

Supporting Information

Theoretical mechanism study on the electrochemical benzylation of [60]fullerene derivatives

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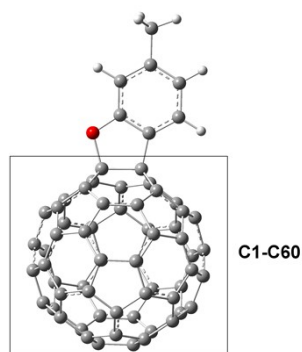
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Computational details of ΔG^\ddagger and ΔG° values

Cartesian Coordinate of computed compounds

Table S1 The calculated nature population analysis (NPA) charge values of **IM2**.



atoms	NPA charge	atoms	NPA charge
C1	-0.08218	C31	-0.03077
C2	-0.03296	C32	-0.02957
C3 (site b)	-0.09544	C33	-0.05012
C4	-0.01921	C34	-0.01887
C5	-0.02960	C35	-0.02023
C6	-0.03227	C36	-0.02146
C7	-0.01925	C37	-0.02322
C8	-0.00808	C38	-0.02134
C9	-0.01801	C39	-0.06018
C10	-0.03922	C40	-0.02612
C11	-0.02140	C41	-0.00875
C12	-0.05104	C42	-0.02193
C13	-0.01410	C43	-0.02988
C14	-0.02460	C44	-0.02274
C15	0.26827	C45	-0.00772
C16 (site a)	-0.12419	C46	-0.02805
C17	-0.02030	C47	-0.01600
C18	-0.03102	C48	-0.01462
C19	-0.03345	C49	-0.06040
C20	-0.03694	C50	-0.00948
C21	-0.01707	C51	-0.05113
C22	-0.02459	C52	-0.01542
C23	-0.09270	C53	-0.01320
C24	-0.01211	C54	-0.01447
C25	-0.03370	C55	-0.04567
C26	-0.01882	C56	-0.01725
C27	-0.01484	C57	-0.06443
C28	-0.02106	C58	-0.03325
C29	-0.02520	C59	0.02050
C30	-0.02546	C60	-0.08536

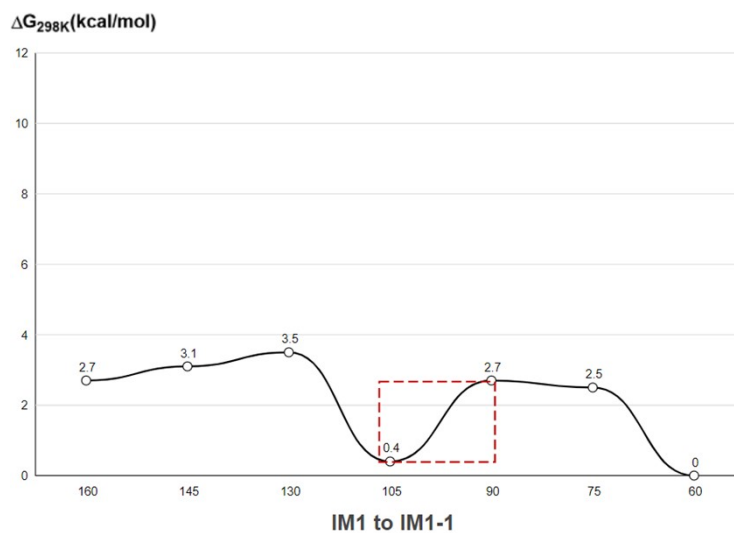


Fig. S1 The energy curve of the rotation of the $C_{\text{benzene}}-C_{\text{C60}}$ bond from **IM1** to **IM1-1**.

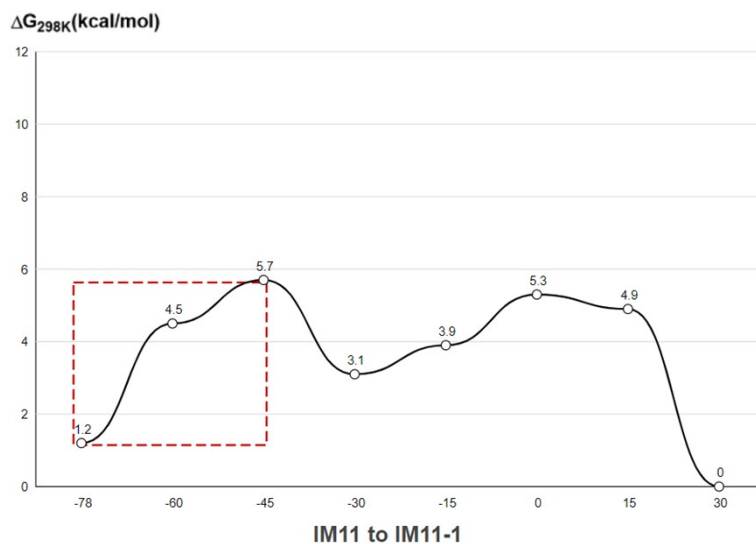


Fig. S2 The energy curve of the rotation of the $C_{\text{benzene}}-C_{\text{C60}}$ bond from **IM11** to **IM11-1**.

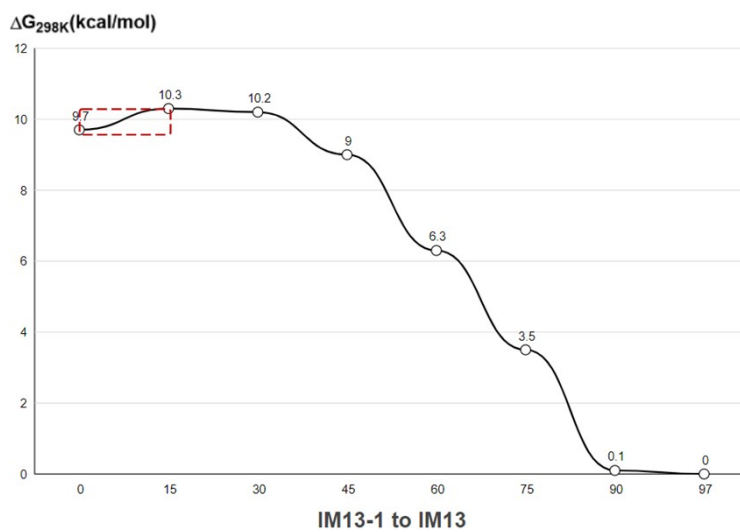


Fig. S3 The energy curve of the rotation of the $C_{\text{benzene}}-C_{\text{C60}}$ bond from **IM13-1** to **IM13**.

Computational details of ΔG^\ddagger and ΔG° values

The free energy in the solution-phase $G(\text{sol})$ has been calculated as follows:

$$G(\text{sol}) = G(\text{gas}) + G(\text{solv})$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas})$$

$$H(\text{gas}) = E(\text{SCF}) + \text{ZPE}$$

$$\Delta E(\text{SCF}) = \Sigma E(\text{SCF}) \text{ for products} - \Sigma E(\text{SCF}) \text{ for reactants}$$

Therefore, the ΔG^\ddagger and ΔG° values can be calculated as follows:

$$\Delta G^\circ(\text{sol}) = \Sigma G(\text{sol}) \text{ for products} - \Sigma G(\text{sol}) \text{ for reactants}$$

$$\Delta G^\ddagger(\text{sol}) = \Sigma G(\text{sol}) \text{ for transition structures} - \Sigma G(\text{sol}) \text{ for relevant intermediates}$$

$G(\text{gas})$ is the free energy in the gas phase, $G(\text{sol})$ is the free energy of solvation as computed using the continuum solvation model, $H(\text{gas})$ is the enthalpy in the gas phase, T is the absolute temperature (298.15 K), $S(\text{gas})$ is the entropy in the gas phase, $E(\text{SCF})$ is the self-consistent field energy, i.e., raw electronic energy as computed from the SCF procedure, and ZPE is the zero-point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model.

Cartesian Coordinate of computed compounds

IM1-1

-2 (charge), 1(multiplicity)

	x	y	z
C	0.92939200	0.82232200	-1.44583400
C	-0.01680700	1.50481500	-2.25518100
C	-0.72600200	2.65155700	-1.82804300
C	-0.56530800	3.04677700	-0.42447300
C	0.77243100	-0.56886700	-1.69310700
C	-0.21019100	-0.76753200	-2.76336300
C	-0.70832600	0.53615800	-3.11682000
C	-2.04860600	0.70922500	-3.46004700
C	-2.11607300	2.78979200	-2.14996700
C	-1.85215100	3.49021600	0.07685800
C	-2.21526200	3.25497000	1.40932900
C	-1.30517200	2.54845400	2.27520600
C	-0.07945900	2.10036700	1.75878700
C	0.43659400	0.79020300	2.11978500
C	1.17154200	0.26437500	1.00057600
C	1.02838200	-1.07971100	0.70163500
C	0.87702300	-1.54637000	-0.68397500
C	-1.05932400	-1.87390600	-2.76079100
C	-0.97387500	-2.85821800	-1.69856900
C	-0.02929900	-2.65634500	-0.67042100
C	-0.41632700	-2.92237700	0.71309400
C	0.24198300	-1.94976500	1.55387500
C	-0.40922900	-1.44135900	2.68535000
C	-0.30843200	-0.03470300	2.97838900
C	-1.60177500	0.41518700	3.48031400
C	-2.08733100	1.67551500	3.13987000

C	-2.81735300	3.32729500	-0.98337200
C	-5.32412500	0.58162500	1.73595100
C	-5.39924200	1.52479700	0.70445000
C	-5.56859300	1.08416700	-0.67506600
C	-5.66938800	-0.28046200	-0.95952400
C	-5.58301500	-1.25550000	0.11245400
C	-4.50786900	-1.54448000	2.31205700
C	-3.84631600	-0.56675600	3.15970800
C	-4.35167900	0.74927400	2.80268000
C	-3.48798400	1.84800300	2.79501700
C	-3.56569600	2.82885500	1.72261100
C	-4.49992800	2.66127700	0.69493600
C	-4.80192400	1.96420300	-1.53697500
C	-4.12030500	1.43306000	-2.64580500
C	-4.22798200	0.01061500	-2.94480700
C	-4.98171700	-0.82637900	-2.12066400
C	-4.47742700	-2.14251000	-1.76429800
C	-4.85258300	-2.40801300	-0.38272700
C	-3.96630900	-3.08890700	0.45671200
C	-3.79506100	-2.65119000	1.83663400
C	-2.49785400	-0.72805300	3.49179600
C	-1.75633000	-1.87898300	2.99927300
C	-2.39636500	-2.81468300	2.17972300
C	-1.70913200	-3.35875700	1.01618600
C	-2.68354800	-3.54882100	-0.04204300
C	-2.31485400	-3.27679700	-1.36964400
C	-3.23965700	-2.56941900	-2.24631800
C	-2.45915700	-1.70147100	-3.11153100
C	-2.94308800	-0.43739200	-3.45397400
C	-4.12374700	2.92524900	-0.68815600
C	-2.78553600	1.86503100	-2.98056800
C	-5.42789800	-0.83630200	1.44066300
C	2.79963400	2.01498400	-0.09719700
C	4.02032800	1.29430100	-0.13623000
C	1.38776400	1.36819900	-0.08199000
C	0.32020900	2.38839800	0.41257000
O	3.98543700	-0.07762800	-0.15288200
C	2.89486200	3.41452000	-0.10248600
C	5.24404900	1.98651400	-0.14697300
H	1.97748200	3.99242400	-0.08091200
H	6.19220500	1.45492200	-0.13991000
C	4.10938700	4.09739400	-0.12500000
C	5.30705100	3.38147200	-0.13941300
H	4.11493400	5.18648200	-0.12157300

C	6.66149600	4.05652300	-0.14980900
H	6.84313000	4.57103600	-1.10459100
H	6.73502700	4.81608800	0.64060600
H	7.46041600	3.32001200	-0.00466900
C	5.21137900	-2.21475800	-0.12415000
C	4.05678000	-2.95916000	-0.36825200
C	6.42011800	-2.88427000	0.13659100
C	4.09825300	-4.35665300	-0.33695500
H	3.12641100	-2.44716400	-0.58290000
C	6.45730600	-4.27702400	0.16026800
H	7.31975800	-2.29039700	0.30335100
C	5.29524800	-5.02115700	-0.07159800
H	3.18601200	-4.92047800	-0.52131300
H	7.39839400	-4.78458000	0.36422100
H	5.32540300	-6.10921000	-0.04621600
Br	8.68792200	0.41057400	0.22657400
C	5.27791900	-0.70961700	-0.16528600
H	5.82788900	-0.39618100	-1.06226700
H	5.88105100	-0.35619300	0.67748100

IM1

-2 1

	x	y	z
C	-2.33206200	-0.60305100	1.29308000
C	-1.68679700	0.10342300	2.33357000
C	-1.38632800	1.48928500	2.26584400
C	-1.65009300	2.16585800	0.99075300
C	-1.74595200	-1.90010000	1.22090800
C	-0.76769900	-2.04840300	2.30084400
C	-0.72649500	-0.78837400	3.00126500
C	0.47563700	-0.29983900	3.50600800
C	-0.12503900	1.96468400	2.74471900
C	-0.56972000	3.10310400	0.73768800
C	-0.12814000	3.34403400	-0.57250100
C	-0.74388400	2.63812100	-1.66702200
C	-1.76094800	1.70822100	-1.39229600
C	-1.80901900	0.43934700	-2.10293200
C	-2.33599100	-0.55850800	-1.21642400
C	-1.78657600	-1.83028500	-1.24469200
C	-1.50549500	-2.55798400	-0.00063400
C	0.39927900	-2.79323100	2.12031000
C	0.65770700	-3.44120300	0.84868800
C	-0.28751100	-3.28620100	-0.18979300
C	0.18668800	-3.05119800	-1.55392600

C	-0.74386600	-2.15524600	-2.19931200
C	-0.27541100	-1.19073600	-3.10670900
C	-0.82592100	0.13961300	-3.06374500
C	0.25571200	1.08540100	-3.31016200
C	0.29568700	2.30370200	-2.63340000
C	0.38026400	2.97764700	1.81454000
C	3.69190900	1.95264800	-1.22093000
C	3.43760200	2.57312000	0.00851500
C	3.71876300	1.86629500	1.25360000
C	4.26013200	0.57698900	1.21172600
C	4.51490400	-0.06365200	-0.06477200
C	3.62764500	-0.09629200	-2.36567200
C	2.69306100	0.80845400	-3.01428500
C	2.73484300	2.07790400	-2.30734900
C	1.55686400	2.80919600	-2.12136000
C	1.29202000	3.45461300	-0.84390400
C	2.21500800	3.32705800	0.20090500
C	2.69584800	2.21053000	2.22114000
C	2.20557700	1.22169500	3.09779700
C	2.76994000	-0.12160400	3.05649600
C	3.77169800	-0.43830600	2.13584800
C	3.73255600	-1.70655800	1.42810200
C	4.19344400	-1.47307200	0.06586400
C	3.59082600	-2.15618400	-0.99480900
C	3.30823000	-1.45467900	-2.24162300
C	1.47693400	0.32407500	-3.50627500
C	1.14493400	-1.08768700	-3.38032200
C	2.04608700	-1.95392300	-2.74895900
C	1.55727300	-2.96603500	-1.82224200
C	2.52421000	-3.10926100	-0.75032600
C	2.06637300	-3.31964400	0.56287000
C	2.69541800	-2.61093400	1.66920700
C	1.65997900	-2.28589600	2.63599100
C	1.69756400	-1.06599100	3.31515400
C	1.75235100	3.09275500	1.56314800
C	0.80106900	1.11351400	3.39250400
C	4.25353300	0.61435100	-1.26611400
C	-4.45894600	0.17411700	0.03587900
C	-5.19176700	-1.08224100	-0.05324800
C	-2.92079100	0.10451200	0.06257900
C	-2.25612500	1.49914200	-0.06241500
O	-4.62268000	-2.21082100	-0.09763700
C	-5.14318500	1.38684300	0.09755800
C	-6.63249200	-0.94156200	-0.08807700

H	-4.57228200	2.31140400	0.16864900
H	-7.19769000	-1.87108400	-0.16298600
C	-6.54018300	1.46513900	0.07167100
C	-7.29098000	0.27728300	-0.02100300
H	-7.03787600	2.43309800	0.12301300
C	-8.80599800	0.33655300	-0.01995700
H	-9.24361600	-0.61111200	-0.35719500
H	-9.21041600	0.54359000	0.98327600
H	-9.18160400	1.13260400	-0.67916800

IM2-1

-2 1

	x	y	z
C	-0.44128600	-2.05162100	-1.14580200
C	0.55240400	-2.97648000	-0.73643300
C	0.86382400	-3.23356800	0.61826500
C	0.21165700	-2.38501200	1.62502900
C	0.03177800	-1.40959400	-2.32242700
C	1.30490600	-2.01511100	-2.72616700
C	1.63228800	-3.00083700	-1.72950200
C	2.95500100	-3.20218600	-1.33884600
C	2.23353800	-3.38995000	1.00754700
C	1.18731200	-2.07860400	2.65532900
C	1.17942900	-0.83196300	3.29693100
C	0.20463300	0.15540000	2.90706800
C	-0.70603300	-0.15144600	1.88319700
C	-1.03411000	0.84319600	0.87730800
C	-1.29123300	0.17265600	-0.36866100
C	-0.82854700	0.75406500	-1.53819800
C	-0.19041000	-0.04544000	-2.59530900
C	2.30807400	-1.24505500	-3.31521700
C	2.09699900	0.17067400	-3.54969000
C	0.86667700	0.74325700	-3.15746000
C	0.87058900	2.04871300	-2.49995800
C	-0.17811800	2.05037200	-1.50647600
C	0.00175500	2.73121600	-0.29473600
C	-0.43994400	2.11166700	0.92899300
C	0.53146900	2.41691300	1.97030600
C	0.84640100	1.46291700	2.93534700
C	2.43943400	-2.69225800	2.27646200
C	4.49900800	1.42628100	2.38764100
C	4.69672900	0.05791900	2.60250800
C	5.34836900	-0.75235300	1.58059400
C	5.78663200	-0.15448000	0.39552900

C	5.57248900	1.26409700	0.17393700
C	3.96621000	3.03886200	0.76466600
C	2.91076500	3.04296300	1.76379600
C	3.24085400	2.04480000	2.76860200
C	2.22737900	1.27202700	3.34297600
C	2.43209200	-0.15154500	3.56641400
C	3.64356800	-0.74327100	3.19390100
C	4.71948800	-2.05936300	1.56070000
C	4.51359300	-2.71447000	0.33492900
C	4.97325600	-2.09311000	-0.90163000
C	5.59147100	-0.84239600	-0.87272500
C	5.26133800	0.15548000	-1.87760300
C	5.25223100	1.45850700	-1.22864100
C	4.30151900	2.41137400	-1.60461100
C	3.64892300	3.22418200	-0.58597100
C	1.58109200	3.22394500	1.37399000
C	1.25064300	3.41855600	-0.03026400
C	2.26925100	3.40969100	-0.98871800
C	2.07361300	2.71815900	-2.25591200
C	3.33629700	2.11984600	-2.64841200
C	3.33392300	0.85688000	-3.26237300
C	4.32719600	-0.13653700	-2.87250100
C	3.69029300	-1.44197200	-2.90845800
C	4.00679800	-2.39966700	-1.94208500
C	3.65070700	-2.04627600	2.54221300
C	3.28157500	-3.41181100	0.06015200
C	4.95217300	2.04813900	1.15610700
C	-2.80718400	-1.99378900	-0.15672400
C	-4.03625000	-1.29642800	-0.11229100
C	-1.38783400	-1.36181800	-0.15041200
C	-0.74578900	-1.44756400	1.26946800
O	-4.02325600	0.07483300	-0.09661200
C	-2.87075200	-3.39515200	-0.16697700
C	-5.24968500	-2.00825200	-0.08841700
H	-1.93755200	-3.94882600	-0.20780200
H	-6.20405600	-1.48756100	-0.04944600
C	-4.07145300	-4.09817300	-0.13555600
C	-5.28420700	-3.40260900	-0.09691200
H	-4.05976100	-5.18713500	-0.14390400
C	-6.62412600	-4.10545700	-0.06834900
H	-6.79240700	-4.68210700	-0.98918700
H	-6.68553300	-4.81586700	0.76783300
H	-7.43805200	-3.37854000	0.03259700
C	-5.20737000	2.21043700	-0.11550300

C	-4.01335400	2.90897900	-0.30336500
C	-6.40480800	2.92553600	0.05876500
C	-4.00740100	4.30737500	-0.30631500
H	-3.09191900	2.35908400	-0.44875300
C	-6.39411300	4.31886600	0.04981400
H	-7.33063000	2.36440700	0.19096100
C	-5.19469600	5.01721300	-0.12917100
H	-3.06655400	4.83516400	-0.44682700
H	-7.32669800	4.86330200	0.18650700
H	-5.18823300	6.10586400	-0.13044200
Br	-8.70087900	-0.37951300	0.20561700
C	-5.31154000	0.70730400	-0.11530100
H	-5.87469200	0.37716900	-0.99758900
H	-5.91151100	0.38224700	0.74193600

IM2

-2 1

	x	y	z
C	2.24664900	1.15191700	-1.18034800
C	1.53087100	2.34826600	-0.94604000
C	1.23773500	2.84101400	0.35822500
C	1.58054100	1.96251400	1.47660300
C	1.65959800	0.49937700	-2.31127900
C	0.61853600	1.35480300	-2.86286800
C	0.52751600	2.50950900	-1.99891800
C	-0.71037800	3.09486800	-1.73011800
C	-0.05559200	3.38847000	0.63052500
C	0.52487000	2.05026300	2.47465100
C	0.17894500	0.93026000	3.23932500
C	0.86620400	-0.32041700	3.02727600
C	1.84821400	-0.39931500	2.01216000
C	1.98280500	-1.57030700	1.19296300
C	2.68640200	-1.23825200	-0.11424600
C	1.90898200	-1.75436700	-1.27613800
C	1.49478400	-0.90009200	-2.36013800
C	-0.53952000	0.81871100	-3.44712000
C	-0.70789300	-0.61882300	-3.49961200
C	0.29351500	-1.44749000	-2.96075800
C	-0.07255800	-2.61041000	-2.17961000
C	0.92610600	-2.76656400	-1.12777900
C	0.51685600	-3.27325000	0.13663200
C	1.04432800	-2.59356200	1.30942300
C	-0.01188000	-2.50372200	2.30870700
C	-0.09555300	-1.39187400	3.15087300
C	-0.49767300	2.92260400	1.94817500

C	-3.57972000	-0.47564600	2.35046900
C	-3.41414700	0.91396900	2.40310500
C	-3.79189300	1.74396400	1.26361100
C	-4.31942200	1.13121100	0.11737100
C	-4.48935400	-0.30652000	0.06405600
C	-3.44873600	-2.36653000	0.95388000
C	-2.45845500	-2.51205100	2.00644800
C	-2.54721000	-1.34739200	2.87798400
C	-1.39067900	-0.80296500	3.44525200
C	-1.21894800	0.63998100	3.50067100
C	-2.21219400	1.47868500	2.98143500
C	-2.83669700	2.82373600	1.14648100
C	-2.40865900	3.25214700	-0.12789600
C	-2.96202700	2.61698800	-1.31920900
C	-3.89433800	1.58503500	-1.19914100
C	-3.80956100	0.42339600	-2.07193200
C	-4.17008400	-0.74769500	-1.28438300
C	-3.49926100	-1.95539300	-1.48794000
C	-3.12248300	-2.78787400	-0.34963600
C	-1.20807500	-3.07356600	1.72960600
C	-0.87427300	-3.52627900	0.37833000
C	-1.84355800	-3.38654800	-0.63930500
C	-1.41651300	-2.91128600	-1.94830000
C	-2.45305900	-2.05160900	-2.49144400
C	-2.09797800	-0.92068500	-3.24236700
C	-2.79652900	0.33866300	-3.02859300
C	-1.82586700	1.41536500	-3.15682400
C	-1.91380200	2.53894000	-2.32387400
C	-1.84752100	2.65123600	2.19496500
C	-1.02657100	3.55920200	-0.38580400
C	-4.13368200	-1.10824000	1.16100800
C	4.43599700	0.46251200	-0.02534100
C	4.99134500	-0.82533400	-0.03556000
C	2.91844300	0.37413100	-0.05769100
C	2.25398200	0.76471000	1.28126300
O	4.09576600	-1.82542500	-0.09459200
C	5.27134900	1.56723400	0.00137700
C	6.37369800	-1.01823900	-0.00471200
H	4.84338900	2.56703000	-0.00680500
H	6.77793700	-2.02805900	-0.01492400
C	6.66331200	1.38666600	0.03413800
C	7.22022200	0.10181700	0.03259300
H	7.32044100	2.25455200	0.05902100
C	8.72147700	-0.08986500	0.06708700

H	9.03988800	-0.65506000	0.95430600
H	9.08106700	-0.64803700	-0.80862900
H	9.24551200	0.87293100	0.08331600

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	x	y	z
C	0.20605200	1.70779500	0.03126300
C	1.07283500	2.71340800	-0.46680200
C	1.65817700	2.66906300	-1.75294000
C	1.45801200	1.44124500	-2.53419500
C	0.48620600	1.55088700	1.41660600
C	1.47565500	2.55227400	1.82690700
C	1.84366900	3.28451100	0.64347600
C	3.15669600	3.71197100	0.45432100
C	3.02464300	3.06671000	-1.91767600
C	2.70114900	1.13512200	-3.21861100
C	3.09642600	-0.19490200	-3.41813300
C	2.26641300	-1.26054900	-2.91547500
C	1.08621600	-0.93902600	-2.22561600
C	0.71643800	-1.67655300	-1.02995900
C	0.03062000	-0.78695600	-0.13203800
C	0.29030500	-0.89050300	1.22502800
C	0.47363600	0.30119100	2.06698000
C	2.42943300	2.25837400	2.80129600
C	2.44585100	0.95437200	3.43573900
C	1.48943400	-0.00294000	3.03225400
C	1.91153100	-1.38876600	2.83990500
C	1.16657700	-1.93093700	1.72761900
C	1.77291800	-2.84123900	0.85124000
C	1.53985500	-2.71172700	-0.56466700
C	2.78178400	-3.02112300	-1.26069800
C	3.13674900	-2.31196500	-2.40603600
C	3.67385200	2.13300400	-2.83698900
C	6.45679200	-1.17721700	-1.25156600
C	6.43106600	0.08566200	-1.85355400
C	6.63538900	1.28163500	-1.04552600
C	6.87029200	1.16028000	0.32706100
C	6.88775300	-0.15150900	0.94876200
C	5.85791300	-2.37520400	0.67850900
C	5.10836800	-2.92323000	-0.43935500
C	5.47870000	-2.18107400	-1.63381600
C	4.51109500	-1.88358400	-2.59753900
C	4.48453700	-0.57098700	-3.22525600

C	5.42434800	0.39429600	-2.84953900
C	5.77981800	2.33439300	-1.55893300
C	5.14964200	3.21711800	-0.66560800
C	5.39620500	3.09303900	0.76608900
C	6.23318800	2.08741000	1.25118000
C	5.86297400	1.34606300	2.44621800
C	6.27081100	-0.03873000	2.25829000
C	5.46035200	-1.06952400	2.74162200
C	5.25477800	-2.26703300	1.93696100
C	3.78500100	-3.33446500	-0.25870500
C	3.15749100	-3.22340000	1.05012500
C	3.88149100	-2.69113200	2.12180600
C	3.24380700	-1.76067500	3.04362900
C	4.22620100	-0.77072200	3.44455100
C	3.82468400	0.56421700	3.61149800
C	4.67082000	1.64019100	3.10982300
C	3.80351700	2.69288000	2.60927600
C	4.15942700	3.40505700	1.46154900
C	5.01505600	1.77949100	-2.65999600
C	3.77662700	3.61523300	-0.85513200
C	6.69846100	-1.30423400	0.17483300
C	-1.77188300	0.76649900	-1.30619800
C	-2.80819600	-0.19435000	-1.29369000
C	-0.30470000	0.55163200	-0.84366800
C	0.64339300	0.41719500	-2.07657400
O	-2.55232100	-1.44104100	-0.78260900
C	-2.08487600	2.03284100	-1.82231600
C	-4.08227600	0.13746000	-1.79348200
H	-1.30413200	2.78760300	-1.83097000
H	-4.88562000	-0.59452500	-1.79810500
C	-3.34529900	2.36183300	-2.31151900
C	-4.36702500	1.40592800	-2.30404000
H	-3.53110900	3.36246200	-2.69733600
C	-5.75926000	1.70818200	-2.81705800
H	-6.25317900	2.47347200	-2.20297400
H	-5.73065000	2.09251400	-3.84592500
H	-6.38305200	0.80769800	-2.79946900
C	-3.33016600	-3.64147800	-0.05961700
C	-2.05362000	-3.97716300	0.39332700
C	-4.38430000	-4.55605000	0.10659300
C	-1.82576900	-5.21391400	1.00522300
H	-1.24219100	-3.27127100	0.27082900
C	-4.15166300	-5.78744400	0.71516100
H	-5.37708600	-4.27487500	-0.24573400

C	-2.87047500	-6.12313800	1.16714000
H	-0.82483200	-5.45751300	1.35455600
H	-4.97508800	-6.48808400	0.84018900
H	-2.69135400	-7.08516900	1.64391200
Br	-7.13555600	-2.20983600	-1.59547100
C	-3.66888600	-2.33839900	-0.73739900
H	-4.51271000	-1.87025500	-0.21844900
H	-4.03111500	-2.53564700	-1.75421500
C	-7.59960300	0.25918300	0.97414800
C	-8.50831300	-0.67695400	1.47195200
C	-9.20975700	-0.41023300	2.64706200
C	-8.99940200	0.79585700	3.32797200
C	-8.08824600	1.72551600	2.83414800
C	-7.37648900	1.46318700	1.65154800
H	-7.07728500	0.00248300	0.05463400
H	-8.62624000	-1.59848300	0.90662500
H	-9.91774100	-1.13743400	3.04000200
H	-9.54313500	1.00703400	4.24684200
H	-7.92685300	2.66543000	3.35882700
C	-6.36366900	2.43156800	1.14283800
H	-5.76909100	2.89460100	1.92915000
H	-5.71892000	2.01375700	0.37224700
Br	-7.22226100	4.03629500	0.24251700

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-2 1

	x	y	z
C	-0.36407500	-1.72145200	-1.81719700
C	0.84560000	-2.38193200	-2.13235600
C	1.54158900	-3.21940500	-1.21487500
C	1.02736000	-3.25135200	0.15471000
C	-0.33109100	-0.42781900	-2.42939900
C	0.87728500	-0.31338700	-3.23369100
C	1.62360300	-1.53439500	-3.03740600
C	3.01735100	-1.50893800	-2.97848800
C	2.96756600	-3.14146400	-1.13035100
C	2.15610400	-3.28136500	1.07229300
C	2.07669200	-2.63877400	2.31313500
C	0.87224900	-1.93299900	2.67686700
C	-0.19123700	-1.86770500	1.74732800
C	-0.97639100	-0.67523100	1.59386600
C	-1.65318000	-0.64564800	0.23340900
C	-1.40590500	0.65132700	-0.45516000
C	-0.83101600	0.71798900	-1.77883400

C	1.55063500	0.90989000	-3.37680100
C	1.03740100	2.08647100	-2.70781800
C	-0.12745400	1.97612600	-1.92403200
C	-0.20486500	2.65174800	-0.64568400
C	-0.97434300	1.80367800	0.25601700
C	-0.64006900	1.78528100	1.63668500
C	-0.60002800	0.47921100	2.27696000
C	0.53055300	0.44746600	3.19449100
C	1.24784500	-0.73477300	3.39222000
C	3.36056800	-3.19984200	0.28035500
C	4.58143800	0.61045800	2.56004100
C	5.07656200	-0.52909500	1.91411100
C	5.59475900	-0.43560700	0.55313300
C	5.58981300	0.80672500	-0.09649800
C	5.07698000	1.98486700	0.57288200
C	3.37685000	2.60953200	2.25584100
C	2.61818400	1.75683000	3.15390200
C	3.36916200	0.52365900	3.35162100
C	2.69788900	-0.69675900	3.47649200
C	3.21182000	-1.88037200	2.80561200
C	4.37638700	-1.79159400	2.03413500
C	5.23019900	-1.64033200	-0.15991700
C	4.84010900	-1.56762000	-1.51315700
C	4.84036300	-0.27455600	-2.18941300
C	5.20746500	0.88184100	-1.49914000
C	4.46137700	2.11529900	-1.69834200
C	4.37526700	2.79260000	-0.41130200
C	3.20600900	3.47056600	-0.05971300
C	2.68613900	3.37986100	1.30164200
C	1.22310300	1.71147800	3.07583800
C	0.50268300	2.52278100	2.09458200
C	1.24620300	3.35333000	1.22783200
C	0.87273000	3.40734900	-0.17823500
C	2.08073000	3.51336100	-0.97739500
C	2.15916500	2.85080500	-2.21206000
C	3.37833300	2.14380400	-2.57796700
C	2.99650200	0.93979400	-3.30073800
C	3.72003500	-0.24483700	-3.11517700
C	4.45982100	-2.47203200	0.74721300
C	3.72698900	-2.33295800	-2.01031300
C	4.58315000	1.90071300	1.88462900
C	-2.40084200	-2.79232200	-0.66475900
C	-3.47857900	-2.09839700	-0.10190500
C	-1.11950000	-1.98589300	-0.52196600

C	-0.13772200	-2.58585500	0.50882400
O	-3.15924600	-0.88766300	0.40824400
C	-2.61943400	-4.03299200	-1.24381200
C	-4.77019000	-2.62407800	-0.10112200
H	-1.78972700	-4.57124500	-1.69605400
H	-5.58894100	-2.05269400	0.32973400
C	-3.91122300	-4.57997100	-1.24555500
C	-4.98748700	-3.88564200	-0.67821200
H	-4.08295600	-5.55624200	-1.69595200
C	-6.37903900	-4.48124400	-0.67748400
H	-6.73066700	-4.68965800	0.34263300
H	-7.11112900	-3.79935700	-1.12998800
H	-6.40987800	-5.42381500	-1.23658900
C	-6.69018500	3.16574900	-0.16930500
C	-6.72593300	4.00352800	-1.28079000
C	-5.74310700	3.89568800	-2.27110100
C	-4.73262900	2.94371900	-2.14225200
C	-4.70089700	2.09448700	-1.03299300
C	-5.67642400	2.20468100	-0.03424000
H	-7.46042600	3.23671700	0.59545300
H	-7.51794700	4.74365300	-1.37570600
H	-5.76678700	4.55490000	-3.13618400
H	-3.95563600	2.85541600	-2.89661600
H	-3.89757400	1.36944000	-0.92905100
C	-5.57212300	1.34277400	1.18514000
H	-4.75726200	0.62182400	1.12568300
H	-5.51670600	1.91489600	2.11111200
Br	-7.23035100	0.22104300	1.46561300

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	x	y	z
C	0.32331500	0.95705000	-1.22234100
C	-0.89197800	1.59745200	-0.88618800
C	-1.30127800	1.84629700	0.44894800
C	-0.47436100	1.26031800	1.51415300
C	0.07379300	0.14024300	-2.36353000
C	-1.30235500	0.35206300	-2.82020700
C	-1.91103600	1.26715800	-1.89099100
C	-3.24913200	1.12366400	-1.52913600
C	-2.67361100	1.63806900	0.80972000
C	-1.36019600	0.75764800	2.54778100
C	-1.03367500	-0.39861700	3.26935800
C	0.18226000	-1.10531800	2.95481000

C	1.00459400	-0.62273800	1.92420500
C	1.62033900	-1.54773600	0.98883000
C	1.72020600	-0.90646600	-0.29488300
C	1.46427700	-1.65884900	-1.42937600
C	0.66117100	-1.12521100	-2.54137100
C	-2.04389800	-0.69539500	-3.36898500
C	-1.45173300	-2.01094600	-3.50879900
C	-0.12548100	-2.20404300	-3.06613000
C	0.20525600	-3.41905100	-2.32595400
C	1.18728900	-3.07781800	-1.32276500
C	1.16461900	-3.71089000	-0.07264200
C	1.38808300	-2.92458300	1.11386700
C	0.50674200	-3.42165600	2.16152000
C	-0.08287200	-2.53350200	3.05844000
C	-2.71970700	0.98561300	2.11751200
C	-3.59264500	-3.52200600	2.46873700
C	-4.15801700	-2.24854400	2.59220300
C	-4.97613400	-1.70691700	1.51351700
C	-5.20310600	-2.46987700	0.36438000
C	-4.60676900	-3.78729400	0.23681000
C	-2.59765400	-5.02130700	0.95821900
C	-1.60921400	-4.67994500	1.96750200
C	-2.22526400	-3.75212600	2.90274700
C	-1.47495400	-2.70116100	3.43747200
C	-2.06321200	-1.37625600	3.56689800
C	-3.37841900	-1.15845200	3.14384300
C	-4.72305000	-0.28241500	1.41689700
C	-4.66711500	0.33112800	0.15441400
C	-4.90524700	-0.46299400	-1.04473600
C	-5.16413800	-1.83079400	-0.94280200
C	-4.54890200	-2.75878000	-1.87830500
C	-4.20638200	-3.96983400	-1.14682300
C	-3.02367200	-4.65000800	-1.44965400
C	-2.20432100	-5.19317300	-0.37434600
C	-0.26919900	-4.51613900	1.60589100
C	0.14040700	-4.69463400	0.22058700
C	-0.81489100	-5.01893900	-0.74792300
C	-0.77748200	-4.37508200	-2.05378900
C	-2.14319300	-4.16556200	-2.49774900
C	-2.46561500	-2.99038700	-3.19271100
C	-3.70073700	-2.28260000	-2.87915200
C	-3.43826900	-0.85818800	-2.99070300
C	-4.02923700	0.03283900	-2.09170100
C	-3.71830300	0.05216500	2.40909800

C	-3.66216400	1.32045600	-0.14981500
C	-3.82526100	-4.31407800	1.27349200
C	2.58793100	1.59626700	-0.19286200
C	3.95926800	1.25718500	-0.14341000
C	1.39187700	0.60633600	-0.17396200
C	0.70873200	0.59635900	1.22880000
O	4.31668500	-0.06610800	-0.12087800
C	2.26984500	2.96222100	-0.22050400
C	4.93459200	2.27124800	-0.12289600
H	1.22134300	3.24147000	-0.26972600
H	5.99456000	2.02906500	-0.08229100
C	3.23506500	3.96408800	-0.19532200
C	4.59071100	3.62275800	-0.14434800
H	2.93018600	5.00947300	-0.21735000
C	5.68991600	4.66225000	-0.11360600
H	5.66928100	5.29300200	-1.01359000
H	5.57988200	5.33432500	0.74899800
H	6.67277700	4.18128100	-0.05347400
C	6.03424700	-1.80322000	-0.14237600
C	5.06590000	-2.80039600	-0.27005300
C	7.38835800	-2.16600100	-0.03757600
C	5.43867600	-4.14821900	-0.28552900
H	4.02368100	-2.52183500	-0.36139300
C	7.75459700	-3.51011600	-0.05701400
H	8.13329100	-1.37430200	0.05103700
C	6.78148700	-4.50859000	-0.17863100
H	4.66973400	-4.91179900	-0.38148900
H	8.80569100	-3.78077600	0.02476400
H	7.07047100	-5.55811900	-0.19043400
Br	8.69188700	1.63160200	0.06703400
C	5.72827700	-0.32795800	-0.13034800
H	6.19098000	0.14976500	-1.00266900
H	6.20890200	0.14001300	0.73624100
C	-2.00818500	7.19354300	-1.35823200
C	-2.68051300	7.49028300	-2.54101100
C	-3.61412300	6.58811800	-3.06004600
C	-3.87010000	5.39252400	-2.38817100
C	-3.19908100	5.09676300	-1.20051300
C	-2.25896900	5.99334400	-0.67679800
H	-1.28424500	7.89540700	-0.95063800
H	-2.47273400	8.42148400	-3.06278800
H	-4.13352300	6.81515600	-3.98805800
H	-4.58437500	4.67896400	-2.78983500
H	-3.39760500	4.16143700	-0.68467900

C	-1.51355900	5.65776100	0.57324700
H	-1.61360700	4.61297300	0.86316400
H	-0.46246200	5.93996300	0.53589000
Br	-2.21577900	6.69929900	2.15274400

IM4

-2 1

	x	y	z
C	1.03734300	1.42466800	1.32298100
C	1.28561000	0.05806100	1.56386300
C	1.61051900	-0.87549100	0.52969200
C	1.50581800	-0.37543100	-0.84265300
C	-0.01412200	1.84750000	2.20316700
C	-0.36668400	0.74241300	3.08054700
C	0.43892800	-0.38635000	2.67210400
C	-0.08977700	-1.67629100	2.70182500
C	1.00445800	-2.17687900	0.54716800
C	0.92996800	-1.42089200	-1.67597300
C	0.09951000	-1.09064100	-2.75434900
C	-0.19814700	0.29269000	-3.02904000
C	0.32102500	1.28943900	-2.16893900
C	-0.45204600	2.44464100	-1.81190000
C	0.06509700	3.06571700	-0.52146800
C	-1.05432000	3.27204900	0.44335400
C	-1.02354700	2.73258300	1.77720200
C	-1.68427800	0.54398100	3.52178200
C	-2.72172200	1.45714000	3.08746700
C	-2.38658000	2.52211600	2.23421700
C	-3.25516900	2.86384600	1.12827700
C	-2.40887800	3.29939500	0.02297700
C	-2.81613400	3.00860800	-1.30792300
C	-1.78480800	2.52008400	-2.20966700
C	-2.35715500	1.47147000	-3.04414200
C	-1.57807800	0.38435400	-3.44843700
C	0.60716200	-2.53438800	-0.81621600
C	-3.79184800	-2.26913600	-2.15306500
C	-2.78708600	-3.15145500	-1.73724600
C	-2.75317800	-3.63231900	-0.36026500
C	-3.73637400	-3.19594700	0.53953400
C	-4.77541500	-2.28339800	0.10849700
C	-5.11967000	-0.43668400	-1.50010100
C	-4.27454600	-0.01291800	-2.60225500
C	-3.46050800	-1.14931000	-3.01380000
C	-2.14207600	-0.95405900	-3.43633100

C	-1.09846800	-1.87051500	-3.00427100
C	-1.41853500	-2.94502400	-2.16637700
C	-1.37128900	-3.73520000	0.05531400
C	-1.00027800	-3.37217900	1.36775800
C	-2.02589000	-2.92381800	2.30342600
C	-3.35942200	-2.84050100	1.89991400
C	-4.17554400	-1.70919400	2.31482200
C	-5.04522500	-1.36048400	1.19981400
C	-5.32921700	-0.02003000	0.93171300
C	-5.36438900	0.46251200	-0.44470500
C	-3.72404600	1.27269400	-2.61866600
C	-3.98986500	2.21340000	-1.52870300
C	-4.81707200	1.79677900	-0.46347000
C	-4.42448800	2.13613400	0.89746000
C	-4.76797000	1.02725500	1.76903900
C	-3.92295000	0.69168800	2.83655300
C	-3.62687400	-0.70593300	3.11572400
C	-2.23719600	-0.79248300	3.53934100
C	-1.45421600	-1.88783700	3.14856400
C	-0.54562100	-3.29270800	-1.05125700
C	0.19596500	-2.61448800	1.62095400
C	-4.81506000	-1.82349900	-1.21725600
C	2.47660300	2.97534500	-0.14630900
C	2.08602000	4.23805100	-0.61321300
C	1.26139100	2.06697600	-0.03877800
C	1.23023800	0.95856500	-1.11339600
O	0.76442800	4.37641800	-0.83174700
C	3.81315500	2.73221000	0.13148100
C	3.01574100	5.25897500	-0.81363100
H	4.13748200	1.76159400	0.49804100
H	2.68327600	6.22883800	-1.17689200
C	4.75767300	3.75089100	-0.06821300
C	4.37031600	5.01174200	-0.53769300
H	5.80712700	3.55600000	0.14485200
C	5.39363300	6.10879800	-0.74024100
H	5.35619300	6.51634600	-1.75981700
H	5.22773400	6.95302600	-0.05586900
H	6.41117000	5.73990000	-0.56712700
C	6.43859100	-3.63761100	0.10654500
C	6.72558900	-4.50357500	-0.94567300
C	5.92633500	-4.49758700	-2.09325600
C	4.84504600	-3.62011100	-2.17906200
C	4.55862100	-2.74942600	-1.12570800
C	5.35201500	-2.75322000	0.02903500

H	7.06398900	-3.63337500	0.99682500
H	7.56975600	-5.18591700	-0.87147600
H	6.14554600	-5.17711800	-2.91389700
H	4.21238100	-3.61163800	-3.06248000
H	3.71178100	-2.07293000	-1.19426400
C	5.01671000	-1.84983200	1.17141200
H	4.03928400	-1.37562000	1.06970500
H	5.10405000	-2.33866000	2.14108200
Br	6.32785400	-0.32192400	1.31217200

IM5

-2 1

	x	y	z
C	-0.81795800	-0.79886000	-2.08062600
C	0.22925700	-1.53339200	-2.67242400
C	0.73229000	-2.75396900	-2.14231700
C	0.21431900	-3.14903000	-0.83258100
C	-0.49405000	0.59132200	-2.21425500
C	0.71347300	0.72621900	-3.03071700
C	1.17768900	-0.60486700	-3.30365500
C	2.54352100	-0.88345200	-3.34315300
C	2.14112200	-2.98994100	-2.13374800
C	1.30900900	-3.69679000	-0.05300200
C	1.36573300	-3.51381100	1.33336400
C	0.33936600	-2.73541900	1.97884300
C	-0.68486000	-2.16358800	1.19429200
C	-1.17273300	-0.84772800	1.47749300
C	-1.92517200	-0.26670600	0.28849000
C	-1.60756500	1.29056500	0.01966400
C	-0.75925400	1.54804000	-1.23946600
C	1.62269100	1.76479600	-2.81207500
C	1.36670500	2.72629100	-1.77023600
C	0.20329500	2.56888500	-0.98912000
C	0.25998300	2.80481800	0.44548700
C	-0.68294500	1.92914100	1.07913300
C	-0.33343400	1.33583200	2.27532400
C	-0.59670100	-0.10358600	2.48152300
C	0.49050900	-0.64913500	3.26334100
C	0.94972600	-1.94833800	3.02216900
C	2.50859300	-3.59786400	-0.85333200
C	4.49348300	-1.09422400	2.46439100
C	4.73895200	-2.02605100	1.44848500
C	5.26539900	-1.58254800	0.16403000
C	5.54090500	-0.22555100	-0.04276900

C	5.27810600	0.73766800	1.00826000
C	3.73338100	1.08616700	2.89608200
C	2.81045200	0.15259500	3.52390500
C	3.28706000	-1.19769100	3.26250400
C	2.37373900	-2.22847900	3.02162600
C	2.63165600	-3.20052100	1.96971500
C	3.79069000	-3.09181900	1.19482400
C	4.66188700	-2.38512400	-0.88012600
C	4.29937300	-1.78598300	-2.09884900
C	4.58472400	-0.36921600	-2.31656600
C	5.18988600	0.39063700	-1.31378900
C	4.72251700	1.74043900	-1.04452700
C	4.77913000	1.95467600	0.39413200
C	3.77761900	2.69879900	1.02560600
C	3.24753300	2.26176600	2.31109800
C	1.43978300	0.41945700	3.51627000
C	0.92843400	1.63783400	2.91135800
C	1.82480400	2.53858300	2.31701300
C	1.47779600	3.14305400	1.05288800
C	2.68717000	3.26309300	0.25337100
C	2.62371900	3.03969700	-1.12604000
C	3.67060800	2.27651300	-1.78969400
C	3.04635000	1.48719400	-2.83932700
C	3.49655200	0.18808700	-3.09452100
C	3.73192700	-3.30336400	-0.24660000
C	3.05853200	-2.10609800	-2.75360200
C	4.77564900	0.31691500	2.24866700
C	-3.04003800	-1.79216600	-1.23655700
C	-3.93807000	-1.25330900	-0.32194000
C	-1.62886500	-1.33091700	-0.91660800
C	-0.78640500	-2.41756400	-0.20832700
O	-3.34133600	-0.41479900	0.59199100
C	-3.51218200	-2.63480500	-2.23763200
C	-5.30498400	-1.52368000	-0.34319200
H	-2.82452000	-3.05646300	-2.96740600
H	-6.00100400	-1.09430800	0.37913400
C	-4.87771300	-2.92266500	-2.28573800
C	-5.77950500	-2.38146000	-1.34958600
H	-5.25864800	-3.58137300	-3.06492600
C	-7.25417500	-2.71358100	-1.42939100
H	-7.41253700	-3.79840600	-1.34512100
H	-7.82440000	-2.21509600	-0.63342800
H	-7.67007400	-2.40725500	-2.40010900
C	-2.84587500	4.47500600	0.71320300

C	-2.79220700	5.84819200	0.47050700
C	-2.78077400	6.32865500	-0.84009200
C	-2.82584600	5.42385100	-1.90219800
C	-2.87910300	4.05193100	-1.65291500
C	-2.88650100	3.55312800	-0.34244900
H	-2.85873200	4.10748000	1.73639600
H	-2.76339100	6.54271600	1.30723000
H	-2.74141300	7.39877100	-1.03187000
H	-2.82145400	5.78524700	-2.92817100
H	-2.91558500	3.35238300	-2.48393800
C	-2.98032500	2.06731800	-0.07228000
H	-3.56989900	1.59419100	-0.86300000
H	-3.52474200	1.89897600	0.85912400
Br	-8.70771600	-0.75976300	1.47068500

IM6

-2 1

	x	y	z
C	1.26570300	1.05546600	1.27873900
C	1.29874000	-0.28751600	1.59728400
C	1.69355400	-1.39882300	0.63266500
C	1.49833600	-0.84704600	-0.80038600
C	0.34355800	1.74430700	2.17692900
C	-0.21353300	0.76002900	3.06565400
C	0.37445000	-0.51809800	2.69548300
C	-0.38469700	-1.67925300	2.78562300
C	0.58902400	-2.48230800	0.64782600
C	0.69763300	-1.76703000	-1.57073500
C	-0.04955400	-1.34701700	-2.67589700
C	-0.08391400	0.05473600	-3.00028900
C	0.61522900	0.96167600	-2.18000500
C	0.06522400	2.24721300	-1.87240100
C	0.68722900	2.81819900	-0.60525100
C	-0.39015100	3.25760100	0.33946800
C	-0.47826800	2.76108800	1.67305200
C	-1.54823500	0.81867400	3.49495200
C	-2.39527000	1.89239500	3.00371200
C	-1.87265200	2.84266700	2.12784800
C	-2.64741100	3.30673500	1.00676000
C	-1.71512100	3.52096300	-0.10169700
C	-2.15394900	3.26872200	-1.42094200
C	-1.22223100	2.56188400	-2.29485000
C	-1.97667800	1.61356800	-3.09153800
C	-1.41277400	0.38501700	-3.45307300
C	0.14882100	-2.77519600	-0.68216400

C	-4.10315300	-1.75665100	-2.11168600
C	-3.28774800	-2.79800600	-1.65079600
C	-3.36252100	-3.22551500	-0.26231900
C	-4.23861900	-2.57608900	0.61355300
C	-5.09085800	-1.50390400	0.13804600
C	-5.06382200	0.31676900	-1.53847200
C	-4.14427800	0.53305600	-2.64137800
C	-3.55845600	-0.74969000	-3.00267900
C	-2.21951400	-0.82020100	-3.40273700
C	-1.37256200	-1.89814600	-2.91820300
C	-1.89878400	-2.86848600	-2.06317700
C	-2.01756700	-3.55114900	0.17832700
C	-1.60319500	-3.22002100	1.47508700
C	-2.52059800	-2.55738200	2.38572200
C	-3.81724300	-2.25084200	1.96863700
C	-4.41271100	-0.97362100	2.33207700
C	-5.19159200	-0.50876800	1.19364200
C	-5.22328400	0.84950400	0.87308600
C	-5.14126400	1.27569600	-0.51620500
C	-3.36183600	1.69085000	-2.68882100
C	-3.45651300	2.69747500	-1.63118400
C	-4.36115500	2.49288000	-0.57206500
C	-3.93002100	2.80522200	0.77973300
C	-4.47349700	1.80104800	1.67887100
C	-3.72361100	1.35544600	2.77014600
C	-3.68649800	-0.06210400	3.10024300
C	-2.34082000	-0.38374100	3.55088500
C	-1.76347600	-1.61949800	3.20278100
C	-1.11746800	-3.32942200	-0.92692700
C	-0.28105300	-2.67990500	1.70332700
C	-5.02080900	-1.09309400	-1.19914500
C	3.02425600	2.31116900	-0.14235300
C	2.86953500	3.59640500	-0.67184900
C	1.66506200	1.62528200	-0.07008700
C	1.44765500	0.49828000	-1.10017500
O	1.58374200	3.94638500	-0.94779500
C	4.29312700	1.86063500	0.19212000
C	3.95414500	4.44063500	-0.88356200
H	4.49216500	0.87694200	0.60884300
H	3.79485300	5.43367000	-1.29768500
C	5.39694300	2.69726900	-0.01724500
C	5.24087600	3.98105000	-0.55090600
H	6.37312300	2.29390700	0.24275100
C	6.44122000	4.87604900	-0.77233900

H	6.54132800	5.16777900	-1.82734600
H	6.36723300	5.80654100	-0.19169000
H	7.36578400	4.37025700	-0.47625600
C	3.08398900	-4.34553700	-0.05941100
C	3.58995300	-5.29591200	-0.94765700
C	4.67622600	-4.97857600	-1.76559400
C	5.25821500	-3.71364600	-1.66926100
C	4.75011200	-2.76026900	-0.78393000
C	3.64005700	-3.05889500	0.02165200
H	2.24730500	-4.60836300	0.58264400
H	3.13715100	-6.28472700	-0.99569900
H	5.07498900	-5.71774000	-2.45862900
H	6.12727600	-3.46457500	-2.27443800
H	5.26603800	-1.81029100	-0.65114600
C	3.10391700	-2.01340900	0.98258200
H	3.84479400	-1.21375800	1.08257500
H	2.99507600	-2.45166800	1.98349500
Br	6.83999900	-0.49298300	1.17463600

IM7

-2 1

	x	y	z
C	0.59599500	-1.39586100	2.39959700
C	1.43943000	-0.61994700	3.22067500
C	1.27425800	0.77896100	3.41965800
C	0.26299200	1.43275400	2.58991900
C	1.42202100	-2.34612800	1.71485000
C	2.78917000	-2.25188500	2.22867500
C	2.80554200	-1.15833100	3.15908800
C	3.91656500	-0.32034500	3.24524900
C	2.42386300	1.62747200	3.43953300
C	0.77891500	2.72198700	2.16699300
C	0.45377700	3.24922000	0.91238600
C	-0.37549900	2.47732600	0.02107100
C	-0.81927600	1.20034700	0.43045100
C	-0.86199900	0.11116500	-0.49812600
C	-0.93533400	-1.22790500	0.22111700
C	-0.01362900	-2.37146500	-0.44234300
C	1.22253000	-2.74472400	0.39666700
C	3.89010000	-2.50091000	1.40474500
C	3.67997600	-2.86656900	0.02735900
C	2.35417100	-2.93976600	-0.44780500
C	2.03341400	-2.43002400	-1.77206300
C	0.69106000	-1.92605300	-1.74240200

C	0.40475300	-0.76513300	-2.43146400
C	-0.40733200	0.28648500	-1.78459800
C	0.10204000	1.57059900	-2.21072800
C	0.11439100	2.65311000	-1.32499100
C	2.12140700	2.84691600	2.68784300
C	3.70794500	3.43141000	-1.59538800
C	3.91178800	3.78035400	-0.25504100
C	4.94127700	3.10586400	0.52503600
C	5.73521100	2.12216700	-0.07551200
C	5.51703600	1.75833900	-1.46179700
C	3.68718100	1.63384600	-3.10737800
C	2.34255000	2.18655300	-3.04204100
C	2.35898600	3.30593900	-2.11156600
C	1.26420800	3.53673900	-1.27306200
C	1.47547600	3.90583000	0.11831100
C	2.77809700	4.01505900	0.61550900
C	4.45499900	2.94312700	1.88013100
C	4.73937700	1.76155300	2.58530900
C	5.56689900	0.73204600	1.95935900
C	6.05214300	0.90847400	0.66235000
C	6.04141400	-0.20262300	-0.27469200
C	5.71106300	0.32532800	-1.59043700
C	4.89874700	-0.41734500	-2.45302100
C	3.86867800	0.25135200	-3.23777500
C	1.23801800	1.33383800	-3.08251900
C	1.41855100	-0.10161200	-3.21876400
C	2.71705000	-0.62747000	-3.29119700
C	3.03073900	-1.82721000	-2.55204500
C	4.38946500	-1.71324700	-2.04492400
C	4.69147800	-2.21004200	-0.77266800
C	5.54708900	-1.44626600	0.12373100
C	5.04880000	-1.63101500	1.47701000
C	5.05865300	-0.55945700	2.37539000
C	3.10824800	3.48415200	1.93214100
C	3.74269300	1.11280000	3.39647200
C	4.53074800	2.40671300	-2.21933600
C	-1.97728200	-1.31249500	2.41345800
C	-2.86310000	-1.71763900	1.42070500
C	-0.67524500	-0.84371900	1.78836000
C	-0.55183000	0.69734100	1.74110400
O	-2.32999500	-1.64661200	0.15609500
C	-2.37919700	-1.35833200	3.74361900
C	-4.15561900	-2.16144800	1.68890100
H	-1.69668100	-1.04916200	4.53197600

H	-4.84900700	-2.44873700	0.89870600
C	-3.66931600	-1.80368000	4.04352100
C	-4.56324200	-2.20335200	3.03358700
H	-3.99600300	-1.83837200	5.08147700
C	-5.94721300	-2.70336100	3.38472000
H	-6.36959800	-2.13359800	4.22288400
H	-6.62510900	-2.63948100	2.52360800
H	-5.91196200	-3.75732200	3.69810400
C	-0.19426800	-5.02660500	-2.69837900
C	0.41660600	-6.14447700	-3.26809700
C	1.01947400	-7.10488200	-2.45381300
C	1.00381600	-6.93664200	-1.06806300
C	0.39126000	-5.81672400	-0.50443300
C	-0.21580300	-4.84156200	-1.30877700
H	-0.66415000	-4.28282100	-3.33729500
H	0.41851900	-6.26562500	-4.34905300
H	1.49486200	-7.97819200	-2.89509300
H	1.46845700	-7.67878500	-0.42264000
H	0.38279700	-5.69049000	0.57508500
C	-0.91237600	-3.64574800	-0.69699400
H	-1.34568900	-3.93538200	0.26495000
H	-1.74735700	-3.34523300	-1.33331400
Br	-7.63308800	-2.64493500	-0.02348200
C	-6.21101100	2.76233300	-2.34018700
C	-7.11437200	1.70681200	-2.45371400
C	-7.06936200	0.64256700	-1.54799500
C	-6.12184400	0.64366300	-0.52217200
C	-5.22096100	1.70120400	-0.40453700
C	-5.25045600	2.76776600	-1.31669200
H	-6.24448000	3.59349900	-3.04281300
H	-7.84888100	1.71075400	-3.25700200
H	-7.73656800	-0.21492200	-1.60816100
H	-6.11443800	-0.20682500	0.15454400
H	-4.47253800	1.69307500	0.38509700
C	-4.24893800	3.86238200	-1.22706800
H	-3.40787900	3.63101300	-0.57604500
H	-3.89437500	4.21246900	-2.19514000
Br	-5.01736200	5.57172500	-0.41619300

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	x	y	z
C	-0.05605200	1.11923200	1.57270900
C	1.21171800	1.66006400	1.63362300

C	1.89136600	2.41306000	0.49722700
C	1.18903700	1.98524800	-0.81449400
C	-0.16800100	0.03406300	2.54411500
C	1.10287900	-0.08763600	3.20734100
C	1.97413500	0.92303200	2.62995700
C	3.32801200	0.65531600	2.46637200
C	3.28780700	1.79235300	0.26059200
C	2.17567900	1.56107400	-1.77755100
C	1.86191600	0.67831600	-2.81590100
C	0.53940700	0.11340400	-2.87262800
C	-0.38740200	0.44812000	-1.86664400
C	-1.29132900	-0.53304100	-1.34629300
C	-1.79781200	-0.13122400	0.03048500
C	-1.62590400	-1.26424400	0.99535500
C	-0.88275900	-1.12081800	2.20721000
C	1.62745800	-1.33391100	3.58206000
C	0.87374800	-2.53405700	3.26474100
C	-0.35201400	-2.43004000	2.60704400
C	-0.69744600	-3.35454900	1.55874400
C	-1.44775200	-2.60436800	0.55086200
C	-1.30806900	-2.95790500	-0.80894700
C	-1.17964700	-1.85685900	-1.75863500
C	-0.19008800	-2.22695200	-2.75213000
C	0.64764300	-1.25625200	-3.31232600
C	3.46483400	1.45459400	-1.11896700
C	3.84942100	-2.91052600	-2.51531500
C	4.58000700	-1.75216100	-2.22368600
C	5.26043100	-1.61986100	-0.94434600
C	5.16382400	-2.64831100	-0.00138200
C	4.41578900	-3.85310300	-0.30372300
C	2.43201500	-4.55772700	-1.60487800
C	1.68365700	-3.81966200	-2.60728800
C	2.56224100	-2.80846600	-3.17644500
C	2.05225200	-1.55288500	-3.52443500
C	2.80846800	-0.35051500	-3.21503800
C	4.04909100	-0.45028600	-2.58180500
C	5.13824900	-0.23846700	-0.51407400
C	4.93121000	0.06177600	0.83843000
C	4.84531700	-1.00869100	1.81668700
C	4.96875800	-2.33756100	1.40744400
C	4.09906700	-3.35481100	1.97813500
C	3.75053500	-4.28560800	0.91453200
C	2.46739500	-4.83152400	0.85388300
C	1.78520900	-4.95686100	-0.42560800

C	0.33181100	-3.52804400	-2.40229500
C	-0.34516600	-3.95970200	-1.17984800
C	0.37813600	-4.68889000	-0.21795100
C	0.19197500	-4.36364500	1.18552000
C	1.47751000	-4.46546600	1.85501200
C	1.81093300	-3.57246900	2.87588100
C	3.14840700	-3.00002100	2.93636300
C	3.02570300	-1.61836700	3.37689300
C	3.86690700	-0.63266500	2.82743300
C	4.39239700	0.47977600	-1.51828700
C	3.99233100	1.09247400	1.22139400
C	3.76192500	-3.98206400	-1.53560100
C	-2.11870800	2.24234800	0.49162600
C	-3.33279700	1.61764000	0.19852200
C	-0.98012600	1.23730900	0.37401100
C	-0.07140500	1.42621700	-0.85818200
O	-3.22887800	0.27706900	-0.06051600
C	-2.10907300	3.59792200	0.79007000
C	-4.53962200	2.30648900	0.18134600
H	-1.20573200	4.15351600	1.02706500
H	-5.46154600	1.78983600	-0.07526100
C	-3.31377700	4.31066700	0.77998200
C	-4.52634300	3.68146700	0.47701700
H	-3.25345700	5.37429900	0.99952300
C	-5.82041100	4.46582200	0.46248700
H	-6.31545300	4.41031000	-0.51666400
H	-6.53624600	4.08002000	1.20158200
H	-5.64021800	5.52150800	0.68920300
C	3.94810800	4.76566700	-0.64814300
C	4.47242400	5.56484900	-1.66522700
C	3.64147100	6.44679700	-2.35906100
C	2.29291500	6.53333200	-2.00997200
C	1.76585900	5.73099100	-0.99530000
C	2.58582400	4.81901500	-0.31241600
H	4.60802200	4.09472400	-0.10441500
H	5.53118800	5.50082500	-1.91006000
H	4.04719500	7.07273400	-3.15222600
H	1.64164100	7.24226300	-2.51657900
H	0.73715700	5.87354400	-0.66606900
C	1.99893500	3.95979600	0.79317000
H	1.01638900	4.35822100	1.06544300
H	2.61988400	4.04335700	1.69495700
Br	-0.74330200	6.86850600	1.39942300
C	-7.18646200	-3.32044600	-0.36771500

C	-7.36437700	-4.28807800	0.61669700
C	-6.51089800	-4.32348600	1.72492300
C	-5.48661800	-3.38459700	1.84022300
C	-5.31133000	-2.40717000	0.85708900
C	-6.15704100	-2.37259100	-0.25798800
H	-7.85551200	-3.28231500	-1.22468500
H	-8.16527100	-5.01805700	0.52111900
H	-6.64498000	-5.08341600	2.49142500
H	-4.81185900	-3.40893400	2.69154000
H	-4.50517300	-1.68392300	0.94210000
C	-5.91814000	-1.36804500	-1.34016400
H	-5.04824100	-0.74034500	-1.15327400
H	-5.87059000	-1.81442500	-2.33265100
Br	-7.45125900	-0.06684600	-1.50179600

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	x	y	z
C	-0.71251000	0.90848100	1.18428700
C	0.37150600	1.69179500	1.44682300
C	0.92253700	2.74290000	0.49784700
C	0.43158600	2.38279800	-0.91913500
C	-0.60920100	-0.32486500	1.96603800
C	0.58922100	-0.23983300	2.76907700
C	1.21584600	1.04500100	2.47644400
C	2.61109300	1.08168000	2.35350400
C	2.44418300	2.51699500	0.32365300
C	1.54714900	2.34258000	-1.82705100
C	1.51106000	1.58398400	-3.00228600
C	0.36198600	0.75691500	-3.25177500
C	-0.68244800	0.73267200	-2.30841900
C	-1.33569500	-0.49719400	-1.99132800
C	-2.08002900	-0.39893000	-0.67279000
C	-1.95361000	-1.71846800	0.24830700
C	-1.06138200	-1.53102300	1.48557400
C	1.35230200	-1.38056600	3.00857600
C	0.91601300	-2.64787400	2.47011500
C	-0.25994300	-2.70410600	1.71379000
C	-0.32148700	-3.52665200	0.52396300
C	-1.17866200	-2.87182500	-0.42799200
C	-0.82971600	-2.90277400	-1.76066400
C	-0.92429100	-1.67378300	-2.57359400
C	0.17668700	-1.67414500	-3.50777500
C	0.80588500	-0.47315300	-3.85748500
C	2.78095600	2.43212400	-1.06254200

C	4.24306400	-1.48853000	-2.99190500
C	4.66705000	-0.25598700	-2.48131900
C	5.21265500	-0.17601400	-1.13645600
C	5.31363600	-1.32938900	-0.35411000
C	4.87983900	-2.60851000	-0.88288600
C	3.19143200	-3.51639400	-2.43704900
C	2.35654200	-2.82206500	-3.40470100
C	3.01283500	-1.57329300	-3.75476100
C	2.25079500	-0.42014100	-3.97592400
C	2.69126400	0.85939900	-3.44689500
C	3.87304500	0.93810400	-2.70835000
C	4.75244900	1.06871900	-0.54262700
C	4.39165500	1.09772900	0.80957000
C	4.50485200	-0.09691800	1.62306800
C	4.96507000	-1.29053300	1.05963300
C	4.33210900	-2.54780700	1.40627900
C	4.26753900	-3.35733700	0.20247000
C	3.15132500	-4.16208900	-0.05125700
C	2.60032800	-4.23576200	-1.39286000
C	0.96478700	-2.86980500	-3.28416200
C	0.34802600	-3.61902400	-2.20183700
C	1.15189000	-4.29894800	-1.28012000
C	0.80761000	-4.25337000	0.11890800
C	2.04050600	-4.16995800	0.88646100
C	2.09084800	-3.38123700	2.03549000
C	3.25721900	-2.55075500	2.30866800
C	2.80044600	-1.32523900	2.92352200
C	3.39687700	-0.10267700	2.56453400
C	3.93225800	1.75475300	-1.50687900
C	3.21415000	1.82024400	1.24267600
C	4.35279900	-2.68837500	-2.17745400
C	-2.90865900	1.72792800	0.14097000
C	-3.91531200	1.00322600	-0.49013200
C	-1.57819400	1.01523600	-0.04482000
C	-0.67080700	1.58863500	-1.15752400
O	-3.47172500	-0.18767200	-1.02257800
C	-3.23396600	2.91501800	0.79153700
C	-5.23834100	1.42867300	-0.55964400
H	-2.48142000	3.46617200	1.34869200
H	-6.01340100	0.85807900	-1.07609700
C	-4.55629100	3.36103400	0.74853000
C	-5.55926500	2.64236400	0.07075000
H	-4.82136900	4.28652100	1.25618200
C	-6.98151900	3.15762200	0.03638300

H	-7.01779000	4.16633500	-0.39878200
H	-7.63221100	2.49688300	-0.55241800
H	-7.39075300	3.23539000	1.05365400
C	-3.63457500	-4.67400200	0.99537900
C	-3.73886700	-5.80640400	1.80394400
C	-3.69987100	-5.68081300	3.19368200
C	-3.55869200	-4.41491600	3.76488400
C	-3.45529400	-3.28584400	2.95144700
C	-3.48742000	-3.39656600	1.55405300
H	-3.67205000	-4.77743100	-0.08639500
H	-3.85565300	-6.78641300	1.34679900
H	-3.78361600	-6.56156600	3.82639300
H	-3.53153300	-4.30309000	4.84620700
H	-3.34863300	-2.30295000	3.40322100
C	-3.40635500	-2.17048400	0.67092700
H	-3.87442000	-1.32462900	1.18284400
H	-3.98237400	-2.33590900	-0.24171700
Br	-8.65058600	0.49526500	-2.06127300
C	2.41255000	5.88010200	0.64419200
C	3.01695900	6.92027500	-0.06262200
C	2.42217700	7.41863600	-1.22350900
C	1.21885100	6.86819800	-1.66888400
C	0.61813700	5.82781000	-0.95824900
C	1.20492800	5.31555500	0.20790700
H	2.87644400	5.49731100	1.54978700
H	3.95260700	7.34372500	0.29615500
H	2.89101200	8.23052500	-1.77521500
H	0.74397200	7.24971000	-2.56997400
H	-0.32047000	5.40515300	-1.30871100
C	0.55673600	4.19176700	0.98301200
H	-0.53270100	4.28148200	0.92241100
H	0.81669300	4.24233900	2.04596800
Br	0.45533900	2.75691400	4.45867300

P2

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	x	y	z
C	-0.49113600	1.94422400	-0.32904100
C	0.79572300	2.33018300	-1.10942300
C	1.18883100	1.79397300	-2.31402800
C	0.54581600	0.56562100	-2.82836700
C	0.14843300	1.73737800	1.05350700
C	1.40769400	2.41876400	1.14215600
C	1.81229800	2.81686700	-0.19692900

C	3.17663500	2.74986700	-0.54054600
C	2.58771500	1.72907500	-2.68882100
C	1.55274500	-0.21893700	-3.50295500
C	1.52980200	-1.61729300	-3.44247200
C	0.50091800	-2.26573500	-2.66688500
C	-0.44858800	-1.48401900	-1.99577100
C	-0.87879400	-1.83236200	-0.65814900
C	-1.16327700	-0.61200300	0.05577000
C	-0.77085800	-0.53001200	1.37387100
C	-0.11661500	0.68535700	1.90019700
C	2.35971200	2.05203900	2.09933500
C	2.08446900	0.95272000	2.98553600
C	0.86396400	0.27285100	2.87397000
C	0.83729200	-1.17302600	2.96471100
C	-0.16806800	-1.66475600	2.04082100
C	0.03806800	-2.87132100	1.36502600
C	-0.32258500	-2.95327900	-0.02800000
C	0.68565000	-3.74911500	-0.70963300
C	1.08681100	-3.41623300	-2.00308900
C	2.81444700	0.49367800	-3.41045700
C	4.70756000	-3.14557200	-1.32923700
C	4.96885200	-2.07259700	-2.18720900
C	5.61291600	-0.87064600	-1.67527600
C	5.96838500	-0.78968200	-0.32610300
C	5.68804300	-1.90238700	0.56589800
C	4.03255400	-3.71306800	0.85091500
C	3.02672400	-4.20766700	-0.07256600
C	3.44537300	-3.85880800	-1.42151000
C	2.49356700	-3.46921900	-2.36772600
C	2.76630100	-2.35570000	-3.26189100
C	3.98089200	-1.66792300	-3.16899100
C	5.02149400	0.27393100	-2.34209900
C	4.80301700	1.45879300	-1.63267600
C	5.17123700	1.54252000	-0.23017700
C	5.74781700	0.44278300	0.41146600
C	5.33481200	0.09275400	1.75995600
C	5.29375600	-1.35509600	1.85424000
C	4.29052000	-1.98294400	2.59993400
C	3.64579800	-3.18343700	2.08576000
C	1.67361400	-4.15693800	0.27523100
C	1.27211900	-3.60966200	1.56068600
C	2.24208800	-3.13103500	2.44714600
C	2.01500400	-1.89357200	3.17560200
C	3.28317600	-1.18740300	3.27432300

C	3.31323000	0.20714900	3.17855100
C	4.35897500	0.86158800	2.40490400
C	3.76951900	2.00831300	1.74198300
C	4.15854400	2.33924500	0.44347300
C	4.01082300	-0.21670700	-3.26306300
C	3.56915100	2.20439100	-1.80926100
C	5.07196300	-3.05636300	0.07493300
C	-2.62683900	0.82509700	-1.55532500
C	-3.84262700	0.23590100	-1.13238700
C	-1.22218700	0.58597700	-0.92716900
C	-0.43674100	-0.05469100	-2.09595300
O	-3.85176000	-0.54810400	-0.01060500
C	-2.67745600	1.60951200	-2.72232000
C	-5.02449700	0.46166700	-1.86398800
H	-1.75437900	2.05020000	-3.08787200
H	-5.96376400	-0.00072300	-1.56670300
C	-3.84780100	1.83969900	-3.43522300
C	-5.04589300	1.25572800	-3.00963100
H	-3.82074100	2.46080500	-4.32826700
C	-6.35166000	1.45057600	-3.74697900
H	-6.70604400	2.48703600	-3.65649900
H	-6.23726900	1.24393500	-4.81956300
H	-7.12558900	0.78921700	-3.34096600
C	-5.04756500	-2.02814400	1.53386600
C	-3.94009100	-2.11441900	2.37869900
C	-6.18773700	-2.80260900	1.80940200
C	-3.96007600	-2.97368700	3.48169500
H	-3.06443200	-1.51088100	2.17336900
C	-6.20461000	-3.65237400	2.91336500
H	-7.04899700	-2.71423700	1.14630700
C	-5.08944800	-3.74524600	3.75324400
H	-3.08536100	-3.03632600	4.12555800
H	-7.09175400	-4.24881500	3.11719600
H	-5.10301200	-4.41443900	4.61157300
Br	-8.30286500	-1.27748800	-1.23448000
C	-5.12711500	-1.12186000	0.33391200
H	-5.84946200	-0.31803200	0.52396600
H	-5.53601300	-1.67871500	-0.51554300
C	-3.52716300	2.84327000	1.17757800
C	-4.26095700	3.02625100	2.35178400
C	-3.72792100	3.77214500	3.40365000
C	-2.46228000	4.34557300	3.26346000
C	-1.72791800	4.16188100	2.09125900
C	-2.24606500	3.39380800	1.03388500

H	-3.96601800	2.28127200	0.36114500
H	-5.25123300	2.58501500	2.43816900
H	-4.29865000	3.91328400	4.31957500
H	-2.04304700	4.94757400	4.06726200
H	-0.75947400	4.64394600	1.96696600
C	-1.42347800	3.23135000	-0.23541800
H	-0.74730800	4.09116500	-0.30013200
H	-2.07324600	3.25998800	-1.11023100
Br	1.33198100	5.66959800	0.40207400

P3

-2 1

	x	y	z
C	0.39528500	1.14676100	-1.48406900
C	-0.70275200	1.91530700	-1.19903700
C	-1.02606400	2.49192200	0.17177400
C	-0.27740100	1.63554400	1.21554300
C	0.10348200	0.32505700	-2.66724500
C	-1.23801000	0.63530200	-3.10808600
C	-1.75261400	1.62003700	-2.18735100
C	-3.08042900	1.57932200	-1.80450000
C	-2.48700000	2.14485900	0.53519800
C	-1.19404800	1.21657900	2.24192600
C	-0.95134500	0.06724500	2.99942200
C	0.20173800	-0.73675400	2.69670600
C	1.05347700	-0.34580400	1.65494000
C	1.57625800	-1.34586000	0.74614700
C	1.69999600	-0.76121600	-0.55711000
C	1.38952400	-1.52853000	-1.66424800
C	0.58178000	-0.96864000	-2.76645000
C	-2.07110500	-0.37137600	-3.61296700
C	-1.57946600	-1.72974600	-3.69781700
C	-0.27378200	-2.02026200	-3.27777200
C	-0.01347700	-3.22193400	-2.50422600
C	1.00530500	-2.91444900	-1.51617200
C	0.94762700	-3.50211800	-0.24740800
C	1.24048400	-2.69619500	0.91157100
C	0.34319300	-3.09627100	1.98096300
C	-0.16834600	-2.13276200	2.85088700
C	-2.55618100	1.56518100	1.85180700
C	-3.74357100	-2.88615600	2.34606900
C	-4.20907500	-1.57034700	2.42952200
C	-5.00225800	-1.00771500	1.34862400
C	-5.29951500	-1.78009100	0.22195300

C	-4.80920900	-3.14432600	0.13106700
C	-2.88306300	-4.49931300	0.86948900
C	-1.85986800	-4.19905400	1.85823100
C	-2.39435900	-3.20578200	2.77215500
C	-1.56331400	-2.18546000	3.25562000
C	-2.04747700	-0.82317300	3.35005400
C	-3.34660500	-0.51681400	2.93478700
C	-4.62318900	0.38619100	1.20371400
C	-4.54636700	0.95208500	-0.07460100
C	-4.85105700	0.14918300	-1.24209700
C	-5.23251300	-1.18980100	-1.10266800
C	-4.70041200	-2.18901300	-2.01577600
C	-4.43879700	-3.39825500	-1.24999700
C	-3.31769800	-4.17964700	-1.54096600
C	-2.52323800	-4.73863500	-0.46177100
C	-0.51588000	-4.14983900	1.47518600
C	-0.14434000	-4.39719100	0.08935600
C	-1.12766700	-4.68805200	-0.85866500
C	-1.05899700	-4.09164100	-2.18337200
C	-2.41403300	-3.78327200	-2.60979700
C	-2.66974400	-2.62697500	-3.34920700
C	-3.83932600	-1.81451000	-3.04875800
C	-3.46114300	-0.41884400	-3.20805000
C	-3.95348100	0.54264300	-2.31644300
C	-3.61169200	0.69122800	2.18251900
C	-3.45130600	1.84105400	-0.40084600
C	-4.04702000	-3.68690300	1.17115300
C	2.77077300	1.63582300	-0.66782300
C	4.08856700	1.20373200	-0.37831200
C	1.48966000	0.77494500	-0.48459500
C	0.84095500	0.87813900	0.93215300
O	4.29814500	-0.09917500	-0.00895800
C	2.62196900	2.95843700	-1.10846600
C	5.16216100	2.10518000	-0.48452300
H	1.63061300	3.29857000	-1.38282400
H	6.17727200	1.79816200	-0.23967500
C	3.68860000	3.84493200	-1.22703000
C	4.98032400	3.42511400	-0.89870000
H	3.50732400	4.86069900	-1.57329600
C	6.18004800	4.34265400	-0.98395200
H	6.30877900	4.73668100	-2.00154900
H	6.06399000	5.20883400	-0.31826800
H	7.09447700	3.80959000	-0.70052200
C	5.84860700	-1.95317800	0.40756700

C	4.85022200	-2.90600800	0.19882200
C	7.11860300	-2.37128300	0.84053100
C	5.10254900	-4.25976900	0.44054100
H	3.87755900	-2.58839400	-0.15431100
C	7.36798900	-3.72242200	1.07298200
H	7.89889900	-1.61957700	0.96304200
C	6.35961300	-4.67302600	0.88069000
H	4.30901600	-4.98709300	0.28272200
H	8.35498200	-4.03527200	1.40796800
H	6.55514500	-5.72688900	1.07006700
Br	8.76383100	1.21794800	0.29985500
C	5.67946900	-0.48088100	0.13870200
H	6.23341400	-0.21135800	-0.76885700
H	6.14842800	0.09813200	0.94059700
C	-1.04314000	5.28300600	-1.84401500
C	-1.77721100	6.12810600	-2.67808200
C	-2.99977500	6.64535200	-2.24586700
C	-3.47580600	6.31294800	-0.97558400
C	-2.74266000	5.46750100	-0.14109300
C	-1.51365400	4.93847200	-0.56857600
H	-0.08799900	4.89002200	-2.18574800
H	-1.39187000	6.38305000	-3.66320200
H	-3.57411600	7.30566100	-2.89289100
H	-4.42362000	6.71715600	-0.62624400
H	-3.09967000	5.21984600	0.85807700
C	-0.72066700	4.02621100	0.34380300
H	-0.94675400	4.26717900	1.38854100
H	0.35276500	4.16453300	0.18046300
Br	-2.80715800	4.07929000	3.38126100

RF5²⁻

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	x	y	z
C	-2.70434500	-1.23543100	-0.00042000
C	-1.91477700	-1.79343000	1.17924600
C	-1.56092500	-1.02703400	2.27516100
C	-1.73367900	0.43080900	2.28065300
C	-1.91449300	-1.79340200	-1.17989300
C	-1.04439900	-2.83734800	-0.72240800
C	-1.04457000	-2.83736100	0.72194500
C	0.13803400	-3.15035600	1.43148100
C	-0.32835300	-1.31233800	3.00359100
C	-0.59948000	0.99465700	3.00696200
C	-0.04014200	2.21361400	2.57875800

C	-0.57041400	2.89064400	1.43541800
C	-1.64841300	2.30802200	0.72082400
C	-1.64825700	2.30803400	-0.72134500
C	-2.24338200	1.08798700	-1.17864100
C	-1.73317400	0.43085300	-2.28121700
C	-1.56041200	-1.02699600	-2.27571800
C	0.13836100	-3.15032900	-1.43168100
C	0.49903700	-2.36472200	-2.57549700
C	-0.32767600	-1.31228900	-3.00387100
C	0.23982600	-0.07524500	-3.47443000
C	-0.59880700	0.99470700	-3.00726000
C	-0.03956300	2.21365600	-2.57890900
C	-0.57009500	2.89066400	-1.43568000
C	0.55909700	3.44964100	-0.69754900
C	0.55893900	3.44962800	0.69755300
C	0.23904500	-0.07530300	3.47430400
C	3.81547400	1.78459000	1.17329600
C	3.46450400	1.03204400	2.29993300
C	3.63216800	-0.40631300	2.29992700
C	4.14729800	-1.05676300	1.17336100
C	4.51118500	-0.27705800	0.00042200
C	3.81573900	1.78461000	-1.17257600
C	2.97332600	2.87583400	-0.71946800
C	2.97316100	2.87582000	0.72001100
C	1.78161300	3.16366400	1.42983200
C	1.41440500	2.38085800	2.58367500
C	2.23298400	1.32932000	3.02875100
C	2.50352900	-0.98108100	3.03018500
C	1.95196000	-2.19628200	2.58446300
C	2.48926500	-2.87144100	1.43079900
C	3.58119100	-2.31449500	0.71950300
C	3.58135700	-2.31448600	-0.71890500
C	4.14756300	-1.05674600	-1.17261100
C	3.63268900	-0.40627400	-2.29928300
C	3.46502300	1.03207900	-2.29930500
C	1.78193400	3.16369000	-1.42955500
C	1.41498600	2.38089900	-2.58349100
C	2.23366500	1.32936800	-3.02839500
C	1.66061500	0.09010100	-3.49081200
C	2.50421300	-0.98103200	-3.02980600
C	1.95254500	-2.19624200	-2.58423300
C	2.48959100	-2.87142400	-1.43045900
C	1.36727200	-3.43489900	-0.69721600
C	1.36710900	-3.43491100	0.69729200

C	1.65982900	0.09004500	3.49101600
C	0.49845500	-2.36476300	2.57538800
C	4.34919800	1.11025200	0.00041500
C	-4.43063400	0.46307500	-0.00035400
C	-4.99088300	-0.81635800	-0.00048600
C	-2.91192100	0.35855900	-0.00040900
C	-2.24359800	1.08795700	1.17795600
O	-4.08420400	-1.81344300	-0.00064200
C	-5.25932200	1.57325900	-0.00056200
C	-6.37022400	-1.01276000	-0.00083000
H	-4.82709300	2.57074900	-0.00092900
H	-6.77527400	-2.02174700	-0.00129000
C	-6.65119100	1.39369800	-0.00080000
C	-7.21332200	0.11100400	-0.00066200
H	-7.30566200	2.26335700	-0.00110000
C	-8.71520200	-0.07559700	0.00232400
H	-9.05593400	-0.61277800	0.89825400
H	-9.23611100	0.88829000	-0.02321900
H	-9.05349700	-0.65910800	-0.86483400

TSa1-1

-2 1

	x	y	z
C	1.16448000	0.82809500	-1.21512000
C	0.30826000	1.07944100	-2.31274000
C	-0.59473300	2.17212900	-2.36614700
C	-0.72660600	2.98279100	-1.15121100
C	1.22679500	-0.58356700	-1.03151300
C	0.47456000	-1.24428900	-2.10074300
C	-0.10657900	-0.20048200	-2.90675800
C	-1.37591600	-0.35818700	-3.45788600
C	-1.91241100	1.97701900	-2.89006500
C	-2.12557000	3.33468400	-0.98406500
C	-2.68459400	3.44102400	0.29763600
C	-1.86255300	3.17941300	1.45157400
C	-0.52182800	2.80551700	1.26259500
C	0.07175400	1.75887000	2.08017800
C	1.04063700	1.05424000	1.28666900
C	1.12579200	-0.32172700	1.41653100
C	1.26553400	-1.18794200	0.23816800
C	-0.22639700	-2.42706300	-1.86295000
C	-0.21303400	-3.02662600	-0.54247000
C	0.50876000	-2.37791700	0.48281100
C	-0.07892300	-2.28842900	1.81857200

C	0.30835400	-1.01989200	2.39075800
C	-0.58729500	-0.31602000	3.20994400
C	-0.70613200	1.11148400	3.05520000
C	-2.11057700	1.46938900	3.21738500
C	-2.67401800	2.47784500	2.43802500
C	-2.86526600	2.70907900	-2.05264300
C	-5.46717300	0.50227300	1.04382500
C	-5.47144200	1.07736600	-0.23240000
C	-5.34536900	0.23133800	-1.41455800
C	-5.23581600	-1.15470800	-1.26508300
C	-5.22308000	-1.74474200	0.06060800
C	-4.52068500	-1.19689600	2.35976100
C	-4.13422400	0.08099500	2.93407100
C	-4.72113300	1.13297600	2.11985200
C	-4.00388800	2.30844100	1.87869600
C	-4.00881000	2.90721200	0.55203100
C	-4.72316100	2.29250100	-0.48235200
C	-4.55166100	0.93556900	-2.40262100
C	-3.62686300	0.22249300	-3.18994700
C	-3.51371400	-1.22314000	-3.03610600
C	-4.29649300	-1.89571900	-2.09612300
C	-3.71172100	-2.94857600	-1.28246800
C	-4.28707800	-2.85412400	0.05195600
C	-3.48605400	-3.10395200	1.17013800
C	-3.61025900	-2.26096500	2.35300800
C	-2.85440400	0.24830100	3.47213700
C	-1.90815800	-0.85776100	3.46776600
C	-2.28324600	-2.08409200	2.90746700
C	-1.34525000	-2.82351800	2.07321700
C	-2.09182500	-3.47406300	1.01242100
C	-1.53213000	-3.54529200	-0.27483000
C	-2.36705600	-3.28900000	-1.44112700
C	-1.55506900	-2.59612400	-2.42717000
C	-2.11731500	-1.58404900	-3.20812600
C	-4.14635900	2.19863200	-1.81756200
C	-2.31636800	0.75112400	-3.46700900
C	-5.35339300	-0.93678100	1.19991600
C	2.63756600	2.60531500	-0.03802800
C	3.88719400	1.90311700	0.14535700
C	1.31121100	1.81515400	-0.04606800
C	0.07127000	2.75127300	-0.04179600
O	3.90627100	0.61664400	0.30294500
C	2.64687600	3.98821400	-0.20955500
C	5.06730600	2.70998500	0.15450700

H	1.69934000	4.50315000	-0.34834500
H	6.02230500	2.21639600	0.31654000
C	3.82552000	4.74176300	-0.21147800
C	5.05067600	4.09217600	-0.02773800
H	3.78618000	5.82059800	-0.35401600
C	6.34941900	4.87130200	-0.05600800
H	6.80516400	4.86804800	-1.05736000
H	6.19372900	5.92108700	0.22435200
H	7.09063700	4.44424400	0.63066400
C	5.18272400	-1.72693000	0.00565600
C	4.74963200	-2.17839800	-1.24927300
C	4.95223500	-2.53452500	1.12886600
C	4.10793700	-3.40721500	-1.37904800
H	4.90779800	-1.54916600	-2.12054700
C	4.31079700	-3.76334800	1.00097400
H	5.28456500	-2.18858100	2.10382300
C	3.88681400	-4.20587200	-0.25455300
H	3.76260500	-3.73563900	-2.35635300
H	4.13021700	-4.37354900	1.88306500
H	3.37232700	-5.15873700	-0.35377100
Br	8.18713400	-1.06767700	0.05302700
C	5.84198800	-0.42786100	0.14472100
H	5.98195100	0.20436900	-0.71289500
H	6.00855300	-0.00918700	1.11942100

TSa1

-2 1

	x	y	z
C	2.48179700	-1.33726200	0.00362300
C	1.82846000	-1.90369600	-1.15630300
C	1.51176400	-1.14355400	-2.29882200
C	1.72644400	0.30061200	-2.29019100
C	1.82620600	-1.90290800	1.16262900
C	0.89156100	-2.92173500	0.72858900
C	0.89300000	-2.92226800	-0.72341600
C	-0.28195500	-3.18555800	-1.42136800
C	0.26953300	-1.37509000	-3.00145800
C	0.62902500	0.93032000	-3.02571600
C	0.12292600	2.17470200	-2.59586500
C	0.67789300	2.81477600	-1.43933900
C	1.70679800	2.16385400	-0.72299100
C	1.70536800	2.16435900	0.72630400
C	2.26014300	0.92460300	1.18250500
C	1.72188100	0.30221700	2.29481100

C	1.50719200	-1.14191900	2.30400700
C	-0.28480200	-3.18454100	1.42435300
C	-0.62109700	-2.37788100	2.58930300
C	0.26353000	-1.37296000	3.00426600
C	-0.26698700	-0.09552600	3.47248300
C	0.62293700	0.93244300	3.02765600
C	0.11771300	2.17651100	2.59593800
C	0.67501900	2.81582900	1.44011400
C	-0.41742400	3.43970500	0.69657200
C	-0.41604400	3.43922900	-0.69843400
C	-0.26001800	-0.09796700	-3.47157300
C	-3.74520200	1.91613800	-1.17789000
C	-3.42592500	1.15214500	-2.30989600
C	-3.64006000	-0.28539900	-2.30504800
C	-4.17791900	-0.90402000	-1.17444000
C	-4.50940400	-0.11346000	-0.00380000
C	-3.74754300	1.91694200	1.17041500
C	-2.84411300	2.96119400	0.72238800
C	-2.84266900	2.96068700	-0.72879400
C	-1.64804700	3.19757200	-1.42331000
C	-1.31277400	2.39921000	-2.59479500
C	-2.18404000	1.39437300	-3.02527600
C	-2.56087800	-0.91768700	-3.05583600
C	-2.04278100	-2.15563400	-2.59858800
C	-2.60425500	-2.79895000	-1.43185600
C	-3.66083000	-2.19342800	-0.72190100
C	-3.66224700	-2.19290800	0.71742300
C	-4.18027600	-0.90319000	1.16804400
C	-3.64466800	-0.28380800	2.29929500
C	-3.43051200	1.15374800	2.30354700
C	-1.65090200	3.19856200	1.41914600
C	-1.31798300	2.40103400	2.59185900
C	-2.19010000	1.39649300	3.02130500
C	-1.66643300	0.11692000	3.47932800
C	-2.56703000	-0.91554700	3.05270700
C	-2.04798300	-2.15380700	2.59734800
C	-2.60710600	-2.79790400	1.42991200
C	-1.52231400	-3.43013200	0.69802200
C	-1.52094300	-3.43066100	-0.69735900
C	-1.65944600	0.11447800	-3.48139100
C	-0.61591000	-2.37972100	-2.58755000
C	-4.30726100	1.27716200	-0.00409000
C	4.44280800	0.26346700	0.00383000
C	5.12659900	-0.99101900	0.00495200

C	2.90826700	0.15792000	0.00356200
C	2.26238000	0.92374000	-1.17721000
O	4.44782800	-2.08901100	0.00510700
C	5.14607500	1.45841900	0.00749000
C	6.55007400	-0.94663500	0.00918100
H	4.59759700	2.39950100	0.01211100
H	7.08246200	-1.89650900	0.01313200
C	6.54787300	1.47287500	0.01211400
C	7.25184100	0.26034900	0.00944200
H	7.08618000	2.41933300	0.01718600
C	8.76677800	0.25577500	-0.02525500
H	9.18223400	-0.55126800	0.59212100
H	9.15356500	0.10716700	-1.04484000
H	9.17930600	1.20437200	0.34124200

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	x	y	z
C	2.33750000	0.01166800	-1.40950800
C	1.72505300	1.14925400	-1.99010800
C	1.44674300	2.33374000	-1.26033900
C	1.70374600	2.30996000	0.18358600
C	1.72630000	-1.14412800	-1.97268100
C	0.76505300	-0.72874800	-3.00044000
C	0.76240000	0.71375000	-3.00910300
C	-0.42414500	1.41451800	-3.22305700
C	0.20461300	3.01563700	-1.45996700
C	0.63861800	3.03788700	0.84961000
C	0.17998200	2.62734500	2.11088800
C	0.76405400	1.46631700	2.73435300
C	1.76825100	0.75613100	2.05253900
C	1.78467000	-0.69861500	2.06530800
C	2.31787200	-1.16156300	0.81310300
C	1.71716400	-2.26358800	0.22154900
C	1.45408200	-2.30462400	-1.22188400
C	-0.41798900	-1.43816500	-3.20556600
C	-0.71140700	-2.61300200	-2.40469700
C	0.21789600	-3.00368700	-1.41672100
C	-0.27550000	-3.43851900	-0.10987500
C	0.65937900	-2.98216900	0.89140600
C	0.19695600	-2.56846200	2.15349500
C	0.77360900	-1.39747100	2.75420700
C	-0.29361700	-0.65880500	3.42162200
C	-0.29785600	0.73483600	3.41288400
C	-0.29552900	3.47042400	-0.15973500

C	-3.67740400	1.19455000	1.98830600
C	-3.38891700	2.32234000	1.21060100
C	-3.66342500	2.30983000	-0.22268800
C	-4.22887200	1.17266700	-0.80925700
C	-4.51791000	0.00351900	-0.00026500
C	-3.67228200	-1.15419100	2.00713000
C	-2.73202700	-0.69743200	3.01608300
C	-2.73554500	0.75655200	3.00530000
C	-1.54113000	1.45625100	3.20036400
C	-1.24152300	2.62950700	2.39283300
C	-2.15016500	3.04619700	1.41203400
C	-2.61783800	3.05120600	-0.89916300
C	-2.13330300	2.59497200	-2.14192300
C	-2.72256000	1.41249100	-2.75445100
C	-3.74398200	0.71549400	-2.10517700
C	-3.74213800	-0.73760700	-2.09611200
C	-4.22069000	-1.17644800	-0.79184200
C	-3.65014500	-2.30064300	-0.18703200
C	-3.37546100	-2.29249500	1.24471800
C	-1.53321500	-1.38836200	3.22169800
C	-1.22597700	-2.57178900	2.43151200
C	-2.13287200	-3.00554700	1.45706200
C	-1.64762700	-3.45980800	0.15848000
C	-2.59824300	-3.04524900	-0.85491200
C	-2.12223300	-2.60873600	-2.10505400
C	-2.71728700	-1.43930000	-2.73615000
C	-1.66061800	-0.71463600	-3.42198600
C	-1.66261800	0.68179500	-3.43010700
C	-1.66935800	3.48461700	0.10800000
C	-0.72481900	2.60387900	-2.44257000
C	-4.26342400	0.01329700	1.38013200
C	4.46442900	0.11468900	0.04464300
C	5.23585100	-1.11885800	0.02283200
C	2.92351100	0.03033100	0.01188100
C	2.27735700	1.20266400	0.78901500
O	4.70546200	-2.26841100	0.00609200
C	5.11067400	1.35031300	0.03681200
C	6.67099000	-0.93524900	0.02641000
H	4.51073600	2.25852900	0.05005200
H	7.26487600	-1.84964500	0.02060000
C	6.50445000	1.47176700	0.02323200
C	7.29202100	0.30533100	0.01581600
H	6.97065900	2.45649600	0.02638200
C	8.80378900	0.40934100	-0.02953700

H	9.17751800	1.18866900	0.65016400
H	9.27862800	-0.53797600	0.25431400
H	9.16973400	0.66819300	-1.03547800

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	x	y	z
C	-0.46108000	1.69915800	0.00291600
C	0.60331500	2.46939100	-0.65996100
C	1.06419600	2.24820700	-1.95550900
C	0.64023400	1.01836400	-2.64990700
C	0.07476100	1.48395900	1.34658500
C	1.20733700	2.35956300	1.58581100
C	1.54249400	2.97454900	0.32603600
C	2.87821300	3.23706800	0.00260600
C	2.44781600	2.47368500	-2.28597500
C	1.76337500	0.52550700	-3.41516900
C	1.97930900	-0.85112700	-3.55936100
C	1.08079900	-1.77365500	-2.90984900
C	0.01844500	-1.27216000	-2.14476100
C	-0.33063300	-1.88637600	-0.87879400
C	-0.81316700	-0.85844500	0.00721900
C	-0.43456600	-0.91593300	1.33421100
C	-0.01406500	0.29447900	2.06087200
C	2.21017100	2.02215200	2.50072100
C	2.13150800	0.77074400	3.21667600
C	1.03944600	-0.07983200	2.96663000
C	1.26723100	-1.51162300	2.83581900
C	0.35685900	-2.02096800	1.83114900
C	0.76077500	-3.05585100	0.97976000
C	0.40926000	-2.98296200	-0.41562500
C	1.53303100	-3.48420300	-1.19262500
C	1.86109100	-2.89582500	-2.41283600
C	2.88300900	1.41656200	-3.18937500
C	5.38768800	-2.11684000	-1.63611800
C	5.45546500	-0.89815800	-2.31895700
C	5.88376100	0.30561200	-1.61792000
C	6.23081600	0.23828300	-0.26573100
C	6.15131300	-1.02768400	0.44260700
C	4.83599600	-3.11568100	0.41938300
C	3.92303000	-3.62892300	-0.58728500
C	4.26523600	-3.01197000	-1.85946100
C	3.25284300	-2.65284100	-2.75278000
C	3.32379400	-1.38513800	-3.46353000

C	4.40468500	-0.52488400	-3.24477100
C	5.10592700	1.42246600	-2.11831600
C	4.68756000	2.43222600	-1.24366000
C	5.04979900	2.36280500	0.16516500
C	5.80384700	1.28959900	0.64291800
C	5.46324000	0.67125800	1.91522700
C	5.68009200	-0.76068100	1.79055500
C	4.80257800	-1.65297100	2.41345700
C	4.37356500	-2.85726100	1.71343000
C	2.58399000	-3.86079900	-0.26237300
C	2.10326700	-3.59361200	1.08435900
C	2.98452300	-3.09742100	2.05026000
C	2.55414700	-2.04075300	2.95369800
C	3.68326500	-1.15656200	3.19022000
C	3.46822000	0.22233900	3.30501100
C	4.38307800	1.15254000	2.65684700
C	3.60084300	2.27208500	2.15973800
C	3.92676600	2.86487100	0.93872700
C	4.18147700	0.90770500	-3.11451900
C	3.35193700	2.98346200	-1.33770400
C	5.74380400	-2.18474600	-0.22906900
C	-2.52270900	0.65512300	-1.29060400
C	-3.63306700	-0.17042700	-0.99830500
C	-1.07060400	0.45922500	-0.77511600
C	-0.22577700	0.13728500	-2.03913500
O	-3.47260800	-1.22850900	-0.14399000
C	-2.72703000	1.70359900	-2.20215600
C	-4.88011400	0.09906000	-1.59312000
H	-1.88066700	2.33163200	-2.46692600
H	-5.74438800	-0.53069500	-1.39201100
C	-3.96103100	1.97036900	-2.78511200
C	-5.06041900	1.15822000	-2.48279800
H	-4.06116100	2.80364300	-3.47699500
C	-6.42678700	1.38472900	-3.09063700
H	-6.87875400	2.31257500	-2.71377000
H	-6.36430500	1.48022500	-4.18292100
H	-7.09850900	0.55346500	-2.84810700
C	-4.37908500	-3.21145100	0.96931200
C	-3.19979100	-3.40037100	1.69194300
C	-5.39937600	-4.17471300	1.05171900
C	-3.03034000	-4.54216000	2.48091500
H	-2.41668600	-2.65436000	1.63719600
C	-5.22822400	-5.30762000	1.84485800
H	-6.31736000	-4.00905900	0.48645100

C	-4.04149500	-5.49933200	2.56079700
H	-2.10120500	-4.67781700	3.03059300
H	-6.02378300	-6.04819500	1.90004700
H	-3.90793400	-6.38833300	3.17460300
Br	-7.90136200	-2.17513900	-1.31662000
C	-4.65648300	-2.00756200	0.10774000
H	-5.41280100	-1.37142300	0.58534300
H	-5.10866300	-2.33644800	-0.83333500
C	-4.03778300	2.46861300	1.20952300
C	-4.91448400	2.02601900	2.19618200
C	-4.53390400	2.05709900	3.54042200
C	-3.27113500	2.54246500	3.89169100
C	-2.39278700	2.98182400	2.90580400
C	-2.75895000	2.94971000	1.54652100
H	-4.34331100	2.45706400	0.16914800
H	-5.89524600	1.65288000	1.91330700
H	-5.21841000	1.70630700	4.30939600
H	-2.97085500	2.57727700	4.93661300
H	-1.41633600	3.37019700	3.18099300
C	-1.82937500	3.39584300	0.51389900
H	-0.96973900	3.97865900	0.79951200
H	-2.18337100	3.51230300	-0.49601900
Br	-2.58136600	6.09737700	0.37984100

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	x	y	z
C	0.83924300	-1.62470400	1.67331000
C	-0.30762300	-2.15884500	2.29739600
C	-1.17004600	-3.10398300	1.67334900
C	-0.90110900	-3.39205900	0.26453200
C	0.93816700	-0.24499600	2.04481500
C	-0.10575500	0.06285300	3.01491500
C	-0.89872000	-1.13220000	3.16214900
C	-2.27928600	-1.04925800	3.33818800
C	-2.58589500	-2.96550900	1.81720200
C	-2.17223300	-3.51085200	-0.43121200
C	-2.29924000	-3.09131200	-1.75974900
C	-1.16136400	-2.51384900	-2.43209100
C	0.04898400	-2.35553700	-1.71996600
C	0.86265700	-1.18845900	-1.90018000
C	1.80518900	-0.98438400	-0.72039100
C	1.77455000	0.45819500	-0.22211200
C	1.34835300	0.75074500	1.14317800

C	-0.71595800	1.32461500	3.05675300
C	-0.30234700	2.34505200	2.12256500
C	0.70001700	2.03796100	1.18201500
C	0.57324200	2.49715200	-0.18557500
C	1.16024700	1.48615800	-1.04121200
C	0.58179400	1.24404600	-2.29698900
C	0.40621400	-0.15501500	-2.69967500
C	-0.85886300	-0.27452800	-3.39883600
C	-1.62788300	-1.43498900	-3.27001400
C	-3.21998300	-3.23810000	0.52590500
C	-4.73454400	0.19940000	-2.13840800
C	-5.13488500	-0.79054500	-1.23215200
C	-5.40458100	-0.44472300	0.15876000
C	-5.26663100	0.88565300	0.57600100
C	-4.84934300	1.90801300	-0.36299300
C	-3.45106500	2.15531300	-2.38250600
C	-2.87903100	1.12873700	-3.23821700
C	-3.68051700	-0.07954400	-3.09431200
C	-3.06854700	-1.33673300	-3.11718300
C	-3.48492600	-2.36541200	-2.17745100
C	-4.49434900	-2.08986300	-1.24882500
C	-4.94852500	-1.53332900	0.99780200
C	-4.32586900	-1.25623400	2.22976100
C	-4.18519300	0.13078700	2.66666800
C	-4.64464400	1.17364400	1.86023000
C	-3.84937100	2.38252600	1.71462600
C	-3.97528100	2.83426400	0.33572900
C	-2.87080200	3.38652500	-0.31787300
C	-2.59773800	3.04423700	-1.70967600
C	-1.49321400	1.02819600	-3.38283700
C	-0.60221500	1.95724600	-2.69468500
C	-1.16417700	2.95425500	-1.87212800
C	-0.55231600	3.22539800	-0.58657000
C	-1.60179400	3.52147300	0.37462100
C	-1.47711000	3.07276400	1.69624900
C	-2.62877200	2.50145700	2.38050800
C	-2.15218500	1.41703200	3.22478300
C	-2.92063100	0.25574300	3.36721900
C	-4.36640000	-2.54251100	0.13102900
C	-3.16329900	-1.98601700	2.66184000
C	-4.59429300	1.58175500	-1.70392100
C	2.64118000	-2.96135200	0.43486400
C	3.60425400	-2.42772800	-0.42389700
C	1.36090300	-2.14428200	0.34526400

C	0.20198300	-2.85683200	-0.38759700
O	3.17434900	-1.36884700	-1.15111800
C	2.97282200	-4.04666200	1.23299200
C	4.90464400	-2.92073700	-0.48614300
H	2.23818800	-4.46218200	1.91881400
H	5.64605400	-2.40698500	-1.09183800
C	4.26571200	-4.58408200	1.15901700
C	5.23640900	-4.02348400	0.31576400
H	4.53036900	-5.43552300	1.78372500
C	6.64088400	-4.58479600	0.26996300
H	6.84541000	-5.09007000	-0.68462100
H	7.38825100	-3.78894500	0.37512400
H	6.80670200	-5.31443100	1.07131400
C	4.02045600	3.56582300	-0.75009200
C	3.97147400	4.88608100	-0.31793300
C	3.98917900	5.18108200	1.04975900
C	4.05014500	4.13967600	1.97840000
C	4.10035900	2.81661300	1.54700000
C	4.09673800	2.50378200	0.17340900
H	4.01091300	3.33598800	-1.81176700
H	3.91462200	5.69093000	-1.04759200
H	3.94652900	6.21439700	1.38748200
H	4.05192400	4.35884800	3.04382800
H	4.14688400	2.00744800	2.26989300
C	4.15648800	1.12964500	-0.27638600
H	4.26998800	0.32546700	0.42765000
H	4.10829500	0.87568300	-1.31889600
Br	6.74853300	0.79878400	-0.64076200

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	x	y	z
C	-0.37675000	1.00750300	1.26878800
C	0.66471000	1.87221400	0.94671000
C	0.97227700	2.32010200	-0.40125700
C	0.27834600	1.51789700	-1.44931200
C	0.02407000	0.23183000	2.42534000
C	1.33340900	0.68884600	2.86637800
C	1.74257800	1.71249500	1.93747400
C	3.07206200	1.81986000	1.56235100
C	2.39192500	2.25257100	-0.76537700
C	1.22995600	1.18770400	-2.48979700
C	1.11491100	0.00760600	-3.23563400
C	0.05605700	-0.91587500	-2.92261500

C	-0.82426000	-0.60709900	-1.87433300
C	-1.23982800	-1.64763000	-0.95149800
C	-1.43338200	-1.05997300	0.34430500
C	-1.03439200	-1.77175800	1.46095000
C	-0.31162600	-1.11227200	2.56407100
C	2.26764400	-0.21056200	3.38739800
C	1.93052700	-1.61520400	3.49840500
C	0.66276300	-2.04723100	3.07439800
C	0.54423600	-3.28474600	2.31641900
C	-0.49985400	-3.10937300	1.32811400
C	-0.37898300	-3.70721500	0.06702600
C	-0.75902100	-2.95473000	-1.10209300
C	0.17984300	-3.26607600	-2.16878500
C	0.58043200	-2.26665700	-3.05429200
C	2.53556600	1.65105200	-2.07329500
C	4.22116900	-2.60486000	-2.53177700
C	4.54086900	-1.24811200	-2.63790400
C	5.26305400	-0.58315400	-1.56055600
C	5.63961800	-1.30618300	-0.42612600
C	5.30132300	-2.71354000	-0.31561800
C	3.54243700	-4.28596400	-1.03593500
C	2.49329400	-4.11653700	-2.02676900
C	2.91261200	-3.07609000	-2.95139300
C	1.97333100	-2.17028500	-3.45375800
C	2.30512800	-0.75880300	-3.56187200
C	3.56592100	-0.30978600	-3.15998600
C	4.74519300	0.76624200	-1.43325500
C	4.59231100	1.33634300	-0.15932200
C	4.98831700	0.58395700	1.02335800
C	5.50079500	-0.70757700	0.89335800
C	5.08586400	-1.74850400	1.81984300
C	4.96054100	-2.98848700	1.06897600
C	3.93224700	-3.88402100	1.37113300
C	3.20897900	-4.54706100	0.29850500
C	1.15208800	-4.20668900	-1.64481000
C	0.80500500	-4.47906500	-0.25652400
C	1.81610700	-4.64275400	0.69386000
C	1.68033000	-4.03980300	2.01188800
C	2.99076800	-3.58285000	2.43835400
C	3.10813700	-2.38855000	3.15681000
C	4.18296800	-1.45624800	2.84360500
C	3.65906400	-0.10896700	2.98773100
C	4.05236100	0.89070500	2.09175500
C	3.68912000	0.92891800	-2.40685400

C	3.41962000	2.10735600	0.16835300
C	4.61099400	-3.35586200	-1.35033400
C	-2.76780000	1.20970400	0.35241500
C	-4.03784900	0.59356200	0.26646700
C	-1.39822200	0.48707800	0.24977900
C	-0.75353900	0.63843800	-1.16293500
O	-4.11037700	-0.77027100	0.13947800
C	-2.74337000	2.60408700	0.49465600
C	-5.20271800	1.38016800	0.31662600
H	-1.77852300	3.09085200	0.58434200
H	-6.18891600	0.92537000	0.24655000
C	-3.89545600	3.38208200	0.53785700
C	-5.14898900	2.76838800	0.44554200
H	-3.81285600	4.46250800	0.63574200
C	-6.44011100	3.55572800	0.48090800
H	-6.54408500	4.10779300	1.42529200
H	-6.47298300	4.29829300	-0.32767800
H	-7.30241300	2.88822600	0.37503600
C	-5.44238000	-2.82137000	0.01538300
C	-4.30101400	-3.61661400	0.12763800
C	-6.69224200	-3.43479600	-0.17979100
C	-4.39662300	-5.00862600	0.03340400
H	-3.33970200	-3.14714700	0.29173000
C	-6.78292300	-4.82220600	-0.26865600
H	-7.57708500	-2.80038300	-0.24592400
C	-5.63536100	-5.61661400	-0.16651800
H	-3.49488200	-5.61164800	0.11707500
H	-7.75535000	-5.28676100	-0.42047200
H	-5.70910400	-6.70011500	-0.24093600
Br	-8.72860400	-0.05460300	0.04559800
C	-5.44002900	-1.31849900	0.12024100
H	-5.98121600	-1.01295000	1.02399600
H	-6.01366500	-0.89240200	-0.70978300
C	0.32837700	5.29261000	1.60076600
C	0.88525300	5.85004400	2.74762100
C	2.22975900	6.23192900	2.76427700
C	3.00979800	6.05318400	1.61918200
C	2.45393000	5.49512700	0.47109400
C	1.10258200	5.10475600	0.44085700
H	-0.72018300	5.00945600	1.58967300
H	0.26804700	5.98762600	3.63223900
H	2.66493000	6.66581900	3.66165500
H	4.05609800	6.35031400	1.62040900
H	3.05983000	5.36825000	-0.42110200

C	0.52693400	4.48694700	-0.75013800
H	1.08521800	4.44593200	-1.66955400
H	-0.53032000	4.28469600	-0.80474000
Br	-0.23581200	6.76247500	-1.92865100

TSa4

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	x	y	z
C	1.25189800	1.23438300	1.30932300
C	1.43847800	-0.14702100	1.42832500
C	1.71797500	-1.01346600	0.30405700
C	1.54143500	-0.37400300	-1.01138900
C	0.28180300	1.65692500	2.29142600
C	-0.10462800	0.50283600	3.07638600
C	0.61151800	-0.63231600	2.53020900
C	0.00383600	-1.88249500	2.47582300
C	0.97257100	-2.26178800	0.23380800
C	0.86515100	-1.30005300	-1.89774600
C	0.02087100	-0.83120500	-2.90962200
C	-0.19895400	0.58637500	-3.04864000
C	0.41929500	1.47028400	-2.13441300
C	-0.26651300	2.63017200	-1.64265500
C	0.34148900	3.10614100	-0.32916000
C	-0.72718400	3.29009700	0.70104700
C	-0.68274900	2.62721500	1.97121900
C	-1.41378800	0.34044800	3.55498100
C	-2.40811000	1.34931200	3.23973700
C	-2.04508600	2.46230100	2.47253400
C	-2.92977100	2.95653600	1.44448600
C	-2.09528300	3.43269200	0.34416800
C	-2.56844400	3.28661700	-0.98411300
C	-1.60492000	2.82077000	-1.97254300
C	-2.27597700	1.88791900	-2.86526700
C	-1.58357900	0.79609000	-3.39805700
C	0.50714100	-2.47038200	-1.12733800
C	-3.91176200	-1.82462200	-2.24689600
C	-2.95080100	-2.79979600	-1.95370700
C	-2.89690200	-3.40334400	-0.62876700
C	-3.80933100	-2.98962300	0.35001700
C	-4.80660500	-1.98226300	0.04683000
C	-5.09325400	0.01931900	-1.37838700
C	-4.26624600	0.48791500	-2.47553000
C	-3.54423300	-0.65383200	-3.02037300
C	-2.23179200	-0.50096800	-3.47825500

C	-1.23360300	-1.51396700	-3.17231800
C	-1.58818600	-2.64009400	-2.42277200
C	-1.50572400	-3.61969100	-0.28393500
C	-1.06511900	-3.39957800	1.03468900
C	-2.01889000	-2.97555200	2.05171100
C	-3.36066400	-2.78158100	1.71878600
C	-4.08759300	-1.64498200	2.26551800
C	-4.97526300	-1.14650400	1.22501300
C	-5.18787600	0.22624100	1.08558500
C	-5.23970900	0.82993700	-0.23899800
C	-3.63513500	1.73373800	-2.40167600
C	-3.79886100	2.58415200	-1.22133300
C	-4.61287500	2.13003400	-0.16456500
C	-4.15081400	2.32376400	1.20102600
C	-4.52514800	1.15948700	1.98357600
C	-3.66719400	0.68066600	2.97996400
C	-3.44541900	-0.75074300	3.12390900
C	-2.04922900	-0.95413800	3.47908800
C	-1.34914400	-2.05470800	2.95779000
C	-0.69685900	-3.13970300	-1.38341200
C	0.18633400	-2.73258000	1.29341300
C	-4.86267100	-1.40352900	-1.22851500
C	2.75107700	2.83725600	-0.03559500
C	2.42292200	4.15288100	-0.38654000
C	1.48401000	1.99342300	0.01466500
C	1.34640400	0.99113900	-1.15184900
O	1.10176500	4.38216000	-0.55639100
C	4.07862700	2.50380100	0.19649200
C	3.39904500	5.13738700	-0.52784900
H	4.37471300	1.50010300	0.48884100
H	3.11021300	6.14941500	-0.80203700
C	5.07024000	3.48565100	0.05651900
C	4.74359700	4.79781600	-0.30546400
H	6.10788600	3.21120600	0.23047300
C	5.82192400	5.84914600	-0.45659400
H	5.85025400	6.25793100	-1.47626600
H	5.65920000	6.69867800	0.22114500
H	6.81217400	5.43474700	-0.23807100
C	4.22795300	-3.89130800	0.77400000
C	4.27790500	-5.19928900	0.30617100
C	4.32546500	-5.45726600	-1.06819200
C	4.32117400	-4.38761500	-1.96793300
C	4.27321800	-3.07709500	-1.50248500
C	4.22432000	-2.80180300	-0.12089500

H	4.19289000	-3.69334800	1.84187400
H	4.27602900	-6.02495000	1.01472000
H	4.35946400	-6.48141200	-1.43318100
H	4.35126600	-4.57676100	-3.03877800
H	4.26898600	-2.24784500	-2.20420600
C	4.16335500	-1.43802100	0.36341600
H	4.13923800	-0.61651100	-0.32912900
H	4.04173800	-1.22634100	1.41103500
Br	6.62648500	-0.83273900	0.70609000

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	x	y	z
C	0.82481600	0.61372400	-1.33697200
C	-0.17399200	1.54842400	-1.57804900
C	-0.65042700	2.51391500	-0.59659700
C	-0.20471000	2.19098100	0.77801100
C	0.52300000	-0.57865600	-2.10975400
C	-0.65326500	-0.31534500	-2.92508000
C	-1.10374800	1.00682400	-2.57987500
C	-2.46118300	1.29030500	-2.52972500
C	-2.10675800	2.63489200	-0.49363300
C	-1.32336400	2.33439400	1.68437400
C	-1.42441500	1.56279900	2.84664400
C	-0.42084500	0.56527300	3.10662900
C	0.62501500	0.38904900	2.17666600
C	1.09545500	-0.92340700	1.85761400
C	1.88307700	-0.92783500	0.55747400
C	1.57220600	-2.19925100	-0.38591900
C	0.75591800	-1.85710900	-1.64319300
C	-1.57428700	-1.32545900	-3.21298300
C	-1.35162000	-2.65198000	-2.69203700
C	-0.21586600	-2.88247500	-1.90166500
C	-0.31094600	-3.72338700	-0.72363100
C	0.61358800	-3.22606800	0.25538500
C	0.23085200	-3.21922100	1.58039000
C	0.49300700	-2.02847700	2.41371200
C	-0.61697200	-1.87085500	3.32535500
C	-1.06429300	-0.59220200	3.67620100
C	-2.50400400	2.62088300	0.89865500
C	-4.59394200	-1.05701800	2.71474700
C	-4.80894400	0.23181500	2.21311500
C	-5.29983200	0.41157200	0.85444100
C	-5.56478000	-0.70520900	0.05647300

C	-5.34057000	-2.04059200	0.57611000
C	-3.85106400	-3.21456900	2.15154200
C	-2.94541200	-2.67020800	3.15140400
C	-3.41045400	-1.33787500	3.50391600
C	-2.48667500	-0.32038200	3.76447100
C	-2.71157800	1.01963100	3.24425100
C	-3.85132100	1.28698700	2.48137200
C	-4.65608100	1.58415000	0.29148200
C	-4.26004200	1.58221800	-1.05531400
C	-4.53678600	0.41646400	-1.88874500
C	-5.17665100	-0.69999200	-1.34610500
C	-4.72522100	-2.03662400	-1.69400900
C	-4.82506300	-2.86545500	-0.50216600
C	-3.84772600	-3.82973700	-0.23884200
C	-3.35274200	-4.01262100	1.11546000
C	-1.57514700	-2.92538100	3.05840900
C	-1.05157200	-3.75293900	1.98353600
C	-1.92908000	-4.28813300	1.03271200
C	-1.54679000	-4.27819200	-0.35837200
C	-2.73183600	-4.00462700	-1.15433900
C	-2.63313000	-3.20319100	-2.29240800
C	-3.65359900	-2.20485100	-2.57451300
C	-2.99336700	-1.04399800	-3.14730800
C	-3.42678800	0.24343100	-2.80540600
C	-3.75113100	2.11347300	1.28677300
C	-2.99094600	2.13386000	-1.45569200
C	-4.86862500	-2.21867300	1.88332000
C	3.05535800	1.07920500	-0.14055300
C	3.91838000	0.17788200	0.47341000
C	1.62777900	0.56390900	-0.05709800
C	0.77166600	1.24281500	1.03752200
O	3.28181200	-0.95245200	0.93738300
C	3.57694900	2.24486000	-0.69496400
C	5.28930900	0.38597600	0.58983900
H	2.93077200	2.95264000	-1.20823300
H	5.95317800	-0.33427400	1.07240400
C	4.94986600	2.48069600	-0.59710000
C	5.81155300	1.56959400	0.04302900
H	5.36498100	3.38849800	-1.03025200
C	7.29517000	1.85175200	0.13705100
H	7.48068000	2.75710000	0.73227000
H	7.83075300	1.01529700	0.60458700
H	7.72145300	2.03379400	-0.85927100
C	2.74379600	-5.37376400	-1.15171700

C	2.68549800	-6.49542400	-1.97944200
C	2.73757900	-6.34639500	-3.36649300
C	2.85137800	-5.06804400	-3.91540400
C	2.90896800	-3.94991100	-3.08238000
C	2.85190200	-4.08266900	-1.68782800
H	2.70864900	-5.49703400	-0.07203100
H	2.60450900	-7.48665200	-1.53917400
H	2.69529800	-7.21942900	-4.01385100
H	2.89863800	-4.93899200	-4.99424400
H	3.00210300	-2.95757100	-3.51634400
C	2.94472500	-2.87257500	-0.78375800
H	3.55668900	-2.10583000	-1.26741100
H	3.46261600	-3.14149900	0.13898100
Br	8.47742900	-1.30391900	1.91222300
C	-1.27159400	5.98964200	0.32545400
C	-1.37310900	6.68530800	1.52702100
C	-0.28885700	6.73174100	2.40735100
C	0.89828100	6.07327100	2.07420700
C	1.00178200	5.37739600	0.87352800
C	-0.08053300	5.32784900	-0.02477000
H	-2.11070600	5.96531000	-0.36419900
H	-2.30118100	7.19406100	1.77783500
H	-0.36887700	7.27406300	3.34664100
H	1.74658800	6.10035000	2.75366000
H	1.92649500	4.86690600	0.61894300
C	0.02030200	4.57670600	-1.26955500
H	0.96297100	4.15823600	-1.58003500
H	-0.78205100	4.58283100	-1.98624200
Br	0.79539900	6.57290400	-2.83585300

TSa6

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	x	y	z
C	-0.97910300	0.76067100	0.93257400
C	-0.02346200	1.58603800	1.47828000
C	0.72546200	2.67579500	0.72043300
C	0.64061500	2.31486900	-0.78205300
C	-1.04751100	-0.47936500	1.70891600
C	-0.08642000	-0.37810800	2.77948200
C	0.57117400	0.90435100	2.62619300
C	1.91815500	1.02992800	2.93461000
C	2.24193600	2.48084900	0.94847600
C	1.96067100	2.32965100	-1.36171300
C	2.27515000	1.58756100	-2.50509900

C	1.27411300	0.71773700	-3.06233600
C	0.02062900	0.62723700	-2.42815200
C	-0.65500100	-0.62965600	-2.32313800
C	-1.70819400	-0.60650300	-1.22010000
C	-1.62511800	-1.86348500	-0.32818500
C	-1.24685400	-1.69603000	1.07443000
C	0.63706300	-1.49108900	3.22594500
C	0.42181200	-2.76843500	2.57846800
C	-0.49580300	-2.85769500	1.53013000
C	-0.19744900	-3.65251000	0.36577300
C	-0.78207800	-2.97822000	-0.77650800
C	-0.11204200	-3.02257100	-1.99483900
C	-0.03338500	-1.77967400	-2.77280700
C	1.27818400	-1.71296400	-3.37740500
C	1.92144500	-0.48015400	-3.53527100
C	2.94249100	2.44560000	-0.29834700
C	5.04287200	-1.36919400	-1.78177700
C	5.25889900	-0.12982400	-1.16701600
C	5.42068900	-0.05125500	0.27648400
C	5.35145100	-1.21458500	1.04796800
C	5.13556600	-2.50056700	0.41313000
C	3.97302300	-3.45241400	-1.54898200
C	3.39801800	-2.77322600	-2.69901300
C	4.06595400	-1.48902500	-2.84696000
C	3.34049600	-0.36578200	-3.25929500
C	3.56144000	0.91953300	-2.61634400
C	4.50441000	1.03345800	-1.59346400
C	4.76253600	1.16024600	0.73472500
C	4.05354200	1.15809900	1.94199400
C	3.99059000	-0.05057400	2.74773100
C	4.63340400	-1.21189500	2.31458400
C	3.97751800	-2.50055700	2.46391300
C	4.28406600	-3.29417000	1.28244400
C	3.31379800	-4.13433300	0.73253900
C	3.14696600	-4.21021600	-0.71012100
C	2.02897600	-2.87785900	-2.95854300
C	1.16976900	-3.67626300	-2.09143200
C	1.73104200	-4.34730600	-0.99403500
C	1.02207300	-4.33155000	0.26669900
C	1.99424100	-4.21243100	1.33986800
C	1.69953300	-3.44925800	2.47129900
C	2.71096100	-2.57398500	3.04594100
C	2.04551300	-1.36782400	3.51364100
C	2.67691600	-0.12121100	3.36564900

C	4.19510100	1.82360800	-0.41316000
C	2.78074100	1.83328700	2.04400800
C	4.97923700	-2.57863700	-0.97677900
C	-2.81123200	1.51527600	-0.73580100
C	-3.59429300	0.70078200	-1.55410800
C	-1.46636500	0.84396800	-0.49738100
C	-0.30934900	1.46389500	-1.30795100
O	-3.02063800	-0.50116500	-1.86481100
C	-3.30189400	2.75014400	-0.33644200
C	-4.85546200	1.08040800	-1.99599000
H	-2.75331600	3.44384700	0.29536800
H	-5.43365200	0.41470400	-2.63145100
C	-4.56962300	3.15340200	-0.77216400
C	-5.35153700	2.33440600	-1.59503400
H	-4.90423800	4.13833100	-0.45490100
C	-6.72602800	2.77810600	-2.04539600
H	-6.85059100	2.66856400	-3.13079500
H	-7.51720300	2.18016000	-1.57219900
H	-6.90253800	3.82714800	-1.78766600
C	2.25285900	5.63937400	0.58383000
C	2.82827400	6.69000300	-0.13269100
C	2.06613000	7.39969700	-1.06263700
C	0.72504600	7.06111600	-1.24988700
C	0.14922700	6.00787100	-0.53598900
C	0.91456300	5.26865600	0.37945600
H	2.85139600	5.10357600	1.31638000
H	3.86941000	6.95572400	0.04087700
H	2.51030000	8.22090000	-1.62253300
H	0.11083300	7.62908700	-1.94515900
H	-0.91815700	5.81031700	-0.61750500
C	0.27504400	4.12660500	1.14759800
H	-0.81415500	4.22320100	1.08340700
H	0.52362100	4.21062600	2.21362300
Br	-3.11283300	6.03164000	1.02149600
C	-3.99360700	-3.35819600	2.15397700
C	-4.50990900	-2.98533100	3.39107700
C	-5.22282600	-1.79023600	3.52325500
C	-5.41852700	-0.97611000	2.40478500
C	-4.90526100	-1.34962700	1.16541000
C	-4.18255300	-2.54740100	1.01879000
H	-3.45379500	-4.29477400	2.04714200
H	-4.35700900	-3.62783100	4.25545600
H	-5.62101900	-1.49445300	4.49124400
H	-5.96754100	-0.04257400	2.49778400

H	-5.06389600	-0.71336400	0.30065600
C	-3.59925900	-2.92726400	-0.26420000
H	-3.89841400	-2.43080400	-1.17121600
H	-3.12344900	-3.88805600	-0.35644900
Br	-5.60136400	-4.65595500	-1.05947600

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	x	y	z
C	-1.38212000	0.19327700	-0.26797600
C	-0.97127300	-0.92799600	0.68176300
C	-0.43851500	-0.69893000	1.95548400
C	-0.04467100	0.63320200	2.37081300
C	-0.79625200	-0.27824300	-1.60233500
C	-0.42786800	-1.65587800	-1.48089700
C	-0.53735400	-2.04729600	-0.07967900
C	0.36504600	-2.99739100	0.44340900
C	0.51598900	-1.64232300	2.50193600
C	1.16553400	0.51037500	3.16104600
C	2.18885300	1.46188200	3.07083600
C	2.05192500	2.57491300	2.14983000
C	0.88388800	2.64628200	1.35452800
C	0.99518100	3.03737300	-0.04498500
C	-0.01158500	2.35643000	-0.79997400
C	0.28258700	1.90489900	-2.07623100
C	-0.11747200	0.54464500	-2.47979600
C	0.56808200	-2.21305500	-2.29100700
C	1.26616500	-1.36009200	-3.22722600
C	0.92982300	-0.00025800	-3.31100800
C	1.98318800	0.99300200	-3.41160300
C	1.57905800	2.16400800	-2.65152100
C	2.55010900	2.88657900	-1.93610400
C	2.24893000	3.33500400	-0.59637400
C	3.44933200	3.24300000	0.21585300
C	3.33538600	2.85386300	1.57256000
C	1.50762700	-0.89941500	3.26208900
C	5.63901800	-0.03465900	1.42442600
C	4.94927300	-0.86402600	2.32368400
C	4.54705700	-2.19923100	1.91718000
C	4.84604200	-2.65548300	0.62220900
C	5.54396800	-1.78836200	-0.31195600
C	5.80677800	0.61567000	-0.84165500
C	5.40893900	1.76749200	-0.08069500
C	5.29415300	1.36791800	1.32135400

C	4.28376700	1.90286800	2.12510300
C	3.57469000	1.04520400	3.06662100
C	3.90425900	-0.31463800	3.15907900
C	3.25137200	-2.47210100	2.49784000
C	2.29278300	-3.19185000	1.76828300
C	2.60133900	-3.65888500	0.42270800
C	3.85418700	-3.39195400	-0.13536200
C	3.96591200	-3.00595500	-1.53954100
C	5.00573600	-2.01869800	-1.64669700
C	4.87291200	-0.93041200	-2.53768000
C	5.27473000	0.39435100	-2.13509300
C	4.48795500	2.69453500	-0.61026300
C	3.93455800	2.46517700	-1.94450200
C	4.32033800	1.34028500	-2.67886000
C	3.32157800	0.59534300	-3.43398900
C	3.66558500	-0.81516900	-3.33622000
C	2.65406300	-1.77423400	-3.23755300
C	2.79654500	-2.90225900	-2.32096000
C	1.50844300	-3.17809100	-1.74650100
C	1.40006200	-3.55005300	-0.38671300
C	2.84686800	-1.30480600	3.26206800
C	0.91025400	-2.76945300	1.77035100
C	5.93146200	-0.50501300	0.07908700
C	-3.09899200	4.79775600	0.97977100
C	-2.02737300	3.94784600	0.73392000
C	-2.21623400	2.60276100	0.38446100
C	-3.55123100	2.14770700	0.27932600
C	-4.64511500	3.02068900	0.55033900
C	-4.43390400	4.33814300	0.90011000
C	-0.99962900	1.67251900	0.17610600
C	-3.80813100	0.81317100	-0.13485200
C	-0.17277700	1.70982000	1.48755600
O	-2.87420900	-0.03291500	-0.46380200
O	-5.05436600	0.41537900	-0.22230400
C	-5.58622200	5.27118400	1.18771200
H	-6.54870500	4.77066900	1.04370600
H	-5.55161600	5.64368900	2.22059500
H	-5.56280300	6.15064000	0.53035500
H	-5.65098000	2.62484000	0.46195200
H	-2.90293200	5.83541900	1.24226800
H	-1.01985400	4.33525900	0.82230400
C	-5.43397100	-0.95832900	-0.62523100
H	-6.34761500	-0.80683300	-1.21517100
H	-4.62660500	-1.36271100	-1.23671800

C	-5.70946800	-1.79715000	0.59884400
C	-7.03836500	-2.06619100	0.95672900
C	-4.66249100	-2.30928300	1.37947500
C	-7.30709600	-2.83779700	2.08994500
H	-7.84290200	-1.68547700	0.32206000
C	-4.93880400	-3.07294200	2.51351500
H	-3.62995200	-2.11252000	1.10068300
C	-6.26360700	-3.33741600	2.87152900
H	-8.33986400	-3.04876600	2.35964400
H	-4.11949000	-3.46369200	3.11250200
H	-6.47887300	-3.93590000	3.75514000
Br	-8.90268800	-0.70135500	-1.91203200

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	x	y	z
C	-2.14599000	0.00100000	-1.39176600
C	-2.75366300	-0.28651700	0.01573400
C	-4.31071500	-0.45287300	-0.01166000
C	-5.26186700	0.59379900	0.03997200
C	-2.05228800	-1.53086200	0.58601800
C	-1.43331400	-1.55194600	1.86455600
C	-1.24765100	-0.39165800	2.64353200
C	-1.61077900	0.89348400	2.02448700
C	-1.37364100	-2.47201700	-0.23019700
C	-0.36521800	-3.17372300	0.57066100
C	-0.40165300	-2.59406800	1.88723600
C	0.77687800	-2.41732300	2.61423000
C	-0.01294000	-0.20531600	3.34592900
C	-0.60608700	1.86958400	2.41141300
C	-0.21641300	2.87690400	1.51926800
C	-0.80965100	2.92554700	0.20639400
C	-1.75125900	1.95402100	-0.15435500
C	-1.71204800	1.36484300	-1.48150500
C	-1.50139500	-0.95634700	-2.16152700
C	-1.13708500	-2.27009500	-1.60743100
C	0.84497300	-3.57149400	0.00225900
C	1.11295300	-3.31414900	-1.39989300
C	0.12979800	-2.64133500	-2.16229200
C	0.54859000	-1.59780600	-3.09800400
C	-0.46351400	-0.56636300	-3.09816600
C	-0.09301500	0.77990800	-3.22722800
C	-0.73918600	1.77078400	-2.40392300
C	0.26030400	2.75852400	-2.01585300

C	0.22570700	3.31779400	-0.73973100
C	0.38411200	1.19681900	3.21780200
C	3.67774600	2.45316800	0.25570900
C	3.41159600	2.18958300	1.60428200
C	3.78268600	0.90318600	2.18077600
C	4.41743300	-0.05759500	1.38689100
C	4.68374300	0.21723000	-0.01358300
C	3.73367600	1.50381600	-1.89182700
C	2.72000100	2.54539300	-1.88939800
C	2.68432300	3.13167000	-0.56054500
C	1.45988400	3.50876100	0.00087000
C	1.18293800	3.23658300	1.40334600
C	2.14264100	2.58230400	2.18507200
C	2.76060500	0.51612500	3.13486300
C	2.37811200	-0.83089100	3.23782000
C	3.03906600	-1.83331300	2.41158100
C	4.03255400	-1.45641200	1.50583400
C	4.06638700	-2.04454300	0.17592000
C	4.47370200	-1.00851000	-0.76240200
C	3.89237000	-0.96124800	-2.03377400
C	3.52179600	0.32368200	-2.61458100
C	1.52787300	2.36082700	-2.59845900
C	1.30729500	1.13460500	-3.35155700
C	2.28662600	0.13476800	-3.34924800
C	1.90060300	-1.26383600	-3.22873000
C	2.90548300	-1.94689600	-2.43286000
C	2.50048100	-2.93606900	-1.52121900
C	3.10677900	-2.98740900	-0.19611700
C	2.07847000	-3.38661200	0.74990800
C	2.04456800	-2.82100400	2.02733700
C	1.73572100	1.54639700	3.12199300
C	0.98889600	-1.20206900	3.37538200
C	4.33445200	1.45574600	-0.57036200
C	-6.15069000	-2.07541800	-0.09126000
C	-4.79187600	-1.77204600	-0.06970200
C	-6.62562400	0.25619700	0.07471500
C	-7.09986500	-1.05214400	-0.01280700
C	-4.99397900	2.12148900	0.00295100
C	-2.20562800	0.95490300	0.77585900
O	-4.17802700	2.50305600	-0.87983000
O	-5.67985200	2.80853100	0.79185000
C	-8.58321400	-1.34850400	-0.03885300
H	-8.80833200	-2.32778700	0.40369200
H	-9.15061600	-0.59004500	0.51388500

H	-8.98112200	-1.36158500	-1.06495700
H	-7.32093800	1.08498800	0.18427800
H	-6.46871400	-3.11677200	-0.14883800
H	-4.07669500	-2.58769400	-0.08292200

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	x	y	z
C	-2.24085200	0.66987800	1.05204400
C	-1.67021100	1.95248300	0.78498900
C	-1.39583600	2.41041600	-0.51234900
C	-1.60325200	1.47908400	-1.62888100
C	-1.61458200	0.16425200	2.21581900
C	-0.70753300	1.18583300	2.76214200
C	-0.75005300	2.30977700	1.86313400
C	0.40037200	3.06109400	1.61191000
C	-0.19637500	3.14461100	-0.77048200
C	-0.53068600	1.68214400	-2.58139400
C	0.00491100	0.60395700	-3.30188200
C	-0.50950200	-0.71875600	-3.06182900
C	-1.52810900	-0.89012400	-2.10701100
C	-1.46549800	-2.01954700	-1.19300500
C	-2.02159000	-1.61296000	0.06274300
C	-1.44975000	-2.07952400	1.23518400
C	-1.26981100	-1.20170900	2.39352900
C	0.48439800	0.83054900	3.38964900
C	0.85483200	-0.56911400	3.52595100
C	-0.01628200	-1.54681100	2.99273600
C	0.56079100	-2.67818700	2.26209300
C	-0.33453600	-3.00744500	1.18070000
C	0.17046700	-3.44438500	-0.05189500
C	-0.41417700	-2.94759900	-1.27151800
C	0.65533900	-2.74247000	-2.23881200
C	0.60933800	-1.65397600	-3.10802100
C	0.34452300	2.70535800	-2.05588900
C	3.90010000	-0.21442700	-2.23738300
C	3.53661300	1.13365800	-2.35072400
C	3.74325200	2.03878400	-1.22647700
C	4.31674400	1.56003400	-0.04466500
C	4.68339500	0.16023400	0.07084700
C	3.97249600	-2.04570400	-0.76880100
C	3.06904600	-2.38016200	-1.85724000
C	3.02305700	-1.24582800	-2.76562500
C	1.81625100	-0.89193000	-3.37847700

C	1.43949200	0.50811900	-3.49990900
C	2.28421000	1.49679700	-2.98249900
C	2.63992000	2.97975900	-1.18314600
C	2.11940400	3.38600600	0.05723700
C	2.71793500	2.89009900	1.28973800
C	3.78912400	1.99618900	1.24069300
C	3.83179900	0.86148700	2.14837000
C	4.39115800	-0.27210200	1.42492700
C	3.88737600	-1.55583500	1.65783800
C	3.68017700	-2.46435000	0.53437100
C	1.90675100	-3.11358100	-1.60057500
C	1.60379800	-3.55015800	-0.24565300
C	2.47409200	-3.22098300	0.79995800
C	1.94451400	-2.78437800	2.08628500
C	2.83216900	-1.77350600	2.62722900
C	2.27435100	-0.67406600	3.30922900
C	2.80058400	0.66426500	3.06843300
C	1.69046900	1.59976900	3.12620200
C	1.64930700	2.69094600	2.25493200
C	1.72539400	2.62960500	-2.25547900
C	0.69614900	3.50138200	0.26419300
C	4.49628100	-0.71273500	-1.01129500
C	-6.15189000	-2.08433900	-0.04053400
C	-4.79156300	-1.77839500	-0.08534300
C	-4.31020900	-0.45907000	-0.07785900
C	-5.26259700	0.58751000	-0.00805200
C	-6.62140200	0.25094400	0.08262800
C	-7.09732100	-1.06131500	0.04855300
C	-2.75872700	-0.24752000	-0.06874300
C	-4.98817400	2.11214200	-0.10656200
C	-2.13963500	0.21872900	-1.42620000
O	-4.19347400	2.43628900	-1.02424000
O	-5.65670500	2.83290800	0.66943800
C	-8.58029400	-1.35726700	0.09544400
H	-8.77589700	-2.38502500	0.42765300
H	-9.10238600	-0.67671900	0.77968200
H	-9.05386000	-1.24031800	-0.89095900
H	-7.31167700	1.08376300	0.19600600
H	-6.46914400	-3.12733800	-0.05507700
H	-4.08518300	-2.60176900	-0.11200600

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C	-0.82987200	1.08329400	-1.24510600
C	-1.07307400	-0.30751000	-1.03224000
C	-1.21497000	-0.87467400	0.24468800
C	-0.98106900	-0.00866300	1.40730800
C	0.07691900	1.19054500	-2.32848300
C	0.32675300	-0.14670600	-2.88744700
C	-0.40105000	-1.08428200	-2.07305600
C	0.12669400	-2.34801200	-1.80271700
C	-0.63421000	-2.15167300	0.52536700
C	-0.28059300	-0.78979100	2.40856400
C	0.68737900	-0.19936600	3.23281600
C	0.99943800	1.19474100	3.05444600
C	0.32890000	1.91946100	2.05397900
C	1.07888300	2.85171300	1.22724300
C	0.50764300	2.84800600	-0.08651600
C	1.34435200	2.95227700	-1.18518000
C	1.12175100	2.14760800	-2.38844600
C	1.57060800	-0.48793900	-3.41365700
C	2.65297300	0.48255500	-3.42665800
C	2.41066200	1.76314100	-2.88182700
C	3.44047600	2.37543900	-2.03978300
C	2.77443800	3.11522700	-0.99630900
C	3.32171800	3.17380600	0.29264500
C	2.45328700	3.04917200	1.43574000
C	3.14687500	2.26876300	2.45139000
C	2.43722400	1.36263800	3.23690100
C	-0.06118900	-2.11262600	1.86960600
C	4.47746300	-1.62286100	2.47606100
C	3.43135000	-2.55369100	2.47161400
C	3.21332400	-3.39671700	1.30254300
C	4.05918400	-3.28230900	0.19547600
C	5.13605500	-2.30893300	0.20150300
C	5.66877200	-0.09545900	1.14707800
C	4.99757800	0.65236300	2.19726400
C	4.25932700	-0.29279600	3.01929700
C	3.00499900	0.05786400	3.52928000
C	1.91817900	-0.90971000	3.52770900
C	2.13147500	-2.18609800	2.99648900
C	1.78479000	-3.57693600	1.12468300
C	1.24226200	-3.60065100	-0.17081300
C	2.12326600	-3.48428300	-1.32609600
C	3.49863400	-3.32597900	-1.14792000
C	4.23446000	-2.37863400	-1.96972700
C	5.25070100	-1.75413500	-1.13468400

C	5.55070300	-0.39957900	-1.30758400
C	5.77110100	0.44643700	-0.13963900
C	4.45062000	1.90886900	1.92044600
C	4.55785700	2.47249500	0.58277700
C	5.19999800	1.74672000	-0.42665300
C	4.63725300	1.70307500	-1.77096900
C	4.87508800	0.38395200	-2.32357700
C	3.87508100	-0.21306700	-3.11388900
C	3.56445500	-1.62629800	-2.93613300
C	2.13475500	-1.79809800	-3.12829600
C	1.42784000	-2.70841600	-2.33952200
C	1.11510900	-2.80927400	2.15887800
C	0.01101500	-2.91226200	-0.47365200
C	5.35672000	-1.50249500	1.32721800
C	-2.66478800	5.51774800	-0.16732000
C	-1.71629200	4.50292200	-0.04239700
C	-2.03537900	3.14163400	-0.17374900
C	-3.38723700	2.81554300	-0.44549100
C	-4.31318300	3.85539200	-0.61259400
C	-3.99109100	5.20622000	-0.46632300
C	-0.86255000	2.10761200	-0.09812700
C	-4.01056900	1.40582300	-0.48364800
C	-0.72446600	1.34461000	1.26057100
O	-3.66224400	0.63203600	0.43839900
O	-4.88730000	1.21724400	-1.37521700
C	-5.04493400	6.28112800	-0.61396500
H	-4.59362500	7.26294400	-0.80443100
H	-5.72997900	6.05869500	-1.44146000
H	-5.66113200	6.37663700	0.29215000
H	-5.32485700	3.56009500	-0.87858700
H	-2.35707100	6.55696500	-0.05211000
H	-0.68747400	4.78966500	0.14670700
C	-5.45254600	-1.72375800	-0.33278300
H	-4.54361700	-2.08431900	0.14318100
H	-5.22318700	-0.89745100	-1.00618700
C	-6.55303500	-1.39100900	0.62772400
C	-7.06710700	-0.08677700	0.64028800
C	-7.05696100	-2.33033200	1.53895000
C	-8.06871000	0.26328700	1.54866700
H	-6.64618500	0.63559200	-0.05619800
C	-8.05686800	-1.97869900	2.44376200
H	-6.67162500	-3.34688200	1.51729300
C	-8.56830300	-0.67742100	2.45083100
H	-8.45585300	1.28028900	1.55348100

H	-8.43763500	-2.71902200	3.14516600
H	-9.34803700	-0.40046700	3.15836900
Br	-6.00632700	-3.27977000	-1.52582200

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	x	y	z
C	-0.57994200	1.54446700	1.31347100
C	-0.81170200	2.19424300	-0.08673200
C	-2.01415700	3.19334300	-0.12313800
C	-3.37712800	2.83999900	-0.25287000
C	0.50270300	2.86253400	-0.52014300
C	1.12660800	2.60035800	-1.76809500
C	0.69777800	1.58013000	-2.64191700
C	-0.36090700	0.68408600	-2.15065300
C	1.52260000	3.22076600	0.39963700
C	2.80911700	3.28226400	-0.30084700
C	2.56074200	2.89082300	-1.66313300
C	3.49707000	2.12846500	-2.36187500
C	1.67495600	0.77428900	-3.31292500
C	-0.03654700	-0.66331700	-2.58325900
C	-0.34017000	-1.76348500	-1.77036700
C	-0.95671500	-1.54194200	-0.48731300
C	-1.22623900	-0.23080000	-0.07653800
C	-0.97737900	0.16572500	1.29769300
C	0.42630700	1.93555800	2.18441600
C	1.49874200	2.85017200	1.76101100
C	3.98885900	2.90797700	0.34199200
C	3.95866200	2.47034000	1.72451000
C	2.71236700	2.42034800	2.38965000
C	2.40930100	1.27308100	3.24398300
C	0.99944900	0.98281500	3.11808900
C	0.55263600	-0.34547400	3.14269700
C	-0.46752300	-0.76266600	2.21414100
C	-0.15390700	-2.11698000	1.77609600
C	-0.39239700	-2.49624700	0.45715900
C	1.21973500	-0.61515800	-3.29423400
C	3.02564400	-3.64952800	-0.33722700
C	3.05610200	-3.21205600	-1.66638600
C	4.11971600	-2.32200000	-2.11474700
C	5.11504500	-1.92130600	-1.21820000
C	5.07519600	-2.37174200	0.16142000
C	3.43031300	-3.00774500	1.88606200
C	2.01333700	-3.30452500	1.75641900

C	1.76313500	-3.70129600	0.38081700
C	0.58261400	-3.30277800	-0.25365100
C	0.61334600	-2.84811600	-1.63586700
C	1.83108000	-2.79851300	-2.32225700
C	3.56006900	-1.38043400	-3.06642300
C	3.99529100	-0.04560000	-3.06444300
C	5.03432800	0.37284900	-2.13141200
C	5.57772400	-0.54134600	-1.22735900
C	5.82947400	-0.14401200	0.14892800
C	5.52039100	-1.27866900	1.00692200
C	4.91408700	-1.06169600	2.24816900
C	3.85100500	-1.95055300	2.70122400
C	1.07171800	-2.52625500	2.43733200
C	1.50822400	-1.42683700	3.28574600
C	2.87346500	-1.14421300	3.40536400
C	3.33589500	0.23615100	3.39351400
C	4.60871000	0.28411900	2.69600800
C	4.89145300	1.37724600	1.86114800
C	5.52585000	1.15249600	0.56781900
C	4.96757900	2.10671900	-0.37512200
C	4.72678700	1.72524500	-1.69790300
C	2.13983000	-1.66213400	-3.17837800
C	3.05929000	1.04301300	-3.21838600
C	4.05780800	-3.23248400	0.59554600
C	-2.67314800	5.55695300	-0.10384300
C	-1.70118000	4.56111700	-0.05692400
C	-4.33428300	3.86362000	-0.35202300
C	-4.02035400	5.21927800	-0.26040600
C	-3.98286800	1.42343700	-0.24024000
C	-0.98714800	0.89854300	-0.93201700
O	-3.70286300	0.70669900	0.75182900
O	-4.77712400	1.16731200	-1.18811900
C	-5.09903200	6.27821100	-0.31294600
H	-4.73724200	7.20094800	-0.78476400
H	-5.97143900	5.92964400	-0.87794400
H	-5.45436800	6.54970300	0.69230700
H	-5.36435200	3.55627600	-0.51512500
H	-2.37398300	6.60312800	-0.03911500
H	-0.65873500	4.85233500	0.01575700
C	-6.41214100	-0.92790600	0.49360600
C	-5.90461000	-2.21298700	-0.08916300
C	-6.33477100	-3.47344600	0.34782400
C	-4.89721000	-2.13211300	-1.06176100
C	-5.76916000	-4.63509400	-0.17545400

H	-7.13198700	-3.53577400	1.08450300
C	-4.32530600	-3.29827400	-1.57539200
H	-4.56935000	-1.14571500	-1.38222200
C	-4.75826800	-4.55069800	-1.13735900
H	-6.11386900	-5.60796800	0.17077600
H	-3.52952500	-3.22185100	-2.31208500
H	-4.30857300	-5.45686100	-1.53849300
H	-6.14802000	-0.06703100	-0.12290200
H	-6.08923400	-0.76054500	1.51951800
Br	-8.43820400	-0.90544300	0.63844600

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	x	y	z
C	-0.89785900	0.27305000	0.96205100
C	-0.19456100	0.15211100	2.19206400
C	0.64351700	1.16006000	2.72351800
C	0.91276000	2.31254900	1.86068300
C	-0.84325800	-1.00397600	0.32477600
C	-0.22167700	-1.97505300	1.22518000
C	0.19041400	-1.25094500	2.39806400
C	1.37584800	-1.58584300	3.05095800
C	1.88660100	0.80045600	3.34419200
C	2.30450100	2.69368200	2.01939000
C	3.03205300	3.20452300	0.93725300
C	2.39283100	3.33137100	-0.34817900
C	1.05922700	2.92069800	-0.48722700
C	0.62441100	2.20386100	-1.67448500
C	-0.42803400	1.29393800	-1.30390300
C	-0.41558500	0.02654400	-1.86325600
C	-0.68123300	-1.17248900	-1.06066900
C	0.55363200	-3.02341200	0.72813700
C	0.74959400	-3.16888900	-0.69995700
C	0.15165300	-2.22433800	-1.55942800
C	0.91489100	-1.71322800	-2.69510000
C	0.55938100	-0.32473900	-2.87975300
C	1.52720500	0.59919300	-3.29304500
C	1.56070000	1.90077800	-2.67598000
C	2.95815100	2.28496800	-2.50923300
C	3.36458800	2.98641300	-1.37639700
C	2.91366100	1.75733100	2.93219200
C	6.01635700	0.65645500	-0.29083800
C	5.81725300	0.78909300	1.08788500
C	5.56457000	-0.39130600	1.90503700

C	5.53480000	-1.65441000	1.30804400
C	5.73347100	-1.78673800	-0.12412200
C	5.33606600	-0.52506300	-2.20451100
C	4.98064400	0.87141500	-2.39158300
C	5.40237500	1.60263600	-1.20744400
C	4.60871900	2.64049900	-0.71124800
C	4.40182500	2.77839100	0.72275300
C	4.99029100	1.86314900	1.60128400
C	4.60765000	-0.03973000	2.93749400
C	3.61707700	-0.96286300	3.31396900
C	3.58748800	-2.28114100	2.69262300
C	4.52211100	-2.61819000	1.71254100
C	4.10271500	-3.35102800	0.52867000
C	4.85464300	-2.83674300	-0.60684600
C	4.23029600	-2.70931700	-1.85077300
C	4.48134300	-1.53059800	-2.67007700
C	3.78241000	1.20842100	-3.02956100
C	2.89423100	0.16381800	-3.51626600
C	3.23788400	-1.17843400	-3.32715900
C	2.22534600	-2.14307600	-2.91954000
C	2.84388900	-3.10245200	-2.02319100
C	2.11442200	-3.58125800	-0.92377300
C	2.76566800	-3.71751800	0.37312800
C	1.79421600	-3.37366100	1.39780300
C	2.19672600	-2.66931300	2.53417200
C	4.23643400	1.34728600	2.73685700
C	2.25653300	-0.54497800	3.55074200
C	5.98514800	-0.65614000	-0.91213100
C	-3.21426700	4.63275500	0.71715100
C	-2.11568500	3.79393500	0.53340900
C	-2.23243400	2.42373100	0.25670500
C	-3.55649600	1.92070400	0.16037600
C	-4.65229100	2.77048200	0.37505800
C	-4.51212800	4.13146400	0.65388100
C	-0.91145000	1.58586100	0.15754500
C	-3.92005900	0.53483000	-0.29461800
C	0.29417800	2.45146000	0.63033300
O	-5.04037300	0.10318000	0.30607500
O	-3.32591600	-0.06954300	-1.16795100
C	-5.72239600	5.00457200	0.88963700
H	-5.45045100	6.06625300	0.90698100
H	-6.47954800	4.86135000	0.10936200
H	-6.20468600	4.76894000	1.84742200
H	-5.64476200	2.33749100	0.30938200

H	-3.04742000	5.68820400	0.92749800
H	-1.12690100	4.22644600	0.62759900
C	-5.64919700	-1.14734300	-0.16016500
H	-6.21966400	-1.50458800	0.70387000
H	-4.83940200	-1.83650400	-0.41072800
C	-6.57074200	-0.91100900	-1.33886300
C	-6.06592100	-0.71488800	-2.63491200
C	-7.95885000	-0.89912700	-1.13431500
C	-6.93235600	-0.49230000	-3.70586300
H	-4.99204900	-0.73127000	-2.79313400
C	-8.82047300	-0.68112200	-2.21298600
H	-8.35162900	-1.09957700	-0.13293200
C	-8.31401200	-0.47182500	-3.49691100
H	-6.52766800	-0.33971100	-4.70480200
H	-9.89550200	-0.68132600	-2.04358400
H	-8.99026200	-0.30139000	-4.33359200
Br	-8.52766700	-2.10489800	2.27754800

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	x	y	z
C	0.04121900	2.11557800	1.26453400
C	-0.95529900	1.73961500	0.12328800
C	-2.25898300	2.58235100	0.27165500
C	-3.58522600	2.15050300	0.04569300
C	-0.24587000	1.94461500	-1.22606300
C	-0.13890800	0.90053700	-2.19118700
C	-0.53666000	-0.42400100	-1.93867800
C	-0.95852400	-0.75560300	-0.57308100
C	0.90894700	2.75830400	-1.35372700
C	1.70418000	2.29688900	-2.50027400
C	1.04363600	1.13085600	-3.02541700
C	1.78815700	0.06148800	-3.52628400
C	0.25811800	-1.51249800	-2.42294800
C	-0.45442400	-2.07794400	-0.25682500
C	-0.04172800	-2.39117500	1.04389500
C	-0.10337200	-1.37504700	2.06344900
C	-0.57202700	-0.09607100	1.72454400
C	0.10401800	1.07796300	2.25117300
C	1.14157600	2.93781900	1.08313600
C	1.58530200	3.34198300	-0.25557000
C	3.09616300	2.37371200	-2.48474600
C	3.78870500	2.92855400	-1.33512500
C	3.01858200	3.36622700	-0.23580400

C	3.47556000	3.04820900	1.11714800
C	2.31019800	2.79141800	1.92912600
C	2.34409800	1.81245900	2.93012900
C	1.21225700	0.93682400	3.10110600
C	1.71249200	-0.39270000	3.42380700
C	1.07151300	-1.51934500	2.91434400
C	0.30265200	-2.54875000	-1.39384400
C	4.01421300	-3.04501500	1.28342000
C	3.34872500	-3.56377900	0.16716300
C	3.79560100	-3.21236400	-1.17481000
C	4.89667700	-2.36811300	-1.34218600
C	5.57785700	-1.82461900	-0.18076800
C	5.09404400	-1.14158200	2.13799500
C	3.92035100	-1.39646100	2.95632200
C	3.25174700	-2.57428600	2.42740600
C	1.85516700	-2.63304100	2.40839900
C	1.16277000	-3.17422400	1.24953100
C	1.90052200	-3.62037100	0.14855100
C	2.62904300	-3.08029400	-2.02765000
C	2.59127900	-2.07467400	-3.00565700
C	3.73957200	-1.19521400	-3.18255600
C	4.86440900	-1.33634100	-2.36866200
C	5.53019200	-0.15716900	-1.83826100
C	5.97548100	-0.46259800	-0.48677200
C	5.91379500	0.52380500	0.50133100
C	5.46892300	0.17452000	1.84513400
C	3.16371900	-0.32805700	3.44551100
C	3.55382200	1.04038200	3.14141300
C	4.68069100	1.28139600	2.34864700
C	4.64730000	2.31344800	1.32015800
C	5.42743600	1.85388800	0.18711400
C	4.97810500	2.14333000	-1.11269700
C	5.04607800	1.11534800	-2.14456800
C	3.88007300	1.26192400	-2.99855200
C	3.23973200	0.13012700	-3.50747900
C	1.45627000	-3.31261300	-1.20440500
C	1.39284800	-1.30176700	-3.23356300
C	5.15788500	-2.16687000	1.11123500
C	-3.17153300	4.76391100	0.93412900
C	-2.09817300	3.90960800	0.70824400
C	-4.66370800	3.01194600	0.32200700
C	-4.48678700	4.32097800	0.76369600
C	-3.97633500	0.86103800	-0.62244900
C	-1.07550100	0.21221700	0.41195100

O	-5.06563200	0.33155300	-0.03950100
O	-3.43020000	0.42220100	-1.61663200
C	-5.66812000	5.21861200	1.05045500
H	-5.57101700	6.18682300	0.54217500
H	-6.60484700	4.75777300	0.72211800
H	-5.76206600	5.42794000	2.12487200
H	-5.66795100	2.63066000	0.16636400
H	-2.97902400	5.78419000	1.26353500
H	-1.09598400	4.28233600	0.88540400
C	-5.77693900	-0.75370100	-0.72030900
C	-5.70613800	-2.01987800	0.09894700
C	-6.88674100	-2.60430200	0.57717600
C	-4.47397400	-2.63172400	0.37062200
C	-6.82427000	-3.78913500	1.31670100
H	-7.84254600	-2.12367600	0.35384100
C	-4.41654400	-3.80849900	1.11626600
H	-3.55726100	-2.18406600	-0.00481200
C	-5.59516900	-4.39164000	1.59128500
H	-7.74532500	-4.23845700	1.68326100
H	-3.45231800	-4.26799500	1.32285600
H	-5.55224300	-5.31188700	2.17190200
H	-5.31509200	-0.88436200	-1.70171900
H	-6.81538300	-0.41500800	-0.82596400
Br	-9.55476500	-0.33999300	-0.78846500

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	x	y	z
C	0.12507600	0.65006900	-1.53620800
C	1.03574700	0.25726300	-0.33452800
C	2.47945100	0.79506000	-0.54621700
C	3.66127300	0.16604400	-0.10318200
C	0.36774500	0.75534900	0.95839600
C	0.07971500	-0.11756600	2.05108600
C	0.23824800	-1.51067600	1.97938600
C	0.60172900	-2.08947700	0.67928300
C	-0.61940000	1.76769000	0.95579500
C	-1.48571000	1.60682000	2.13328000
C	-1.04183100	0.42283100	2.82110600
C	-1.96376700	-0.42470100	3.43826300
C	-0.73422900	-2.37256300	2.58235600
C	-0.12873100	-3.33225400	0.52410600
C	-0.59008200	-3.73550300	-0.73470800
C	-0.34928300	-2.88762000	-1.87493300

C	0.33761400	-1.67731400	-1.69344400
C	-0.12087500	-0.48140700	-2.38120800
C	-0.81224800	1.66981000	-1.49080500
C	-1.17743700	2.32193200	-0.22687300
C	-2.84078100	1.92264700	2.07374200
C	-3.42383100	2.43772800	0.84525000
C	-2.58761700	2.58770600	-0.28281500
C	-3.09191600	2.17905100	-1.59387600
C	-1.98894800	1.61770500	-2.33617800
C	-2.19435400	0.53805500	-3.20456500
C	-1.23515300	-0.53677300	-3.23337800
C	-1.96140900	-1.78878800	-3.39325000
C	-1.52979300	-2.93460000	-2.72885000
C	-0.95911200	-3.50994100	1.69322000
C	-4.69742500	-3.69526900	-0.98659100
C	-4.13559800	-4.17282600	0.20309100
C	-4.51497900	-3.57577400	1.47678900
C	-5.44940200	-2.53697300	1.50738400
C	-6.02373800	-2.03992400	0.27003300
C	-5.42312100	-1.76105700	-2.10498000
C	-4.31202600	-2.32201600	-2.85506700
C	-3.86243600	-3.51880400	-2.16266000
C	-2.49819800	-3.81778300	-2.10273700
C	-1.91344000	-4.31596500	-0.86701100
C	-2.71982800	-4.47878600	0.26402800
C	-3.34401400	-3.53920800	2.33393300
C	-3.13102000	-2.43716900	3.17561400
C	-4.10596400	-1.35481500	3.21028200
C	-5.23659700	-1.40160400	2.39333600
C	-5.68378600	-0.20405700	1.70015500
C	-6.17486700	-0.60114000	0.38870500
C	-5.93735100	0.22127500	-0.71596400
C	-5.55960500	-0.37321400	-1.99263300
C	-3.37842800	-1.47541300	-3.45923500
C	-3.52095700	-0.03179500	-3.34293800
C	-4.58916000	0.50418900	-2.61618100
C	-4.37494700	1.63939100	-1.72793800
C	-5.22492200	1.47552100	-0.56467800
C	-4.73216600	1.84948900	0.69759000
C	-4.98151500	0.99269100	1.85091900
C	-3.80986500	1.04289500	2.70758000
C	-3.38029400	-0.10680200	3.37416200
C	-2.22953100	-4.07931800	1.57627400
C	-1.81498400	-1.86217900	3.33115300

C	-5.66833700	-2.61642900	-0.95678600
C	3.88876400	2.56670400	-1.49477800
C	2.63806800	1.99978000	-1.25119200
C	4.92112200	0.71677300	-0.39465800
C	5.05989700	1.92614100	-1.07647700
C	3.74670600	-1.01687000	0.81550600
C	0.88269900	-1.29215500	-0.41798500
O	4.59613800	-1.93917100	0.31685700
O	3.22232200	-1.08872000	1.90986700
C	6.43931000	2.48898300	-1.33660900
H	6.52294900	3.52354500	-0.97635800
H	7.20109900	1.88103900	-0.83473600
H	6.66691500	2.50616500	-2.41192700
H	5.81782100	0.20422700	-0.04346000
H	3.93522300	3.51858700	-2.02182400
H	1.76121800	2.50936100	-1.63577500
C	5.19736500	-2.85939500	1.26725900
C	5.77285200	-4.01935100	0.49665100
C	7.01745200	-3.88594800	-0.13798500
C	5.07775500	-5.23029900	0.39733800
C	7.54882600	-4.95933100	-0.85451000
H	7.55656600	-2.93954200	-0.04822200
C	5.61224100	-6.30249200	-0.32032900
H	4.10887500	-5.33062400	0.88288600
C	6.85187100	-6.16741500	-0.94838100
H	8.51591200	-4.85026100	-1.34106900
H	5.06099500	-7.23819600	-0.39004100
H	7.27258000	-7.00073900	-1.50885500
H	4.43597300	-3.17997500	1.98282700
H	5.98942000	-2.29781700	1.77560600
Br	8.26472600	-0.51101700	0.87333000
C	1.50936900	7.31661900	1.16584200
C	0.99740800	8.32577500	1.97725500
C	-0.34690300	8.30184200	2.36183400
C	-1.17212900	7.26383500	1.92864700
C	-0.65903200	6.25288900	1.11344500
C	0.68733800	6.26794100	0.72718000
H	2.55164400	7.33758700	0.85705400
H	1.64670200	9.13054400	2.31405600
H	-0.74581600	9.08790900	2.99884000
H	-2.21702700	7.23450400	2.22680400
H	-1.29951700	5.43911100	0.78304500
C	1.23604200	5.15498400	-0.10600800
H	2.17724700	4.75019000	0.26300400

H	0.51790500	4.35114800	-0.25766800
Br	1.69424500	5.77587400	-1.96405900

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	x	y	z
C	-1.27364000	-1.77423100	-1.92044300
C	-0.07275300	-0.89765800	-1.45376400
C	1.23259900	-1.39220200	-2.13779700
C	2.49303800	-1.50224400	-1.51741000
C	-0.40982100	0.57705100	-1.72865700
C	-0.37207600	1.56613200	-0.70518900
C	-0.16630800	1.26219200	0.65433500
C	-0.12372400	-0.15549000	1.02951000
C	-1.41881100	0.95938600	-2.65087100
C	-1.95034500	2.27524300	-2.27170500
C	-1.29156900	2.65553600	-1.04944500
C	-1.98711600	3.34724900	-0.05752000
C	-0.91837100	1.95153700	1.66043400
C	-0.80849400	-0.30660700	2.29948700
C	-1.55257500	-1.46020600	2.57422800
C	-1.64725900	-2.49183000	1.57260600
C	-0.99634500	-2.30974300	0.34259700
C	-1.66876400	-2.68820500	-0.88908300
C	-2.21540000	-1.35647900	-2.84586700
C	-2.28380100	0.04085300	-3.29065300
C	-3.29145500	2.59388900	-2.48063800
C	-4.18774900	1.62945500	-3.09321100
C	-3.67053800	0.36583900	-3.45149200
C	-4.46837800	-0.82849500	-3.17490600
C	-3.56314600	-1.89098900	-2.80699400
C	-3.92869100	-2.82832800	-1.83205300
C	-2.95712800	-3.24341100	-0.85155900
C	-3.64007700	-3.40013800	0.42584200
C	-3.00117700	-3.03130900	1.60742900
C	-1.30654000	0.99119600	2.69208000
C	-5.58778900	-0.69916200	2.84002400
C	-4.72209600	0.23736400	3.41631000
C	-4.79593500	1.63804500	3.01976000
C	-5.74080600	2.04236000	2.07279900
C	-6.63101700	1.06600800	1.47126700
C	-6.66323500	-1.31833700	0.84533600
C	-5.75125900	-2.38843300	1.21334300
C	-5.08533700	-2.00512900	2.44775900

C	-3.73731700	-2.32205700	2.63958700
C	-2.83725800	-1.34929600	3.23964300
C	-3.32391000	-0.09158300	3.60962800
C	-3.45017100	2.18095700	2.99691000
C	-3.08369100	3.09303300	1.99461800
C	-4.06977700	3.51803300	1.00908000
C	-5.36602200	3.00277100	1.04505500
C	-6.03068200	2.61912500	-0.18991500
C	-6.81619900	1.42284900	0.07652900
C	-6.90468800	0.42303800	-0.89589900
C	-6.83292500	-0.97844600	-0.50159200
C	-5.04081000	-3.07262900	0.22324100
C	-5.21848800	-2.72028800	-1.17750900
C	-6.09316400	-1.68628500	-1.52737200
C	-5.71752500	-0.72379200	-2.55532500
C	-6.23764000	0.57574800	-2.17504000
C	-5.46233700	1.72089300	-2.42432500
C	-5.37222500	2.76576800	-1.41160500
C	-4.02568700	3.30990000	-1.44981500
C	-3.38739500	3.67829000	-0.26382600
C	-2.53860300	1.10568700	3.34178500
C	-1.80059500	3.00451800	1.33913300
C	-6.57040900	-0.28001100	1.85644200
C	2.24585000	-2.33610000	-4.15711900
C	1.14975000	-1.81667600	-3.47368500
C	3.58295500	-2.07456900	-2.19567000
C	3.48372600	-2.49309800	-3.52398900
C	2.83479000	-0.92227600	-0.17852500
C	-0.16692600	-1.16365500	0.07924700
O	3.33296300	-1.86114100	0.65364700
O	2.77013000	0.25930300	0.10403300
C	4.67937700	-3.09290200	-4.22857300
H	4.86014900	-2.59857600	-5.19288200
H	5.58085600	-3.00158500	-3.61125200
H	4.51875900	-4.15962800	-4.44085800
H	4.54318200	-2.17877200	-1.69100100
H	2.12701300	-2.64062400	-5.19652200
H	0.19680700	-1.74833700	-3.98781400
C	3.90885500	-1.36653900	1.88687000
C	4.58799900	-2.51444600	2.58858300
C	5.69288200	-3.14981300	2.00121500
C	4.13400000	-2.94575900	3.83993900
C	6.32240500	-4.20078400	2.66773600
H	6.06774600	-2.84200900	1.02242100

C	4.77211100	-3.99352500	4.50833500
H	3.27144900	-2.45989400	4.29225100
C	5.86940300	-4.62434500	3.92056300
H	7.17399300	-4.68411800	2.19517600
H	4.40726200	-4.31796400	5.48083000
H	6.36782000	-5.44382600	4.43544600
H	3.11228800	-0.93149200	2.49953500
H	4.61594000	-0.56943000	1.63654400
Br	7.29476800	-2.54044500	-1.33952200
C	5.90699800	2.00003200	-0.10396700
C	6.67258600	0.86228700	-0.36408800
C	8.00884800	0.80888500	0.03487500
C	8.58334000	1.90209000	0.69109200
C	7.82105300	3.03847100	0.95477800
C	6.47390000	3.09596100	0.56413600
H	4.85859800	2.02108600	-0.39251100
H	6.26754800	-0.01011400	-0.87067900
H	8.55770100	-0.10595200	-0.17589800
H	9.62534100	1.86787300	1.00358100
H	8.26633800	3.89582400	1.45647500
C	5.63102900	4.27475400	0.90650000
H	4.58426700	4.14013100	0.64103300
H	5.72235700	4.59368800	1.94419600
Br	6.17176600	5.96041300	-0.09679100

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	x	y	z
C	-0.39245400	0.29111700	-2.34796700
C	0.64002700	0.43781600	-1.18825400
C	2.04732600	0.76008100	-1.76364400
C	3.27966100	0.22566000	-1.33403000
C	0.14583900	1.53480700	-0.22952600
C	-0.03621600	1.29628100	1.16347800
C	0.08542200	0.02373800	1.75007000
C	0.27103900	-1.11880600	0.84819100
C	-0.81704900	2.50168400	-0.62368800
C	-1.54028200	2.97651700	0.56299400
C	-1.04856900	2.21931300	1.68384400
C	-1.91154700	1.83119900	2.70904200
C	-0.83558000	-0.37783800	2.77272100
C	-0.50191200	-2.23034000	1.36746200
C	-1.11664200	-3.13801500	0.49676600
C	-0.99005700	-2.94445500	-0.92543000

C	-0.25644800	-1.84724100	-1.40214200
C	-0.76183100	-1.08211800	-2.53009400
C	-1.29355800	1.28241600	-2.70160600
C	-1.49664500	2.47098700	-1.86332800
C	-2.88660100	3.33147100	0.48584600
C	-3.59494600	3.25132500	-0.77868300
C	-2.89373700	2.79110000	-1.91344700
C	-3.55641800	1.85780300	-2.82340300
C	-2.56163700	0.93224000	-3.31172300
C	-2.89355800	-0.40907300	-3.54106100
C	-1.97005300	-1.44294300	-3.14643200
C	-2.74116900	-2.56477900	-2.62778700
C	-2.26313000	-3.29489600	-1.54262300
C	-1.19227200	-1.77750200	2.55308200
C	-5.22237000	-2.90801900	0.63496100
C	-4.53676300	-2.81432700	1.85099300
C	-4.75024000	-1.66422800	2.72041000
C	-5.64855300	-0.66348800	2.34032400
C	-6.35127000	-0.76048000	1.07353300
C	-6.02585200	-1.67091700	-1.19374500
C	-5.02454000	-2.60103400	-1.68727600
C	-4.52685700	-3.36651000	-0.55577200
C	-3.17263300	-3.70611600	-0.48685500
C	-2.46002100	-3.61019500	0.77726900
C	-3.13138800	-3.16315000	1.91902000
C	-3.48606200	-1.32037300	3.34498000
C	-3.14867500	0.02736500	3.54081600
C	-4.08715200	1.07095300	3.14834600
C	-5.30656700	0.73402200	2.55941400
C	-5.80310000	1.49925900	1.42653300
C	-6.45303300	0.57387300	0.51022100
C	-6.32786700	0.76297800	-0.86873500
C	-6.11603600	-0.38606500	-1.74029400
C	-4.14779300	-2.20983100	-2.70276900
C	-4.24114900	-0.87375700	-3.27127000
C	-5.20334700	0.02033300	-2.79030900
C	-4.85912200	1.41907000	-2.56980600
C	-5.57099600	1.88388900	-1.39433500
C	-4.92699700	2.76531100	-0.51032100
C	-5.06024100	2.57031400	0.92825900
C	-3.79474400	2.92590200	1.54662400
C	-3.31768900	2.19102700	2.63387500
C	-2.48153400	-2.23494200	2.83461400
C	-1.80972500	0.50455500	3.28405300

C	-6.15559400	-1.86808100	0.23907900
C	3.28977800	2.09384300	-3.40480400
C	2.09619500	1.69024300	-2.81722300
C	4.47580900	0.60405100	-1.97148600
C	4.51192700	1.55442100	-2.99034400
C	3.48934300	-0.63885200	-0.11999300
C	0.44618700	-0.95509800	-0.51745300
O	4.17245600	-1.74478600	-0.43418700
O	3.16837200	-0.30084100	1.00703100
C	5.82027300	2.02434300	-3.57770400
H	6.12350300	2.96789600	-3.10480300
H	6.61989000	1.29525400	-3.41235300
H	5.73785800	2.20638500	-4.65623300
H	5.40207900	0.14986700	-1.63054200
H	3.26797800	2.83732500	-4.19943700
H	1.16728300	2.11392000	-3.18243300
C	4.72652600	-2.57460300	0.64331200
C	4.26679900	-4.00163000	0.47056600
C	5.21525600	-5.02488900	0.33996700
C	2.90176900	-4.32173100	0.46728900
C	4.79127100	-6.35088700	0.21176800
H	6.27729600	-4.76602100	0.34450200
C	2.48411500	-5.64486700	0.33061000
H	2.16328400	-3.53113300	0.57217600
C	3.43122600	-6.66540300	0.20369100
H	5.53384000	-7.14023300	0.11164100
H	1.42102000	-5.87531300	0.32611900
H	3.10719900	-7.69968600	0.09900200
H	4.38790500	-2.15043600	1.59130300
H	5.81939000	-2.50082500	0.56301400
Br	8.45760400	-3.20969700	0.49899600
C	3.45685600	2.91204800	2.26918700
C	3.57138600	2.97529000	3.66043100
C	3.64731900	4.20857700	4.30628100
C	3.60494800	5.38831000	3.55611700
C	3.48604800	5.32907400	2.17028600
C	3.41112500	4.09125300	1.51413600
H	3.38357700	1.94423400	1.77860400
H	3.60079700	2.05236100	4.23298800
H	3.73881100	4.25399100	5.38915800
H	3.66443700	6.35408000	4.05327800
H	3.47085300	6.24360800	1.58228000
C	3.21734700	4.00685300	0.03283000
H	3.23418800	2.98549000	-0.33637700

H	2.31915800	4.51418100	-0.31697000
Br	4.69009400	4.93594500	-0.98743100

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	x	y	z
C	-2.12362200	-0.91666200	1.21349800
C	-1.49036100	-0.30865900	2.34087300
C	-1.22508900	1.07246600	2.37029000
C	-1.58093700	1.92299600	1.27077100
C	-1.49770900	-2.16434700	0.98606700
C	-0.50666300	-2.39338100	2.03720600
C	-0.51002100	-1.22993400	2.89272600
C	0.68864400	-0.77176400	3.46342600
C	0.01542400	1.54270900	2.95589700
C	-0.53740600	2.86945700	1.10371300
C	-0.10526000	3.33757100	-0.16554300
C	-0.68786000	2.68535600	-1.32576300
C	-1.69161000	1.72865600	-1.19153000
C	-1.64703000	0.54961000	-2.00045100
C	-2.13396300	-0.56825300	-1.25412200
C	-1.54721500	-1.81347000	-1.43593500
C	-1.25999500	-2.70251200	-0.31061600
C	0.68267400	-3.07093000	1.76731400
C	0.95349400	-3.57201800	0.42633000
C	-0.00933800	-3.34406100	-0.58474500
C	0.45411300	-2.92682100	-1.91010400
C	-0.50715000	-1.98904700	-2.43923100
C	-0.08740000	-0.90800700	-3.22178200
C	-0.68189700	0.39032200	-3.02163700
C	0.35203000	1.38918200	-3.16334100
C	0.35233900	2.51062200	-2.33073200
C	0.45491400	2.66392600	2.15367800
C	3.77978800	2.14804500	-0.99940000
C	3.49453400	2.60502100	0.30070600
C	3.82135000	1.76253200	1.44674600
C	4.40291500	0.50806100	1.25288000
C	4.67850700	0.02996700	-0.09259300
C	3.76791800	0.23650900	-2.37521800
C	2.79585300	1.17351900	-2.90553000
C	2.79540200	2.35135400	-2.04700100
C	1.58965300	3.00309000	-1.76839900
C	1.29898000	3.49183500	-0.41985400
C	2.26303000	3.29572500	0.59224400

C	2.79242400	1.94420900	2.45651200
C	2.36525900	0.85045400	3.22386700
C	2.97013700	-0.45811200	3.01929700
C	3.96631600	-0.62554800	2.05622900
C	3.96196600	-1.80072100	1.19691300
C	4.40629800	-1.39323200	-0.12773200
C	3.82974500	-1.97924200	-1.26331400
C	3.50406200	-1.13856700	-2.41032100
C	1.59985800	0.70661200	-3.45956300
C	1.32567100	-0.72154000	-3.49612600
C	2.26006000	-1.62274100	-2.97308100
C	1.81816000	-2.75681100	-2.17014200
C	2.79955400	-2.98665100	-1.12622900
C	2.35303700	-3.36881200	0.15532800
C	2.95909700	-2.76186200	1.33578200
C	1.92736300	-2.59775900	2.34674700
C	1.92584400	-1.46126200	3.16731400
C	1.81418200	2.86835500	1.90998600
C	0.95931500	0.65105000	3.49693200
C	4.37228300	0.84075900	-1.19601000
C	-6.08056400	-2.05335600	0.00506900
C	-4.73060200	-1.73701900	0.05380600
C	-4.29138200	-0.39896700	0.05006900
C	-5.26634300	0.60107500	0.00369200
C	-6.63387600	0.27113900	-0.03248200
C	-7.06470400	-1.04856700	-0.03522600
C	-2.78567400	-0.11275200	0.08411800
C	-4.92118200	2.04967500	0.01360000
C	-2.42722800	1.47126700	0.12064000
O	-3.64287900	2.39582500	0.10104300
O	-5.78435100	2.91885400	-0.03316500
C	-8.53461700	-1.40122700	-0.07266000
H	-8.84809200	-1.93853100	0.83353100
H	-9.15466800	-0.50175900	-0.15430800
H	-8.77535900	-2.05080200	-0.92555800
H	-7.34239800	1.09392500	-0.05755200
H	-6.38218400	-3.10055700	0.00176100
H	-3.99243600	-2.53082000	0.09598500

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	x	y	z
C	-1.15524100	0.83144600	-0.99658800
C	-1.26074500	1.84702800	0.18044700

C	-2.68292000	2.41782400	0.22309600
C	-3.00255300	3.70776400	-0.21233200
C	-0.93470400	1.07791000	1.46781800
C	0.09044300	1.48040000	2.38333600
C	1.02896800	2.46549800	2.03206800
C	0.99382500	3.11201100	0.75341300
C	-1.09070200	-0.31947700	1.57811500
C	-0.20574000	-0.81062300	2.63444400
C	0.52781000	0.32455900	3.14572400
C	1.86358600	0.17461800	3.55220200
C	2.41102100	2.30891800	2.45078400
C	2.33451700	3.28332400	0.32129000
C	2.73795500	3.15156100	-1.03362900
C	1.72759200	2.68190500	-1.96612200
C	0.41127100	2.47329900	-1.56275900
C	-0.28664100	1.31356900	-2.02368600
C	-1.33628500	-0.53892400	-0.84812700
C	-1.38553900	-1.17384200	0.47035700
C	0.40548300	-2.05943700	2.53604300
C	0.16254700	-2.90783000	1.37389800
C	-0.69148700	-2.42726900	0.35643400
C	-0.29639900	-2.62747300	-1.03818900
C	-0.70429900	-1.46100300	-1.78266200
C	0.08229500	-0.97869300	-2.83420500
C	0.28244600	0.44093500	-2.98017200
C	1.64464800	0.66580500	-3.40394700
C	2.35486300	1.75969600	-2.90379900
C	3.23186000	2.81095900	1.37107700
C	5.26501100	-0.09098800	-1.58163400
C	5.46746600	0.71789000	-0.44801000
C	5.49034800	0.10654400	0.87634400
C	5.30096700	-1.26938300	1.01853000
C	5.07259000	-2.10032300	-0.15308600
C	4.05151800	-1.94059000	-2.39157900
C	3.63251500	-0.77007900	-3.13861200
C	4.37538600	0.37594800	-2.62905000
C	3.73905100	1.61639600	-2.51539000
C	3.96000200	2.46490100	-1.34310900
C	4.83201600	2.00783900	-0.33261000
C	4.87555700	1.02978600	1.81646000
C	4.07449800	0.53767100	2.85611500
C	3.87600500	-0.89708500	3.00234000
C	4.47617800	-1.78087400	2.10416200
C	3.72992600	-2.92143800	1.59282200

C	4.10431000	-3.11925700	0.20035100
C	3.13857600	-3.53523900	-0.72672400
C	3.11603100	-2.92549600	-2.05114700
C	2.29697400	-0.62647200	-3.52628500
C	1.32462400	-1.64897100	-3.17152000
C	1.72923200	-2.77250500	-2.44247600
C	0.89959100	-3.28244700	-1.35726300
C	1.77236500	-3.76937500	-0.30717200
C	1.40240700	-3.55646300	1.03664400
C	2.41166200	-3.13105800	2.00084800
C	1.78756100	-2.22144400	2.94779700
C	2.50317300	-1.11696300	3.43226000
C	4.44329700	2.19062300	1.05857000
C	2.83009800	1.19330600	3.19455100
C	5.05747200	-1.51644400	-1.42815800
C	-5.05540100	2.04308000	0.64304800
C	-3.73932000	1.60253100	0.66878800
C	-4.33722200	4.15149400	-0.22495400
C	-5.38090600	3.33292300	0.18826200
C	-1.95866000	4.69276100	-0.60594400
C	-0.13563000	2.95234500	-0.21988000
O	-0.68122800	4.34774300	-0.46160200
O	-2.24071000	5.82162500	-0.98782300
C	-6.81585500	3.80913000	0.16579700
H	-6.88946900	4.82522900	-0.23731500
H	-7.44878300	3.15761600	-0.45195300
H	-7.25702700	3.81730900	1.17213400
H	-4.52029600	5.16681400	-0.56462400
H	-5.83703900	1.36625000	0.98274800
H	-3.52129800	0.61048800	1.04858600
C	-4.79484900	-1.80913700	-1.62157700
C	-5.36179300	-1.80823300	-2.89787300
C	-6.52563900	-2.53406900	-3.15217600
C	-7.12590300	-3.26648700	-2.12296900
C	-6.56010400	-3.27006100	-0.85074000
C	-5.38833300	-2.54418900	-0.58713800
H	-3.88471200	-1.24711700	-1.42973500
H	-4.88611000	-1.23836500	-3.69139800
H	-6.96448000	-2.53203900	-4.14741000
H	-8.03358300	-3.83482600	-2.31438100
H	-7.03119100	-3.82845400	-0.04454400
C	-4.76065300	-2.57535000	0.76868200
H	-4.75497700	-3.57013700	1.21290400
H	-3.75987800	-2.14028400	0.79454400

Br	-5.82742200	-1.49150500	2.09508800
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	x	y	z
C	-0.04970600	2.12954500	1.20928800
C	-0.77909200	2.17393000	-0.16471700
C	-1.81315200	3.30683200	-0.16978800
C	-3.19456000	3.10053500	-0.22939300
C	0.28440000	2.43480400	-1.24299100
C	0.47930700	1.58201100	-2.37296500
C	-0.13658800	0.32142100	-2.45163100
C	-0.98323000	-0.15920800	-1.39295900
C	1.52307000	3.05006200	-0.94704100
C	2.50209900	2.65185000	-1.95916200
C	1.84211300	1.73579700	-2.85887200
C	2.54979700	0.65606300	-3.41001300
C	0.59729100	-0.79238200	-3.01627000
C	-0.72741400	-1.54470800	-1.23341100
C	-0.73011500	-2.19971800	0.02895900
C	-0.85337500	-1.34134600	1.19527300
C	-1.07193000	0.02881400	1.06819000
C	-0.36696000	0.93326800	1.92449300
C	1.15738100	2.76877500	1.45725300
C	1.97407000	3.31943000	0.37577600
C	3.84500900	2.47274700	-1.62583800
C	4.29749200	2.69108800	-0.25913700
C	3.34495700	3.07530000	0.71256600
C	3.40095600	2.44584500	2.03386100
C	2.04551200	2.26878500	2.49657400
C	1.69416000	1.14175000	3.24753300
C	0.44959500	0.46543900	2.97832600
C	0.66779300	-0.95641400	3.11111200
C	0.03396100	-1.84141300	2.23620400
C	0.23716300	-1.96292100	-2.24478000
C	3.04981800	-3.59521600	1.02390600
C	2.61064200	-3.77254200	-0.30055200
C	3.43156400	-3.28093300	-1.40274700
C	4.64009000	-2.63172000	-1.14194900
C	5.08254800	-2.43367600	0.22881100
C	4.12352900	-2.08104000	2.47278000
C	2.75962800	-2.25170300	2.93662700
C	2.09282400	-3.18111800	2.03353300
C	0.75228100	-2.97180400	1.69246200

C	0.29166300	-3.17009900	0.31893500
C	1.22594800	-3.57729900	-0.65498300
C	2.54902300	-2.79177400	-2.44820900
C	2.90154400	-1.65056100	-3.18426900
C	4.16111900	-0.97327700	-2.91031500
C	5.01042900	-1.45252000	-1.91239500
C	5.67230300	-0.52322700	-1.00851400
C	5.71921400	-1.13372100	0.31190600
C	5.55541000	-0.33434000	1.45122300
C	4.73676900	-0.82480700	2.55406000
C	2.05942100	-1.16616400	3.47110700
C	2.69662000	0.13894400	3.55629600
C	4.00868800	0.30335700	3.09860500
C	4.37480900	1.48546600	2.32769800
C	5.34546000	1.09238000	1.32345500
C	5.27925100	1.68217800	0.04550500
C	5.45603100	0.84948700	-1.13903000
C	4.58155200	1.35323000	-2.18559700
C	3.93820700	0.45821600	-3.05036400
C	1.18757500	-2.94652300	-1.96774000
C	1.91300900	-0.64208400	-3.49268600
C	4.29918400	-2.91111300	1.28981600
C	-2.24526400	5.70458900	-0.09884000
C	-1.35828300	4.63810900	-0.10818000
C	-4.08730100	4.18897600	-0.23436800
C	-3.63581100	5.49962900	-0.16630300
C	-3.78776300	1.73990600	-0.29704800
C	-1.42976700	0.69236800	-0.25263600
O	-2.98052000	0.69247200	-0.30243800
O	-5.00545700	1.57095800	-0.35504800
C	-4.59457400	6.66856500	-0.16626600
H	-5.63461800	6.32674500	-0.19959500
H	-4.47658600	7.28964800	0.73227200
H	-4.43277100	7.32672200	-1.03115900
H	-5.14795900	3.96338400	-0.29019700
H	-1.85500900	6.72027100	-0.04154200
H	-0.29070200	4.82577800	-0.06742400
C	-7.07023900	-3.44278000	-0.64073400
C	-6.36250200	-4.64140600	-0.61871000
C	-4.97294700	-4.63204200	-0.45119500
C	-4.29777800	-3.42086900	-0.30281900
C	-5.00935300	-2.21715000	-0.31654800
C	-6.39968700	-2.21883600	-0.49035100
H	-8.15251600	-3.44598000	-0.75093000

H	-6.89269700	-5.58519200	-0.73171100
H	-4.41951900	-5.56829600	-0.43680700
H	-3.21805100	-3.39466500	-0.17729600
H	-4.47611000	-1.27591600	-0.21342300
C	-7.12288900	-0.91212000	-0.58143700
H	-6.47638000	-0.05469700	-0.39475900
H	-7.66768400	-0.78783200	-1.51782200
Br	-8.60238800	-0.75602700	0.79228500

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	x	y	z
C	-1.22773200	0.56866100	-0.87266900
C	-1.38744300	1.63503100	0.25421400
C	-2.84771600	2.11115300	0.32543100
C	-3.28457600	3.22790700	-0.40783300
C	-0.89915100	0.93183800	1.52401200
C	0.07761100	1.51719200	2.43345900
C	0.90141900	2.54905200	1.96459300
C	0.75422900	3.14238300	0.68374500
C	-0.94663400	-0.43559300	1.73089800
C	0.02059300	-0.77774900	2.76144300
C	0.65595600	0.45101900	3.20475500
C	2.01417200	0.44380800	3.56449600
C	2.32006000	2.56489300	2.34844800
C	2.06020100	3.41880700	0.19165700
C	2.42347400	3.26707800	-1.16294300
C	1.43084000	2.65342100	-2.03848400
C	0.16443300	2.32425800	-1.57053100
C	-0.43728500	1.09032400	-1.95388300
C	-1.30127900	-0.79669900	-0.67988300
C	-1.42360400	-1.46388600	0.71131800
C	0.75179900	-1.95970200	2.71709000
C	0.56584400	-2.86871300	1.56695200
C	-0.34906100	-2.56604500	0.57682700
C	0.00964800	-2.75779400	-0.79306500
C	-0.56145600	-1.66795200	-1.56398600
C	0.13847200	-1.18062700	-2.67133600
C	0.19299600	0.24054300	-2.88383600
C	1.50343800	0.57863600	-3.37961500
C	2.11700600	1.76078200	-2.95030300
C	3.04489000	3.10058900	1.22685400
C	5.24625400	0.27745700	-1.67682500
C	5.40232100	1.14769100	-0.58727700

C	5.54547300	0.60792600	0.75660400
C	5.49613400	-0.77080700	0.96894700
C	5.31384700	-1.67425600	-0.15616800
C	4.20396300	-1.72130400	-2.36232400
C	3.63979900	-0.63411900	-3.13912500
C	4.27666400	0.60220500	-2.70778000
C	3.52337600	1.77645500	-2.61993500
C	3.69953800	2.69130100	-1.49171700
C	4.65206000	2.38210400	-0.50272800
C	4.86423400	1.50689800	1.67518500
C	4.16203700	0.99079900	2.76677000
C	4.10513100	-0.44762700	2.98393400
C	4.76412800	-1.30901900	2.10603800
C	4.11793400	-2.54000200	1.67439600
C	4.46060500	-2.76361400	0.27717700
C	3.52363300	-3.31973400	-0.59990400
C	3.38789400	-2.77969800	-1.94363100
C	2.28028400	-0.64313200	-3.47079500
C	1.43250500	-1.73864700	-3.02885900
C	1.97828400	-2.78615300	-2.28524700
C	1.24557500	-3.32001100	-1.14904500
C	2.19532400	-3.64975300	-0.11453200
C	1.85842500	-3.41739700	1.22520400
C	2.83869700	-2.85187500	2.13612200
C	2.14988700	-1.96754100	3.06624800
C	2.77541200	-0.77498900	3.47866300
C	4.30099600	2.59303300	0.89061500
C	2.86213000	1.53535100	3.11459600
C	5.18429500	-1.15430800	-1.44990400
C	-5.18165300	1.64148900	0.86735600
C	-3.82171100	1.36898000	1.00068700
C	-4.65498800	3.50321300	-0.53880000
C	-5.62452300	2.70331300	0.06134000
C	-2.33765600	4.24025200	-0.92272500
C	-0.39048600	2.83190800	-0.24288700
O	-1.05159700	4.12176800	-0.51950900
O	-2.66661600	5.22843400	-1.55460200
C	-7.10273900	2.95829400	-0.11123900
H	-7.30497800	3.51107200	-1.03658100
H	-7.64807000	2.00428900	-0.11854800
H	-7.50161500	3.55462900	0.72229500
H	-4.93480000	4.37542500	-1.12278900
H	-5.92346800	0.98926100	1.32785800
H	-3.50859400	0.55000300	1.63384800

C	-4.92156400	-2.42233100	-0.18681300
C	-5.74444000	-3.12263300	-1.07046200
C	-5.27102700	-4.27534500	-1.69699300
C	-3.97987800	-4.73207400	-1.41463500
C	-3.16713500	-4.03896900	-0.51643800
C	-3.62161100	-2.86166000	0.10094600
H	-5.35061000	-1.54750700	0.29732900
H	-6.75349100	-2.74458100	-1.21729800
H	-5.90457300	-4.82586700	-2.39038900
H	-3.60475000	-5.63869700	-1.88665900
H	-2.17645000	-4.42230100	-0.28926900
C	-2.80623000	-2.10151200	1.13164300
H	-2.57579600	-2.75603400	1.98337600
H	-3.44008500	-1.30918300	1.52787700
Br	-8.10517400	-0.63996400	0.63545100

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	x	y	z
C	-0.33009900	2.56898300	0.85439700
C	-1.51728800	1.68896700	0.35231600
C	-2.88240800	2.39302800	0.25384700
C	-3.98314800	2.00297000	1.03301600
C	-1.13704400	1.23727000	-1.05420400
C	-1.11395000	-0.12955600	-1.48122600
C	-1.20816300	-1.19843500	-0.60723800
C	-1.57274100	-1.05576600	0.87677000
C	-0.26224600	1.95930800	-1.88026300
C	0.27593000	1.06152200	-2.90997700
C	-0.27345800	-0.24331400	-2.66952000
C	0.49104800	-1.38845400	-2.90424900
C	-0.38007900	-2.33881800	-0.82127900
C	-0.45890300	-1.94723300	1.48470900
C	0.34873900	-1.59028000	2.54855300
C	0.39262200	-0.18518500	2.99419500
C	-0.33378400	0.76626200	2.32267600
C	0.20394500	2.06309500	2.07872400
C	0.53043300	3.27430100	0.01479600
C	0.54343700	3.04378800	-1.42632800
C	1.57627200	1.20790800	-3.38246200
C	2.42858300	2.26397600	-2.85900800
C	1.90056900	3.12684900	-1.86718400
C	2.74505000	3.48047000	-0.72570600
C	1.89221400	3.56914300	0.43758600

C	2.36528700	3.15803100	1.68871600
C	1.49596700	2.39190300	2.54252800
C	2.28117500	1.38388600	3.21278700
C	1.73691300	0.11464200	3.43311900
C	0.09829900	-2.79909100	0.47198400
C	4.39337500	-1.85584500	1.79412500
C	3.57624400	-2.86695700	1.27098100
C	3.59547100	-3.13837500	-0.15972000
C	4.44038100	-2.40457900	-0.99813000
C	5.28534000	-1.36054500	-0.44756800
C	5.29074400	0.27916000	1.39651200
C	4.43318400	0.37217900	2.56169500
C	3.86924800	-0.94854900	2.80318200
C	2.54363900	-1.07104800	3.22388500
C	1.68779600	-2.11724500	2.68475700
C	2.20401500	-2.99556700	1.72187300
C	2.24338900	-3.45996000	-0.58018500
C	1.77711200	-3.01247500	-1.82090900
C	2.65808100	-2.25793800	-2.70179400
C	3.95990500	-1.95581700	-2.29683500
C	4.51096600	-0.63375700	-2.54295700
C	5.33809300	-0.27000000	-1.40136200
C	5.35039700	1.05608700	-0.95305400
C	5.33585800	1.33427000	0.47771000
C	3.65571900	1.51648800	2.76877600
C	3.70691100	2.61673800	1.81732700
C	4.52558600	2.51690500	0.68892600
C	4.04061200	2.96607600	-0.61049400
C	4.57215200	2.07642400	-1.62580800
C	3.75041100	1.72061400	-2.71129700
C	3.73703300	0.33624000	-3.18274300
C	2.38803000	0.02227200	-3.60793000
C	1.85562900	-1.25080900	-3.37541500
C	1.38436200	-3.35025500	0.58761200
C	0.44160500	-2.47538900	-1.95922800
C	5.27559900	-1.09996000	0.93094800
C	-4.39925000	3.79749300	-1.02340700
C	-3.10984200	3.34213800	-0.74876300
C	-5.28230800	2.41888400	0.71525200
C	-5.51528400	3.30099400	-0.33935000
C	-3.80949600	1.18368700	2.24223800
C	-1.53614000	0.47344100	1.43955800
O	-2.59369300	0.59797900	2.43312700
O	-4.63718400	1.04936200	3.11957700

C	-6.92748500	3.61171900	-0.76207000
H	-7.52337900	4.01970000	0.06530600
H	-6.95490800	4.33025400	-1.59034800
H	-7.39389700	2.66499600	-1.07601500
H	-6.10813700	1.99625800	1.27498800
H	-4.54540100	4.50910900	-1.83492700
H	-2.28201700	3.68570900	-1.36047900
C	-4.38119900	-3.00654200	-0.47686500
C	-4.78233000	-4.22596900	-1.02700000
C	-4.20708600	-5.42265400	-0.59716300
C	-3.23947900	-5.39547400	0.40964700
C	-2.84279500	-4.17873600	0.96607100
C	-3.39015300	-2.96651900	0.51739700
H	-4.89254500	-2.09150500	-0.78083600
H	-5.56174600	-4.22977100	-1.78515000
H	-4.52027600	-6.37132700	-1.02989400
H	-2.79585100	-6.32239400	0.76879100
H	-2.10219800	-4.17159000	1.76121000
C	-3.02572500	-1.63166400	1.13957600
H	-3.16796100	-1.67804700	2.22278400
H	-3.74426900	-0.90058800	0.75712300
Br	-7.08426500	-0.15530400	-0.88956100

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	x	y	z
C	-0.66090700	1.17416000	-0.86620500
C	0.34307300	1.43585300	0.29902200
C	0.69493300	2.93156700	0.36657700
C	1.79735400	3.45295600	-0.33412700
C	-0.36747600	0.90620000	1.54823200
C	0.26015000	-0.00868200	2.49492900
C	1.37412200	-0.74811200	2.08199100
C	2.00907600	-0.56509300	0.82239900
C	-1.74038700	0.84078700	1.70061000
C	-2.04198600	-0.13969200	2.73305400
C	-0.78449400	-0.66424700	3.23367900
C	-0.69232300	-2.01321300	3.61479000
C	1.49279000	-2.15442500	2.48687800
C	2.40859100	-1.85263400	0.36031200
C	2.34278800	-2.24359100	-0.99336000
C	1.68225900	-1.31683600	-1.90648900
C	1.23075500	-0.07630500	-1.47211500
C	-0.03294500	0.41524200	-1.91269700

C	-2.03411000	1.13413200	-0.72700000
C	-2.76373700	1.21695700	0.63498400
C	-3.15614000	-0.96726500	2.65409300
C	-4.03097800	-0.87258200	1.46749000
C	-3.76584300	0.05183400	0.47569100
C	-3.87243400	-0.33918100	-0.89457100
C	-2.80416000	0.31160300	-1.63141700
C	-2.21675300	-0.35867000	-2.70784200
C	-0.78898000	-0.29656900	-2.86381300
C	-0.32359000	-1.58026400	-3.32501300
C	0.88732400	-2.08686400	-2.84122200
C	2.13104400	-2.84606200	1.39847000
C	-0.38008800	-5.31207700	-1.57647900
C	0.45579000	-5.38230000	-0.45228200
C	-0.12332900	-5.55317100	0.87150700
C	-1.50871900	-5.61711200	1.02933100
C	-2.37811500	-5.52501700	-0.13247500
C	-2.42962900	-4.45080500	-2.35605100
C	-1.36269000	-3.80716100	-3.09847400
C	-0.09598000	-4.33257500	-2.60978100
C	1.00705000	-3.48261100	-2.48791400
C	1.88715800	-3.56803600	-1.32330000
C	1.61927400	-4.52941000	-0.33208500
C	0.67797600	-4.78702400	1.81297700
C	0.06216300	-4.11721800	2.87265500
C	-1.38327000	-4.17864700	3.03318200
C	-2.15078100	-4.91768500	2.13283800
C	-3.41338500	-4.38352900	1.64411600
C	-3.55168400	-4.76128000	0.24476900
C	-4.14738600	-3.88448200	-0.66737900
C	-3.56829600	-3.72155300	-1.99198900
C	-1.47184800	-2.45777100	-3.45165900
C	-2.65063300	-1.69924200	-3.06618900
C	-3.67834500	-2.32175700	-2.35591200
C	-4.31536100	-1.62200600	-1.25236300
C	-4.60601000	-2.58260000	-0.21628300
C	-4.45689600	-2.21058200	1.12594400
C	-3.84905000	-3.12900700	2.07337700
C	-3.06162600	-2.35709300	3.02505300
C	-1.83959500	-2.87513200	3.49382600
C	1.74361000	-4.14413100	1.06248700
C	0.48201400	-2.77220200	3.22126400
C	-1.82003500	-5.36899200	-1.40721200
C	0.02042800	5.22520800	0.86289700

C	-0.14584800	3.84862800	1.00445000
C	1.96513200	4.84008800	-0.47422300
C	1.06879500	5.74641800	0.08640900
C	2.90413100	2.58958400	-0.78773400
C	1.63398700	0.53321000	-0.13443800
O	2.87814300	1.30304500	-0.37561900
O	3.89359800	2.99358300	-1.37971100
C	1.20967600	7.23841800	-0.09496600
H	1.78215700	7.47623300	-0.99945500
H	0.21549600	7.70347900	-0.14724800
H	1.73626200	7.69173200	0.75723500
H	2.83272600	5.18548900	-1.02898200
H	-0.70505500	5.91567800	1.29287500
H	-0.95729100	3.47823600	1.61645500
C	-3.96388100	4.61788100	-0.34943700
C	-4.68136800	5.37127500	-1.27998000
C	-5.75085300	4.79533300	-1.96535500
C	-6.10908900	3.47102800	-1.69494400
C	-5.40052600	2.72701800	-0.75034800
C	-4.30389600	3.28615300	-0.07315000
H	-3.15817200	5.12431800	0.17823400
H	-4.38362300	6.40811700	-1.41738200
H	-6.31342000	5.37397500	-2.69597100
H	-6.95089700	3.01518100	-2.21351700
H	-5.70935000	1.70799500	-0.53565200
C	-3.53113700	2.54737200	1.00503000
H	-4.20393100	2.27431600	1.82941900
H	-2.81121500	3.24795700	1.42644800
Br	-2.47727800	7.92198700	0.52580500
C	7.73196300	1.46183300	0.80020700
C	8.11969200	1.71890000	2.11375400
C	7.31744100	1.30079300	3.17888100
C	6.12623500	0.62413100	2.91712800
C	5.74017000	0.36004300	1.60134300
C	6.53845700	0.77894600	0.52854200
H	8.36284100	1.77289900	-0.02761100
H	9.05021800	2.24850300	2.30663500
H	7.61915100	1.50335100	4.20408000
H	5.48940600	0.29793100	3.73548400
H	4.79983100	-0.14738500	1.40433300
C	6.04073500	0.55451000	-0.87104200
H	5.28227900	-0.22365100	-0.91999000
H	5.64798000	1.46039800	-1.33385100
Br	7.48880400	-0.06602000	-2.11734900

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	x	y	z
C	0.53670800	0.49296300	-2.17277800
C	1.27925600	-0.59580800	-1.33568500
C	2.77442000	-0.78438000	-1.64867900
C	3.28318500	-1.98188200	-2.17617300
C	1.17002900	-0.14753100	0.11758100
C	0.65627300	-0.96529000	1.17725700
C	-0.01318600	-2.15563900	0.95629400
C	-0.08563000	-2.85287100	-0.40961900
C	1.01673500	1.19212000	0.49696400
C	0.46357600	1.24550500	1.85668700
C	0.25620300	-0.10852300	2.28844700
C	-0.83894500	-0.43561000	3.09175400
C	-1.16488700	-2.45380800	1.74341300
C	-1.60809000	-3.14512200	-0.44808900
C	-2.43963100	-2.87634200	-1.51911600
C	-1.96791200	-2.00262600	-2.60933800
C	-0.72440100	-1.42729000	-2.53182900
C	-0.50855000	-0.08473200	-2.95711300
C	0.38866800	1.82066900	-1.77540300
C	0.70711400	2.24690400	-0.41513000
C	-0.41814800	2.25384200	2.23396900
C	-0.80624800	3.28172800	1.27902600
C	-0.26704900	3.22319900	-0.02961800
C	-1.15334700	3.47825100	-1.16471300
C	-0.74512200	2.60567000	-2.24145000
C	-1.70311600	2.05410600	-3.09935500
C	-1.57987100	0.67155500	-3.47905700
C	-2.89869600	0.08798800	-3.52425200
C	-3.08852100	-1.22890800	-3.09382700
C	-2.16196200	-3.05572300	0.87404300
C	-5.72510900	-0.56056200	-0.59883900
C	-5.34474000	-1.53374200	0.33447900
C	-5.05891900	-1.14148200	1.70664200
C	-5.18165800	0.19730800	2.09052700
C	-5.57710100	1.20007000	1.11781400
C	-5.38296800	1.65571900	-1.30016700
C	-4.96957900	0.78299400	-2.38155100
C	-5.17327000	-0.59107400	-1.94458700
C	-4.24404300	-1.57427400	-2.29022200
C	-3.84315500	-2.58826400	-1.32623000

C	-4.38889200	-2.55982700	-0.03587200
C	-3.94653200	-1.94307100	2.18619300
C	-2.98228700	-1.36571400	3.01763400
C	-3.11200200	0.02593200	3.42758000
C	-4.18551700	0.79257200	2.96961000
C	-3.96929500	2.16225000	2.53463400
C	-4.83705900	2.41593900	1.39387500
C	-4.37573500	3.21275500	0.33955700
C	-4.66382700	2.82735100	-1.03619600
C	-3.85658500	1.11436500	-3.16135700
C	-3.11270800	2.33624300	-2.89242300
C	-3.50778600	3.16763600	-1.84102400
C	-2.50790800	3.76061900	-0.96161800
C	-3.05600900	3.80956700	0.38074000
C	-2.20643200	3.54381400	1.46994000
C	-2.68616200	2.71136500	2.57238700
C	-1.57296300	1.91893800	3.05270100
C	-1.77816600	0.60044000	3.47462100
C	-3.52564300	-2.80586900	1.09430000
C	-1.57586800	-1.64369500	2.82124100
C	-5.86027400	0.82526000	-0.20395200
C	5.07004300	-0.06844400	-1.29719200
C	3.69961900	0.18810200	-1.25479900
C	4.65639400	-2.25654300	-2.16144000
C	5.57167000	-1.31307400	-1.69501600
C	2.40014700	-2.97652400	-2.80386700
C	0.41388100	-1.93868500	-1.66404400
O	1.05691900	-2.82575600	-2.62199500
O	2.76586800	-3.87732600	-3.52956500
C	7.02387600	-1.68467900	-1.54507200
H	7.45984800	-2.02874600	-2.49248500
H	7.62293300	-0.84230800	-1.17852900
H	7.07877300	-2.51844500	-0.82860100
H	4.98662500	-3.24158800	-2.46855900
H	5.76068300	0.69764000	-0.94770700
H	3.34764500	1.13247800	-0.85302800
C	1.79165500	-5.29048400	1.62083600
C	1.73926800	-6.19022100	2.68777800
C	0.57825400	-6.92066000	2.94510300
C	-0.52966500	-6.76360100	2.10938500
C	-0.47702300	-5.87092000	1.03808200
C	0.67378100	-5.10602300	0.79085500
H	2.73202500	-4.78245300	1.39804400
H	2.62371600	-6.32478200	3.30583100

H	0.54021200	-7.61969100	3.77886900
H	-1.43521700	-7.34155400	2.28511700
H	-1.33851700	-5.77229600	0.38324200
C	0.78929300	-4.17385300	-0.40067500
H	0.56105000	-4.72101500	-1.31952900
H	1.83940900	-3.87395000	-0.46452100
Br	5.42477800	-4.50992900	0.39190100
C	3.32230900	3.93975500	2.02056000
C	3.88534600	3.54045500	3.23384900
C	5.25119400	3.70735000	3.46113900
C	6.05683400	4.27537500	2.46917400
C	5.49666200	4.66729600	1.25649700
C	4.12411600	4.50033200	1.01848000
H	2.26042500	3.79820600	1.84419700
H	3.25340700	3.08522500	3.99114700
H	5.69083700	3.38671600	4.40228400
H	7.12344300	4.40129600	2.63892300
H	6.12046800	5.11104600	0.48388200
C	3.52782100	4.86633600	-0.30047700
H	4.13642700	4.55327300	-1.14761600
H	2.50522700	4.51162500	-0.41837700
Br	3.41097800	6.86965300	-0.54398400

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	x	y	z
C	-1.45564300	0.80614500	-0.18131900
C	-1.17758500	-0.25777100	0.88488700
C	-0.55038100	0.00838100	2.08864200
C	0.11858200	1.28532100	2.31823400
C	-1.00551000	0.06668200	-1.44438900
C	-0.91337400	-1.33830100	-1.16750200
C	-1.02214900	-1.53385200	0.25873700
C	-0.28284100	-2.56623100	0.89080200
C	0.25457200	-1.02469600	2.73692000
C	1.32332200	1.00371900	3.09620600
C	2.49805200	1.73476000	2.84856600
C	2.52016600	2.74274700	1.83207000
C	1.35237100	2.96352200	1.05416700
C	1.45943500	3.15783900	-0.37027600
C	0.30851500	2.57975500	-1.00389600
C	0.44903900	1.91823200	-2.20448700
C	-0.22597700	0.63079400	-2.42874500
C	-0.07130900	-2.16442900	-1.93840100

C	0.74319600	-1.58021500	-2.96191300
C	0.68079200	-0.19826900	-3.21318100
C	1.87715800	0.55149100	-3.49144600
C	1.75143800	1.83442400	-2.85386600
C	2.86697600	2.44688700	-2.25113400
C	2.72241500	3.12893000	-1.00428000
C	3.92030400	2.85170400	-0.20870500
C	3.81253800	2.66099900	1.16891700
C	1.38278900	-0.40501300	3.38267100
C	5.53527300	-0.59775900	1.32865100
C	4.74547500	-1.16313200	2.33322200
C	4.07550900	-2.43040100	2.10866900
C	4.21728200	-3.09264700	0.88648600
C	5.03670200	-2.50457700	-0.16045200
C	5.70495300	-0.27192000	-0.98883200
C	5.59216800	1.02795300	-0.36132900
C	5.48184900	0.83053200	1.06081500
C	4.61066500	1.63582700	1.82729700
C	3.79151900	1.05212000	2.85988700
C	3.84701400	-0.32775000	3.12458000
C	2.77339400	-2.36117700	2.76509000
C	1.66662600	-2.97376100	2.14676100
C	1.81431500	-3.66166900	0.88935200
C	3.07381900	-3.73023300	0.25233000
C	3.18078800	-3.53854800	-1.16996400
C	4.38263600	-2.77333000	-1.43197300
C	4.40662700	-1.79609300	-2.43635500
C	5.07412400	-0.53426500	-2.21350500
C	4.82036600	2.03577100	-0.99630300
C	4.16037500	1.76245600	-2.25113300
C	4.27663900	0.50529900	-2.86389000
C	3.14161600	-0.11411900	-3.50354200
C	3.20384900	-1.52584400	-3.22431400
C	2.03609700	-2.26223500	-2.96284600
C	2.01580900	-3.27702100	-1.93754600
C	0.72745200	-3.19908900	-1.27977800
C	0.62225200	-3.38639000	0.09838600
C	2.64600900	-1.07490200	3.39829600
C	0.37638800	-2.28798000	2.13641300
C	5.68099000	-1.28400500	0.05572500
C	-2.19823700	5.76972600	0.50182600
C	-1.31922400	4.70856900	0.33956100
C	-1.77930300	3.38674900	0.18436700
C	-3.16460200	3.19694600	0.18610800

C	-4.05117200	4.27598300	0.35885000
C	-3.59046000	5.57418100	0.52324600
C	-0.76271400	2.23094800	0.06551900
C	-3.76569000	1.86534100	-0.03753500
C	0.14432600	2.25380800	1.33012200
O	-2.95462400	0.84607500	-0.30111800
O	-4.97754600	1.67789900	-0.03119800
C	-4.53830500	6.73534600	0.71576800
H	-5.58183200	6.40847000	0.65673500
H	-4.39507900	7.21633300	1.69303000
H	-4.38749900	7.51158000	-0.04643900
H	-5.11387200	4.05399000	0.35139500
H	-1.79566500	6.77526800	0.61700800
H	-0.25278700	4.89813600	0.33920700
C	-7.08483000	-0.80263200	0.26510600
H	-7.74575600	-0.43353200	1.04945500
H	-6.41394600	-0.01356100	-0.07129000
C	-6.37126200	-2.05993300	0.64373500
C	-7.06870100	-3.16184600	1.16335200
C	-4.97530200	-2.12231100	0.53970200
C	-6.38312900	-4.30200600	1.57263100
H	-8.15423600	-3.12246700	1.22599700
C	-4.28585800	-3.26381100	0.95924100
H	-4.42127800	-1.27351200	0.14816700
C	-4.98823300	-4.35350900	1.47335000
H	-6.93407100	-5.15133800	1.97169800
H	-3.20179000	-3.28658400	0.88720600
H	-4.45090100	-5.24136000	1.79817600
Br	-8.36944500	-1.08658700	-1.27532500

P4'

-2 1

	x	y	z
C	1.23421300	-0.61212200	-0.79617400
C	1.02234800	0.91982300	-0.59163100
C	2.22423800	1.82907000	-1.01219800
C	3.59399800	1.61406700	-0.70288600
C	-0.21862900	1.30084600	-1.38617600
C	-1.24963100	2.06172100	-0.92740100
C	-1.36449300	2.57377500	0.49399000
C	-0.48434400	1.66435700	1.38004300
C	-0.65496700	0.57704800	-2.57779400
C	-2.03005900	0.93256500	-2.83722900
C	-2.41836700	1.88534200	-1.81049200

C	-3.69219700	1.80660400	-1.26151200
C	-2.77286300	2.20965500	1.02516700
C	-1.26753400	1.16238800	2.47947800
C	-0.93733600	-0.03432100	3.12471000
C	0.16164300	-0.81189400	2.61832800
C	0.86369100	-0.34801800	1.50250800
C	1.26503500	-1.28319100	0.46903000
C	0.76200200	-1.30816800	-1.89967900
C	-0.17479700	-0.68818700	-2.85918900
C	-2.92057600	-0.03838100	-3.29293300
C	-2.44838000	-1.38797700	-3.53559400
C	-1.09798400	-1.70319000	-3.31540400
C	-0.74682900	-2.94967200	-2.65835700
C	0.39679400	-2.70272300	-1.79404600
C	0.50339300	-3.37241400	-0.56973800
C	0.95138100	-2.64466200	0.58975700
C	0.19752800	-3.11645500	1.73967700
C	-0.18817900	-2.21732800	2.73289200
C	-2.66501500	1.49951300	2.26219100
C	-3.80635300	-2.94586300	2.65516500
C	-4.25273100	-1.64201200	2.89009100
C	-5.17859400	-1.01145800	1.96055000
C	-5.61785300	-1.70851200	0.83295900
C	-5.15291500	-3.06142300	0.58771500
C	-3.15425000	-4.45620000	0.97625200
C	-2.00785700	-4.21857000	1.83605600
C	-2.41105600	-3.28640700	2.87430100
C	-1.51716200	-2.30314000	3.31242600
C	-1.98213000	-0.94888000	3.55606800
C	-3.32347500	-0.62465500	3.34635700
C	-4.81627300	0.39109300	1.85436200
C	-4.89338600	1.03578500	0.61308500
C	-5.36018500	0.31388600	-0.55628800
C	-5.72071300	-1.03232100	-0.45190700
C	-5.33293400	-1.96898600	-1.49019800
C	-4.97119600	-3.21988900	-0.84563000
C	-3.90257700	-3.97844300	-1.33191700
C	-2.97486600	-4.60099100	-0.40407300
C	-0.72578800	-4.13667200	1.28354300
C	-0.53985200	-4.29236400	-0.15165700
C	-1.64259000	-4.51957800	-0.97690200
C	-1.74653100	-3.84016600	-2.25876700
C	-3.14438600	-3.51008200	-2.48153500
C	-3.48390100	-2.30438100	-3.10012500

C	-4.60167800	-1.51370100	-2.59418200
C	-4.25736500	-0.11536800	-2.72491300
C	-4.61075100	0.78651300	-1.70867400
C	-3.67796400	0.63032300	2.70470900
C	-3.85162700	1.94758400	0.19454800
C	-4.26508600	-3.66983100	1.48166000
C	2.91889900	3.77550100	-2.33590000
C	1.93063000	2.92501000	-1.84241700
C	4.57460500	2.46540100	-1.23821400
C	4.26538300	3.55938000	-2.04759500
C	4.11744500	0.58894700	0.26426500
C	0.58368700	0.92875900	0.90529000
O	5.31522200	0.12506100	-0.12025000
O	3.55702300	0.27806800	1.30188500
C	5.34949300	4.47591800	-2.56422800
H	5.53765800	5.30317800	-1.86603400
H	6.29637000	3.94120700	-2.69349500
H	5.07067500	4.92003700	-3.52663100
H	5.61136400	2.25599200	-0.99687300
H	2.61607200	4.60835600	-2.96705700
H	0.90828000	3.14120100	-2.13811200
C	6.10752600	-0.66804600	0.82640300
C	6.18773900	-2.10680000	0.37515900
C	7.43443300	-2.66759200	0.06668400
C	5.03306400	-2.89704700	0.28048400
C	7.51386200	-4.00479400	-0.33303100
H	8.32993500	-2.04727200	0.15709200
C	5.11702300	-4.22746200	-0.12815000
H	4.06678600	-2.46727900	0.53191100
C	6.36128300	-4.78556600	-0.43648900
H	8.48575000	-4.43378600	-0.56897400
H	4.21206600	-4.82686300	-0.20277800
H	6.42868000	-5.82496700	-0.75372400
H	5.63139900	-0.58106300	1.80558800
H	7.10282200	-0.20615000	0.83961900
Br	9.81057600	0.09643300	0.83038300
C	-0.26138700	4.72132900	2.92476900
C	-0.48254700	5.30989900	4.17091100
C	-1.70475600	5.92453300	4.44954300
C	-2.70145900	5.94559600	3.47184700
C	-2.47537700	5.35571700	2.22766300
C	-1.25329500	4.73319400	1.93343800
H	0.69376500	4.24642800	2.71411200
H	0.30261700	5.28913400	4.92311600

H	-1.87814800	6.38501800	5.41966300
H	-3.65656600	6.42465800	3.67621700
H	-3.25209100	5.37765600	1.46723300
C	-1.01746500	4.10356300	0.58033300
H	0.03529000	4.20534800	0.29536700
H	-1.59168400	4.60871400	-0.20311000
Br	-1.66892100	4.40764100	-2.98767600

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	x	y	z
C	-0.26246400	1.29878500	-1.51669900
C	0.95966300	1.01820500	-0.60984700
C	2.12283300	1.99442300	-0.98553900
C	3.49564800	1.80370200	-0.69486900
C	0.45080200	1.07138700	0.83600800
C	0.68597900	-0.02045900	1.79369600
C	1.15250400	-1.25074300	1.37649000
C	1.40019800	-1.48403200	-0.05940600
C	-0.68220900	1.74290000	1.22190000
C	-1.20068700	1.13907100	2.45763100
C	-0.33051300	0.04447100	2.81717200
C	-0.85355700	-1.12149200	3.38600400
C	0.61266400	-2.46522900	1.94332200
C	0.99824200	-2.84342800	-0.34706200
C	0.39629000	-3.16401200	-1.56820400
C	0.15405200	-2.11437400	-2.52692700
C	0.52489400	-0.79770400	-2.21058200
C	-0.36965100	0.29733200	-2.53451200
C	-1.36911600	2.01673300	-1.13780200
C	-1.57584100	2.55449500	0.29659200
C	-2.56020500	1.04880100	2.69475800
C	-3.51170800	1.55218000	1.68390100
C	-3.04955000	2.13904200	0.52005800
C	-3.67007600	1.79742200	-0.72781900
C	-2.63969200	1.72136300	-1.74533800
C	-2.75389000	0.77958900	-2.77384500
C	-1.58110200	0.05235000	-3.19045200
C	-1.97252500	-1.31075400	-3.48830900
C	-1.12475900	-2.37543900	-3.16864600
C	0.51232900	-3.44925200	0.88108400
C	-3.53614900	-4.29668000	-1.13886200
C	-2.62945400	-4.76653400	-0.18210600
C	-2.87190400	-4.52794400	1.22966600

C	-4.01006500	-3.82482000	1.63403100
C	-4.94902700	-3.33189100	0.64216700
C	-4.96688700	-2.51491200	-1.68934300
C	-3.93283300	-2.59607300	-2.70775800
C	-3.05155300	-3.70060000	-2.37065200
C	-1.67474400	-3.58761400	-2.59665800
C	-0.73141200	-4.07838400	-1.60148200
C	-1.20160400	-4.65363200	-0.41924200
C	-1.59208800	-4.27018200	1.87110000
C	-1.49857300	-3.32361000	2.89300900
C	-2.68458500	-2.58952500	3.31401300
C	-3.91151900	-2.83411500	2.69473500
C	-4.78686300	-1.72549100	2.35018600
C	-5.43199000	-2.03622300	1.08365700
C	-5.66887100	-1.02267800	0.15232700
C	-5.42902800	-1.26464500	-1.26396200
C	-3.40250700	-1.42459900	-3.25477700
C	-3.88184600	-0.12673100	-2.80781600
C	-4.88536000	-0.04911300	-1.83583200
C	-4.78157400	0.93837900	-0.77698300
C	-5.27030100	0.34266900	0.44365500
C	-4.63039100	0.63829400	1.65300000
C	-4.39097100	-0.41517200	2.62549800
C	-3.11619000	-0.15699400	3.27324200
C	-2.27977800	-1.22766800	3.61734600
C	-0.56055800	-4.34132100	0.84867600
C	-0.37033400	-2.41106400	2.94042500
C	-4.71918800	-3.56524400	-0.71894400
C	2.74452700	4.03548100	-2.19041200
C	1.78607200	3.12669600	-1.74895300
C	4.44966300	2.71419200	-1.18052600
C	4.10107000	3.84253100	-1.92189900
C	4.03574600	0.73133000	0.20339100
C	1.21029100	-0.47572400	-0.98804800
O	5.21772000	0.27084800	-0.23977500
O	3.49323000	0.37439500	1.23388000
C	5.15070200	4.80779400	-2.42126000
H	4.93120000	5.83535400	-2.10474700
H	6.14499700	4.54428800	-2.04703100
H	5.19693200	4.81387600	-3.51828100
H	5.49315800	2.52366000	-0.95198900
H	2.40620800	4.89409800	-2.76670400
H	0.75882800	3.32904000	-2.04212600
C	5.99292600	-0.62848900	0.61468400

C	6.28371400	-1.91374000	-0.12471600
C	7.59107000	-2.41877100	-0.14026000
C	5.26214900	-2.63094300	-0.76274000
C	7.85980600	-3.63135800	-0.78137200
H	8.38494400	-1.84832400	0.34895200
C	5.53741800	-3.83648500	-1.40763700
H	4.24723600	-2.24176300	-0.75850000
C	6.84017400	-4.34271400	-1.41615300
H	8.87828500	-4.01461700	-0.78912200
H	4.73397600	-4.38071400	-1.89985900
H	7.05635900	-5.28467100	-1.91756100
H	5.40926500	-0.80880800	1.52080300
H	6.92342600	-0.10766300	0.87550600
Br	9.55843200	0.15375600	1.65728700
C	-0.78276200	4.73824300	2.81377000
C	-1.12577200	5.30273600	4.04309400
C	-2.39820100	5.84422200	4.23585500
C	-3.32118900	5.81722800	3.18853900
C	-2.97310800	5.25107300	1.96139600
C	-1.70034800	4.69909200	1.75317600
H	0.21162800	4.32311300	2.66908300
H	-0.39613400	5.32132400	4.84944700
H	-2.66657500	6.28673300	5.19268500
H	-4.31365400	6.24164900	3.32459300
H	-3.69150200	5.24134300	1.14536900
C	-1.33027200	4.10254700	0.41496500
H	-0.26603600	4.26275800	0.21350900
H	-1.86321200	4.58671000	-0.41057400
Br	-1.59304400	4.61549200	-3.05460400

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	x	y	z
C	-0.15715900	1.05630000	-1.89334500
C	0.88675100	1.08075000	-0.74263800
C	2.18730900	1.71611900	-1.33411900
C	3.50689800	1.27517500	-1.07941300
C	0.31730300	1.82969600	0.59691800
C	0.09738200	0.87277100	1.78648700
C	0.54916200	-0.42729100	1.85832600
C	1.03338100	-1.10733300	0.63910200
C	-1.12014600	2.35967500	0.44741600
C	-1.86409900	2.13685400	1.64356900
C	-1.11822700	1.21433700	2.47808600

C	-1.79999800	0.29299600	3.28250200
C	-0.16016700	-1.40979100	2.64739400
C	0.62275000	-2.49024500	0.71311000
C	0.24525700	-3.18772000	-0.43980800
C	0.23915200	-2.49472600	-1.70346100
C	0.61086800	-1.14443300	-1.74312500
C	-0.13569300	-0.21226000	-2.56393200
C	-1.29839900	1.82422100	-1.94955100
C	-1.79106300	2.52944200	-0.74795900
C	-3.26883800	2.13294700	1.66443600
C	-3.96983800	2.27464400	0.41416700
C	-3.23839500	2.44945700	-0.76757100
C	-3.64251000	1.73989400	-1.96348700
C	-2.44731300	1.35995000	-2.69301300
C	-2.41346100	0.14613000	-3.38838500
C	-1.22167100	-0.66325700	-3.32665400
C	-1.62300200	-2.05814200	-3.26062400
C	-0.90777300	-2.95686600	-2.46874600
C	-0.11359200	-2.68079800	1.94842300
C	-3.74665300	-4.17222600	-0.44293900
C	-3.05818200	-4.30760900	0.76645600
C	-3.54833500	-3.63982200	1.96400200
C	-4.70636300	-2.85871400	1.90386200
C	-5.41765900	-2.71357100	0.64382700
C	-4.95329200	-2.66165300	-1.78121200
C	-3.75720600	-3.04937000	-2.50841000
C	-3.01125800	-3.98361600	-1.68093100
C	-1.61399100	-3.93757500	-1.66319200
C	-0.89874500	-4.07988400	-0.40497400
C	-1.60898000	-4.25937800	0.78540500
C	-2.40116700	-3.17761700	2.72145300
C	-2.45198200	-1.95359600	3.39418000
C	-3.65832900	-1.14036000	3.33194400
C	-4.76693500	-1.58879500	2.60463400
C	-5.51024000	-0.65469900	1.77490100
C	-5.91352900	-1.34984200	0.56466400
C	-5.91143000	-0.67737200	-0.66043000
C	-5.42158600	-1.34661800	-1.85766900
C	-3.07600100	-2.10528700	-3.28250300
C	-3.56438000	-0.73808900	-3.36338900
C	-4.71498000	-0.36728600	-2.66078700
C	-4.76430600	0.90587500	-1.96062000
C	-5.50916100	0.71446500	-0.72816300
C	-5.11674100	1.38496600	0.43424100

C	-5.11859300	0.68544200	1.70904200
C	-3.96668600	1.14679500	2.46696600
C	-3.25576400	0.25111900	3.26906900
C	-1.20144500	-3.55415800	1.99064300
C	-1.30918700	-1.05924800	3.36745600
C	-4.94810500	-3.35614100	-0.50441800
C	3.11098500	3.30637100	-2.94700700
C	2.02896200	2.75221700	-2.26926700
C	4.58092800	1.81163300	-1.81077500
C	4.40844800	2.82367900	-2.75458900
C	3.90508300	0.37842600	0.05780500
C	1.05829900	-0.44697400	-0.56770300
O	4.87392900	-0.47074300	-0.30747400
O	3.45099200	0.48023400	1.18640500
C	5.58130900	3.37625700	-3.53002900
H	5.51499900	4.46630600	-3.63045700
H	6.53120000	3.13507700	-3.04242600
H	5.61902500	2.96008700	-4.54632000
H	5.57680700	1.43301400	-1.60293100
H	2.92755600	4.12869800	-3.63555200
H	1.04704900	3.18765300	-2.43801500
C	5.58099900	-1.23609100	0.72408600
C	5.64991800	-2.68454400	0.30377100
C	6.89641400	-3.30124100	0.13251700
C	4.47983100	-3.43062700	0.10295500
C	6.95974200	-4.64985300	-0.23071700
H	7.80409400	-2.71177600	0.28748200
C	4.54801700	-4.77292300	-0.26750900
H	3.51053100	-2.95647100	0.23534100
C	5.79254600	-5.38780100	-0.43404600
H	7.93199200	-5.12098100	-0.36117300
H	3.63080200	-5.33715700	-0.42322500
H	5.84821200	-6.43654000	-0.72152800
H	5.03501400	-1.10807300	1.66166400
H	6.58712400	-0.80328500	0.80747400
Br	9.31323300	-0.59606700	0.84704400
C	1.27920400	3.59455500	3.44847700
C	0.90360900	4.40255700	4.52348400
C	0.08626900	5.51399200	4.30965800
C	-0.34802800	5.81172400	3.01562000
C	0.02689800	5.00492000	1.94014400
C	0.84395200	3.88158400	2.14740400
H	1.92313500	2.73376800	3.61435300
H	1.25376000	4.16508300	5.52582800

H	-0.20657100	6.14640100	5.14552900
H	-0.98071600	6.67871500	2.83864300
H	-0.30834500	5.23810000	0.92924800
C	1.27302500	3.02852200	0.97434900
H	2.26210400	2.60402600	1.16203500
H	1.32726700	3.66921400	0.09112700
Br	-0.91137100	5.06195600	-1.97914700

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C	0.07437700	1.30211100	-1.88584500
C	1.41655600	1.12532600	-1.09473200
C	2.50533200	2.20889600	-1.25371200
C	3.62796100	2.01895800	-2.07549900
C	0.97965400	1.10336400	0.36134000
C	1.40866100	0.08126800	1.31526000
C	1.92854200	-1.11659300	0.89920500
C	2.41801200	-1.41757800	-0.51874800
C	-0.11404000	1.76016200	0.86672700
C	-0.44558200	1.16936200	2.16933500
C	0.51971700	0.14023200	2.45393300
C	0.14270900	-1.02233500	3.13066600
C	1.51525800	-2.32520700	1.57024400
C	1.73298000	-2.79484200	-0.70786100
C	0.98703600	-3.15930900	-1.80829300
C	0.54479200	-2.13244500	-2.76705200
C	0.83046500	-0.81074200	-2.52497800
C	-0.11232200	0.21418800	-2.80225200
C	-1.05767600	1.92392800	-1.38837300
C	-1.15751000	2.49622200	0.03819400
C	-1.76027200	1.01379900	2.57057300
C	-2.84811700	1.42359400	1.66202200
C	-2.56199900	1.99320900	0.43972700
C	-3.31163700	1.61069700	-0.72371500
C	-2.36958100	1.52580500	-1.83400900
C	-2.54038000	0.54585000	-2.81533700
C	-1.37742400	-0.12889400	-3.31615400
C	-1.70937300	-1.51393000	-3.53710100
C	-0.75924300	-2.50240600	-3.25584400
C	1.37691200	-3.35931700	0.56794500
C	-2.80479800	-4.51741600	-0.94426100
C	-1.77409400	-4.90550500	-0.08152500
C	-1.87699000	-4.62808300	1.33992200

C	-3.00461900	-3.97270200	1.84377500
C	-4.07415300	-3.57226000	0.94733600
C	-4.39198700	-2.84285000	-1.39463100
C	-3.48020900	-2.89880800	-2.51855700
C	-2.49114100	-3.92597600	-2.23720500
C	-1.15644700	-3.73161900	-2.59999500
C	-0.08195700	-4.12994100	-1.70310300
C	-0.38599900	-4.71819300	-0.47182900
C	-0.55232500	-4.26921400	1.82296000
C	-0.41048100	-3.27693400	2.79236800
C	-1.58298000	-2.59961600	3.32444300
C	-2.85433200	-2.93713800	2.85504000
C	-3.83242100	-1.89805600	2.57749600
C	-4.58737100	-2.29208400	1.39968400
C	-4.98240400	-1.32919700	0.46597300
C	-4.88610100	-1.60862400	-0.95570100
C	-3.09429500	-1.71074300	-3.15568600
C	-3.61353200	-0.43107000	-2.70864500
C	-4.48515000	-0.38002900	-1.61861000
C	-4.34310100	0.65562200	-0.61498400
C	-4.64465100	0.07004400	0.66557200
C	-3.90564800	0.44731800	1.79224100
C	-3.48987000	-0.55416100	2.75853800
C	-2.16988200	-0.19783300	3.24749500
C	-1.23308000	-1.20283400	3.53312100
C	0.36360900	-4.32228800	0.69526200
C	0.65228300	-2.29264000	2.67094200
C	-3.97670200	-3.84358600	-0.42302000
C	3.52164200	4.29896100	-0.51954800
C	2.47081500	3.38361900	-0.49711200
C	4.69425100	2.92296200	-2.06777700
C	4.67494200	4.06437400	-1.26981700
C	3.79734500	0.82076500	-2.90769300
C	1.95129500	-0.32597400	-1.62641200
O	3.01655200	-0.25270700	-2.61458400
O	4.58514300	0.70700500	-3.82318400
C	5.91463700	4.90258900	-1.11325300
H	6.41274800	5.08671800	-2.07302200
H	5.70135700	5.86821600	-0.64020600
H	6.60327000	4.33119800	-0.47379300
H	5.56754100	2.67748700	-2.66091900
H	3.46551500	5.17857400	0.11868400
H	1.64289200	3.56385500	0.17249700
C	5.30861100	-1.87613700	1.58863000

C	5.92413400	-2.70271000	2.53170900
C	5.87905500	-4.09146200	2.39898900
C	5.22888900	-4.65543600	1.29909100
C	4.61657500	-3.83120400	0.35419100
C	4.63035000	-2.43473000	0.49409300
H	5.41460700	-0.79273700	1.65523500
H	6.45485600	-2.25080600	3.36669200
H	6.36001400	-4.73082400	3.13716900
H	5.20232800	-5.73603000	1.17213300
H	4.12440400	-4.27738600	-0.50688900
C	4.00026300	-1.52609800	-0.54416100
H	4.27766100	-1.86826800	-1.54415500
H	4.42197500	-0.52107400	-0.41468700
Br	6.48358600	1.51338500	0.58518800
C	-2.63116000	5.13348100	1.76574500
C	-2.86122600	5.72558300	3.00892900
C	-1.81564600	5.89489100	3.91927900
C	-0.53093900	5.46913300	3.57670400
C	-0.29978300	4.87791800	2.33344400
C	-1.34244400	4.70105700	1.41219100
H	-3.43948600	5.01010700	1.04558100
H	-3.86524000	6.05822400	3.26436300
H	-1.99899900	6.35657700	4.88767300
H	0.29345400	5.59543800	4.27522200
H	0.70567500	4.55147500	2.07752000
C	-1.10541400	4.06951700	0.05571400
H	-0.13633800	4.37981400	-0.34570700
H	-1.88423800	4.40317500	-0.63986500
Br	-4.44623200	4.29271600	-1.49288800

RL6²⁻

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	x	y	z
C	-2.45096600	1.44374900	-0.09460700
C	-1.57438300	1.91404300	-1.26067500
C	-1.25890200	1.13148000	-2.35064900
C	-1.52828000	-0.31111500	-2.33936300
C	-1.62551500	1.94831800	1.09583700
C	-0.68757200	2.93140300	0.64520900
C	-0.65531900	2.91068400	-0.79682900
C	0.55525500	3.14490100	-1.48576800
C	0.00484000	1.32771600	-3.05267000
C	-0.41638600	-0.95669600	-3.03005300
C	0.05596900	-2.20106200	-2.57195600

C	-0.54034200	-2.81952200	-1.43056800
C	-1.58656300	-2.15163700	-0.74729500
C	-1.61725500	-2.13182700	0.69303700
C	-2.14804100	-0.87492500	1.12383000
C	-1.62202000	-0.24669000	2.23567700
C	-1.35345800	1.19245400	2.21853400
C	0.49572900	3.18659000	1.37736200
C	0.78272200	2.39885600	2.54033300
C	-0.11890400	1.40922900	2.96681600
C	0.35762700	0.14471000	3.46335900
C	-0.53950000	-0.87417500	2.98909100
C	-0.05003200	-2.12977800	2.58552000
C	-0.60041900	-2.78247100	1.43833200
C	0.50288900	-3.42438000	0.73251300
C	0.53380600	-3.44498900	-0.66132200
C	0.50053200	0.04983700	-3.49208400
C	3.89920200	-2.00507300	-1.08502300
C	3.62202900	-1.24632900	-2.22882000
C	3.88294000	0.17688000	-2.24301100
C	4.41499700	0.80953400	-1.11284100
C	4.70234300	0.02398900	0.07721100
C	3.85119900	-1.97183200	1.26050500
C	2.94777500	-3.01206500	0.80091800
C	2.97960300	-3.03336100	-0.63752500
C	1.78590200	-3.25356100	-1.37040300
C	1.49538900	-2.46447300	-2.54186900
C	2.38950600	-1.47414200	-2.98162900
C	2.80910800	0.81306500	-3.00465900
C	2.32724000	2.06626200	-2.58638800
C	2.88298700	2.72254800	-1.42946500
C	3.92256100	2.10654600	-0.68844600
C	3.89041800	2.12547700	0.75048500
C	4.36645800	0.84043200	1.23269600
C	3.78770100	0.24071200	2.35632900
C	3.52668300	-1.18449100	2.37036200
C	1.72686000	-3.21113900	1.48872000
C	1.38852500	-2.39395900	2.62680800
C	2.26525200	-1.39200300	3.07828300
C	1.76409800	-0.11259300	3.51192200
C	2.68477800	0.89597700	3.05557000
C	2.22049100	2.13699500	2.58216400
C	2.82281900	2.75897400	1.43045400
C	1.75357300	3.38318800	0.66593500
C	1.78492600	3.36441600	-0.72804200

C	1.90750000	-0.20767400	-3.47258900
C	0.88918900	2.32904000	-2.61536300
C	4.45061800	-1.34990300	0.09079600
C	-6.11662700	-2.04969600	-0.06521600
C	-4.76395300	-1.74542600	-0.11746900
C	-4.30489200	-0.41442200	-0.07429300
C	-5.27696400	0.58627900	0.01022300
C	-6.64633600	0.27107000	0.06900800
C	-7.09210700	-1.04259900	0.03619700
C	-2.78811400	-0.12557800	-0.08031000
C	-4.92272300	2.02538000	-0.00500900
C	-2.10542000	-0.90790000	-1.23680700
O	-3.63932300	2.34953400	-0.14999700
O	-5.76020100	2.91292700	0.06361100
C	-8.56311300	-1.38413700	0.10080000
H	-8.79354600	-2.02036900	0.96619700
H	-9.17574400	-0.47973500	0.18085900
H	-8.89241700	-1.93140800	-0.79310900
H	-7.34374500	1.10079600	0.13474400
H	-6.42452100	-3.09409000	-0.10132200
H	-4.04143400	-2.54953400	-0.18720100

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	x	y	z
C	2.29885300	1.36325100	0.07045300
C	1.59672800	1.87989600	1.23673300
C	1.28683000	1.09946900	2.36106000
C	1.52493100	-0.33662300	2.32048600
C	1.62336600	1.93482800	-1.08541400
C	0.67622600	2.92882600	-0.63649300
C	0.65968300	2.89446000	0.81395600
C	-0.52536900	3.13538300	1.50552400
C	0.02754600	1.29734500	3.05267500
C	0.41888800	-0.99621700	3.02043200
C	-0.06642700	-2.23229600	2.55246700
C	0.51250200	-2.83673000	1.38961200
C	1.53672000	-2.14932600	0.70295900
C	1.55347000	-2.11545100	-0.74454300
C	2.11108100	-0.86740700	-1.16843200
C	1.57650900	-0.22808700	-2.27461700
C	1.33870300	1.20814400	-2.25200700
C	-0.49303100	3.20287300	-1.34252900
C	-0.80423500	2.42105300	-2.52821600

C	0.09562400	1.43947700	-2.96207800
C	-0.40950000	0.17188800	-3.46900300
C	0.48723400	-0.85335100	-3.03015700
C	-0.00772200	-2.10987200	-2.63198700
C	0.54542400	-2.76903100	-1.48610600
C	-0.54914900	-3.42380800	-0.77248300
C	-0.56502200	-3.45710000	0.62136500
C	-0.48804200	0.00735400	3.48761200
C	-3.91906000	-1.99557500	1.09582600
C	-3.62638200	-1.25455600	2.24876000
C	-3.86195800	0.17702500	2.27615900
C	-4.39226700	0.81786400	1.15450800
C	-4.69747400	0.05077900	-0.03991600
C	-3.89279200	-1.94013900	-1.25329200
C	-2.98304600	-2.98390900	-0.81706900
C	-2.99945600	-3.01816700	0.63152400
C	-1.80843000	-3.25410500	1.33724600
C	-1.49994200	-2.47919600	2.52985900
C	-2.38884600	-1.49742400	2.97788100
C	-2.79463000	0.80314300	3.05318800
C	-2.28891600	2.05585200	2.63158500
C	-2.84479100	2.72249500	1.47503800
C	-3.88741800	2.12221700	0.73839000
C	-3.87095100	2.15616300	-0.70054300
C	-4.36622600	0.87334900	-1.18958600
C	-3.80998700	0.28584700	-2.32795500
C	-3.57456600	-1.14570400	-2.36312800
C	-1.77627900	-3.18634900	-1.50582700
C	-1.44128400	-2.35649600	-2.65322400
C	-2.32046200	-1.35434700	-3.07453400
C	-1.80927100	-0.06157100	-3.49723100
C	-2.72558500	0.94736300	-3.04974800
C	-2.23002900	2.17841600	-2.55801800
C	-2.81202200	2.78966000	-1.38397900
C	-1.74295300	3.41403300	-0.62449300
C	-1.75891300	3.38102300	0.77026300
C	-1.88801100	-0.22641800	3.47256200
C	-0.86278200	2.29885000	2.64550600
C	-4.47350100	-1.33333200	-0.07010300
C	6.04314100	-2.11578300	0.02897600
C	4.70949700	-1.73238000	0.05209800
C	4.30628500	-0.38136900	0.03863700
C	5.32570900	0.58724300	0.00103300
C	6.67173100	0.17855700	-0.02821300

C	7.06166300	-1.15475200	-0.01406300
C	2.75931100	-0.12210900	0.04040800
C	5.12193300	2.09657600	0.00445200
C	2.08615900	-0.92333200	1.19815000
O	3.91892200	2.52591200	0.11745600
O	6.11982800	2.83053500	-0.08406500
C	8.51978800	-1.55444700	-0.03616300
H	8.73958600	-2.24756700	-0.86002700
H	9.16632200	-0.67830700	-0.15609300
H	8.81850800	-2.06141100	0.89261200
H	7.40552300	0.97823700	-0.06265900
H	6.29211500	-3.17684000	0.04223500
H	3.95507800	-2.50935200	0.07941400

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	x	y	z
C	-1.50773100	0.50571800	-0.32076300
C	-1.20143900	-0.43027100	0.84335400
C	-0.62768300	0.00327800	2.04190000
C	-0.07958000	1.33511200	2.17122400
C	-0.98631100	-0.29849200	-1.51256600
C	-0.77865300	-1.65957600	-1.09872500
C	-0.91990900	-1.73153000	0.34527200
C	-0.11787000	-2.64594600	1.07415300
C	0.23360500	-0.90506300	2.78865200
C	1.12681500	1.23590200	2.98761400
C	2.24567500	2.03016800	2.70542700
C	2.21931300	2.94864100	1.59012400
C	1.05283900	2.98653000	0.77625900
C	1.19300100	3.05516900	-0.66474400
C	0.10387800	2.34044600	-1.27433100
C	0.33116000	1.59981200	-2.41228200
C	-0.23233200	0.23496000	-2.52978800
C	0.14116800	-2.47323300	-1.76604700
C	0.92293800	-1.92277700	-2.84063700
C	0.74616000	-0.58096900	-3.21839500
C	1.89513300	0.24276000	-3.51785100
C	1.64293100	1.57562600	-3.02202900
C	2.69510400	2.32303100	-2.45620900
C	2.46210100	3.07861300	-1.25992900
C	3.66465300	3.00733600	-0.42390200
C	3.51719500	2.92805100	0.97221300
C	1.30101600	-0.14009300	3.39842900

C	5.48916900	-0.16423900	1.46907900
C	4.72324300	-0.69725800	2.50902600
C	4.16430000	-2.03603300	2.38669000
C	4.39417900	-2.78187900	1.22708600
C	5.18021400	-2.22118400	0.14271500
C	5.69957700	-0.02270100	-0.87282600
C	5.45985200	1.30467500	-0.37685900
C	5.31001700	1.22289600	1.06442200
C	4.37017800	2.01603200	1.73136200
C	3.58098600	1.46647700	2.81458100
C	3.75088200	0.12595200	3.20411200
C	2.85196500	-2.02489300	3.00452800
C	1.81083400	-2.77141000	2.42240100
C	2.04853300	-3.54189800	1.22005300
C	3.31531900	-3.55330400	0.62462700
C	3.45504400	-3.49168100	-0.81691600
C	4.59301600	-2.66300900	-1.11575200
C	4.57310400	-1.77488400	-2.21135900
C	5.12751900	-0.45276700	-2.09180600
C	4.63214200	2.19804700	-1.10750900
C	4.02890600	1.75074700	-2.35438300
C	4.26763400	0.46011600	-2.83523500
C	3.19163600	-0.30643200	-3.43714700
C	3.36949500	-1.68579600	-3.03386700
C	2.26005800	-2.48684200	-2.74183400
C	2.28891800	-3.41295300	-1.62224700
C	0.98905500	-3.39884900	-1.01065100
C	0.85199600	-3.45757400	0.38569500
C	2.59888700	-0.69301900	3.50378700
C	0.48074400	-2.19856600	2.31258600
C	5.71724600	-0.93732800	0.26027000
C	-2.68083800	5.42761200	-0.07917900
C	-1.71573500	4.43275600	-0.17825900
C	-2.05735700	3.07072000	-0.18018300
C	-3.42682000	2.75558400	-0.10215500
C	-4.40411100	3.77477600	0.02659000
C	-4.05045200	5.11118300	0.04281300
C	-0.95002700	1.99572000	-0.19341800
C	-3.87107800	1.38517600	-0.23331400
C	-0.09488200	2.21350900	1.08648600
O	-3.02132400	0.42247000	-0.48889200
O	-5.10903600	1.10692900	-0.15662200
C	-5.08683700	6.20224800	0.17575400
H	-6.09837600	5.78572000	0.22369300

H	-4.92808400	6.80007900	1.08351600
H	-5.05073600	6.89754500	-0.67383400
H	-5.44428200	3.47451400	0.09708500
H	-2.36923900	6.47051900	-0.09093000
H	-0.67230900	4.71553000	-0.24465500
C	-5.81404200	-0.52913300	-0.57492200
H	-6.66633300	-0.08171000	-1.05522300
H	-5.03466300	-0.89365400	-1.22632900
C	-5.97911700	-1.13299900	0.75759000
C	-7.19352300	-0.99794800	1.44876400
C	-4.90525900	-1.78019900	1.38668800
C	-7.33309100	-1.50336400	2.73714100
H	-8.03338400	-0.52570900	0.94753100
C	-5.04639700	-2.28572800	2.67855000
H	-3.95554900	-1.87410400	0.86905900
C	-6.25817000	-2.14869400	3.35784700
H	-8.28283900	-1.40209200	3.25801800
H	-4.20396500	-2.78180300	3.15324600
H	-6.36680000	-2.54348700	4.36577200
Br	-7.32431700	-2.47730700	-1.90485400

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-2 1

	x	y	z
C	0.61513000	1.65489900	-1.37475100
C	1.00096100	2.12706200	0.06110000
C	2.21506800	3.10241000	0.05101300
C	3.55256900	2.78579400	0.35530800
C	-0.23487200	2.78361000	0.69782700
C	-0.74867300	2.38518600	1.96173900
C	-0.27706800	1.25728300	2.66110000
C	0.69815900	0.39993100	1.96832900
C	-1.32340800	3.26770500	-0.07108000
C	-2.53558400	3.27677800	0.75458700
C	-2.17396800	2.72067000	2.03191100
C	-3.06690700	1.90328900	2.72522700
C	-1.21417100	0.40108500	3.32824300
C	0.36713600	-0.98125300	2.27092900
C	0.55172400	-1.98313700	1.31104400
C	1.05201700	-1.62682200	0.00784900
C	1.33235500	-0.28458200	-0.27125700
C	0.97099300	0.27724600	-1.56059200
C	-0.45224600	2.17418400	-2.09225200
C	-1.44314000	3.06135400	-1.46380400

C	-3.78259800	3.01086900	0.19110200
C	-3.90044500	2.74072300	-1.23024000
C	-2.72549600	2.73949700	-2.01618900
C	-2.54767300	1.69499100	-3.02421300
C	-1.14366900	1.35413800	-3.06956800
C	-0.74847500	0.02820200	-3.29326000
C	0.33887700	-0.52295600	-2.52451800
C	0.01975600	-1.91067900	-2.21763300
C	0.36737000	-2.44686600	-0.98010100
C	-0.81316700	-0.98675300	3.10400400
C	-2.99890400	-3.60267600	0.00784900
C	-2.88751200	-3.32523200	1.37498500
C	-3.87134500	-2.46875300	2.02506400
C	-4.93134200	-1.93970400	1.28302200
C	-5.03855200	-2.22408100	-0.13688300
C	-3.58798400	-2.69050000	-2.07552200
C	-2.17760700	-3.03507900	-2.12136400
C	-1.81239100	-3.59879900	-0.83156500
C	-0.56428400	-3.30914700	-0.27434800
C	-0.44691400	-3.02119600	1.14753500
C	-1.59167400	-3.02380200	1.95129400
C	-3.18995400	-1.66106600	3.01976700
C	-3.57519200	-0.32617100	3.21586600
C	-4.68132200	0.22597100	2.44373100
C	-5.34172800	-0.56006000	1.49803000
C	-5.70572600	0.00451000	0.20811100
C	-5.52103500	-1.02729000	-0.80200000
C	-5.02887700	-0.67944000	-2.06352600
C	-4.04611400	-1.53466500	-2.71825700
C	-1.27751700	-2.20717300	-2.79823600
C	-1.75224700	-1.00476200	-3.46661900
C	-3.11093200	-0.67549100	-3.41683200
C	-3.52020200	0.70560800	-3.19936100
C	-4.71877900	0.70215100	-2.38028200
C	-4.88001000	1.69502900	-1.39993400
C	-5.39680700	1.33363500	-0.08492200
C	-4.71755300	2.15416500	0.90287400
C	-4.36631800	1.61165800	2.14155000
C	-1.77661200	-1.99014800	2.95977500
C	-2.58975700	0.71346100	3.40227000
C	-4.09831100	-3.05227300	-0.76462700
C	2.88478400	5.43964500	-0.27343300
C	1.91814400	4.44242000	-0.26122500
C	4.50638000	3.82110100	0.39076300

C	4.20967900	5.14261000	0.06934900
C	4.17166100	1.40792700	0.62538100
C	1.21572600	0.74161100	0.72958100
O	4.11575000	0.60012700	-0.36954900
O	4.77859000	1.25054300	1.69814300
C	5.27716400	6.21342300	0.08149400
H	4.94244200	7.11357600	0.61422200
H	6.19118900	5.85598100	0.56812200
H	5.54940700	6.52799700	-0.93633000
H	5.51802100	3.55486400	0.68651300
H	2.60151900	6.45989500	-0.53078000
H	0.89037300	4.70845200	-0.48574300
C	5.75049000	-0.72680500	-0.34770200
C	5.07529800	-1.93642600	0.13278000
C	4.74083800	-2.97541400	-0.74929100
C	4.73850600	-2.06237200	1.49027300
C	4.09689900	-4.11944000	-0.28611400
H	5.01823100	-2.88699900	-1.79596700
C	4.09499300	-3.20866000	1.95155300
H	4.94746600	-1.22782400	2.15249300
C	3.77471200	-4.24284400	1.06837800
H	3.84259500	-4.91623800	-0.98171300
H	3.82639500	-3.28897300	3.00244100
H	3.26337900	-5.13254800	1.42960900
H	6.19025700	-0.04469700	0.35712100
H	5.79212900	-0.50463700	-1.39834100
Br	8.08736900	-1.66286000	-0.71648400

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	x	y	z
C	-0.81316200	1.07179100	-1.39318900
C	-0.94162500	-0.34958100	-1.39250400
C	-1.15021700	-1.10402400	-0.22573000
C	-1.10138200	-0.39605500	1.06000500
C	0.17883600	1.40337100	-2.35174300
C	0.60102500	0.18407200	-3.05602300
C	-0.10784900	-0.91437700	-2.45377500
C	0.50840500	-2.15667400	-2.29975600
C	-0.47857000	-2.35758200	-0.05872500
C	-0.42688800	-1.25476200	2.01559100
C	0.40145200	-0.71211200	3.00681400
C	0.59835300	0.71413500	3.05032200
C	-0.04145200	1.51893700	2.09307900

C	0.69068300	2.61528900	1.48032000
C	0.24510400	2.75484800	0.12562300
C	1.16493800	3.07977200	-0.85694600
C	1.12958500	2.43831900	-2.17363400
C	1.91499900	0.02148900	-3.49084800
C	2.89854600	1.06623200	-3.26060700
C	2.48960500	2.23228400	-2.57781400
C	3.37578300	2.79881900	-1.55969000
C	2.55072800	3.32644500	-0.50074800
C	2.96944400	3.24295300	0.83370800
C	2.01547100	2.88798400	1.85373000
C	2.68237800	2.02913400	2.82263000
C	1.99116100	0.96736400	3.40278000
C	-0.03747500	-2.46548200	1.32985500
C	4.36029100	-1.70774300	2.46411300
C	3.41079800	-2.70818600	2.22609000
C	3.38092000	-3.39193300	0.93924600
C	4.30976800	-3.05346700	-0.04889700
C	5.28677300	-2.00882800	0.19917600
C	5.52087900	0.08304700	1.48189400
C	4.68987600	0.61799300	2.54738800
C	3.97091000	-0.49016500	3.15530100
C	2.64803600	-0.31695600	3.57470800
C	1.66076500	-1.35760200	3.33000300
C	2.03944100	-2.52440900	2.65828700
C	1.99690000	-3.65605100	0.59122400
C	1.58037600	-3.53673800	-0.74403600
C	2.54893200	-3.18698600	-1.77537500
C	3.88133200	-2.94850600	-1.43639400
C	4.59835500	-1.83885600	-2.04359200
C	5.47120600	-1.26133900	-1.03165000
C	5.65923600	0.12311500	-0.98919100
C	5.69158200	0.80889300	0.29752000
C	4.05666700	1.85366000	2.38613500
C	4.23391200	2.60855400	1.15435900
C	5.03063500	2.08777900	0.12910300
C	4.59968200	2.19153100	-1.25963500
C	5.00885400	0.98739900	-1.95569000
C	4.14725400	0.43186500	-2.91898200
C	3.95365600	-1.01234900	-2.96549000
C	2.56964800	-1.26700800	-3.32623800
C	1.88091100	-2.33254500	-2.74249700
C	1.16691800	-3.10090500	1.64411000
C	0.32297900	-2.91278300	-1.07786000

C	5.32570100	-1.35537200	1.43863800
C	-3.15780200	5.13144500	0.09607400
C	-2.12974300	4.19402800	0.17989100
C	-2.29463900	2.84676100	-0.18083700
C	-3.57413000	2.45896100	-0.64377000
C	-4.58345900	3.42562600	-0.75916800
C	-4.41250700	4.76001400	-0.38681000
C	-1.04103700	1.91512500	-0.12765600
C	-4.06129100	1.04842900	-0.99388400
C	-0.95888400	0.98001600	1.12438000
O	-3.84888800	0.18127300	-0.07402500
O	-4.71537100	0.90142800	-2.03984000
C	-5.54990200	5.75078200	-0.49070800
H	-5.18098700	6.78326700	-0.52414100
H	-6.15021400	5.57728500	-1.39192500
H	-6.23331600	5.67639100	0.36742900
H	-5.53609200	3.09439800	-1.16354500
H	-2.96743800	6.16282600	0.39142200
H	-1.15764000	4.53304500	0.52046700
C	-5.00992000	-1.53368500	-0.34824100
H	-4.17240000	-2.07426000	0.05576500
H	-5.02623600	-1.30581700	-1.39912300
C	-6.08351200	-1.04873600	0.52971200
C	-7.10776100	-0.23736900	0.01447900
C	-6.09005300	-1.35283000	1.89955200
C	-8.11282500	0.24788900	0.84816800
H	-7.08169200	0.02499800	-1.03827600
C	-7.09548100	-0.86738200	2.73185900
H	-5.30142000	-1.98205400	2.30257600
C	-8.11475900	-0.06577800	2.21014900
H	-8.89733700	0.87884700	0.43442000
H	-7.08399900	-1.11343200	3.79193300
H	-8.90025800	0.31497200	2.86039900
Br	-6.03991600	-3.77023000	-0.87036000

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	x	y	z
C	-0.69533000	-0.99600800	1.64773700
C	-0.90581700	0.52589100	1.36543700
C	-2.25009800	1.01571800	1.99246800
C	-3.55569800	0.72911400	1.52015900
C	0.30718800	1.27883400	1.92099500
C	1.06931100	2.17268000	1.17380500

C	0.86452700	2.43749700	-0.23441300
C	-0.00118900	1.42052100	-0.88994700
C	1.15451300	0.72910800	2.95614300
C	2.45888300	1.37146000	2.88740400
C	2.41085300	2.27534900	1.76644100
C	3.52622800	2.45038800	0.96149600
C	2.09035100	2.46381600	-1.04325100
C	0.60977000	1.02727000	-2.14053600
C	0.42850200	-0.25587800	-2.66743400
C	-0.33680700	-1.21419100	-1.91372700
C	-0.87398200	-0.83140300	-0.67926500
C	-0.84352700	-1.75475200	0.43943400
C	0.12753800	-1.48525600	2.64771700
C	1.06308200	-0.60005300	3.36591400
C	3.62203100	0.65394800	3.17227400
C	3.53375800	-0.74147300	3.55365600
C	2.26840900	-1.34950000	3.62629300
C	2.08892800	-2.69527000	3.09965400
C	0.77150900	-2.77390600	2.50100000
C	0.57220100	-3.54114400	1.34630800
C	-0.25913400	-3.02131700	0.29086500
C	0.33192700	-3.40276700	-0.98274700
C	0.29642500	-2.51532300	-2.05739700
C	1.89834100	1.67533400	-2.24193100
C	3.92378700	-2.42889600	-2.73814100
C	4.00320100	-1.08015900	-3.09923700
C	4.92877600	-0.19401100	-2.40548100
C	5.73982800	-0.69618400	-1.38504300
C	5.65150800	-2.09523400	-1.00765800
C	3.98758800	-3.91403700	-0.91735800
C	2.66762200	-3.99881200	-1.51774300
C	2.62785100	-3.07851500	-2.64244100
C	1.46342400	-2.35208500	-2.90638900
C	1.54633600	-0.94879900	-3.28057600
C	2.79472900	-0.32717700	-3.37405900
C	4.29666800	1.10559100	-2.27023800
C	4.47666000	1.84928400	-1.09476500
C	5.32597000	1.32718700	-0.03220400
C	5.94308500	0.08295200	-0.17338400
C	5.98738200	-0.83714600	0.95184400
C	5.80627900	-2.18503700	0.43385200
C	5.05730800	-3.11373200	1.16057400
C	4.13158300	-3.99819200	0.47197600
C	1.54054800	-4.15580200	-0.70586700

C	1.68963600	-4.24147900	0.74012800
C	2.96060400	-4.15953300	1.31380400
C	3.16478100	-3.37624400	2.52331700
C	4.46677100	-2.74004000	2.43594500
C	4.63857000	-1.44392100	2.93225200
C	5.42122200	-0.47561600	2.17511700
C	4.78920200	0.82339000	2.32558500
C	4.74132300	1.70653100	1.24203400
C	2.97564100	1.01887400	-2.85273000
C	3.37199100	2.55381900	-0.48963000
C	4.76476900	-2.94884600	-1.67377900
C	-3.28125300	2.03700800	3.97175600
C	-2.16138100	1.67576600	3.22643900
C	-4.67283700	1.06684300	2.30103400
C	-4.56596200	1.72943800	3.52510200
C	-3.91429600	0.19039500	0.15873800
C	-0.76821100	0.51371400	-0.18232400
O	-4.85924400	-0.75092500	0.25914400
O	-3.47007400	0.63253600	-0.88779000
C	-5.79871300	2.11546300	4.30762700
H	-6.21303800	3.06836500	3.95149300
H	-6.58754900	1.36275000	4.20466500
H	-5.57364200	2.23458800	5.37366000
H	-5.65549100	0.80322400	1.92187900
H	-3.14386300	2.55780900	4.91757200
H	-1.18034300	1.91355500	3.61992000
C	-5.57864300	-1.17987100	-0.94897000
C	-5.20623600	-2.59728700	-1.30702700
C	-6.12422700	-3.63259200	-1.08400600
C	-3.95431000	-2.89182700	-1.86550600
C	-5.78033500	-4.94655200	-1.41363900
H	-7.10580300	-3.38628100	-0.67143300
C	-3.61237300	-4.20582500	-2.18451500
H	-3.24876700	-2.08528900	-2.04868000
C	-4.52749500	-5.23784100	-1.95687000
H	-6.49830900	-5.74589400	-1.24116100
H	-2.63345600	-4.42196800	-2.60667800
H	-4.26292900	-6.26425900	-2.20567900
H	-5.32456400	-0.48027700	-1.74793400
H	-6.64078100	-1.11067000	-0.68229400
Br	-9.16614100	-1.77726900	0.01728200
C	-1.79161000	3.88157900	-2.05255900
C	-2.25604200	3.88066900	-3.36554800
C	-1.49985400	4.47171400	-4.38046200

C	-0.26827500	5.05887500	-4.07350700
C	0.19957200	5.05796600	-2.76326300
C	-0.55872900	4.47846300	-1.72930100
H	-2.37670500	3.39666700	-1.27652000
H	-3.20745800	3.40815800	-3.59430500
H	-1.86402100	4.46937100	-5.40529500
H	0.32687100	5.52004600	-4.85855800
H	1.14658700	5.53146800	-2.51938000
C	-0.05562400	4.45545700	-0.36024400
H	-0.71465700	4.20508000	0.45524300
H	0.88821800	4.91011000	-0.11474200
Br	-0.73039400	6.95356400	0.36769400

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	x	y	z
C	0.25094600	0.55185600	2.30722300
C	-0.78720300	0.66009500	1.15178400
C	-2.16106200	1.06041000	1.76616700
C	-3.43608400	0.62851900	1.33574500
C	-0.27322500	1.66960700	0.04783000
C	-0.00673900	1.16140400	-1.29740800
C	-0.23466300	-0.14870800	-1.70776900
C	-0.54894800	-1.15632500	-0.68247500
C	0.90019400	2.48934200	0.34283000
C	1.66405100	2.72658100	-0.87027000
C	1.09800200	1.88922800	-1.89684600
C	1.91977300	1.30848000	-2.86762800
C	0.63404400	-0.76750700	-2.67331900
C	0.10847700	-2.38926900	-1.05611000
C	0.62501800	-3.24810400	-0.07961200
C	0.51815100	-2.87181700	1.30676400
C	-0.10328000	-1.65854900	1.63959200
C	0.47608100	-0.81753100	2.66983800
C	1.24052900	1.48017500	2.55690100
C	1.56809900	2.52160500	1.56796900
C	3.04209900	2.96562600	-0.82940900
C	3.73362100	2.96638900	0.43921300
C	2.99332200	2.71900800	1.60934800
C	3.55120700	1.84510500	2.63363500
C	2.46509200	1.08833400	3.21927600
C	2.66406400	-0.23865900	3.61788200
C	1.64258900	-1.21658700	3.33795600
C	2.29691000	-2.46401400	2.97257900

C	1.74789300	-3.26978100	1.97698000
C	0.84279100	-2.15421600	-2.28145100
C	4.73200900	-3.44576500	-0.19332600
C	4.05987700	-3.43011300	-1.41939400
C	4.39269000	-2.42473100	-2.41974500
C	5.38806500	-1.48027500	-2.15448100
C	6.07804200	-1.49312400	-0.87593200
C	5.65569900	-2.08181600	1.48306100
C	4.56579200	-2.84082900	2.07213600
C	3.99406600	-3.68416700	1.03505100
C	2.61276500	-3.89489000	0.99007400
C	1.91476100	-3.88153100	-0.28506400
C	2.62730300	-3.64647100	-1.46469900
C	3.16913100	-2.03059000	-3.09164300
C	2.97439900	-0.69452800	-3.46171600
C	4.01088300	0.29020000	-3.18498700
C	5.19063000	-0.09400400	-2.54455200
C	5.76233400	0.75032900	-1.50722200
C	6.31154000	-0.11538200	-0.47716700
C	6.20417500	0.24975800	0.86740700
C	5.87216100	-0.75526600	1.86883600
C	3.73241900	-2.24335300	3.02171600
C	3.95875400	-0.86405600	3.42383600
C	5.00674500	-0.13499000	2.85237400
C	4.80370300	1.25165500	2.45823400
C	5.55554900	1.49262900	1.23883900
C	5.01735800	2.32404700	0.24846200
C	5.13005000	1.94436500	-1.15311200
C	3.90445300	2.34530800	-1.82257500
C	3.35500100	1.53390300	-2.81695500
C	2.07529100	-2.77534700	-2.49183200
C	1.68729600	-0.05690100	-3.27506900
C	5.76301800	-2.45988600	0.08417800
C	-3.28632800	2.52388100	3.37613500
C	-2.13208600	1.98203100	2.82430900
C	-4.59401400	1.14136200	1.94602800
C	-4.54733100	2.12733500	2.92941100
C	-3.70639000	-0.21283200	0.12080900
C	-0.70301500	-0.80889100	0.64477100
O	-4.62728200	-1.15048500	0.38056500
O	-3.20988900	0.00202700	-0.97316000
C	-5.79727300	2.82191500	3.40331800
H	-5.90196800	3.75936900	2.84059200
H	-6.69205400	2.21526100	3.23000200

H	-5.74759200	3.07299700	4.46989500
H	-5.55652500	0.79114800	1.58650700
H	-3.19974100	3.28979500	4.14327600
H	-1.17452500	2.32287400	3.20036500
C	-5.22150100	-1.90586000	-0.72890700
C	-4.82913600	-3.36205400	-0.63899300
C	-5.81702100	-4.34170300	-0.47175200
C	-3.48580800	-3.75006600	-0.74039800
C	-5.45333100	-5.69001100	-0.40506200
H	-6.86431800	-4.03487700	-0.41019000
C	-3.12685500	-5.09497700	-0.66373200
H	-2.71900800	-2.99395300	-0.88243300
C	-4.11348300	-6.07093600	-0.49502900
H	-6.22727200	-6.44429100	-0.27727200
H	-2.07878500	-5.37726800	-0.73765600
H	-3.83594600	-7.12222900	-0.43671900
H	-4.87499200	-1.45042000	-1.65931800
H	-6.30698200	-1.78878900	-0.62621000
Br	-9.01764400	-2.48557100	-0.58293600
C	-2.24408900	3.18854100	-2.64387600
C	-2.05555900	3.63790400	-3.94726800
C	-1.23222700	4.73938000	-4.20128200
C	-0.59570100	5.38830900	-3.14013200
C	-0.78102900	4.94055400	-1.83468800
C	-1.61386000	3.83899500	-1.56469500
H	-2.87318000	2.32606800	-2.44189400
H	-2.55129100	3.12693600	-4.76906500
H	-1.08727500	5.08916700	-5.22107300
H	0.04403100	6.24703500	-3.33082200
H	-0.30686100	5.45806400	-1.00573100
C	-1.80706900	3.35297600	-0.20870100
H	-2.60488000	2.66048100	-0.00743800
H	-1.38111700	3.87809800	0.62796200
Br	-3.72892600	5.15922300	0.62621400

TSb3

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	x	y	z
C	-0.05862000	1.00033900	-1.55184600
C	0.99613600	0.86590700	-0.41291400
C	2.15475600	1.89235700	-0.62755600
C	3.51987700	1.73354600	-0.29069600
C	0.25258100	1.05303300	0.91938400
C	0.33224800	0.07894400	1.98981500

C	0.90837800	-1.17347600	1.80799100
C	1.38028800	-1.54192900	0.46299600
C	-0.97938100	1.69879700	1.02138900
C	-1.68358500	1.20628700	2.21734900
C	-0.85319400	0.19692900	2.82499300
C	-1.42861000	-0.92960300	3.41941100
C	0.30328800	-2.33997600	2.39801300
C	1.07597900	-2.94094300	0.26057400
C	0.70294400	-3.41220000	-1.00347800
C	0.60125700	-2.47843400	-2.09541100
C	0.88047500	-1.12193900	-1.86604100
C	0.02743700	-0.10584100	-2.45874700
C	-1.26294400	1.66455200	-1.41035800
C	-1.74202700	2.19301100	-0.10844600
C	-3.06412100	1.07252700	2.22640400
C	-3.84596200	1.43097400	1.04095400
C	-3.17552900	1.89610500	-0.09382100
C	-3.58876100	1.41392700	-1.39781900
C	-2.40067700	1.27029600	-2.20885600
C	-2.30109400	0.23163300	-3.14131400
C	-1.05372500	-0.47550100	-3.27262300
C	-1.35307700	-1.88315900	-3.48479600
C	-0.54515100	-2.86203000	-2.90885600
C	0.40933700	-3.43724600	1.44719800
C	-3.21022700	-4.68165400	-1.11222700
C	-2.46477500	-5.00844500	0.02639800
C	-2.94857800	-4.63171800	1.34455700
C	-4.15905500	-3.94636500	1.47372000
C	-4.92762400	-3.60123000	0.29094500
C	-4.57201300	-3.03025000	-2.08236200
C	-3.38088400	-3.16881700	-2.90258600
C	-2.53844300	-4.18981100	-2.30282300
C	-1.14865800	-4.03681000	-2.30757800
C	-0.37314100	-4.37894500	-1.12466000
C	-1.02247700	-4.84909800	0.01945100
C	-1.80531000	-4.25605200	2.16037000
C	-1.91313100	-3.19763600	3.06815300
C	-3.17571600	-2.48407900	3.20449800
C	-4.27242000	-2.84852100	2.42175900
C	-5.11035000	-1.82423800	1.81893900
C	-5.52064800	-2.29305500	0.50379600
C	-5.61931200	-1.38897800	-0.55650400
C	-5.13762300	-1.76775200	-1.87896600
C	-2.79773600	-2.03836600	-3.48196600

C	-3.38519400	-0.72565500	-3.26810400
C	-4.53229100	-0.59493700	-2.47980700
C	-4.64500000	0.50325800	-1.53010500
C	-5.32865300	0.01795000	-0.35231700
C	-4.91066200	0.46723800	0.91092500
C	-4.81185000	-0.47515600	2.01740600
C	-3.67362200	-0.09471300	2.83607000
C	-2.87169200	-1.07987100	3.42156200
C	-0.61611600	-4.37810800	1.33573300
C	-0.83874300	-2.23516300	3.20884000
C	-4.46849800	-3.96979600	-0.97908100
C	2.69966900	4.14714900	-1.44881900
C	1.79703100	3.11412700	-1.22114100
C	4.43653500	2.75998800	-0.58782300
C	4.05395700	3.97757900	-1.14868700
C	4.08886200	0.58922100	0.49756900
C	1.34101800	-0.64377500	-0.58951300
O	5.31765700	0.26447800	0.06447500
O	3.53171400	0.07997900	1.45397700
C	5.06294600	5.06848300	-1.42066600
H	4.73367900	6.02681200	-1.00074900
H	6.03982800	4.82457700	-0.99132500
H	5.20275600	5.22265300	-2.49894000
H	5.47914500	2.59062600	-0.33946600
H	2.31876700	5.08493800	-1.84802900
H	0.77276200	3.27709800	-1.52768800
C	6.13232200	-0.65535200	0.86509900
C	6.25423800	-1.99416900	0.17578700
C	7.51411900	-2.45835000	-0.22551000
C	5.12210800	-2.78982500	-0.05178300
C	7.62799500	-3.70416200	-0.84975400
H	8.39411900	-1.84111000	-0.02730600
C	5.23993800	-4.02742300	-0.68298200
H	4.14670600	-2.43633300	0.27095000
C	6.49721600	-4.48820100	-1.08485100
H	8.61016600	-4.05862400	-1.15634600
H	4.35098800	-4.63005300	-0.85726200
H	6.59199200	-5.45526600	-1.57618800
H	5.65497400	-0.75031000	1.84313600
H	7.11379300	-0.17622600	0.96286100
Br	9.86255700	0.12266300	1.06641700
C	-1.90751700	5.19964900	2.03331900
C	-2.75467100	5.70559800	3.01480900
C	-4.07749800	6.03210100	2.70295600

C	-4.54598600	5.84541200	1.39926800
C	-3.70091300	5.33724400	0.41771900
C	-2.36520100	5.00980300	0.71614800
H	-0.87805900	4.95026000	2.27470200
H	-2.38251100	5.84635300	4.02669400
H	-4.73873700	6.42769400	3.47039200
H	-5.57404200	6.09648600	1.14861700
H	-4.06354500	5.19815900	-0.59710200
C	-1.48319800	4.46115000	-0.30297300
H	-0.44360700	4.29724300	-0.08410100
H	-1.81622900	4.36142700	-1.32154000
Br	-0.45324800	6.66047300	-1.35240300

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-2 1

	x	y	z
C	-0.32742900	2.68886700	0.55707800
C	-1.49256700	1.95099700	-0.16963700
C	-2.66795600	2.92449900	-0.31810300
C	-3.73223700	2.95595000	0.58833000
C	-0.95275100	1.50284800	-1.52753000
C	-0.97094600	0.14121800	-1.97044300
C	-1.27957700	-0.91297100	-1.10677400
C	-1.71210500	-0.71137500	0.27675700
C	0.13495400	2.14067600	-2.16111600
C	0.76061200	1.20017100	-3.09631400
C	0.05421000	-0.04986600	-2.98566100
C	0.74470000	-1.26507000	-3.10842100
C	-0.55384300	-2.14911900	-1.22352200
C	-0.98119500	-1.72457400	1.03330300
C	-0.37333000	-1.50071200	2.27451400
C	-0.27433100	-0.11416100	2.73770300
C	-0.81102000	0.91851300	1.99281000
C	-0.08957400	2.14258600	1.85339700
C	0.71323600	3.32752400	-0.10537900
C	0.95084700	3.12375000	-1.53202700
C	2.13585500	1.22039400	-3.32292700
C	2.97842400	2.18426700	-2.63172800
C	2.36822600	3.08588200	-1.72711100
C	3.02781300	3.34374400	-0.44575800
C	1.99791700	3.49972800	0.55505900
C	2.20014800	3.03404200	1.85823300
C	1.12781700	2.35229000	2.53802800
C	1.69013500	1.27078800	3.30981800

C	1.00201300	0.05784100	3.40456500
C	-0.35303800	-2.65363100	0.11753900
C	3.70966200	-2.14583600	2.19984800
C	2.89606700	-3.05986800	1.51346200
C	3.14324800	-3.32211300	0.10013100
C	4.18648900	-2.66864800	-0.56160100
C	5.01932700	-1.71662500	0.15225400
C	4.85495200	-0.10002800	2.00787400
C	3.81881100	0.06455700	3.00846800
C	3.10224500	-1.19956300	3.12076500
C	1.71783900	-1.19762200	3.31041200
C	0.86733200	-2.15182300	2.60589900
C	1.46471000	-3.07157800	1.72351700
C	1.86222300	-3.50943200	-0.55781800
C	1.66575500	-3.01423000	-1.85293200
C	2.75345700	-2.33793700	-2.54621100
C	3.98513200	-2.16605000	-1.91334400
C	4.69330300	-0.90053000	-2.02764200
C	5.33685800	-0.62762100	-0.75110500
C	5.40073000	0.68802700	-0.27603400
C	5.15857600	0.95364700	1.13675500
C	3.12798500	1.27609700	3.10892800
C	3.44448600	2.37198200	2.20559300
C	4.43626600	2.20578100	1.23345400
C	4.23092400	2.70980500	-0.11938500
C	4.84595200	1.78024100	-1.04897900
C	4.20085700	1.51615500	-2.27140200
C	4.13765200	0.14390100	-2.76924600
C	2.86111700	-0.03512300	-3.43487200
C	2.17721400	-1.25151700	-3.32387500
C	0.82818200	-3.32670200	0.44837200
C	0.43202300	-2.34910200	-2.20995500
C	4.78950000	-1.46736500	1.51301400
C	-3.65106700	4.85345500	-1.42886300
C	-2.65314900	3.89110800	-1.33740200
C	-4.73807100	3.93073400	0.48937200
C	-4.71674100	4.89277100	-0.51383100
C	-3.88889200	1.92389700	1.64279400
C	-1.81628300	0.71585400	0.85667000
O	-3.13754300	0.81306700	1.52902900
O	-4.71747400	1.99661000	2.53104300
C	-5.80895400	5.93076600	-0.63536700
H	-6.48414000	5.89748200	0.22624000
H	-5.39653100	6.94647700	-0.70070700

H	-6.41706900	5.77307100	-1.53665300
H	-5.54368600	3.89449200	1.21647400
H	-3.60491200	5.59138900	-2.22904500
H	-1.84320800	3.88194300	-2.05832300
C	-3.53874800	-3.55786900	-1.34743800
C	-3.34554900	-4.93121300	-1.47692200
C	-3.32365200	-5.74890800	-0.34526300
C	-3.49561600	-5.17904500	0.92076700
C	-3.68882500	-3.80830800	1.05114400
C	-3.72142400	-2.97097200	-0.08114500
H	-3.56967800	-2.92462600	-2.22859200
H	-3.20820000	-5.36438800	-2.46523300
H	-3.16973000	-6.82119700	-0.44681500
H	-3.47562700	-5.80782500	1.80836400
H	-3.82497100	-3.36587200	2.03401800
C	-3.92551600	-1.54035100	0.06063900
H	-4.16538900	-1.10779800	1.01556700
H	-4.01349900	-0.91313900	-0.80944000
Br	-6.61004500	-1.57213700	-0.27918700

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-2 1

	x	y	z
C	1.23193600	1.05289700	1.07786400
C	1.35518700	2.04957300	-0.11374600
C	2.75673900	2.67424100	-0.11793800
C	3.01434800	3.95935500	0.37251100
C	1.09820100	1.23287500	-1.38362800
C	0.12311900	1.60078100	-2.37575100
C	-0.86194700	2.55320800	-2.07033200
C	-0.90598500	3.23208000	-0.81634900
C	1.32556200	-0.14849900	-1.46971600
C	0.50623300	-0.68311000	-2.55557100
C	-0.24035300	0.41856100	-3.12601300
C	-1.54976100	0.21382400	-3.59008500
C	-2.22394400	2.34776600	-2.55637400
C	-2.27359900	3.36309600	-0.44991700
C	-2.73304800	3.24294600	0.88321500
C	-1.75207200	2.82525300	1.87450100
C	-0.41404400	2.65083100	1.53719200
C	0.30098600	1.52646400	2.05464800
C	1.46357600	-0.31107400	0.96922300
C	1.63814800	-0.98186200	-0.33018200
C	-0.07201900	-1.94552100	-2.46434400

C	0.13941300	-2.76064800	-1.26340600
C	0.91908200	-2.24273600	-0.22250300
C	0.47309100	-2.42847700	1.14657300
C	0.81111500	-1.23091700	1.88312900
C	-0.03560600	-0.76053200	2.89151000
C	-0.28852500	0.65359700	2.99704500
C	-1.67420100	0.84049100	3.35283600
C	-2.39474800	1.90158600	2.79632800
C	-3.10885600	2.84622700	-1.53147700
C	-5.17966100	-0.06684900	1.38260500
C	-5.35477400	0.71024100	0.22492100
C	-5.30074500	0.07508600	-1.08465900
C	-5.05659200	-1.29538100	-1.19133100
C	-4.85788400	-2.09645400	0.00607500
C	-3.94958400	-1.86118100	2.28760800
C	-3.60322600	-0.66308000	3.02808100
C	-4.35550200	0.44792200	2.46073200
C	-3.75402000	1.70567600	2.34976300
C	-3.94681900	2.52092200	1.14978200
C	-4.75840900	2.02231400	0.11221100
C	-4.66672100	1.00048000	-2.01130300
C	-3.80670700	0.51625500	-3.00305100
C	-3.55168300	-0.91274000	-3.11215300
C	-4.16532000	-1.79917500	-2.22607700
C	-3.40748200	-2.90502700	-1.65778800
C	-3.83951800	-3.08822000	-0.28047900
C	-2.91096200	-3.45564900	0.70092500
C	-2.96850700	-2.82120300	2.01086700
C	-2.29121600	-0.46873000	3.47119400
C	-1.27171100	-1.46571100	3.18215200
C	-1.60629800	-2.61752800	2.46361700
C	-0.71172900	-3.12091300	1.42951300
C	-1.51738400	-3.64743600	0.34942000
C	-1.09357400	-3.45082700	-0.97738400
C	-2.06444400	-3.07564800	-1.99750700
C	-1.42326700	-2.16308700	-2.93217600
C	-2.15335500	-1.09207100	-3.47444000
C	-4.31326100	2.19278900	-1.26153800
C	-2.56552800	1.20709300	-3.29088700
C	-4.91719100	-1.48803500	1.26664000
C	5.15848500	2.37913900	-0.43826100
C	3.85430900	1.91470300	-0.55069500
C	4.33379900	4.43594600	0.46678700
C	5.42086800	3.65735200	0.08410900

C	1.92251300	4.90490800	0.71751900
C	0.18250400	3.12988700	0.21424000
O	0.66549500	4.53212900	0.45038000
O	2.13337900	6.03012300	1.14566500
C	6.83934700	4.16537900	0.20818800
H	6.86790000	5.15478900	0.67819700
H	7.45556200	3.48616900	0.81114300
H	7.32616500	4.24628500	-0.77297800
H	4.47268200	5.44380300	0.84716100
H	5.96843300	1.71727100	-0.74097500
H	3.68140700	0.94007400	-0.98695500
C	4.12519600	-3.05593700	1.66135900
C	4.09378500	-4.30000000	2.28375000
C	3.98574700	-5.46711300	1.52245100
C	3.90470500	-5.37538400	0.12843300
C	3.93340400	-4.13421700	-0.49613700
C	4.04658200	-2.94727200	0.25761600
H	4.20985100	-2.14976400	2.25438700
H	4.14954700	-4.36040700	3.36833800
H	3.95810900	-6.43900000	2.01001600
H	3.81475300	-6.27840100	-0.47144200
H	3.87357200	-4.06458300	-1.57875800
C	4.07492300	-1.65288600	-0.38370900
H	3.93797600	-1.55584500	-1.44677400
H	4.16636200	-0.75947100	0.20609500
Br	6.59657100	-1.28636000	-0.90420500

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-2 1

	x	y	z
C	-0.69519100	0.83998700	1.99698600
C	-1.57855300	-0.14065700	1.16011900
C	-3.10459200	-0.02647100	1.33605600
C	-3.87042800	-1.04796600	1.91958300
C	-1.25260900	0.18554200	-0.29231000
C	-0.85994500	-0.80813200	-1.27252900
C	-0.46457300	-2.07742100	-0.91870300
C	-0.63961100	-2.68212600	0.47785800
C	-0.82482300	1.43004600	-0.73273700
C	-0.17165700	1.26660400	-2.03995100
C	-0.21443700	-0.13005000	-2.38226900
C	0.84385200	-0.72426800	-3.07279600
C	0.65586000	-2.66903300	-1.59519500
C	0.78339500	-3.26544900	0.66018500

C	1.57119900	-3.09729500	1.78048800
C	1.21131100	-2.07417100	2.77888600
C	0.12233900	-1.26690900	2.56230600
C	0.15388600	0.11729700	2.89456300
C	-0.25291900	2.07963600	1.54364400
C	-0.43361900	2.52715600	0.14250400
C	0.92048400	2.03938100	-2.40082400
C	1.44985800	3.02974400	-1.45754800
C	0.83186900	3.17279800	-0.21235000
C	1.65332500	3.32663300	0.96713300
C	0.98945800	2.63324500	2.05012400
C	1.75141000	1.97129800	3.01847200
C	1.31923800	0.67430900	3.46162000
C	2.48324200	-0.15543100	3.65281100
C	2.42899200	-1.51081900	3.31112300
C	1.43758000	-3.39389100	-0.61320800
C	5.32187800	-1.56744100	1.02271300
C	4.81723400	-2.50477400	0.11317800
C	4.72242800	-2.16452800	-1.29637900
C	5.14161300	-0.90749600	-1.74189300
C	5.66485500	0.06138400	-0.79540100
C	5.39555700	0.71768100	1.57054900
C	4.73307900	0.02415600	2.65779000
C	4.68066200	-1.38983000	2.31647200
C	3.54531200	-2.13812600	2.63404000
C	3.01461300	-3.11255100	1.69138800
C	3.64652800	-3.29334800	0.45624600
C	3.50097300	-2.75424800	-1.82188400
C	2.74383400	-2.06044500	-2.76666300
C	3.18232300	-0.75483900	-3.23857200
C	4.35524400	-0.18870900	-2.73337100
C	4.39282000	1.22326000	-2.39224400
C	5.21031400	1.37874800	-1.19762100
C	4.85650100	2.32409000	-0.23025900
C	4.95703000	1.98882700	1.18273600
C	3.65621800	0.62739100	3.31659600
C	3.20166200	1.95079700	2.91655200
C	3.84021800	2.61344900	1.86566100
C	3.05221400	3.32891700	0.87258600
C	3.68844400	3.16515800	-0.41428200
C	2.88478600	2.99837300	-1.55366000
C	3.25425200	2.01287300	-2.56502900
C	2.03716700	1.42872000	-3.09450000
C	2.00058000	0.06831000	-3.43092800

C	2.83569300	-3.44198800	-0.72815400
C	1.29680100	-2.03362200	-2.66912600
C	5.76218300	-0.26650800	0.56334100
C	-5.19134800	1.06194900	0.71829800
C	-3.79787200	1.04958100	0.77608800
C	-5.26489700	-1.05837800	1.80971200
C	-5.94762200	-0.01886000	1.18044700
C	-3.25274700	-2.14579200	2.67291800
C	-1.03067200	-1.60421600	1.63156000
O	-1.89796100	-2.28223200	2.57766700
O	-3.83508500	-2.90142900	3.42133000
C	-7.42489000	-0.14280400	0.91575100
H	-7.98777100	-0.38561900	1.82614600
H	-7.84198300	0.77586300	0.48762300
H	-7.56111200	-0.97053200	0.20529600
H	-5.79746500	-1.92130100	2.19005400
H	-5.69200800	1.90645900	0.24856100
H	-3.24505300	1.86196200	0.32344300
C	-2.47827300	-4.87259100	-1.73061700
C	-2.37898700	-5.86098200	-2.71279300
C	-1.41362000	-6.86469500	-2.61798400
C	-0.55526400	-6.88999600	-1.51662100
C	-0.65558800	-5.90593900	-0.53234200
C	-1.60164800	-4.87421800	-0.63417800
H	-3.28360400	-4.13773000	-1.77238500
H	-3.07507500	-5.84887400	-3.54842100
H	-1.33998500	-7.63198100	-3.38672900
H	0.18867000	-7.67846100	-1.41894400
H	0.00668900	-5.94149000	0.32947100
C	-1.74728400	-3.81804700	0.44454500
H	-1.74645100	-4.29542800	1.42759000
H	-2.72769000	-3.34387600	0.31317500
Br	-5.69006800	-3.19229400	-0.79228200
C	-1.08451500	5.44820000	-1.97705300
C	-1.21261600	5.65809500	-3.34695500
C	-2.22133700	5.01269200	-4.06706800
C	-3.10360700	4.15713000	-3.40143600
C	-2.97853600	3.94877400	-2.03127500
C	-1.96716300	4.59122800	-1.29283000
H	-0.30834300	5.96062800	-1.41649100
H	-0.52241000	6.32739100	-3.85562600
H	-2.31847100	5.17347400	-5.13832000
H	-3.89065300	3.64790200	-3.95201700
H	-3.67134300	3.28668200	-1.52038600

C	-1.81578000	4.35381000	0.13700600
H	-2.55967500	3.80274900	0.68703100
H	-1.07232800	4.88398200	0.70598700
Br	-3.24616400	6.42955700	1.00137900

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	x	y	z
C	1.45253800	-0.35805100	1.07391100
C	1.32980600	0.96453600	0.25689400
C	2.67243700	1.71176200	0.26788400
C	2.99085200	2.56376600	1.33878300
C	0.88413900	0.51070400	-1.12800300
C	-0.26506200	1.08574700	-1.82555800
C	-1.22191300	1.79066500	-1.11310900
C	-1.07969300	2.23345000	0.26984800
C	1.17156000	-0.71806700	-1.68085100
C	0.21119900	-0.98394100	-2.74911000
C	-0.67597400	0.15468200	-2.84680500
C	-2.02619000	-0.03448800	-3.17001300
C	-2.62697200	1.59909000	-1.44057600
C	-2.40367000	1.95883200	0.84791600
C	-2.61719300	1.38040600	2.09697800
C	-1.46345200	0.78567000	2.78071300
C	-0.21039900	0.83528400	2.20394200
C	0.65279600	-0.29505600	2.26264100
C	1.77012000	-1.59076700	0.53799800
C	1.91414400	-1.84914800	-0.97906600
C	-0.26889600	-2.26210900	-2.99744900
C	0.17168700	-3.37156500	-2.12714800
C	1.08174200	-3.14392900	-1.11237900
C	0.86507000	-3.73887500	0.16904500
C	1.27229700	-2.78246600	1.18290600
C	0.57440300	-2.73841700	2.39400700
C	0.26243500	-1.45449900	2.95899000
C	-1.04864900	-1.51997200	3.55239800
C	-1.90270200	-0.41579300	3.45017600
C	-3.36250300	1.69011600	-0.20636800
C	-4.77491100	-2.13887100	1.90478500
C	-5.18385400	-1.08230600	1.08216400
C	-5.31543900	-1.28843400	-0.35110400
C	-5.01881800	-2.53349200	-0.91004500
C	-4.58394400	-3.62675200	-0.05819400
C	-3.32844900	-3.99087600	2.03844900

C	-2.92761900	-3.03964400	3.05641400
C	-3.81625800	-1.89007400	2.96922100
C	-3.30822600	-0.60297800	3.16179500
C	-3.74099600	0.50155300	2.31189400
C	-4.68127000	0.26130700	1.29898700
C	-4.88204900	-0.07120400	-1.01925600
C	-4.17391400	-0.14825800	-2.21956000
C	-3.86327300	-1.44555300	-2.80222900
C	-4.27897100	-2.61322500	-2.16095000
C	-3.38057900	-3.75351600	-2.07394200
C	-3.57305700	-4.38122100	-0.77443600
C	-2.48485000	-4.92746100	-0.08860200
C	-2.35789800	-4.72513100	1.34584400
C	-1.57071900	-2.85637600	3.34568300
C	-0.56291500	-3.61527600	2.62235200
C	-0.95181800	-4.53258400	1.64513500
C	-0.21429900	-4.60677000	0.39458800
C	-1.15516800	-4.85555600	-0.66971500
C	-0.96581200	-4.23428600	-1.90991500
C	-2.10119300	-3.67523300	-2.62664500
C	-1.66463000	-2.46585700	-3.30504300
C	-2.53481000	-1.36536500	-3.39084800
C	-4.48153100	0.87698700	0.00654200
C	-3.02845800	0.71529000	-2.44262900
C	-4.46369900	-3.43033100	1.32301900
C	4.97952800	1.91874500	-0.49247700
C	3.67811600	1.44800900	-0.66629300
C	4.29871000	3.03928400	1.51005600
C	5.31905500	2.70317800	0.62254900
C	1.94547800	3.10029600	2.23052800
C	0.17179500	1.79425300	1.07964300
O	0.66334600	2.97951800	1.76500900
O	2.14283600	3.73915100	3.24063700
C	6.74182400	3.16351000	0.82090600
H	6.92085000	3.46309400	1.86010300
H	7.43414600	2.35853200	0.53643000
H	6.96807700	4.02922500	0.18267700
H	4.48943500	3.68984900	2.35861100
H	5.76958300	1.61322900	-1.17716500
H	3.44795000	0.84864600	-1.53837600
C	5.58315400	-2.35493600	-0.45550100
C	6.57274600	-3.12683200	0.15550700
C	6.34613900	-4.47945800	0.40847800
C	5.13419700	-5.05895100	0.02033200

C	4.15492200	-4.28949000	-0.60948800
C	4.35902500	-2.91884000	-0.84068900
H	5.82722800	-1.31429000	-0.66331000
H	7.51428800	-2.63643200	0.39011800
H	7.11127100	-5.08667900	0.88889600
H	4.95263400	-6.11784200	0.19630400
H	3.23243000	-4.76421400	-0.93156000
C	3.36047800	-2.04294400	-1.57617300
H	3.20582600	-2.42246300	-2.59575300
H	3.80936300	-1.05616400	-1.68396500
Br	8.19653400	0.16978700	-0.95969400
C	-2.03015300	4.83374500	-2.15533600
C	-3.13533700	5.15250100	-2.93987400
C	-4.36812800	5.42540400	-2.34160100
C	-4.48330500	5.37548500	-0.94986500
C	-3.37802400	5.05662300	-0.16549500
C	-2.12907000	4.78733500	-0.75312000
H	-1.06929400	4.63654100	-2.62223700
H	-3.03430300	5.18947100	-4.02212100
H	-5.23157400	5.67440800	-2.95444200
H	-5.43809600	5.58767100	-0.47400200
H	-3.46598900	5.03262400	0.91706900
C	-0.97220000	4.44017000	0.07041600
H	-1.00303900	4.56260400	1.13884700
H	0.00602400	4.38081000	-0.37767600
Br	-0.17359500	7.02972800	0.29847200

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	x	y	z
C	-2.23528700	0.17060300	1.24075200
C	-1.68491800	1.46135800	1.50458800
C	-1.41865300	2.39655700	0.49165000
C	-1.61408600	1.97378400	-0.90020800
C	-1.60517500	-0.74684600	2.11293000
C	-0.70847100	-0.01555100	3.02034000
C	-0.76450000	1.37237200	2.64060500
C	0.38013500	2.16972000	2.70247600
C	-0.22347500	3.18487300	0.54671600
C	-0.55218200	2.54593200	-1.69160900
C	-0.01154400	1.84733100	-2.78365900
C	-0.51403600	0.53465800	-3.08394800
C	-1.53177700	-0.00933000	-2.27627200
C	-1.45714900	-1.40831900	-1.88479600

C	-2.01256500	-1.53745400	-0.57107000
C	-1.42648900	-2.41920700	0.32389300
C	-1.24987700	-2.06842900	1.73528400
C	0.48925200	-0.57978800	3.45628800
C	0.87146900	-1.91601500	3.02837700
C	0.00768500	-2.61082800	2.15116400
C	0.59097800	-3.35793700	1.03372900
C	-0.30545900	-3.24239400	-0.09015800
C	0.19856200	-3.15078800	-1.39455700
C	-0.39577800	-2.21970300	-2.32014400
C	0.66959000	-1.64019300	-3.12743400
C	0.61234500	-0.29699400	-3.49439200
C	0.31659400	3.28936700	-0.80698700
C	3.89502800	0.71090100	-2.12680000
C	3.51878900	1.99078500	-1.69876800
C	3.72274500	2.38060100	-0.30861400
C	4.30341200	1.47947600	0.58863100
C	4.68238700	0.15090700	0.14246100
C	3.98691200	-1.55093400	-1.50008400
C	3.08271000	-1.43639300	-2.63246400
C	3.02467900	-0.03600800	-3.01916800
C	1.81287400	0.51966700	-3.44301900
C	1.42297100	1.84981700	-3.00026600
C	2.26244100	2.56320100	-2.13689000
C	2.61132700	3.21810900	0.10276400
C	2.09215800	3.09806900	1.40256100
C	2.69772800	2.16065300	2.33868700
C	3.77618400	1.36812600	1.94150800
C	3.83144600	-0.03256900	2.32768500
C	4.39840000	-0.78346400	1.21609000
C	3.90589900	-2.05926200	0.92286300
C	3.70308100	-2.45280700	-0.46803200
C	1.92645300	-2.22053600	-2.68577400
C	1.63206800	-3.15926500	-1.61369900
C	2.50337100	-3.26278700	-0.52305100
C	1.97444700	-3.37374300	0.83073800
C	2.85549100	-2.65053700	1.72729700
C	2.29188900	-1.91518000	2.78869200
C	2.80603100	-0.58632000	3.09610100
C	1.68765000	0.24119200	3.51746900
C	1.63443600	1.58746300	3.14790800
C	1.69660700	3.31186100	-1.02094500
C	0.66781800	3.11060800	1.63783000
C	4.49772300	-0.22543500	-1.19593500

C	-6.13569400	-2.08395700	-0.08128300
C	-4.77988700	-1.76750300	-0.16733000
C	-4.30794800	-0.44434600	-0.15879400
C	-5.26491600	0.59304100	-0.03282200
C	-6.61776100	0.24469000	0.09420400
C	-7.08552400	-1.07029600	0.05255900
C	-2.75628700	-0.23568700	-0.14976900
C	-5.00921200	2.12269800	-0.08762000
C	-2.15068600	0.73379700	-1.21456700
O	-4.27880200	2.49421800	-1.04219600
O	-5.62642600	2.80495300	0.76082000
C	-8.56425100	-1.37791000	0.13778200
H	-8.74312700	-2.40402100	0.48423600
H	-9.07517800	-0.69516200	0.82808700
H	-9.06271800	-1.27495600	-0.83797100
H	-7.31172000	1.06829700	0.24554700
H	-6.44557000	-3.12902100	-0.10377700
H	-4.06890700	-2.58354800	-0.23529500