

optimization-xyz

InZn-1

SCF Energy = -4826.66547559 au

In	-0.04550000	-0.70339000	-0.04052100
Zn	0.13109900	1.84630500	-0.10660400
Si	-0.89512500	-3.66376000	-1.37157800
O	-0.27899500	-4.26650100	0.05377500
N	-1.30660900	-1.98615600	-1.13329700
C	-2.54747400	-1.48184700	-1.56908900
C	-2.71003600	-0.97772100	-2.88342000
C	-3.96641800	-0.52199200	-3.29421300
H	-4.09073100	-0.14123800	-4.31222100
C	-5.05709800	-0.54035500	-2.43351600
H	-6.03348000	-0.18421000	-2.77149100
C	-4.89553900	-1.01978800	-1.13612200
H	-5.75447500	-1.03669100	-0.46126400
C	-3.66288600	-1.49648500	-0.68798100
C	-1.53958900	-0.92205100	-3.84344600
H	-0.67723800	-1.33525800	-3.30042900
C	-1.19510800	0.51606800	-4.22765400
H	-0.31168600	0.54819800	-4.88512800
H	-0.97528400	1.12278400	-3.33537100
H	-2.02637800	1.00637400	-4.75955000
C	-1.77369600	-1.78778400	-5.07976000
H	-0.88209500	-1.79933500	-5.72696500
H	-2.61747500	-1.41384300	-5.68189000
H	-2.00448700	-2.82665800	-4.79938400
C	-3.49911000	-2.03036000	0.72175300
H	-2.67152900	-2.75445400	0.68044200
C	-3.08919600	-0.92062000	1.68914800
H	-2.86860900	-1.31799600	2.69251600
H	-3.87874700	-0.16225900	1.78248700
H	-2.19607700	-0.36908700	1.34709600
C	-4.72530600	-2.76634400	1.24993900
H	-4.49357600	-3.24803300	2.21259800
H	-5.05857000	-3.54735500	0.54981500
H	-5.57450600	-2.08598000	1.42484300
C	-2.42327500	-4.64022700	-1.82435600
H	-2.87607500	-4.26354600	-2.75450100
H	-3.18279300	-4.57225000	-1.03099800
H	-2.16788500	-5.70170600	-1.96623500
C	0.43950200	-3.90193400	-2.66854400
H	0.07188600	-3.67026600	-3.67973400
H	0.79656400	-4.94381600	-2.66219200
H	1.30132700	-3.24890700	-2.46426100
C	2.86953800	2.47479900	-0.99918800
C	3.18687700	2.22842300	-2.34634000
C	4.46350200	1.75566800	-2.65637500
H	4.71515700	1.56914800	-3.70478800
C	5.41723500	1.50033600	-1.66699400

optimization-xyz

C	5.05752800	1.71853400	-0.33543500
H	5.77748600	1.50330100	0.45873900
C	3.79500800	2.19773100	0.02056200
C	2.16581100	2.46726100	-3.41817100
H	2.54736900	2.16558100	-4.40298100
H	1.86428900	3.52539900	-3.47985000
H	1.24499400	1.89720700	-3.21966400
C	6.76247300	0.93510000	-2.01839900
H	7.09056400	1.25764400	-3.01717900
H	6.73277100	-0.16838800	-2.02552700
H	7.53014100	1.23496900	-1.29046300
C	3.42278300	2.41268400	1.45607100
H	4.27874700	2.23288300	2.11814700
H	2.62949800	1.71051800	1.76099500
H	3.04182800	3.42992700	1.63687200
N	1.60291200	3.02488800	-0.66149700
C	1.46940300	4.35019000	-0.67929200
C	2.66028800	5.19565600	-1.04610200
H	3.49032800	5.00764200	-0.34811100
H	2.41059100	6.26270200	-1.02268100
H	3.04037600	4.93777300	-2.04530000
C	0.28311000	5.03462000	-0.36562000
H	0.32751600	6.11683000	-0.47713100
Si	0.50196600	-3.72419200	1.41833200
N	1.03541900	-2.08651600	1.12496400
C	2.25646700	-1.63119400	1.66574600
C	2.30868100	-1.04413300	2.95478900
C	3.53422900	-0.59649000	3.45635400
H	3.57257000	-0.14117400	4.44983800
C	4.70414400	-0.72143100	2.71607600
H	5.65548300	-0.37118700	3.12454600
C	4.65513400	-1.30358200	1.45270600
H	5.57628400	-1.40588200	0.87456300
C	3.45349000	-1.76678800	0.91433900
C	1.04386400	-0.87505800	3.77061500
H	0.27735700	-1.48936100	3.27976700
C	0.54771500	0.56781400	3.72273700
H	-0.40197700	0.68191000	4.26898900
H	0.36929600	0.88365500	2.68213900
H	1.28112800	1.26496500	4.15997300
C	1.18863600	-1.36876000	5.20674400
H	0.22008400	-1.32785200	5.72976700
H	1.89896900	-0.75684200	5.78552100
H	1.54754000	-2.40891500	5.23487200
C	3.41016200	-2.39148800	-0.46575200
H	2.53955500	-3.06338600	-0.47446200
C	3.17518100	-1.32817400	-1.53519200
H	3.08867400	-1.77426200	-2.53876100
H	3.99369800	-0.59654300	-1.55048700

optimization-xyz

H	2.25603700	-0.74595700	-1.35022600
C	4.64179600	-3.22416900	-0.80331500
H	4.48923900	-3.76152800	-1.75218000
H	4.85270100	-3.96731200	-0.01941200
H	5.54221800	-2.60071500	-0.92649300
C	1.96342400	-4.83368500	1.78746000
H	2.53915600	-4.45265300	2.64544000
H	2.64557900	-4.90957900	0.92809300
H	1.60958800	-5.84725000	2.03260800
C	-0.73431600	-3.88663300	2.82305200
H	-0.26676400	-3.70846800	3.80369300
H	-1.15313900	-4.90555700	2.82511200
H	-1.56960900	-3.17989700	2.70910100
C	-2.44081100	2.87607600	0.89051600
C	-2.63305700	2.92055800	2.28267300
C	-3.88248000	2.56280100	2.79682900
H	-4.03257200	2.59177700	3.88037800
C	-4.93956600	2.17713500	1.96990300
C	-4.71677900	2.14426900	0.59097300
H	-5.52393100	1.83425600	-0.07825900
C	-3.48164600	2.47730500	0.03365100
C	-1.53444200	3.38776700	3.19125600
H	-1.70888600	3.06214000	4.22574100
H	-1.46020400	4.48864200	3.20043300
H	-0.55376100	3.01464100	2.86694300
C	-6.25924700	1.75035800	2.54374500
H	-6.42624900	2.17923600	3.54217400
H	-6.30460700	0.65226400	2.64687200
H	-7.09683800	2.04912800	1.89642600
C	-3.25845500	2.40329900	-1.44495100
H	-4.20473100	2.27026300	-1.98325300
H	-2.63031200	1.53319700	-1.69702400
H	-2.74891100	3.29714000	-1.83492500
N	-1.18242200	3.24225300	0.33968200
C	-0.94105300	4.52998600	0.10354900
C	-2.04013300	5.53055900	0.34429100
H	-2.92933100	5.27040000	-0.24966300
H	-1.71794700	6.54442700	0.08000500
H	-2.36307800	5.52223700	1.39532600

InZn-2

SCF Energy = -5230.26742947 au

In	1.23182800	-0.53529300	-0.05571700
Zn	-2.00840500	0.71980900	-0.31810200
Si	2.72645000	-1.81953700	-2.60504600
Si	4.46427000	-1.18833400	-0.03630900
O	3.98713900	-1.79329000	-1.51562100
N	1.23195800	-1.83511000	-1.69270600
N	3.18997700	-0.13063500	0.52641500

	optimization-xyz		
N	-0.40241500	0.41884300	0.64246000
N	-2.61317600	2.11449500	-1.56386200
N	-3.73325500	-0.20575500	-0.09084900
C	0.28183900	-2.85401700	-1.92722900
C	-0.63363600	-2.74290300	-3.00608200
C	-1.42967100	-3.83734700	-3.35458100
H	-2.11021100	-3.75163800	-4.20618600
C	-1.37911100	-5.02459100	-2.63683200
H	-1.99761800	-5.87660600	-2.92850500
C	-0.55270300	-5.10353000	-1.52236600
H	-0.53661500	-6.02394000	-0.93389100
C	0.27098900	-4.03972900	-1.14388000
C	-0.79973400	-1.44747000	-3.77269800
H	-0.11110700	-0.72479300	-3.30988600
C	-0.41786400	-1.57657100	-5.24569700
H	-1.08525500	-2.27654300	-5.77358600
H	0.61035200	-1.94715800	-5.36660600
H	-0.48948300	-0.60187600	-5.75439200
C	-2.22635300	-0.91827800	-3.62492000
H	-2.49818600	-0.76006300	-2.57049900
H	-2.96204000	-1.62394700	-4.04127100
H	-2.35494200	0.03928300	-4.14941500
C	1.15510300	-4.20894600	0.07554000
H	1.47800000	-3.20024800	0.38859100
C	2.42178600	-4.99948200	-0.25478500
H	3.07039800	-4.45083600	-0.95075300
H	2.16067600	-5.96650200	-0.71334700
H	3.00757900	-5.20361300	0.65447700
C	0.41300100	-4.83961500	1.25291700
H	0.22021600	-5.91065000	1.08404600
H	-0.55380500	-4.34837500	1.43470200
H	1.01623300	-4.76227100	2.17084100
C	2.85769300	-0.26867500	-3.65149100
H	3.87853000	-0.14994300	-4.04726000
H	2.61875400	0.62972300	-3.06386200
H	2.15940700	-0.30470500	-4.50149900
C	2.88178800	-3.33874400	-3.67839000
H	2.77277400	-4.26327700	-3.09449600
H	3.87133100	-3.34678900	-4.16117500
H	2.11257700	-3.35225000	-4.46454800
C	6.06384300	-0.24102700	-0.22547400
H	5.99743600	0.49641400	-1.03854100
H	6.88897400	-0.93243100	-0.45640600
H	6.31380600	0.29741600	0.70221500
C	4.73347300	-2.67406500	1.07254300
H	5.31406300	-3.44372900	0.54075100
H	3.77574700	-3.12112100	1.37614200
H	5.28019200	-2.40038000	1.98596600
C	3.44017300	1.06068500	1.25577600

	optimization-xyz		
C	3.64232800	2.28309700	0.56356600
C	3.84058000	3.46129400	1.28673000
H	3.98425900	4.40133100	0.74836300
C	3.85106700	3.46073400	2.67681600
H	3.99751800	4.39199000	3.22907300
C	3.68320800	2.26033100	3.35489400
H	3.70665300	2.25272600	4.44755200
C	3.49104600	1.05600800	2.67152300
C	3.59903300	2.33397900	-0.94803500
H	3.74241400	1.30291900	-1.30045500
C	4.70537100	3.18656100	-1.56142500
H	5.69638800	2.89117300	-1.18560700
H	4.57064400	4.25781600	-1.34271100
H	4.70742800	3.07730500	-2.65748000
C	2.22748900	2.80060900	-1.42674700
H	2.01250900	3.82241600	-1.07847000
H	1.40895000	2.17036100	-1.04064600
H	2.16759300	2.80186800	-2.52571400
C	3.39662100	-0.23043800	3.46290900
H	3.10030200	-1.01625300	2.75164200
C	4.76735100	-0.59959300	4.03411700
H	5.08417400	0.13633700	4.79065200
H	5.54225400	-0.61715400	3.25326900
H	4.74206300	-1.58940100	4.51755700
C	2.34608900	-0.16961000	4.56727100
H	1.36792700	0.14099300	4.17793400
H	2.63064600	0.54088400	5.35967800
H	2.22718800	-1.15627800	5.04304700
C	-0.57276600	0.70407500	2.00982600
C	-0.86278100	-0.32101900	2.94310400
C	-1.19833000	0.00689500	4.25793600
H	-1.44349700	-0.80304400	4.95195600
C	-1.21948600	1.32691800	4.71012200
C	-0.83275400	2.32234400	3.80839400
H	-0.78053900	3.36146900	4.14905500
C	-0.49263000	2.03931100	2.48383400
C	-0.75106000	-1.75004100	2.52501900
H	-1.07129800	-2.43232000	3.32345100
H	0.30019800	-2.00446400	2.28534000
H	-1.34505700	-1.96366300	1.62635900
C	-1.64026800	1.66502800	6.11081400
H	-1.44647100	0.83192100	6.80258000
H	-2.72030800	1.88715900	6.16234900
H	-1.10985000	2.55163900	6.48921800
C	0.02028400	3.11900700	1.58455300
H	1.10929100	3.00897500	1.45125200
H	-0.16816900	4.11778600	2.00258300
H	-0.41701000	3.07134100	0.57927500
C	-3.81072700	2.03925400	-2.14587900

	optimization-xyz		
C	-4.77060200	1.05142700	-1.87572100
H	-5.69082100	1.12760800	-2.45309700
C	-4.78031500	0.08108700	-0.85429100
C	-4.20249100	3.11116100	-3.12857600
H	-3.41656000	3.26387400	-3.88211900
H	-4.32693100	4.07719100	-2.61530000
H	-5.14319100	2.85997600	-3.63261800
C	-6.08330300	-0.62764100	-0.60049500
H	-6.44744900	-0.38881200	0.41083800
H	-5.95756800	-1.71927200	-0.62972900
H	-6.84606700	-0.33166500	-1.33010200
C	-1.86958200	3.31684400	-1.70713600
C	-0.87526500	3.43908500	-2.69124500
C	-0.17686800	4.64361600	-2.79294800
H	0.59337500	4.73935500	-3.56398600
C	-0.41855900	5.71621000	-1.93253900
C	-1.40212700	5.56078100	-0.95335400
H	-1.60403900	6.38341600	-0.26089300
C	-2.13479500	4.37968200	-0.82325700
C	-0.57384400	2.29525900	-3.60910900
H	-1.42225000	2.06894100	-4.27424300
H	-0.37359900	1.37403500	-3.04183100
H	0.30098300	2.50652400	-4.23844000
C	0.39086300	6.97668200	-2.02959300
H	0.60952600	7.23713300	-3.07583800
H	1.35969900	6.86156800	-1.51460600
H	-0.12776800	7.82777000	-1.56571400
C	-3.16289700	4.22485500	0.25804300
H	-4.15529900	3.96498700	-0.14272000
H	-3.26037400	5.14873400	0.84375500
H	-2.88751400	3.41488300	0.95397300
C	-3.88387000	-1.12434700	0.98348600
C	-4.14469600	-0.63258600	2.27392000
C	-4.26033600	-1.54473800	3.32515100
H	-4.45669300	-1.16081300	4.33055700
C	-4.12004200	-2.92007000	3.13189600
C	-3.85798000	-3.37732700	1.83817000
H	-3.73542600	-4.45018900	1.66094000
C	-3.72783400	-2.50329300	0.75697900
C	-4.25191300	0.84190300	2.52309400
H	-4.89100900	1.34471400	1.78172900
H	-3.25536500	1.31499800	2.47552000
H	-4.65378300	1.04330100	3.52510400
C	-4.19694900	-3.87447400	4.28820000
H	-4.85905200	-3.49720100	5.08110500
H	-3.20156400	-4.02656300	4.73968800
H	-4.56525100	-4.86208600	3.97441500
C	-3.37187100	-3.01757500	-0.60264600
H	-2.35096500	-2.71358300	-0.88533700

optimization-xyz
H -4.03546800 -2.63317600 -1.39137300
H -3.39979400 -4.11377100 -0.63380300