|  |  |
| --- | --- |
| Conformer | Coordinates |
| opt\_4e\_CS\_4 | C 1.38579400 -0.25823000 -0.64365100  C 0.89290700 1.05224700 -0.64128900  C -0.47075100 1.33516200 -0.63204400  C -1.38566200 0.25822100 -0.64362000  C -0.89277400 -1.05225700 -0.64126700  C 0.47088300 -1.33516800 -0.63207200  C -2.84264800 0.49510400 -0.68193800  N -3.69200500 -0.45198300 -0.66801600  C -5.10018400 -0.11157000 -0.72888000  C -5.93903400 -0.73284900 0.43853400  C 2.84277300 -0.49512800 -0.68187100  N 3.69214000 0.45195400 -0.66796300  C 5.10033100 0.11151100 -0.72859200  C 5.93906600 0.73322700 0.43866000  H 1.61209200 1.86171500 -0.64747200  C -0.90789100 2.76757800 -0.63478500  H -1.61195800 -1.86172500 -0.64747700  C 0.90803800 -2.76758800 -0.63488100  H -3.15880500 1.54440900 -0.73187500  C -5.79165000 -0.69966400 -2.00372700  H 3.15890100 -1.54444600 -0.73174500  C 5.79194700 0.69909600 -2.00360100  C -0.78781700 3.50950500 -1.79207800  C -1.16779700 4.86928800 -1.83911400  C -1.66687100 5.48607000 -0.72046300  C -1.79989300 4.77198500 0.49807000  C -1.41224900 3.39333000 0.55132100  C -1.53544900 2.70590000 1.78885500  C -2.02573100 3.33868700 2.90600900  C -2.41776100 4.69494600 2.84790200  C -2.30405600 5.39251000 1.67094500  C 1.41205000 -3.39347600 0.55129500  C 1.79969700 -4.77212700 0.49800200  C 1.66703900 -5.48606400 -0.72065800  C 1.16832800 -4.86914100 -1.83939300  C 0.78833700 -3.50935900 -1.79231000  C 1.53494300 -2.70616000 1.78892100  C 2.02490600 -3.33906800 2.90614600  C 2.41690700 -4.69533400 2.84801400  C 2.30351600 -5.39278200 1.67095600  H -0.40062500 3.03362000 -2.68604600  H -1.06402800 5.41909000 -2.76772900  H -1.96370000 6.52919500 -0.75037900  H -1.23135000 1.66830400 1.84606300  H -2.10964200 2.79573300 3.84068200  H -2.80375100 5.18231900 3.73611000  H -2.59757700 6.43593800 1.62039100  H 1.96386500 -6.52919000 -0.75060700  H 1.06485000 -5.41882800 -2.76810800  H 0.40141400 -3.03336500 -2.68633600  H 1.23086600 -1.66855700 1.84613300  H 2.10859300 -2.79620500 3.84089200  H 2.80263800 -5.18280400 3.73628100  H 2.59703000 -6.43620900 1.62038100  C 6.96848200 1.52124600 -1.43350900  C 5.63934000 2.25733100 0.45633300  C 6.36205500 2.80007000 -0.81309800  C 7.38924900 0.69499900 -0.17902600  C 8.45664100 1.38070900 0.69215000  C 7.92926300 -0.70855400 -0.50970500  C 5.71619900 0.03988600 1.77439100  C -6.96820900 -1.52163600 -1.43345200  C -7.38915900 -0.69489300 -0.17935100  C -5.71636200 -0.03896000 1.77400900  H -5.21836800 0.98075300 -0.70327000  H 5.21851700 -0.98079800 -0.70256000  H -5.09480200 -1.32375800 -2.56675700  H -6.12255500 0.10167200 -2.66806400  H 5.09519200 1.32300700 -2.56695200  H 6.12287200 -0.10251800 -2.66759600  H 7.76586400 1.71089600 -2.15667200  H 6.02946100 2.71238300 1.37005100  H 4.56553800 2.43673200 0.43357600  H 7.13388200 3.53010500 -0.55884800  H 5.67398600 3.29003700 -1.50597800  H 8.66145000 0.78591300 1.58745200  H 8.18035400 2.38219100 1.01955600  H 9.39675600 1.46264700 0.13724500  H 7.27546700 -1.29969100 -1.15023100  H 8.09984400 -1.28285600 0.40608500  H 8.89375100 -0.62301100 -1.02032500  H 5.94034700 -1.02992300 1.71790300  H 4.67371800 0.13987200 2.09112500  H 6.34158300 0.47619100 2.55878100  H -7.76550300 -1.71160300 -2.15662900  C -7.92915000 0.70851500 -0.51068300  C -8.45667300 -1.38026400 0.69193500  H -5.94081000 1.03076500 1.71712600  H -4.67385800 -0.13852800 2.09080300  H -6.34163500 -0.47515500 2.55854600  C -5.63928000 -2.25694600 0.45684600  C -6.36181900 -2.80019600 -0.81246100  H -7.27521100 1.29945100 -1.15124700  H -8.10000200 1.28315000 0.40484800  H -8.89350300 0.62274000 -1.02152200  H -8.18048000 -2.38166600 1.01966200  H -9.39674800 -1.46230700 0.13697800  H -8.66151500 -0.78518400 1.58704000  H -6.02951700 -2.71162500 1.37069900  H -4.56547500 -2.43635000 0.43429800  H -7.13365400 -3.53016000 -0.55802600  H -5.67363300 -3.29039900 -1.50505800 |
| opt\_4e\_CS\_8 | C -0.25946800 1.38630900 -0.19783100  C 1.05206700 0.89431300 -0.19698100  C 1.33487000 -0.46967400 -0.19166600  C 0.25946800 -1.38630900 -0.19783100  C -1.05206700 -0.89431300 -0.19698100  C -1.33487000 0.46967400 -0.19166600  C 0.50251600 -2.84281800 -0.22233700  N -0.43838300 -3.69947300 -0.19079700  C -0.08469200 -5.10577400 -0.21462700  C -0.76651200 -5.90175500 -1.37784900  C -0.50251600 2.84281800 -0.22233700  N 0.43838300 3.69947300 -0.19079700  C 0.08469200 5.10577400 -0.21462700  C 0.76651200 5.90175500 -1.37784900  H 1.86282300 1.61254700 -0.19969900  C 2.76741100 -0.90830800 -0.20459400  H -1.86282300 -1.61254700 -0.19969900  C -2.76741100 0.90830800 -0.20459400  H 1.55310900 -3.15488500 -0.27504600  C -0.58666300 -5.85945000 1.06226600  H -1.55310900 3.15488500 -0.27504600  C 0.58666300 5.85945000 1.06226600  C 3.48680400 -0.84093700 -1.38051400  C 4.84518700 -1.22756400 -1.43722100  C 5.48260100 -1.68059100 -0.30938400  C 4.79100200 -1.75828500 0.92738700  C 3.41451000 -1.36341700 0.98961200  C 2.74805900 -1.43514400 2.24304400  C 3.39985600 -1.88045400 3.36907600  C 4.75515600 -2.27704000 3.30332800  C 5.43213400 -2.21463500 2.10945500  C -3.41451000 1.36341700 0.98961200  C -4.79100200 1.75828500 0.92738700  C -5.48260100 1.68059100 -0.30938400  C -4.84518700 1.22756400 -1.43722100  C -3.48680400 0.84093700 -1.38051400  C -2.74805900 1.43514400 2.24304400  C -3.39985600 1.88045400 3.36907600  C -4.75515600 2.27704000 3.30332800  C -5.43213400 2.21463500 2.10945500  H 2.99569800 -0.48981400 -2.28135100  H 5.37768600 -1.16538600 -2.37964500  H 6.52431800 -1.98179300 -0.34702300  H 1.71132400 -1.12830800 2.30552800  H 2.87303700 -1.92569300 4.31571400  H 5.25800800 -2.62661100 4.19805200  H 6.47404600 -2.51280500 2.05323900  H -6.52431800 1.98179300 -0.34702300  H -5.37768600 1.16538600 -2.37964500  H -2.99569800 0.48981400 -2.28135100  H -1.71132400 1.12830800 2.30552800  H -2.87303700 1.92569300 4.31571400  H -5.25800800 2.62661100 4.19805200  H -6.47404600 2.51280500 2.05323900  C 1.42475600 7.02475700 0.49141600  C 2.29273300 5.62811100 -1.29181800  C 2.74805900 6.41663200 -0.02640600  C 0.66977900 7.37684400 -0.82610800  C 1.38922400 8.41923900 -1.70056000  C -0.76105700 7.90214300 -0.60597700  C 0.15744700 5.61495300 -2.74253300  C -1.42475600 -7.02475700 0.49141600  C -0.66977900 -7.37684400 -0.82610800  C -0.15744700 -5.61495300 -2.74253300  H 1.00491300 -5.21034600 -0.31315600  H -1.00491300 5.21034600 -0.31315600  H -1.18496900 -5.19759900 1.69190700  H 0.25772700 -6.20550700 1.66249100  H 1.18496900 5.19759900 1.69190700  H -0.25772700 6.20550700 1.66249100  H 1.55787600 7.85570200 1.18916000  H 2.79446700 5.98726600 -2.19382800  H 2.49081200 4.55981500 -1.21098900  H 3.47857600 7.19089200 -0.27283700  H 3.20858700 5.76878100 0.72322300  H 0.84130100 8.58149300 -2.63391500  H 2.41066200 8.14568600 -1.96306500  H 1.42927500 9.38111600 -1.17907100  H -1.37072900 7.27818600 0.04700100  H -1.28781200 7.99432100 -1.56083900  H -0.72556500 8.90132300 -0.15976000  H -0.91605500 5.82989300 -2.76021100  H 0.28705000 4.56180400 -3.01041700  H 0.63425500 6.21288600 -3.52494800  H -1.55787600 -7.85570200 1.18916000  C 0.76105700 -7.90214300 -0.60597700  C -1.38922400 -8.41923900 -1.70056000  H 0.91605500 -5.82989300 -2.76021100  H -0.28705000 -4.56180400 -3.01041700  H -0.63425500 -6.21288600 -3.52494800  C -2.29273300 -5.62811100 -1.29181800  C -2.74805900 -6.41663200 -0.02640600  H 1.37072900 -7.27818600 0.04700100  H 1.28781200 -7.99432100 -1.56083900  H 0.72556500 -8.90132300 -0.15976000  H -2.41066200 -8.14568600 -1.96306500  H -1.42927500 -9.38111600 -1.17907100  H -0.84130100 -8.58149300 -2.63391500  H -2.79446700 -5.98726600 -2.19382800  H -2.49081200 -4.55981500 -1.21098900  H -3.47857600 -7.19089200 -0.27283700  H -3.20858700 -5.76878100 0.72322300 |
| opt\_4e\_CS\_16 | C -0.00189200 1.41010900 -0.19328400  C 1.19748300 0.68693000 -0.19145600  C 1.22693100 -0.70576600 -0.18539800  C 0.00189200 -1.41010900 -0.19328400  C -1.19748300 -0.68693000 -0.19145600  C -1.22693100 0.70576600 -0.18539800  C -0.02701900 -2.88632700 -0.22487000  N -1.10983500 -3.55433200 -0.18330500  C -1.02460700 -5.00151700 -0.21852800  C -1.84507000 -5.64646200 -1.38594300  C 0.02701900 2.88632700 -0.22487000  N 1.10983500 3.55433200 -0.18330500  C 1.02460700 5.00151700 -0.21852800  C 1.84507000 5.64646200 -1.38594300  H 2.12544200 1.24549400 -0.19252100  C 2.55576600 -1.39737600 -0.19244900  H -2.12544200 -1.24549400 -0.19252100  C -2.55576600 1.39737600 -0.19244900  H 0.94770200 -3.38589900 -0.28940400  C -1.65636400 -5.65855400 1.05352400  H -0.94770200 3.38589900 -0.28940400  C 1.65636400 5.65855400 1.05352400  C 3.28480400 -1.45116000 -1.36309000  C 4.54927700 -2.08015700 -1.41644800  C 5.08420100 -2.65310600 -0.29007500  C 4.38113300 -2.61383100 0.94188200  C 3.09977000 -1.97418800 1.00071900  C 2.42440400 -1.93076800 2.25049000  C 2.97625100 -2.49689200 3.37553900  C 4.23561600 -3.13572700 3.31264900  C 4.91989000 -3.18956300 2.12275100  C -3.09977000 1.97418800 1.00071900  C -4.38113300 2.61383100 0.94188200  C -5.08420100 2.65310600 -0.29007500  C -4.54927700 2.08015700 -1.41644800  C -3.28480400 1.45116000 -1.36309000  C -2.42440400 1.93076800 2.25049000  C -2.97625100 2.49689200 3.37553900  C -4.23561600 3.13572700 3.31264900  C -4.91989000 3.18956300 2.12275100  H 2.87262300 -1.00842100 -2.26307900  H 5.09094200 -2.10813500 -2.35524500  H 6.05328700 -3.13984700 -0.32487700  H 1.46220300 -1.43753700 2.31137700  H 2.44452200 -2.45098900 4.31935900  H 4.66013600 -3.57846200 4.20669100  H 5.88977100 -3.67331300 2.06876500  H -6.05328700 3.13984700 -0.32487700  H -5.09094200 2.10813500 -2.35524500  H -2.87262300 1.00842100 -2.26307900  H -1.46220300 1.43753700 2.31137700  H -2.44452200 2.45098900 4.31935900  H -4.66013600 3.57846200 4.20669100  H -5.88977100 3.67331300 2.06876500  C 2.69739100 6.64324600 0.47612300  C 3.29365200 5.09450200 -1.29191600  C 3.88517000 5.79453200 -0.03126700  C 2.02319300 7.11882500 -0.84709600  C 2.92535800 8.00081500 -1.72874600  C 0.71557400 7.90386000 -0.63501300  C 1.19748300 5.46517200 -2.75107800  C -2.69739100 -6.64324600 0.47612300  C -2.02319300 -7.11882500 -0.84709600  C -1.19748300 -5.46517200 -2.75107800  H 0.02601400 -5.30738500 -0.32072400  H -0.02601400 5.30738500 -0.32072400  H -2.12124700 -4.90107200 1.68795600  H -0.89072900 -6.15889500 1.65057800  H 2.12124700 4.90107200 1.68795600  H 0.89072900 6.15889500 1.65057800  H 2.98150300 7.44047200 1.16787100  H 3.85584500 5.34516100 -2.19497000  H 3.28772200 4.00881300 -1.20143200  H 4.74786800 6.41689100 -0.28067300  H 4.21484800 5.07867500 0.72541500  H 2.41234200 8.26606600 -2.65827600  H 3.87147100 7.53288200 -1.99839300  H 3.15629300 8.93665300 -1.20948200  H 0.00168200 7.41250300 0.02537400  H 0.21320400 8.08168300 -1.59091500  H 0.93777300 8.88399200 -0.20075700  H 0.18240300 5.87488400 -2.77614200  H 1.13046300 4.40385900 -3.00943100  H 1.77957200 5.95727700 -3.53605100  H -2.98150300 -7.44047200 1.16787100  C -0.71557400 -7.90386000 -0.63501300  C -2.92535800 -8.00081500 -1.72874600  H -0.18240300 -5.87488400 -2.77614200  H -1.13046300 -4.40385900 -3.00943100  H -1.77957200 -5.95727700 -3.53605100  C -3.29365200 -5.09450200 -1.29191600  C -3.88517000 -5.79453200 -0.03126700  H -0.00168200 -7.41250300 0.02537400  H -0.21320400 -8.08168300 -1.59091500  H -0.93777300 -8.88399200 -0.20075700  H -3.87147100 -7.53288200 -1.99839300  H -3.15629300 -8.93665300 -1.20948200  H -2.41234200 -8.26606600 -2.65827600  H -3.85584500 -5.34516100 -2.19497000  H -3.28772200 -4.00881300 -1.20143200  H -4.74786800 -6.41689100 -0.28067300  H -4.21484800 -5.07867500 0.72541500 |
| opt\_4e\_CS\_25 | C -1.24035800 0.90580600 -0.58014400  C -0.34668500 1.98471200 -0.64425300  C 1.03673400 1.84028100 -0.53618300  C 1.55690000 0.54316700 -0.36215200  C 0.66679400 -0.53906200 -0.29175100  C -0.71383100 -0.39594500 -0.39259700  C 3.01260300 0.30846400 -0.27900200  N 3.51089700 -0.84450000 -0.07645300  C 4.95439100 -0.96822500 -0.01454400  C 5.53733400 -1.97577700 -1.06267000  C -2.66673900 1.25179900 -0.73641600  N -3.64249900 0.43856100 -0.74464500  C -4.97202300 0.98905200 -0.93848100  C -5.98038800 0.61648300 0.19804500  H -0.75068700 2.98243800 -0.78289100  C 1.89979100 3.05977400 -0.63448200  H 1.08914200 -1.52709600 -0.15533000  C -1.53689600 -1.64478900 -0.31579500  H 3.65151900 1.19155000 -0.40506000  C 5.43430500 -1.56860200 1.34822100  H -2.84060100 2.33323900 -0.86480800  C -5.66775300 0.41979900 -2.21953400  C 2.09031900 3.65531400 -1.86523100  C 2.88088200 4.81797200 -2.00785900  C 3.47936400 5.38508100 -0.91091600  C 3.30663000 4.81839600 0.37855100  C 2.50201800 3.64171100 0.52819500  C 2.32767700 3.10555000 1.83295100  C 2.92432900 3.68915900 2.92568600  C 3.72640200 4.84301200 2.77379100  C 3.90902000 5.39353000 1.52856400  C -2.07728100 -2.09347100 0.93006300  C -2.78687300 -3.33730200 0.97197800  C -2.93762600 -4.09294100 -0.21956000  C -2.40106000 -3.64408800 -1.40023400  C -1.69341800 -2.42205900 -1.44312100  C -1.93479200 -1.35794800 2.13693600  C -2.46440500 -1.82052000 3.31839600  C -3.16501100 -3.04792400 3.35738700  C -3.31990000 -3.78615400 2.20937100  H 1.63144100 3.21312500 -2.74268800  H 3.01345700 5.25458400 -2.99136100  H 4.09069400 6.27552000 -1.01404500  H 1.71113700 2.22469800 1.96197700  H 2.77753500 3.26393100 3.91220300  H 4.19243900 5.29319300 3.64305500  H 4.51861300 6.28282600 1.40565200  H -3.47789800 -5.03314900 -0.18000900  H -2.51185300 -4.22708700 -2.30789400  H -1.27231600 -2.08436700 -2.38356500  H -1.39730500 -0.41771600 2.11902800  H -2.34400600 -1.24250300 4.22803000  H -3.57731600 -3.40358800 4.29510800  H -3.85563900 -4.72973000 2.23194600  C -7.01328200 -0.12699100 -1.69043000  C -5.96270300 -0.92987800 0.33995800  C -6.69727300 -1.43796300 -0.93645200  C -7.35627700 0.86155600 -0.53333200  C -8.58355100 0.44915400 0.29870900  C -7.61009500 2.30692800 -1.00033400  C -5.72449200 1.36065800 1.50086800  C 6.28068000 -2.79123900 0.92966800  C 6.93041900 -2.31865600 -0.40612500  C 5.53829800 -1.43391400 -2.48464300  H 5.41735700 0.01445800 -0.18192700  H -4.90791100 2.08536300 -1.00021600  H 4.58019500 -1.85680000 1.96438600  H 6.01082800 -0.83261700 1.91304100  H -5.05917300 -0.36594600 -2.67137600  H -5.79840500 1.20452200 -2.96838200  H -7.78154200 -0.22754000 -2.46169000  H -6.47986700 -1.23420200 1.25314900  H -4.94146300 -1.29977400 0.40723600  H -7.60798100 -1.98853500 -0.68855300  H -6.07252300 -2.10358200 -1.53637100  H -8.74400500 1.15476100 1.11957700  H -8.50534200 -0.54696200 0.73238400  H -9.48326500 0.46929100 -0.32496300  H -6.83470300 2.70980700 -1.65151900  H -7.70236000 2.97932500 -0.14161300  H -8.55482700 2.35779800 -1.55124500  H -5.73639000 2.44644800 1.35920100  H -4.74749000 1.09022400 1.91214300  H -6.47646700 1.11040300 2.25504900  H 6.98305100 -3.12461500 1.69805300  C 7.89485800 -1.12809800 -0.24742200  C 7.71292200 -3.41845200 -1.14570500  H 6.09531800 -0.49445300 -2.56016000  H 4.51672600 -1.23981800 -2.82568900  H 5.98528100 -2.14830100 -3.18240200  C 4.76860800 -3.31487000 -0.89338200  C 5.29252700 -3.88287700 0.46084300  H 7.48304500 -0.28912500 0.31303200  H 8.20509700 -0.75030400 -1.22670000  H 8.80142500 -1.45238100 0.27362500  H 7.12408500 -4.30900600 -1.36244500  H 8.57497300 -3.73079700 -0.54733600  H 8.10066200 -3.03988500 -2.09647100  H 4.99002300 -3.98737700 -1.72585100  H 3.69234700 -3.14693500 -0.88643000  H 5.78952300 -4.84694000 0.32932600  H 4.49006400 -4.03247900 1.18689500 |
| opt\_4e\_CS\_29 | C -1.24674000 0.86890900 -0.71897400  C -0.36141000 1.95507400 -0.77189900  C 1.01779600 1.82370500 -0.60838400  C 1.54232100 0.53387000 -0.39712900  C 0.66107200 -0.55689400 -0.35154200  C -0.71579600 -0.42638200 -0.50555700  C 2.99612400 0.31724100 -0.25476900  N 3.50321200 -0.83147000 -0.04972000  C 4.94466900 -0.93238700 0.07195100  C 5.59005800 -1.90674300 -0.97066300  C -2.67465900 1.19485400 -0.90271500  N -3.64865700 0.39800300 -0.73069200  C -4.98778300 0.90604000 -0.96363900  C -5.92701300 0.79255400 0.28396500  H -0.76895100 2.94707500 -0.93889300  C 1.87597800 3.04817200 -0.69164000  H 1.08787200 -1.54062100 -0.19802600  C -1.53378100 -1.68104900 -0.48442800  H 3.62663400 1.21133400 -0.33893800  C 5.37809500 -1.55365300 1.44081000  H -2.85236000 2.24082000 -1.20406200  C -5.75146900 0.07912100 -2.05011100  C 2.14358000 3.60402500 -1.92642100  C 2.93044000 4.77093200 -2.05514200  C 3.44740100 5.38185900 -0.94033800  C 3.19437800 4.85581500 0.35311000  C 2.39359800 3.67474600 0.48813300  C 2.13975200 3.17762800 1.79534800  C 2.65646900 3.80365300 2.90529700  C 3.45395900 4.96270000 2.76876000  C 3.71281100 5.47535800 1.52079000  C -2.01167200 -2.22871800 0.74686900  C -2.72422900 -3.47129100 0.72444400  C -2.93834300 -4.12812300 -0.51496700  C -2.46063400 -3.58554500 -1.68166600  C -1.75180800 -2.36373600 -1.66179100  C -1.81008000 -1.58966200 1.99950300  C -2.28189400 -2.14540700 3.16528100  C -2.98186900 -3.37360300 3.14130600  C -3.19644000 -4.01803700 1.94712300  H 1.74847700 3.12797100 -2.81710600  H 3.12455300 5.17633100 -3.04178200  H 4.05504200 6.27605600 -1.03237000  H 1.52632600 2.29273300 1.91185600  H 2.44986000 3.40810800 3.89345200  H 3.85650400 5.44645500 3.65158900  H 4.31990300 6.36785400 1.40914300  H -3.47868200 -5.06911800 -0.52371400  H -2.61840700 -4.09435700 -2.62629300  H -1.37678100 -1.95126900 -2.59198900  H -1.27529400 -0.64813900 2.02889600  H -2.11819000 -1.63980600 4.11057900  H -3.34838100 -3.80315200 4.06703400  H -3.73376400 -4.96063500 1.92101300  C -7.05702400 -0.33894700 -1.33715000  C -5.88663300 -0.68573400 0.75772700  C -6.68498300 -1.45604500 -0.33649900  C -7.34431700 0.87668000 -0.40362100  C -8.52109100 0.65823100 0.56422700  C -7.63675800 2.18756200 -1.15806000  C -5.60526700 1.80420600 1.37412500  C 6.27326500 -2.74551400 1.03329000  C 6.96387300 -2.23035200 -0.26623600  C 5.63180700 -1.33945000 -2.38211400  H 5.39634000 0.06151400 -0.05526400  H -4.93243600 1.96347800 -1.26132400  H 4.50441000 -1.87888100 2.00926000  H 5.90825800 -0.81773200 2.04932200  H -5.16290000 -0.78632400 -2.36055300  H -5.93499100 0.68671500 -2.93955300  H -7.86770700 -0.60297500 -2.02141400  H -6.35155800 -0.78291100 1.74181500  H -4.85944800 -1.03600900 0.84669200  H -7.57461600 -1.93895800 0.07503500  H -6.08715000 -2.23669900 -0.81207500  H -8.64865400 1.52769800 1.21643400  H -8.40949200 -0.21755700 1.20256200  H -9.45192100 0.53929200 -0.00001300  H -6.90220100 2.43585300 -1.92362900  H -7.68729100 3.03110100 -0.46248500  H -8.61083000 2.12044900 -1.65330000  H -5.65457700 2.83254900 1.00120300  H -4.59637100 1.64198000 1.76573400  H -6.29950000 1.71644600 2.21515300  H 6.95255100 -3.07693500 1.82292400  C 7.89307200 -1.02260100 -0.04409200  C 7.79974000 -3.29658400 -0.99696600  H 6.16260900 -0.38258800 -2.42040800  H 4.61898300 -1.16946200 -2.76014400  H 6.12685000 -2.02830700 -3.07313700  C 4.84473900 -3.26511500 -0.85586000  C 5.33258600 -3.85109100 0.50378800  H 7.44101400 -0.20835600 0.52149500  H 8.22949200 -0.61288300 -1.00158200  H 8.78760500 -1.33896000 0.50201100  H 7.23995200 -4.19431400 -1.25731800  H 8.64428900 -3.60433500 -0.37179200  H 8.21627900 -2.88829900 -1.92298100  H 5.10783700 -3.91522000 -1.69393900  H 3.76562400 -3.11820900 -0.88308100  H 5.85963400 -4.79866500 0.36996300  H 4.50832200 -4.03748700 1.19601700 |
| opt\_4e\_CS\_30 | C 1.56786600 0.51528200 -0.36942500  C 0.68268400 -0.57149200 -0.31369700  C -0.69261400 -0.43719600 -0.47436500  C -1.21770100 0.85802900 -0.70454600  C -0.32839200 1.93949400 -0.76732600  C 1.04934500 1.80365500 -0.60042600  C -2.64294000 1.18421300 -0.90355000  N -3.61613400 0.38388000 -0.74895500  C -4.95337700 0.88586200 -1.00103500  C -5.90952700 0.76174700 0.23260000  C 3.01889500 0.29593700 -0.20909300  N 3.52220400 -0.85872400 -0.03252200  C 4.96034800 -0.96514100 0.11604100  C 5.62446800 -1.90852800 -0.94301800  H 1.10570900 -1.55370800 -0.14306100  C -1.51548800 -1.68837300 -0.43890300  H -0.73037100 2.93065200 -0.95102700  C 1.91542000 3.02165000 -0.70399000  H -2.81762200 2.23043800 -1.20586700  C -5.69395900 0.05478300 -2.10010100  H 3.64829500 1.19368600 -0.25250800  C 5.36332400 -1.63072500 1.47340300  C -1.68843600 -2.41326200 -1.59791100  C -2.40200200 -3.63217100 -1.60172800  C -2.92941500 -4.12920500 -0.43712800  C -2.76288800 -3.42788400 0.78500100  C -2.04593800 -2.18818700 0.79077900  C -1.89298400 -1.50317600 2.02503800  C -2.41506700 -2.01276000 3.18957600  C -3.11947600 -3.23786200 3.18255500  C -3.28802100 -3.92577200 2.00627900  C 2.34718000 3.72463700 0.46661200  C 3.15467800 4.89854200 0.31296900  C 3.50383100 5.33724400 -0.99023300  C 3.07235000 4.65087400 -2.09647300  C 2.27611900 3.49303300 -1.94946600  C 2.00363100 3.30838100 1.78110900  C 2.43649400 4.00865800 2.88151400  C 3.23550300 5.16387000 2.72772400  C 3.58388700 5.59629900 1.47202900  H -1.27376800 -2.03639300 -2.52608800  H -2.52397100 -4.17437000 -2.53287400  H -3.47417500 -5.06756900 -0.43288500  H -1.35452100 -0.56363000 2.03974500  H -2.28717100 -1.47308500 4.12137800  H -3.52579000 -3.63090000 4.10783000  H -3.82877800 -4.86655000 1.99299600  H 4.11655000 6.22636000 -1.09605600  H 3.33980100 4.99035200 -3.09073900  H 1.94520000 2.95846700 -2.83289100  H 1.38896700 2.42597000 1.90884200  H 2.16276400 3.67469300 3.87601500  H 3.57038900 5.70705800 3.60419200  H 4.19546200 6.48381800 1.34680700  C 6.26154600 -2.81359900 1.04691300  C 4.87052600 -3.26553700 -0.88631000  C 5.32681900 -3.89651600 0.46334100  C 6.98161500 -2.26090000 -0.22125400  C 7.82754100 -3.30781300 -0.96775900  C 7.91114000 -1.06640700 0.06061100  C 5.69620000 -1.29758600 -2.33457000  C -7.00365700 -0.38006400 -1.40564500  C -7.31774800 0.83062500 -0.47443700  C -5.61399300 1.77555800 1.32780100  H -4.90069700 1.94442100 -1.29577900  H 5.41652900 0.03114400 0.03017900  H -5.09131800 -0.80252100 -2.40538400  H -5.87290400 0.66345900 -2.98961300  H 4.47659800 -1.96893500 2.01305500  H 5.88421800 -0.91675600 2.11500700  H 6.92263100 -3.17352500 1.83933900  H 5.14651200 -3.89057000 -1.73909300  H 3.79357800 -3.10939500 -0.93015300  H 5.85178800 -4.84234600 0.31120000  H 4.48767500 -4.09961900 1.13247600  H 8.26206500 -2.87418900 -1.87366000  H 7.26980400 -4.19535700 -1.26463500  H 8.65943300 -3.63680800 -0.33674900  H 7.44766500 -0.26647600 0.63711000  H 8.27593200 -0.63105500 -0.87471700  H 8.78814200 -1.40449300 0.62158600  H 6.22924400 -0.34131400 -2.33239600  H 4.69141800 -1.11317000 -2.72664100  H 6.20336300 -1.96596300 -3.03661800  H -7.80186700 -0.65245100 -2.10104000  C -7.61416500 2.13947700 -1.23035300  C -8.50516400 0.59699000 0.47643600  H -5.66707300 2.80355900 0.95477600  H -4.60987200 1.62154900 1.73424100  H -6.32018300 1.68064000 2.15783900  C -5.85888500 -0.71639500 0.70530200  C -6.63167400 -1.49415900 -0.40164600  H -6.87013700 2.39850000 -1.98299600  H -7.68605200 2.98028600 -0.53353500  H -8.57895300 2.06171200 -1.74160600  H -8.39481700 -0.28185400 1.11058000  H -9.42733800 0.47409600 -0.10072600  H -8.64811700 1.46127000 1.13221600  H -6.33720500 -0.82027000 1.68219800  H -4.82954700 -1.05457100 0.80826700  H -7.52072000 -1.98940400 -0.00393000  H -6.01664700 -2.26574100 -0.86975400 |
| opt\_4e\_CS\_44 | C -1.22879700 0.88623000 -0.58716200  C -0.33335400 1.96353800 -0.65473600  C 1.04896300 1.81694300 -0.53957500  C 1.56629000 0.52160300 -0.34868100  C 0.67482700 -0.55961700 -0.27803300  C -0.70467500 -0.41531100 -0.39046700  C 3.02051900 0.29074700 -0.23845300  N 3.52081700 -0.86556600 -0.06139800  C 4.96291000 -0.98223800 0.03592900  C 5.58219800 -1.94508600 -1.03256600  C -2.65424400 1.23326600 -0.74984800  N -3.63165600 0.42167900 -0.75160400  C -4.96015200 0.97253600 -0.95111600  C -5.97065600 0.60724500 0.18574000  H -0.73474200 2.96047700 -0.80618300  C 1.91818000 3.03165000 -0.65327500  H 1.09496800 -1.54696800 -0.13018500  C -1.53002500 -1.66287800 -0.31597200  H 3.65661900 1.18133400 -0.31866600  C 5.41078700 -1.63061400 1.38753000  H -2.82575100 2.31373100 -0.88941800  C -5.65431400 0.39667900 -2.23001300  C 2.20235600 3.54605500 -1.90208100  C 3.00201700 4.70073300 -2.05918500  C 3.51512300 5.34053100 -0.95896900  C 3.24533500 4.85713100 0.34762400  C 2.43297600 3.68767500 0.51117000  C 2.16724200 3.22926100 1.83004500  C 2.67995600 3.88391900 2.92511900  C 3.48552900 5.03373300 2.76099800  C 3.75886600 5.50714900 1.50072500  C -2.06822000 -2.11513400 0.92940700  C -2.78060100 -3.35743300 0.96837000  C -2.93605700 -4.10810200 -0.22566700  C -2.40143900 -3.65588700 -1.40594600  C -1.69121400 -2.43530400 -1.44592500  C -1.92132900 -1.38432200 2.13856300  C -2.44914900 -1.85004300 3.31955200  C -3.15234200 -3.07603500 3.35569200  C -3.31165900 -3.80966200 2.20535800  H 1.80863900 3.04794700 -2.78122300  H 3.20819900 5.07427800 -3.05589000  H 4.13191600 6.22588400 -1.07288200  H 1.54833900 2.35108200 1.96699700  H 2.46467900 3.51783400 3.92273300  H 3.88427000 5.54068000 3.63246600  H 4.37391500 6.39126100 1.36801500  H -3.47830600 -5.04725800 -0.18840200  H -2.51569700 -4.23520600 -2.31552600  H -1.27166000 -2.09493000 -2.38608600  H -1.38178900 -0.44523600 2.12263000  H -2.32542000 -1.27561800 4.23100800  H -3.56319800 -3.43424000 4.29307500  H -3.84950500 -4.75207800 2.22574300  C -7.00157000 -0.14506000 -1.70026100  C -5.95489300 -0.93844600 0.33573800  C -6.68849000 -1.45241400 -0.93889900  C -7.34482400 0.85058000 -0.54929500  C -8.57449700 0.44547100 0.28284900  C -7.59473900 2.29378700 -1.02500400  C -5.71606100 1.35809500 1.48499000  C 6.28281400 -2.82753100 0.94649800  C 6.96173700 -2.29846900 -0.35341700  C 5.61207700 -1.35312600 -2.43409700  H 5.42270400 0.00910000 -0.08168000  H -4.89483200 2.06839000 -1.01912900  H 4.54254600 -1.95317900 1.96572000  H 5.96101000 -0.91138300 1.99818700  H -5.04602700 -0.39274500 -2.67578600  H -5.78222100 1.17694700 -2.98397600  H -7.76862600 -0.24865500 -2.47231900  H -6.47335200 -1.23755300 1.24990500  H -4.93409600 -1.30907700 0.40599300  H -7.60024900 -2.00042600 -0.68940000  H -6.06379000 -2.12200600 -1.53441400  H -8.73570000 1.15664200 1.09876900  H -8.49891400 -0.54787400 0.72325600  H -9.47283300 0.46296000 -0.34287800  H -6.81766000 2.69089600 -1.67780300  H -7.68624800 2.97145800 -0.17036100  H -8.53875300 2.34372300 -1.57722700  H -5.72593000 2.44308300 1.33719400  H -4.74028200 1.08847300 1.89967700  H -6.46991100 1.11324400 2.23907500  H 6.96870800 -3.18184300 1.72030800  C 7.90950700 -1.10676000 -0.12315800  C 7.77384000 -3.36203500 -1.11413000  H 6.15451800 -0.40249100 -2.46253600  H 4.59656800 -1.16370800 -2.79529400  H 6.08898400 -2.03569400 -3.14383600  C 4.82215300 -3.29628100 -0.93159900  C 5.31937200 -3.91088100 0.41184200  H 7.47384200 -0.29394200 0.45736800  H 8.24315200 -0.68880700 -1.07805900  H 8.80428900 -1.44294800 0.41054300  H 7.19983100 -4.24897500 -1.38016900  H 8.62406500 -3.68927300 -0.50684900  H 8.18113100 -2.94360500 -2.03969300  H 5.06756100 -3.93492700 -1.78377200  H 3.74460500 -3.13650800 -0.94320000  H 5.83091200 -4.86355200 0.25584900  H 4.50177500 -4.09685000 1.11208600 |
| opt\_4e\_CS\_52 | C 1.25781900 0.93449000 -0.22255000  C 0.36458600 2.01081600 -0.31182100  C -1.01315500 1.84897600 -0.46111900  C -1.52574100 0.54003300 -0.52718000  C -0.63652300 -0.54139000 -0.42634800  C 0.73686300 -0.38324600 -0.26722100  C -2.97173700 0.29483100 -0.70005100  N -3.46263100 -0.87650100 -0.77436500  C -4.89458300 -1.01699400 -0.95052100  C -5.57592900 -1.86437700 0.17835300  C 2.68556300 1.29322900 -0.11852700  N 3.65971500 0.47958500 -0.15514800  C 5.00124100 1.02035900 -0.04501300  C 5.92573700 0.64483200 -1.25213400  H 0.76357500 3.01938300 -0.27137600  C -1.87808400 3.06787900 -0.56516500  H -1.05453100 -1.53965800 -0.46829200  C 1.56272200 -1.62729100 -0.16449300  H -3.60770900 1.18684300 -0.76649800  C -5.24922200 -1.81730200 -2.24803500  H 2.86185700 2.37684700 -0.01447900  C 5.77525600 0.43246600 1.18152500  C -2.02400300 3.69882100 -1.78374300  C -2.80934200 4.86626000 -1.91906800  C -3.44560700 5.40172200 -0.82736700  C -3.32235900 4.79443900 0.44923500  C -2.52721700 3.61044800 0.59033600  C -2.41333500 3.02267300 1.87950500  C -3.05054500 3.57121700 2.96746300  C -3.83633900 4.73756800 2.82532200  C -3.96656700 5.33311200 1.59419400  C 2.05024500 -2.09404800 1.09768600  C 2.78133900 -3.32455000 1.14711700  C 2.99700300 -4.05661800 -0.04965800  C 2.50175900 -3.59768700 -1.24377000  C 1.77870600 -2.38466500 -1.29609400  C 1.83100600 -1.39286500 2.31278800  C 2.31515100 -1.87018700 3.50801700  C 3.04451600 -3.08026400 3.55313700  C 3.26852000 -3.78875600 2.39761600  H -1.52881200 3.28642200 -2.65597100  H -2.90453700 5.33413200 -2.89247900  H -4.04998100 6.29751000 -0.92514000  H -1.81177100 2.12995000 1.99916300  H -2.95035100 3.10765900 3.94249800  H -4.33390100 5.16016500 3.69096400  H -4.56691700 6.22969700 1.47892900  H 3.55343000 -4.98696200 -0.00245900  H 2.66155300 -4.16184400 -2.15593900  H 1.39705900 -2.03481200 -2.24882000  H 1.26985600 -0.46675200 2.29181500  H 2.13574900 -1.31746500 4.42363200  H 3.42150700 -3.44786900 4.50106400  H 3.82190700 -4.72198700 2.42499000  C 7.06627100 -0.14061200 0.55542400  C 5.86783400 -0.89881000 -1.41130100  C 6.66823300 -1.43638700 -0.18678000  C 7.35294600 0.85249800 -0.61202700  C 8.51481800 0.42312900 -1.52530500  C 7.66604200 2.28808900 -0.15151800  C 5.60071200 1.41304500 -2.52485700  C -6.12479400 -2.97960400 -1.72995900  C -6.89974400 -2.32340300 -0.54688700  C -5.71672600 -1.11350100 1.49424400  H -5.36592800 -0.02434900 -0.97520300  H 4.95117600 2.11686500 0.02758000  H -4.34313000 -2.17759800 -2.73942600  H -5.77741600 -1.18127800 -2.96201900  H 5.18518700 -0.33930500 1.67846400  H 5.97933300 1.21327400 1.91788400  H 7.88317000 -0.26803000 1.27065300  H 6.32539500 -1.19978100 -2.35721300  H 4.83676100 -1.24945400 -1.42039100  H 7.54607800 -2.00849400 -0.49692300  H 6.06492600 -2.08955500 0.44718600  H 8.63331800 1.12747000 -2.35453900  H 8.39354200 -0.57124100 -1.95316500  H 9.45359100 0.42759400 -0.96187200  H 6.93891100 2.70198700 0.54656700  H 7.72221800 2.96467400 -1.01010200  H 8.64231800 2.31453200 0.34322500  H 5.65096400 2.49595500 -2.37068300  H 4.59051300 1.17567400 -2.87245000  H 6.29294600 1.15482300 -3.33186800  H -6.75004800 -3.43776700 -2.50080200  C -7.84348600 -1.18393000 -0.97396000  C -7.74878700 -3.31283100 0.27097500  H -6.29039600 -0.18927300 1.37189000  H -4.73522800 -0.84158800 1.89440200  H -6.21943200 -1.72559300 2.24900400  C -4.79322500 -3.20107400 0.28606100  C -5.17892700 -3.97042100 -1.01379400  H -7.37493200 -0.43032200 -1.60658400  H -8.25177600 -0.67108400 -0.09762900  H -8.69170000 -1.59419200 -1.53137200  H -7.18176600 -4.15131500 0.67355000  H -8.54836600 -3.72435800 -0.35359900  H -8.22757300 -2.80408200 1.11333900  H -5.09482200 -3.74741500 1.18312400  H -3.72197600 -3.01852900 0.35980700  H -5.67860200 -4.91627500 -0.79182800  H -4.30826300 -4.20551300 -1.63040100 |
| opt\_4e\_CS\_55 | C -1.31472700 -0.17002400 -0.61768100  C -0.77897700 1.12323000 -0.61839000  C 0.58366600 1.36429200 -0.46140900  C 1.45263400 0.26223100 -0.29999400  C 0.91559300 -1.03094600 -0.28923800  C -0.44747200 -1.27151200 -0.44231800  C 2.91060200 0.45466600 -0.16853400  N 3.72225600 -0.51722400 -0.04498200  C 5.13564100 -0.21947100 0.08068600  C 6.01352100 -0.89491300 -1.02715200  C -2.76415400 -0.36675400 -0.83548200  N -3.57506500 0.60981100 -0.89157700  C -4.98528600 0.39304100 -1.18756700  C -5.88732400 1.50345500 -0.55958600  H -1.46281600 1.95133700 -0.75713400  C 1.07420000 2.77916900 -0.51042100  H 1.59924800 -1.86016700 -0.15660200  C -0.93386000 -2.68821700 -0.43619000  H 3.26207900 1.49360600 -0.18636000  C 5.74095500 -0.79769300 1.40237200  H -3.08275600 -1.40651600 -0.95880900  C -5.67419300 -0.93640200 -0.72562600  C 1.17565200 3.41542000 -1.73053600  C 1.61007000 4.75603500 -1.82931300  C 1.94001300 5.45990100 -0.69951400  C 1.84443500 4.85546900 0.58034400  C 1.40290600 3.49600300 0.68509200  C 1.30111400 2.91735400 1.97890300  C 1.62615000 3.63599500 3.10425200  C 2.06800500 4.97393100 2.99788800  C 2.17160600 5.56704100 1.76401800  C -1.59019600 -3.24470900 0.70925000  C -2.01687900 -4.61233100 0.66959600  C -1.77550400 -5.38332800 -0.49651300  C -1.13452200 -4.83197300 -1.57632800  C -0.71271300 -3.48418400 -1.54161100  C -1.82591400 -2.49918700 1.89592400  C -2.45672200 -3.06741100 2.97688600  C -2.88467800 -4.41337700 2.93160200  C -2.66649400 -5.16552800 1.80398600  H 0.92046500 2.87044100 -2.63244700  H 1.68103400 5.22198700 -2.80566100  H 2.27591900 6.48926800 -0.76786400  H 0.95680300 1.89483400 2.07099200  H 1.54036900 3.17591300 4.08227200  H 2.32104400 5.53002500 3.89355400  H 2.50584300 6.59557600 1.67538500  H -2.10360400 -6.41726900 -0.51706300  H -0.94809500 -5.42521600 -2.46442000  H -0.21018700 -3.06117600 -2.40421400  H -1.49496400 -1.46940500 1.94348700  H -2.62416000 -2.48128800 3.87350600  H -3.38122600 -4.84952300 3.79104400  H -2.98712600 -6.20140500 1.76417200  C -6.90270500 -0.43546800 0.06685400  C -5.65439500 1.43695000 0.97382800  C -6.37100000 0.12237000 1.40788200  C -7.31467000 0.85683700 -0.70260400  C -8.43744600 1.65617700 -0.01881300  C -7.77390700 0.60190700 -2.14956900  C -5.66203300 2.88078700 -1.16385500  C 6.92213200 -1.66531000 0.91315800  C 7.43057700 -0.88272400 -0.33621500  C 5.88280600 -0.22815800 -2.38834100  H 5.29154800 0.86744600 0.03486800  H -5.05504500 0.48615100 -2.27744500  H 4.99679000 -1.38959200 1.93872500  H 6.05913400 0.00783600 2.06781400  H -5.02184200 -1.53999500 -0.09111500  H -5.95623400 -1.55987800 -1.57679300  H -7.69121000 -1.18442500 0.17628300  H -6.08008100 2.31284400 1.46923500  H -4.58684400 1.43271500 1.19937200  H -7.18301200 0.31847500 2.11163300  H -5.69311500 -0.58457800 1.89214500  H -8.64615100 2.57637900 -0.57278400  H -8.21343100 1.93701800 1.00979600  H -9.36182500 1.06958700 -0.00671600  H -7.07917200 0.00473600 -2.74024800  H -7.92570500 1.54840100 -2.67709400  H -8.73383700 0.07567900 -2.14895500  H -5.85806000 2.88773000 -2.24107800  H -4.62452500 3.19066400 -1.01664500  H -6.30713200 3.63160000 -0.69785700  H 7.67513500 -1.85964000 1.68131800  C 7.99454400 0.51279600 -0.01069100  C 8.52089200 -1.62101700 -1.13267400  H 6.14808900 0.83289400 -2.34481800  H 4.85429500 -0.29579800 -2.75561800  H 6.52783700 -0.70765200 -3.13042800  C 5.66859000 -2.40947300 -1.02453000  C 6.31265100 -2.94203500 0.29114800  H 7.33002500 1.13414700 0.58873000  H 8.22115800 1.06276300 -0.92936900  H 8.93304000 0.41217300 0.54362000  H 8.22580800 -2.61563900 -1.46463200  H 9.42103500 -1.73138600 -0.51952100  H 8.80383800 -1.04737500 -2.02058700  H 6.08806500 -2.89817300 -1.90732500  H 4.58988700 -2.55686600 -1.04974400  H 7.07639200 -3.69706700 0.09072800  H 5.57782200 -3.39778200 0.95871600 |

|  |  |
| --- | --- |
| Conformer | Coordinates |
| opt\_4e\_CS\_4 | C 1.38579400 -0.25823000 -0.64365100  C 0.89290700 1.05224700 -0.64128900  C -0.47075100 1.33516200 -0.63204400  C -1.38566200 0.25822100 -0.64362000  C -0.89277400 -1.05225700 -0.64126700  C 0.47088300 -1.33516800 -0.63207200  C -2.84264800 0.49510400 -0.68193800  N -3.69200500 -0.45198300 -0.66801600  C -5.10018400 -0.11157000 -0.72888000  C -5.93903400 -0.73284900 0.43853400  C 2.84277300 -0.49512800 -0.68187100  N 3.69214000 0.45195400 -0.66796300  C 5.10033100 0.11151100 -0.72859200  C 5.93906600 0.73322700 0.43866000  H 1.61209200 1.86171500 -0.64747200  C -0.90789100 2.76757800 -0.63478500  H -1.61195800 -1.86172500 -0.64747700  C 0.90803800 -2.76758800 -0.63488100  H -3.15880500 1.54440900 -0.73187500  C -5.79165000 -0.69966400 -2.00372700  H 3.15890100 -1.54444600 -0.73174500  C 5.79194700 0.69909600 -2.00360100  C -0.78781700 3.50950500 -1.79207800  C -1.16779700 4.86928800 -1.83911400  C -1.66687100 5.48607000 -0.72046300  C -1.79989300 4.77198500 0.49807000  C -1.41224900 3.39333000 0.55132100  C -1.53544900 2.70590000 1.78885500  C -2.02573100 3.33868700 2.90600900  C -2.41776100 4.69494600 2.84790200  C -2.30405600 5.39251000 1.67094500  C 1.41205000 -3.39347600 0.55129500  C 1.79969700 -4.77212700 0.49800200  C 1.66703900 -5.48606400 -0.72065800  C 1.16832800 -4.86914100 -1.83939300  C 0.78833700 -3.50935900 -1.79231000  C 1.53494300 -2.70616000 1.78892100  C 2.02490600 -3.33906800 2.90614600  C 2.41690700 -4.69533400 2.84801400  C 2.30351600 -5.39278200 1.67095600  H -0.40062500 3.03362000 -2.68604600  H -1.06402800 5.41909000 -2.76772900  H -1.96370000 6.52919500 -0.75037900  H -1.23135000 1.66830400 1.84606300  H -2.10964200 2.79573300 3.84068200  H -2.80375100 5.18231900 3.73611000  H -2.59757700 6.43593800 1.62039100  H 1.96386500 -6.52919000 -0.75060700  H 1.06485000 -5.41882800 -2.76810800  H 0.40141400 -3.03336500 -2.68633600  H 1.23086600 -1.66855700 1.84613300  H 2.10859300 -2.79620500 3.84089200  H 2.80263800 -5.18280400 3.73628100  H 2.59703000 -6.43620900 1.62038100  C 6.96848200 1.52124600 -1.43350900  C 5.63934000 2.25733100 0.45633300  C 6.36205500 2.80007000 -0.81309800  C 7.38924900 0.69499900 -0.17902600  C 8.45664100 1.38070900 0.69215000  C 7.92926300 -0.70855400 -0.50970500  C 5.71619900 0.03988600 1.77439100  C -6.96820900 -1.52163600 -1.43345200  C -7.38915900 -0.69489300 -0.17935100  C -5.71636200 -0.03896000 1.77400900  H -5.21836800 0.98075300 -0.70327000  H 5.21851700 -0.98079800 -0.70256000  H -5.09480200 -1.32375800 -2.56675700  H -6.12255500 0.10167200 -2.66806400  H 5.09519200 1.32300700 -2.56695200  H 6.12287200 -0.10251800 -2.66759600  H 7.76586400 1.71089600 -2.15667200  H 6.02946100 2.71238300 1.37005100  H 4.56553800 2.43673200 0.43357600  H 7.13388200 3.53010500 -0.55884800  H 5.67398600 3.29003700 -1.50597800  H 8.66145000 0.78591300 1.58745200  H 8.18035400 2.38219100 1.01955600  H 9.39675600 1.46264700 0.13724500  H 7.27546700 -1.29969100 -1.15023100  H 8.09984400 -1.28285600 0.40608500  H 8.89375100 -0.62301100 -1.02032500  H 5.94034700 -1.02992300 1.71790300  H 4.67371800 0.13987200 2.09112500  H 6.34158300 0.47619100 2.55878100  H -7.76550300 -1.71160300 -2.15662900  C -7.92915000 0.70851500 -0.51068300  C -8.45667300 -1.38026400 0.69193500  H -5.94081000 1.03076500 1.71712600  H -4.67385800 -0.13852800 2.09080300  H -6.34163500 -0.47515500 2.55854600  C -5.63928000 -2.25694600 0.45684600  C -6.36181900 -2.80019600 -0.81246100  H -7.27521100 1.29945100 -1.15124700  H -8.10000200 1.28315000 0.40484800  H -8.89350300 0.62274000 -1.02152200  H -8.18048000 -2.38166600 1.01966200  H -9.39674800 -1.46230700 0.13697800  H -8.66151500 -0.78518400 1.58704000  H -6.02951700 -2.71162500 1.37069900  H -4.56547500 -2.43635000 0.43429800  H -7.13365400 -3.53016000 -0.55802600  H -5.67363300 -3.29039900 -1.50505800 |
| opt\_4e\_CS\_8 | C -0.25946800 1.38630900 -0.19783100  C 1.05206700 0.89431300 -0.19698100  C 1.33487000 -0.46967400 -0.19166600  C 0.25946800 -1.38630900 -0.19783100  C -1.05206700 -0.89431300 -0.19698100  C -1.33487000 0.46967400 -0.19166600  C 0.50251600 -2.84281800 -0.22233700  N -0.43838300 -3.69947300 -0.19079700  C -0.08469200 -5.10577400 -0.21462700  C -0.76651200 -5.90175500 -1.37784900  C -0.50251600 2.84281800 -0.22233700  N 0.43838300 3.69947300 -0.19079700  C 0.08469200 5.10577400 -0.21462700  C 0.76651200 5.90175500 -1.37784900  H 1.86282300 1.61254700 -0.19969900  C 2.76741100 -0.90830800 -0.20459400  H -1.86282300 -1.61254700 -0.19969900  C -2.76741100 0.90830800 -0.20459400  H 1.55310900 -3.15488500 -0.27504600  C -0.58666300 -5.85945000 1.06226600  H -1.55310900 3.15488500 -0.27504600  C 0.58666300 5.85945000 1.06226600  C 3.48680400 -0.84093700 -1.38051400  C 4.84518700 -1.22756400 -1.43722100  C 5.48260100 -1.68059100 -0.30938400  C 4.79100200 -1.75828500 0.92738700  C 3.41451000 -1.36341700 0.98961200  C 2.74805900 -1.43514400 2.24304400  C 3.39985600 -1.88045400 3.36907600  C 4.75515600 -2.27704000 3.30332800  C 5.43213400 -2.21463500 2.10945500  C -3.41451000 1.36341700 0.98961200  C -4.79100200 1.75828500 0.92738700  C -5.48260100 1.68059100 -0.30938400  C -4.84518700 1.22756400 -1.43722100  C -3.48680400 0.84093700 -1.38051400  C -2.74805900 1.43514400 2.24304400  C -3.39985600 1.88045400 3.36907600  C -4.75515600 2.27704000 3.30332800  C -5.43213400 2.21463500 2.10945500  H 2.99569800 -0.48981400 -2.28135100  H 5.37768600 -1.16538600 -2.37964500  H 6.52431800 -1.98179300 -0.34702300  H 1.71132400 -1.12830800 2.30552800  H 2.87303700 -1.92569300 4.31571400  H 5.25800800 -2.62661100 4.19805200  H 6.47404600 -2.51280500 2.05323900  H -6.52431800 1.98179300 -0.34702300  H -5.37768600 1.16538600 -2.37964500  H -2.99569800 0.48981400 -2.28135100  H -1.71132400 1.12830800 2.30552800  H -2.87303700 1.92569300 4.31571400  H -5.25800800 2.62661100 4.19805200  H -6.47404600 2.51280500 2.05323900  C 1.42475600 7.02475700 0.49141600  C 2.29273300 5.62811100 -1.29181800  C 2.74805900 6.41663200 -0.02640600  C 0.66977900 7.37684400 -0.82610800  C 1.38922400 8.41923900 -1.70056000  C -0.76105700 7.90214300 -0.60597700  C 0.15744700 5.61495300 -2.74253300  C -1.42475600 -7.02475700 0.49141600  C -0.66977900 -7.37684400 -0.82610800  C -0.15744700 -5.61495300 -2.74253300  H 1.00491300 -5.21034600 -0.31315600  H -1.00491300 5.21034600 -0.31315600  H -1.18496900 -5.19759900 1.69190700  H 0.25772700 -6.20550700 1.66249100  H 1.18496900 5.19759900 1.69190700  H -0.25772700 6.20550700 1.66249100  H 1.55787600 7.85570200 1.18916000  H 2.79446700 5.98726600 -2.19382800  H 2.49081200 4.55981500 -1.21098900  H 3.47857600 7.19089200 -0.27283700  H 3.20858700 5.76878100 0.72322300  H 0.84130100 8.58149300 -2.63391500  H 2.41066200 8.14568600 -1.96306500  H 1.42927500 9.38111600 -1.17907100  H -1.37072900 7.27818600 0.04700100  H -1.28781200 7.99432100 -1.56083900  H -0.72556500 8.90132300 -0.15976000  H -0.91605500 5.82989300 -2.76021100  H 0.28705000 4.56180400 -3.01041700  H 0.63425500 6.21288600 -3.52494800  H -1.55787600 -7.85570200 1.18916000  C 0.76105700 -7.90214300 -0.60597700  C -1.38922400 -8.41923900 -1.70056000  H 0.91605500 -5.82989300 -2.76021100  H -0.28705000 -4.56180400 -3.01041700  H -0.63425500 -6.21288600 -3.52494800  C -2.29273300 -5.62811100 -1.29181800  C -2.74805900 -6.41663200 -0.02640600  H 1.37072900 -7.27818600 0.04700100  H 1.28781200 -7.99432100 -1.56083900  H 0.72556500 -8.90132300 -0.15976000  H -2.41066200 -8.14568600 -1.96306500  H -1.42927500 -9.38111600 -1.17907100  H -0.84130100 -8.58149300 -2.63391500  H -2.79446700 -5.98726600 -2.19382800  H -2.49081200 -4.55981500 -1.21098900  H -3.47857600 -7.19089200 -0.27283700  H -3.20858700 -5.76878100 0.72322300 |
| opt\_4e\_CS\_16 | C -0.00189200 1.41010900 -0.19328400  C 1.19748300 0.68693000 -0.19145600  C 1.22693100 -0.70576600 -0.18539800  C 0.00189200 -1.41010900 -0.19328400  C -1.19748300 -0.68693000 -0.19145600  C -1.22693100 0.70576600 -0.18539800  C -0.02701900 -2.88632700 -0.22487000  N -1.10983500 -3.55433200 -0.18330500  C -1.02460700 -5.00151700 -0.21852800  C -1.84507000 -5.64646200 -1.38594300  C 0.02701900 2.88632700 -0.22487000  N 1.10983500 3.55433200 -0.18330500  C 1.02460700 5.00151700 -0.21852800  C 1.84507000 5.64646200 -1.38594300  H 2.12544200 1.24549400 -0.19252100  C 2.55576600 -1.39737600 -0.19244900  H -2.12544200 -1.24549400 -0.19252100  C -2.55576600 1.39737600 -0.19244900  H 0.94770200 -3.38589900 -0.28940400  C -1.65636400 -5.65855400 1.05352400  H -0.94770200 3.38589900 -0.28940400  C 1.65636400 5.65855400 1.05352400  C 3.28480400 -1.45116000 -1.36309000  C 4.54927700 -2.08015700 -1.41644800  C 5.08420100 -2.65310600 -0.29007500  C 4.38113300 -2.61383100 0.94188200  C 3.09977000 -1.97418800 1.00071900  C 2.42440400 -1.93076800 2.25049000  C 2.97625100 -2.49689200 3.37553900  C 4.23561600 -3.13572700 3.31264900  C 4.91989000 -3.18956300 2.12275100  C -3.09977000 1.97418800 1.00071900  C -4.38113300 2.61383100 0.94188200  C -5.08420100 2.65310600 -0.29007500  C -4.54927700 2.08015700 -1.41644800  C -3.28480400 1.45116000 -1.36309000  C -2.42440400 1.93076800 2.25049000  C -2.97625100 2.49689200 3.37553900  C -4.23561600 3.13572700 3.31264900  C -4.91989000 3.18956300 2.12275100  H 2.87262300 -1.00842100 -2.26307900  H 5.09094200 -2.10813500 -2.35524500  H 6.05328700 -3.13984700 -0.32487700  H 1.46220300 -1.43753700 2.31137700  H 2.44452200 -2.45098900 4.31935900  H 4.66013600 -3.57846200 4.20669100  H 5.88977100 -3.67331300 2.06876500  H -6.05328700 3.13984700 -0.32487700  H -5.09094200 2.10813500 -2.35524500  H -2.87262300 1.00842100 -2.26307900  H -1.46220300 1.43753700 2.31137700  H -2.44452200 2.45098900 4.31935900  H -4.66013600 3.57846200 4.20669100  H -5.88977100 3.67331300 2.06876500  C 2.69739100 6.64324600 0.47612300  C 3.29365200 5.09450200 -1.29191600  C 3.88517000 5.79453200 -0.03126700  C 2.02319300 7.11882500 -0.84709600  C 2.92535800 8.00081500 -1.72874600  C 0.71557400 7.90386000 -0.63501300  C 1.19748300 5.46517200 -2.75107800  C -2.69739100 -6.64324600 0.47612300  C -2.02319300 -7.11882500 -0.84709600  C -1.19748300 -5.46517200 -2.75107800  H 0.02601400 -5.30738500 -0.32072400  H -0.02601400 5.30738500 -0.32072400  H -2.12124700 -4.90107200 1.68795600  H -0.89072900 -6.15889500 1.65057800  H 2.12124700 4.90107200 1.68795600  H 0.89072900 6.15889500 1.65057800  H 2.98150300 7.44047200 1.16787100  H 3.85584500 5.34516100 -2.19497000  H 3.28772200 4.00881300 -1.20143200  H 4.74786800 6.41689100 -0.28067300  H 4.21484800 5.07867500 0.72541500  H 2.41234200 8.26606600 -2.65827600  H 3.87147100 7.53288200 -1.99839300  H 3.15629300 8.93665300 -1.20948200  H 0.00168200 7.41250300 0.02537400  H 0.21320400 8.08168300 -1.59091500  H 0.93777300 8.88399200 -0.20075700  H 0.18240300 5.87488400 -2.77614200  H 1.13046300 4.40385900 -3.00943100  H 1.77957200 5.95727700 -3.53605100  H -2.98150300 -7.44047200 1.16787100  C -0.71557400 -7.90386000 -0.63501300  C -2.92535800 -8.00081500 -1.72874600  H -0.18240300 -5.87488400 -2.77614200  H -1.13046300 -4.40385900 -3.00943100  H -1.77957200 -5.95727700 -3.53605100  C -3.29365200 -5.09450200 -1.29191600  C -3.88517000 -5.79453200 -0.03126700  H -0.00168200 -7.41250300 0.02537400  H -0.21320400 -8.08168300 -1.59091500  H -0.93777300 -8.88399200 -0.20075700  H -3.87147100 -7.53288200 -1.99839300  H -3.15629300 -8.93665300 -1.20948200  H -2.41234200 -8.26606600 -2.65827600  H -3.85584500 -5.34516100 -2.19497000  H -3.28772200 -4.00881300 -1.20143200  H -4.74786800 -6.41689100 -0.28067300  H -4.21484800 -5.07867500 0.72541500 |
| opt\_4e\_CS\_25 | C -1.24035800 0.90580600 -0.58014400  C -0.34668500 1.98471200 -0.64425300  C 1.03673400 1.84028100 -0.53618300  C 1.55690000 0.54316700 -0.36215200  C 0.66679400 -0.53906200 -0.29175100  C -0.71383100 -0.39594500 -0.39259700  C 3.01260300 0.30846400 -0.27900200  N 3.51089700 -0.84450000 -0.07645300  C 4.95439100 -0.96822500 -0.01454400  C 5.53733400 -1.97577700 -1.06267000  C -2.66673900 1.25179900 -0.73641600  N -3.64249900 0.43856100 -0.74464500  C -4.97202300 0.98905200 -0.93848100  C -5.98038800 0.61648300 0.19804500  H -0.75068700 2.98243800 -0.78289100  C 1.89979100 3.05977400 -0.63448200  H 1.08914200 -1.52709600 -0.15533000  C -1.53689600 -1.64478900 -0.31579500  H 3.65151900 1.19155000 -0.40506000  C 5.43430500 -1.56860200 1.34822100  H -2.84060100 2.33323900 -0.86480800  C -5.66775300 0.41979900 -2.21953400  C 2.09031900 3.65531400 -1.86523100  C 2.88088200 4.81797200 -2.00785900  C 3.47936400 5.38508100 -0.91091600  C 3.30663000 4.81839600 0.37855100  C 2.50201800 3.64171100 0.52819500  C 2.32767700 3.10555000 1.83295100  C 2.92432900 3.68915900 2.92568600  C 3.72640200 4.84301200 2.77379100  C 3.90902000 5.39353000 1.52856400  C -2.07728100 -2.09347100 0.93006300  C -2.78687300 -3.33730200 0.97197800  C -2.93762600 -4.09294100 -0.21956000  C -2.40106000 -3.64408800 -1.40023400  C -1.69341800 -2.42205900 -1.44312100  C -1.93479200 -1.35794800 2.13693600  C -2.46440500 -1.82052000 3.31839600  C -3.16501100 -3.04792400 3.35738700  C -3.31990000 -3.78615400 2.20937100  H 1.63144100 3.21312500 -2.74268800  H 3.01345700 5.25458400 -2.99136100  H 4.09069400 6.27552000 -1.01404500  H 1.71113700 2.22469800 1.96197700  H 2.77753500 3.26393100 3.91220300  H 4.19243900 5.29319300 3.64305500  H 4.51861300 6.28282600 1.40565200  H -3.47789800 -5.03314900 -0.18000900  H -2.51185300 -4.22708700 -2.30789400  H -1.27231600 -2.08436700 -2.38356500  H -1.39730500 -0.41771600 2.11902800  H -2.34400600 -1.24250300 4.22803000  H -3.57731600 -3.40358800 4.29510800  H -3.85563900 -4.72973000 2.23194600  C -7.01328200 -0.12699100 -1.69043000  C -5.96270300 -0.92987800 0.33995800  C -6.69727300 -1.43796300 -0.93645200  C -7.35627700 0.86155600 -0.53333200  C -8.58355100 0.44915400 0.29870900  C -7.61009500 2.30692800 -1.00033400  C -5.72449200 1.36065800 1.50086800  C 6.28068000 -2.79123900 0.92966800  C 6.93041900 -2.31865600 -0.40612500  C 5.53829800 -1.43391400 -2.48464300  H 5.41735700 0.01445800 -0.18192700  H -4.90791100 2.08536300 -1.00021600  H 4.58019500 -1.85680000 1.96438600  H 6.01082800 -0.83261700 1.91304100  H -5.05917300 -0.36594600 -2.67137600  H -5.79840500 1.20452200 -2.96838200  H -7.78154200 -0.22754000 -2.46169000  H -6.47986700 -1.23420200 1.25314900  H -4.94146300 -1.29977400 0.40723600  H -7.60798100 -1.98853500 -0.68855300  H -6.07252300 -2.10358200 -1.53637100  H -8.74400500 1.15476100 1.11957700  H -8.50534200 -0.54696200 0.73238400  H -9.48326500 0.46929100 -0.32496300  H -6.83470300 2.70980700 -1.65151900  H -7.70236000 2.97932500 -0.14161300  H -8.55482700 2.35779800 -1.55124500  H -5.73639000 2.44644800 1.35920100  H -4.74749000 1.09022400 1.91214300  H -6.47646700 1.11040300 2.25504900  H 6.98305100 -3.12461500 1.69805300  C 7.89485800 -1.12809800 -0.24742200  C 7.71292200 -3.41845200 -1.14570500  H 6.09531800 -0.49445300 -2.56016000  H 4.51672600 -1.23981800 -2.82568900  H 5.98528100 -2.14830100 -3.18240200  C 4.76860800 -3.31487000 -0.89338200  C 5.29252700 -3.88287700 0.46084300  H 7.48304500 -0.28912500 0.31303200  H 8.20509700 -0.75030400 -1.22670000  H 8.80142500 -1.45238100 0.27362500  H 7.12408500 -4.30900600 -1.36244500  H 8.57497300 -3.73079700 -0.54733600  H 8.10066200 -3.03988500 -2.09647100  H 4.99002300 -3.98737700 -1.72585100  H 3.69234700 -3.14693500 -0.88643000  H 5.78952300 -4.84694000 0.32932600  H 4.49006400 -4.03247900 1.18689500 |
| opt\_4e\_CS\_29 | C -1.24674000 0.86890900 -0.71897400  C -0.36141000 1.95507400 -0.77189900  C 1.01779600 1.82370500 -0.60838400  C 1.54232100 0.53387000 -0.39712900  C 0.66107200 -0.55689400 -0.35154200  C -0.71579600 -0.42638200 -0.50555700  C 2.99612400 0.31724100 -0.25476900  N 3.50321200 -0.83147000 -0.04972000  C 4.94466900 -0.93238700 0.07195100  C 5.59005800 -1.90674300 -0.97066300  C -2.67465900 1.19485400 -0.90271500  N -3.64865700 0.39800300 -0.73069200  C -4.98778300 0.90604000 -0.96363900  C -5.92701300 0.79255400 0.28396500  H -0.76895100 2.94707500 -0.93889300  C 1.87597800 3.04817200 -0.69164000  H 1.08787200 -1.54062100 -0.19802600  C -1.53378100 -1.68104900 -0.48442800  H 3.62663400 1.21133400 -0.33893800  C 5.37809500 -1.55365300 1.44081000  H -2.85236000 2.24082000 -1.20406200  C -5.75146900 0.07912100 -2.05011100  C 2.14358000 3.60402500 -1.92642100  C 2.93044000 4.77093200 -2.05514200  C 3.44740100 5.38185900 -0.94033800  C 3.19437800 4.85581500 0.35311000  C 2.39359800 3.67474600 0.48813300  C 2.13975200 3.17762800 1.79534800  C 2.65646900 3.80365300 2.90529700  C 3.45395900 4.96270000 2.76876000  C 3.71281100 5.47535800 1.52079000  C -2.01167200 -2.22871800 0.74686900  C -2.72422900 -3.47129100 0.72444400  C -2.93834300 -4.12812300 -0.51496700  C -2.46063400 -3.58554500 -1.68166600  C -1.75180800 -2.36373600 -1.66179100  C -1.81008000 -1.58966200 1.99950300  C -2.28189400 -2.14540700 3.16528100  C -2.98186900 -3.37360300 3.14130600  C -3.19644000 -4.01803700 1.94712300  H 1.74847700 3.12797100 -2.81710600  H 3.12455300 5.17633100 -3.04178200  H 4.05504200 6.27605600 -1.03237000  H 1.52632600 2.29273300 1.91185600  H 2.44986000 3.40810800 3.89345200  H 3.85650400 5.44645500 3.65158900  H 4.31990300 6.36785400 1.40914300  H -3.47868200 -5.06911800 -0.52371400  H -2.61840700 -4.09435700 -2.62629300  H -1.37678100 -1.95126900 -2.59198900  H -1.27529400 -0.64813900 2.02889600  H -2.11819000 -1.63980600 4.11057900  H -3.34838100 -3.80315200 4.06703400  H -3.73376400 -4.96063500 1.92101300  C -7.05702400 -0.33894700 -1.33715000  C -5.88663300 -0.68573400 0.75772700  C -6.68498300 -1.45604500 -0.33649900  C -7.34431700 0.87668000 -0.40362100  C -8.52109100 0.65823100 0.56422700  C -7.63675800 2.18756200 -1.15806000  C -5.60526700 1.80420600 1.37412500  C 6.27326500 -2.74551400 1.03329000  C 6.96387300 -2.23035200 -0.26623600  C 5.63180700 -1.33945000 -2.38211400  H 5.39634000 0.06151400 -0.05526400  H -4.93243600 1.96347800 -1.26132400  H 4.50441000 -1.87888100 2.00926000  H 5.90825800 -0.81773200 2.04932200  H -5.16290000 -0.78632400 -2.36055300  H -5.93499100 0.68671500 -2.93955300  H -7.86770700 -0.60297500 -2.02141400  H -6.35155800 -0.78291100 1.74181500  H -4.85944800 -1.03600900 0.84669200  H -7.57461600 -1.93895800 0.07503500  H -6.08715000 -2.23669900 -0.81207500  H -8.64865400 1.52769800 1.21643400  H -8.40949200 -0.21755700 1.20256200  H -9.45192100 0.53929200 -0.00001300  H -6.90220100 2.43585300 -1.92362900  H -7.68729100 3.03110100 -0.46248500  H -8.61083000 2.12044900 -1.65330000  H -5.65457700 2.83254900 1.00120300  H -4.59637100 1.64198000 1.76573400  H -6.29950000 1.71644600 2.21515300  H 6.95255100 -3.07693500 1.82292400  C 7.89307200 -1.02260100 -0.04409200  C 7.79974000 -3.29658400 -0.99696600  H 6.16260900 -0.38258800 -2.42040800  H 4.61898300 -1.16946200 -2.76014400  H 6.12685000 -2.02830700 -3.07313700  C 4.84473900 -3.26511500 -0.85586000  C 5.33258600 -3.85109100 0.50378800  H 7.44101400 -0.20835600 0.52149500  H 8.22949200 -0.61288300 -1.00158200  H 8.78760500 -1.33896000 0.50201100  H 7.23995200 -4.19431400 -1.25731800  H 8.64428900 -3.60433500 -0.37179200  H 8.21627900 -2.88829900 -1.92298100  H 5.10783700 -3.91522000 -1.69393900  H 3.76562400 -3.11820900 -0.88308100  H 5.85963400 -4.79866500 0.36996300  H 4.50832200 -4.03748700 1.19601700 |
| opt\_4e\_CS\_30 | C 1.56786600 0.51528200 -0.36942500  C 0.68268400 -0.57149200 -0.31369700  C -0.69261400 -0.43719600 -0.47436500  C -1.21770100 0.85802900 -0.70454600  C -0.32839200 1.93949400 -0.76732600  C 1.04934500 1.80365500 -0.60042600  C -2.64294000 1.18421300 -0.90355000  N -3.61613400 0.38388000 -0.74895500  C -4.95337700 0.88586200 -1.00103500  C -5.90952700 0.76174700 0.23260000  C 3.01889500 0.29593700 -0.20909300  N 3.52220400 -0.85872400 -0.03252200  C 4.96034800 -0.96514100 0.11604100  C 5.62446800 -1.90852800 -0.94301800  H 1.10570900 -1.55370800 -0.14306100  C -1.51548800 -1.68837300 -0.43890300  H -0.73037100 2.93065200 -0.95102700  C 1.91542000 3.02165000 -0.70399000  H -2.81762200 2.23043800 -1.20586700  C -5.69395900 0.05478300 -2.10010100  H 3.64829500 1.19368600 -0.25250800  C 5.36332400 -1.63072500 1.47340300  C -1.68843600 -2.41326200 -1.59791100  C -2.40200200 -3.63217100 -1.60172800  C -2.92941500 -4.12920500 -0.43712800  C -2.76288800 -3.42788400 0.78500100  C -2.04593800 -2.18818700 0.79077900  C -1.89298400 -1.50317600 2.02503800  C -2.41506700 -2.01276000 3.18957600  C -3.11947600 -3.23786200 3.18255500  C -3.28802100 -3.92577200 2.00627900  C 2.34718000 3.72463700 0.46661200  C 3.15467800 4.89854200 0.31296900  C 3.50383100 5.33724400 -0.99023300  C 3.07235000 4.65087400 -2.09647300  C 2.27611900 3.49303300 -1.94946600  C 2.00363100 3.30838100 1.78110900  C 2.43649400 4.00865800 2.88151400  C 3.23550300 5.16387000 2.72772400  C 3.58388700 5.59629900 1.47202900  H -1.27376800 -2.03639300 -2.52608800  H -2.52397100 -4.17437000 -2.53287400  H -3.47417500 -5.06756900 -0.43288500  H -1.35452100 -0.56363000 2.03974500  H -2.28717100 -1.47308500 4.12137800  H -3.52579000 -3.63090000 4.10783000  H -3.82877800 -4.86655000 1.99299600  H 4.11655000 6.22636000 -1.09605600  H 3.33980100 4.99035200 -3.09073900  H 1.94520000 2.95846700 -2.83289100  H 1.38896700 2.42597000 1.90884200  H 2.16276400 3.67469300 3.87601500  H 3.57038900 5.70705800 3.60419200  H 4.19546200 6.48381800 1.34680700  C 6.26154600 -2.81359900 1.04691300  C 4.87052600 -3.26553700 -0.88631000  C 5.32681900 -3.89651600 0.46334100  C 6.98161500 -2.26090000 -0.22125400  C 7.82754100 -3.30781300 -0.96775900  C 7.91114000 -1.06640700 0.06061100  C 5.69620000 -1.29758600 -2.33457000  C -7.00365700 -0.38006400 -1.40564500  C -7.31774800 0.83062500 -0.47443700  C -5.61399300 1.77555800 1.32780100  H -4.90069700 1.94442100 -1.29577900  H 5.41652900 0.03114400 0.03017900  H -5.09131800 -0.80252100 -2.40538400  H -5.87290400 0.66345900 -2.98961300  H 4.47659800 -1.96893500 2.01305500  H 5.88421800 -0.91675600 2.11500700  H 6.92263100 -3.17352500 1.83933900  H 5.14651200 -3.89057000 -1.73909300  H 3.79357800 -3.10939500 -0.93015300  H 5.85178800 -4.84234600 0.31120000  H 4.48767500 -4.09961900 1.13247600  H 8.26206500 -2.87418900 -1.87366000  H 7.26980400 -4.19535700 -1.26463500  H 8.65943300 -3.63680800 -0.33674900  H 7.44766500 -0.26647600 0.63711000  H 8.27593200 -0.63105500 -0.87471700  H 8.78814200 -1.40449300 0.62158600  H 6.22924400 -0.34131400 -2.33239600  H 4.69141800 -1.11317000 -2.72664100  H 6.20336300 -1.96596300 -3.03661800  H -7.80186700 -0.65245100 -2.10104000  C -7.61416500 2.13947700 -1.23035300  C -8.50516400 0.59699000 0.47643600  H -5.66707300 2.80355900 0.95477600  H -4.60987200 1.62154900 1.73424100  H -6.32018300 1.68064000 2.15783900  C -5.85888500 -0.71639500 0.70530200  C -6.63167400 -1.49415900 -0.40164600  H -6.87013700 2.39850000 -1.98299600  H -7.68605200 2.98028600 -0.53353500  H -8.57895300 2.06171200 -1.74160600  H -8.39481700 -0.28185400 1.11058000  H -9.42733800 0.47409600 -0.10072600  H -8.64811700 1.46127000 1.13221600  H -6.33720500 -0.82027000 1.68219800  H -4.82954700 -1.05457100 0.80826700  H -7.52072000 -1.98940400 -0.00393000  H -6.01664700 -2.26574100 -0.86975400 |
| opt\_4e\_CS\_44 | C -1.22879700 0.88623000 -0.58716200  C -0.33335400 1.96353800 -0.65473600  C 1.04896300 1.81694300 -0.53957500  C 1.56629000 0.52160300 -0.34868100  C 0.67482700 -0.55961700 -0.27803300  C -0.70467500 -0.41531100 -0.39046700  C 3.02051900 0.29074700 -0.23845300  N 3.52081700 -0.86556600 -0.06139800  C 4.96291000 -0.98223800 0.03592900  C 5.58219800 -1.94508600 -1.03256600  C -2.65424400 1.23326600 -0.74984800  N -3.63165600 0.42167900 -0.75160400  C -4.96015200 0.97253600 -0.95111600  C -5.97065600 0.60724500 0.18574000  H -0.73474200 2.96047700 -0.80618300  C 1.91818000 3.03165000 -0.65327500  H 1.09496800 -1.54696800 -0.13018500  C -1.53002500 -1.66287800 -0.31597200  H 3.65661900 1.18133400 -0.31866600  C 5.41078700 -1.63061400 1.38753000  H -2.82575100 2.31373100 -0.88941800  C -5.65431400 0.39667900 -2.23001300  C 2.20235600 3.54605500 -1.90208100  C 3.00201700 4.70073300 -2.05918500  C 3.51512300 5.34053100 -0.95896900  C 3.24533500 4.85713100 0.34762400  C 2.43297600 3.68767500 0.51117000  C 2.16724200 3.22926100 1.83004500  C 2.67995600 3.88391900 2.92511900  C 3.48552900 5.03373300 2.76099800  C 3.75886600 5.50714900 1.50072500  C -2.06822000 -2.11513400 0.92940700  C -2.78060100 -3.35743300 0.96837000  C -2.93605700 -4.10810200 -0.22566700  C -2.40143900 -3.65588700 -1.40594600  C -1.69121400 -2.43530400 -1.44592500  C -1.92132900 -1.38432200 2.13856300  C -2.44914900 -1.85004300 3.31955200  C -3.15234200 -3.07603500 3.35569200  C -3.31165900 -3.80966200 2.20535800  H 1.80863900 3.04794700 -2.78122300  H 3.20819900 5.07427800 -3.05589000  H 4.13191600 6.22588400 -1.07288200  H 1.54833900 2.35108200 1.96699700  H 2.46467900 3.51783400 3.92273300  H 3.88427000 5.54068000 3.63246600  H 4.37391500 6.39126100 1.36801500  H -3.47830600 -5.04725800 -0.18840200  H -2.51569700 -4.23520600 -2.31552600  H -1.27166000 -2.09493000 -2.38608600  H -1.38178900 -0.44523600 2.12263000  H -2.32542000 -1.27561800 4.23100800  H -3.56319800 -3.43424000 4.29307500  H -3.84950500 -4.75207800 2.22574300  C -7.00157000 -0.14506000 -1.70026100  C -5.95489300 -0.93844600 0.33573800  C -6.68849000 -1.45241400 -0.93889900  C -7.34482400 0.85058000 -0.54929500  C -8.57449700 0.44547100 0.28284900  C -7.59473900 2.29378700 -1.02500400  C -5.71606100 1.35809500 1.48499000  C 6.28281400 -2.82753100 0.94649800  C 6.96173700 -2.29846900 -0.35341700  C 5.61207700 -1.35312600 -2.43409700  H 5.42270400 0.00910000 -0.08168000  H -4.89483200 2.06839000 -1.01912900  H 4.54254600 -1.95317900 1.96572000  H 5.96101000 -0.91138300 1.99818700  H -5.04602700 -0.39274500 -2.67578600  H -5.78222100 1.17694700 -2.98397600  H -7.76862600 -0.24865500 -2.47231900  H -6.47335200 -1.23755300 1.24990500  H -4.93409600 -1.30907700 0.40599300  H -7.60024900 -2.00042600 -0.68940000  H -6.06379000 -2.12200600 -1.53441400  H -8.73570000 1.15664200 1.09876900  H -8.49891400 -0.54787400 0.72325600  H -9.47283300 0.46296000 -0.34287800  H -6.81766000 2.69089600 -1.67780300  H -7.68624800 2.97145800 -0.17036100  H -8.53875300 2.34372300 -1.57722700  H -5.72593000 2.44308300 1.33719400  H -4.74028200 1.08847300 1.89967700  H -6.46991100 1.11324400 2.23907500  H 6.96870800 -3.18184300 1.72030800  C 7.90950700 -1.10676000 -0.12315800  C 7.77384000 -3.36203500 -1.11413000  H 6.15451800 -0.40249100 -2.46253600  H 4.59656800 -1.16370800 -2.79529400  H 6.08898400 -2.03569400 -3.14383600  C 4.82215300 -3.29628100 -0.93159900  C 5.31937200 -3.91088100 0.41184200  H 7.47384200 -0.29394200 0.45736800  H 8.24315200 -0.68880700 -1.07805900  H 8.80428900 -1.44294800 0.41054300  H 7.19983100 -4.24897500 -1.38016900  H 8.62406500 -3.68927300 -0.50684900  H 8.18113100 -2.94360500 -2.03969300  H 5.06756100 -3.93492700 -1.78377200  H 3.74460500 -3.13650800 -0.94320000  H 5.83091200 -4.86355200 0.25584900  H 4.50177500 -4.09685000 1.11208600 |
| opt\_4e\_CS\_52 | C 1.25781900 0.93449000 -0.22255000  C 0.36458600 2.01081600 -0.31182100  C -1.01315500 1.84897600 -0.46111900  C -1.52574100 0.54003300 -0.52718000  C -0.63652300 -0.54139000 -0.42634800  C 0.73686300 -0.38324600 -0.26722100  C -2.97173700 0.29483100 -0.70005100  N -3.46263100 -0.87650100 -0.77436500  C -4.89458300 -1.01699400 -0.95052100  C -5.57592900 -1.86437700 0.17835300  C 2.68556300 1.29322900 -0.11852700  N 3.65971500 0.47958500 -0.15514800  C 5.00124100 1.02035900 -0.04501300  C 5.92573700 0.64483200 -1.25213400  H 0.76357500 3.01938300 -0.27137600  C -1.87808400 3.06787900 -0.56516500  H -1.05453100 -1.53965800 -0.46829200  C 1.56272200 -1.62729100 -0.16449300  H -3.60770900 1.18684300 -0.76649800  C -5.24922200 -1.81730200 -2.24803500  H 2.86185700 2.37684700 -0.01447900  C 5.77525600 0.43246600 1.18152500  C -2.02400300 3.69882100 -1.78374300  C -2.80934200 4.86626000 -1.91906800  C -3.44560700 5.40172200 -0.82736700  C -3.32235900 4.79443900 0.44923500  C -2.52721700 3.61044800 0.59033600  C -2.41333500 3.02267300 1.87950500  C -3.05054500 3.57121700 2.96746300  C -3.83633900 4.73756800 2.82532200  C -3.96656700 5.33311200 1.59419400  C 2.05024500 -2.09404800 1.09768600  C 2.78133900 -3.32455000 1.14711700  C 2.99700300 -4.05661800 -0.04965800  C 2.50175900 -3.59768700 -1.24377000  C 1.77870600 -2.38466500 -1.29609400  C 1.83100600 -1.39286500 2.31278800  C 2.31515100 -1.87018700 3.50801700  C 3.04451600 -3.08026400 3.55313700  C 3.26852000 -3.78875600 2.39761600  H -1.52881200 3.28642200 -2.65597100  H -2.90453700 5.33413200 -2.89247900  H -4.04998100 6.29751000 -0.92514000  H -1.81177100 2.12995000 1.99916300  H -2.95035100 3.10765900 3.94249800  H -4.33390100 5.16016500 3.69096400  H -4.56691700 6.22969700 1.47892900  H 3.55343000 -4.98696200 -0.00245900  H 2.66155300 -4.16184400 -2.15593900  H 1.39705900 -2.03481200 -2.24882000  H 1.26985600 -0.46675200 2.29181500  H 2.13574900 -1.31746500 4.42363200  H 3.42150700 -3.44786900 4.50106400  H 3.82190700 -4.72198700 2.42499000  C 7.06627100 -0.14061200 0.55542400  C 5.86783400 -0.89881000 -1.41130100  C 6.66823300 -1.43638700 -0.18678000  C 7.35294600 0.85249800 -0.61202700  C 8.51481800 0.42312900 -1.52530500  C 7.66604200 2.28808900 -0.15151800  C 5.60071200 1.41304500 -2.52485700  C -6.12479400 -2.97960400 -1.72995900  C -6.89974400 -2.32340300 -0.54688700  C -5.71672600 -1.11350100 1.49424400  H -5.36592800 -0.02434900 -0.97520300  H 4.95117600 2.11686500 0.02758000  H -4.34313000 -2.17759800 -2.73942600  H -5.77741600 -1.18127800 -2.96201900  H 5.18518700 -0.33930500 1.67846400  H 5.97933300 1.21327400 1.91788400  H 7.88317000 -0.26803000 1.27065300  H 6.32539500 -1.19978100 -2.35721300  H 4.83676100 -1.24945400 -1.42039100  H 7.54607800 -2.00849400 -0.49692300  H 6.06492600 -2.08955500 0.44718600  H 8.63331800 1.12747000 -2.35453900  H 8.39354200 -0.57124100 -1.95316500  H 9.45359100 0.42759400 -0.96187200  H 6.93891100 2.70198700 0.54656700  H 7.72221800 2.96467400 -1.01010200  H 8.64231800 2.31453200 0.34322500  H 5.65096400 2.49595500 -2.37068300  H 4.59051300 1.17567400 -2.87245000  H 6.29294600 1.15482300 -3.33186800  H -6.75004800 -3.43776700 -2.50080200  C -7.84348600 -1.18393000 -0.97396000  C -7.74878700 -3.31283100 0.27097500  H -6.29039600 -0.18927300 1.37189000  H -4.73522800 -0.84158800 1.89440200  H -6.21943200 -1.72559300 2.24900400  C -4.79322500 -3.20107400 0.28606100  C -5.17892700 -3.97042100 -1.01379400  H -7.37493200 -0.43032200 -1.60658400  H -8.25177600 -0.67108400 -0.09762900  H -8.69170000 -1.59419200 -1.53137200  H -7.18176600 -4.15131500 0.67355000  H -8.54836600 -3.72435800 -0.35359900  H -8.22757300 -2.80408200 1.11333900  H -5.09482200 -3.74741500 1.18312400  H -3.72197600 -3.01852900 0.35980700  H -5.67860200 -4.91627500 -0.79182800  H -4.30826300 -4.20551300 -1.63040100 |
| opt\_4e\_CS\_55 | C -1.31472700 -0.17002400 -0.61768100  C -0.77897700 1.12323000 -0.61839000  C 0.58366600 1.36429200 -0.46140900  C 1.45263400 0.26223100 -0.29999400  C 0.91559300 -1.03094600 -0.28923800  C -0.44747200 -1.27151200 -0.44231800  C 2.91060200 0.45466600 -0.16853400  N 3.72225600 -0.51722400 -0.04498200  C 5.13564100 -0.21947100 0.08068600  C 6.01352100 -0.89491300 -1.02715200  C -2.76415400 -0.36675400 -0.83548200  N -3.57506500 0.60981100 -0.89157700  C -4.98528600 0.39304100 -1.18756700  C -5.88732400 1.50345500 -0.55958600  H -1.46281600 1.95133700 -0.75713400  C 1.07420000 2.77916900 -0.51042100  H 1.59924800 -1.86016700 -0.15660200  C -0.93386000 -2.68821700 -0.43619000  H 3.26207900 1.49360600 -0.18636000  C 5.74095500 -0.79769300 1.40237200  H -3.08275600 -1.40651600 -0.95880900  C -5.67419300 -0.93640200 -0.72562600  C 1.17565200 3.41542000 -1.73053600  C 1.61007000 4.75603500 -1.82931300  C 1.94001300 5.45990100 -0.69951400  C 1.84443500 4.85546900 0.58034400  C 1.40290600 3.49600300 0.68509200  C 1.30111400 2.91735400 1.97890300  C 1.62615000 3.63599500 3.10425200  C 2.06800500 4.97393100 2.99788800  C 2.17160600 5.56704100 1.76401800  C -1.59019600 -3.24470900 0.70925000  C -2.01687900 -4.61233100 0.66959600  C -1.77550400 -5.38332800 -0.49651300  C -1.13452200 -4.83197300 -1.57632800  C -0.71271300 -3.48418400 -1.54161100  C -1.82591400 -2.49918700 1.89592400  C -2.45672200 -3.06741100 2.97688600  C -2.88467800 -4.41337700 2.93160200  C -2.66649400 -5.16552800 1.80398600  H 0.92046500 2.87044100 -2.63244700  H 1.68103400 5.22198700 -2.80566100  H 2.27591900 6.48926800 -0.76786400  H 0.95680300 1.89483400 2.07099200  H 1.54036900 3.17591300 4.08227200  H 2.32104400 5.53002500 3.89355400  H 2.50584300 6.59557600 1.67538500  H -2.10360400 -6.41726900 -0.51706300  H -0.94809500 -5.42521600 -2.46442000  H -0.21018700 -3.06117600 -2.40421400  H -1.49496400 -1.46940500 1.94348700  H -2.62416000 -2.48128800 3.87350600  H -3.38122600 -4.84952300 3.79104400  H -2.98712600 -6.20140500 1.76417200  C -6.90270500 -0.43546800 0.06685400  C -5.65439500 1.43695000 0.97382800  C -6.37100000 0.12237000 1.40788200  C -7.31467000 0.85683700 -0.70260400  C -8.43744600 1.65617700 -0.01881300  C -7.77390700 0.60190700 -2.14956900  C -5.66203300 2.88078700 -1.16385500  C 6.92213200 -1.66531000 0.91315800  C 7.43057700 -0.88272400 -0.33621500  C 5.88280600 -0.22815800 -2.38834100  H 5.29154800 0.86744600 0.03486800  H -5.05504500 0.48615100 -2.27744500  H 4.99679000 -1.38959200 1.93872500  H 6.05913400 0.00783600 2.06781400  H -5.02184200 -1.53999500 -0.09111500  H -5.95623400 -1.55987800 -1.57679300  H -7.69121000 -1.18442500 0.17628300  H -6.08008100 2.31284400 1.46923500  H -4.58684400 1.43271500 1.19937200  H -7.18301200 0.31847500 2.11163300  H -5.69311500 -0.58457800 1.89214500  H -8.64615100 2.57637900 -0.57278400  H -8.21343100 1.93701800 1.00979600  H -9.36182500 1.06958700 -0.00671600  H -7.07917200 0.00473600 -2.74024800  H -7.92570500 1.54840100 -2.67709400  H -8.73383700 0.07567900 -2.14895500  H -5.85806000 2.88773000 -2.24107800  H -4.62452500 3.19066400 -1.01664500  H -6.30713200 3.63160000 -0.69785700  H 7.67513500 -1.85964000 1.68131800  C 7.99454400 0.51279600 -0.01069100  C 8.52089200 -1.62101700 -1.13267400  H 6.14808900 0.83289400 -2.34481800  H 4.85429500 -0.29579800 -2.75561800  H 6.52783700 -0.70765200 -3.13042800  C 5.66859000 -2.40947300 -1.02453000  C 6.31265100 -2.94203500 0.29114800  H 7.33002500 1.13414700 0.58873000  H 8.22115800 1.06276300 -0.92936900  H 8.93304000 0.41217300 0.54362000  H 8.22580800 -2.61563900 -1.46463200  H 9.42103500 -1.73138600 -0.51952100  H 8.80383800 -1.04737500 -2.02058700  H 6.08806500 -2.89817300 -1.90732500  H 4.58988700 -2.55686600 -1.04974400  H 7.07639200 -3.69706700 0.09072800  H 5.57782200 -3.39778200 0.95871600 |