

**Computational rationalization of the selective C-H and C-F activations of
fluoroaromatic imines and ketones by Cobalt Complexes**

Electronic supplementary information (ESI)

Jingjing Li, Dongju Zhang^{*}, Hongjian Sun, and Xiaoyan Li^{*}

*Key Lab of Colloid and Interface Chemistry, Ministry of Education, Institute of
Theoretical Chemistry, Shandong University, Jinan, 250100, P. R. China
Email: zhangdj@sdu.edu.cn*

**Cartesian Coordinates of all stationary points optimized at the B3LYP/6-31G(d,
p) level of theory**

A			
C	-1.08140200	0.24653200	0.22036200
C	-2.08352700	0.87243100	-0.53053800
C	-3.30134700	0.27027600	-0.82453200
H	-4.02913100	0.80984400	-1.41959300
C	-3.54600300	-1.01541000	-0.34166900
H	-4.49305400	-1.49956900	-0.55714400
C	-2.58506400	-1.68288100	0.41860700
H	-2.75218300	-2.67889000	0.81229400
C	-1.37985300	-1.04191100	0.67841600
C	0.20540200	0.94354700	0.56502800
C	1.49042900	0.34138700	0.11044000
C	1.53077400	-0.68365400	-0.84559300
H	0.60761500	-1.06461300	-1.27023100
C	2.75116100	-1.20813200	-1.27251100
H	2.76655400	-1.99832400	-2.01755400
C	3.94585900	-0.71907800	-0.74432900
H	4.89612000	-1.13052000	-1.07281200
C	3.91536900	0.30265700	0.21055100
H	4.84298700	0.68580600	0.62625900
C	2.69984300	0.83060000	0.63289000
F	-1.85387800	2.11610000	-0.99614100
F	-0.45437000	-1.68320300	1.41743500
H	2.65917100	1.62540900	1.36934400
N	0.23157800	2.03986500	1.22848900
H	-0.71473800	2.33754900	1.47563900
2¹A			
C	3.08471700	-0.67041200	-0.33617600
C	3.15158900	-1.89786700	0.35974100
C	4.26574100	-2.72113300	0.39880000
H	4.22256000	-3.63812300	0.97650400
C	5.41924300	-2.33166800	-0.28640500
H	6.30393700	-2.95933100	-0.26687700

C	5.42557700	-1.12846000	-0.99634100
H	6.29351400	-0.79669000	-1.55568400
C	4.28147800	-0.34417800	-1.01353700
C	1.86056500	0.14361500	-0.40081100
C	1.90889400	1.58300400	-0.20248000
C	0.82993800	2.40664800	-0.61088400
H	0.00227100	1.94716300	-1.14099000
C	0.84130100	3.78235200	-0.39503500
H	0.00490800	4.38487700	-0.74308000
C	1.92245800	4.39601100	0.24595900
H	1.92990200	5.46859400	0.41617800
C	2.99945000	3.60023300	0.65820800
H	3.84866300	4.05698300	1.16048700
C	2.99689000	2.22818100	0.43953300
C	-1.53638800	-3.33429600	-1.69696400
H	-1.80312800	-4.39437200	-1.62272800
H	-0.46175500	-3.25354400	-1.88455800
H	-2.05433500	-2.89508300	-2.55419500
C	-3.75130200	-2.89313100	0.04537200
H	-4.34672900	-2.46682400	-0.76766800
H	-4.13966800	-2.49988800	0.98929700
H	-3.87707000	-3.98141900	0.03689100
C	-1.17041100	-3.47620300	1.12412500
H	-1.48483200	-3.16230300	2.12393600
H	-0.08587200	-3.35883400	1.06241400
H	-1.43254100	-4.53147000	0.98892600
C	-3.38076200	0.18014700	-3.04260400
H	-4.17057700	0.74025200	-3.55529900
H	-3.70816100	-0.85644500	-2.91938200
H	-2.48131800	0.17719200	-3.66467000
C	-4.66812800	0.99833300	-0.62903600
H	-4.61656200	1.55492000	0.31133600
H	-5.02514200	-0.01001400	-0.40251900
H	-5.38836000	1.49053200	-1.29223100
C	-2.74180200	2.69177200	-1.85746500
H	-1.85053700	2.79498000	-2.48257700
H	-2.59197200	3.29338200	-0.95658400
H	-3.60699400	3.07946900	-2.40603500
C	0.13955600	0.28798600	2.96148000
H	0.05936800	0.58486700	4.01289100
H	0.94445300	0.85286200	2.48428500
H	0.40132400	-0.77104600	2.89561700
C	-1.68016800	2.40843200	2.35397800
H	-2.66710900	2.71598700	1.99335300
H	-0.92263100	2.97685800	1.80782900
H	-1.60745400	2.64358400	3.42146100
C	-2.68800600	-0.12012400	3.19396800
H	-2.56685600	-1.20583400	3.25044200
H	-3.69688100	0.08933900	2.82584700

H	-2.58696700	0.29404100	4.20331600
F	2.06110700	-2.29597300	1.07592300
F	4.31368200	0.79123300	-1.74375900
H	3.83629400	1.63459500	0.78730100
N	0.67053600	-0.47644800	-0.60860700
P	-1.97099700	-2.39033300	-0.15335800
P	-2.96864100	0.90838800	-1.38186600
P	-1.42880600	0.59688100	2.02481200
Co	-1.22661900	-0.11587300	-0.20963900
H	0.84217400	-1.45238400	-0.82657800

²TS2^a

C	-2.19086400	-0.77865300	-0.45589800
C	-2.71718700	-1.56192400	-1.50007700
C	-3.57195900	-2.64249000	-1.31549300
H	-3.92717500	-3.18578500	-2.18436200
C	-3.96868800	-2.97842000	-0.02065700
H	-4.64124500	-3.81389400	0.14473300
C	-3.50198800	-2.22970000	1.05939600
H	-3.78910700	-2.45240300	2.08132400
C	-2.64343900	-1.16448800	0.81224300
C	-1.22605000	0.34365300	-0.73929100
C	-1.72583000	1.73794900	-0.52207700
C	-1.08763900	2.81175700	-1.18050200
H	-0.23785700	2.58309700	-1.81421000
C	-1.52934900	4.12505000	-1.03828300
H	-1.01621000	4.92292400	-1.57059700
C	-2.62855300	4.42143800	-0.22688200
H	-2.97404900	5.44508800	-0.11386800
C	-3.28153900	3.37406700	0.42467300
H	-4.14649600	3.57910200	1.05086400
C	-2.84423000	2.05706800	0.27702400
C	2.85229800	-1.30411000	-2.72723100
H	3.66741200	-1.14294800	-3.44117400
H	1.89811900	-1.32769400	-3.25963400
H	2.99018000	-2.27730200	-2.24758300
C	4.51736900	-0.02324700	-0.78411200
H	4.67066200	-0.93206800	-0.19640600
H	4.68939400	0.83558600	-0.12874100
H	5.25534600	0.00325100	-1.59346700
C	2.87053100	1.53983900	-2.50766100
H	2.97506500	2.42857600	-1.87890200
H	1.93298600	1.63075300	-3.06133900
H	3.71003900	1.49793900	-3.21033400
C	0.23239400	-3.54921700	-0.03405400
H	0.39695900	-4.51601000	0.45440900
H	0.62770000	-3.58916500	-1.05283700
H	-0.84051200	-3.35867000	-0.10107500
C	2.74615500	-2.91220200	1.13052200

H	3.35548900	-2.25256200	1.75552400
H	3.24799800	-3.02185400	0.16458400
H	2.69244600	-3.89784600	1.60622100
C	0.37110400	-2.43372000	2.59735600
H	-0.64311700	-2.03557500	2.64674600
H	0.98123300	-1.88747800	3.32358900
H	0.36613500	-3.49325500	2.87561000
F	-2.39168300	-1.24956800	-2.77549600
F	-2.19905500	-0.47051200	1.89660200
H	-3.38589400	1.27202200	0.79003000
N	-0.24402500	0.10870900	-1.66768100
P	2.77522300	0.02815300	-1.43695500
P	1.05529500	-2.16300600	0.88761700
Co	0.86298100	-0.02193200	-0.20993200
H	-0.35643600	0.12899500	-2.67090300
P	1.33131600	1.36748200	1.59658900
C	1.75859500	3.12164700	1.15628900
H	1.91570900	3.73849800	2.04803300
H	2.67018700	3.13991500	0.55105200
H	0.94455400	3.54631600	0.56360100
C	2.75228100	0.97647700	2.73591900
H	3.68029100	0.90173100	2.16194200
H	2.87532900	1.74395800	3.50790200
H	2.58230700	0.01392100	3.22696400
C	-0.01390200	1.65185300	2.83789700
H	0.29023800	2.37450300	3.60306400
H	-0.90296900	2.01923500	2.32040900
H	-0.27494000	0.70582000	3.31743800

²IV^a

C	1.97563700	1.25240300	-0.35076600
C	1.41596200	2.19654500	-1.23948400
C	1.52564400	3.57185700	-1.08526900
H	1.08946400	4.22049700	-1.83764400
C	2.23126600	4.08352900	0.00857000
H	2.33546100	5.15576400	0.13768500
C	2.80335700	3.20461600	0.93103200
H	3.34607700	3.55666000	1.80154400
C	2.66095000	1.83867700	0.73439300
C	1.86521800	-0.20214600	-0.54332400
C	3.05337900	-1.04454100	-0.50094400
C	2.94622000	-2.44940000	-0.32854900
H	1.97098700	-2.89172800	-0.14481600
C	4.06780300	-3.27323300	-0.34488800
H	3.94462000	-4.34449900	-0.20299700
C	5.34541500	-2.73574600	-0.52135500
H	6.22022200	-3.37918300	-0.53111200
C	5.47699500	-1.34988700	-0.68002200
H	6.46209300	-0.91235200	-0.82255100

C	4.36138400	-0.52344400	-0.67117300
C	-3.16919800	-1.74411800	-2.64723300
H	-3.65079400	-2.64997000	-3.03161200
H	-2.37468400	-1.44063000	-3.33487100
H	-3.91006900	-0.93984200	-2.61368800
C	-3.92191800	-2.67283200	-0.05505400
H	-4.65593400	-1.87496100	0.09122200
H	-3.61626900	-3.03255700	0.93211900
H	-4.39666900	-3.49753900	-0.59795900
C	-1.49762800	-3.57486000	-1.25446500
H	-1.08886100	-3.94472400	-0.30976600
H	-0.66004700	-3.37692100	-1.92995200
H	-2.12753600	-4.35256600	-1.69953700
C	-2.55369400	2.29828200	-2.18148600
H	-3.12944800	3.22728500	-2.25966700
H	-2.99848800	1.54777200	-2.84144300
H	-1.52830500	2.46805700	-2.51659700
C	-4.32898500	1.57168700	-0.06262900
H	-4.47127400	1.35195600	0.99926800
H	-4.79698500	0.76748600	-0.63802300
H	-4.83388200	2.51446300	-0.30068700
C	-2.04071500	3.17459800	0.49317800
H	-1.00191500	3.43274100	0.27101600
H	-2.12054900	2.98296800	1.56745900
H	-2.68392900	4.02371400	0.23711900
C	-0.53793800	-2.24633300	2.74738100
H	-0.43810700	-2.33184400	3.83511900
H	0.43428400	-2.43046300	2.28259700
H	-1.23468100	-3.01382300	2.39681800
C	0.06412000	0.50894300	3.15306400
H	-0.23185800	1.55774000	3.05708300
H	1.05911500	0.39973800	2.71492700
H	0.11059700	0.24961300	4.21645900
C	-2.63751300	-0.40603200	3.33289400
H	-3.41947500	-1.09091300	2.99160300
H	-3.03252600	0.61254600	3.27059800
H	-2.40601600	-0.62834200	4.38068400
F	0.75728900	1.74893700	-2.33534900
F	3.18618300	1.01317600	1.67301600
H	4.49083600	0.54318300	-0.82579200
N	0.63132600	-0.71864700	-0.77338100
P	-2.43960000	-1.99875900	-0.95593100
P	-2.50970600	1.64150200	-0.44503100
P	-1.14077500	-0.56492800	2.23652600
Co	-1.13216400	-0.21048800	-0.08770800
H	0.71907700	-1.66323400	-1.13849500
${}^2V^a$			
C	3.01754100	-0.98027500	0.34315400

C	3.20603700	-1.87556200	1.42206300
C	4.39216600	-2.58847300	1.57602200
H	4.50617000	-3.25888500	2.42433200
C	5.43762400	-2.43363100	0.66238000
H	6.36237200	-2.99051800	0.78209300
C	5.27518300	-1.54670500	-0.40753400
H	6.07548300	-1.41793000	-1.13192700
C	4.09113200	-0.83579500	-0.56549600
C	1.73340300	-0.29657500	0.13927600
C	1.67032200	1.00513300	-0.51651600
C	0.60227400	1.44073100	-1.33730900
C	0.49418100	2.69393500	-1.91748100
H	-0.35766800	2.90387700	-2.55578300
C	1.50164300	3.63533200	-1.69453000
H	1.44377300	4.62069400	-2.14387600
C	2.58393800	3.28810900	-0.87961500
H	3.37856200	3.99012500	-0.65145700
C	2.63953700	2.02522200	-0.31379700
C	-1.98140500	-3.02400100	-2.01292600
H	-2.72126000	-3.63894900	-2.53760700
H	-1.29826600	-3.67530900	-1.46064500
H	-1.38913900	-2.46928000	-2.74599500
C	-4.03423700	-1.04643700	-1.95585500
H	-3.52574300	-0.41757300	-2.69241600
H	-4.70254700	-0.40830000	-1.37027800
H	-4.63187400	-1.79787200	-2.48362700
C	-3.83939200	-2.96112300	0.16606600
H	-4.48206300	-2.37231900	0.82643100
H	-3.20779900	-3.59927700	0.79102200
H	-4.46602000	-3.59656200	-0.46832700
C	-1.54309300	2.14790300	2.62107600
H	-2.11968400	2.98157200	3.03712500
H	-0.62764400	2.53275600	2.16349700
H	-1.24959300	1.47398700	3.43097400
C	-3.05576500	2.56518200	0.22710800
H	-3.75445800	2.17024500	-0.51588100
H	-2.18966000	2.96925700	-0.30440000
H	-3.54320200	3.37354200	0.78284100
C	-4.06184600	0.83728400	2.28184700
H	-3.86157900	0.09758600	3.06271600
H	-4.80976200	0.41716100	1.60283400
H	-4.47489600	1.73839400	2.74782000
N	0.58129900	-0.87238800	0.57229100
P	-2.76928900	-1.82240100	-0.83683100
P	-2.49544200	1.19348000	1.34630300
Co	-1.29089500	-0.49538200	0.33747100
H	0.79297800	-1.77773800	0.98360800
F	-0.40563200	0.55305900	-1.63760600
F	3.67580800	1.77144300	0.51377200

H	3.97538300	-0.17485200	-1.41902600
H	2.42711400	-1.98001800	2.17302300
²TS3^a			
C	1.39554800	1.22665100	-0.28103700
C	0.00430700	1.40817100	-0.67619100
C	-0.43337600	2.73712300	-1.01331400
H	-1.44114400	2.87258300	-1.39393600
C	0.40261200	3.81429800	-0.86720000
H	0.03489000	4.81531100	-1.07996900
C	1.75477200	3.65370800	-0.45602200
H	2.42503200	4.49722800	-0.34261300
C	2.20752700	2.38488300	-0.19362100
C	1.73597900	-0.06899500	0.21279800
C	3.12240200	-0.59559500	0.31522500
C	3.50442100	-1.35595100	1.43369500
H	2.80271200	-1.48501400	2.25332100
C	4.78114000	-1.91020300	1.51725600
H	5.06448100	-2.48248700	2.39629800
C	5.69547800	-1.72086400	0.47930700
H	6.69000200	-2.15345200	0.54194100
C	5.32650200	-0.96725400	-0.63798600
H	6.03260600	-0.81703700	-1.44982900
C	4.05432200	-0.40530700	-0.71817500
C	-3.61465200	-2.52761700	-1.24513200
H	-3.75796600	-3.53304900	-1.65567100
H	-3.72272000	-1.79708100	-2.05211300
H	-4.39863900	-2.33641000	-0.50643100
C	-1.92194700	-3.76693500	0.70303400
H	-2.64255200	-3.59723500	1.50857300
H	-0.93018100	-3.85597800	1.15596200
H	-2.16733700	-4.70886400	0.20059700
C	-0.84644500	-2.93662700	-1.83136300
H	0.16773600	-3.06275100	-1.44364900
H	-0.80163800	-2.17264000	-2.61174200
H	-1.19483100	-3.88304000	-2.25817400
C	-4.18468800	1.58553500	-0.49374300
H	-5.00678200	2.13703400	-0.02495100
H	-4.59413200	0.73374700	-1.04433300
H	-3.68363200	2.23955100	-1.21209200
C	-4.07851200	0.08555600	1.94196900
H	-3.50066500	-0.24478300	2.81020300
H	-4.49756800	-0.80081000	1.45791000
H	-4.90051000	0.72215100	2.28587900
C	-2.62319900	2.52728500	1.72705300
H	-1.98874500	3.18940200	1.13338000
H	-2.07283100	2.26397500	2.63492200
H	-3.54715700	3.04609800	2.00366900
F	-0.39842300	0.47200500	-1.81472600

F	3.49306100	2.24581200	0.21745700
H	3.76677300	0.17631200	-1.58776300
N	0.71031500	-0.83891600	0.57300300
P	-1.94023800	-2.32502200	-0.46769300
P	-2.95677600	0.98239400	0.76269300
Co	-1.11864900	-0.20121800	0.14527700
H	1.00643600	-1.78557400	0.79821400
²VI^a			
C	1.37374400	1.23458400	-0.40377600
C	0.05160800	1.68887200	-0.67054500
C	-0.11639500	3.00253200	-1.12734300
H	-1.11174400	3.35954400	-1.38183800
C	0.97156300	3.86565700	-1.28714700
H	0.81842900	4.87981300	-1.64911600
C	2.26483300	3.44062500	-0.97453200
H	3.12749700	4.09182500	-1.06219000
C	2.44256800	2.13663300	-0.53647600
C	1.49553600	-0.17260500	0.01640300
C	2.78516600	-0.92151200	0.08261400
C	3.09589700	-1.67935500	1.22148900
H	2.43537900	-1.64248800	2.08369300
C	4.25486000	-2.45511100	1.26338700
H	4.49134800	-3.02443700	2.15778400
C	5.10709100	-2.49638400	0.15933400
H	6.00732600	-3.10353900	0.18792500
C	4.79981100	-1.75181600	-0.98266300
H	5.45713400	-1.78509200	-1.84669700
C	3.65321200	-0.96163900	-1.01926200
C	-1.91533700	-2.79125100	-1.63317000
H	-2.58585300	-3.52164600	-2.09772200
H	-1.26871600	-3.30609100	-0.91650400
H	-1.29822500	-2.29657400	-2.38543700
C	-3.90727600	-2.37226600	0.40311300
H	-4.64144100	-1.70370900	0.86102000
H	-3.28810200	-2.79196700	1.20192100
H	-4.44285600	-3.19130400	-0.08872800
C	-4.05397500	-0.92893300	-2.09368000
H	-3.46305400	-0.41893000	-2.85688000
H	-4.78468900	-0.22888400	-1.67731800
H	-4.58230300	-1.78575300	-2.52392100
C	-0.54431700	1.61062700	2.70161000
H	-0.90353500	2.11228100	3.60584600
H	0.21257200	2.23011100	2.21602900
H	-0.07801900	0.66112300	2.97597600
C	-2.70244200	2.96003100	1.37461900
H	-3.61691300	2.89248700	0.77813200
H	-2.01206300	3.63594600	0.86532600
H	-2.94797300	3.37082900	2.35930400

C	-3.13982800	0.42863000	2.61696000
H	-2.78422200	-0.57864400	2.84966800
H	-4.10279200	0.34012200	2.10709900
H	-3.28742900	0.97825100	3.55248500
F	-1.23454800	0.00982400	-2.30369400
F	3.70555100	1.75972100	-0.21506700
H	3.41730900	-0.38300500	-1.90643800
N	0.37513200	-0.77480500	0.28031600
P	-2.84227700	-1.43260700	-0.79730300
P	-1.92165300	1.28633300	1.51042000
Co	-1.30558000	0.33239300	-0.46828800
H	0.51151700	-1.76201500	0.49317200

²II^a

C	2.82834700	-0.78054300	0.08788600
C	2.95993300	-1.78011000	1.08282500
C	4.15593300	-2.38041200	1.44049300
H	4.14991300	-3.12630200	2.22788300
C	5.33276100	-1.99645600	0.79266000
H	6.27965100	-2.45230800	1.06170100
C	5.27690600	-1.02456300	-0.20946800
H	6.15986700	-0.71187600	-0.75615200
C	4.05577600	-0.45905100	-0.54182500
C	1.54405900	-0.18987900	-0.29068900
C	1.42025900	1.21682600	-0.65292100
C	0.34535400	1.65658300	-1.47102800
C	0.13941000	3.01349900	-1.73700800
H	-0.67599600	3.31076200	-2.39269400
C	0.98786100	3.97931200	-1.19610200
H	0.82879200	5.03384600	-1.40136900
C	2.06577000	3.56335800	-0.39747500
H	2.73890200	4.30311800	0.02847600
C	2.28105500	2.21710700	-0.13597300
C	-2.30491500	-3.14251700	-1.95003700
H	-3.06635900	-3.89877300	-2.17077100
H	-1.45449500	-3.62297100	-1.45826200
H	-1.94423900	-2.71283600	-2.88881300
C	-4.46946800	-1.27925000	-1.80753600
H	-4.17149700	-0.78032100	-2.73449100
H	-5.05201100	-0.56789900	-1.21476600
H	-5.10314100	-2.13716700	-2.05670700
C	-3.71262100	-2.78138300	0.51112100
H	-4.26802100	-2.11996400	1.18122900
H	-2.92041500	-3.26061200	1.09324200
H	-4.38985500	-3.55246100	0.12800700
C	-0.93469700	1.95669700	2.40990100
H	-1.33314300	2.65784200	3.15150400
H	-0.17859500	2.45914200	1.80067000
H	-0.44788700	1.12316700	2.92354900

C	-3.07699500	2.86204200	0.74087500
H	-3.97285000	2.63056100	0.15706000
H	-2.38142700	3.40873000	0.09816700
H	-3.35773600	3.49876700	1.58646200
C	-3.49288100	0.66509700	2.53903200
H	-3.09148700	-0.22355300	3.03416600
H	-4.41761100	0.38111700	2.02767900
H	-3.72705100	1.41899700	3.29837400
F	1.84583400	-2.17526900	1.75603800
F	4.04447600	0.44028200	-1.55131600
H	3.10589900	1.92358900	0.50564300
N	0.39768200	-0.91670400	-0.25463200
P	-2.95274800	-1.78634600	-0.86033300
P	-2.26051100	1.29162800	1.30008900
Co	-1.39406900	-0.16475900	-0.26426000
H	0.58051700	-1.89197600	-0.05043800
H	-0.25862900	0.91230100	-1.98912600

²TS1^a

C	2.77462700	-0.61618600	0.16516800
C	3.16757700	-0.97201100	1.46155000
C	4.43669900	-1.44175500	1.77576000
H	4.67207100	-1.68836200	2.80474300
C	5.37119400	-1.57728700	0.74859100
H	6.36767900	-1.94444200	0.97228000
C	5.03277900	-1.24851100	-0.56408100
H	5.73527600	-1.35303000	-1.38301500
C	3.75109200	-0.77783100	-0.82604100
C	1.39437600	-0.12811700	-0.13063400
C	1.13560500	1.17669300	-0.71223900
C	-0.24176200	1.43897300	-1.01176500
C	-0.52854500	2.71481100	-1.56259900
H	-1.55302700	2.95372300	-1.84242100
C	0.46191400	3.66727000	-1.76274700
H	0.19845900	4.64119900	-2.17031800
C	1.80575800	3.38827700	-1.45059900
H	2.57481700	4.13680400	-1.61661500
C	2.13622300	2.14444800	-0.93644700
C	-2.00980900	-2.91668400	-2.08088700
H	-2.68511800	-3.74953100	-2.30693800
H	-1.08134300	-3.31020600	-1.65804600
H	-1.75513600	-2.38975000	-3.00372800
C	-4.35810300	-1.32302900	-1.75562900
H	-4.14752800	-0.74010500	-2.65652500
H	-4.99425400	-0.71786700	-1.10285200
H	-4.90116200	-2.23229000	-2.03613600
C	-3.37249900	-2.88297800	0.41851500
H	-3.97606000	-2.33706600	1.14881100
H	-2.51837100	-3.31575600	0.94842200

H	-3.97366100	-3.69618700	-0.00390900
C	-0.56711700	1.49029800	2.57286100
H	-0.86665700	1.99652200	3.49648700
H	0.05642300	2.15991100	1.97498900
H	0.03340500	0.61015100	2.81397100
C	-2.92268000	2.59835400	1.38399300
H	-3.90000200	2.43468600	0.91992200
H	-2.34016500	3.25224600	0.72933500
H	-3.06770300	3.09125200	2.35122700
C	-3.07861000	0.15111300	2.84641300
H	-2.60701200	-0.78591000	3.15638100
H	-4.05895900	-0.08738000	2.42285800
H	-3.22148400	0.78367000	3.72962900
F	2.26877500	-0.84791300	2.46467300
F	3.42739700	-0.47794400	-2.09735500
H	3.16990400	1.92266500	-0.68463700
N	0.34856300	-0.86241400	0.13568900
P	-2.75964500	-1.70758800	-0.89011800
P	-2.02734300	0.98205900	1.55586600
Co	-1.44594800	0.05138900	-0.42196500
H	0.58799900	-1.77025500	0.52916000
H	-0.94077500	0.28522900	-1.85703400

²III^a

C	2.76020800	-0.63871600	0.16482000
C	3.17746900	-0.90453100	1.47346400
C	4.44254500	-1.38399300	1.78987700
H	4.70066400	-1.55974600	2.82788200
C	5.34362400	-1.62208600	0.75139800
H	6.33591900	-1.99965100	0.97637300
C	4.97893200	-1.38157500	-0.57353100
H	5.65677500	-1.56462500	-1.39940400
C	3.70327000	-0.89549400	-0.83707600
C	1.37921800	-0.14680500	-0.13660100
C	1.13502900	1.17329900	-0.71504200
C	-0.23256800	1.47989800	-0.97490300
C	-0.48650000	2.74964000	-1.52996200
H	-1.50931800	3.03349400	-1.77353400
C	0.53717600	3.66024700	-1.79612600
H	0.29951500	4.63134100	-2.22625900
C	1.87297200	3.33617500	-1.51912900
H	2.66665400	4.04842000	-1.72572400
C	2.16998000	2.09065200	-0.98068800
C	-1.94169200	-3.17184800	-1.50351700
H	-2.63335100	-3.98459700	-1.75005500
H	-1.20196500	-3.54186800	-0.78776100
H	-1.41024100	-2.85188300	-2.40209600
C	-4.16377700	-1.44010700	-2.03605900
H	-3.70857200	-1.07952800	-2.96126200

H	-4.85227700	-0.66961500	-1.67593600
H	-4.73038000	-2.35576700	-2.23689000
C	-3.80516600	-2.55619200	0.55823900
H	-4.54256300	-1.86050700	0.96888100
H	-3.13812300	-2.85733500	1.37121600
H	-4.33128000	-3.44194900	0.18558100
C	-0.49796100	1.73828600	2.41382300
H	-0.80040600	2.21186900	3.35344300
H	0.00172000	2.47317800	1.77899100
H	0.21557900	0.93775700	2.62285800
C	-3.02571000	2.55096100	1.34056500
H	-4.00596200	2.26555500	0.94716400
H	-2.56084600	3.23961000	0.63011100
H	-3.16276100	3.06217600	2.29948000
C	-2.81783900	0.15412500	2.88514800
H	-2.22829200	-0.71819900	3.18222700
H	-3.79590600	-0.19832700	2.54736900
H	-2.95729300	0.79927000	3.75939300
F	2.30756400	-0.67896100	2.48479000
F	3.34976900	-0.67474400	-2.11606000
H	3.20199800	1.83300900	-0.75704800
N	0.34137200	-0.88094800	0.12587700
P	-2.82495400	-1.71185200	-0.78326800
P	-1.95267300	1.04707000	1.50273300
Co	-1.46733300	0.06304600	-0.51547600
H	0.58626000	-1.78653400	0.52283000
H	-1.29400200	-0.19769800	-1.99985800
1			
C	1.55749500	1.30568200	0.08336300
C	0.13964100	1.53853500	0.03139400
C	-0.26207900	2.89199600	0.07249400
H	-1.31728400	3.13986900	0.01744200
C	0.63934000	3.95012000	0.18496000
H	0.27798600	4.97585400	0.20576800
C	2.01386500	3.70353200	0.28751700
H	2.74236100	4.49844700	0.40371100
C	2.44007800	2.38989200	0.24446600
C	1.91887400	-0.09368700	0.00014100
C	3.27843700	-0.68544400	-0.07128500
C	4.23876300	-0.23337300	-0.99359400
H	4.00967500	0.61625500	-1.62722700
C	5.47228900	-0.87026400	-1.10555400
H	6.19733700	-0.51029400	-1.83035100
C	5.77981300	-1.96709100	-0.29574700
H	6.74527500	-2.45738300	-0.38223800
C	4.83901200	-2.42388200	0.62822400
H	5.07145100	-3.26732000	1.27273700
C	3.60072300	-1.79101900	0.73649700

C	-0.98652200	1.64971600	-3.07400000
H	-1.58862500	2.03685500	-3.90405100
H	-0.21852100	0.97816000	-3.46907200
H	-0.48166300	2.47495700	-2.56975600
C	-3.41577300	1.92957000	-1.59190800
H	-3.08213200	2.76267800	-0.97055300
H	-4.23535600	1.42638100	-1.06934100
H	-3.79133100	2.32862100	-2.54123400
C	-2.91017500	-0.37914400	-3.08606000
H	-3.71641900	-0.94277900	-2.61006200
H	-2.20803100	-1.08740300	-3.53366200
H	-3.34574600	0.22563700	-3.88920600
C	-2.40539700	2.08915900	2.42181500
H	-2.71314600	2.11790100	3.47275900
H	-3.25916100	2.36798500	1.79734000
H	-1.60956400	2.81744700	2.26257000
C	-3.25419400	-0.54963700	2.70387300
H	-3.06189400	-1.62489700	2.72187700
H	-4.15180500	-0.37523700	2.10246100
H	-3.45348100	-0.22042100	3.72972200
C	-0.55652500	0.13213900	3.30748000
H	0.31668200	0.74983300	3.08187000
H	-0.23249800	-0.91226800	3.30954900
H	-0.94208300	0.39318100	4.29973400
C	-1.07340300	-3.29683800	-1.59883600
H	-1.33764800	-4.35411400	-1.48794600
H	0.01339900	-3.21002200	-1.67940400
H	-1.50552200	-2.92184100	-2.52862600
C	-1.07405000	-3.36773900	1.22467300
H	-1.44902300	-3.00166900	2.18276600
H	0.01791700	-3.33316300	1.26451400
H	-1.38884300	-4.40859900	1.09476300
C	-3.47960000	-2.77396000	-0.17962500
H	-3.96650300	-2.36806500	-1.06871900
H	-3.98678600	-2.36633900	0.69623000
H	-3.59467200	-3.86299400	-0.18399300
F	3.77446900	2.16506700	0.37533700
H	2.88065500	-2.13588800	1.47414100
N	0.85782300	-0.87707400	-0.05547600
H	1.12727300	-1.85413100	-0.15323800
P	-2.02485200	0.70942100	-1.85042700
P	-1.81414600	0.38448800	1.95960700
P	-1.68707500	-2.28493100	-0.16170300
Co	-0.92036400	-0.11353900	-0.06203200
3^b			
C	2.04876300	1.36338300	-0.10668000
C	3.30650600	1.72212200	0.44977200
C	3.65759700	3.04972200	0.65624400

H	4.62897300	3.27892100	1.08795400
C	2.77813300	4.09108600	0.32781000
H	3.05870500	5.12573100	0.48981700
C	1.52919400	3.76472700	-0.21215200
H	0.83225000	4.55382500	-0.48067300
C	1.17131200	2.43525300	-0.42194700
C	1.63435400	-0.01515100	-0.29444000
C	2.60943700	-1.11344100	-0.28554700
C	3.84265400	-1.08454700	-0.98543200
C	4.74435500	-2.13641600	-1.02604000
H	5.65989300	-2.01262800	-1.59513300
C	4.43918800	-3.33006200	-0.36674000
H	5.13414900	-4.16445700	-0.39177200
C	3.22803000	-3.44265200	0.31989600
H	2.94969600	-4.34457200	0.85291300
C	2.36256700	-2.36030800	0.33888700
C	-2.02791300	0.22808800	3.61384300
H	-1.79877400	0.70525000	4.57164700
H	-1.89371300	-0.85086800	3.72352200
H	-3.07188400	0.42589200	3.36082000
C	0.73309600	0.30996600	2.95683100
H	1.53818600	0.86400900	2.46968400
H	0.87494900	-0.75089000	2.73505700
H	0.78562700	0.47607900	4.03831300
C	-0.88641100	2.67272000	2.68075300
H	-1.87212100	3.09534400	2.47082500
H	-0.14919500	3.17040900	2.04684400
H	-0.63547600	2.84755900	3.73271200
C	-4.28780300	-2.05267200	0.08627600
H	-4.63450600	-3.09051900	0.15740100
H	-4.60438100	-1.63911300	-0.87612400
H	-4.76458300	-1.45987400	0.87197500
C	-1.87209600	-3.12647400	-1.04232200
H	-0.81008400	-3.33768200	-0.88737100
H	-1.99269800	-2.70309600	-2.04439200
H	-2.42220800	-4.07201300	-0.99061100
C	-2.17516700	-2.98494900	1.75809200
H	-2.66571300	-2.53985100	2.62613600
H	-1.10360000	-3.06019300	1.95652500
H	-2.58112100	-3.99226400	1.60947000
N	0.32225300	-0.31719500	-0.47386300
H	0.23376100	-1.29143500	-0.73526800
P	-0.89805500	0.86310300	2.28697700
P	-2.44195600	-1.91828000	0.25814500
Co	-1.48577400	0.42409600	0.06826100
C	-3.22026200	1.39111800	0.45910400
H	-3.04598900	2.47562700	0.39727300
H	-4.02160900	1.15249000	-0.25440600
H	-3.63953600	1.19214900	1.45361600

P	-1.95121200	0.80823700	-2.22874300
C	-0.68351000	0.24138300	-3.44909100
H	0.29000700	0.64588500	-3.16663600
H	-0.60562800	-0.84911600	-3.42074700
H	-0.93681300	0.55304100	-4.46815400
C	-2.09734800	2.60883300	-2.64985700
H	-2.88619400	3.05754600	-2.04166500
H	-1.15668000	3.11798400	-2.42242800
H	-2.32845500	2.75478200	-3.70967200
C	-3.51308400	0.16000300	-2.99693300
H	-3.49964600	-0.93314200	-3.00550900
H	-4.37629500	0.48914900	-2.41395400
H	-3.62246800	0.51371500	-4.02608100
H	0.20334200	2.20170300	-0.84993200
H	4.00162900	0.94251600	0.74245800
F	4.15461500	0.02793800	-1.68532700
F	1.20239800	-2.51309300	1.05020900

¹H^b

C	1.20831900	1.34116600	-0.63259400
C	2.15482600	2.37388800	-0.44298700
C	1.82547200	3.68873100	-0.71726500
H	2.55558100	4.47639100	-0.55504700
C	0.54082600	4.00909000	-1.21139700
H	0.29314100	5.04376000	-1.43385400
C	-0.39101800	3.01114000	-1.43309000
H	-1.36165700	3.25677400	-1.85331600
C	-0.09600600	1.65896800	-1.12966700
C	1.40062900	-0.02387600	-0.21882000
C	2.72846400	-0.61834600	0.06395000
C	3.83197000	-0.46697100	-0.79377100
C	5.08003700	-1.02530800	-0.54583300
H	5.87865600	-0.86543900	-1.26127700
C	5.26194300	-1.78662700	0.60832700
H	6.22983800	-2.23067600	0.81680000
C	4.20082100	-1.98562100	1.49256400
H	4.30730500	-2.57179700	2.39818100
C	2.97404800	-1.40642900	1.20126500
C	-3.00817300	0.07503400	2.69860600
H	-3.15013300	0.60190100	3.64889800
H	-2.64728800	-0.93646400	2.90572800
H	-3.97202600	-0.00358800	2.18826500
C	-0.33263700	1.10612500	2.71061700
H	0.39828200	1.77027300	2.24095500
H	0.14257900	0.13130800	2.84086000
H	-0.60918300	1.51416200	3.68849000
C	-2.46892200	2.67572800	1.65809200
H	-3.44707300	2.71021900	1.17254800
H	-1.79453900	3.33928400	1.11010000

H	-2.56584600	3.02910400	2.69009600
C	-2.60525300	-2.31089100	-2.68153800
H	-3.10607500	-3.27261000	-2.84122100
H	-1.62834100	-2.32666500	-3.17274500
H	-3.20012000	-1.51726600	-3.14040600
C	-1.50251200	-3.49059000	-0.33845200
H	-1.35627900	-3.48258200	0.74632500
H	-0.52127800	-3.55320800	-0.81842600
H	-2.07417300	-4.38522800	-0.60686700
C	-4.07915700	-2.27971900	-0.24209500
H	-4.75668800	-1.49267900	-0.58084500
H	-4.07305700	-2.27470800	0.85123100
H	-4.45142600	-3.24866400	-0.59175700
N	0.28568200	-0.72491600	-0.07833800
H	0.44561500	-1.67952500	0.22651600
P	-1.80080900	0.94961100	1.59046800
P	-2.37030000	-1.93291000	-0.87722800
Co	-1.44872100	0.04850100	-0.38779400
C	-3.14996400	0.89309800	-1.07432900
H	-3.03190700	1.98316300	-1.11002600
H	-3.38123600	0.56987200	-2.10044300
H	-4.04933700	0.69831400	-0.47260400
H	-0.63610000	0.88039100	-1.74222400
H	3.13604600	2.13435500	-0.04393000
F	3.67277900	0.23823700	-1.92957300
F	1.95686300	-1.61772200	2.07298400

³II^b

C	1.80017300	1.35103200	-0.31553300
C	2.88415500	1.86748500	0.42493900
C	3.19148800	3.22508500	0.39615600
H	4.02671500	3.59767900	0.98295100
C	2.43375600	4.10616800	-0.38074000
H	2.67820600	5.16413000	-0.40708900
C	1.36236200	3.60858700	-1.12858000
H	0.77623300	4.27832800	-1.75250900
C	1.04336000	2.25267000	-1.09281500
C	1.45003100	-0.07670200	-0.27957200
C	2.48127200	-1.09138300	0.03806100
C	3.76642600	-1.09894800	-0.53957800
C	4.73024000	-2.05994000	-0.26607500
H	5.69183300	-1.99320000	-0.76242700
C	4.42578200	-3.09330900	0.62126300
H	5.16673800	-3.85404600	0.84364400
C	3.16592000	-3.15020700	1.21948200
H	2.89563400	-3.93309000	1.91916800
C	2.23756800	-2.16483200	0.91789400
C	-3.59507800	1.37652300	2.00890600
H	-3.71919700	2.06354900	2.85289500

H	-3.66248800	0.34972200	2.38019900
H	-4.41197000	1.53656600	1.29918200
C	-0.77491700	1.47635700	2.54926300
H	0.22153700	1.75781200	2.19875100
H	-0.73175400	0.43442000	2.87859200
H	-1.05286000	2.11426700	3.39529100
C	-2.00262600	3.45781900	0.87210200
H	-2.76724200	3.69874700	0.12806800
H	-1.03411100	3.77794800	0.47988100
H	-2.21526800	4.00392100	1.79739900
C	-2.38211200	-3.07630400	-1.69599700
H	-2.97681700	-3.99299400	-1.62022400
H	-1.32124800	-3.34123900	-1.64774200
H	-2.56330800	-2.60194600	-2.66394900
C	-2.57479900	-2.93168000	1.15790500
H	-2.95187200	-2.40221200	2.03831200
H	-1.50856600	-3.11893100	1.31589000
H	-3.10052200	-3.88921600	1.07216400
C	-4.63627100	-1.78685700	-0.49328600
H	-4.89653100	-1.27641000	-1.42438800
H	-5.04767400	-1.20539100	0.33691000
H	-5.09066400	-2.78321400	-0.48740000
N	0.20013500	-0.46380400	-0.50383600
H	0.15932000	-1.47937100	-0.51852000
P	-1.97134900	1.62440800	1.14194600
P	-2.78936100	-1.86336300	-0.35171400
Co	-1.61959700	0.25566200	-0.84594000
C	-2.44343500	0.86187500	-2.60500300
H	-2.00629300	1.80660800	-2.95956000
H	-2.30586800	0.12434900	-3.40824600
H	-3.52603500	1.02979800	-2.49838000
H	0.22198500	1.87483400	-1.69423100
H	3.47956500	1.19812800	1.03832800
F	4.07701900	-0.13185600	-1.42427300
F	1.02649100	-2.23838000	1.52961000

¹TS1^b

C	1.20168400	1.43190200	-0.40973500
C	2.23210500	2.39425600	-0.43939200
C	1.92356000	3.72706800	-0.64875400
H	2.70761100	4.47819600	-0.66950400
C	0.57879600	4.09559300	-0.84399100
H	0.33334400	5.14249700	-1.01093900
C	-0.43932900	3.15060100	-0.82583500
H	-1.46031100	3.47728400	-0.99517800
C	-0.17905500	1.77929500	-0.58770500
C	1.41483600	0.02390600	-0.18252600
C	2.76153600	-0.59222600	-0.00930300
C	3.71911500	-0.60222800	-1.03099700

C	4.97227100	-1.18767500	-0.89225300
H	5.66305700	-1.16420500	-1.72724300
C	5.29856100	-1.79261200	0.32177700
C	4.38274400	-1.81140300	1.37437800
H	4.61252400	-2.26878500	2.32983600
C	3.14266500	-1.21520400	1.18435700
C	-3.51100300	0.45227500	2.50423100
H	-3.52954900	0.51426200	3.59718500
H	-4.12699100	-0.39308700	2.18641100
H	-3.94508700	1.36215600	2.08417700
C	-1.23812300	-1.24521700	2.84509500
H	-0.17205800	-1.41280100	2.67489400
H	-1.78498400	-2.13130400	2.50781100
H	-1.41108600	-1.11547500	3.91896300
C	-0.89849300	1.58830100	2.77766100
H	-1.21117200	2.55493700	2.37439000
H	0.17547000	1.48845700	2.59974000
H	-1.09312000	1.55932700	3.85505000
C	-3.16801600	-1.13693800	-2.95258900
H	-3.71919500	-1.99010600	-3.36295000
H	-2.33287500	-0.88911600	-3.61289000
H	-3.82696900	-0.26683300	-2.90596200
C	-1.55709500	-3.04816700	-1.57355700
H	-1.22715500	-3.48478900	-0.62510900
H	-0.67061200	-2.81876200	-2.17149900
H	-2.16005700	-3.79200700	-2.10495100
C	-4.02427300	-2.18014200	-0.44096200
H	-4.74650200	-1.37725000	-0.26970700
H	-3.75612200	-2.61065800	0.52877800
H	-4.49723200	-2.95678500	-1.05170600
N	0.32739200	-0.69890000	-0.13769800
H	0.48482800	-1.69069500	0.01730300
P	-1.78315900	0.23970800	1.87041900
P	-2.50720800	-1.48085600	-1.25755600
Co	-1.38458900	0.28025900	-0.36596400
C	-3.02463200	1.40976600	-0.65599900
H	-3.00456600	2.29059000	-0.00121600
H	-3.06079600	1.77389300	-1.68959500
H	-3.97121500	0.88810700	-0.45582900
H	-0.87054300	0.81143900	-1.66995300
H	3.26440200	2.08986000	-0.28703400
H	6.27297100	-2.25318800	0.44870600
F	3.40140700	-0.03105400	-2.20675700
F	2.26353900	-1.22667300	2.21304400
¹III^b			
C	1.21565500	1.39030800	-0.51709800
C	2.27457900	2.31272500	-0.62685700
C	1.99584200	3.64378800	-0.89883500

H	2.79966600	4.36880600	-0.98814100
C	0.65930600	4.03801800	-1.06433900
H	0.43515000	5.07954800	-1.28698300
C	-0.38522600	3.11946000	-0.95175500
H	-1.40135600	3.47247700	-1.10061100
C	-0.15548500	1.76190200	-0.66177800
C	1.41277800	-0.01963200	-0.24578400
C	2.75633900	-0.63029700	-0.01780200
C	3.67556300	-0.82954800	-1.05269700
C	4.92308000	-1.41077800	-0.85532900
H	5.58663700	-1.54313500	-1.70214200
C	5.27994800	-1.80737000	0.43399100
C	4.40170000	-1.62683600	1.50364600
H	4.65779600	-1.92085500	2.51500800
C	3.16568900	-1.04471500	1.25282300
C	-3.39480000	0.79487200	2.46602700
H	-3.39011000	0.93046800	3.55240200
H	-4.07817700	-0.01966400	2.21192700
H	-3.76653200	1.70550400	1.99070600
C	-1.23435800	-1.04742600	2.86590400
H	-0.17747100	-1.27416800	2.70506400
H	-1.82472800	-1.92003500	2.57100400
H	-1.39635700	-0.85802500	3.93236300
C	-0.69739800	1.73848300	2.64271700
H	-0.91461700	2.70045900	2.17239500
H	0.36325900	1.52505500	2.48711700
H	-0.90123400	1.79728300	3.71721600
C	-3.41557600	-1.39278100	-2.70301300
H	-4.01936600	-2.27043100	-2.95680700
H	-2.63462300	-1.25350400	-3.45438500
H	-4.04679500	-0.50140800	-2.70841800
C	-1.70002800	-3.15856500	-1.25670900
H	-1.30617500	-3.49814100	-0.29320400
H	-0.85795000	-3.00067700	-1.93652600
H	-2.34236600	-3.94568600	-1.66477800
C	-4.06637400	-2.12934700	-0.02757800
H	-4.76377600	-1.29716700	0.10240300
H	-3.72695400	-2.44829200	0.96245100
H	-4.59733600	-2.96208100	-0.50115900
N	0.33086700	-0.73703600	-0.18600300
H	0.49017200	-1.72295900	0.00454600
P	-1.69957400	0.41739000	1.82194500
P	-2.61763600	-1.55737800	-1.04334300
Co	-1.38342700	0.26548800	-0.47965100
C	-2.98910100	1.41876300	-0.82406700
H	-2.94610700	2.31720100	-0.19645000
H	-3.00709200	1.74571100	-1.86850200
H	-3.95009200	0.92917800	-0.60689200
H	-1.13712800	0.30504100	-1.92567900

H	3.30330800	1.98471700	-0.49852300
H	6.25041800	-2.26116700	0.60716700
F	3.32367100	-0.45227000	-2.29466800
F	2.31652300	-0.85876500	2.29046600
¹TS2^b			
C	1.21757700	1.40199100	-0.46758500
C	2.22344900	2.38639900	-0.43854700
C	1.88528300	3.72259400	-0.60616400
H	2.65446600	4.48950400	-0.58780800
C	0.54059800	4.07024800	-0.79912100
H	0.27143600	5.11606500	-0.93380800
C	-0.45503800	3.09152700	-0.81395800
H	-1.48471400	3.40922200	-0.95951900
C	-0.16290300	1.72404000	-0.64595500
C	1.44569800	-0.01717900	-0.27089800
C	2.77373600	-0.62858300	0.00618000
C	3.86352100	-0.50898600	-0.86769700
C	5.10461200	-1.08592800	-0.62448400
H	5.89895300	-0.95444000	-1.35030700
C	5.28496400	-1.82536100	0.54431500
C	4.23337100	-1.98671400	1.44731900
H	4.34292200	-2.55510900	2.36382000
C	3.01238800	-1.39306000	1.15673800
C	-2.83602400	2.23333100	1.89715200
H	-2.94488700	2.47468100	2.95959900
H	-3.83165700	2.11350800	1.45912500
H	-2.33843000	3.06312700	1.38904200
C	-2.75297000	-0.46627200	2.78403100
H	-2.21730900	-1.41809600	2.85163200
H	-3.75388700	-0.66515800	2.39055200
H	-2.85230400	-0.05034000	3.79279200
C	-0.36463900	1.06624200	2.70241200
H	0.17705800	1.91162400	2.27239300
H	0.31159100	0.20782700	2.71396200
H	-0.66021400	1.30859100	3.72875900
C	-2.47380600	-2.36549600	-2.65165300
H	-3.01300300	-3.30995200	-2.78287500
H	-1.44038800	-2.48643200	-2.98718600
H	-2.93720600	-1.59714200	-3.27587500
C	-1.84485800	-3.33141200	-0.04468100
H	-1.85061900	-3.19218800	1.03973900
H	-0.81632000	-3.53574000	-0.35724000
H	-2.45510100	-4.20574900	-0.29307200
C	-4.28285300	-1.91417600	-0.49094100
H	-4.81522100	-1.09884600	-0.98732400
H	-4.43315500	-1.80890500	0.58648000
H	-4.71091100	-2.86856800	-0.81554800
N	0.36004200	-0.74514500	-0.31031300

H	0.52573400	-1.73177700	-0.12965600
P	-1.83868000	0.69040000	1.64158900
P	-2.47229600	-1.79790000	-0.88682200
Co	-1.34935900	0.18395100	-0.57478900
C	-2.86041400	1.18694500	-1.66715600
H	-3.37935500	1.63843600	-0.81640200
H	-2.58231200	2.00114700	-2.34224500
H	-3.57433000	0.55107500	-2.19986500
H	-1.56485600	0.49399900	-1.98843200
H	3.26149800	2.10793700	-0.28000300
H	6.24759200	-2.28177400	0.75095400
F	3.69447200	0.18252200	-2.00990700
F	1.99795300	-1.56314300	2.03907100

¹IV^b

C	2.94654600	-0.36618700	0.23871700
C	4.00392300	-0.20915200	-0.66833000
C	5.30430000	-0.62340100	-0.40595900
H	6.06826600	-0.47283300	-1.16018100
C	5.58158800	-1.23291400	0.81770700
H	6.59146500	-1.56222800	1.03997800
C	4.56642200	-1.42762300	1.75513300
H	4.75084400	-1.89739900	2.71452700
C	3.28256500	-0.99812600	1.44547500
C	1.55690200	0.07298400	-0.04939800
C	1.15272900	1.43667400	-0.36156400
C	2.02845300	2.51121400	-0.57935900
H	3.10110500	2.38471300	-0.46478800
C	1.51624500	3.74771700	-0.96492200
H	2.18396600	4.58668100	-1.13954000
C	0.13615500	3.89079800	-1.14115400
H	-0.26832400	4.84906300	-1.46147800
C	-0.72904200	2.81894000	-0.88662400
H	-1.79755200	2.98739200	-1.01756800
C	-0.26747400	1.56359700	-0.45292400
C	-3.75232100	-2.82769700	-0.44549200
H	-3.96725800	-3.67618000	-1.10421200
H	-4.54211100	-2.08104600	-0.56921200
H	-3.77012500	-3.17509500	0.59149300
C	-2.27228300	-1.82635300	-2.66700500
H	-1.31283400	-1.50395000	-3.07909100
H	-3.00303300	-1.03785900	-2.86571700
H	-2.59327200	-2.74665700	-3.16765300
C	-1.04327500	-3.59730000	-0.78553200
H	-0.92824000	-3.93859600	0.24803400
H	-0.05122000	-3.36817400	-1.18496100
H	-1.47871900	-4.41002300	-1.37638000
F	3.74309000	0.34953600	-1.86659100
F	2.30653000	-1.19407900	2.35842800

N	0.55496100	-0.77163500	-0.00239500
H	0.82264500	-1.71427300	0.26891100
P	-2.09814800	-2.06364300	-0.83183800
Co	-1.21910000	-0.09976000	-0.12625400
P	-2.87249400	0.85179900	0.98014800
C	-2.32809300	2.20804500	2.12103200
H	-1.54679400	1.81849900	2.77907200
H	-1.89434300	3.02360500	1.54034800
H	-3.15978500	2.58392700	2.72701600
C	-4.35143100	1.65200000	0.17481200
H	-5.03540100	2.08342200	0.91420700
H	-4.01845100	2.44380600	-0.50157900
H	-4.89358300	0.90953500	-0.41854800
C	-3.73376200	-0.25285400	2.20491400
H	-2.98546200	-0.73045500	2.84358300
H	-4.42848500	0.31315400	2.83511800
H	-4.28816500	-1.03767700	1.68591200

³2

C	3.38661900	0.17036800	-0.04112400
C	4.14923500	-0.33987700	1.01164600
C	5.50477800	-0.07529000	1.16641500
H	6.03853900	-0.50164000	2.00809900
C	6.13604900	0.73865600	0.22407200
H	7.19435000	0.95666000	0.32548600
C	5.41892200	1.27829500	-0.84487000
H	5.88607900	1.91389200	-1.58845500
C	4.06445000	0.98457500	-0.95126400
C	1.91113500	-0.08877900	-0.15311200
C	1.40471700	-1.32751000	-0.76270700
C	2.31884600	-2.27763600	-1.25960300
H	3.38892300	-2.09271300	-1.20326400
C	1.85816600	-3.45905300	-1.82925700
H	2.55835600	-4.19537500	-2.21421200
C	0.47966200	-3.67767500	-1.89718300
H	0.10067500	-4.59672100	-2.34162700
C	-0.41160700	-2.72041800	-1.39992300
H	-1.47275800	-2.94953400	-1.48565000
C	-0.01146400	-1.50392400	-0.80911500
C	-2.95246700	3.32734200	-1.13505700
H	-2.74866600	4.36614100	-1.41814100
H	-3.69779700	3.32161600	-0.33455300
H	-3.37829100	2.81084000	-2.00037000
C	-0.29670900	2.85675900	-2.01120400
H	-0.65223200	2.32416100	-2.89858300
H	0.71520400	2.50377200	-1.80009300
H	-0.27551000	3.93116700	-2.22657000
C	-0.81469600	3.69084800	0.67825200
H	0.17558800	3.41081400	1.04531300

H	-1.49928500	3.69516900	1.53168400
H	-0.76224600	4.70295000	0.26119900
C	-2.80147200	0.25062700	3.35380800
H	-2.71343700	-0.09196400	4.39121900
H	-3.72744400	-0.15147800	2.93119800
H	-2.87996900	1.34231700	3.34995100
C	-1.28987400	-2.08434100	2.71292600
H	-0.40285300	-2.51287300	2.23983700
H	-2.16346600	-2.58590400	2.28799900
H	-1.26029200	-2.26934700	3.79260100
C	0.04167400	0.33839600	3.37364800
H	0.07211200	1.43183500	3.34396500
H	0.98822000	-0.03855800	2.97885300
H	-0.06827900	0.01521100	4.41470300
F	3.52683400	-1.11543500	1.92492300
F	3.36442000	1.51010500	-1.98006200
N	1.07676600	0.78526800	0.30234500
H	1.55942700	1.58588100	0.71241900
P	-1.40691900	2.44705600	-0.57572200
P	-1.35117500	-0.27364300	2.30274600
Co	-1.15466400	0.09129800	-0.03865300
P	-3.44490900	-0.66340000	-0.71741100
C	-3.57274800	-0.89675200	-2.55949900
H	-3.44484600	0.07171000	-3.05315300
H	-2.76132300	-1.54744900	-2.89462700
H	-4.53439500	-1.32468500	-2.86470000
C	-4.02476000	-2.33175500	-0.12210700
H	-4.93948300	-2.65686600	-0.63095100
H	-3.24273400	-3.07770500	-0.27913200
H	-4.22607400	-2.27878300	0.95240600
C	-5.02240300	0.28832300	-0.41492200
H	-4.96045200	1.27497900	-0.88031300
H	-5.90083100	-0.23223600	-0.81334400
H	-5.15881600	0.43348500	0.66118000
³TS3^b			
C	1.67091900	1.14022500	-0.62640000
C	1.10963300	1.97802800	-1.61417500
C	1.24428200	3.35768700	-1.64006200
H	0.79175400	3.91571500	-2.45242400
C	1.98438900	3.98527100	-0.63470700
H	2.10628800	5.06333800	-0.64044400
C	2.56292700	3.21936100	0.37895800
H	3.12873900	3.66844300	1.18781600
C	2.39284400	1.84138700	0.36175600
C	1.44283800	-0.31500600	-0.61574600
C	2.52697700	-1.25423800	-0.40355500
C	2.24570100	-2.62680600	-0.17771900
H	1.20647800	-2.93264500	-0.13738200

C	3.26703400	-3.55288500	-0.00408400
H	3.01810900	-4.59566900	0.17645300
C	4.60757000	-3.15461600	-0.05651300
H	5.40428800	-3.88034800	0.07921800
C	4.90849400	-1.80837600	-0.29399200
H	5.94515300	-1.48703500	-0.35488000
C	3.89403700	-0.87554000	-0.46583500
C	-3.00817000	1.17493400	-2.02773300
H	-3.76679100	1.27884400	-2.81094300
H	-2.01329200	1.32426800	-2.45363200
H	-3.17026000	1.95141100	-1.27429100
C	-4.82690900	-0.58424600	-0.64952000
H	-4.99550100	0.14644200	0.14666600
H	-5.01876400	-1.57821300	-0.23770000
H	-5.52989300	-0.38883000	-1.46599300
C	-3.09707600	-1.62038400	-2.68645900
H	-3.24143600	-2.65004200	-2.34713900
H	-2.13648200	-1.56871700	-3.20721500
H	-3.89534300	-1.36064100	-3.38979700
C	-1.21952700	2.32381800	1.69077500
H	-1.20173600	2.91134700	2.61512300
H	-2.08366700	2.63080800	1.09444400
H	-0.31680600	2.53467500	1.11378900
C	-2.78405500	0.45744100	3.19116600
H	-2.90005700	-0.55515700	3.58405600
H	-3.69642600	0.70975100	2.64314700
H	-2.66369000	1.15737100	4.02466400
C	0.07406700	0.25676600	3.22256500
H	1.02328000	0.41340700	2.70507700
H	0.05233600	-0.77308600	3.59022900
H	0.01086800	0.94103600	4.07549100
F	0.41813700	1.40333900	-2.63137500
F	2.91792500	1.13736600	1.39387800
H	4.15501600	0.15484900	-0.68201900
N	0.14650400	-0.77745100	-0.85793500
P	-3.06806000	-0.48898500	-1.21712400
P	-1.33172900	0.50791100	2.04323300
Co	-1.36321700	-0.96445400	0.26679700
H	-0.03178100	-0.88082700	-1.85648600
C	-2.43116600	-2.28456900	1.28515400
H	-2.58796500	-3.14078200	0.60974300
H	-1.81960200	-2.64232800	2.12825900
H	-3.40805300	-1.98471100	1.68079300
³V^b			
C	-1.32259500	-0.74492700	-0.91298000
C	-2.37347200	-1.70771100	-0.88657700
C	-2.45852000	-2.81261300	-1.71383000
H	-3.30584900	-3.47995200	-1.59797200

C	-1.44381200	-3.05900800	-2.64690000
H	-1.49508200	-3.91873400	-3.30552000
C	-0.35292300	-2.18349300	-2.70183500
H	0.46433300	-2.32821300	-3.40044800
C	-0.32106800	-1.08671100	-1.86129800
C	-1.27753200	0.41602400	-0.03711800
C	-2.50256700	1.14756100	0.31254600
C	-3.62253800	1.20369800	-0.55035700
H	-3.59677600	0.65628200	-1.48741900
C	-4.73868200	1.97047000	-0.24021600
H	-5.57684500	1.99575800	-0.93207200
C	-4.78674700	2.71909600	0.94238700
H	-5.65977200	3.31968900	1.18038700
C	-3.69445300	2.67725800	1.81136600
H	-3.71893200	3.23769900	2.74289400
C	-2.57504400	1.90688000	1.50540400
C	2.18821600	-1.95334600	3.14898100
H	1.90578400	-2.83884300	3.72731300
H	2.08901200	-1.07051800	3.78767900
H	3.23269000	-2.03838200	2.84395300
C	-0.56472100	-1.79121200	2.46002700
H	-1.35757200	-1.77036200	1.71216500
H	-0.67871600	-0.90247400	3.08613400
H	-0.67363700	-2.68527700	3.08241100
C	1.21038900	-3.40423200	0.84494700
H	2.20698900	-3.53097100	0.41514800
H	0.47765500	-3.45213500	0.03538600
H	1.01613600	-4.21496000	1.55448900
C	3.44770700	1.66444100	-2.20377800
H	3.80041300	2.59785100	-2.65350100
H	2.76899200	1.16139700	-2.89669700
H	4.29882000	1.00568700	-2.01965300
C	1.33107700	3.26591300	-1.12764000
H	0.83971100	3.69121200	-0.24838200
H	0.56184800	2.79602900	-1.74457200
H	1.81288000	4.07332800	-1.68830300
C	3.78549900	2.95836900	0.35154100
H	4.62585200	2.31593000	0.62616700
H	3.31984100	3.32244300	1.27217900
H	4.16005100	3.81525100	-0.21761700
F	-3.33276500	-1.57230900	0.06250500
F	0.77987400	-0.27381900	-1.97005500
H	-1.75633600	1.85658500	2.21824900
N	-0.08680700	0.85205000	0.45622300
H	-0.19466800	1.78010100	0.85298000
P	1.10129100	-1.75123700	1.66296500
P	2.55257600	1.97628600	-0.61891000
Co	1.72287600	0.07057200	0.39998800
C	3.55407800	-0.73965600	0.20401700

H	3.69638800	-0.95042100	-0.86609400
H	4.36850400	-0.06871300	0.51428000
H	3.73255800	-1.68645900	0.72818200
³TS4^b			
C	1.51858600	1.21474800	-0.30879900
C	2.57452600	2.14755700	-0.20036300
C	2.43908500	3.47155400	-0.54095500
H	3.27435900	4.15002300	-0.41491600
C	1.18215000	3.90417800	-1.02734000
H	1.05510800	4.95365900	-1.28286900
C	0.11690600	3.04200700	-1.17459100
H	-0.82601400	3.40687800	-1.56263200
C	0.24333100	1.67297900	-0.80201500
C	1.54670700	-0.15794200	0.11115000
C	2.77811300	-0.98066600	0.25376100
C	3.78076700	-0.95567600	-0.72842500
H	3.67778900	-0.28502300	-1.57489500
C	4.88647500	-1.79708700	-0.62848700
H	5.64964200	-1.77574000	-1.40105800
C	5.01689900	-2.66367000	0.45982300
H	5.88421000	-3.31286700	0.53891800
C	4.03099600	-2.68866400	1.44765100
H	4.13167500	-3.35086800	2.30288800
C	2.91628500	-1.85751500	1.34132100
C	-3.82064500	0.62439700	2.71596500
H	-3.90330700	0.77513400	3.79793800
H	-4.50108100	-0.17919900	2.41835900
H	-4.13678800	1.53732300	2.20392800
C	-1.71930100	-1.24492400	3.29423200
H	-0.67371200	-1.53664900	3.16097600
H	-2.34742100	-2.09597500	3.01319700
H	-1.88960400	-1.01726700	4.35212300
C	-1.12203600	1.54278700	3.03304000
H	-1.35367000	2.50173800	2.56177300
H	-0.05490300	1.35349100	2.88943100
H	-1.34069100	1.60425300	4.10473300
C	-2.59875800	-1.07117400	-3.18117100
H	-2.93619800	-1.89880000	-3.81332900
H	-1.64963100	-0.66893800	-3.54384700
H	-3.33293800	-0.26180300	-3.21716400
C	-1.45030100	-3.18494200	-1.60166200
H	-1.33170000	-3.65803800	-0.62184500
H	-0.45467500	-2.98661800	-2.00842000
H	-1.97411300	-3.87998300	-2.26644300
C	-4.04652300	-2.13727000	-0.91685700
H	-4.70485800	-1.26688000	-0.84570500
H	-4.00092500	-2.61057800	0.06845700
H	-4.47423400	-2.84921400	-1.63058600

F	3.76462900	1.73175000	0.30164100
F	-0.14124000	0.69978300	-2.18018400
H	2.15740900	-1.86634400	2.11904800
N	0.36116200	-0.69421900	0.31978000
H	0.39418700	-1.69416900	0.50049100
P	-2.08945500	0.20492400	2.19045600
P	-2.35486800	-1.57620300	-1.42290700
Co	-1.23568600	0.40066600	-0.34188600
C	-2.69726400	1.73475000	-0.72621700
H	-2.58150100	2.61627400	-0.08524600
H	-2.64699600	2.05191800	-1.77243300
H	-3.67569000	1.27866000	-0.52510800

¹VI^b

C	1.42014500	1.21614500	-0.34995600
C	2.46926200	2.14294200	-0.46979500
C	2.27370100	3.42124000	-0.96532100
H	3.11670100	4.09904700	-1.04081800
C	0.98080200	3.78336300	-1.34911600
H	0.80759400	4.77722000	-1.75568600
C	-0.08762500	2.89387500	-1.20552900
H	-1.07385800	3.22178400	-1.51547700
C	0.09103300	1.60652800	-0.68547200
C	1.56539500	-0.16070700	0.13081300
C	2.85943300	-0.88631700	0.27814700
C	3.77638900	-0.94037000	-0.78270500
H	3.56949600	-0.39210500	-1.69577200
C	4.93335800	-1.70790900	-0.67191300
H	5.62967200	-1.75268500	-1.50418900
C	5.20089200	-2.41517400	0.50335900
H	6.10898000	-3.00486300	0.58945600
C	4.29892600	-2.35970900	1.56645500
H	4.50412700	-2.90028900	2.48598500
C	3.13004400	-1.60663800	1.45088100
C	-3.67075600	1.06952400	1.91093000
H	-3.86987500	1.46577800	2.91163500
H	-4.13941800	0.08697300	1.81908000
H	-4.11791000	1.73071300	1.16579300
C	-1.30905700	-0.08096500	3.05435900
H	-0.21828800	-0.13764100	3.06155400
H	-1.70241200	-1.09759300	2.96575300
H	-1.65501100	0.35180300	3.99855600
C	-1.27141800	2.61267400	2.09501200
H	-1.59541100	3.34398600	1.35153500
H	-0.17963700	2.62799400	2.12052100
H	-1.66465300	2.89164600	3.07775000
C	-3.32194400	-1.90257500	-2.22407700
H	-3.63466400	-2.91666800	-2.49193900
H	-2.60901000	-1.50913800	-2.95046100

H	-4.19741800	-1.24987600	-2.19541700
C	-1.25823700	-3.27479600	-0.79788100
H	-0.81434700	-3.54412500	0.16588600
H	-0.47874400	-2.92201900	-1.47634100
H	-1.74542200	-4.16239600	-1.21328700
C	-3.71391800	-2.60051700	0.54020100
H	-4.57200700	-1.92622100	0.62050700
H	-3.29160800	-2.73600400	1.54100500
H	-4.07373200	-3.57103100	0.18208600
F	3.72447100	1.81065200	-0.07705400
F	-0.69813500	-0.53568800	-2.08687200
H	2.43150000	-1.55851300	2.28203700
N	0.44485300	-0.76947900	0.36982000
H	0.56608000	-1.75035800	0.60938100
P	-1.85226500	0.93068800	1.60102600
P	-2.44214700	-1.86884400	-0.60614300
Co	-1.20112700	0.17167500	-0.43359500
C	-2.67440000	1.20829700	-1.25522700
H	-2.74566800	2.23765600	-0.88508000
H	-2.42995500	1.22530800	-2.31997200
H	-3.65639900	0.74071400	-1.11690600

B

C	-1.09194300	0.22349400	0.19347800
C	-2.11122700	0.90966400	-0.47718600
C	-3.35024000	0.34131600	-0.74760800
H	-4.09255100	0.92071800	-1.28436100
C	-3.59964000	-0.96153200	-0.31445100
H	-4.56504200	-1.41692500	-0.51065200
C	-2.62170500	-1.68398900	0.36954300
H	-2.79361200	-2.69325700	0.72543400
C	-1.39356000	-1.07764900	0.60479300
C	0.20436100	0.91689500	0.55140800
C	1.50034900	0.32374800	0.10945700
C	1.57530600	-0.73289700	-0.80966000
H	0.66653500	-1.15825700	-1.22228200
C	2.81571200	-1.22579100	-1.21232400
H	2.86729200	-2.04030200	-1.92869700
C	3.98866200	-0.67230900	-0.69522600
H	4.95440400	-1.06043900	-1.00651700
C	3.92169100	0.38286100	0.22070200
H	4.83445000	0.81409300	0.62123600
C	2.68528200	0.88162100	0.61680700
F	-1.87073500	2.15973900	-0.90550200
F	-0.45096700	-1.77035600	1.27653800
H	2.60657400	1.70445200	1.31934500
O	0.15987400	1.95910800	1.18609600

³I^c

C	-1.92360300	1.47493200	-0.19919500
C	-3.26660200	1.88227100	-0.45913800
C	-3.62884600	3.21946700	-0.49188400
H	-4.66381500	3.48184200	-0.69752300
C	-2.68270000	4.23402500	-0.27692100
H	-2.97335900	5.27968800	-0.30296200
C	-1.35431000	3.86558300	-0.03732600
H	-0.60046400	4.63289200	0.12724500
C	-0.98027900	2.52608700	-0.00258700
C	-1.52634600	0.08963800	-0.17443900
C	-2.53464600	-0.99902800	-0.23514900
C	-3.60315400	-1.11870900	0.67173400
C	-4.50890400	-2.17142400	0.67628800
H	-5.30036600	-2.18218700	1.41760200
C	-4.35543400	-3.19698100	-0.25808600
H	-5.05058600	-4.03007400	-0.27094400
C	-3.30222900	-3.14989300	-1.17460100
H	-3.15693500	-3.92235300	-1.92190000
C	-2.43065600	-2.07096000	-1.14063600
C	3.12963200	0.37285600	-3.11486200
H	3.16334600	0.86738200	-4.09108200
H	2.99941600	-0.70010100	-3.27269400
H	4.08083100	0.53386100	-2.60148000
C	0.27117700	0.71680000	-3.16473900
H	-0.57704100	1.28608000	-2.77748800
H	0.00188300	-0.33944700	-3.11759400
H	0.46372500	1.01051200	-4.20168900
C	1.98395100	2.85621100	-2.29209400
H	2.88029300	3.16337600	-1.74717600
H	1.12292800	3.38251700	-1.87264300
H	2.09053100	3.13130000	-3.34651700
C	3.94074800	-2.61007100	0.37089400
H	4.05019200	-3.69959600	0.34610500
H	4.24762100	-2.24472000	1.35533000
H	4.61556400	-2.16931100	-0.36893500
C	1.23874500	-3.11736900	1.20877500
H	0.17663400	-2.91292500	1.05219600
H	1.48960000	-2.85986300	2.24146900
H	1.43154800	-4.18517400	1.05914600
C	1.83431000	-2.98398200	-1.54432200
H	2.47029900	-2.62261300	-2.35677700
H	0.79009000	-2.80610600	-1.81163700
H	2.00032800	-4.06079800	-1.42857000
P	1.73497700	1.03327400	-2.08794700
P	2.20072400	-2.06107200	0.02397000
Co	1.56804700	0.36933300	0.14567300
C	3.39170600	1.14309900	0.44146600
H	3.32048800	2.21996700	0.65790600
H	3.90766600	0.67001500	1.28586400

H	4.05455600	1.03128100	-0.42588500
P	1.19404600	0.56012700	2.46178400
C	-0.37760300	-0.14455100	3.13010400
H	-1.23159400	0.27875500	2.59701300
H	-0.39032500	-1.22516500	2.97086000
H	-0.47768900	0.06224800	4.20073300
C	1.11057700	2.31107500	3.06047200
H	2.03642500	2.82972200	2.79708000
H	0.27571500	2.82063100	2.57296600
H	0.97112300	2.35377900	4.14553100
C	2.45270600	-0.13864600	3.63098900
H	2.55067800	-1.21735900	3.48319000
H	3.42563500	0.32119900	3.44192300
H	2.16713200	0.04862600	4.67126900
H	0.05977500	2.27683700	0.18571500
H	-4.02049000	1.12931700	-0.66128300
F	-3.74389800	-0.16434700	1.62201200
F	-1.43801000	-2.04664800	-2.06848100
O	-0.28963700	-0.32932700	-0.12061100

³II^c

C	-1.21027100	-1.21246000	-0.66947200
C	-2.14096200	-2.28043700	-0.53418600
C	-2.11200600	-3.44812600	-1.27832600
H	-2.86996500	-4.20032200	-1.08799700
C	-1.09695000	-3.64451800	-2.21997100
H	-1.06086300	-4.55347300	-2.81015900
C	-0.12122500	-2.65495900	-2.38171800
H	0.68423700	-2.75296300	-3.10171300
C	-0.20238300	-1.50192000	-1.62237800
C	-1.25506600	0.00848500	0.13459000
C	-2.51695900	0.66507500	0.48123700
C	-3.71802900	0.47784600	-0.24291600
H	-3.73521100	-0.20347700	-1.08717200
C	-4.87201800	1.18073300	0.08470200
H	-5.77674800	1.02056500	-0.49630400
C	-4.87440000	2.09816700	1.14149100
H	-5.77852000	2.64463000	1.39401000
C	-3.69440200	2.30418900	1.86353400
H	-3.68057300	3.01151500	2.68936100
C	-2.53573200	1.60658200	1.53898200
C	3.32503100	-1.23518600	2.75924600
H	3.46508900	-2.15126300	3.34201100
H	3.01262900	-0.43268300	3.43384900
H	4.27484300	-0.94728300	2.30321600
C	0.58837200	-2.03514500	2.41790600
H	-0.21044700	-2.33667800	1.73754100
H	0.21288500	-1.20322900	3.01873800
H	0.84704800	-2.87305700	3.07309300

C	2.60832800	-2.99445700	0.58456600
H	3.54105200	-2.79164000	0.05258500
H	1.85327800	-3.29228100	-0.14788800
H	2.76720300	-3.81433700	1.29224000
C	2.85751800	3.38622400	-1.65485200
H	2.55040300	4.37880800	-1.99886800
H	3.20947500	2.80602000	-2.51226300
H	3.69165800	3.49036200	-0.95616300
C	0.13358600	2.56142700	-2.11109800
H	-0.79176300	2.17981200	-1.67437200
H	0.40582300	1.92068900	-2.95332100
H	-0.02557900	3.58327400	-2.46981400
C	0.87367900	3.72990100	0.41309700
H	1.64138200	3.88130000	1.17773500
H	-0.02100000	3.32402100	0.89013600
H	0.63856300	4.69302100	-0.05112900
F	-3.09388300	-2.18242300	0.41931000
F	0.77418400	-0.56076100	-1.84542500
H	-1.62322600	1.76046300	2.10418300
P	2.04509200	-1.45937400	1.44311700
P	1.46087700	2.49874500	-0.83130800
Co	1.75883000	0.41454200	0.14535000
C	3.71470700	0.43892300	-0.22212100
H	3.90370100	0.74656200	-1.25827200
H	4.20782500	1.17460300	0.43242600
H	4.23436800	-0.51715400	-0.07869300
O	-0.15913700	0.58219700	0.57282100

³TS1^c

C	1.39407800	1.32828400	-0.12062700
C	2.45382200	2.25415200	0.05522800
C	2.31220100	3.59906800	-0.17303100
H	3.14484900	4.26762500	0.01055600
C	1.05052200	4.07058900	-0.61278800
H	0.92252300	5.13776800	-0.77846500
C	-0.01653200	3.22462800	-0.81647800
H	-0.96350500	3.62220800	-1.15978900
C	0.11399900	1.82783700	-0.56719300
C	1.40894900	-0.07205800	0.18077700
C	2.62187100	-0.93122600	0.25441900
C	3.71398900	-0.74727400	-0.60767600
H	3.70377800	0.07050800	-1.31922200
C	4.79609600	-1.62449000	-0.56955000
H	5.63049300	-1.47928800	-1.24946300
C	4.80874400	-2.68655800	0.33727400
H	5.65763500	-3.36369500	0.37081900
C	3.72457500	-2.87959600	1.19737700
H	3.72927500	-3.70510900	1.90352700
C	2.63314500	-2.01628800	1.14567100

C	-3.85445500	0.23487400	2.74202000
H	-3.97891100	0.01776100	3.80824500
H	-4.58343900	-0.35099300	2.17432900
H	-4.06814900	1.29311100	2.56700700
C	-1.92674000	-1.91080300	2.66640800
H	-0.92282300	-2.23389400	2.38019200
H	-2.64901300	-2.54293800	2.14147800
H	-2.05942200	-2.04300700	3.74551100
C	-1.09578700	0.74671500	3.37366000
H	-1.24378100	1.82439800	3.26059800
H	-0.04463800	0.52979100	3.16690500
H	-1.32977600	0.45825400	4.40400200
C	-2.83555300	-0.75814300	-3.18088000
H	-2.95209200	-1.50884000	-3.96924000
H	-2.22989200	0.07521300	-3.54551900
H	-3.81882700	-0.37049700	-2.90039000
C	-0.44659000	-2.16455200	-2.41207700
H	0.09268000	-2.71436900	-1.63720800
H	0.17686900	-1.32832900	-2.73591300
H	-0.66137100	-2.82654600	-3.25716700
C	-2.99162000	-2.91740800	-1.25648800
H	-3.98061100	-2.60379300	-0.90870000
H	-2.50279400	-3.46720900	-0.44692900
H	-3.11825900	-3.59042200	-2.11117100
F	3.64385700	1.80987600	0.52849200
F	-0.23651300	0.98100400	-2.07705900
H	1.78015700	-2.16695000	1.79880000
P	-2.14454900	-0.14886100	2.13744000
P	-1.97586300	-1.42745500	-1.69129200
Co	-1.33396800	0.52399900	-0.22234700
C	-2.80415300	1.82541500	-0.55240400
H	-2.76262600	2.62771200	0.19207600
H	-2.71807100	2.24345400	-1.55797800
H	-3.74829600	1.27646800	-0.44525300
O	0.28648700	-0.64856900	0.35559700
13			
C	1.38452700	1.26176400	-0.30254000
C	2.42836200	2.20588400	-0.37161700
C	2.22879600	3.49489100	-0.83218300
H	3.06471200	4.18470500	-0.86383200
C	0.94008900	3.85823500	-1.23453800
H	0.76855100	4.86278300	-1.61464900
C	-0.12339400	2.95957100	-1.13649400
H	-1.10821400	3.28676500	-1.45258400
C	0.05787000	1.66008500	-0.64801700
C	1.50986900	-0.12089500	0.17097700
C	2.78890900	-0.87235600	0.31605900
C	3.80645700	-0.78888200	-0.64567600

H	3.69753200	-0.11609400	-1.48866000
C	4.94185600	-1.58918400	-0.53478300
H	5.71780200	-1.52981500	-1.29219500
C	5.08313900	-2.46239600	0.54580200
H	5.97540500	-3.07546300	0.63610900
C	4.07279700	-2.55212000	1.50681400
H	4.17764900	-3.23313700	2.34645900
C	2.92363100	-1.77556000	1.38185800
C	-3.76563600	0.74144300	1.86057600
H	-4.04023500	1.14712600	2.83938500
H	-4.04950200	-0.31223000	1.81996300
H	-4.31624900	1.27504100	1.08264000
C	-1.22609700	0.04132800	3.01283600
H	-0.14349400	0.18443800	3.01589400
H	-1.42161600	-1.03107500	2.93435600
H	-1.64435600	0.41722600	3.95190700
C	-1.67008000	2.68139500	1.98194300
H	-2.13441100	3.31920200	1.22613000
H	-0.59847200	2.89152300	1.98107900
H	-2.09009300	2.92115000	2.96395600
C	-3.13092400	-2.06177300	-2.27056300
H	-3.34166700	-3.10127800	-2.54101400
H	-2.46588400	-1.60213500	-3.00384000
H	-4.06800900	-1.49999100	-2.23935300
C	-0.90313900	-3.18505400	-0.85552700
H	-0.37830300	-3.32665200	0.09154900
H	-0.20922900	-2.74675700	-1.57443000
H	-1.28312800	-4.14544800	-1.21858000
C	-3.42651600	-2.83214200	0.48777600
H	-4.36181100	-2.27134400	0.57924000
H	-2.98259000	-2.92546100	1.48389500
H	-3.66338400	-3.83642200	0.12045500
F	3.67504100	1.88751200	0.05237600
F	-0.58247100	-0.45317500	-2.08348100
H	2.12128000	-1.85571100	2.10796100
P	-1.95165500	0.90859800	1.55040800
P	-2.25303900	-1.94710500	-0.65437400
Co	-1.19753900	0.20846800	-0.46698900
C	-2.66861000	1.17071900	-1.34084600
H	-2.82128500	2.18561700	-0.95545000
H	-2.37128900	1.22160200	-2.39060800
H	-3.61649500	0.62796300	-1.25563000
O	0.45577300	-0.73573600	0.45085500
¹III^c			
C	1.18272900	1.42678300	-0.50676200
C	2.12596600	2.46414800	-0.28488600
C	1.77162200	3.77921900	-0.48440800
H	2.48762800	4.57372900	-0.29620600

C	0.46574300	4.10007400	-0.94808100
H	0.20222600	5.14247800	-1.11025700
C	-0.45680200	3.11222500	-1.20711700
H	-1.43500500	3.37197400	-1.60020100
C	-0.15495400	1.73547200	-0.96413300
C	1.38055900	0.05271800	-0.20352000
C	2.70566300	-0.57240200	0.05488100
C	3.81901700	-0.37588400	-0.77746800
C	5.04719600	-0.99394900	-0.57410200
H	5.85738100	-0.79710400	-1.26687900
C	5.19191400	-1.86067900	0.50834000
H	6.14345600	-2.35233100	0.68340600
C	4.11827100	-2.10112200	1.36658900
H	4.20052500	-2.76533200	2.21934200
C	2.90969600	-1.46310200	1.12118600
C	-3.61131900	0.80316100	2.17821800
H	-3.69252700	1.07253400	3.23625700
H	-4.11277500	-0.15378500	2.01459500
H	-4.11841800	1.55827900	1.57367200
C	-1.16698700	-0.50858000	2.90570000
H	-0.09395100	-0.62897900	2.74853800
H	-1.63515300	-1.48699300	2.76433000
H	-1.35480000	-0.16837200	3.92983100
C	-1.16525900	2.28542300	2.26941300
H	-1.56071600	3.10053000	1.65804800
H	-0.07853300	2.28393000	2.15246800
H	-1.41860800	2.46059200	3.32044800
C	-2.74341600	-2.02521700	-2.80764500
H	-3.19450000	-3.00021100	-3.02322200
H	-1.83961300	-1.90658400	-3.41183500
H	-3.44365700	-1.23456500	-3.08973300
C	-1.23779700	-3.32655400	-0.74096900
H	-0.98618900	-3.40284100	0.31998500
H	-0.30183400	-3.20122100	-1.28945800
H	-1.73456000	-4.24756700	-1.06402300
C	-3.88735500	-2.38823300	-0.22193800
H	-4.65698800	-1.62524800	-0.36351400
H	-3.73389400	-2.52561300	0.85248200
H	-4.24164700	-3.33307800	-0.64779400
P	-1.84127600	0.67701300	1.65337200
P	-2.30208100	-1.83595700	-1.01559500
Co	-1.40264400	0.18800300	-0.44925800
C	-3.06793600	1.10080500	-1.07145300
H	-3.14687100	2.12411700	-0.67967300
H	-3.02670600	1.17516600	-2.16820000
H	-4.00575100	0.59029600	-0.81553000
O	0.34472600	-0.70164300	-0.15659400
H	-0.58104800	1.01009700	-1.75232800
H	3.11909800	2.21537900	0.07738300

F	1.89423700	-1.70032200	1.97713400
F	3.69332600	0.43433400	-1.84679300
¹TS2^c			
C	1.17153000	1.49968100	-0.31923100
C	2.22003600	2.45192200	-0.29544100
C	1.92389700	3.79672400	-0.36604400
H	2.71468500	4.54034100	-0.34450700
C	0.57231200	4.19804500	-0.47497000
H	0.34026800	5.25994700	-0.52723200
C	-0.45929800	3.27523400	-0.51499400
H	-1.48035200	3.62926500	-0.61613200
C	-0.21472400	1.87871500	-0.41920200
C	1.36268500	0.08761200	-0.21993300
C	2.70480200	-0.56271800	-0.07612100
C	3.66920600	-0.54779300	-1.08711400
C	4.89398800	-1.19667600	-0.97521100
H	5.59558100	-1.15201900	-1.80025400
C	5.17681800	-1.89210900	0.20034700
H	6.12825000	-2.40321900	0.30679800
C	4.24895900	-1.93605400	1.24256200
H	4.44818200	-2.46223500	2.16902500
C	3.03820000	-1.27672400	1.07844200
C	-3.38175700	0.26621300	2.63250600
H	-3.37492400	0.09194700	3.71339100
H	-4.11166300	-0.40223400	2.16824800
H	-3.69652800	1.29374800	2.43547300
C	-1.30751600	-1.71890700	2.52513400
H	-0.27830000	-1.95556800	2.24776100
H	-1.96777500	-2.45898300	2.06420300
H	-1.41291100	-1.78089700	3.61352600
C	-0.63348000	1.01090200	2.98305500
H	-0.80677300	2.06747100	2.76399000
H	0.41246100	0.78506000	2.75961500
H	-0.82047900	0.81946500	4.04501500
C	-3.09938100	-0.86438800	-3.07005700
H	-3.60507200	-1.69863700	-3.56803600
H	-2.25521900	-0.53351800	-3.68063300
H	-3.79371300	-0.02550300	-2.97536900
C	-1.45537500	-2.82612800	-1.77484200
H	-1.10817000	-3.27842800	-0.84222800
H	-0.57241800	-2.51900100	-2.34054500
H	-2.01758800	-3.56831100	-2.35161900
C	-3.99954500	-2.11190600	-0.67125000
H	-4.73729700	-1.33574900	-0.44934200
H	-3.75080600	-2.62398300	0.26314700
H	-4.44748500	-2.83800200	-1.35820300
P	-1.71104700	-0.02432600	1.89106600
P	-2.47516600	-1.32840500	-1.38980700

Co	-1.39860900	0.38302600	-0.32782800
C	-3.04995600	1.49421100	-0.43614100
H	-3.00722400	2.31449200	0.29148300
H	-3.14759800	1.93802100	-1.43372100
H	-3.96585800	0.92505500	-0.22778600
O	0.35111500	-0.66851500	-0.22570400
H	-0.92616600	1.06583100	-1.58285500
H	3.25115300	2.11982300	-0.21105500
F	2.14865800	-1.30115100	2.09669500
F	3.39045900	0.11538100	-2.22592000

¹IV^c

C	1.18577800	1.44924500	-0.42326800
C	2.25398500	2.37474000	-0.46660500
C	1.98137900	3.71827300	-0.64696300
H	2.78593600	4.44664000	-0.68356900
C	0.64242800	4.12914500	-0.78835700
H	0.42633600	5.18556900	-0.93638800
C	-0.40731200	3.21546800	-0.74360300
H	-1.42151700	3.58313000	-0.86921700
C	-0.18560600	1.83723500	-0.54818600
C	1.36915400	0.03408600	-0.23404000
C	2.71487600	-0.59960200	-0.03078500
C	3.67325300	-0.67807900	-1.04384000
C	4.89901400	-1.31297900	-0.87680300
H	5.59699800	-1.34581200	-1.70543700
C	5.18776200	-1.89311700	0.35847500
H	6.14022000	-2.39123700	0.50833600
C	4.26561500	-1.83790000	1.40528700
H	4.47071200	-2.27298600	2.37661800
C	3.05312700	-1.19802600	1.18533200
C	-3.40262200	0.66084700	2.49051100
H	-3.41091400	0.67834400	3.58501000
H	-4.11211200	-0.09367100	2.14084100
H	-3.73082000	1.63136200	2.11127200
C	-1.30995300	-1.29410900	2.72595300
H	-0.28060500	-1.57469200	2.49197800
H	-1.96982100	-2.09883200	2.38977000
H	-1.41638400	-1.18426400	3.81062100
C	-0.67133400	1.47821100	2.78474100
H	-0.84017000	2.48949700	2.40681500
H	0.38223000	1.23244200	2.62703400
H	-0.88975200	1.44464200	3.85725200
C	-3.28915100	-1.31985900	-2.83392000
H	-3.82790400	-2.21948600	-3.14938800
H	-2.50016700	-1.09225700	-3.55467200
H	-3.97795400	-0.47184000	-2.81362200
C	-1.48363500	-3.03145300	-1.40461700
H	-1.06271300	-3.34279900	-0.44532500

H	-0.65001400	-2.78338200	-2.06598100
H	-2.05855000	-3.85752900	-1.83580700
C	-3.96447800	-2.21389600	-0.21587700
H	-4.71244500	-1.42925000	-0.07105600
H	-3.63511200	-2.55833400	0.76841700
H	-4.43088900	-3.05285400	-0.74295300
P	-1.71462500	0.28154100	1.83251500
P	-2.52347600	-1.52020800	-1.16325600
Co	-1.38834900	0.33863900	-0.48415900
C	-3.00325400	1.46359100	-0.77674100
H	-2.98416500	2.32225700	-0.09499900
H	-3.02148400	1.84734400	-1.80123400
H	-3.94622900	0.92859300	-0.59447500
O	0.36775500	-0.72063700	-0.20100000
H	-1.13652700	0.46163800	-1.92464400
H	3.27957500	2.03306300	-0.35591000
F	2.16776200	-1.12211600	2.20456300
F	3.38723800	-0.12281400	-2.23656700

¹TS3^c

C	1.14103100	1.46851900	-0.42130500
C	2.13805500	2.46922600	-0.37206900
C	1.78648200	3.79565000	-0.55092600
H	2.54221500	4.57500700	-0.51967100
C	0.43684000	4.12423300	-0.77625700
H	0.16064100	5.16679100	-0.92203600
C	-0.54691600	3.13950500	-0.80803200
H	-1.57706800	3.44309700	-0.97827600
C	-0.24414300	1.77235700	-0.62693500
C	1.38524600	0.05956800	-0.23979500
C	2.72263000	-0.54354300	0.05191400
C	3.83272400	-0.39398700	-0.78787600
C	5.06025500	-0.99923100	-0.54375500
H	5.87417600	-0.84459600	-1.24274000
C	5.19963900	-1.79730700	0.59113100
C	4.12345700	-1.98844700	1.45902700
H	4.20367000	-2.60185100	2.34914400
C	2.91512100	-1.36947700	1.16779000
C	-2.89947300	2.19154100	1.87013600
H	-3.07596700	2.39257400	2.93180200
H	-3.86492900	2.12082400	1.35987000
H	-2.34455900	3.02524400	1.43283900
C	-2.94728100	-0.53623400	2.66413300
H	-2.43323700	-1.49778500	2.75063200
H	-3.91890100	-0.70889700	2.19142200
H	-3.11528000	-0.13876000	3.67120400
C	-0.50732000	0.92999400	2.76803600
H	0.07782200	1.77207200	2.39004400
H	0.14485800	0.05339700	2.78904400

H	-0.84702700	1.15444000	3.78467100
C	-1.93099600	-2.49788900	-2.65977000
H	-2.30419600	-3.51581900	-2.81767400
H	-0.85453000	-2.47238800	-2.84798400
H	-2.41163500	-1.82265500	-3.37299900
C	-1.50029700	-3.25814700	0.06466100
H	-1.81701900	-3.16583200	1.10704400
H	-0.41395900	-3.15162600	0.03209000
H	-1.79062100	-4.24607900	-0.30751700
C	-4.05919500	-2.24894800	-0.76872600
H	-4.62984900	-1.55390500	-1.39055900
H	-4.36708600	-2.10375400	0.26999600
H	-4.30117000	-3.27381000	-1.06866600
P	-1.93350900	0.62828500	1.62081200
P	-2.24682500	-1.89301800	-0.93779300
Co	-1.37164300	0.21679100	-0.59103700
C	-2.89693200	1.13502300	-1.70416600
H	-3.43405700	1.57318700	-0.85756800
H	-2.65849900	1.95284300	-2.39072100
H	-3.57593100	0.45249800	-2.22325900
H	-1.57622700	0.50884100	-2.01160400
H	3.17522500	2.20198800	-0.19364100
H	6.15103200	-2.27596200	0.79980700
F	3.70204100	0.35485600	-1.90053900
F	1.88461500	-1.55939000	2.01892900
O	0.39850100	-0.72188500	-0.29134800

¹V^c

C	2.89713200	-0.17785300	0.16598800
C	3.94377000	0.21112800	-0.67913900
C	5.24940800	-0.24282900	-0.53322200
H	6.00708100	0.09534400	-1.23073200
C	5.53810700	-1.13244900	0.50105800
H	6.55249000	-1.49531900	0.63208200
C	4.53101300	-1.56448500	1.36536700
H	4.72699800	-2.25442200	2.17812400
C	3.23974100	-1.09052200	1.17558500
C	1.48237500	0.26133900	-0.01005900
C	1.02058100	1.62554700	-0.06771000
C	1.86845000	2.75129600	-0.02298300
H	2.93835500	2.62999500	0.11610100
C	1.32944100	4.01990700	-0.16866300
H	1.96685200	4.89870200	-0.14045600
C	-0.05326400	4.14758900	-0.36909200
H	-0.48317200	5.13790100	-0.50774700
C	-0.88534200	3.02670500	-0.37742800
H	-1.94805900	3.20206200	-0.52418400
C	-0.40761200	1.71073600	-0.19424400
C	-3.18543100	-3.17483000	-0.94922800

H	-2.99084800	-4.19547100	-1.29521700
H	-3.75063300	-2.64509900	-1.72196700
H	-3.80053500	-3.22553500	-0.04746100
C	-0.63741400	-2.69059500	-2.12826700
H	0.38040900	-2.31494400	-2.00699500
H	-1.08693300	-2.19214200	-2.99164200
H	-0.61199900	-3.77049700	-2.31056500
C	-0.81681000	-3.40287300	0.64864300
H	-1.42382300	-3.41915500	1.55868400
H	0.16589900	-2.99898200	0.90154500
H	-0.71343800	-4.42626200	0.27173500
F	3.67151000	1.04296200	-1.70419100
F	2.27779200	-1.51001900	2.01986500
P	-1.59870900	-2.27458300	-0.59769700
Co	-1.24344100	-0.04801100	-0.16239400
P	-3.22886900	0.66606400	0.46143700
C	-3.16841900	1.81950500	1.91366500
H	-2.70178300	1.29695600	2.75338400
H	-2.55013200	2.68656400	1.67756100
H	-4.17130300	2.14760700	2.20833700
C	-4.32890300	1.58948700	-0.72397200
H	-5.23334000	1.96248100	-0.23076600
H	-3.79177200	2.42992000	-1.16840400
H	-4.62006400	0.91499400	-1.53468000
C	-4.47231900	-0.55581300	1.11184700
H	-4.00710200	-1.18346200	1.87729200
H	-5.33578900	-0.04543500	1.55159200
H	-4.82374000	-1.20110700	0.30362300
O	0.61027800	-0.64913200	-0.08508000

³VI^c

C	-1.21027100	-1.21246000	-0.66947200
C	-2.14096200	-2.28043700	-0.53418600
C	-2.11200600	-3.44812600	-1.27832600
H	-2.86996500	-4.20032200	-1.08799700
C	-1.09695000	-3.64451800	-2.21997100
H	-1.06086300	-4.55347300	-2.81015900
C	-0.12122500	-2.65495900	-2.38171800
H	0.68423700	-2.75296300	-3.10171300
C	-0.20238300	-1.50192000	-1.62237800
C	-1.25506600	0.00848500	0.13459000
C	-2.51695900	0.66507500	0.48123700
C	-3.71802900	0.47784600	-0.24291600
H	-3.73521100	-0.20347700	-1.08717200
C	-4.87201800	1.18073300	0.08470200
H	-5.77674800	1.02056500	-0.49630400
C	-4.87440000	2.09816700	1.14149100
H	-5.77852000	2.64463000	1.39401000
C	-3.69440200	2.30418900	1.86353400

H	-3.68057300	3.01151500	2.68936100
C	-2.53573200	1.60658200	1.53898200
C	3.32503100	-1.23518600	2.75924600
H	3.46508900	-2.15126300	3.34201100
H	3.01262900	-0.43268300	3.43384900
H	4.27484300	-0.94728300	2.30321600
C	0.58837200	-2.03514500	2.41790600
H	-0.21044700	-2.33667800	1.73754100
H	0.21288500	-1.20322900	3.01873800
H	0.84704800	-2.87305700	3.07309300
C	2.60832800	-2.99445700	0.58456600
H	3.54105200	-2.79164000	0.05258500
H	1.85327800	-3.29228100	-0.14788800
H	2.76720300	-3.81433700	1.29224000
C	2.85751800	3.38622400	-1.65485200
H	2.55040300	4.37880800	-1.99886800
H	3.20947500	2.80602000	-2.51226300
H	3.69165800	3.49036200	-0.95616300
C	0.13358600	2.56142700	-2.11109800
H	-0.79176300	2.17981200	-1.67437200
H	0.40582300	1.92068900	-2.95332100
H	-0.02557900	3.58327400	-2.46981400
C	0.87367900	3.72990100	0.41309700
H	1.64138200	3.88130000	1.17773500
H	-0.02100000	3.32402100	0.89013600
H	0.63856300	4.69302100	-0.05112900
F	-3.09388300	-2.18242300	0.41931000
F	0.77418400	-0.56076100	-1.84542500
H	-1.62322600	1.76046300	2.10418300
P	2.04509200	-1.45937400	1.44311700
P	1.46087700	2.49874500	-0.83130800
Co	1.75883000	0.41454200	0.14535000
C	3.71470700	0.43892300	-0.22212100
H	3.90370100	0.74656200	-1.25827200
H	4.20782500	1.17460300	0.43242600
H	4.23436800	-0.51715400	-0.07869300
O	-0.15913700	0.58219700	0.57282100
³VI^c			
C	3.37638500	0.13201600	-0.10729900
C	4.12793800	-0.43521600	0.92086500
C	5.47835300	-0.16807800	1.11226500
H	6.00543800	-0.64135700	1.93281800
C	6.11133800	0.71292300	0.23396500
H	7.16594700	0.93445300	0.36286000
C	5.40138700	1.31459000	-0.80666100
H	5.87114200	2.00226200	-1.50060500
C	4.05097100	1.01777900	-0.94745600
C	1.88132300	-0.09268900	-0.22552400

C	1.35389600	-1.35850300	-0.74321200
C	2.25592100	-2.34559500	-1.19968200
H	3.32690700	-2.16300500	-1.17286300
C	1.77913800	-3.54935500	-1.69696500
H	2.46572700	-4.31237400	-2.05257200
C	0.39513800	-3.75783100	-1.73421500
H	0.00403800	-4.69665400	-2.12332000
C	-0.48321100	-2.77089800	-1.28053400
H	-1.54686100	-2.99520100	-1.33965300
C	-0.06593800	-1.52506600	-0.76136000
C	-2.85330000	3.41295900	-0.99439700
H	-2.60564400	4.45114600	-1.24240600
H	-3.54369100	3.40914800	-0.14590000
H	-3.36570200	2.96498400	-1.85135600
C	-0.28272700	2.81565200	-2.06185000
H	-0.69260200	2.31118300	-2.94216500
H	0.72668500	2.43546000	-1.89098100
H	-0.23771300	3.89299700	-2.25790500
C	-0.55508400	3.53435500	0.68819600
H	0.42254800	3.12153700	0.94442200
H	-1.17465500	3.55304400	1.58980300
H	-0.43620200	4.55915500	0.31883700
C	-2.54469400	0.63326700	3.36931200
H	-2.41574400	0.36350800	4.42381200
H	-3.55218100	0.34467400	3.05402100
H	-2.46287000	1.72017500	3.27214400
C	-1.46766900	-1.95023400	2.82387800
H	-0.70720400	-2.55479500	2.32304400
H	-2.44719000	-2.33561700	2.52833800
H	-1.35904600	-2.05255200	3.90933500
C	0.27188800	0.26595500	3.17894900
H	0.47928400	1.33125300	3.04865400
H	1.11590300	-0.28941900	2.76351800
H	0.18839600	0.04376000	4.24875600
F	3.50081400	-1.27508800	1.77500100
F	3.35948200	1.59720800	-1.95262500
P	-1.33088000	2.42313000	-0.57888600
P	-1.28346500	-0.18695900	2.26702900
Co	-1.23598800	0.06195000	-0.09513300
P	-3.49670000	-0.64575800	-0.68340200
C	-3.65649100	-0.92196400	-2.51655200
H	-3.48675400	0.02509300	-3.03812500
H	-2.88289200	-1.62199700	-2.84242500
H	-4.64142400	-1.31028400	-2.79915000
C	-4.12501600	-2.27536000	-0.03572400
H	-5.04895200	-2.58799100	-0.53526900
H	-3.36583700	-3.04952900	-0.16694000
H	-4.32510000	-2.18115300	1.03592400
C	-5.02749200	0.37679900	-0.38297200

H	-4.92560400	1.35159200	-0.86623900
H	-5.93141600	-0.11179600	-0.76412700
H	-5.14724500	0.54716700	0.69143700
O	1.16161200	0.84002400	0.14777600
C			
C	1.51251500	0.11139300	-0.22073900
C	2.65435100	0.55105400	0.46207200
C	3.81144300	-0.21456500	0.54135600
H	4.65894100	0.17132100	1.09739600
C	3.85058900	-1.45391500	-0.09791500
H	4.75410500	-2.05400900	-0.04762700
C	2.73461400	-1.91898300	-0.79660500
H	2.76575000	-2.87950600	-1.30093000
C	1.57660200	-1.14386600	-0.84669400
C	0.31364500	1.00919900	-0.36664100
C	-1.05663900	0.44108000	-0.16514000
C	-1.29833900	-0.76128000	0.51851500
H	-0.46833200	-1.33718500	0.91276200
C	-2.60021400	-1.21644300	0.71877300
H	-2.80769600	-2.13745400	1.25233400
C	-3.65455500	-0.45773600	0.22206300
C	-3.45165100	0.74302300	-0.45560900
H	-4.30614500	1.30224600	-0.82092800
C	-2.14898300	1.18947100	-0.63766500
F	2.63261900	1.73472900	1.09683900
H	-1.94735100	2.12632000	-1.14572400
O	0.46364100	2.18563800	-0.66563300
H	0.71080600	-1.50028300	-1.39610300
F	-4.91367300	-0.89552400	0.40530100
C'			
C	-1.63791900	0.44458900	-0.00817500
C	-2.71281500	1.05182200	-0.67953000
C	-3.93280500	0.40052900	-0.83130200
H	-4.74296300	0.88340200	-1.36833600
C	-4.11356900	-0.87228400	-0.28114500
H	-5.06462300	-1.38532800	-0.38788700
C	-3.07663900	-1.48582600	0.41975600
H	-3.19202000	-2.46104600	0.88021300
C	-1.86153400	-0.82092600	0.54431400
C	-0.37044800	1.24228600	0.15174500
C	0.96960300	0.59471700	0.03118300
C	1.17052000	-0.63610100	-0.61244700
H	0.32666400	-1.18177100	-1.01936700
C	2.45207100	-1.15987500	-0.76019900
H	2.62883300	-2.10424000	-1.26296900
C	3.52796500	-0.44316600	-0.24608700
C	3.36602100	0.78312100	0.39449700

H	4.23553000	1.30729000	0.77583100
C	2.08248500	1.30099000	0.51852400
H	1.91505300	2.26143800	0.99363300
O	-0.45958100	2.45055400	0.33852200
F	4.76807700	-0.94984200	-0.37659100
H	-2.55999200	2.05009900	-1.07612700
F	-0.88446000	-1.42499600	1.25548200
3rd			
C	2.23172000	-0.58338900	-0.30467400
C	3.61985500	-0.53132200	-0.61834600
C	4.45027400	-1.63138200	-0.46341100
H	5.50489800	-1.57832400	-0.71419100
C	3.91776800	-2.83193700	0.00650600
C	2.56485900	-2.94849400	0.30475900
H	2.17458900	-3.89781300	0.65930200
C	1.73758400	-1.83968500	0.14151000
C	1.34161600	0.55015200	-0.48860100
C	1.84266200	1.92004800	-0.70543700
C	2.91157000	2.50829000	-0.00123600
C	3.33007200	3.81701600	-0.19265700
H	4.15827800	4.19075300	0.40087100
C	2.65840700	4.62449500	-1.11389400
H	2.97777000	5.64999900	-1.27164200
C	1.56531100	4.09879500	-1.81128100
H	1.02908100	4.71674500	-2.52640300
C	1.16725000	2.78225500	-1.60273600
C	-3.32864700	-2.20664400	-2.42658700
H	-3.25309200	-2.79524900	-3.34644800
H	-3.84492200	-1.27019600	-2.65128500
H	-3.92815900	-2.76068500	-1.70028400
C	-0.75239300	-1.16213600	-3.17355000
H	0.29249700	-1.00617200	-2.89974400
H	-1.17910100	-0.19047800	-3.43413100
H	-0.81415400	-1.82675700	-4.04146200
C	-0.96519500	-3.58139300	-1.63693400
H	-1.48562500	-4.13860800	-0.85297800
H	0.09744700	-3.53947000	-1.38550800
H	-1.08565200	-4.10780500	-2.58953200
C	-4.65001500	1.29983700	0.48495100
H	-5.18229900	2.23068600	0.26196800
H	-4.63576600	1.14757600	1.56791500
H	-5.19778300	0.46213300	0.04337600
C	-2.27788500	2.92639700	0.48295300
H	-1.26546200	3.07913200	0.09953100
H	-2.22948700	2.90775500	1.57531800
H	-2.91366500	3.76460900	0.17783400
C	-3.19663000	1.78009800	-1.93281300
H	-3.72189800	0.97959700	-2.46078400

H	-2.22885500	1.93238600	-2.41787100
H	-3.78517600	2.69988400	-2.02018700
P	-1.64974700	-1.86195800	-1.71935400
P	-2.90878100	1.30394500	-0.15941000
Co	-1.43565800	-0.65914500	0.29812400
C	-2.80295800	-1.89092800	1.09866300
H	-2.33677400	-2.85726400	1.34540700
H	-3.25804500	-1.50431200	2.01813600
H	-3.63136300	-2.09360300	0.40907000
P	-0.75682900	-0.13579700	2.47937400
C	0.55931500	1.13540300	2.73561100
H	1.46814100	0.85662600	2.19931800
H	0.22245300	2.09588100	2.33823200
H	0.78771000	1.24824200	3.80055200
C	-0.08115800	-1.58527100	3.41220800
H	-0.82366800	-2.38761300	3.42140100
H	0.81870200	-1.94953300	2.91040400
H	0.16994700	-1.31515000	4.44304200
C	-2.05853000	0.45969000	3.65892100
H	-2.48609300	1.40060300	3.30362500
H	-2.86270700	-0.27545900	3.73279700
H	-1.63382900	0.62327400	4.65457100
H	0.68261600	-1.94104300	0.37432100
H	4.04274500	0.38274700	-1.01747300
F	3.54635100	1.78971500	0.96378500
O	0.04108100	0.41134100	-0.56863400
F	4.73009600	-3.90627300	0.15910800
H	0.32404200	2.36989000	-2.14607200

¹II^d

C	1.28893000	1.12811400	-0.38467200
C	2.25813300	2.12615500	-0.10057700
C	1.96623600	3.45977600	-0.26810700
H	2.68253800	4.24172700	-0.04250300
C	0.68583100	3.81349700	-0.75835500
C	-0.27970300	2.89521300	-1.07227700
H	-1.22548800	3.23391900	-1.47956300
C	-0.03184300	1.50175100	-0.85732400
C	1.43083200	-0.25904100	-0.10254200
C	2.70032900	-0.96999200	0.19521100
C	3.91829600	-0.72275100	-0.45411000
C	5.07858400	-1.43461400	-0.17222700
H	5.98461800	-1.19429400	-0.71812300
C	5.04108700	-2.44488400	0.78770200
H	5.94352700	-3.00387000	1.01600700
C	3.84101600	-2.73790000	1.44214400
H	3.80364200	-3.52827300	2.18554100
C	2.69167300	-2.01433200	1.13985100
C	-3.23550500	-0.26000300	2.49350200

H	-3.42490600	0.14180500	3.49471900
H	-3.01529200	-1.32814700	2.57770300
H	-4.13782500	-0.14235700	1.88727300
C	-0.46206400	0.37096700	2.88963800
H	0.43138400	0.89559500	2.54024900
H	-0.22014100	-0.69205700	2.96842400
H	-0.73892900	0.75252600	3.87781100
C	-2.28104700	2.37261800	1.92795000
H	-3.18961900	2.60132900	1.36600900
H	-1.48088500	3.01410700	1.55016100
H	-2.44993000	2.58529600	2.98844700
C	-1.96250900	-2.52823100	-2.73301800
H	-2.39761000	-3.50746100	-2.96389500
H	-0.88785000	-2.55757900	-2.93253200
H	-2.40813800	-1.77550400	-3.38942300
C	-1.53545400	-3.49771200	-0.07113300
H	-1.81756700	-3.45002500	0.98497000
H	-0.44656900	-3.44700500	-0.13096500
H	-1.88880600	-4.44564800	-0.49001400
C	-4.05807800	-2.34104600	-0.80866700
H	-4.60402600	-1.59806800	-1.39506300
H	-4.36395200	-2.23807800	0.23590900
H	-4.32791800	-3.34234900	-1.16018100
P	-1.82327700	0.60329800	1.65621700
P	-2.23754000	-2.03528600	-0.96445900
Co	-1.34692500	-0.00262100	-0.39011200
C	-2.99814900	0.90329900	-1.05733400
H	-2.93666900	1.99315100	-0.95330100
H	-3.11483100	0.68600600	-2.12974800
H	-3.92606100	0.58508800	-0.56309300
O	0.35501500	-0.96109800	-0.06967000
H	-0.47139700	0.81773000	-1.67326400
H	3.23049200	1.83688600	0.28225600
F	3.98655900	0.22127600	-1.41874800
F	0.42960500	5.13193000	-0.92200400
H	1.75227800	-2.23923800	1.63302900

¹TS1^d

C	1.31184800	1.17378800	-0.18306300
C	2.36026300	2.11994500	-0.08775800
C	2.10455600	3.46216000	-0.27507600
H	2.87782000	4.21858500	-0.20591600
C	0.78299600	3.84141300	-0.57362500
C	-0.26604500	2.95237500	-0.67338100
H	-1.25275200	3.33602300	-0.90733800
C	-0.04920700	1.57051200	-0.45057200
C	1.45682100	-0.23930600	0.01954300
C	2.74853900	-0.95827200	0.23404600
C	3.88840700	-0.77134700	-0.55640100

C	5.06346100	-1.48757000	-0.35671400
H	5.90868000	-1.30016500	-1.01011500
C	5.11528000	-2.43387200	0.66529800
C	3.98979700	-2.66476700	1.46132000
H	4.02303200	-3.40786100	2.25186300
C	2.82155600	-1.94261500	1.23501200
C	-3.72581700	-0.00739700	2.26929300
H	-3.89130600	0.12054200	3.34400500
H	-4.11159600	-0.98320400	1.96473200
H	-4.28041200	0.76202800	1.72725700
C	-1.20093800	-1.16482800	2.96823500
H	-0.11109100	-1.09205000	2.93672600
H	-1.48118100	-2.16143900	2.61581200
H	-1.53723800	-1.04219900	4.00318500
C	-1.46847500	1.67354900	2.73897800
H	-1.91715800	2.52860100	2.22654100
H	-0.38323300	1.79968600	2.70379400
H	-1.80026200	1.66222600	3.78259500
C	-2.81352600	-1.34745800	-3.06454200
H	-3.27175500	-2.22612000	-3.53113100
H	-1.94802500	-1.03279900	-3.65344600
H	-3.53219000	-0.52420100	-3.05922400
C	-1.17481500	-3.16377700	-1.56939000
H	-0.85717600	-3.54390600	-0.59534100
H	-0.27655000	-2.86016200	-2.11221200
H	-1.68358500	-3.96005100	-2.12292300
C	-3.79557800	-2.49265600	-0.64763100
H	-4.57955800	-1.74142400	-0.51809600
H	-3.57681600	-2.93197200	0.33040200
H	-4.16977900	-3.28163100	-1.30896500
P	-1.92799600	0.11900000	1.84462700
P	-2.26529900	-1.68652500	-1.32923900
Co	-1.28785600	0.12504200	-0.32724200
C	-2.88454800	1.24354800	-0.77427000
H	-2.95554400	2.12265900	-0.11976900
H	-2.80650800	1.60762700	-1.80516500
H	-3.83370300	0.69761000	-0.68453600
O	0.40546900	-0.94474300	0.04255800
H	-0.64595000	0.65512400	-1.58398200
H	1.93577300	-2.12773500	1.83326600
F	0.54246300	5.15893600	-0.75298100
H	3.36897800	1.79575500	0.14349100
H	6.02986900	-2.99499600	0.83153500
F	3.85748500	0.10990400	-1.57908600
¹III^d			
C	1.32119800	1.15257900	-0.19463600
C	2.39367900	2.06945000	-0.10601300
C	2.16885700	3.41797600	-0.31153100

H	2.96010000	4.15661100	-0.25145600
C	0.86107500	3.81976100	-0.61420600
C	-0.21106900	2.94508700	-0.69097100
H	-1.18848800	3.35174200	-0.92910500
C	-0.02405900	1.57215700	-0.45862100
C	1.45270100	-0.27139200	0.01212800
C	2.74309000	-0.99274000	0.24407300
C	3.88108300	-0.83352100	-0.55434500
C	5.05008900	-1.55602700	-0.34118900
H	5.89483000	-1.39263800	-1.00156200
C	5.09648600	-2.47726500	0.70365200
C	3.97223000	-2.67860800	1.50941500
H	4.00194400	-3.40248000	2.31767800
C	2.80928400	-1.95256400	1.26856600
C	-3.71643800	0.24430400	2.19164400
H	-3.89118400	0.48173600	3.24613300
H	-4.11301600	-0.75207900	1.98347600
H	-4.25557700	0.96260100	1.56920000
C	-1.21169600	-0.90471800	2.98796400
H	-0.12026700	-0.85985400	2.94867100
H	-1.51566300	-1.91822500	2.71096500
H	-1.54009000	-0.70011500	4.01235800
C	-1.44311000	1.91334200	2.57439100
H	-1.86187800	2.74124900	1.99664300
H	-0.35568600	2.02033500	2.56306800
H	-1.80463300	1.97164400	3.60625800
C	-3.05568700	-1.61790200	-2.86206900
H	-3.51989600	-2.55022800	-3.20001600
H	-2.25697800	-1.33478400	-3.55168700
H	-3.80157100	-0.81946200	-2.86857600
C	-1.20380300	-3.22532300	-1.37601200
H	-0.78740800	-3.50774500	-0.40640400
H	-0.37129800	-2.92636800	-2.01707700
H	-1.71813700	-4.08421400	-1.81914300
C	-3.76574600	-2.57363300	-0.27415300
H	-4.57969700	-1.85035200	-0.17137600
H	-3.45215200	-2.88216600	0.72761500
H	-4.14225200	-3.45170200	-0.80972900
P	-1.91241600	0.31157200	1.77476900
P	-2.33934500	-1.78080700	-1.16558700
Co	-1.27594600	0.11556000	-0.45381900
C	-2.81799100	1.25538300	-0.99724500
H	-2.89907400	2.13993400	-0.35158500
H	-2.68289900	1.60524800	-2.02494000
H	-3.78073800	0.72837000	-0.94061100
O	0.40742400	-0.97232400	0.03644600
H	-0.86731000	0.12625300	-1.86512500
H	1.92362700	-2.11534300	1.87372600
F	0.64552800	5.13653200	-0.82522300

H	3.39574900	1.72648800	0.12791600
H	6.00642000	-3.04277300	0.88027300
F	3.85333500	0.02315900	-1.59665000
¹TS2^d			
C	1.28920500	1.17070900	-0.24679700
C	2.32479900	2.12653800	-0.13454300
C	2.04952400	3.47177300	-0.30066000
H	2.81535600	4.23559800	-0.22614500
C	0.72579600	3.83760800	-0.57727200
C	-0.31264400	2.92509100	-0.67062100
H	-1.30802600	3.30647500	-0.87815500
C	-0.07341800	1.54748000	-0.49719100
C	1.46090200	-0.25170600	-0.07268500
C	2.74737300	-0.94834100	0.22803900
C	3.92909000	-0.75813600	-0.49678000
C	5.09772900	-1.45998100	-0.22297100
H	5.97691500	-1.27073400	-0.82937500
C	5.10050400	-2.39545000	0.81050500
C	3.93388700	-2.62786800	1.54449300
H	3.92947600	-3.36079000	2.34527800
C	2.77362200	-1.91973000	1.24436900
C	-2.74478300	2.14166000	1.89035800
H	-3.00291500	2.32149200	2.93909200
H	-3.65384300	2.21992000	1.28602600
H	-2.04798000	2.91254800	1.55259000
C	-3.20665600	-0.57422300	2.57134100
H	-2.83602000	-1.60004900	2.65582200
H	-4.15329500	-0.59804600	2.02318600
H	-3.39756500	-0.18812100	3.57875000
C	-0.61477500	0.54077700	2.91686200
H	0.17084400	1.21541100	2.56768700
H	-0.17767100	-0.45533700	3.03285300
H	-0.97965600	0.88347600	3.89090200
C	-1.86921500	-2.60291700	-2.66621800
H	-2.27958000	-3.60118000	-2.85419800
H	-0.78544300	-2.62327700	-2.80696600
H	-2.28786500	-1.89928300	-3.39095000
C	-1.59615600	-3.41491700	0.06264500
H	-1.91809900	-3.29710000	1.10107400
H	-0.50483600	-3.38411800	0.04046100
H	-1.94838700	-4.38188700	-0.31083900
C	-4.06694600	-2.27808000	-0.86722700
H	-4.57619300	-1.54861800	-1.50284800
H	-4.41368200	-2.13248200	0.15914300
H	-4.34312100	-3.28603500	-1.19393600
P	-1.97032500	0.47358300	1.65095000
P	-2.23446600	-2.00503200	-0.95196800
Co	-1.28267400	0.05613300	-0.52856400

C	-2.69054400	1.04919700	-1.73066400
H	-3.29174300	1.45166600	-0.90964400
H	-2.36880200	1.89598500	-2.34345200
H	-3.33896300	0.41975700	-2.34739000
H	-1.39437500	0.36339200	-1.95682000
H	3.34109700	1.81611600	0.08166900
H	6.00925500	-2.94588500	1.03445800
F	3.94690300	0.11396000	-1.52854600
O	0.42630300	-0.97355900	-0.12622800
H	1.85856100	-2.10249000	1.79796200
F	0.45936500	5.15285100	-0.74365600

¹IV^d

C	1.14705000	1.35055300	0.00516300
C	2.00019600	2.47336800	-0.02617200
C	1.47339400	3.74057600	-0.21403900
H	2.09131800	4.63058200	-0.24941800
C	0.08891700	3.84140400	-0.37306800
C	-0.76821700	2.75043400	-0.31251000
H	-1.82610200	2.96082200	-0.43311700
C	-0.28617200	1.44537600	-0.08802700
C	1.60139600	-0.00983700	0.15026100
C	3.00806500	-0.45850500	0.35498700
C	4.08141500	-0.08323200	-0.46007600
C	5.37474400	-0.55098900	-0.25787200
H	6.16052000	-0.22833900	-0.93239100
C	5.62024700	-1.43073900	0.79551800
C	4.56975400	-1.84304100	1.62031000
H	4.75573700	-2.53212900	2.43818900
C	3.28088500	-1.37007000	1.39097500
C	-4.21698000	1.35885700	-0.65187000
H	-5.12897100	1.73159900	-0.17281600
H	-4.49561100	0.68236200	-1.46526800
H	-3.67620700	2.19994400	-1.09093200
C	-4.37871900	-0.77810900	1.19785000
H	-3.91958600	-1.39717700	1.97382200
H	-4.71807600	-1.43208400	0.39152000
H	-5.24911300	-0.26721200	1.62305400
C	-3.09046800	1.60854600	1.99546700
H	-2.46984200	2.47466200	1.76131600
H	-2.63535100	1.09318700	2.84587000
H	-4.09677500	1.93980800	2.27422900
C	-0.56991900	-2.74669100	-2.16092200
H	-0.57232500	-3.80062400	-2.45988600
H	0.45794300	-2.41252800	-2.00449100
H	-1.00580200	-2.14568000	-2.96369400
C	-0.76369600	-3.75118900	0.51789500
H	-1.34283700	-3.82648000	1.44296000
H	0.24502500	-3.41704600	0.76936200

H	-0.71845700	-4.73776200	0.04408900
C	-3.12526300	-3.30377600	-1.03354900
H	-3.68135900	-2.68623000	-1.74512600
H	-3.74123400	-3.44006700	-0.14107900
H	-2.94734400	-4.28501900	-1.48617000
P	-3.13190700	0.44237800	0.55232200
P	-1.52239100	-2.47434800	-0.59254500
Co	-1.13622400	-0.29365500	-0.00732200
H	3.07249300	2.35648100	0.08479900
H	6.62805000	-1.79754100	0.96498700
F	3.86565100	0.73838000	-1.51137100
O	0.71451800	-0.91371500	0.17371800
H	2.45582000	-1.68859500	2.01954200
F	-0.43735100	5.07110800	-0.57529400

¹₄

C	-3.29157900	-0.08577000	0.06446900
C	-3.86456700	-1.09599700	-0.72275000
C	-5.20675300	-1.44127200	-0.64363800
H	-5.58723200	-2.22349400	-1.29191900
C	-6.02935800	-0.76664100	0.26039900
H	-7.07988500	-1.03152100	0.33239100
C	-5.49758800	0.24280100	1.06500000
H	-6.13045500	0.76487800	1.77606600
C	-4.14730300	0.57627800	0.96374100
C	-1.83849700	0.21416700	-0.01037700
C	-1.26267000	1.52949900	-0.08032100
C	-2.01152300	2.72191800	-0.22324000
H	-3.09433700	2.67674900	-0.29033500
C	-1.37735700	3.94844700	-0.30041800
H	-1.92003600	4.88024400	-0.41441100
C	0.02110000	3.95471000	-0.23680900
C	0.77974700	2.80255600	-0.11975500
H	1.85646100	2.92626300	-0.09013200
C	0.17979700	1.52355900	-0.04835700
C	2.58336200	-3.62392200	0.10108000
H	2.33798500	-4.68757200	0.19006200
H	3.23290000	-3.34196400	0.93329400
H	3.13787900	-3.47350400	-0.82785600
C	0.08443100	-3.38056800	-1.27377500
H	0.56941900	-3.19048900	-2.23433300
H	-0.90931800	-2.92990400	-1.29505400
H	-0.00048500	-4.46308900	-1.12870000
C	0.14360000	-3.29776200	1.55543200
H	-0.84278700	-2.83115800	1.59575500
H	0.67368100	-3.07075200	2.48405400
H	0.03226200	-4.38400800	1.46949600
C	3.12988400	-1.01473400	2.73554000
H	3.45251200	-0.68050700	3.72793300

H	4.00645600	-1.07050200	2.08303000
H	2.71336600	-2.02039000	2.83069400
C	2.80694800	1.73659100	2.31038600
H	2.15284900	2.59432300	2.14651500
H	3.65378600	1.81440700	1.62273500
H	3.18260300	1.76682400	3.33891600
C	0.66661300	0.24755400	3.41047800
H	0.13079900	-0.70147800	3.49708800
H	-0.06803600	1.02582300	3.18619400
H	1.15319700	0.47461500	4.36626600
F	-3.10022600	-1.74764300	-1.62839200
P	1.04256700	-2.58411300	0.09784200
P	1.87616600	0.15567600	1.99715600
Co	0.91533700	-0.26615500	0.02978300
P	2.14253200	0.11607900	-1.80411800
C	1.23485100	0.90427500	-3.22283800
H	0.42026600	0.24430600	-3.53533500
H	0.79363300	1.84493400	-2.88622500
H	1.89312500	1.09455700	-4.07828400
C	3.61858800	1.25151900	-1.69637000
H	4.09243400	1.38516600	-2.67554700
H	3.32389000	2.23137800	-1.31768000
H	4.34989900	0.82282400	-1.00483600
C	2.98916900	-1.25850200	-2.74210200
H	2.26677100	-2.01739000	-3.05329500
H	3.48661900	-0.86868800	-3.63704800
H	3.74274400	-1.73604500	-2.10993700
O	-1.02267500	-0.75786400	0.00684200
H	-3.73019500	1.34653100	1.60420000
F	0.65468800	5.15107200	-0.30610700
$3V^d$			
C	-2.36268600	-0.32943000	-0.20586000
C	-3.73693200	-0.13771500	0.12841200
C	-4.62772700	-1.19760800	0.21586300
H	-5.66888400	-1.03486000	0.47609600
C	-4.17514500	-2.49751200	-0.01626800
C	-2.84070700	-2.74736800	-0.31783200
H	-2.51289600	-3.76933800	-0.48416600
C	-1.95245800	-1.67888500	-0.40655900
C	-1.40129400	0.75432700	-0.27675500
C	-1.83504200	2.16505900	-0.32181900
C	-2.90815900	2.61580400	-1.12698300
C	-3.25792300	3.96044800	-1.21840800
H	-4.08490200	4.25631000	-1.85774600
C	-2.53791000	4.92768800	-0.51137300
H	-2.80212100	5.97837200	-0.57912200
C	-1.46723600	4.52568300	0.29192900
H	-0.88866100	5.23671600	0.87311500

C	-1.14244700	3.18073300	0.36787200
C	1.92710200	-0.94795900	3.61128000
H	1.53331200	-1.25654000	4.58505900
H	2.25936100	0.08978900	3.68438900
H	2.78761200	-1.57227600	3.36081300
C	-0.68277300	0.02763700	2.97670900
H	-1.62288400	-0.15816000	2.45332500
H	-0.40288500	1.06683100	2.79399300
H	-0.82728200	-0.13872100	4.04923500
C	-0.07154500	-2.76690900	2.67301200
H	0.67585400	-3.52976600	2.44014900
H	-0.94895600	-2.93588000	2.04375100
H	-0.36176800	-2.85664400	3.72489100
C	4.73542100	0.62402400	-0.05594700
H	5.37008600	1.51651500	-0.07869000
H	4.85941900	0.07706700	-0.99409100
H	5.07189100	-0.02991400	0.75406000
C	2.65718400	2.32496800	-1.10461100
H	1.64328200	2.71013900	-0.97737000
H	2.72353000	1.87411000	-2.09856700
H	3.37739500	3.14787600	-1.04244300
C	3.09171600	2.15614200	1.68516300
H	3.42128800	1.58395700	2.55638000
H	2.11580400	2.59745500	1.89688100
H	3.81401600	2.96070600	1.50778000
P	0.62253500	-1.09161200	2.30293500
P	2.94340700	1.04230800	0.20420700
Co	1.26885700	-0.84607900	0.07626400
C	2.55155100	-2.36511500	0.36160900
H	2.01088900	-3.32297000	0.31921000
H	3.33922200	-2.40276300	-0.40209000
H	3.06595100	-2.32327200	1.32974000
P	1.42346400	-1.27244000	-2.23889600
C	0.35496800	-0.22962100	-3.32490200
H	-0.68645800	-0.35284400	-3.01995500
H	0.61318000	0.82229200	-3.18621100
H	0.46354600	-0.50189700	-4.37976100
C	0.91120900	-2.98674200	-2.72354300
H	1.53094700	-3.71237600	-2.19037700
H	-0.13239000	-3.15233300	-2.44337200
H	1.01480500	-3.14788900	-3.80153400
C	3.06718400	-1.16360500	-3.08945100
H	3.44956000	-0.14101700	-3.04076300
H	3.78354500	-1.82298200	-2.59290000
H	2.98553900	-1.45670300	-4.14107400
H	-0.91257900	-1.88145400	-0.63650200
H	-4.09786300	0.86111700	0.34466800
F	-0.11703200	2.84348700	1.20367600
O	-0.11232700	0.55262900	-0.34069400

F	-5.04771600	-3.53183400	0.06687000
H	-3.45648300	1.88148600	-1.70821800
³VI^d			
C	1.14380600	1.80099800	-0.40003500
C	2.09474800	2.64954800	0.23651100
C	1.99953400	4.03526000	0.20760500
H	2.75368200	4.62992100	0.71547300
C	0.93772000	4.66725600	-0.45069200
C	-0.03628900	3.87661200	-1.06915700
H	-0.88318900	4.31104900	-1.59039300
C	0.08651400	2.50104500	-1.03174700
C	1.22596900	0.34435300	-0.36744900
C	2.50206600	-0.36906500	-0.24765400
C	3.75240800	0.16858500	-0.64016400
C	4.92517600	-0.57378600	-0.54869500
H	5.87959600	-0.16098300	-0.85892400
C	4.86666600	-1.87910400	-0.06813600
C	3.65894400	-2.46102900	0.30393400
H	3.64767100	-3.48549800	0.66247700
C	2.49151400	-1.71186200	0.20515700
C	-2.68510000	0.48252900	3.41633500
H	-2.49707600	0.15962500	4.44536700
H	-3.69992100	0.19844100	3.12749600
H	-2.61733300	1.57257000	3.36531100
C	-1.62005000	-2.06682000	2.62976900
H	-0.85703400	-2.61797000	2.07432900
H	-2.60301900	-2.42779900	2.31475400
H	-1.49499700	-2.25989700	3.70036700
C	0.14514600	0.16807800	3.02362800
H	0.30581900	1.24755100	2.95573300
H	0.95711200	-0.32446100	2.48300200
H	0.17253400	-0.13376800	4.07583600
C	-2.25154000	-1.01550500	-3.18539900
H	-2.54284500	-1.81853900	-3.87054600
H	-1.20385800	-0.75465000	-3.35608700
H	-2.85973900	-0.13004300	-3.39041700
C	-1.50349400	-3.08934900	-1.34474000
H	-1.70910300	-3.60121800	-0.40012000
H	-0.44006100	-2.84060900	-1.37634400
H	-1.75496500	-3.75918200	-2.17354800
C	-4.21421300	-2.07314200	-1.36220000
H	-4.87386700	-1.20884300	-1.47605700
H	-4.42491400	-2.52972900	-0.39074800
H	-4.43434700	-2.80015600	-2.15075700
P	-1.47290800	-0.26449500	2.23781000
P	-2.45421200	-1.50584700	-1.41255300
Co	-1.67747900	0.21167200	-0.00726800
C	-3.43182000	1.08978200	0.16202200

H	-3.31464600	2.00872900	0.75712700
H	-3.76338100	1.38623600	-0.84479600
H	-4.23281400	0.49481400	0.61895000
O	0.14822200	-0.39821800	-0.43190600
H	2.90599300	2.18722600	0.78709200
H	1.53888500	-2.15250000	0.47526000
F	-0.91107200	1.78456100	-1.65870400
H	3.80173100	1.17044000	-1.05149800
H	0.86077000	5.74912500	-0.47844500
F	6.00774300	-2.60127900	0.02641400

³TS3^d

C	0.94066400	1.74950300	0.02402900
C	1.81974600	2.82983100	0.30884300
C	1.36911600	4.12959400	0.26507200
H	2.03102600	4.95315800	0.51336800
C	0.01810800	4.38307100	-0.08874800
H	-0.33934400	5.41039900	-0.11006100
C	-0.85656800	3.36494100	-0.39696000
H	-1.87764800	3.59514600	-0.67731900
C	-0.43174900	2.00562700	-0.33783900
C	1.27135900	0.36426100	0.14192000
C	2.66280400	-0.16368600	0.14110800
C	3.68165000	0.41895300	-0.63197400
H	3.46054000	1.28793500	-1.24158800
C	4.96337600	-0.12768800	-0.65428900
H	5.75568600	0.30343000	-1.25646900
C	5.21910300	-1.26183300	0.10832100
C	4.23278600	-1.87275300	0.87783900
H	4.47590000	-2.75907200	1.45395700
C	2.95481100	-1.32335500	0.87935500
C	-3.76970000	-0.82792500	2.86315000
H	-3.77705700	-1.23998200	3.87804200
H	-4.41326000	-1.44277300	2.22693600
H	-4.19037400	0.18131600	2.88652000
C	-1.47908400	-2.50488700	2.36483300
H	-0.45566600	-2.57338900	1.98802400
H	-2.10414000	-3.17813500	1.77089800
H	-1.50732600	-2.82591400	3.41161500
C	-1.12708800	0.12014600	3.47422700
H	-1.48389400	1.15144500	3.54659000
H	-0.06920300	0.15056500	3.20109700
H	-1.23652300	-0.36666600	4.44927400
C	-2.95747300	-0.82657500	-3.17403500
H	-2.96528500	-1.47350000	-4.05744600
H	-2.57921400	0.16292600	-3.44256700
H	-3.97873600	-0.71205400	-2.80006600
C	-0.26623700	-1.73213700	-2.71362700
H	0.43320000	-2.24787700	-2.05148200

H	0.13229400	-0.73710300	-2.92440400
H	-0.38621600	-2.29836900	-3.64284800
C	-2.49243600	-3.20719600	-1.59918700
H	-3.50128900	-3.18409500	-1.17604900
H	-1.84026500	-3.73991400	-0.90105300
H	-2.52211600	-3.76088200	-2.54365900
F	-0.66970400	1.30460700	-1.92385100
H	2.16404400	-1.78644800	1.45923800
P	-2.06300100	-0.76119500	2.14024100
P	-1.86677500	-1.47624200	-1.83250600
Co	-1.55135900	0.38157100	-0.13610800
C	-3.27604400	1.37917500	-0.22946000
H	-3.35256500	2.07240200	0.61492900
H	-3.34382100	1.92936000	-1.17101200
H	-4.07893300	0.63377500	-0.16404400
O	0.32310100	-0.48234500	0.23982100
H	2.84086200	2.61761500	0.61046600
F	6.45803500	-1.79214200	0.09651500

¹VII^d

C	2.78499800	-0.11975400	0.18341500
C	3.74920700	0.22290400	-0.77867600
C	5.05583900	-0.25144200	-0.67583500
H	5.80849900	-0.01120400	-1.41864000
C	5.38997900	-1.05941500	0.40517700
C	4.45768500	-1.42518300	1.37258800
H	4.76168500	-2.06332100	2.19519300
C	3.15214300	-0.96318400	1.24530500
C	1.36121500	0.30462900	0.06359900
C	0.94059700	1.63232600	-0.38588300
C	1.82309700	2.72762600	-0.50179800
H	2.87217800	2.61646800	-0.24700300
C	1.34238200	3.96145600	-0.91824000
H	2.01292800	4.81124100	-1.00556700
C	-0.01806900	4.09536800	-1.22297100
C	-0.89542900	3.01739900	-1.08144100
H	-1.94164700	3.16714200	-1.33028300
C	-0.45516500	1.76315900	-0.63847100
C	-0.38784800	-3.17213500	-0.95090800
H	-0.57606100	-4.18489100	-1.32133200
H	0.20769500	-3.21504400	-0.03664000
H	0.15443400	-2.58289300	-1.69181000
C	-2.85632100	-3.40783100	0.50878700
H	-3.87420300	-3.04780600	0.68450600
H	-2.33739100	-3.45557000	1.47148800
H	-2.91382700	-4.42130400	0.09742100
C	-2.86926100	-2.51012700	-2.22393600
H	-2.35045500	-1.90133400	-2.96623100
H	-3.90001400	-2.15795600	-2.13311800

H	-2.87163100	-3.56296000	-2.52373300
C	-0.94038500	0.46369100	2.99570500
H	-1.38616100	0.72977900	3.95926300
H	-0.08173000	1.11307400	2.80736400
H	-0.58298500	-0.56798200	3.03145400
C	-2.72545200	2.38908300	1.84565500
H	-3.57140400	2.58839500	1.18351000
H	-1.92092700	3.07864400	1.58331600
H	-3.03543700	2.56133100	2.88106300
C	-3.61560200	-0.28724900	2.25267500
H	-3.35321000	-1.33798600	2.39143300
H	-4.42643300	-0.22908600	1.52172100
H	-3.96344200	0.12289700	3.20608600
P	-1.95649700	-2.25506300	-0.64301000
P	-2.15359800	0.64836800	1.61332500
Co	-1.37627000	0.08121000	-0.43630600
C	-3.06386600	0.68856600	-1.23572700
H	-3.90152700	0.02551100	-0.98639600
H	-3.33968500	1.70953300	-0.95525700
H	-2.87266400	0.64753200	-2.30993400
H	3.46742400	0.83354800	-1.62907000
O	0.48050000	-0.52870600	0.37536500
H	-0.39792200	5.05525000	-1.56658000
H	2.39952000	-1.24933800	1.97207900
F	-0.70950800	-0.41841200	-2.09455200
F	6.65424500	-1.50976300	0.51724000