

Electronic Supplementary Information

The Cp*Si⁺ Cation as a Stoichiometric Source of Silicon

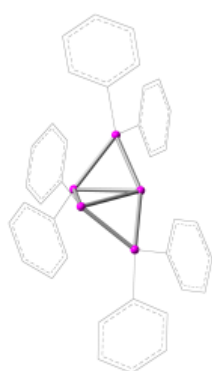
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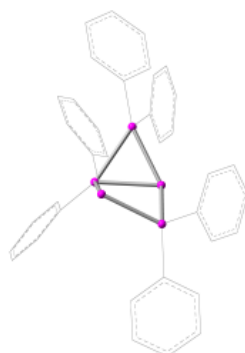
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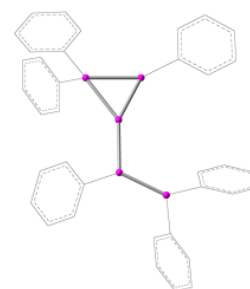
DFT Calculations [B3LYP/6-31G(d,p)]:



3Ph



3'Ph



8Ph

E_{abs} [Hartree]	-2836.855621	-2836.860541	-2836.818826
E_{rel} [kcal mol ⁻¹]	0.00	-3.08	+23.10
H [Hartree]	-2836.816448	-2836.820749	-2836.778337
H [kcal mol ⁻¹]	0.00	-2.70	+23.92
G [Hartree]	-2836.935491	-2836.939868	-2836.902506
G [kcal mol ⁻¹]	0.00	-2.75	+20.70
Symmetry	C_1 ^[1]	C_1	C_1
NIMAG	1	0	0

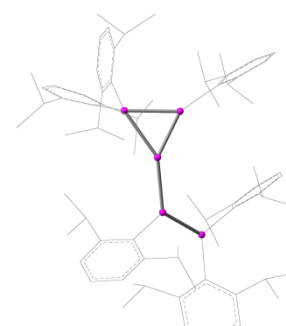
[1] In order to be the transition state of the degenerate rearrangement **3Ph** would in fact have to be C_2 symmetric as it is the case for the hydrogen substituted model system. This discrepancy is very likely due to a slight rotation of one or more of the phenyl substituents. We decided to ignore it due to (1) the obvious shortcomings of the phenyl substituted model and (2) the presumably more significant error caused by the inadequate modelling of dispersive forces by the B3LYP functional.



3Dip



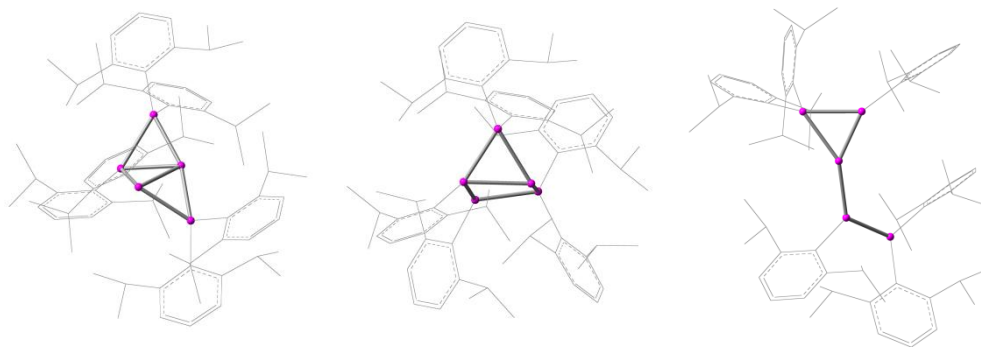
3Dip'



8Dip

E_{abs} [Hartree]	-4251.143991	-4251.137974	-4251.130838
E_{rel} [kcal mol ⁻¹]	0.00	+3.78	+8.25
H [Hartree]	-4251.054394	-4251.048000	-4251.039754
H [kcal mol ⁻¹]	0.00	+4.01	+9.19
G [Hartree]	-4251.264735	-4251.259848	-4251.259441
G [kcal mol ⁻¹]	0.00	+3.07	+3.32
Symmetry	C_2	C_1	C_1
NIMAG	0	0	0

DFT Calculations [ω B97XD/6-311g(d,p)]:



	3Dip	3Dip'	8Dip
E_{abs} [Hartree]	-4250.961977	-4250.952440	-4250.906190
E_{rel} [kcal mol ⁻¹]	0.00	+5.98	+35.01
H [Hartree]	-4250.876130	-4250.866168	-4250.818339
H [kcal mol ⁻¹]	0.00	+6.25	+36.26
G[Hartree]	-4251.075376	-4251.064611	-4251.025808
G [kcal mol ⁻¹]	0.00	+6.75	+31.10
Symmetry	C ₂	C ₁	C ₁
NIMAG	1 ^[2]	0	0

[1] With the ω B97XD functional **3Dip** retains a small imaginary eigen frequency. This frequency involves the rotation of two methyl groups of the *ortho*-isopropyl substituents and thus no rearrangement of the silicon framework. Despite two attempts to eliminate this imaginary frequency, we were unsuccessful and abandoned further attempts due to the large computational cost.

Cartesian coordinates of calculated stationary points [B3LYP/6-31G(d,p)]

Compound 3Ph

Transition state C₁

0 1

Si	-2.25893700	-0.30393000	0.51312000
Si	-0.92285700	0.65856300	-1.11109300
Si	0.92286900	-0.65851800	-1.11108600
Si	2.25891300	0.30391900	0.51318300
Si	-0.00002500	0.00003500	1.02999800
C	-2.95079200	-2.05125800	0.34928100
C	-3.38438700	-2.54158200	-0.89509800
C	-3.92054400	-3.82520400	-1.01520000
H	-4.25039300	-4.18471600	-1.98580000
C	-4.02655700	-4.64552000	0.10869500
C	-3.59609300	-4.17842400	1.35287200
H	-3.67209800	-4.81554200	2.22957400
C	-3.06397500	-2.89452300	1.47093800
C	-3.47348200	0.80540100	1.43308300
C	-4.75742100	0.34777800	1.78223300
C	-5.66508700	1.18277800	2.43630000
H	-6.65092700	0.80858800	2.69806100
C	-5.30681400	2.49310000	2.75360600
C	-4.03701900	2.96644300	2.41419300
H	-3.75266500	3.98614700	2.65791800
C	-3.13205800	2.13146300	1.76200200
C	-1.17501600	2.41001300	-1.77667900
C	-2.25631200	2.67422800	-2.63780700
C	-2.47351000	3.95416900	-3.14964800
H	-3.31634300	4.13670700	-3.81061000
C	-1.60742900	4.99587800	-2.81451600
C	-0.52729300	4.75218700	-1.96361500
H	0.15016300	5.55890900	-1.69737200
C	-0.31512900	3.47376700	-1.44712900
C	1.17501600	-2.40997300	-1.77667100
C	2.25621700	-2.67413400	-2.63793500
C	2.47344900	-3.95407500	-3.14975900
H	3.31621000	-4.13657000	-3.81082400
C	1.60749500	-4.99584100	-2.81447600
C	0.52744600	-4.75220100	-1.96344900
H	-0.14992000	-5.55896500	-1.69710100
C	0.31525200	-3.47378100	-1.44697800
C	3.47343900	-0.80543700	1.43313500
C	4.75741400	-0.34784700	1.78219700
C	5.66508000	-1.18285000	2.43625800
H	6.65094900	-0.80868700	2.69795000
C	5.30676800	-2.49314000	2.75365300
C	4.03693700	-2.96645000	2.41432800
H	3.75255400	-3.98612900	2.65812000
C	3.13197800	-2.13146800	1.76213800
C	2.95079200	2.05124400	0.34937800
C	3.06364100	2.89463300	1.47097400
C	3.59578400	4.17852500	1.35291800
H	3.67152900	4.81574200	2.22957000
C	4.02660400	4.64548600	0.10881300

C	3.92092600	3.82504400	-1.01502100
H	4.25105300	4.18445100	-1.98556500
C	3.38474700	2.54143000	-0.89493100
H	-4.43937200	-5.64610500	0.01621000
H	-2.72665000	-2.54834800	2.44487700
H	-3.29397100	-1.91644600	-1.77961000
H	-2.14812600	2.51476100	1.50464200
H	-6.01254700	3.14333200	3.26286600
H	-5.05234500	-0.66975800	1.54317300
H	-1.77358600	5.99259900	-3.21365300
H	-2.93740300	1.87226400	-2.91212300
H	0.52486600	3.30179200	-0.78170200
H	1.77368200	-5.99256400	-3.21359300
H	2.93720600	-1.87212400	-2.91237300
H	-0.52467900	-3.30184200	-0.78146000
H	4.43943200	5.64606700	0.01633600
H	2.72603200	2.54856300	2.44485100
H	3.29459000	1.91619400	-1.77939900
H	6.01249800	-3.14337300	3.26291500
H	2.14801900	-2.51474000	1.50484000
H	5.05236300	0.66966800	1.54307200

Compound 3'Ph

Local minimum C₁

0 1

Si	-2.32849800	0.23741000	-0.44284100
Si	-0.92522600	-0.06379800	1.39129200
Si	0.92704000	1.19532600	0.81110100
Si	2.02485400	-0.23342600	-0.64478700
Si	-0.12764900	0.56639600	-1.17761500
C	-3.33171700	1.83269600	-0.49172800
C	-3.61215500	2.56492900	0.67494700
C	-4.35527200	3.74572700	0.62210300
H	-4.56038600	4.29626200	1.53586100
C	-4.83147500	4.21754100	-0.60096900
C	-4.56291900	3.50498600	-1.77217200
H	-4.92853100	3.87002500	-2.72780600
C	-3.82080500	2.32617700	-1.71718900
C	-3.32491200	-1.20346800	-1.13487800
C	-4.72553600	-1.12636000	-1.25134700
C	-5.46467300	-2.19855100	-1.75380600
H	-6.54502200	-2.11883400	-1.83528900
C	-4.81688300	-3.36797300	-2.15303300
C	-3.42713900	-3.46357500	-2.04648600
H	-2.91830200	-4.37132200	-2.35795200
C	-2.69118200	-2.39309800	-1.54213900
C	-0.72270400	-1.84706500	1.98864000
C	0.45701800	-2.26398200	2.63380400
C	0.56817900	-3.54049500	3.18340400
H	1.49429900	-3.84098400	3.66480400
C	-0.50597300	-4.42931200	3.11240400
C	-1.69196200	-4.03120100	2.49226900
H	-2.53548700	-4.71420500	2.43969500
C	-1.80004800	-2.75437400	1.94198500

C	1.34411300	2.83848900	1.63071200
C	0.53574900	3.37044900	2.65053900
C	0.84270900	4.59621900	3.24101700
H	0.20528200	4.99180700	4.02700700
C	1.96982200	5.30948200	2.82897700
C	2.78845400	4.79115900	1.82359300
H	3.66901700	5.33991400	1.50122700
C	2.48023500	3.56677800	1.23110900
C	3.29803800	0.51432600	-1.83654200
C	4.45172600	-0.20272100	-2.20131000
C	5.39404400	0.34160000	-3.07684800
H	6.27626700	-0.23382300	-3.34393500
C	5.20306400	1.61628700	-3.60911300
C	4.06279100	2.34470600	-3.26159600
H	3.90378000	3.33762900	-3.67309700
C	3.12511300	1.79945700	-2.38616300
C	2.56025000	-1.98431400	-0.18044800
C	1.94096100	-3.11381700	-0.74138600
C	2.36438200	-4.40369900	-0.41749500
H	1.86855600	-5.26307900	-0.85995800
C	3.42028400	-4.58906600	0.47545300
C	4.05216900	-3.48003100	1.04206300
H	4.87615200	-3.61811500	1.73681100
C	3.62454200	-2.19221700	0.71749800
H	2.21184800	6.26185200	3.29209500
H	-0.33858300	2.81918200	2.98718800
H	3.12788700	3.17752800	0.44979000
H	-3.61565200	1.78808800	-2.63937000
H	-5.40804100	5.13723600	-0.64364800
H	-3.24514400	2.20727800	1.63290300
H	-0.42241600	-5.42276200	3.54413800
H	1.30080900	-1.58353300	2.70362800
H	-2.73477500	-2.46308500	1.47155200
H	-1.61108200	-2.48204300	-1.46039800
H	-5.39117000	-4.20156700	-2.54726400
H	-5.24320100	-0.21951700	-0.95253900
H	1.11708000	-2.98522100	-1.43857400
H	4.12466700	-1.33962800	1.17141700
H	3.74980300	-5.59257800	0.72946900
H	5.93544900	2.04002500	-4.29044000
H	4.61754300	-1.19837300	-1.80121000
H	2.24235000	2.38102100	-2.13140500

Compound 8Ph

Local minimum C₁

0 1			
Si	1.89131200	1.58286800	-0.51803500
Si	0.58462000	-0.07670100	-0.09986800
C	2.05726400	3.43404100	-0.75056800
C	0.91763000	4.25266400	-0.87456600
C	1.04873300	5.62833500	-1.05641100
C	2.31676300	6.21119800	-1.11758100
C	3.45604400	5.41258000	-0.99595900
C	3.32872100	4.03616100	-0.81597000
H	0.15963700	6.24566600	-1.14916300

H	4.44388300	5.86223300	-1.04212400
Si	-3.27152000	0.22939900	-0.07263200
Si	-1.48551200	-0.98877800	0.35218100
C	-3.28442300	2.06808000	0.28133000
C	-2.30720600	2.68119300	1.09249500
C	-2.30776700	4.05971800	1.30210100
C	-3.28699300	4.86050900	0.70916700
C	-4.26340500	4.27445000	-0.09796700
C	-4.26089700	2.89617000	-0.31104500
C	-4.98557800	-0.52334900	-0.16158200
C	-6.08520800	0.05771300	0.50246600
C	-7.35280000	-0.51907300	0.43167100
C	-7.54996200	-1.68963800	-0.30347700
C	-6.47385700	-2.28077200	-0.96905500
C	-5.20747000	-1.70254900	-0.90181700
C	-1.58323900	-2.85593700	0.10273400
C	-2.54039300	-3.61337200	0.80656900
C	-2.61319500	-4.99791300	0.65601700
C	-1.71968300	-5.65862500	-0.18928200
C	-0.75542200	-4.92688900	-0.88471400
C	-0.68811600	-3.54096500	-0.74164300
H	-1.54729600	4.50715800	1.93546000
H	-5.02730200	4.89043300	-0.56402900
H	-8.18604600	-0.05693000	0.95356600
H	-6.62214800	-3.18961700	-1.54513000
H	-3.36181700	-5.56148500	1.20586500
H	-0.05572300	-5.43422500	-1.54289000
H	-1.77151300	-6.73786800	-0.30146200
H	-3.23400000	-3.11627900	1.47941400
H	0.06440900	-2.98671100	-1.29578900
H	-8.53774000	-2.13816700	-0.35869700
H	-5.94729500	0.96590800	1.08183300
H	-4.38064700	-2.17119300	-1.42790000
H	-3.29087700	5.93340100	0.87877000
H	-5.02853000	2.46098100	-0.94518300
H	-1.54567200	2.07357700	1.57251100
H	2.41691000	7.28343800	-1.25969800
H	-0.07463600	3.81416600	-0.82241400
H	4.22310100	3.42557300	-0.72249300
Si	2.89316900	-0.41157700	0.05967200
C	3.69786300	-0.69058300	1.75168200
C	5.09235000	-0.83625400	1.88411400
C	2.92372100	-0.70449700	2.92559800
C	5.68699200	-0.98593300	3.13768800
H	5.72240500	-0.83836000	0.99860900
C	3.51281400	-0.86243500	4.18002600
H	1.84475900	-0.58828600	2.85576300
C	4.89774400	-1.00132500	4.28887600
H	6.76557200	-1.09296400	3.21543100
H	2.89220000	-0.87718400	5.07176700
H	5.35924300	-1.12148300	5.26508700
C	3.84397300	-1.41186500	-1.23854400
C	4.39902500	-2.66702600	-0.92295500
C	3.97080400	-0.95497200	-2.56243900
C	5.05238100	-3.43222100	-1.89036900
H	4.32538800	-3.05138400	0.09077900

C	4.62774400	-1.71348100	-3.53111800
H	3.54476200	0.00654300	-2.83834600
C	5.17004400	-2.95596700	-3.19698500
H	5.47092400	-4.39873100	-1.62294000
H	4.71745700	-1.33534900	-4.54583900
H	5.68164800	-3.54884400	-3.95009900

Compound 3Dip

Local minimum C₂

0 1

Si	2.31493500	0.45948900	0.55856000
Si	0.97674800	-0.64794800	-1.12563100
Si	-0.97674800	0.64794800	-1.12563100
Si	-2.31493500	-0.45948900	0.55856000
Si	0.00000000	0.00000000	0.90099200
C	-3.04317400	-2.26562700	0.38873500
C	-3.26690200	-2.91048900	-0.86908700
C	-3.34138500	-3.01293300	1.57008500
C	-3.68555300	-4.24966100	-0.90136700
C	-3.78254100	-4.33879700	1.47979700
C	-3.93509200	-4.97052700	0.25510700
H	-3.83232300	-4.73092700	-1.86279300
H	-4.01046400	-4.88545000	2.38916300
H	-4.26015700	-6.00587000	0.20251700
C	3.04317400	2.26562700	0.38873500
C	3.26690200	2.91048900	-0.86908700
C	3.34138500	3.01293300	1.57008500
C	3.68555300	4.24966100	-0.90136700
C	3.78254100	4.33879700	1.47979700
C	3.93509200	4.97052700	0.25510700
H	3.83232300	4.73092700	-1.86279300
H	4.01046400	4.88545000	2.38916300
H	4.26015700	6.00587000	0.20251700
C	3.51604400	-0.69416800	1.56622600
C	4.75673900	-1.04051900	0.95593500
C	3.24588800	-1.21841700	2.87093900
C	5.65775600	-1.89166700	1.61038400
C	4.17794200	-2.07126600	3.47870800
C	5.37221100	-2.41608800	2.86196300
H	6.59794600	-2.14421700	1.12980100
H	3.96150600	-2.47246300	4.46380700
H	6.07555800	-3.08049500	3.35611600
C	-3.51604400	0.69416800	1.56622600
C	-4.75673900	1.04051900	0.95593500
C	-3.24588800	1.21841700	2.87093900
C	-5.65775600	1.89166700	1.61038400
C	-4.17794200	2.07126600	3.47870800
C	-5.37221100	2.41608800	2.86196300
H	-6.59794600	2.14421700	1.12980100
H	-3.96150600	2.47246300	4.46380700
H	-6.07555800	3.08049500	3.35611600
C	1.49627900	-2.34629000	-1.92970300
C	1.86796700	-2.37943300	-3.30774900
C	1.55517900	-3.56971400	-1.19552900
C	2.26222500	-3.58669400	-3.90050000

C	1.92958600	-4.75493300	-1.84488000
C	2.28473600	-4.77391400	-3.18468300
H	2.55548400	-3.59562500	-4.94551000
H	1.95209800	-5.68083400	-1.27914700
H	2.58303700	-5.70222200	-3.66416100
C	-1.49627900	2.34629000	-1.92970300
C	-1.86796700	2.37943300	-3.30774900
C	-1.55517900	3.56971400	-1.19552900
C	-2.26222500	3.58669400	-3.90050000
C	-1.92958600	4.75493300	-1.84488000
C	-2.28473600	4.77391400	-3.18468300
H	-2.55548400	3.59562500	-4.94551000
H	-1.95209800	5.68083400	-1.27914700
H	-2.58303700	5.70222200	-3.66416100
C	-3.14942100	-2.25073400	-2.24602700
H	-2.87666400	-1.20222300	-2.10809800
C	-3.27468100	-2.43863700	2.98333100
H	-2.75841200	-1.47887800	2.94062600
C	3.14942100	2.25073400	-2.24602700
H	2.87666400	1.20222300	-2.10809800
C	3.27468100	2.43863700	2.98333100
H	2.75841200	1.47887800	2.94062600
C	1.89350600	-1.15831400	-4.22606200
H	1.47938300	-0.30305900	-3.67773100
C	1.24917800	-3.71037000	0.29328000
H	1.04170300	-2.71307100	0.68860900
C	-1.89350600	1.15831400	-4.22606200
H	-1.47938300	0.30305900	-3.67773100
C	-1.24917800	3.71037000	0.29328000
H	-1.04170300	2.71307100	0.68860900
C	-2.00044900	0.91312600	3.71340300
H	-1.43363500	0.12404400	3.21517500
C	-5.21010400	0.49824100	-0.39886400
H	-4.39824700	-0.10417400	-0.82137700
C	5.21010400	-0.49824100	-0.39886400
H	4.39824700	0.10417400	-0.82137700
C	2.00044900	-0.91312600	3.71340300
H	1.43363500	-0.12404400	3.21517500
C	-2.45587400	4.28244000	1.06216400
H	-3.35360500	3.67844900	0.91331000
H	-2.24388200	4.31238500	2.13461400
H	-2.68135700	5.30680500	0.74659000
C	0.00000000	4.57643800	0.53784700
H	0.22142900	4.63326000	1.60904000
H	0.87948300	4.17262500	0.03292500
H	-0.15239900	5.60123800	0.18128800
C	3.33393800	-0.80126800	-4.63814100
H	3.79187000	-1.61293100	-5.21358400
H	3.34307300	0.09535200	-5.26741700
H	3.96645400	-0.61657600	-3.76720300
C	1.03096600	-1.37279100	-5.48321900
H	-0.00950000	-1.58449900	-5.22288000
H	1.05389400	-0.48346900	-6.11837200
H	1.39924700	-2.21025300	-6.08389400
C	-1.03096600	1.37279100	-5.48321900
H	0.00950000	1.58449900	-5.22288000

H	-1.05389400	0.48346900	-6.11837200
H	-1.39924700	2.21025300	-6.08389400
C	-3.33393800	0.80126800	-4.63814100
H	-3.79187000	1.61293100	-5.21358400
H	-3.34307300	-0.09535200	-5.26741700
H	-3.96645400	0.61657600	-3.76720300
C	2.45587400	-4.28244000	1.06216400
H	3.35360500	-3.67844900	0.91331000
H	2.24388200	-4.31238500	2.13461400
H	2.68135700	-5.30680500	0.74659000
C	0.00000000	-4.57643800	0.53784700
H	-0.22142900	-4.63326000	1.60904000
H	-0.87948300	-4.17262500	0.03292500
H	0.15239900	-5.60123800	0.18128800
C	-1.06598500	2.12990800	3.83066700
H	-1.57930800	2.98015600	4.29282100
H	-0.20135900	1.88465400	4.45607800
H	-0.69405500	2.44867900	2.85478200
C	-2.34616600	0.40478900	5.12862500
H	-1.43663300	0.05780700	5.63146900
H	-2.77586000	1.19491300	5.75298000
H	-3.05874300	-0.42169500	5.10660100
C	-5.50520400	1.62085800	-1.41098100
H	-5.79067600	1.19431800	-2.37827400
H	-6.33428900	2.25467300	-1.07948000
H	-4.63270300	2.26135100	-1.56438100
C	-6.43050900	-0.42917600	-0.23208200
H	-6.76824300	-0.80899600	-1.20178500
H	-6.19399000	-1.28602300	0.40507600
H	-7.27186400	0.10586200	0.22038000
C	1.06598500	-2.12990800	3.83066700
H	1.57930800	-2.98015600	4.29282100
H	0.20135900	-1.88465400	4.45607800
H	0.69405500	-2.44867900	2.85478200
C	2.34616600	-0.40478900	5.12862500
H	1.43663300	-0.05780700	5.63146900
H	2.77586000	-1.19491300	5.75298000
H	3.05874300	0.42169500	5.10660100
C	5.50520400	-1.62085800	-1.41098100
H	5.79067600	-1.19431800	-2.37827400
H	6.33428900	-2.25467300	-1.07948000
H	4.63270300	-2.26135100	-1.56438100
C	6.43050900	0.42917600	-0.23208200
H	6.76824300	0.80899600	-1.20178500
H	6.19399000	1.28602300	0.40507600
H	7.27186400	-0.10586200	0.22038000
C	-4.69852400	-2.18155000	3.51883900
H	-4.67029300	-1.78247600	4.53830400
H	-5.23681400	-1.46656600	2.89149700
H	-5.27520100	-3.11243100	3.54401400
C	-2.48324700	-3.32835500	3.96092000
H	-1.49071900	-3.56820800	3.57156600
H	-2.35811800	-2.81681100	4.92102200
H	-2.99979800	-4.27141400	4.16550800
C	-4.49839600	-2.29349100	-2.99542000
H	-4.42193400	-1.76202400	-3.94786600

H	-4.80033900	-3.32154000	-3.21918500
H	-5.30161300	-1.83585500	-2.41351500
C	-2.05536600	-2.90046300	-3.11215000
H	-1.97719400	-2.38053300	-4.07337700
H	-1.07756600	-2.87030400	-2.62865200
H	-2.28769700	-3.94884700	-3.32801800
C	2.48324700	3.32835500	3.96092000
H	1.49071900	3.56820800	3.57156600
H	2.35811800	2.81681100	4.92102200
H	2.99979800	4.27141400	4.16550800
C	4.69852400	2.18155000	3.51883900
H	4.67029300	1.78247600	4.53830400
H	5.23681400	1.46656600	2.89149700
H	5.27520100	3.11243100	3.54401400
C	2.05536600	2.90046300	-3.11215000
H	1.97719400	2.38053300	-4.07337700
H	1.07756600	2.87030400	-2.62865200
H	2.28769700	3.94884700	-3.32801800
C	4.49839600	2.29349100	-2.99542000
H	5.30161300	1.83585500	-2.41351500
H	4.42193400	1.76202400	-3.94786600
H	4.80033900	3.32154000	-3.21918500

Compound 3Dip'

Local minimum C₁

0 1

Si	-2.11343400	-0.72027200	0.21825300
Si	-1.02338600	1.35971600	-0.23328500
Si	1.15966100	1.17021400	0.61094800
Si	1.89305000	-1.03359900	-0.17716100
Si	-0.21013300	-0.73142200	-1.26291100
C	-1.73100800	2.98034000	-1.04336500
C	-1.71193100	4.22907900	-0.35619400
C	-2.32516600	2.93906900	-2.34373100
C	-2.24590600	5.37236300	-0.96681400
C	-2.82924800	4.11710100	-2.91179400
C	-2.79385900	5.32911800	-2.23917700
H	-2.23016000	6.31523800	-0.42978800
H	-3.26086200	4.07729600	-3.90655000
H	-3.19421900	6.22822200	-2.69920400
C	2.30736600	2.74691500	0.49627700
C	2.72654700	3.29844600	1.74832500
C	2.72180400	3.40563100	-0.69359700
C	3.50152200	4.46595600	1.77254400
C	3.48593100	4.57888300	-0.61614100
C	3.87442000	5.11390900	0.60385200
H	3.81305600	4.87822900	2.72744200
H	3.78649700	5.07790700	-1.53201600
H	4.46737500	6.02343700	0.64302900
C	3.46674700	-0.87965000	-1.35114000
C	4.74349000	-0.69557100	-0.73855200
C	3.43504600	-0.99565800	-2.78307300
C	5.90517600	-0.60898700	-1.51912800
C	4.62806100	-0.88772200	-3.51293500

C	5.85614900	-0.69194200	-2.90133600
H	6.86549800	-0.48009200	-1.03054100
H	4.58802200	-0.96385000	-4.59472200
H	6.76335300	-0.61367900	-3.49399000
C	-3.68024600	-1.07694600	-0.92009400
C	-4.92245000	-0.45547500	-0.58778200
C	-3.67601200	-1.96544700	-2.04762700
C	-6.06804000	-0.68199500	-1.36370900
C	-4.85141100	-2.15119700	-2.79178600
C	-6.04051000	-1.51656000	-2.46879700
H	-6.99769600	-0.19151700	-1.09195200
H	-4.83056300	-2.81911700	-3.64677100
H	-6.93386500	-1.67789400	-3.06572100
C	-2.49120900	-1.30887300	2.04419500
C	-2.64203500	-2.71484500	2.24248100
C	-2.63718900	-0.46475200	3.18963700
C	-2.87446900	-3.23406100	3.52263100
C	-2.87169300	-1.03615300	4.44958900
C	-2.98005900	-2.40643200	4.62938200
H	-2.97985800	-4.30716100	3.64887100
H	-2.96956500	-0.38646000	5.31324600
H	-3.15573800	-2.82182000	5.61783800
C	2.10728300	-2.62043100	0.94639300
C	2.24299400	-3.87439100	0.27133600
C	2.14392300	-2.63973400	2.37343400
C	2.38902400	-5.06169200	1.00035800
C	2.28908700	-3.85868800	3.05397700
C	2.40727400	-5.06619300	2.38623500
H	2.48869800	-6.00097300	0.46548000
H	2.30709100	-3.85488800	4.13879600
H	2.51469900	-5.99633000	2.93714800
C	-1.16522900	4.43435400	1.05424300
H	-0.72210300	3.49143700	1.39604400
C	-2.44468900	1.68999300	-3.21614400
H	-2.14595600	0.82092800	-2.62530500
C	2.38541600	2.70060000	3.11825700
H	1.80355400	1.78313600	2.95633800
C	2.40800900	2.89913000	-2.09624200
H	1.86039400	1.95354900	-1.99645400
C	-2.56243500	1.06512400	3.19030900
H	-2.50519700	1.40966100	2.15342800
C	-2.62009000	-3.74095300	1.11104900
H	-2.38101500	-3.22194500	0.17850700
C	2.03535800	-1.41698300	3.28268200
H	1.97151400	-0.52467300	2.65367400
C	2.26922900	-4.04519900	-1.24734000
H	2.12487800	-3.07035200	-1.71272900
C	-2.48521200	-2.78864200	-2.55968200
H	-1.65344200	-2.66888000	-1.85909500
C	-5.12948900	0.45536700	0.62099300
H	-4.17676300	0.55450800	1.14215400
C	2.19809600	-1.26228400	-3.65349300
H	1.34632900	-1.47375800	-3.00374600
C	4.97004400	-0.63919400	0.77255500
H	3.99694800	-0.59829200	1.27235400
C	-4.01427500	-4.37915600	0.94377200

H	-4.00784300	-5.13789300	0.15479800
H	-4.76621300	-3.62758800	0.68697200
H	-4.33249900	-4.87299500	1.86759800
C	-1.53651000	-4.81537300	1.31262200
H	-1.49698400	-5.48190700	0.44437200
H	-1.74193200	-5.43714600	2.19031600
H	-0.54919000	-4.36660100	1.44464500
C	1.12506400	-4.94483600	-1.75148800
H	1.21628300	-5.96936400	-1.37639200
H	1.13244700	-4.99267500	-2.84576000
H	0.15209800	-4.56022000	-1.43338500
C	3.64112400	-4.57467200	-1.71258700
H	4.44154900	-3.87791700	-1.44967700
H	3.66082400	-4.71819400	-2.79735900
H	3.86957500	-5.54116200	-1.25252700
C	3.26430000	-1.26395100	4.20090400
H	3.38636700	-2.13071800	4.85802400
H	3.14906900	-0.38569400	4.84208300
H	4.19011700	-1.14867300	3.63249500
C	-3.80293700	1.71705500	3.83660900
H	-3.75678000	2.80464300	3.72892200
H	-3.85799000	1.50409100	4.90881700
H	-4.73220700	1.36909100	3.38482200
C	0.75586100	-1.47702400	4.13488700
H	0.65478000	-0.56972000	4.73844000
H	0.77820500	-2.32815100	4.82379400
H	-0.13526900	-1.57630300	3.51415300
C	-1.30116800	1.56511300	3.91124500
H	-1.27237700	1.20866600	4.94641800
H	-1.28608500	2.65796700	3.93702700
H	-0.39456200	1.22068200	3.41035600
C	3.64930800	2.31210900	3.90700400
H	3.37631200	1.89216300	4.88041000
H	4.28386300	3.18424700	4.09443700
H	4.24815400	1.57415500	3.37193900
C	-2.30165200	4.79679800	2.03065600
H	-2.74303000	5.76633800	1.77706200
H	-1.92639100	4.86530900	3.05765800
H	-3.10271100	4.05356400	2.00405300
C	1.52228200	3.64784900	3.97215700
H	1.25167800	3.16720700	4.91803300
H	0.60068400	3.92781500	3.46022400
H	2.06513800	4.56840000	4.21251000
C	-0.06708000	5.51506800	1.08833900
H	0.75549300	5.27506700	0.41190000
H	0.34347700	5.61847700	2.09621900
H	-0.46749100	6.49258700	0.80102600
C	3.70708300	2.61774800	-2.87627900
H	3.48361300	2.19942600	-3.86073700
H	4.34901300	1.91213000	-2.34453600
H	4.27627200	3.53962700	-3.03496200
C	-3.88680600	1.43928900	-3.69449600
H	-4.58715700	1.39169200	-2.85828500
H	-3.94174300	0.48571600	-4.22739500
H	-4.23034000	2.21889100	-4.38276500
C	-1.49324400	1.77122800	-4.42417300

H	-1.74758900	2.61948100	-5.06924300
H	-1.56151500	0.86106800	-5.02946100
H	-0.45564400	1.89043300	-4.10748800
C	1.51620000	3.88367600	-2.87675200
H	0.57138700	4.07182200	-2.36191100
H	1.28909200	3.48861200	-3.87243700
H	2.02263800	4.84505200	-3.01569800
C	-1.99641700	-2.29189700	-3.93393400
H	-1.14243400	-2.89014900	-4.27113800
H	-2.78430400	-2.38067300	-4.68977900
H	-1.67514600	-1.24957300	-3.88729800
C	1.80364100	-0.03869100	-4.49779000
H	2.61191700	0.25300200	-5.17740800
H	0.92252000	-0.26862700	-5.10513400
H	1.55950000	0.81982900	-3.87092200
C	2.36434900	-2.47877800	-4.58781400
H	1.40592800	-2.70472000	-5.06793100
H	3.08694300	-2.28936500	-5.38859200
H	2.69289400	-3.37045300	-4.05210200
C	-2.79002500	-4.29830100	-2.64294200
H	-3.53920000	-4.52276700	-3.40920300
H	-1.88019800	-4.84568600	-2.91079900
H	-3.15823200	-4.69464600	-1.69540500
C	-5.56549400	1.87749800	0.21977300
H	-5.65217400	2.51305500	1.10800600
H	-4.84137100	2.33986200	-0.45706400
H	-6.54052000	1.87856500	-0.27911100
C	5.75005600	0.61763600	1.20307700
H	5.23457000	1.53422800	0.90402900
H	5.87424100	0.63162400	2.29063500
H	6.75457500	0.63941100	0.76934000
C	-6.13198900	-0.18059700	1.60604200
H	-6.31515100	0.47593000	2.46221500
H	-7.09894100	-0.36334900	1.12705600
H	-5.75812500	-1.13605000	1.98517400
C	5.68930300	-1.91527300	1.25617900
H	6.67462900	-2.00694800	0.78677300
H	5.84172700	-1.89171800	2.34024700
H	5.11396400	-2.81254400	1.01490400

Compound 8Dip

Local minimum C₁

0 1

Si	-1.99276500	1.42220200	0.54492400
Si	-0.62325300	-0.24116000	0.41633600
C	-2.23408200	3.31554200	0.55179300
C	-2.06822500	4.02971700	-0.66631400
C	-2.11779800	5.42894300	-0.64405700
C	-2.34879400	6.12246000	0.53924900
C	-2.56137600	5.42126200	1.72149000
C	-2.51608900	4.02197800	1.74913200
H	-1.97853700	5.98217000	-1.56806300
H	-2.77326200	5.96887800	2.63515600
Si	3.41330700	0.16341700	-0.08176200
Si	1.61119600	-1.01986900	0.40240400

C	3.23656200	1.95090200	-0.73652600
C	3.48935600	2.19842800	-2.11381100
C	3.43014400	3.50834600	-2.60675800
C	3.10890300	4.57267400	-1.77326100
C	2.85341100	4.33846100	-0.42677700
C	2.92398300	3.04939500	0.11718000
C	5.23746200	-0.47411500	-0.15543500
C	5.61638000	-1.67879700	-0.82079200
C	6.97451700	-1.98758300	-0.98235200
C	7.97699200	-1.16175000	-0.49761200
C	7.62201700	-0.00581700	0.18210000
C	6.28088500	0.34969200	0.37030300
C	1.82200100	-2.74992500	1.20381400
C	1.42006300	-3.91734000	0.49575300
C	1.65098700	-5.18098300	1.05287500
C	2.26210300	-5.31936200	2.29334800
C	2.61627800	-4.18350100	3.01077700
C	2.39371000	-2.89723300	2.49967800
H	3.63295000	3.69481900	-3.65733900
H	2.60362800	5.17593400	0.21722200
H	7.24920000	-2.90199800	-1.49836700
H	8.40094900	0.63463000	0.58445100
H	1.34241700	-6.07003700	0.51068800
H	3.06353100	-4.29510500	3.99418800
H	2.44404800	-6.30743800	2.70714500
H	9.02244400	-1.42228900	-0.63703600
H	3.05909800	5.58289700	-2.17018900
H	-2.38038600	7.20859400	0.53709200
Si	-2.96548800	-0.60840900	-0.05635400
C	-3.80017800	-0.30912300	-1.77872200
C	-5.03182300	0.41105700	-1.79037900
C	-3.19837800	-0.64371000	-3.02075500
C	-5.61698800	0.76327700	-3.01426300
C	-3.80948200	-0.25285000	-4.22028200
C	-5.01339000	0.44098200	-4.22433300
H	-6.56095600	1.30090200	-3.01907300
H	-3.33904400	-0.50398800	-5.16658300
H	-5.47879900	0.72768100	-5.16333500
C	-4.08383100	-1.83833100	0.96833000
C	-4.82935500	-2.86608800	0.30967100
C	-4.30227400	-1.66317400	2.37147600
C	-5.84599100	-3.54349000	0.99975200
C	-5.31488700	-2.38201200	3.01923400
C	-6.11113100	-3.29167600	2.33681900
H	-6.42417200	-4.30127100	0.47968800
H	-5.47954900	-2.23216700	4.08050500
H	-6.90587500	-3.82424400	2.85200900
C	2.67340800	2.90693700	1.62100300
H	2.97789100	1.89488900	1.91504300
C	3.84173200	1.08486300	-3.09786500
H	3.76513500	0.13070200	-2.56024300
C	-1.84497400	3.33170700	-2.00582400
H	-1.99381000	2.25589300	-1.84583200
C	-2.84211800	3.31282400	3.05979100
H	-2.66677700	2.23833000	2.90714500
C	-1.88658700	-1.42133700	-3.12177200

H	-1.62474500	-1.76447200	-2.11459600
C	-5.77715200	0.83640000	-0.51974800
H	-5.18064300	0.54204000	0.34916700
C	-4.53981900	-3.39082100	-1.10064800
C	-5.70188100	-3.18251300	-2.08914000
H	-3.66922700	-2.86123900	-1.49114400
C	-4.17279800	-4.89081500	-1.05128700
C	-3.40864800	-0.79261900	3.25089200
H	-2.95080200	-0.02858400	2.61842200
C	-4.14849500	-0.06235900	4.38444300
C	-2.25664900	-1.64122700	3.82522900
C	2.74767300	-1.71790300	3.40448100
H	2.47572100	-0.80070400	2.87310400
C	0.65214300	-3.85880300	-0.82255500
H	0.64330500	-2.81345200	-1.15992400
C	6.03917000	1.62788200	1.16729000
H	4.96169200	1.75759100	1.27480200
C	4.64078800	-2.71086600	-1.38011400
H	3.62232000	-2.35887000	-1.19277500
C	-2.86926800	3.76528300	-3.07047800
H	-3.89540400	3.62755900	-2.71948200
H	-2.74422800	4.81700100	-3.35089000
H	-2.74274300	3.16354400	-3.97585200
C	-0.40654000	3.52567500	-2.51459100
H	-0.18644900	4.58578400	-2.68197300
H	0.32781400	3.14347400	-1.80146100
H	-0.26274700	3.00154400	-3.46562200
C	-4.33154100	3.49526000	3.41312200
H	-4.58028700	2.95926800	4.33404800
H	-4.56945300	4.55346200	3.56635300
H	-4.97859000	3.12238700	2.61349400
C	-1.94820500	3.75667700	4.23084700
H	-2.11124200	4.80941900	4.48527900
H	-2.17374200	3.16647300	5.12557300
H	-0.88860300	3.62890700	3.99648700
C	-5.95526700	2.36492600	-0.43881900
H	-6.58451800	2.74078200	-1.25262300
H	-6.44258400	2.64081800	0.50316400
H	-4.99576400	2.88649700	-0.48752700
C	-7.13775700	0.12709500	-0.37793700
H	-7.63494100	0.44383100	0.54539500
H	-7.80372900	0.36935200	-1.21344500
H	-7.01923100	-0.95818600	-0.33973700
C	-0.73229500	-0.52451800	-3.60544900
H	-0.92915600	-0.13872900	-4.61202600
H	-0.58945600	0.32720800	-2.93511700
H	0.20597800	-1.08873700	-3.63916400
C	-2.00349400	-2.67017400	-4.01728600
H	-2.19460300	-2.40253300	-5.06163300
H	-1.06867700	-3.24076400	-3.99629600
H	-2.81317300	-3.33027700	-3.69273000
C	3.48268400	3.90523200	2.47218100
H	4.54793000	3.88800000	2.23337700
H	3.12838600	4.93226800	2.33541100
H	3.36832600	3.66443400	3.53449500
C	1.18286200	3.03388400	1.96417800

H	0.78940200	4.01417900	1.67626100
H	0.59320900	2.27045800	1.45478700
H	1.03355700	2.91092400	3.04254800
C	5.28952100	1.20987200	-3.60700400
H	5.53196500	0.38393500	-4.28461900
H	5.43572700	2.14484500	-4.15903100
H	6.00432400	1.18952000	-2.77978000
C	2.84473100	1.00804400	-4.26810300
H	3.07544700	0.15017700	-4.90914300
H	1.81901800	0.89812700	-3.90646500
H	2.88654700	1.90616400	-4.89357600
C	1.27736500	-4.68965200	-1.95619100
H	0.67072000	-4.60356800	-2.86401900
H	2.28691300	-4.35106800	-2.19477800
H	1.32959000	-5.75335200	-1.70111000
C	-0.80642600	-4.29137400	-0.59672900
H	-0.85613100	-5.33804600	-0.27720500
H	-1.29129500	-3.68500300	0.17319900
H	-1.38141300	-4.19958300	-1.52213400
C	4.25682900	-1.64496500	3.69743500
H	4.83665700	-1.56469900	2.77313400
H	4.48307400	-0.77279600	4.32125800
H	4.60622400	-2.53330900	4.23524100
C	1.93017900	-1.74265800	4.71026200
H	0.85617800	-1.76815700	4.50380900
H	2.17269500	-2.61530900	5.32637800
H	2.14151000	-0.84841000	5.30709800
C	6.58770600	2.86658600	0.43321800
H	6.12154600	2.98580200	-0.54832200
H	6.39846300	3.77780100	1.00995500
H	7.67039200	2.79124700	0.28758600
C	6.61661600	1.52904900	2.59332200
H	7.70839700	1.44768500	2.58263200
H	6.35946100	2.42275300	3.17191700
H	6.22251200	0.65646600	3.12171300
C	4.79669200	-2.87935200	-2.90508200
H	4.05839900	-3.58828600	-3.29395200
H	4.65883200	-1.92914400	-3.42950400
H	5.78741500	-3.26336300	-3.16962800
C	4.81559100	-4.06077200	-0.65528700
H	4.66517300	-3.95247200	0.42184100
H	4.09500900	-4.79692900	-1.02029000
H	5.81786600	-4.47100900	-0.81732700
H	-5.94602000	-2.12706000	-2.21486700
H	-6.60333000	-3.70469200	-1.75015700
H	-5.44002700	-3.58724100	-3.07303500
H	-5.04353200	-5.50645100	-0.80368500
H	-3.39993800	-5.09647200	-0.30764100
H	-3.80690200	-5.22424500	-2.02882000
H	-4.49416000	-0.74640500	5.16657600
H	-5.01730700	0.48869700	4.01230300
H	-3.47265600	0.65108800	4.86759000
H	-1.66162000	-2.09440400	3.02721300
H	-2.64571300	-2.44716400	4.45788900
H	-1.58971300	-1.02097700	4.43485500

Cartesian coordinates of calculated stationary points [ω B97XD/6-311g (d,p)]

Compound 3Dip

Local minimum C₂

0 1

Si	0.73256200	-2.16263900	0.52737200
Si	-0.48030200	-1.03472100	-1.13561100
Si	0.48030200	1.03472100	-1.13561100
Si	-0.73256200	2.16263900	0.52737200
Si	0.00000000	0.00000000	0.87745500
C	-2.58557700	2.62281800	0.36683300
C	-3.24547300	2.74493500	-0.88097100
C	-3.36441300	2.74522700	1.54550700
C	-4.63615900	2.87035000	-0.91437800
C	-4.74413200	2.90191800	1.46390500
C	-5.38756600	2.93403300	0.24069400
H	-5.14007500	2.92728600	-1.87228500
H	-5.32743300	2.99274800	2.37220100
H	-6.46659300	3.02876900	0.18860700
C	2.58557700	-2.62281800	0.36683300
C	3.24547300	-2.74493500	-0.88097100
C	3.36441300	-2.74522700	1.54550700
C	4.63615900	-2.87035000	-0.91437800
C	4.74413200	-2.90191800	1.46390500
C	5.38756600	-2.93403300	0.24069400
H	5.14007500	-2.92728600	-1.87228500
H	5.32743300	-2.99274800	2.37220100
H	6.46659300	-3.02876900	0.18860700
C	-0.27180700	-3.43007100	1.54564800
C	-0.49687600	-4.68240100	0.93570800
C	-0.77524400	-3.21152500	2.85579900
C	-1.18420900	-5.68438500	1.61965000
C	-1.47386800	-4.23500800	3.49299100
C	-1.67481800	-5.46487800	2.89176300
H	-1.34244000	-6.64709700	1.14583300
H	-1.87081400	-4.06784500	4.48813800
H	-2.21544000	-6.24658800	3.41385800
C	0.27180700	3.43007100	1.54564800
C	0.49687600	4.68240100	0.93570800
C	0.77524400	3.21152500	2.85579900
C	1.18420900	5.68438500	1.61965000
C	1.47386800	4.23500800	3.49299100
C	1.67481800	5.46487800	2.89176300
H	1.34244000	6.64709700	1.14583300
H	1.87081400	4.06784500	4.48813800
H	2.21544000	6.24658800	3.41385800
C	-2.06473300	-1.78417900	-1.89199400
C	-2.06684500	-2.11371100	-3.26681200
C	-3.21281200	-2.08696100	-1.12200700
C	-3.18874700	-2.71352300	-3.83573900
C	-4.32327200	-2.66113900	-1.73886800
C	-4.31740100	-2.97863300	-3.08393300
H	-3.18008700	-2.98237600	-4.88588100
H	-5.20855000	-2.87192500	-1.14993000
H	-5.18653300	-3.43719400	-3.54281000

C	2.06473300	1.78417900	-1.89199400
C	2.06684500	2.11371100	-3.26681200
C	3.21281200	2.08696100	-1.12200700
C	3.18874700	2.71352300	-3.83573900
C	4.32327200	2.66113900	-1.73886800
C	4.31740100	2.97863300	-3.08393300
H	3.18008700	2.98237600	-4.88588100
H	5.20855000	2.87192500	-1.14993000
H	5.18653300	3.43719400	-3.54281000
C	-2.55584700	2.79467700	-2.23831900
H	-1.47785500	2.78936500	-2.08100900
C	-2.74374000	2.79680400	2.93046300
H	-1.76815400	2.31462800	2.88101900
C	2.55584700	-2.79467700	-2.23831900
H	1.47785500	-2.78936500	-2.08100900
C	2.74374000	-2.79680400	2.93046300
H	1.76815400	-2.31462800	2.88101900
C	-0.86629500	-1.90491100	-4.17779300
H	-0.12975900	-1.28693000	-3.65154000
C	-3.33053000	-1.80304400	0.36475300
H	-2.33341900	-1.56311000	0.73349400
C	0.86629500	1.90491100	-4.17779300
H	0.12975900	1.28693000	-3.65154000
C	3.33053000	1.80304400	0.36475300
H	2.33341900	1.56311000	0.73349400
C	0.60642800	1.91918400	3.65490400
H	-0.13811700	1.30050500	3.15496800
C	0.00000000	5.01684900	-0.46323900
H	-0.46023400	4.12286200	-0.89572900
C	0.00000000	-5.01684900	-0.46323900
H	0.46023400	-4.12286200	-0.89572900
C	-0.60642800	-1.91918400	3.65490400
H	0.13811700	-1.30050500	3.15496800
C	3.82272500	3.01538200	1.15850300
H	3.22323100	3.90203200	0.94429300
H	3.74838800	2.81316300	2.22922200
H	4.86999700	3.24560400	0.94162800
C	4.22605800	0.58615400	0.60681000
H	4.28106200	0.34835200	1.67336000
H	3.85005400	-0.29286700	0.08301600
H	5.24458400	0.77850100	0.25496300
C	-0.20727800	-3.25103400	-4.49177500
H	-0.88910100	-3.89587700	-5.05452300
H	0.69515600	-3.10735200	-5.09308600
H	0.06710000	-3.77636800	-3.57507400
C	-1.23137200	-1.17471300	-5.47218700
H	-1.64736900	-0.18608600	-5.26570200
H	-0.34433300	-1.05502800	-6.09676900
H	-1.96633500	-1.73290300	-6.05740500
C	1.23137200	1.17471300	-5.47218700
H	1.64736900	0.18608600	-5.26570200
H	0.34433300	1.05502800	-6.09676900
H	1.96633500	1.73290300	-6.05740500
C	0.20727800	3.25103400	-4.49177500
H	0.88910100	3.89587700	-5.05452300
H	-0.69515600	3.10735200	-5.09308600

H	-0.06710000	3.77636800	-3.57507400
C	-3.82272500	-3.01538200	1.15850300
H	-3.22323100	-3.90203200	0.94429300
H	-3.74838800	-2.81316300	2.22922200
H	-4.86999700	-3.24560400	0.94162800
C	-4.22605800	-0.58615400	0.60681000
H	-4.28106200	-0.34835200	1.67336000
H	-3.85005400	0.29286700	0.08301600
H	-5.24458400	-0.77850100	0.25496300
C	1.89653300	1.09609700	3.70335400
H	2.70881300	1.65956100	4.17327300
H	1.73718400	0.18537000	4.28744800
H	2.22494400	0.79590500	2.70677700
C	0.09443900	2.15934200	5.08044700
H	-0.18237700	1.20552300	5.53972900
H	0.85654600	2.61458400	5.71880500
H	-0.78139000	2.80913800	5.09087300
C	1.15226500	5.40194500	-1.39881000
H	0.77403200	5.58693700	-2.40797000
H	1.65074200	6.31512200	-1.06136600
H	1.89857500	4.60581800	-1.45597200
C	-1.08017700	6.10239400	-0.41052600
H	-1.39321600	6.38367300	-1.41938600
H	-1.95887100	5.75225300	0.13831800
H	-0.70688400	7.00449500	0.08230600
C	-1.89653300	-1.09609700	3.70335400
H	-2.70881300	-1.65956100	4.17327300
H	-1.73718400	-0.18537000	4.28744800
H	-2.22494400	-0.79590500	2.70677700
C	-0.09443900	-2.15934200	5.08044700
H	0.18237700	-1.20552300	5.53972900
H	-0.85654600	-2.61458400	5.71880500
H	0.78139000	-2.80913800	5.09087300
C	-1.15226500	-5.40194500	-1.39881000
H	-0.77403200	-5.58693700	-2.40797000
H	-1.65074200	-6.31512200	-1.06136600
H	-1.89857500	-4.60581800	-1.45597200
C	1.08017700	-6.10239400	-0.41052600
H	1.39321600	-6.38367300	-1.41938600
H	1.95887100	-5.75225300	0.13831800
H	0.70688400	-7.00449500	0.08230600
C	-2.53436000	4.26247700	3.33671600
H	-2.06402600	4.33911200	4.32090000
H	-1.89815700	4.78651400	2.62079700
H	-3.49878500	4.77806400	3.38139500
C	-3.54654600	2.04576400	3.99739300
H	-3.81128300	1.04013500	3.66355800
H	-2.95884100	1.95592200	4.91493300
H	-4.46869300	2.57165800	4.25911900
C	-2.91153000	4.09091700	-2.97861400
H	-2.34661000	4.16814400	-3.90934700
H	-3.97278300	4.12828600	-3.23788700
H	-2.69011400	4.96721100	-2.36733300
C	-2.88889700	1.57018200	-3.09257300
H	-2.34995300	1.61669600	-4.04390200
H	-2.61283000	0.64403700	-2.58765500

H	-3.95837000	1.51757600	-3.31692700
C	3.54654600	-2.04576400	3.99739300
H	3.81128300	-1.04013500	3.66355800
H	2.95884100	-1.95592200	4.91493300
H	4.46869300	-2.57165800	4.25911900
C	2.53436000	-4.26247700	3.33671600
H	2.06402600	-4.33911200	4.32090000
H	1.89815700	-4.78651400	2.62079700
H	3.49878500	-4.77806400	3.38139500
C	2.88889700	-1.57018200	-3.09257300
H	2.34995300	-1.61669600	-4.04390200
H	2.61283000	-0.64403700	-2.58765500
H	3.95837000	-1.51757600	-3.31692700
C	2.91153000	-4.09091700	-2.97861400
H	2.69011400	-4.96721100	-2.36733300
H	2.34661000	-4.16814400	-3.90934700
H	3.97278300	-4.12828600	-3.23788700

Compound 3Dip'

Local minimum C₁

0 1

Si	-2.05227500	-0.65306700	0.23636600
Si	-1.04424300	1.37650000	-0.23668700
Si	1.08415100	1.10952000	0.49445500
Si	1.80812200	-1.05125600	-0.11327100
Si	-0.20490500	-0.72309800	-1.26394800
C	-1.72372700	2.92807500	-1.10561100
C	-1.58108100	4.21676400	-0.54816400
C	-2.44517400	2.78421400	-2.31903800
C	-2.14803700	5.31449600	-1.19668100
C	-2.98457300	3.91097300	-2.93298300
C	-2.84318800	5.17068000	-2.38013600
H	-2.04037500	6.30249600	-0.76380100
H	-3.52237700	3.79883400	-3.86695000
H	-3.27401700	6.03642300	-2.87080800
C	2.27956800	2.58085500	0.26670800
C	2.72145500	3.19326700	1.46351000
C	2.75172100	3.07711700	-0.96493100
C	3.59166000	4.27965500	1.40495100
C	3.61240000	4.17396900	-0.98032200
C	4.03140900	4.77633400	0.19256500
H	3.92945300	4.74682000	2.32382000
H	3.96311700	4.56495000	-1.92852900
H	4.70379700	5.62646200	0.16073600
C	3.33323300	-0.95903400	-1.31073000
C	4.58857500	-0.63332900	-0.74573900
C	3.29648000	-1.28706700	-2.70179400
C	5.74665700	-0.65847600	-1.52480100
C	4.47860100	-1.26975900	-3.43981400
C	5.69903800	-0.96948900	-2.86700800
H	6.70320900	-0.43088400	-1.06923000
H	4.44175000	-1.50233400	-4.49753000
H	6.60427800	-0.97680600	-3.46406900

C	-3.58662000	-1.13018400	-0.83926900
C	-4.81690100	-0.49007600	-0.56275800
C	-3.56642400	-2.10831000	-1.87351800
C	-5.95289800	-0.77668100	-1.31874300
C	-4.72899600	-2.36058700	-2.60235400
C	-5.91438100	-1.69998000	-2.34267600
H	-6.88373300	-0.26476200	-1.09954700
H	-4.70569700	-3.09773600	-3.39700800
H	-6.80158500	-1.91134900	-2.92935800
C	-2.37755900	-1.06345200	2.08225700
C	-2.46122100	-2.43808500	2.40161600
C	-2.54225100	-0.12216700	3.13277000
C	-2.61920900	-2.85052500	3.72281300
C	-2.71183800	-0.58127900	4.43914600
C	-2.73155400	-1.92850200	4.74440400
H	-2.67086900	-3.90954100	3.94998300
H	-2.82013200	0.13788200	5.24314400
H	-2.85102000	-2.25562700	5.77155900
C	2.00452800	-2.51779600	1.11260400
C	2.08806500	-3.80721900	0.53094500
C	2.04150100	-2.43088700	2.52654100
C	2.15472000	-4.94532100	1.33117400
C	2.05048700	-3.60166800	3.28787500
C	2.10650700	-4.85251900	2.70704800
H	2.22498500	-5.92145900	0.86444200
H	2.02580000	-3.52954000	4.36834500
H	2.12060500	-5.74524500	3.32257500
C	-0.84361200	4.51114100	0.74818400
H	-0.42390900	3.57657100	1.13603500
C	-2.60938000	1.46228700	-3.05040100
H	-2.40907600	0.64864100	-2.35319600
C	2.30377400	2.72431200	2.85252000
H	1.61621600	1.87694900	2.74316200
C	2.35891400	2.47713300	-2.30116400
H	1.83530800	1.53579200	-2.10319200
C	-2.53284800	1.39824500	2.98342100
H	-2.51879400	1.64929700	1.91988800
C	-2.47289300	-3.52485700	1.34044900
H	-2.22731100	-3.07167500	0.37763900
C	2.08836000	-1.13536600	3.32226400
H	2.30574100	-0.31783000	2.63105900
C	2.14390200	-4.04831400	-0.96637200
H	2.02368900	-3.09702500	-1.47581200
C	-2.35876400	-2.94749400	-2.29069700
H	-1.54482700	-2.75870100	-1.58763100
C	-5.00340000	0.49947000	0.57556400
H	-4.04946700	0.61888800	1.08378900
C	2.05602600	-1.67039800	-3.51424900
H	1.23841400	-1.89453400	-2.83197800
C	4.78949500	-0.27892300	0.72122800
H	3.80926300	-0.13545200	1.18670300
C	-3.88855300	-4.10558200	1.22599200
H	-3.92634000	-4.92013400	0.49859900
H	-4.59880100	-3.33629900	0.91110600
H	-4.22128200	-4.50653700	2.18792600
C	-1.41723800	-4.60365500	1.58207100

H	-1.39304900	-5.30540200	0.74281800
H	-1.62291800	-5.18168500	2.48762700
H	-0.42667100	-4.15785100	1.68398400
C	0.98895700	-4.92871800	-1.44892300
H	1.04945600	-5.94422400	-1.04748700
H	0.99122100	-4.99855300	-2.54073100
H	0.03330500	-4.50214800	-1.13440400
C	3.52193100	-4.59458900	-1.35693700
H	4.29990700	-3.86322900	-1.12189300
H	3.57786200	-4.81363800	-2.42537600
H	3.74682800	-5.51951200	-0.81857900
C	3.19568100	-1.15253600	4.38397100
H	3.02832500	-1.92565300	5.13885300
H	3.22561100	-0.19639400	4.90830500
H	4.17640700	-1.33011100	3.93780800
C	-3.77802400	2.05740300	3.58953500
H	-3.78055800	3.12844400	3.36996900
H	-3.80225800	1.95054200	4.67724600
H	-4.69549800	1.62630200	3.19338400
C	0.73448800	-0.84493900	3.96643600
H	0.76114300	0.10457100	4.50962800
H	0.45683900	-1.63301600	4.67409800
H	-0.05265800	-0.79014500	3.21482100
C	-1.27701600	2.00248600	3.60823400
H	-1.19410900	1.73705900	4.66630300
H	-1.30278300	3.09054100	3.53575400
H	-0.38427500	1.64178400	3.09962400
C	3.50034200	2.22626200	3.66527000
H	3.18455400	1.96521100	4.67866800
H	4.27294300	2.99583700	3.74534000
H	3.95051100	1.34370700	3.20999800
C	-1.81391500	5.05849700	1.80124500
H	-2.24216500	6.01240100	1.48190200
H	-1.30385800	5.23045500	2.75360400
H	-2.63920100	4.36311200	1.96986700
C	1.55733700	3.81244400	3.62936600
H	1.19583200	3.41623900	4.58220700
H	0.69780500	4.18088900	3.07153800
H	2.21177400	4.66195000	3.84437300
C	0.31838000	5.48341000	0.51408000
H	1.01576000	5.09547800	-0.22997900
H	0.87530100	5.65220600	1.43797200
H	-0.04738800	6.45331700	0.16568900
C	3.59287800	2.15090700	-3.14863300
H	3.30396200	1.61098900	-4.05141900
H	4.29921700	1.53159400	-2.59359300
H	4.10881500	3.06184100	-3.46541900
C	-4.02061000	1.22592600	-3.59384300
H	-4.78062900	1.41098600	-2.83303100
H	-4.11769700	0.18417300	-3.90973900
H	-4.23883100	1.85662900	-4.46109300
C	-1.57028300	1.36599100	-4.17013900
H	-1.68661500	2.19210400	-4.87905000
H	-1.67929700	0.42741700	-4.71983800
H	-0.56129700	1.40431500	-3.75979400
C	1.40132500	3.40173600	-3.06140500

H	0.48204700	3.58425200	-2.50087000
H	1.13012700	2.96197600	-4.02533300
H	1.87644800	4.36815400	-3.25733900
C	-1.86058500	-2.54562600	-3.68351000
H	-0.93870500	-3.08456800	-3.92524100
H	-2.60485000	-2.78458400	-4.44969000
H	-1.64421900	-1.47787300	-3.72681800
C	1.57621600	-0.51360200	-4.39297800
H	2.33203700	-0.25262500	-5.14054400
H	0.65854700	-0.79580800	-4.91661000
H	1.35743500	0.37436900	-3.80181200
C	2.24671500	-2.91576100	-4.38962100
H	1.27830300	-3.22362300	-4.79495400
H	2.90312200	-2.72707200	-5.24353100
H	2.66137200	-3.75258500	-3.82942300
C	-2.63358300	-4.45544000	-2.24963200
H	-3.42320400	-4.74776800	-2.94671700
H	-1.73048600	-5.00246600	-2.53286700
H	-2.92923100	-4.78254400	-1.25282000
C	-5.40508100	1.89467600	0.08756800
H	-5.47763600	2.58317300	0.93492000
H	-4.66219700	2.29625200	-0.60681500
H	-6.37517000	1.88601100	-0.41847500
C	5.55531500	1.04027300	0.88628600
H	5.04737500	1.86179200	0.37592800
H	5.64567200	1.29924800	1.94381600
H	6.57042600	0.96631900	0.48733800
C	-5.99377600	-0.06995600	1.60018000
H	-6.20289200	0.65008400	2.39457200
H	-6.94916000	-0.32142200	1.13235300
H	-5.58948900	-0.97657100	2.05872600
C	5.49382300	-1.42754700	1.45385100
H	6.45431700	-1.65417700	0.98176900
H	5.69342500	-1.15748700	2.49445800
H	4.88542900	-2.33572300	1.44297000

Compound 8Dip

Local minimum C₁

0 1

Si	-1.96384400	1.34006400	0.65593300
Si	-0.63599700	-0.31109300	0.62912500
C	-2.18376900	3.19308000	0.47479800
C	-1.98646700	3.77528200	-0.79167200
C	-2.05690800	5.16223100	-0.90595200
C	-2.34011700	5.95337900	0.19575700
C	-2.56950900	5.37049000	1.43281500
C	-2.49370900	3.98952500	1.58985400
H	-1.89266600	5.62999000	-1.87042900
H	-2.81416700	6.00039700	2.28082200
Si	3.23199000	0.19477900	0.01358200
Si	1.54515400	-1.03423800	0.55181500
C	3.04102500	1.93290500	-0.69709800
C	3.32750000	2.10546000	-2.06796200
C	3.31273500	3.38494400	-2.61754300
C	3.00473200	4.48648000	-1.83810000

C	2.71419400	4.32083600	-0.49484600
C	2.73854100	3.06096500	0.09924700
C	5.03579100	-0.39520300	-0.10400800
C	5.41312300	-1.58510300	-0.76934400
C	6.76324400	-1.83113500	-1.02113500
C	7.74822700	-0.95071000	-0.61898500
C	7.39087100	0.19098900	0.07389100
C	6.05635500	0.47964700	0.34412800
C	1.86178400	-2.72230300	1.34874900
C	1.48798400	-3.90339500	0.67112900
C	1.77894600	-5.14091300	1.23935100
C	2.44522200	-5.23025000	2.44957600
C	2.79036400	-4.07562000	3.12921400
C	2.48742300	-2.81684700	2.61138400
H	3.53794400	3.52221400	-3.66961200
H	2.46410300	5.19013700	0.10314500
H	7.04954200	-2.73831100	-1.54122700
H	8.16362800	0.87231900	0.41227700
H	1.48657400	-6.05152000	0.72849600
H	3.29165500	-4.15323200	4.08817500
H	2.68093600	-6.20130800	2.87104000
H	8.79103700	-1.16009600	-0.83021400
H	2.98668600	5.47683900	-2.27980300
H	-2.39572600	7.03117400	0.08730400
Si	-2.88046500	-0.64306600	0.01470700
C	-3.52040400	-0.35741700	-1.75869500
C	-4.70620700	0.39993200	-1.89331100
C	-2.82070500	-0.74934000	-2.91594800
C	-5.17864200	0.71288900	-3.16671000
C	-3.31160900	-0.39549200	-4.17174000
C	-4.48998100	0.31964300	-4.30115800
H	-6.10048700	1.27523700	-3.27371700
H	-2.77013800	-0.68937600	-5.06483900
H	-4.86826800	0.57517100	-5.28495500
C	-4.13675200	-1.76996300	0.92758800
C	-4.80258500	-2.79088200	0.20951100
C	-4.56779500	-1.49208900	2.25311600
C	-5.94363300	-3.38900800	0.74870500
C	-5.70902700	-2.11337500	2.75165000
C	-6.41642800	-3.03343300	1.99495600
H	-6.46339100	-4.15371100	0.18162800
H	-6.05423400	-1.88327300	3.75158400
H	-7.31317500	-3.49453800	2.39435700
C	2.41693300	2.97160500	1.58592600
H	2.63789400	1.95147400	1.91890300
C	3.68606000	0.93532800	-2.97033900
H	3.48391400	0.00994800	-2.41723600
C	-1.68139300	2.94139000	-2.02529300
H	-1.89590700	1.89387300	-1.78719400
C	-2.82660300	3.36022100	2.93079700
H	-2.40130000	2.34598800	2.93944400
C	-1.52836400	-1.54881800	-2.84844800
H	-1.39114300	-1.87968400	-1.81491700
C	-5.52146700	0.88641700	-0.69960200
H	-4.98652000	0.63559700	0.21895000
C	-4.30640300	-3.35911000	-1.11452300

C	-5.27390800	-3.11671500	-2.27757200
H	-3.35851200	-2.87811000	-1.35710600
C	-4.01637700	-4.86032600	-0.97433800
C	-3.75844300	-0.60737900	3.18780800
H	-3.36624300	0.22723400	2.60011700
C	-4.54685200	-0.00529100	4.35136000
C	-2.55694000	-1.39565000	3.72668600
C	2.82965700	-1.60036500	3.45792100
H	2.40578500	-0.72313700	2.96328300
C	0.70366300	-3.87550500	-0.63190200
H	0.77694800	-2.86313000	-1.05164000
C	5.77866300	1.75130300	1.12625400
H	4.70862600	1.79339800	1.33490500
C	4.44222500	-2.66359200	-1.22385500
H	3.42486700	-2.33751700	-0.99905200
C	-2.57193600	3.29995100	-3.21762300
H	-3.62896900	3.28224600	-2.94333100
H	-2.33434700	4.28967900	-3.62019700
H	-2.42542900	2.56771300	-4.01568500
C	-0.19808400	3.03670400	-2.38865300
H	0.09019600	4.07403700	-2.58205300
H	0.43712100	2.66039500	-1.58268000
H	0.01447400	2.45582200	-3.29053700
C	-4.34898000	3.23027900	3.06578300
H	-4.62229500	2.81494900	4.03817900
H	-4.82450400	4.21063300	2.96486400
H	-4.75577900	2.57830300	2.28706600
C	-2.22047800	4.09906400	4.12532800
H	-2.69253300	5.07374100	4.27953100
H	-2.36907300	3.51934600	5.04029400
H	-1.14839600	4.25877900	3.98845500
C	-5.67980900	2.41124200	-0.70115100
H	-6.25048500	2.75684500	-1.56826700
H	-6.21446400	2.73666500	0.19629800
H	-4.70843100	2.91142800	-0.71310000
C	-6.87802100	0.17896300	-0.61746000
H	-7.43086400	0.52080400	0.26227600
H	-7.48755600	0.38741800	-1.50229200
H	-6.74903100	-0.90208700	-0.53447300
C	-0.32101900	-0.67455000	-3.19961000
H	-0.39262300	-0.30878000	-4.22934400
H	-0.25857300	0.18915100	-2.53349000
H	0.61220000	-1.23845200	-3.10112500
C	-1.56839900	-2.80642900	-3.72077700
H	-1.67228300	-2.56246000	-4.78123800
H	-0.63921700	-3.36979200	-3.60560400
H	-2.40237700	-3.45748500	-3.44486400
C	3.23778900	3.93243100	2.45224700
H	4.31020900	3.81081700	2.29871300
H	2.98641900	4.97635400	2.24492200
H	3.02447000	3.74968400	3.50917000
C	0.92387700	3.19767500	1.81365200
H	0.62166100	4.20997700	1.52673400
H	0.34704300	2.49825500	1.21266200
H	0.66044300	3.04325200	2.86459700
C	5.17578100	0.94888000	-3.33082900

H	5.43237600	0.07819900	-3.94139200
H	5.42357200	1.84809500	-3.90371800
H	5.80250600	0.92985900	-2.43668200
C	2.81093200	0.88106800	-4.22579300
H	2.99127400	-0.05032400	-4.77062500
H	1.75174400	0.92671400	-3.96795100
H	3.03247400	1.70846800	-4.90619500
C	1.23975900	-4.83953400	-1.69342700
H	0.68946900	-4.71479600	-2.62893000
H	2.29560000	-4.66433900	-1.89774800
H	1.12149700	-5.88333800	-1.38992300
C	-0.77343500	-4.16904500	-0.35512700
H	-0.88792900	-5.16561200	0.08246800
H	-1.20844200	-3.44685800	0.34088900
H	-1.34747100	-4.14371500	-1.28342400
C	4.34285000	-1.38451500	3.54526500
H	4.78356800	-1.26452500	2.55180700
H	4.56657000	-0.48742700	4.13104700
H	4.83539900	-2.23340600	4.03006500
C	2.18898700	-1.67856300	4.84806100
H	1.11025400	-1.83641300	4.77091100
H	2.60781600	-2.49310000	5.44640200
H	2.36072300	-0.74583000	5.39317500
C	6.15476800	2.99423400	0.31098300
H	5.62735700	3.01679800	-0.64475700
H	5.90649000	3.91020500	0.85353200
H	7.22997600	3.00967400	0.10879300
C	6.48107200	1.74461200	2.48923900
H	7.56822600	1.78938100	2.37991600
H	6.17383100	2.61332300	3.07881100
H	6.23582200	0.84233400	3.05306000
C	4.51500000	-2.89188300	-2.73892200
H	3.76658800	-3.62253400	-3.05588400
H	4.32951300	-1.96346200	-3.28512300
H	5.49405200	-3.27080300	-3.04564400
C	4.70167700	-3.95430400	-0.43581300
H	4.57286400	-3.78566600	0.63631100
H	4.00705800	-4.74263600	-0.73031100
H	5.71720600	-4.32373700	-0.60560000
H	-5.47004600	-2.05529400	-2.42811700
H	-6.22874300	-3.62094300	-2.09948200
H	-4.85566600	-3.51542200	-3.20668700
H	-4.94053600	-5.43246800	-0.85529000
H	-3.38117000	-5.06457100	-0.11071700
H	-3.51113700	-5.23404500	-1.87047600
H	-4.83978100	-0.76381200	5.08327200
H	-5.44826900	0.50931700	4.00975400
H	-3.91909100	0.71887700	4.87805100
H	-1.94376400	-1.79657700	2.91714900
H	-2.90201100	-2.23372800	4.34090100
H	-1.92035500	-0.75334500	4.34334100