7.71749000	-5.77207500	-0.08678400
C	-7.89452000	-1.16678100	-0.11390100
H	8.90112200	3.82379400	0.03684600
H	8.89527300	1.37052200	-0.11194000
H	8.90763600	-1.07624100	-0.26178000
H	8.93788200	-3.52944600	-0.41193900
H	-8.98126200	-3.62421000	-0.06262900
H	-8.98104300	-1.16641400	-0.08611400
H	-8.99508200	1.28696300	-0.11319000
H	-9.02340500	3.74453900	-0.13806100
C	0.80118600	-0.22871600	2.86300600
C	-0.44403600	-0.75651200	2.96598800
C	-0.27904400	-2.17898100	2.86535000
C	1.05231700	-2.38890700	2.71110200
O	1.72442000	-1.21113400	2.70825200
H	1.18526200	0.77992200	2.86869900
H	-1.36995000	-0.20991400	3.08064700
H	-1.05377200	-2.93292100	2.88886100
H	1.65657100	-3.27399900	2.58146600

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C	-5.09303900	1.32401900	-0.23987800
C	-5.81387900	2.54027100	-0.23316200
C	-3.63866800	1.32689500	-0.26167800
C	-7.93049400	1.30100200	-0.19125100
C	-7.25044900	2.51738400	-0.21484500
C	-5.13032400	3.80836500	-0.24483300
C	-2.94953800	2.57250900	-0.25039900
C	-7.96213100	3.77330600	-0.22054000
C	-5.85572500	4.98212200	-0.25007600
C	-3.65717300	3.80047300	-0.24388200
C	-1.51602100	2.58432900	-0.23934900
C	-7.28243700	4.95675100	-0.23955600
H	-5.36154700	5.95072100	-0.26144200
C	-2.94460400	4.99852100	-0.24034800
C	-0.78832000	1.34534300	-0.28030500
C	-0.82420400	3.81634600	-0.20084100
H	-7.81327400	5.90810300	-0.24575600
C	-1.56059200	5.00588200	-0.22114100
H	-3.47955000	5.94595700	-0.25205500

C	0.63728500	1.35329600	-0.28019800
C	0.63748900	3.82092200	-0.14166400
H	-1.05730800	5.96331600	-0.23086900
C	1.34749600	2.59820500	-0.20055700
C	1.36292400	5.01133000	-0.01558500
C	2.78092200	2.60883100	-0.16688100
C	2.74681200	5.02786300	0.01952200
H	0.84027800	5.95792600	0.06694500
C	3.48640000	1.37159800	-0.24079400
C	3.47185900	3.84059500	-0.06311100
H	3.26021800	5.98069100	0.11516800
C	4.94207100	1.38531500	-0.22496300
C	4.94349800	3.86150800	-0.03652800
C	5.64806200	2.60428300	-0.12512300
C	5.66196500	5.03447200	0.06551800
C	7.08532200	2.60533400	-0.11084200
H	5.15016300	5.99896900	0.13456400
C	7.09093200	5.03452900	0.08388800
C	7.78476300	3.86296000	-0.00215600
C	7.78016600	1.39936700	-0.20230200
H	7.60693100	5.99213700	0.16728300
C	7.83163700	-3.52059300	-0.60362700
C	7.79584100	-1.05729700	-0.40270900
C	7.15252300	-4.70018200	-0.69647300
C	7.11639400	-2.27127300	-0.50086100
C	7.09279600	0.16701100	-0.30590900
C	5.72347200	-4.71713800	-0.69015300
H	7.68050500	-5.65156300	-0.77596400
C	5.67904500	-2.28734500	-0.49961100
C	5.65562400	0.15846300	-0.31289400
C	4.99022600	-3.55292800	-0.59351900
H	5.22380500	-5.68761500	-0.76398700
C	4.95769800	-1.07686300	-0.40792800
C	3.51830000	-3.54956900	-0.57675600
C	3.50183900	-1.08081300	-0.40615200
C	2.80816900	-4.74580800	-0.65805300
C	2.81194800	-2.32536800	-0.48528600
C	2.80039700	0.14206200	-0.33065800
C	1.42360400	-4.74541400	-0.62422800
H	3.33318800	-5.69258000	-0.75099000
C	1.37913800	-2.33147200	-0.45646300
C	1.34760000	0.13297000	-0.33728000
C	0.68502200	-3.56342800	-0.49795900
H	0.91126300	-5.69776700	-0.70740900
C	0.65244100	-1.09567000	-0.38929400
C	-0.77396400	-3.57743100	-0.40401600
C	-0.77239300	-1.10653800	-0.37841600
C	-1.48971500	-4.77648000	-0.31880200
C	-1.48292500	-2.35530000	-0.37775500
C	-1.48540200	0.11458700	-0.32385800

C	-2.87270500	-4.78938100	-0.25549800
H	-0.97005500	-5.72490800	-0.28940100
C	-2.91469400	-2.36387000	-0.30938800
C	-2.93948900	0.10433300	-0.29105500
C	-3.60342200	-3.60220200	-0.26173800
H	-3.39183400	-5.74387900	-0.19612000
C	-3.62141500	-1.12861300	-0.27963600
C	-5.07530800	-3.63143900	-0.20784700
C	-5.07491600	-1.14693300	-0.23292800
C	-5.78265000	-4.81559200	-0.16990900
C	-5.77737300	-2.37347200	-0.20054900
C	-5.79015100	0.08348200	-0.22147900
C	-7.20891800	-4.81088500	-0.12536300
H	-5.27440800	-5.77685300	-0.17498700
C	-7.21374600	-2.37142100	-0.15972000
C	-7.23172800	0.07295000	-0.19001300
C	-7.90612100	-3.63754300	-0.12126800
H	-7.72516100	-5.76980400	-0.09595900
C	-7.91186100	-1.16519000	-0.15799500
H	8.87505700	3.84895300	0.00930100
H	8.87279200	1.39941200	-0.19410800
H	8.88840900	-1.04421300	-0.40005200
H	8.92174200	-3.49367100	-0.60510900
H	-8.99301500	-3.62463900	-0.08919500
H	-8.99808100	-1.16701600	-0.13130400
H	-9.01683500	1.28704900	-0.17359800
H	-9.04916300	3.74459600	-0.20995600
C	0.65327300	-0.02799000	2.94716400
C	-0.59222800	-0.57232300	2.86003100
C	-0.56149900	-2.00186800	2.79029900
C	0.70663300	-2.49830300	2.82587700
H	0.92352700	1.01800900	2.99816900
H	-1.50321700	0.01679100	2.82734000
H	-1.44644400	-2.62379700	2.69912300
H	1.02266300	-3.53128300	2.77677700
S	1.88132300	-1.23988300	2.95467500

Graphene-U6C

C	-4.95258000	1.37051900	-0.26590000
C	-5.66088600	2.59104100	-0.22445200
C	-3.49636700	1.35812200	-0.28022700
C	-7.79111300	1.38086900	-0.24470700
C	-7.09821300	2.59063500	-0.21662500
C	-4.95890300	3.85241300	-0.18888800
C	-2.79317000	2.59690400	-0.23759400
C	-7.79972300	3.85145800	-0.17884400
C	-5.67875300	5.02819800	-0.15360300
C	-3.48716300	3.83127700	-0.19025300
C	-1.35910100	2.58663900	-0.24005900
C	-7.10794400	5.02683500	-0.14912500

H	-5.16903600	5.99541500	-0.12772900
C	-2.76508700	5.02150200	-0.14259100
C	-0.64713100	1.34229700	-0.29459400
C	-0.65163800	3.81192600	-0.18487100
H	-7.62553100	5.98664100	-0.12094800
C	-1.38060900	5.00540000	-0.13831500
H	-3.28170300	5.97682900	-0.10487800
C	0.77915700	1.33559000	-0.27458100
C	0.81101900	3.80639600	-0.17093600
H	-0.86212000	5.95656500	-0.09473700
C	1.50452200	2.57430200	-0.20695400
C	1.54712900	4.99468000	-0.11700600
C	2.93808300	2.56364400	-0.17623600
C	2.93093200	4.98842200	-0.09029500
H	1.04478100	5.95227300	-0.09349500
C	3.62922400	1.31997100	-0.20483100
C	3.64408800	3.79166500	-0.11539200
H	3.46396500	5.93590700	-0.04639300
C	5.08378800	1.31895900	-0.16741100
C	5.11635500	3.80135400	-0.07796300
C	5.80243800	2.53432600	-0.10491900
C	5.83952000	4.97467500	-0.01707800
C	7.23870300	2.51417900	-0.06802600
H	5.34316100	5.94255200	0.00397400
C	7.26615600	4.95189700	0.02012000
C	7.94792600	3.76996500	-0.00389000
C	7.92142200	1.29953200	-0.09455200
H	7.79433300	5.90360000	0.06821400
C	7.91142500	-3.63461600	-0.28707200
C	7.90927900	-1.16432400	-0.18847800
C	7.21791200	-4.80814900	-0.35193800
C	7.21465300	-2.37070300	-0.25351700
C	7.22471000	0.07167700	-0.15850300
C	5.79105800	-4.81416000	-0.38727000
H	7.73673000	-5.76583300	-0.37830500
C	5.77817500	-2.37401000	-0.28902100
C	5.78400800	0.08020800	-0.19456800
C	5.07945100	-3.63259600	-0.35703700
H	5.28524100	-5.77589600	-0.43917500
C	5.07168300	-1.15034500	-0.25873400
C	3.60727300	-3.60562800	-0.39082800
C	3.61736300	-1.13429400	-0.29321700
C	2.88202600	-4.79351200	-0.46030500
C	2.91343300	-2.36955500	-0.35821700
C	2.93183200	0.09710300	-0.26891300
C	1.49803700	-4.78362800	-0.48115100
H	3.40569300	-5.74647600	-0.49906200
C	1.48002000	-2.36311700	-0.38899600
C	1.47838900	0.10530500	-0.31032600
C	0.77417800	-3.58730800	-0.43226200

H	0.98558400	-5.73412000	-0.54488000
C	0.76712900	-1.11678200	-0.36954400
C	-0.68763500	-3.57843900	-0.41651000
C	-0.65883500	-1.10838500	-0.38370500
C	-1.42589300	-4.76601100	-0.38009000
C	-1.38315800	-2.34581300	-0.40787900
C	-1.35569600	0.12024400	-0.34708900
C	-2.81102900	-4.76991300	-0.36356900
H	-0.91512900	-5.72216800	-0.35506600
C	-2.81618300	-2.34306800	-0.38637500
C	-2.80777800	0.12721800	-0.33278200
C	-3.52174700	-3.57207200	-0.37472500
H	-3.33620400	-5.72103300	-0.33937900
C	-3.50773700	-1.09873100	-0.35304700
C	-4.99362800	-3.58019400	-0.36654200
C	-4.96415300	-1.09789300	-0.32926700
C	-5.72419300	-4.74971700	-0.38413800
C	-5.68399600	-2.31219800	-0.34267800
C	-5.66436900	0.13948800	-0.29293500
C	-7.15332900	-4.73547300	-0.37643000
H	-5.22341600	-5.72167800	-0.40509400
C	-7.12123500	-2.29894000	-0.33152000
C	-7.10135900	0.14591500	-0.28027600
C	-7.83429500	-3.55372400	-0.35061500
H	-7.67967500	-5.69079000	-0.39185200
C	-7.80277700	-1.08281400	-0.30249600
H	9.03490200	3.74237800	0.02412100
H	9.00796800	1.28666100	-0.06678800
H	8.99589200	-1.16421400	-0.16106200
H	8.99865400	-3.61988300	-0.25977000
H	-8.92421000	-3.52857700	-0.34399200
H	-8.89486400	-1.07114100	-0.29545900
H	-8.88328600	1.37915300	-0.23842600
H	-8.88985000	3.83606900	-0.17483100
H	-3.12475700	-1.15371500	2.81053900
C	-2.03894900	-1.17519400	2.81981900
C	-1.31861000	0.01691700	2.85332300
C	-1.36624500	-2.39447200	2.78277200
C	0.07465400	-0.00945200	2.84626400
H	-1.84347800	0.96851400	2.86258000
C	0.02701800	-2.42206400	2.77464100
H	-1.92825600	-3.32351800	2.73682100
C	0.74665700	-1.22942600	2.80873700
H	0.63830900	0.92001300	2.85527800
H	0.55431500	-3.37139700	2.72655000
H	1.83428200	-1.24981500	2.77886400

Graphene-U6N

C	-5.07770300	1.32098400	-0.16980500
C	-5.79565200	2.53873600	-0.10747000

C	-3.62425200	1.32141400	-0.21418800
C	-7.91482100	1.30263700	-0.08083500
C	-7.23165500	2.51744700	-0.06372400
C	-5.11035600	3.80416900	-0.08804100
C	-2.93227200	2.56688500	-0.18946300
C	-7.93928700	3.77385600	-0.00235700
C	-5.83126400	4.97989900	-0.02987200
C	-3.63749700	3.79353700	-0.12862900
C	-1.49894400	2.57791800	-0.22148500
C	-7.25662400	4.95603200	0.01285800
H	-5.33476900	5.94653500	-0.01550200
C	-2.92321800	4.99114000	-0.10402600
C	-0.77310300	1.33640000	-0.28923300
C	-0.80505400	3.80797700	-0.18666300
H	-7.78532500	5.90740800	0.05820200
C	-1.54048400	4.99802700	-0.13127300
H	-3.45771900	5.93808300	-0.05914600
C	0.65147300	1.34172400	-0.30340900
C	0.65810900	3.81186100	-0.20012700
H	-1.03780600	5.95530900	-0.10585600
C	1.36479200	2.58883800	-0.24850200
C	1.38820200	5.00714300	-0.15842200
C	2.79855200	2.59822100	-0.23862700
C	2.77076100	5.02286500	-0.15489900
H	0.86872100	5.95812600	-0.12477700
C	3.50191300	1.35566700	-0.27353100
C	3.49226400	3.82982000	-0.19090000
H	3.28750300	5.97783100	-0.11959700
C	4.95628900	1.36746200	-0.25012900
C	4.96384200	3.84925300	-0.17612600
C	5.66584800	2.58906900	-0.20278400
C	5.68545500	5.02487000	-0.13475700
C	7.10271700	2.58833800	-0.18040100
H	5.17421100	5.99279600	-0.11496800
C	7.11373000	5.02396700	-0.11533500
C	7.80517800	3.84744000	-0.13630700
C	7.79494400	1.37665900	-0.20020700
H	7.63198200	5.98367200	-0.08249300
C	7.83723400	-3.55690100	-0.31959900
C	7.80582600	-1.08638500	-0.26115500
C	7.15576300	-4.73852200	-0.35972500
C	7.12425500	-2.30263700	-0.30356800
C	7.10501400	0.14292300	-0.24459100
C	5.72739800	-4.75021100	-0.38535500
H	7.68181900	-5.69444900	-0.37210700
C	5.68700000	-2.31440800	-0.33037800
C	5.66729300	0.13722700	-0.27108300
C	4.99585600	-3.58013400	-0.37147300
H	5.22443500	-5.72224300	-0.41630900
C	4.96664400	-1.09864300	-0.31782800

C	3.52450600	-3.57187000	-0.39623100
C	3.51228300	-1.09932600	-0.34524900
C	2.81386700	-4.77236900	-0.41604700
C	2.82012700	-2.34590700	-0.39650800
C	2.81383800	0.12634700	-0.33043700
C	1.43145900	-4.76773300	-0.43757800
H	3.33896000	-5.72338700	-0.41052200
C	1.38715800	-2.34805300	-0.42418700
C	1.35921900	0.12043500	-0.35391000
C	0.69173400	-3.57739700	-0.44525100
H	0.91985300	-5.72362700	-0.44180100
C	0.66189000	-1.10701400	-0.39612000
C	-0.77090300	-3.58723400	-0.44623600
C	-0.76193400	-1.11530300	-0.38768100
C	-1.49532100	-4.78565500	-0.47276300
C	-1.47622700	-2.36436500	-0.40279300
C	-1.47302100	0.10678200	-0.32484100
C	-2.87797400	-4.79374200	-0.44305500
H	-0.98373000	-5.73732900	-0.52221600
C	-2.90966300	-2.36939300	-0.36217900
C	-2.92837100	0.09905000	-0.27955700
C	-3.60346100	-3.60391800	-0.38202300
H	-3.40397400	-5.74629900	-0.46604900
C	-3.61340000	-1.13196800	-0.29656400
C	-5.07601400	-3.63117600	-0.33883400
C	-5.06635900	-1.14804800	-0.25231100
C	-5.78596100	-4.81486600	-0.35941200
C	-5.77295700	-2.37377900	-0.27181900
C	-5.77789700	0.08262100	-0.18816300
C	-7.21139600	-4.80699700	-0.31439400
H	-5.28072000	-5.77552300	-0.41155800
C	-7.20925400	-2.36865200	-0.22675900
C	-7.22069900	0.07434700	-0.14316400
C	-7.90507400	-3.63294200	-0.24975300
H	-7.73131000	-5.76410000	-0.33329900
C	-7.90347100	-1.16190900	-0.16270100
H	8.89572700	3.83215100	-0.12014100
H	8.88819000	1.37513000	-0.18058900
H	8.89899000	-1.07595800	-0.23923100
H	8.92757200	-3.53330000	-0.29829400
H	-8.99152200	-3.61820300	-0.21525700
H	-8.98888700	-1.16201300	-0.12855500
H	-9.00022600	1.29058800	-0.04735100
H	-9.02559100	3.74675100	0.03034700
C	1.30691300	-0.06363600	2.80867400
C	-0.08521500	-0.01257600	2.82359200
C	-0.79059700	-1.21098800	2.78857000
C	-0.07400400	-2.40272300	2.74414700
C	1.31735400	-2.33854200	2.73494900
N	2.01090300	-1.19757400	2.76401700

H	-1.87881100	-1.21542600	2.76967400
H	1.88764500	0.85731300	2.81481600
H	-0.59973200	0.94373000	2.84367300
H	-0.58052500	-3.36228900	2.69773400
H	1.90667100	-3.25263300	2.68313600

Graphene-U6O

C	-5.03302200	1.34599100	-0.18038400
C	-5.74638400	2.56463400	-0.10374000
C	-3.57909800	1.34165900	-0.22130600
C	-7.87024400	1.33721200	-0.09853300
C	-7.18252300	2.54889900	-0.06189300
C	-5.05567700	3.82789800	-0.06795800
C	-2.88270200	2.58328800	-0.18691300
C	-7.88593600	3.80689500	0.01745200
C	-5.77308600	5.00438300	0.00692300
C	-3.58328600	3.81281700	-0.11274900
C	-1.44942100	2.58934600	-0.22591200
C	-7.19908500	4.98598200	0.04997500
H	-5.27296200	5.96948000	0.03444900
C	-2.86472500	5.00688500	-0.07806800
C	-0.72884600	1.34687800	-0.29462400
C	-0.75115500	3.81781700	-0.19067100
H	-7.72374700	5.93889900	0.10930400
C	-1.48156700	5.00889200	-0.11412900
H	-3.39451900	5.95545200	-0.01769700
C	0.69645300	1.34721300	-0.30853300
C	0.71143400	3.81758300	-0.22297400
H	-0.97516400	5.96370300	-0.07486200
C	1.41395800	2.59014200	-0.26259300
C	1.44575100	5.00968000	-0.21058300
C	2.84786000	2.59438500	-0.25508600
C	2.82957400	5.02020100	-0.21238300
H	0.92998300	5.96339700	-0.19867000
C	3.54619100	1.35047800	-0.27226000
C	3.54672000	3.82517300	-0.22671400
H	3.35000800	5.97390400	-0.19875000
C	5.00138900	1.35636800	-0.24151600
C	5.01846200	3.83917500	-0.21060000
C	5.71515800	2.57488200	-0.21181000
C	5.74424800	5.01212600	-0.19020200
C	7.15210100	2.56818300	-0.18283600
H	5.23808600	5.98223900	-0.19120300
C	7.17292800	5.00490800	-0.16596000
C	7.85939100	3.82573400	-0.16059800
C	7.83919800	1.35420700	-0.17642500
H	7.69489900	5.96284100	-0.15084800
C	7.86040200	-3.58144400	-0.21395400
C	7.83965200	-1.11007700	-0.19400700
C	7.17449700	-4.76039700	-0.24745300

C	7.15302800	-2.32363700	-0.22502000
C	7.14416900	0.12222800	-0.20307500
C	5.74633800	-4.76727700	-0.29553700
H	7.69640200	-5.71843800	-0.23893900
C	5.71630700	-2.33007700	-0.26945500
C	5.70725000	0.12220900	-0.24028400
C	5.02050100	-3.59426200	-0.30750800
H	5.24075500	-5.73729900	-0.32345400
C	5.00179700	-1.11179800	-0.27643900
C	3.54974900	-3.57983700	-0.36116900
C	3.54667500	-1.10634600	-0.32057000
C	2.83393900	-4.77546500	-0.39515500
C	2.85023500	-2.34892300	-0.37432300
C	2.85293700	0.12280900	-0.31870300
C	1.45060400	-4.76498600	-0.44776200
H	3.35444100	-5.72909700	-0.37691500
C	1.41795600	-2.34455500	-0.42823600
C	1.39995300	0.12224400	-0.35241000
C	0.71727200	-3.57298600	-0.47167500
H	0.93474200	-5.71876500	-0.45639700
C	0.69873200	-1.10251700	-0.40674800
C	-0.74437500	-3.57581500	-0.50351700
C	-0.72599800	-1.10564500	-0.39493300
C	-1.47294500	-4.76824800	-0.58199800
C	-1.44482600	-2.35039000	-0.43969900
C	-1.43274500	0.11959300	-0.33373200
C	-2.85637700	-4.77138200	-0.56295900
H	-0.96495600	-5.71958000	-0.66401600
C	-2.87851100	-2.35024700	-0.41541200
C	-2.88748500	0.11732900	-0.29658600
C	-3.57725300	-3.58157400	-0.46928700
H	-3.38518000	-5.72068900	-0.62139600
C	-3.57724500	-1.11145600	-0.33344400
C	-5.04972800	-3.60300800	-0.43242800
C	-5.03092900	-1.12204100	-0.29912600
C	-5.76537900	-4.78216200	-0.47687300
C	-5.74240000	-2.34339000	-0.34429900
C	-5.73799700	0.11050700	-0.21869100
C	-7.19145400	-4.76997200	-0.43634700
H	-5.26377000	-5.74443300	-0.54412200
C	-7.17875400	-2.33387900	-0.30439900
C	-7.17977300	0.10728600	-0.17862000
C	-7.88022200	-3.59450400	-0.35267800
H	-7.71478500	-5.72472500	-0.47407800
C	-7.86833900	-1.12561700	-0.22128400
H	8.94952700	3.80584900	-0.14000600
H	8.93169200	1.34792100	-0.15083600
H	8.93196600	-1.10377800	-0.16199400
H	8.95015300	-3.56173200	-0.17806100
H	-8.96697700	-3.57583200	-0.32129300

H	-8.95431300	-1.12178900	-0.19017800
H	-8.95621300	1.32859500	-0.06700700
H	-8.97261100	3.78337400	0.04955000
C	0.84042300	-0.04787800	2.73996700
C	-0.48212600	-0.01195100	2.87562300
C	-1.32767600	-1.25682700	2.93072700
C	-0.43923800	-2.46028900	2.75845300
C	0.88167000	-2.36544300	2.62885300
H	-1.87465900	-1.31156200	3.88425400
H	1.47353300	0.83060700	2.69545000
H	-0.96102800	0.96070000	2.94303800
H	-0.88415100	-3.45060600	2.72966600
H	1.54532700	-3.21260500	2.49873800
O	1.58915500	-1.19125200	2.61983000
H	-2.10792700	-1.23289400	2.15227200

Graphene-U6S

C	-5.05948000	1.35338000	-0.25639400
C	-5.77684600	2.57240900	-0.21578100
C	-3.60598000	1.35273400	-0.29628800
C	-7.89628200	1.33725300	-0.16847100
C	-7.21292200	2.55216200	-0.17525700
C	-5.09094600	3.83771900	-0.21596900
C	-2.91297800	2.59829000	-0.28018500
C	-7.92030400	3.80973100	-0.14183200
C	-5.81169600	5.01452900	-0.18442100
C	-3.61770600	3.82587700	-0.24427900
C	-1.47951500	2.60738700	-0.29491500
C	-7.23726400	4.99179500	-0.14814000
H	-5.31497200	5.98113100	-0.18621700
C	-2.90246200	5.02337200	-0.23479000
C	-0.75447000	1.36512900	-0.34918700
C	-0.78468400	3.83678400	-0.25824600
H	-7.76587200	5.94402900	-0.12476800
C	-1.51942900	5.02845000	-0.24181700
H	-3.43669200	5.97134400	-0.21785000
C	0.66950600	1.36859800	-0.34921800
C	0.67812800	3.83812300	-0.22968000
H	-1.01540700	5.98542000	-0.23555800
C	1.38376500	2.61425300	-0.27711700
C	1.40848600	5.03062500	-0.14223600
C	2.81711800	2.62078000	-0.24084200
C	2.79085600	5.04336200	-0.10929300
H	0.88954300	5.98113900	-0.09016100
C	3.51935000	1.37794600	-0.28856300
C	3.51144500	3.85020200	-0.15792700
H	3.30785300	5.99633800	-0.03990900
C	4.97382200	1.38718400	-0.25486200
C	4.98273100	3.86643200	-0.11766900
C	5.68376800	2.60621700	-0.16920600

C	5.70500100	5.03909700	-0.03219200
C	7.12049100	2.60290200	-0.13264700
H	5.19472400	6.00688500	0.00854300
C	7.13306300	5.03548100	0.00640000
C	7.82356800	3.85935200	-0.04200900
C	7.81175800	1.39186700	-0.18510700
H	7.65169700	5.99308600	0.07535900
C	7.85138700	-3.53438900	-0.48635800
C	7.82112300	-1.06785500	-0.33259100
C	7.16945100	-4.71302700	-0.57532500
C	7.13901000	-2.28123500	-0.42330000
C	7.12124900	0.16067400	-0.27484800
C	5.74108500	-4.72297000	-0.60565700
H	7.69508200	-5.66806600	-0.62390300
C	5.70184500	-2.29123100	-0.45423700
C	5.68379000	0.15717500	-0.30787800
C	5.01001800	-3.55406200	-0.54757600
H	5.23775600	-5.69274800	-0.67616800
C	4.98263900	-1.07625300	-0.39550800
C	3.53846400	-3.54462100	-0.57241000
C	3.52793200	-1.07531300	-0.41934700
C	2.82663800	-4.74100700	-0.66463300
C	2.83507000	-2.31978000	-0.50828800
C	2.83075800	0.15092400	-0.37210600
C	1.44388100	-4.73562700	-0.67342500
H	3.35103000	-5.69021200	-0.73013000
C	1.40173300	-2.32048900	-0.51788400
C	1.37619500	0.14622100	-0.39786400
C	0.70512200	-3.54811100	-0.58387200
H	0.93198100	-5.68818300	-0.75212000
C	0.67813300	-1.07979200	-0.45810900
C	-0.75640000	-3.55838200	-0.53960600
C	-0.74504600	-1.08677600	-0.44896700
C	-1.48003800	-4.75719900	-0.53002000
C	-1.46072000	-2.33563000	-0.47797200
C	-1.45524900	0.13625400	-0.38974400
C	-2.86188300	-4.76534700	-0.47043900
H	-0.96764800	-5.70934900	-0.55919300
C	-2.89325200	-2.34044100	-0.41966300
C	-2.91062300	0.13017900	-0.35082100
C	-3.58716900	-3.57468600	-0.41591800
H	-3.38765700	-5.71826600	-0.46328500
C	-3.59623200	-1.10145500	-0.35627700
C	-5.05899300	-3.60107100	-0.35158300
C	-5.04872400	-1.11670300	-0.30345000
C	-5.76882600	-4.78496500	-0.34246200
C	-5.75530800	-2.34266100	-0.29875000
C	-5.75981000	0.11503300	-0.25513600
C	-7.19372500	-4.77612900	-0.28312800
H	-5.26406900	-5.74641500	-0.38251400

C	-7.19128600	-2.33647200	-0.24331000
C	-7.20257600	0.10781900	-0.20679100
C	-7.88700000	-3.60102000	-0.23545400
H	-7.71363800	-5.73342000	-0.27799400
C	-7.88520400	-1.12868500	-0.19890000
H	8.91383200	3.84209700	-0.01331500
H	8.90481000	1.38845800	-0.15703300
H	8.91419700	-1.05918900	-0.30575900
H	8.94166700	-3.51231200	-0.46091100
H	-8.97310900	-3.58562200	-0.19169200
H	-8.97042800	-1.12812600	-0.15931600
H	-8.98170600	1.32613700	-0.13513700
H	-9.00674400	3.78361200	-0.11282800
C	0.71076200	0.13614600	2.80109900
C	-0.61931800	0.06589100	2.77008600
C	-1.44083600	-1.19101100	2.86656700
C	-0.64971100	-2.45155800	2.64795700
C	0.67884000	-2.55546400	2.66944000
H	-1.94580100	-1.23273400	3.84585500
H	1.22796400	1.08759100	2.72077500
H	-1.17020500	0.99873700	2.65508700
H	-1.22273700	-3.35461400	2.44062100
H	1.17317200	-3.50665600	2.49735700
H	-2.26049200	-1.14623300	2.13194600
S	1.81746000	-1.23248600	2.91848800

Graphene-CH₄

C	5.00289600	-1.20116600	-0.07891500
C	5.71752000	-2.41993100	-0.07283800
C	3.54772900	-1.19591000	-0.08829500
C	7.84142000	-1.19414500	-0.06573800
C	7.15436200	-2.40655000	-0.06562700
C	5.02639300	-3.68515000	-0.07432200
C	2.85198700	-2.43695200	-0.09576300
C	7.85976200	-3.66621100	-0.05884400
C	5.74626100	-4.86180300	-0.06828700
C	3.55389000	-3.66920500	-0.08365900
C	1.41842000	-2.44108400	-0.11158200
C	7.17377500	-4.84576900	-0.06010800
H	5.24632000	-5.82844900	-0.06985000
C	2.83635600	-4.86311200	-0.07446600
C	0.69780600	-1.19957700	-0.11344500
C	0.72026500	-3.67141500	-0.10724300
H	7.69854400	-5.80061600	-0.05514900
C	1.45192500	-4.86293700	-0.08204900
H	3.36547000	-5.81350800	-0.05710700
C	-0.72956900	-1.20077300	-0.10077700
C	-0.74246600	-3.67183200	-0.12139500
H	0.94536600	-5.81851700	-0.06260500
C	-1.44628400	-2.44328100	-0.10658800

C	-1.47509500	-4.86341200	-0.15087700
C	-2.88019700	-2.44835600	-0.10276600
C	-2.85976800	-4.87435400	-0.15000400
H	-0.95980100	-5.81674700	-0.17938800
C	-3.57964700	-1.20790300	-0.08098700
C	-3.57828500	-3.68155300	-0.12196300
H	-3.37981600	-5.82833600	-0.17251300
C	-5.03579700	-1.21578400	-0.07321400
C	-5.04999100	-3.69843300	-0.11588600
C	-5.74798400	-2.43453700	-0.09000700
C	-5.77329400	-4.87247000	-0.13296400
C	-7.18522300	-2.42966300	-0.08158000
H	-5.26697700	-5.84128000	-0.15266700
C	-7.20243900	-4.86647000	-0.12542900
C	-7.89054000	-3.68882500	-0.10036500
C	-7.87426400	-1.21769800	-0.05549300
H	-7.72308900	-5.82481000	-0.14000500
C	-7.90160400	3.71748900	0.03202100
C	-7.87794800	1.24641100	-0.01133400
C	-7.21706100	4.89737900	0.04607100
C	-7.19252700	2.46060400	0.00420900
C	-7.18062800	0.01548500	-0.03814400
C	-5.78798400	4.90802000	0.03287700
H	-7.74055100	5.85404400	0.06736800
C	-5.75533300	2.47011000	-0.00772000
C	-5.74361600	0.01780800	-0.04807300
C	-5.06120500	3.73632100	0.00637100
H	-5.28458500	5.87847500	0.04435700
C	-5.03945800	1.25365400	-0.03299100
C	-3.58952800	3.72421200	-0.00889200
C	-3.58328600	1.25041100	-0.04454800
C	-2.87470000	4.91939900	0.00133300
C	-2.88761700	2.49323600	-0.03347400
C	-2.88740300	0.02236300	-0.06726300
C	-1.49003100	4.91293400	-0.01371000
H	-3.39757400	5.87187700	0.02213600
C	-1.45389400	2.49299700	-0.04818900
C	-1.43505300	0.02460200	-0.07914300
C	-0.75370000	3.72364800	-0.04021900
H	-0.97797200	5.86834800	-0.00262900
C	-0.73354300	1.25251400	-0.06982600
C	0.70905100	3.72785900	-0.05753500
C	0.69423400	1.25577300	-0.08151600
C	1.43746500	4.92142100	-0.05957400
C	1.41116300	2.49963500	-0.07219400
C	1.40112400	0.02921300	-0.10025000
C	2.82201500	4.92567500	-0.06924700
H	0.92853500	5.87588200	-0.05397400
C	2.84487700	2.49952900	-0.07971900
C	2.85437200	0.03166100	-0.09270500

C	3.54311300	3.73397400	-0.07733700
H	3.34831200	5.87779300	-0.06945600
C	3.54411100	1.26079300	-0.08568600
C	5.01560100	3.75424800	-0.08196700
C	4.99938500	1.27018400	-0.08140500
C	5.73207800	4.93295800	-0.08532100
C	5.71043700	2.49103800	-0.08067100
C	5.70762500	0.03556000	-0.07747000
C	7.15968100	4.92108000	-0.08557600
H	5.22933000	5.89815600	-0.08739100
C	7.14730200	2.48182400	-0.07856800
C	7.14815100	0.03762100	-0.07212800
C	7.84908100	3.74352900	-0.08161300
H	7.68168900	5.87744300	-0.08851100
C	7.83785600	1.27140000	-0.07370800
H	-8.98046700	-3.67015300	-0.09402600
H	-8.96613600	-1.21268600	-0.04835100
H	-8.96978300	1.23788300	-0.00287500
H	-8.99143300	3.69527300	0.04144700
H	8.93675100	3.72385100	-0.08083800
H	8.92513100	1.26629900	-0.07116800
H	8.92865600	-1.18590200	-0.06095300
H	8.94734600	-3.64338400	-0.05286900
C	0.84117600	-1.22111600	3.14708800
H	0.27366600	-0.35060000	2.81189200
H	0.35816000	-2.13307700	2.79051500
H	1.85564900	-1.16871000	2.74210800
H	0.88704000	-1.23172500	4.23783900

Graphene-NH₃

C	-5.01601500	1.24020900	-0.07150900
C	-5.72850600	2.46041800	-0.07125200
C	-3.56088000	1.23268700	-0.07591700
C	-7.85429600	1.23741700	-0.06456100
C	-7.16546800	2.44861800	-0.06858700
C	-5.03603800	3.72444800	-0.07367700
C	-2.86342400	2.47267400	-0.07633300
C	-7.86856400	3.70968000	-0.07018500
C	-5.75323700	4.90269000	-0.07527800
C	-3.56331400	3.70591100	-0.07375700
C	-1.42954500	2.47561000	-0.07661400
C	-7.18068300	4.88811500	-0.07364800
H	-5.25232700	5.86827800	-0.07738800
C	-2.84358900	4.89856600	-0.07031700
C	-0.71084300	1.23235500	-0.08437300
C	-0.72921000	3.70465700	-0.07145300
H	-7.70421300	5.84360000	-0.07494500
C	-1.45905600	4.89720400	-0.06859400
H	-3.37189600	5.84957700	-0.06804100
C	0.71688700	1.23059300	-0.07850500

C	0.73404100	3.70207800	-0.06721300
H	-0.95221600	5.85248200	-0.06447600
C	1.43597700	2.47414500	-0.07018300
C	1.46926600	4.89359600	-0.05893700
C	2.86973600	2.47656300	-0.06435800
C	2.85290000	4.90267700	-0.05328700
H	0.95491500	5.84785500	-0.05618100
C	3.56744400	1.23324900	-0.06683700
C	3.56947000	3.70745300	-0.05532100
H	3.37393900	5.85598100	-0.04595800
C	5.02259400	1.23831400	-0.06053400
C	5.04099200	3.72111300	-0.04800500
C	5.73726300	2.45688600	-0.05096600
C	5.76716500	4.89421800	-0.03738800
C	7.17447700	2.44991500	-0.04352700
H	5.26116900	5.86438900	-0.03390600
C	7.19586900	4.88669900	-0.02993900
C	7.88218300	3.70734000	-0.03290100
C	7.86141700	1.23590100	-0.04578700
H	7.71826600	5.84453100	-0.02131600
C	7.88191000	-3.69973000	-0.06650200
C	7.86132400	-1.22825000	-0.05700800
C	7.19549500	-4.87902200	-0.07338300
C	7.17431100	-2.44220700	-0.06530000
C	7.16586600	0.00386900	-0.05538000
C	5.76678700	-4.88636300	-0.07924300
H	7.71782300	-5.83693200	-0.07385400
C	5.73710000	-2.44901200	-0.07175500
C	5.72838300	0.00396100	-0.06246200
C	5.04070400	-3.71314500	-0.07876700
H	5.26071000	-5.85649500	-0.08354700
C	5.02254900	-1.23033700	-0.07066800
C	3.56917500	-3.69929800	-0.08333700
C	3.56743100	-1.22511700	-0.07589500
C	2.85249100	-4.89448400	-0.09028600
C	2.86962800	-2.46830400	-0.08138900
C	2.87384100	0.00407700	-0.07486900
C	1.46887600	-4.88530900	-0.09082200
H	3.37349200	-5.84782500	-0.09429700
C	1.43574500	-2.46565000	-0.08396100
C	1.42013900	0.00410700	-0.08207700
C	0.73376800	-3.69367600	-0.08422800
H	0.95438300	-5.83947100	-0.09746900
C	0.71674300	-1.22216300	-0.08594600
C	-0.72948500	-3.69612100	-0.07714300
C	-0.71093400	-1.22373200	-0.09094800
C	-1.45932400	-4.88854100	-0.06288200
C	-1.42970900	-2.46682700	-0.08089900
C	-1.41616200	0.00428400	-0.08516800
C	-2.84390500	-4.88976600	-0.05838300

H	-0.95249200	-5.84378100	-0.05300400
C	-2.86369500	-2.46383600	-0.07398200
C	-2.87022200	0.00440000	-0.07942900
C	-3.56358100	-3.69714400	-0.06487400
H	-3.37222700	-5.84071700	-0.04816600
C	-3.56104300	-1.22394400	-0.07368700
C	-5.03629600	-3.71559800	-0.06002000
C	-5.01615400	-1.23136700	-0.06731900
C	-5.75354200	-4.89379300	-0.05454100
C	-5.72868000	-2.45152600	-0.06145600
C	-5.72231700	0.00445500	-0.06740700
C	-7.18100100	-4.87912300	-0.04995100
H	-5.25271200	-5.85942500	-0.05338900
C	-7.16564800	-2.43961000	-0.05688100
C	-7.16360100	0.00451700	-0.06330300
C	-7.86880300	-3.70065200	-0.05108500
H	-7.70457100	-5.83457800	-0.04543700
C	-7.85437500	-1.22838500	-0.05816400
H	8.97251000	3.68733000	-0.02681700
H	8.95417600	1.22943900	-0.03953100
H	8.95409100	-1.22191300	-0.05110800
H	8.97225100	-3.67987000	-0.06126500
H	-8.95625100	-3.67929100	-0.04748600
H	-8.94126200	-1.22168800	-0.05489000
H	-8.94118100	1.23083700	-0.06207700
H	-8.95601100	3.68839700	-0.06842100
N	-0.13407400	-0.19048200	3.18000700
H	-1.15087600	-0.13460800	3.15263100
H	0.10786900	-1.03645000	2.66791900
H	0.19832500	0.58189000	2.60564200

Graphene-CO₂

C	-5.02122200	1.29653300	-0.12290700
C	-5.73418400	2.51574500	-0.10495400
C	-3.56579000	1.28951300	-0.12352900
C	-7.85965400	1.29317300	-0.12281200
C	-7.17109200	2.50454500	-0.10552100
C	-5.04108500	3.78014100	-0.08551600
C	-2.86834700	2.52867600	-0.10229600
C	-7.87494700	3.76504200	-0.08753000
C	-5.75961400	4.95729700	-0.06846900
C	-3.56861600	3.76209200	-0.08377500
C	-1.43448800	2.53080100	-0.09901500
C	-7.18738500	4.94342400	-0.06974500
H	-5.25838500	5.92333900	-0.05338600
C	-2.84951500	4.95456500	-0.06480100
C	-0.71549700	1.28938300	-0.12235500
C	-0.73432700	3.76038400	-0.07497400
H	-7.71069700	5.89901800	-0.05594600
C	-1.46471800	4.95232700	-0.06108400

H	-3.37702100	5.90589100	-0.05237700
C	0.71232800	1.28827400	-0.12193600
C	0.72837700	3.75864800	-0.06706800
H	-0.95736300	5.90758200	-0.04734000
C	1.43062600	2.52925400	-0.09282800
C	1.46255300	4.94880300	-0.03362900
C	2.86442300	2.53214300	-0.08995000
C	2.84745500	4.95774600	-0.03028800
H	0.94909600	5.90311300	-0.00773100
C	3.56226000	1.29135700	-0.11697100
C	3.56438900	3.76437300	-0.05913000
H	3.36868600	5.91100100	-0.00366100
C	5.01850800	1.29687400	-0.11493100
C	5.03613500	3.77918600	-0.05692500
C	5.73239100	2.51430900	-0.08638900
C	5.76095500	4.95196700	-0.02802200
C	7.16964400	2.50724500	-0.08590600
H	5.25611900	5.92135400	-0.00488800
C	7.19016500	4.94371200	-0.02721700
C	7.87667900	3.76527400	-0.05540300
C	7.85696100	1.29443700	-0.11434300
H	7.71209400	5.90114800	-0.00359500
C	7.87759200	-3.64029400	-0.22187200
C	7.85713100	-1.16941500	-0.16998700
C	7.19156000	-4.81916800	-0.24325200
C	7.17009100	-2.38248100	-0.19400900
C	7.16151000	0.06246600	-0.14223600
C	5.76239900	-4.82795400	-0.23758300
H	7.71384400	-5.77647000	-0.26474900
C	5.73282800	-2.38999200	-0.19084700
C	5.72449100	0.06223100	-0.14181100
C	5.03717900	-3.65532000	-0.21172100
H	5.25779200	-5.79764700	-0.25427200
C	5.01858500	-1.17258800	-0.16707600
C	3.56551700	-3.64124200	-0.20442800
C	3.56237300	-1.16717500	-0.16821600
C	2.84878400	-4.83492700	-0.21457400
C	2.86517600	-2.40891800	-0.18651300
C	2.86834800	0.06213100	-0.14445200
C	1.46388500	-4.82642500	-0.20706400
H	3.37024900	-5.78829900	-0.22763100
C	1.43148700	-2.40717900	-0.18503600
C	1.41624300	0.06255500	-0.14787600
C	0.72928700	-3.63638100	-0.19199500
H	0.95068000	-5.78111100	-0.21468700
C	0.71327300	-1.16506700	-0.17167700
C	-0.73330700	-3.63849800	-0.18442300
C	-0.71622200	-1.16618900	-0.17456500
C	-1.46338000	-4.83005600	-0.18383000
C	-1.43420200	-2.40891800	-0.17792900

C	-1.42121000	0.06178800	-0.14724300
C	-2.84842700	-4.83267100	-0.18341000
H	-0.95587300	-5.78525800	-0.18233200
C	-2.86800600	-2.40672500	-0.17369900
C	-2.87410900	0.06144000	-0.14420200
C	-3.56800400	-3.64066600	-0.18039000
H	-3.37545700	-5.78430500	-0.18481900
C	-3.56528400	-1.16732000	-0.15968000
C	-5.04041300	-3.65878400	-0.18231200
C	-5.02087900	-1.17483600	-0.15633300
C	-5.75877000	-4.83602800	-0.19653600
C	-5.73353800	-2.39427700	-0.16941200
C	-5.72748000	0.06070900	-0.13987000
C	-7.18658300	-4.82236200	-0.19822000
H	-5.25737800	-5.80209400	-0.20681900
C	-7.17047400	-2.38335200	-0.16983600
C	-7.16768300	0.06065900	-0.13951600
C	-7.87420900	-3.64399500	-0.18526500
H	-7.70974700	-5.77806400	-0.21008700
C	-7.85930100	-1.17214900	-0.15545600
H	8.96652800	3.74493200	-0.05535200
H	8.94874300	1.28770300	-0.11479500
H	8.94895900	-1.16239800	-0.17206700
H	8.96744600	-3.61947600	-0.22531500
H	-8.96192100	-3.62270700	-0.18625200
H	-8.94674200	-1.16545400	-0.15609800
H	-8.94705000	1.28627400	-0.12326000
H	-8.96263900	3.74369900	-0.08847100
C	0.01670000	-1.27216400	2.81705600
O	0.00713700	-0.10926600	2.84374700
O	0.03437300	-2.43548600	2.79888500

Graphene-H₂O

C	5.02463400	-1.23327400	-0.05807200
C	5.73946800	-2.45203200	-0.05966700
C	3.56947900	-1.22788000	-0.06327600
C	7.86370900	-1.23146400	-0.04108700
C	7.17674800	-2.44556400	-0.05104700
C	5.04300200	-3.71583800	-0.07010800
C	2.87207000	-2.47190500	-0.07250900
C	7.88452200	-3.70288700	-0.05226200
C	5.76942400	-4.88895400	-0.07061300
C	3.57134300	-3.70215800	-0.07787600
C	1.43822800	-2.46851300	-0.07600200
C	7.19809400	-4.88220600	-0.06182400
H	5.26271300	-5.85922000	-0.07740400
C	2.85543400	-4.89816600	-0.09305900
C	0.72001200	-1.22475000	-0.07844200
C	0.73723400	-3.69645300	-0.07998400
H	7.72032300	-5.84027900	-0.06248300

C	1.47221900	-4.88849100	-0.09486700
H	3.37638400	-5.85142200	-0.10325100
C	-0.70563300	-1.22698700	-0.08783900
C	-0.72587900	-3.70026800	-0.06814200
H	0.95727200	-5.84234100	-0.11061900
C	-1.42613900	-2.47182800	-0.07591000
C	-1.45591700	-4.89351000	-0.04492200
C	-2.86050100	-2.46858400	-0.07048400
C	-2.83988200	-4.89418000	-0.04048700
H	-0.94874400	-5.84858200	-0.02658300
C	-3.55825100	-1.22755700	-0.07451300
C	-3.56012300	-3.70100000	-0.05515300
H	-3.36925900	-5.84472800	-0.02346800
C	-5.01276100	-1.23509600	-0.06458600
C	-5.03322800	-3.71963900	-0.05028500
C	-5.72508500	-2.45648200	-0.05381000
C	-5.74950400	-4.89896600	-0.04197000
C	-7.16202300	-2.44375700	-0.04679600
H	-5.24861000	-5.86384800	-0.04023700
C	-7.17627400	-4.88349100	-0.03593200
C	-7.86450000	-3.70488800	-0.03787800
C	-7.85092000	-1.23246800	-0.04848000
H	-7.70032300	-5.83857500	-0.02969100
C	-7.86461000	3.70593600	-0.06447200
C	-7.85096800	1.23347300	-0.05735100
C	-7.17636300	4.88454800	-0.06982700
C	-7.16210200	2.44484300	-0.06366500
C	-7.16136300	0.00055000	-0.05685900
C	-5.74962000	4.90002400	-0.07370700
H	-7.70044500	5.83963800	-0.07103700
C	-5.72518200	2.45754100	-0.06924200
C	-5.71882400	0.00051400	-0.06453200
C	-5.03329000	3.72068500	-0.07286100
H	-5.24870800	5.86489300	-0.07750000
C	-5.01278700	1.23614300	-0.07164600
C	-3.56016900	3.70204000	-0.07409000
C	-3.55829900	1.22863600	-0.07974600
C	-2.84000100	4.89538600	-0.06673000
C	-2.86037600	2.46977700	-0.07997500
C	-2.86748900	0.00061000	-0.08505200
C	-1.45612300	4.89468400	-0.06545800
H	-3.36947200	5.84601500	-0.06045300
C	-1.42606900	2.47296100	-0.08017900
C	-1.41219200	0.00070700	-0.09000300
C	-0.72591000	3.70130300	-0.07367600
H	-0.94915600	5.84997900	-0.05615100
C	-0.70541600	1.22834000	-0.08700200
C	0.73719500	3.69752800	-0.07283600
C	0.71998400	1.22608500	-0.07725200
C	1.47222300	4.88956700	-0.07285100

C	1.43819500	2.46964800	-0.06992100
C	1.42176600	0.00084200	-0.07136800
C	2.85544900	4.89932700	-0.06496000
H	0.95746700	5.84361000	-0.07958100
C	2.87198100	2.47308200	-0.06129900
C	2.87558300	0.00066500	-0.06388900
C	3.57133200	3.70333300	-0.05681700
H	3.37631700	5.85268300	-0.06407100
C	3.56950000	1.22923900	-0.05678500
C	5.04298200	3.71700000	-0.04519300
C	5.02466900	1.23447000	-0.05010800
C	5.76937900	4.89007100	-0.03549500
C	5.73950300	2.45316700	-0.04264000
C	5.73053700	0.00056900	-0.04941600
C	7.19807400	4.88327900	-0.02438000
H	5.26265400	5.86035700	-0.03577000
C	7.17682300	2.44662600	-0.03250700
C	7.16817200	0.00052500	-0.04071900
C	7.88455600	3.70398600	-0.02306600
H	7.72022900	5.84136500	-0.01666500
C	7.86375300	1.23255600	-0.03138500
H	-8.95163100	-3.68369300	-0.03312200
H	-8.93725800	-1.22613100	-0.04349100
H	-8.93730100	1.22718700	-0.05291200
H	-8.95173300	3.68478200	-0.06102700
H	8.97502200	3.68427600	-0.01452000
H	8.95686600	1.22626300	-0.02313400
H	8.95683500	-1.22528600	-0.03342000
H	8.97500900	-3.68321300	-0.04507400
O	-0.20618600	-0.01305400	2.86552800
H	-0.65475000	-0.83146000	2.61229600
H	-0.84123800	0.67598900	2.62617200

Graphene-H₂

C	-5.01947600	1.23514800	-0.01358500
C	-5.73348400	2.45279400	-0.01295000
C	-3.56315400	1.22950300	-0.01444500
C	-7.85801600	1.23240500	-0.01262600
C	-7.17074100	2.44554000	-0.01264900
C	-5.03754600	3.71818300	-0.01261900
C	-2.86567600	2.47101000	-0.01384300
C	-7.87789500	3.70388900	-0.01240400
C	-5.76239900	4.89128000	-0.01245400
C	-3.56580800	3.70347500	-0.01251300
C	-1.43187300	2.46855500	-0.01425200
C	-7.19159600	4.88278500	-0.01237900
H	-5.25776600	5.86095400	-0.01234800
C	-2.84909100	4.89743500	-0.01093500
C	-0.71355200	1.22714300	-0.01660400
C	-0.72976200	3.69835900	-0.01259100

H	-7.71368900	5.84038400	-0.01227400
C	-1.46422600	4.88887100	-0.01081500
H	-3.37076800	5.85084300	-0.00962000
C	0.71454600	1.22822300	-0.01651400
C	0.73301500	3.70011200	-0.01274700
H	-0.95099000	5.84363500	-0.00925700
C	1.43340400	2.47053300	-0.01427400
C	1.46350200	4.89227300	-0.01141700
C	2.86722600	2.46819500	-0.01400300
C	2.84821000	4.89447200	-0.01157700
H	0.95602800	5.84760100	-0.01023000
C	3.56459800	1.22856200	-0.01457100
C	3.56737800	3.70175000	-0.01286200
H	3.37576400	5.84585700	-0.01055500
C	5.02003000	1.23586900	-0.01366300
C	5.03981600	3.71983000	-0.01288000
C	5.73293800	2.45539100	-0.01306500
C	5.75828500	4.89722000	-0.01269100
C	7.16982500	2.44432800	-0.01262700
H	5.25689700	5.86333400	-0.01267200
C	7.18600700	4.88350800	-0.01247600
C	7.87359500	3.70496800	-0.01238400
C	7.85856900	1.23289700	-0.01245900
H	7.70928000	5.83920800	-0.01235700
C	7.87358400	-3.70469500	-0.01178500
C	7.85856900	-1.23261500	-0.01226600
C	7.18598300	-4.88322700	-0.01179900
C	7.16982500	-2.44404800	-0.01233800
C	7.16678300	0.00014000	-0.01270600
C	5.75825800	-4.89692800	-0.01230600
H	7.70924200	-5.83893400	-0.01140100
C	5.73294100	-2.45510700	-0.01296400
C	5.72654600	0.00014600	-0.01339600
C	5.03979800	-3.71953400	-0.01282000
H	5.25686800	-5.86304100	-0.01226000
C	5.02004300	-1.23558100	-0.01366800
C	3.56735900	-3.70143700	-0.01319600
C	3.56461900	-1.22828200	-0.01468600
C	2.84818500	-4.89415200	-0.01219100
C	2.86720900	-2.46787600	-0.01438100
C	2.87311700	0.00012900	-0.01527300
C	1.46347600	-4.89193400	-0.01230900
H	3.37572800	-5.84554500	-0.01111400
C	1.43337600	-2.47016800	-0.01501400
C	1.42000500	0.00010100	-0.01688300
C	0.73300400	-3.69976500	-0.01372600
H	0.95599700	-5.84726000	-0.01118700
C	0.71449800	-1.22793200	-0.01711100
C	-0.72975200	-3.69800800	-0.01376600
C	-0.71348600	-1.22684000	-0.01716800

C	-1.46420900	-4.88852700	-0.01247800
C	-1.43184000	-2.46818500	-0.01505700
C	-1.41705700	0.00011300	-0.01693500
C	-2.84907200	-4.89710600	-0.01241900
H	-0.95096800	-5.84328800	-0.01146600
C	-2.86566000	-2.47067900	-0.01443800
C	-2.86912900	0.00014000	-0.01525300
C	-3.56579200	-3.70314700	-0.01335600
H	-3.37074500	-5.85051700	-0.01146300
C	-3.56317300	-1.22920600	-0.01467600
C	-5.03753000	-3.71786900	-0.01309000
C	-5.01948700	-1.23484400	-0.01375300
C	-5.76237400	-4.89097400	-0.01274400
C	-5.73348800	-2.45249500	-0.01319900
C	-5.72551100	0.00015300	-0.01345200
C	-7.19156800	-4.88248800	-0.01238300
H	-5.25772900	-5.86064200	-0.01272800
C	-7.17074200	-2.44524700	-0.01271600
C	-7.16251800	0.00014700	-0.01289800
C	-7.87788400	-3.70359800	-0.01233900
H	-7.71365700	-5.84009100	-0.01212200
C	-7.85801600	-1.23210800	-0.01261700
H	8.96131700	3.68368600	-0.01213400
H	8.94599400	1.22613200	-0.01209000
H	8.94599300	-1.22585300	-0.01181000
H	8.96130600	-3.68342200	-0.01135000
H	-8.96770900	-3.68307200	-0.01201400
H	-8.94972300	-1.22525400	-0.01226800
H	-8.94972500	1.22554600	-0.01235900
H	-8.96772200	3.68334500	-0.01225300
H	0.04438100	0.02041400	2.66902200
H	-0.06685200	-0.08985900	3.39088400

XYZ coordinates (in Å) of graphene-metal ion complexes optimized at M06-2X/6-31G* level

Graphene-Be²⁺

C	4.98614700	-1.22329300	-0.02857600
C	5.71027500	-2.45037200	-0.02549400
C	3.56285100	-1.22611000	-0.03436500
C	7.81738200	-1.21430900	-0.01913300
C	7.14330800	-2.43888700	-0.02112700
C	5.02727100	-3.68892500	-0.02686200
C	2.85522200	-2.47365900	-0.03499400
C	7.86734800	-3.65614800	-0.01892200
C	5.78900500	-4.86157100	-0.02504600
C	3.56750300	-3.69594900	-0.03022400
C	1.42927500	-2.47100100	-0.03916100
C	7.19062000	-4.85302200	-0.02112000
H	5.29678800	-5.82713200	-0.02703500

C	2.83719400	-4.89306500	-0.02811800
C	0.70947200	-1.22597300	-0.04611300
C	0.72671400	-3.69321000	-0.03546600
H	7.73099900	-5.79288300	-0.01983400
C	1.46320000	-4.89021000	-0.03016400
H	3.34319600	-5.85029800	-0.02357000
C	-0.70971900	-1.22598000	-0.04591400
C	-0.72696600	-3.69321500	-0.03572700
H	0.95837800	-5.84741700	-0.02708300
C	-1.42952700	-2.47100500	-0.03888500
C	-1.46345500	-4.89021600	-0.03161200
C	-2.85547700	-2.47365900	-0.03486900
C	-2.83745000	-4.89307000	-0.02955300
H	-0.95863900	-5.84743000	-0.02982100
C	-3.56310500	-1.22611200	-0.03390500
C	-3.56775800	-3.69595400	-0.03054800
H	-3.34345200	-5.85030700	-0.02618900
C	-4.98640300	-1.22329400	-0.02836300
C	-5.02752600	-3.68892600	-0.02681200
C	-5.71052900	-2.45037200	-0.02532600
C	-5.78926100	-4.86157100	-0.02464000
C	-7.14356400	-2.43888700	-0.02081100
H	-5.29704400	-5.82713300	-0.02635800
C	-7.19087600	-4.85302200	-0.02054100
C	-7.86760300	-3.65614800	-0.01845700
C	-7.81763600	-1.21431000	-0.01880800
H	-7.73125500	-5.79288300	-0.01901200
C	-7.86760400	3.65616300	-0.01845300
C	-7.81763500	1.21432800	-0.01880700
C	-7.19088000	4.85303800	-0.02053100
C	-7.14356300	2.43890600	-0.02080800
C	-7.12108400	0.00001000	-0.02113800
C	-5.78926600	4.86159000	-0.02462800
H	-7.73126200	5.79289700	-0.01899800
C	-5.71052800	2.45039200	-0.02532200
C	-5.68403100	0.00001000	-0.02611300
C	-5.02752400	3.68894800	-0.02680600
H	-5.29705800	5.82715600	-0.02633600
C	-4.98640200	1.22331400	-0.02836000
C	-3.56775000	3.69597400	-0.03054100
C	-3.56310400	1.22612800	-0.03389800
C	-2.83742900	4.89308700	-0.02955600
C	-2.85547400	2.47367400	-0.03485500
C	-2.85555400	0.00000700	-0.03814000
C	-1.46343300	4.89022500	-0.03160700
H	-3.34341700	5.85032900	-0.02621200
C	-1.42952500	2.47101300	-0.03885800
C	-1.41429700	0.00000400	-0.04531800
C	-0.72696200	3.69321800	-0.03570100
H	-0.95859900	5.84743200	-0.02983300

C	-0.70971900	1.22598800	-0.04588700
C	0.72670800	3.69321300	-0.03542700
C	0.70947100	1.22598000	-0.04608600
C	1.46317700	4.89021800	-0.03010500
C	1.42927200	2.47100900	-0.03912800
C	1.41405200	0.00000400	-0.04633400
C	2.83717100	4.89308200	-0.02806000
H	0.95833600	5.84741900	-0.02700100
C	2.85521900	2.47367400	-0.03496900
C	2.85529800	0.00000700	-0.03857900
C	3.56749500	3.69597000	-0.03018900
H	3.34315900	5.85032100	-0.02349200
C	3.56285000	1.22612700	-0.03435300
C	5.02726900	3.68894700	-0.02683900
C	4.98614600	1.22331300	-0.02856700
C	5.78901100	4.86159100	-0.02502900
C	5.71027400	2.45039300	-0.02548000
C	5.68377700	0.00001000	-0.02636700
C	7.19062500	4.85303800	-0.02111100
H	5.29680300	5.82715500	-0.02701700
C	7.14330800	2.43890600	-0.02112000
C	7.12083200	0.00001000	-0.02141400
C	7.86735000	3.65616300	-0.01891600
H	7.73100700	5.79289700	-0.01982900
C	7.81738200	1.21432800	-0.01913100
H	-8.95329100	-3.62691400	-0.01508900
H	-8.90580400	-1.20491200	-0.01522400
H	-8.90580400	1.20493000	-0.01522300
H	-8.95329300	3.62692700	-0.01508700
H	8.95303900	3.62692700	-0.01565300
H	8.90555000	1.20493300	-0.01562500
H	8.90555000	-1.20491400	-0.01562500
H	8.95303700	-3.62691500	-0.01565300
Be	0.01448300	-0.00088200	3.31348800

Graphene-Ca²⁺

C	4.99407200	-1.22656000	-0.08486200
C	5.71601600	-2.45560700	-0.06115200
C	3.57023400	-1.22816400	-0.09823100
C	7.82346800	-1.21706600	-0.06190400
C	7.14852700	-2.44185200	-0.05005300
C	5.03278900	-3.69540600	-0.04977800
C	2.86166400	-2.47429300	-0.09967500
C	7.86657500	-3.66239100	-0.02868800
C	5.78767200	-4.87159000	-0.03138500
C	3.57256000	-3.69761900	-0.06315000
C	1.43499200	-2.47605900	-0.13177200
C	7.18861400	-4.85866700	-0.02040500
H	5.29550900	-5.83675800	-0.02926400
C	2.83759200	-4.89077100	-0.03231500

C	0.71633100	-1.23217200	-0.17134300
C	0.72723800	-3.69689600	-0.10827000
H	7.73078800	-5.79763200	-0.00690500
C	1.46234800	-4.89134200	-0.04757000
H	3.34379000	-5.84687300	0.01221500
C	-0.71212000	-1.23087500	-0.13598900
C	-0.72771100	-3.69748500	-0.13925900
H	0.95725300	-5.84753900	-0.00783900
C	-1.43483000	-2.47695900	-0.13230600
C	-1.46329500	-4.89232500	-0.17638900
C	-2.86157800	-2.47380200	-0.14431900
C	-2.83839200	-4.89136200	-0.18253500
H	-0.95859900	-5.84899100	-0.20910200
C	-3.56978700	-1.22753900	-0.14050300
C	-3.57285800	-3.69742900	-0.15911300
H	-3.34534100	-5.84762800	-0.21146600
C	-4.99383800	-1.22611700	-0.12414300
C	-5.03309000	-3.69518600	-0.15646600
C	-5.71592300	-2.45534300	-0.13469400
C	-5.78823600	-4.87118100	-0.16999300
C	-7.14840800	-2.44171400	-0.12503500
H	-5.29633400	-5.83632500	-0.18709400
C	-7.18921800	-4.85836200	-0.16259800
C	-7.86684500	-3.66211700	-0.13975500
C	-7.82328900	-1.21709600	-0.10145300
H	-7.73153300	-5.79725300	-0.17485300
C	-7.86660300	3.66219200	-0.02899200
C	-7.82354100	1.21687000	-0.06252100
C	-7.18862700	4.85845500	-0.02037400
C	-7.14857500	2.44164500	-0.05040500
C	-7.13171100	-0.00002100	-0.08694900
C	-5.78768300	4.87135700	-0.03115100
H	-7.73078500	5.79742800	-0.00683500
C	-5.71606400	2.45537400	-0.06137400
C	-5.69204700	-0.00002300	-0.09890700
C	-5.03282300	3.69516300	-0.04958800
H	-5.29550600	5.83651700	-0.02877800
C	-4.99412900	1.22633000	-0.08521000
C	-3.57259000	3.69733900	-0.06284500
C	-3.57027200	1.22789700	-0.09765700
C	-2.83757200	4.89044100	-0.03157400
C	-2.86172000	2.47402300	-0.10029400
C	-2.86694600	-0.00071100	-0.13075700
C	-1.46231300	4.89101500	-0.04703100
H	-3.34374000	5.84654900	0.01323200
C	-1.43500500	2.47571800	-0.13093400
C	-1.42330600	0.00169800	-0.15397700
C	-0.72725000	3.69660300	-0.10854700
H	-0.95719500	5.84718100	-0.00683600
C	-0.71637800	1.23200000	-0.17447400

C	0.72770400	3.69720400	-0.13949500
C	0.71199900	1.23061400	-0.13305200
C	1.46322700	4.89204800	-0.17743100
C	1.43478700	2.47669000	-0.13360800
C	1.42328900	-0.00182800	-0.15724500
C	2.83833100	4.89113400	-0.18377300
H	0.95849300	5.84868000	-0.21069800
C	2.86152000	2.47358700	-0.14410900
C	2.86682600	0.00046300	-0.12898700
C	3.57280000	3.69722800	-0.15983500
H	3.34526900	5.84739600	-0.21295100
C	3.56968000	1.22732100	-0.14127100
C	5.03301800	3.69497500	-0.15708300
C	4.99372500	1.22591400	-0.12396600
C	5.78816700	4.87097400	-0.17075700
C	5.71582600	2.45513500	-0.13473200
C	5.69195000	-0.00017700	-0.09862800
C	7.18914100	4.85815600	-0.16312200
H	5.29625800	5.83610900	-0.18827600
C	7.14831200	2.44151300	-0.12494300
C	7.13161800	-0.00018200	-0.08652500
C	7.86675800	3.66190700	-0.13980400
H	7.73147000	5.79703700	-0.17550100
C	7.82318300	1.21689700	-0.10095500
H	-8.95244900	-3.63535800	-0.13344500
H	-8.91090800	-1.20963700	-0.09451100
H	-8.91112400	1.20906500	-0.05444900
H	-8.95219700	3.63558000	-0.02146000
H	8.95236100	3.63514500	-0.13334100
H	8.91080400	1.20944300	-0.09392400
H	8.91105100	-1.20923800	-0.05376900
H	8.95216800	-3.63576700	-0.02104100
Ca	0.00063200	0.00266500	2.47523900

Graphene-K⁺

C	-5.00104800	1.22869200	-0.10072500
C	-5.72089400	2.45900100	-0.09555500
C	-3.57402100	1.22734700	-0.11550700
C	-7.83103500	1.22065100	-0.08144600
C	-7.15427600	2.44316700	-0.08699100
C	-5.03567300	3.70182200	-0.10122500
C	-2.86455400	2.47041800	-0.11596700
C	-7.86304900	3.67096700	-0.08539300
C	-5.78072000	4.88168600	-0.10067500
C	-3.57475700	3.69652900	-0.10749600
C	-1.43567100	2.47275700	-0.12716500
C	-7.18239900	4.86393300	-0.09304700
H	-5.28693600	5.84541700	-0.10982300
C	-2.83866100	4.88783400	-0.10463800
C	-0.71462100	1.22982900	-0.14209000

C	-0.72775900	3.69606500	-0.11828000
H	-7.72574400	5.80311200	-0.09456100
C	-1.46274700	4.89016800	-0.10868200
H	-3.34745900	5.84362000	-0.09958000
C	0.71428400	1.22987600	-0.15027000
C	0.72732000	3.69605400	-0.11818500
H	-0.95796500	5.84741700	-0.10882400
C	1.43523300	2.47265200	-0.12406500
C	1.46230100	4.89010300	-0.10570000
C	2.86419400	2.47036200	-0.11743700
C	2.83822900	4.88771800	-0.10102000
H	0.95751500	5.84734400	-0.10354700
C	3.57370400	1.22733400	-0.11375900
C	3.57438400	3.69646100	-0.10594500
H	3.34699400	5.84351600	-0.09451900
C	5.00078200	1.22868100	-0.10195200
C	5.03533100	3.70180800	-0.10039000
C	5.72059100	2.45898000	-0.09605500
C	5.78034900	4.88167600	-0.09978200
C	7.15398600	2.44315300	-0.08798900
H	5.28657200	5.84541200	-0.10819900
C	7.18204400	4.86392600	-0.09278000
C	7.86272000	3.67098100	-0.08618800
C	7.83077500	1.22065900	-0.08346400
H	7.72537800	5.80311200	-0.09421800
C	7.86272200	-3.67097200	-0.08619700
C	7.83077600	-1.22065000	-0.08346700
C	7.18204600	-4.86391700	-0.09279400
C	7.15398700	-2.44314400	-0.08799500
C	7.14534100	0.00000400	-0.08713900
C	5.78035200	-4.88166800	-0.09979500
H	7.72538100	-5.80310300	-0.09423500
C	5.72059200	-2.45897300	-0.09606100
C	5.70228200	0.00000400	-0.09666100
C	5.03533300	-3.70180100	-0.10040000
H	5.28657600	-5.84540400	-0.10821700
C	5.00078300	-1.22867400	-0.10195600
C	3.57438500	-3.69645400	-0.10595400
C	3.57370400	-1.22732600	-0.11376300
C	2.83822900	-4.88771100	-0.10102700
C	2.86419500	-2.47035500	-0.11744600
C	2.86925200	0.00000400	-0.12668500
C	1.46230100	-4.89009600	-0.10570900
H	3.34699300	-5.84350900	-0.09452300
C	1.43523300	-2.47264500	-0.12407700
C	1.42449200	0.00000400	-0.14243900
C	0.72732000	-3.69604700	-0.11819900
H	0.95751400	-5.84733700	-0.10355300
C	0.71428400	-1.22986900	-0.15028600
C	-0.72775900	-3.69605800	-0.11829500

C	-0.71462100	-1.22982200	-0.14210500
C	-1.46274700	-4.89016100	-0.10870100
C	-1.43567100	-2.47275000	-0.12717700
C	-1.42487500	0.00000400	-0.14967000
C	-2.83866100	-4.88782700	-0.10465400
H	-0.95796500	-5.84741000	-0.10885100
C	-2.86455500	-2.47041100	-0.11597400
C	-2.86943500	0.00000400	-0.12103300
C	-3.57475800	-3.69652200	-0.10750300
H	-3.34745900	-5.84361300	-0.09960200
C	-3.57402100	-1.22734000	-0.11551000
C	-5.03567500	-3.70181400	-0.10122500
C	-5.00104800	-1.22868400	-0.10072700
C	-5.78072200	-4.88167800	-0.10066800
C	-5.72089400	-2.45899300	-0.09555500
C	-5.70253200	0.00000400	-0.09570000
C	-7.18240200	-4.86392400	-0.09303800
H	-5.28694000	-5.84541000	-0.10981300
C	-7.15427600	-2.44315800	-0.08698800
C	-7.14558900	0.00000400	-0.08552500
C	-7.86305100	-3.67095800	-0.08538600
H	-7.72574700	-5.80310300	-0.09454700
C	-7.83103500	-1.22064200	-0.08144500
H	8.94845400	3.64785000	-0.08160200
H	8.91783200	1.21574700	-0.07844600
H	8.91783200	-1.21573800	-0.07845000
H	8.94845500	-3.64784000	-0.08161200
H	-8.94878200	-3.64779400	-0.08041800
H	-8.91809200	-1.21571500	-0.07623300
H	-8.91809100	1.21572400	-0.07623600
H	-8.94878000	3.64780300	-0.08042700
K	0.00414300	-0.00009200	2.53309500

Graphene-Li⁺

C	-5.00240700	1.22925600	-0.01007000
C	-5.72206200	2.45935400	-0.00899100
C	-3.57555200	1.22820500	-0.01369300
C	-7.83156700	1.22063500	-0.00807800
C	-7.15527100	2.44328500	-0.00857100
C	-5.03722400	3.70244400	-0.00932600
C	-2.86603100	2.47152300	-0.01224500
C	-7.86463500	3.67082100	-0.00907100
C	-5.78252200	4.88181600	-0.01014700
C	-3.57626600	3.69754900	-0.00922700
C	-1.43820400	2.47716000	-0.01398200
C	-7.18438300	4.86389000	-0.01017300
H	-5.28909300	5.84577700	-0.01249000
C	-2.83949700	4.88812100	-0.00668900
C	-0.71715400	1.23420500	-0.03133800
C	-0.72811300	3.69822300	-0.01035100

H	-7.72776400	5.80296800	-0.01174900
C	-1.46321800	4.89163100	-0.00640800
H	-3.34827200	5.84390500	-0.00540300
C	0.71714500	1.23419300	-0.03250700
C	0.72810000	3.69821100	-0.01040800
H	-0.95901900	5.84905400	-0.00576300
C	1.43818000	2.47712100	-0.01338200
C	1.46320300	4.89161200	-0.00625500
C	2.86601900	2.47150800	-0.01249200
C	2.83948600	4.88809400	-0.00643200
H	0.95900600	5.84903600	-0.00549400
C	3.57556400	1.22820700	-0.01328900
C	3.57626100	3.69753000	-0.00909300
H	3.34825500	5.84388200	-0.00511600
C	5.00242300	1.22925100	-0.01017800
C	5.03722500	3.70243300	-0.00926600
C	5.72207200	2.45934500	-0.00902800
C	5.78251500	4.88180500	-0.01013500
C	7.15528100	2.44328200	-0.00864400
H	5.28908400	5.84576600	-0.01244700
C	7.18438000	4.86388700	-0.01020400
C	7.86463800	3.67082500	-0.00916600
C	7.83158400	1.22063700	-0.00824300
H	7.72775200	5.80296900	-0.01181400
C	7.86463700	-3.67082400	-0.00912900
C	7.83158400	-1.22063700	-0.00823100
C	7.18437900	-4.86388600	-0.01015500
C	7.15528100	-2.44328200	-0.00862100
C	7.14596800	0.00000000	-0.00856900
C	5.78251500	-4.88180500	-0.01008900
H	7.72775200	-5.80296900	-0.01175300
C	5.72207100	-2.45934400	-0.00900700
C	5.70317800	0.00000000	-0.00981300
C	5.03722400	-3.70243300	-0.00923500
H	5.28908400	-5.84576600	-0.01239000
C	5.00242300	-1.22925000	-0.01016900
C	3.57626000	-3.69752900	-0.00907000
C	3.57556300	-1.22820600	-0.01328200
C	2.83948600	-4.88809300	-0.00640600
C	2.86601900	-2.47150800	-0.01248100
C	2.87440300	0.00000000	-0.01627100
C	1.46320200	-4.89161100	-0.00623700
H	3.34825400	-5.84388100	-0.00508200
C	1.43818000	-2.47712000	-0.01337800
C	1.42962100	0.00000100	-0.03279600
C	0.72810000	-3.69821000	-0.01040400
H	0.95900500	-5.84903500	-0.00547300
C	0.71714500	-1.23419100	-0.03251700
C	-0.72811300	-3.69822200	-0.01035700
C	-0.71715400	-1.23420300	-0.03134900

C	-1.46321800	-4.89163000	-0.00641700
C	-1.43820400	-2.47715900	-0.01399300
C	-1.42960200	0.00000100	-0.03403900
C	-2.83949700	-4.88812000	-0.00670600
H	-0.95901900	-5.84905300	-0.00576900
C	-2.86603100	-2.47152300	-0.01226100
C	-2.87435800	0.00000000	-0.01539200
C	-3.57626500	-3.69754800	-0.00924900
H	-3.34827100	-5.84390400	-0.00542100
C	-3.57555200	-1.22820500	-0.01370200
C	-5.03722400	-3.70244300	-0.00935800
C	-5.00240700	-1.22925500	-0.01008000
C	-5.78252200	-4.88181500	-0.01019700
C	-5.72206200	-2.45935300	-0.00901300
C	-5.70315700	0.00000000	-0.00979200
C	-7.18438300	-4.86388900	-0.01022700
H	-5.28909200	-5.84577700	-0.01255400
C	-7.15527100	-2.44328400	-0.00859600
C	-7.14595000	0.00000000	-0.00847800
C	-7.86463500	-3.67082100	-0.00911200
H	-7.72776400	-5.80296700	-0.01181800
C	-7.83156700	-1.22063500	-0.00809100
H	8.95033500	3.64730300	-0.00972700
H	8.91863400	1.21540400	-0.00849700
H	8.91863400	-1.21540400	-0.00848400
H	8.95033500	-3.64730300	-0.00968800
H	-8.95033300	-3.64729400	-0.00965900
H	-8.91861800	-1.21539900	-0.00835600
H	-8.91861800	1.21539900	-0.00834200
H	-8.95033300	3.64729400	-0.00961600
Li	-0.00005500	-0.00005700	1.76966500

Graphene-Mg²⁺

C	-4.98620700	1.22340600	-0.09092200
C	-5.71032600	2.45048900	-0.08563900
C	-3.56293700	1.22621800	-0.09976500
C	-7.81740800	1.21442300	-0.07603800
C	-7.14334200	2.43900200	-0.07877900
C	-5.02732300	3.68902600	-0.08724500
C	-2.85530400	2.47378100	-0.10075800
C	-7.86738900	3.65624700	-0.07472700
C	-5.78906400	4.86167600	-0.08343200
C	-3.56757700	3.69604500	-0.09278700
C	-1.42939700	2.47113000	-0.10715700
C	-7.19066400	4.85312500	-0.07734200
H	-5.29685300	5.82723800	-0.08553400
C	-2.83725400	4.89315300	-0.08960800
C	-0.70959300	1.22609900	-0.11925100
C	-0.72684500	3.69329600	-0.10048500
H	-7.73104100	5.79298500	-0.07464200

C	-1.46329400	4.89030900	-0.09238200
H	-3.34325400	5.85037300	-0.08303100
C	0.70954200	1.22608800	-0.11914500
C	0.72680100	3.69329000	-0.10032200
H	-0.95843200	5.84748100	-0.08772000
C	1.42935000	2.47112600	-0.10719600
C	1.46324600	4.89030300	-0.09163200
C	2.85525500	2.47378500	-0.10069400
C	2.83720500	4.89315400	-0.08878700
H	0.95837300	5.84746600	-0.08638400
C	3.56289500	1.22622300	-0.09978900
C	3.56752900	3.69604700	-0.09258200
H	3.34319800	5.85037200	-0.08143900
C	4.98616100	1.22340700	-0.09084800
C	5.02727700	3.68902600	-0.08734300
C	5.71028400	2.45049200	-0.08561200
C	5.78902100	4.86167600	-0.08408800
C	7.14329800	2.43900400	-0.07879100
H	5.29681600	5.82723900	-0.08678000
C	7.19062200	4.85312600	-0.07801000
C	7.86734700	3.65625000	-0.07499300
C	7.81736300	1.21442400	-0.07594300
H	7.73099700	5.79298900	-0.07568800
C	7.86732500	-3.65604300	-0.07517700
C	7.81735800	-1.21421000	-0.07604900
C	7.19059100	-4.85291600	-0.07810300
C	7.14328700	-2.43878700	-0.07897600
C	7.12082100	0.00010900	-0.07968100
C	5.78899000	-4.86145200	-0.08416400
H	7.73095600	-5.79278300	-0.07569300
C	5.71027400	-2.45026300	-0.08581100
C	5.68377400	0.00011400	-0.08745400
C	5.02726500	-3.68879400	-0.08758800
H	5.29675900	-5.82700700	-0.08663500
C	4.98615800	-1.22317600	-0.09097300
C	3.56752800	-3.69580900	-0.09296300
C	3.56289100	-1.22598300	-0.09987500
C	2.83721600	-4.89291800	-0.08951200
C	2.85525500	-2.47354800	-0.10095000
C	2.85538700	0.00012000	-0.10736400
C	1.46325600	-4.89007500	-0.09227800
H	3.34322400	-5.85013500	-0.08261300
C	1.42935300	-2.47089600	-0.10739600
C	1.41421800	0.00011600	-0.11914000
C	0.72680200	-3.69306500	-0.10066500
H	0.95839900	-5.84724800	-0.08728800
C	0.70954900	-1.22586400	-0.11942200
C	-0.72684500	-3.69305900	-0.10067500
C	-0.70958500	-1.22585500	-0.11936000
C	-1.46329200	-4.89007400	-0.09234000

C	-1.42939100	-2.47089000	-0.10741000
C	-1.41426300	0.00011700	-0.11907300
C	-2.83725000	-4.89292400	-0.08950300
H	-0.95841700	-5.84723800	-0.08747700
C	-2.85529800	-2.47355000	-0.10090600
C	-2.85543100	0.00011500	-0.10734800
C	-3.56756800	-3.69581400	-0.09293400
H	-3.34325300	-5.85014000	-0.08254400
C	-3.56293700	-1.22599100	-0.09988200
C	-5.02731100	-3.68879800	-0.08755600
C	-4.98620500	-1.22317900	-0.09099000
C	-5.78904500	-4.86145200	-0.08412800
C	-5.71032000	-2.45026500	-0.08582100
C	-5.68382000	0.00011300	-0.08753700
C	-7.19064600	-4.85291000	-0.07804900
H	-5.29682900	-5.82701200	-0.08662100
C	-7.14333600	-2.43878500	-0.07899200
C	-7.12086700	0.00010900	-0.07979700
C	-7.86737800	-3.65603600	-0.07515300
H	-7.73101700	-5.79277300	-0.07561200
C	-7.81740500	-1.21420800	-0.07613500
H	8.95302800	3.62700900	-0.06990500
H	8.90552400	1.20503100	-0.07043700
H	8.90551900	-1.20482300	-0.07055100
H	8.95300700	-3.62680900	-0.07012400
H	-8.95305900	-3.62680400	-0.07009100
H	-8.90556600	-1.20481900	-0.07066500
H	-8.90556900	1.20503100	-0.07056900
H	-8.95307100	3.62700800	-0.06968700
Mg	0.00085700	-0.00430600	3.46692000

Graphene-Na⁺

C	5.00212700	-1.22903500	-0.05085500
C	5.72182700	-2.45918400	-0.05007900
C	3.57506100	-1.22796600	-0.05438000
C	7.83170700	-1.22065300	-0.04855500
C	7.15517000	-2.44321500	-0.04957700
C	5.03673900	-3.70222600	-0.05131500
C	2.86557500	-2.47104000	-0.05398000
C	7.86422900	-3.67091700	-0.05091100
C	5.78195900	-4.88178700	-0.05314200
C	3.57577100	-3.69722400	-0.05113100
C	1.43693700	-2.47506000	-0.05552400
C	7.18376800	-4.86391400	-0.05309200
H	5.28835400	-5.84565100	-0.05706100
C	2.83928400	-4.88813700	-0.04905500
C	0.71599300	-1.23222900	-0.06722300
C	0.72780900	-3.69755600	-0.05293400
H	7.72713100	-5.80304400	-0.05589700
C	1.46310600	-4.89116400	-0.04934700

H	3.34807900	-5.84392500	-0.04873000
C	-0.71595600	-1.23223600	-0.06737800
C	-0.72778000	-3.69756200	-0.05276100
H	0.95870600	-5.84857100	-0.05060000
C	-1.43690600	-2.47505900	-0.05545900
C	-1.46307700	-4.89116300	-0.04855600
C	-2.86554600	-2.47103300	-0.05396600
C	-2.83926100	-4.88812800	-0.04822900
H	-0.95868700	-5.84857500	-0.04918800
C	-3.57503100	-1.22796800	-0.05438300
C	-3.57574200	-3.69722200	-0.05088300
H	-3.34806500	-5.84391400	-0.04730600
C	-5.00210100	-1.22903700	-0.05085300
C	-5.03670700	-3.70222700	-0.05131900
C	-5.72179500	-2.45918300	-0.05007600
C	-5.78191200	-4.88178800	-0.05343200
C	-7.15514000	-2.44321600	-0.04964200
H	-5.28829900	-5.84564900	-0.05761200
C	-7.18372400	-4.86391800	-0.05345700
C	-7.86419000	-3.67092600	-0.05112000
C	-7.83167700	-1.22065700	-0.04858700
H	-7.72708200	-5.80305000	-0.05646900
C	-7.86419100	3.67093000	-0.05109300
C	-7.83167700	1.22066000	-0.04857800
C	-7.18372500	4.86392200	-0.05342000
C	-7.15514000	2.44322000	-0.04962400
C	-7.14613400	0.00000200	-0.04873200
C	-5.78191200	4.88179200	-0.05339700
H	-7.72708200	5.80305400	-0.05642500
C	-5.72179500	2.45918600	-0.05005900
C	-5.70320500	0.00000200	-0.05004900
C	-5.03670700	3.70223000	-0.05129300
H	-5.28829900	5.84565300	-0.05756800
C	-5.00210200	1.22904100	-0.05084400
C	-3.57574300	3.69722600	-0.05085900
C	-3.57503100	1.22797200	-0.05437400
C	-2.83926300	4.88813300	-0.04820000
C	-2.86554600	2.47103700	-0.05394900
C	-2.87210500	0.00000200	-0.05686600
C	-1.46307900	4.89116800	-0.04853200
H	-3.34806800	5.84391800	-0.04726900
C	-1.43690600	2.47506400	-0.05544400
C	-1.42742000	0.00000300	-0.06828500
C	-0.72778000	3.69756700	-0.05274700
H	-0.95869000	5.84858000	-0.04915900
C	-0.71595600	1.23224200	-0.06736300
C	0.72781000	3.69756100	-0.05293100
C	0.71599300	1.23223500	-0.06721000
C	1.46310700	4.89116900	-0.04935900
C	1.43693700	2.47506600	-0.05552200

C	1.42745000	0.00000300	-0.06827900
C	2.83928600	4.88814100	-0.04907600
H	0.95870900	5.84857600	-0.05061900
C	2.86557500	2.47104500	-0.05398600
C	2.87213500	0.00000200	-0.05668500
C	3.57577200	3.69722800	-0.05114800
H	3.34808200	5.84392900	-0.04876100
C	3.57506100	1.22797100	-0.05438500
C	5.03674000	3.70223000	-0.05133700
C	5.00212700	1.22903800	-0.05086100
C	5.78196000	4.88179000	-0.05317500
C	5.72182700	2.45918800	-0.05009400
C	5.70323100	0.00000200	-0.05007900
C	7.18376900	4.86391700	-0.05312700
H	5.28835500	5.84565500	-0.05710000
C	7.15517000	2.44321900	-0.04959400
C	7.14616200	0.00000200	-0.04874900
C	7.86423000	3.67092000	-0.05093800
H	7.72713200	5.80304700	-0.05594100
C	7.83170700	1.22065600	-0.04856400
H	-8.94991200	-3.64759200	-0.05195600
H	-8.91873700	-1.21557900	-0.04919900
H	-8.91873700	1.21558200	-0.04918900
H	-8.94991300	3.64759600	-0.05192900
H	8.94995200	3.64758000	-0.05174000
H	8.91876800	1.21557900	-0.04914500
H	8.91876700	-1.21557600	-0.04913500
H	8.94995100	-3.64757700	-0.05171100
Na	-0.00066500	-0.00008600	2.19179600

Graphene-NH₄⁺

C	-4.99535800	1.22087900	-0.06327500
C	-5.71498700	2.45118000	-0.05628400
C	-3.56826200	1.21946000	-0.08883500
C	-7.82497800	1.21269200	-0.02706800
C	-7.14834200	2.43511300	-0.03907600
C	-5.02984500	3.69421600	-0.06922400
C	-2.85869300	2.46224200	-0.09675900
C	-7.85665200	3.66332400	-0.03655200
C	-5.77440700	4.87428200	-0.06841100
C	-3.56899600	3.68855700	-0.08284000
C	-1.42930600	2.46393700	-0.11706500
C	-7.17607300	4.85618500	-0.05229800
H	-5.28083800	5.83799900	-0.08557900
C	-2.83281200	4.87977400	-0.07931200
C	-0.70837300	1.22113600	-0.13635900
C	-0.72194200	3.68813100	-0.10302500
H	-7.71959700	5.79528400	-0.05413100
C	-1.45698100	4.88218400	-0.08604500
H	-3.34172700	5.83543300	-0.06795000

C	0.72029700	1.22158700	-0.13134400
C	0.73297000	3.68857400	-0.09975700
H	-0.95210300	5.83936600	-0.08098000
C	1.44058900	2.46434400	-0.09809400
C	1.46787100	4.88278700	-0.08756600
C	2.86990800	2.46262900	-0.08221800
C	2.84365100	4.88041100	-0.07488300
H	0.96301400	5.83996900	-0.09438100
C	3.57893400	1.21982500	-0.07198900
C	3.57968800	3.68896800	-0.06966400
H	3.35241600	5.83622000	-0.07101000
C	5.00581000	1.22145400	-0.05559600
C	5.04047400	3.69441600	-0.05528800
C	5.72566800	2.45176100	-0.04789000
C	5.78565500	4.87435800	-0.05007600
C	7.15895700	2.43627700	-0.03389100
H	5.29183600	5.83809700	-0.05922800
C	7.18720100	4.85696400	-0.03707600
C	7.86782900	3.66387200	-0.02876600
C	7.83573300	1.21363600	-0.02689300
H	7.73042500	5.79618900	-0.03529100
C	7.86843200	-3.67709400	-0.02647500
C	7.83572900	-1.22718200	-0.02587000
C	7.18794400	-4.87023600	-0.03299200
C	7.15904500	-2.44980600	-0.03140400
C	7.14998000	-0.00674500	-0.03243600
C	5.78637100	-4.88780000	-0.04369100
H	7.73124300	-5.80942000	-0.03108300
C	5.72568800	-2.46553100	-0.04336900
C	5.70709300	-0.00686300	-0.04647200
C	5.04065600	-3.70818500	-0.04868400
H	5.29260600	-5.85156500	-0.05020300
C	5.00549900	-1.23532600	-0.05182800
C	3.57989800	-3.70341500	-0.05908400
C	3.57866100	-1.23417500	-0.06540700
C	2.84429000	-4.89502000	-0.06309900
C	2.86946500	-2.47767300	-0.06822300
C	2.87424600	-0.00721000	-0.08299800
C	1.46861000	-4.89722400	-0.07034300
H	3.35310400	-5.85080700	-0.06324400
C	1.44136700	-2.48046900	-0.07407600
C	1.43048300	-0.00664300	-0.10027400
C	0.73367600	-3.70292900	-0.07433500
H	0.96374000	-5.85436700	-0.07828300
C	0.72002900	-1.23730000	-0.09943100
C	-0.72137000	-3.70289800	-0.07304700
C	-0.70978300	-1.23761000	-0.10785700
C	-1.45580000	-4.89690600	-0.05344600
C	-1.42951500	-2.47999400	-0.08943000
C	-1.41861800	-0.00839000	-0.13692600

C	-2.83184000	-4.89522600	-0.04999400
H	-0.95072400	-5.85390400	-0.04122700
C	-2.85810500	-2.47827100	-0.07828400
C	-2.86288600	-0.00829900	-0.09537000
C	-3.56822400	-3.70447600	-0.06279600
H	-3.34024500	-5.85110200	-0.03390200
C	-3.56789700	-1.23591700	-0.08073300
C	-5.02915400	-3.71009600	-0.05540600
C	-4.99493100	-1.23697200	-0.05769400
C	-5.77378700	-4.89006700	-0.05485500
C	-5.71465900	-2.46726600	-0.04757700
C	-5.69671100	-0.00810400	-0.05153600
C	-7.17551300	-4.87221400	-0.04225400
H	-5.27987400	-5.85364500	-0.06904500
C	-7.14804700	-2.45135600	-0.03326700
C	-7.13981600	-0.00817200	-0.03321000
C	-7.85639900	-3.67951800	-0.02980900
H	-7.71880800	-5.81145300	-0.04376700
C	-7.82491900	-1.22904300	-0.02466700
H	8.95353900	3.64067400	-0.01974300
H	8.92278700	1.20861800	-0.01786800
H	8.92279700	-1.22209900	-0.01745100
H	8.95414000	-3.65354200	-0.01896000
H	-8.94210400	-3.65662300	-0.02061700
H	-8.91191200	-1.22424100	-0.01454800
H	-8.91196300	1.20784200	-0.01596900
H	-8.94233900	3.64036900	-0.02516900
N	-0.23317300	0.31162500	2.64707300
H	-1.24218800	0.35039400	2.45342500
H	0.18431100	-0.37566600	1.98869600
H	0.17682100	1.22945000	2.43044400
H	-0.05264600	0.04594300	3.61994100

Graphene-NMe₄⁺

C	5.13201000	-1.22750500	-0.21863300
C	5.85279200	-2.45755500	-0.20189800
C	3.70593600	-1.22647700	-0.25550800
C	7.96222400	-1.21961600	-0.14901600
C	7.28573700	-2.44268300	-0.16679900
C	5.16786700	-3.69942100	-0.22145700
C	2.99716300	-2.47006500	-0.27418000
C	7.99622300	-3.66879700	-0.15238600
C	5.91506800	-4.87863000	-0.20601200
C	3.70762100	-3.69559600	-0.25815100
C	1.56947300	-2.47011100	-0.31043300
C	7.31606200	-4.86230300	-0.17202600
H	5.42116700	-5.84228900	-0.22295200
C	2.97383100	-4.88820700	-0.28169700
C	0.84961500	-1.22795900	-0.33839500
C	0.86413300	-3.69402000	-0.32433700

H	7.85888600	-5.80168900	-0.16286800
C	1.59880200	-4.88888000	-0.31316800
H	3.48248600	-5.84412800	-0.27900600
C	-0.57495100	-1.22898700	-0.38190100
C	-0.58988900	-3.69532100	-0.34957500
H	1.09365800	-5.84575200	-0.33829000
C	-1.29623700	-2.47177100	-0.38339200
C	-1.32487500	-4.88985500	-0.33715800
C	-2.72603700	-2.47142700	-0.40883100
C	-2.70041200	-4.88872000	-0.36201000
H	-0.81988400	-5.84666500	-0.30711400
C	-3.43678200	-1.22801500	-0.42918700
C	-3.43660400	-3.69781100	-0.39990000
H	-3.20959000	-5.84430100	-0.35097600
C	-4.86503200	-1.23032600	-0.43689100
C	-4.89772300	-3.70481800	-0.42697600
C	-5.58403100	-2.46135100	-0.43793900
C	-5.64006300	-4.88580900	-0.44023800
C	-7.01790900	-2.44486500	-0.45478500
H	-5.14552300	-5.84907800	-0.44335900
C	-7.04198400	-4.86695800	-0.45939000
C	-7.72384800	-3.67504400	-0.46441800
C	-7.69544800	-1.22316600	-0.46253000
H	-7.58531700	-5.80631000	-0.47288300
C	-7.72425900	3.67260600	-0.47008800
C	-7.69559000	1.22073000	-0.46436300
C	-7.04252600	4.86459600	-0.46690700
C	-7.01819500	2.44251100	-0.45820600
C	-7.01194500	-0.00117500	-0.45642300
C	-5.64060800	4.88363200	-0.44701400
H	-7.58594400	5.80386700	-0.48250900
C	-5.58432500	2.45918300	-0.44076700
C	-5.56792500	-0.00107800	-0.44336600
C	-4.89817200	3.70274500	-0.43102200
H	-5.14614500	5.84693400	-0.45216600
C	-4.86518800	1.22825200	-0.43817500
C	-3.43708100	3.69592700	-0.40229700
C	-3.43692000	1.22611000	-0.43041300
C	-2.70112200	4.88693200	-0.36257400
C	-2.72632900	2.46965600	-0.41086800
C	-2.73030500	-0.00092100	-0.43095900
C	-1.32560500	4.88825000	-0.33671800
H	-3.21050100	5.84239300	-0.35034600
C	-1.29654800	2.47018000	-0.38483200
C	-1.28415700	-0.00081600	-0.40645300
C	-0.59043100	3.69381600	-0.35007800
H	-0.82076700	5.84508600	-0.30483700
C	-0.57510800	1.22746200	-0.38243800
C	0.86359300	3.69271800	-0.32483100
C	0.84942400	1.22664400	-0.33835500

C	1.59807000	4.88769800	-0.31439500
C	1.56910000	2.46891000	-0.31061000
C	1.55689300	-0.00060600	-0.31779200
C	2.97309600	4.88724300	-0.28290300
H	1.09277200	5.84446700	-0.34047400
C	2.99678500	2.46909000	-0.27440600
C	2.99979600	-0.00049300	-0.27445100
C	3.70705000	3.69474100	-0.25873700
H	3.48162400	5.84323300	-0.28090500
C	3.70574700	1.22561000	-0.25561300
C	5.16728900	3.69880400	-0.22197200
C	5.13181700	1.22687900	-0.21877700
C	5.91429500	4.87813900	-0.20663000
C	5.85240500	2.45704800	-0.20222500
C	5.83320900	-0.00025700	-0.20073800
C	7.31528700	4.86204200	-0.17265000
H	5.42023300	5.84171600	-0.22362100
C	7.28535200	2.44241300	-0.16712700
C	7.27531200	-0.00013700	-0.16514000
C	7.99563800	3.66864200	-0.15288200
H	7.85796400	5.80151600	-0.16359400
C	7.96203100	1.21945100	-0.14917900
H	-8.80955100	-3.65343300	-0.48067900
H	-8.78232900	-1.21935000	-0.47763600
H	-8.78246700	1.21676100	-0.47971400
H	-8.80995300	3.65085000	-0.48679600
H	9.08112700	3.64463700	-0.12783100
H	9.04898500	1.21409800	-0.12411900
H	9.04917700	-1.21408400	-0.12395300
H	9.08170800	-3.64460800	-0.12732200
N	-1.43495300	0.00722500	3.48909600
C	-2.15115500	-1.20861800	2.98211900
H	-3.18381600	-1.17749500	3.33319900
H	-2.12584600	-1.19759300	1.89219800
H	-1.64502700	-2.09688500	3.36335500
C	-2.12008100	1.23509800	2.96831300
H	-3.14367100	1.25052800	3.34592200
H	-1.57256500	2.11406700	3.31219300
H	-2.12336600	1.19458100	1.87902600
C	-0.01730900	-0.01378300	3.00126800
H	0.49492200	0.87263500	3.37886400
H	0.46543400	-0.91971200	3.37132000
H	-0.02648900	-0.00905700	1.91134800
C	-1.45217800	0.01612900	4.98267400
H	-0.93455700	0.90974200	5.33440800
H	-2.48875500	0.02399200	5.32241200
H	-0.94455700	-0.87886300	5.34530700

Graphene-OH₃⁺

C	-5.00236300	1.23060100	-0.05684000
C	-5.72148900	2.46041100	-0.05352300
C	-3.57490500	1.22944100	-0.06093600
C	-7.83185200	1.22287800	-0.05105200
C	-7.15489000	2.44498700	-0.05180400
C	-5.03566800	3.70337000	-0.05382300
C	-2.86465400	2.47084000	-0.06204000
C	-7.86337200	3.67320400	-0.05252100
C	-5.78032300	4.88300800	-0.05644600
C	-3.57468700	3.69754400	-0.05244400
C	-1.43491100	2.47352000	-0.06062800
C	-7.18234700	4.86570700	-0.05561700
H	-5.28649800	5.84675900	-0.06204400
C	-2.83786700	4.88772200	-0.04229000
C	-0.71540300	1.23256700	-0.08338800
C	-0.72613200	3.69774900	-0.05481100
H	-7.72519200	5.80512500	-0.05884900
C	-1.46138400	4.89068200	-0.04254400
H	-3.34631500	5.84368500	-0.03471400
C	0.71666900	1.23355400	-0.06112300
C	0.72889800	3.69923400	-0.05408500
H	-0.95718800	5.84811700	-0.03546400
C	1.43772600	2.47628600	-0.06060600
C	1.46436300	4.89260700	-0.05116000
C	2.86677900	2.47247900	-0.05760000
C	2.84069800	4.88968000	-0.05267700
H	0.96016000	5.85008900	-0.05306200
C	3.57522400	1.22983400	-0.06389800
C	3.57703100	3.69886700	-0.05655900
H	3.34943500	5.84547100	-0.05235100
C	5.00212100	1.23019000	-0.05988700
C	5.03788700	3.70326800	-0.06045100
C	5.72244300	2.45983600	-0.06062200
C	5.78386500	4.88235900	-0.06384400
C	7.15573600	2.44351300	-0.06333200
H	5.29066200	5.84644700	-0.06593600
C	7.18567900	4.86402800	-0.06763900
C	7.86562000	3.67073800	-0.06687900
C	7.83153400	1.22058000	-0.06189400
H	7.72934000	5.80295900	-0.07178900
C	7.86361600	-3.67016800	-0.04654400
C	7.83029500	-1.22034900	-0.05529400
C	7.18348700	-4.86334600	-0.04123400
C	7.15387700	-2.44289000	-0.05163800
C	7.14498800	0.00047900	-0.05899000
C	5.78170500	-4.88105000	-0.04194900
H	7.72684700	-5.80243300	-0.03672600
C	5.72060100	-2.45858600	-0.05244400
C	5.70227300	0.00076500	-0.05885300

C	5.03602600	-3.70179200	-0.04976700
H	5.28802800	-5.84490800	-0.03658700
C	5.00093500	-1.22842100	-0.05642000
C	3.57542100	-3.69744700	-0.05469800
C	3.57406400	-1.22732300	-0.06153300
C	2.83917000	-4.88822700	-0.06299400
C	2.86521900	-2.47107800	-0.05399100
C	2.87132600	0.00186100	-0.05993100
C	1.46293100	-4.89098700	-0.06734300
H	3.34790400	-5.84400400	-0.07016800
C	1.43684700	-2.47593400	-0.06001000
C	1.42943000	0.00312300	-0.08069200
C	0.72771400	-3.69749900	-0.06196300
H	0.95852100	-5.84825700	-0.08129800
C	0.71567700	-1.23084900	-0.05149100
C	-0.72778500	-3.69575700	-0.06592000
C	-0.71831700	-1.23026300	-0.09014200
C	-1.46289700	-4.88826500	-0.05594500
C	-1.43681700	-2.47170200	-0.06928900
C	-1.42725300	0.00139500	-0.07383200
C	-2.83969000	-4.88508500	-0.05651400
H	-0.95892400	-5.84580800	-0.04858800
C	-2.86614100	-2.46845700	-0.07103100
C	-2.87165500	0.00120400	-0.07324100
C	-3.57641700	-3.69519800	-0.06368600
H	-3.34816300	-5.84104800	-0.05103800
C	-3.57541100	-1.22677100	-0.06499300
C	-5.03747600	-3.70045000	-0.06304500
C	-5.00294400	-1.22752000	-0.06036700
C	-5.78263800	-4.87967800	-0.06613600
C	-5.72262100	-2.45710800	-0.05961500
C	-5.70380300	0.00164600	-0.05616800
C	-7.18467800	-4.86170500	-0.06369700
H	-5.28921700	-5.84362900	-0.07299700
C	-7.15598700	-2.44102800	-0.05658100
C	-7.14658800	0.00196400	-0.05275300
C	-7.86508200	-3.66890800	-0.05849700
H	-7.72799000	-5.80085000	-0.06728200
C	-7.83239700	-1.21860300	-0.05321600
H	8.95130000	3.64684200	-0.07043900
H	8.91857700	1.21470700	-0.06432700
H	8.91737700	-1.21534600	-0.05637900
H	8.94930700	-3.64641400	-0.04737400
H	-8.95077700	-3.64566600	-0.05718800
H	-8.91942000	-1.21339100	-0.05188600
H	-8.91887900	1.21815500	-0.05030600
H	-8.94908200	3.65050000	-0.05235600
H	-0.95166000	-0.05087400	2.34204400
H	0.39972300	-0.73150300	1.88775100
H	0.37123400	0.80204500	2.22879300

O	0.01458800	-0.06680600	2.55287600
Graphene-OMe ₃ ⁺			
C	-5.10802100	1.22727900	-0.16138800
C	-5.82883600	2.45731400	-0.15028100
C	-3.68178500	1.22624300	-0.18665700
C	-7.93858400	1.21953400	-0.11565300
C	-7.26196000	2.44261000	-0.12767400
C	-5.14379700	3.69908900	-0.16314500
C	-2.97279800	2.46984100	-0.19845000
C	-7.97276100	3.66854000	-0.11922700
C	-5.89128100	4.87820600	-0.15422800
C	-3.68329600	3.69539700	-0.18636800
C	-1.54490300	2.46996900	-0.22305600
C	-7.29250400	4.86210600	-0.13271300
H	-5.39729400	5.84190000	-0.16656300
C	-2.94922200	4.88796600	-0.20043000
C	-0.82491000	1.22768000	-0.24664400
C	-0.83932000	3.69378600	-0.22995000
H	-7.83528800	5.80149900	-0.12814000
C	-1.57395300	4.88864200	-0.22094000
H	-3.45770100	5.84396100	-0.19872800
C	0.60024400	1.22853600	-0.27938600
C	0.61495600	3.69505600	-0.24729400
H	-1.06863600	5.84555400	-0.23900500
C	1.32144600	2.47140200	-0.27892000
C	1.35008600	4.88943100	-0.23133500
C	2.75147400	2.47096700	-0.30103300
C	2.72580500	4.88811400	-0.25239800
H	0.84522500	5.84630500	-0.20209300
C	3.46234500	1.22725000	-0.31860800
C	3.46227600	3.69739200	-0.29003700
H	3.23501100	5.84362100	-0.23854300
C	4.89100900	1.22960300	-0.32284400
C	4.92354400	3.70428600	-0.31451300
C	5.60977400	2.46044300	-0.32306500
C	5.66572500	4.88506200	-0.32733500
C	7.04370100	2.44375300	-0.33602400
H	5.17141500	5.84843000	-0.33286800
C	7.06787700	4.86594700	-0.34309700
C	7.74961200	3.67412800	-0.34509000
C	7.72118300	1.22218700	-0.34034300
H	7.61129900	5.80522100	-0.35611000
C	7.74965700	-3.67389900	-0.33988100
C	7.72119300	-1.22198100	-0.33853100
C	7.06796400	-4.86575800	-0.33687100
C	7.04370300	-2.44355000	-0.33312700
C	7.03772900	0.00010100	-0.33468600
C	5.66581900	-4.88490300	-0.32312300
H	7.61145300	-5.80502200	-0.34757400

C	5.60975800	-2.46026300	-0.32153400
C	5.59375300	0.00009900	-0.32625200
C	4.92354900	-3.70411300	-0.31331900
H	5.17158500	-5.84831600	-0.32731300
C	4.89089400	-1.22942100	-0.32228700
C	3.46224100	-3.69723300	-0.29242900
C	3.46233300	-1.22712200	-0.31849200
C	2.72565000	-4.88798500	-0.25991900
C	2.75152800	-2.47066800	-0.30270300
C	2.75578000	-0.00007000	-0.32028000
C	1.34987600	-4.88935800	-0.24066800
H	3.23475100	-5.84358400	-0.24914200
C	1.32127400	-2.47124900	-0.28227500
C	1.30949800	0.00002600	-0.29877600
C	0.61474700	-3.69503500	-0.25323700
H	0.84501500	-5.84634000	-0.21546800
C	0.60000300	-1.22831500	-0.28114600
C	-0.83945300	-3.69369800	-0.23426600
C	-0.82497600	-1.22752800	-0.24803200
C	-1.57412800	-4.88852900	-0.22501700
C	-1.54494700	-2.46979900	-0.22532200
C	-1.53255700	-0.00000700	-0.23253500
C	-2.94936400	-4.88781700	-0.20269000
H	-1.06887700	-5.84545800	-0.24393600
C	-2.97286400	-2.46968800	-0.19928900
C	-2.97582000	0.00005300	-0.20052100
C	-3.68338400	-3.69523500	-0.18705900
H	-3.45787000	-5.84379800	-0.20094900
C	-3.68181300	-1.22609500	-0.18680900
C	-5.14386400	-3.69891900	-0.16221100
C	-5.10806400	-1.22710900	-0.16116000
C	-5.89133500	-4.87802700	-0.15181900
C	-5.82889400	-2.45712700	-0.14942900
C	-5.80927900	0.00008600	-0.14926700
C	-7.29254700	-4.86190200	-0.12932900
H	-5.39736000	-5.84173300	-0.16360700
C	-7.26201500	-2.44240100	-0.12611100
C	-7.25149400	0.00009700	-0.12566700
C	-7.97280400	-3.66833400	-0.11640600
H	-7.83532500	-5.80129400	-0.12358900
C	-7.93862100	-1.21931200	-0.11471800
H	8.83533100	3.65252700	-0.35823300
H	8.80806700	1.21834200	-0.35196400
H	8.80808300	-1.21815400	-0.34960100
H	8.83538900	-3.65227900	-0.35183700
H	-9.05843700	-3.64410500	-0.10013100
H	-9.02574100	-1.21374600	-0.09850000
H	-9.02570900	1.21400300	-0.09969000
H	-9.05840200	3.64431800	-0.10355400
O	1.44207800	0.00113400	3.44973500

C	2.11115400	1.24797400	3.04745200
H	1.45744800	2.06020700	3.35943100
H	3.05392000	1.27066800	3.59097000
H	2.25942400	1.23207400	1.96652800
C	2.19251700	-1.20323700	3.06321900
H	3.20862400	-1.05631600	3.42479600
H	1.71059600	-2.03541600	3.57249400
H	2.15680900	-1.30501500	1.97745000
C	0.02317600	-0.04922800	3.06825100
H	-0.35289600	-1.00649100	3.42399000
H	-0.45707200	0.77779200	3.58775700
H	-0.05164400	0.04388600	1.98423100

Graphene-SMe₃⁺

C	4.93867500	-1.08243500	-0.39861800
C	5.66543600	-2.30841600	-0.44136800
C	3.51089800	-1.08741200	-0.41340700
C	7.76889300	-1.05869300	-0.37884600
C	7.09910500	-2.28370800	-0.43346300
C	4.98768500	-3.55507600	-0.49615800
C	2.80899700	-2.33491400	-0.46254100
C	7.81345400	-3.50783600	-0.48371800
C	5.73813600	-4.73036300	-0.54723500
C	3.52655900	-3.55725100	-0.49530700
C	1.37867300	-2.34432800	-0.45911200
C	7.13976300	-4.70324900	-0.54119900
H	5.25032400	-5.69563700	-0.60210600
C	2.79723500	-4.75289700	-0.52439700
C	0.64960500	-1.10496900	-0.40959600
C	0.67905300	-3.57338000	-0.49060300
H	7.68915100	-5.63803300	-0.58581100
C	1.42137300	-4.76354300	-0.52137400
H	3.31249900	-5.70488500	-0.55236000
C	-0.77700400	-1.11416600	-0.38731200
C	-0.77652600	-3.58150900	-0.47069700
H	0.92180500	-5.72331800	-0.55099200
C	-1.48977700	-2.36156200	-0.41442800
C	-1.50421300	-4.78092600	-0.49324700
C	-2.91814500	-2.37092600	-0.37859900
C	-2.87933000	-4.78835700	-0.46252300
H	-0.99356200	-5.73375900	-0.54762300
C	-3.63408800	-1.13263600	-0.31867400
C	-3.62090000	-3.60124600	-0.40426400
H	-3.38281900	-5.74663900	-0.48962700
C	-5.06030500	-1.14406800	-0.28519600
C	-5.08121800	-3.61559100	-0.37215700
C	-5.77318600	-2.37847500	-0.31204100
C	-5.82017400	-4.79956600	-0.40059400
C	-7.20629700	-2.37272800	-0.28084100
H	-5.32106900	-5.75925800	-0.45258300

C	-7.22128500	-4.79177600	-0.37037400
C	-7.90837300	-3.60356400	-0.31096600
C	-7.89040200	-1.15505400	-0.22377500
H	-7.75906800	-5.73377400	-0.39703400
C	-7.95252100	3.73187100	-0.06718500
C	-7.90528000	1.28363000	-0.14318800
C	-7.27870300	4.92877900	-0.04585400
C	-7.23570500	2.51017000	-0.11907000
C	-7.21170800	0.06881400	-0.19728200
C	-5.87765500	4.95462400	-0.07360300
H	-7.82681800	5.86443600	-0.00795900
C	-5.80265600	2.53463600	-0.14841900
C	-5.76920300	0.07827800	-0.22835400
C	-5.12443000	3.78044300	-0.12413400
H	-5.38925700	5.92101800	-0.05592500
C	-5.07480700	1.30974100	-0.20313100
C	-3.66392300	3.78521800	-0.15208200
C	-3.64833000	1.31811000	-0.23410500
C	-2.93635100	4.98149600	-0.12779000
C	-2.94628100	2.56500900	-0.20535200
C	-2.93519300	0.09753600	-0.29258600
C	-1.56110000	4.99107200	-0.14647000
H	-3.45039000	5.93388800	-0.09333400
C	-1.51826800	2.57439700	-0.22896500
C	-1.49215200	0.10773400	-0.32789800
C	-0.81937200	3.80149600	-0.19275600
H	-1.06146200	5.95089600	-0.12793400
C	-0.79044400	1.33824800	-0.29267100
C	0.63473700	3.81079500	-0.19964000
C	0.63510200	1.34834700	-0.31140500
C	1.36195800	5.00868700	-0.14615300
C	1.34867000	2.59281100	-0.25487800
C	1.35192800	0.12702900	-0.36844800
C	2.73747700	5.01569000	-0.14664800
H	0.85108100	5.96175300	-0.10246600
C	2.77727800	2.60084800	-0.25504100
C	2.79675000	0.13519400	-0.36968900
C	3.48024900	3.82955100	-0.19929500
H	3.24034300	5.97370900	-0.10415500
C	3.49517200	1.36361300	-0.30670500
C	4.94136000	3.84426500	-0.19618000
C	4.92303500	1.37301500	-0.29778100
C	5.67815900	5.02800600	-0.14858300
C	5.63529200	2.60650800	-0.24206700
C	5.63341600	0.14945900	-0.34254000
C	7.08009700	5.01833700	-0.14327000
H	5.17812900	5.98791100	-0.11688500
C	7.06908700	2.59895000	-0.23537200
C	7.07704800	0.15772700	-0.33288100
C	7.76905400	3.83107100	-0.18453100

H	7.61733800	5.96051100	-0.10713100
C	7.75409800	1.38193200	-0.27961700
H	-8.99407000	-3.58705500	-0.28901700
H	-8.97736900	-1.15729800	-0.20219800
H	-8.99217200	1.27125700	-0.12190000
H	-9.03791100	3.70131200	-0.04658300
H	8.85495100	3.81524800	-0.18168000
H	8.84111800	1.38409800	-0.27577700
H	8.85585300	-1.04802900	-0.37543200
H	8.89909300	-3.47910500	-0.48044900
S	0.74089900	-1.22259800	3.75620100
C	-0.04993700	-2.61490800	2.91678100
H	0.47983300	-3.52330600	3.20944200
H	-1.08706600	-2.66235800	3.25401700
H	0.00470800	-2.46145900	1.83747900
C	-0.09543800	0.17923100	2.97919100
H	-1.13434100	0.17540700	3.31441000
H	0.40129900	1.09120700	3.31605100
H	-0.03234800	0.07691300	1.89450500
C	2.34919500	-1.17805300	2.93032200
H	2.86696800	-0.27482000	3.25904200
H	2.90895700	-2.06204600	3.24143700
H	2.19974400	-1.16991000	1.84909100