Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Stereocontrol in the synthesis of cyclic amino acids: a new ligand for directed hydrogenation through hydrogen bonding

Vasudeva Rao Gandi, Bao Nguyen Do Doan,

Sivarajan Kasinathan, Roderick W. Bates*

Division of Chemistry and Biological Chemistry,

School of Physical and Mathematical Sciences,

Nanyang Technological University, 21 Nanyang Link, Singapore 637371
FAX +65 6791 1961 e-mail: roderick@ntu.edu.sg

Computational Details

The DFT calculations were performed using Gaussian 16.[1] The geometry of each gas phase minimum was optimized using the Becke, 3-parameter, Lee-Yang-Parr B3LYP[2] method with mixed basis sets of Stuttgart-Dresden[3] effective core potential SDD for Rh and Pople's basis set 6-31+G(d,p)[4] for rest of the atoms. Frequency calculations were carried out at that level to ensure convergence (all positive eigenvalues for minima and single negative for saddle points). Thermochemical corrections and zero point vibrational energies, as well as the infrared, were determined at the gas phase B3LYP/6-31+G(d,p)+SDD level using the unscaled frequencies. Solvation energies were considered with single point calculations with the SMD[5] model (dichloromethane parameters) on gas phase optimized structures using the Minnesota functional M06-L with mixed Ahlrichs[6] basis sets of QZVP for Rh and def2TZVP for rest of the atoms. Empirical Dispersion Correction was also taken into consideration for solvation energies using Grimme's dispersion[7] with the original D3 damping function.
List on pages S4 – S7 are: Calculation results, including energies, thermal free energy corrections, enthalpy corrections, sum of electronic and thermal free energies (Gibbs free energy), solvation energy, sum of electronic and thermal free energies with solvation energy, and cartesian coordinate of gas phase optimized complex. Three dimensional views of all the transition structures were prepared using CYLview.[8]

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Complex	Energy	$G_{correction}$	$H_{correction}$	G	$\Delta G_{solvation}$	ΔG_{sol}
A	-2485.99148184	0.561983	0.682993	-2485.429499	-57.02	-2485.965827
B	-2485.98276703	0.560919	0.682806	-2485.421848	-55.13	-2485.963845

All of energy values are in hartrees, except for $\Delta G_{solvation}$ in kcal/mol

Complex A

C	-1.26487200	-1.68810900	-2.55024500
C	-0.86519500	-2.65952300	-1.66542000
H	-0.21154200	-3.48853100	-1.92007700
C	-2.48582900	-0.98394500	-2.00131400
H	-3.36146700	-1.30197300	-2.58931200
H	-2.42344300	0.10818600	-2.04340800
C	-1.77780200	-2.72150400	-0.45178600
H	-2.41956200	-3.61381000	-0.52566500
N	-2.56397300	-1.45360100	-0.59429100
S	-4.16295600	-1.55999500	0.03943500
O	-5.04454300	-2.18084800	-0.96031100
O	-3.99772900	-2.17468900	1.36254600
C	-4.63744200	0.15317400	0.21324600
C	-5.47453900	2.80377900	0.54019800
C	-4.14263100	0.90025700	1.28621900
C	-5.54806800	0.70166600	-0.69379600
C	-5.95367500	2.02592700	-0.52567700
C	-4.56286800	2.22026600	1.43711600
H	-3.45674100	0.45129900	1.99657000
H	-5.94374600	0.09374500	-1.50026600
H	-6.66520500	2.45506200	-1.22585000
H	-4.19050700	2.80342400	2.27503300
C	-5.96024800	4.21860500	0.74036900
H	-6.15200100	4.71550400	-0.21517800
H	-5.23683500	4.81733500	1.30108200
H	-6.90035800	4.22580800	1.30573800
C	-1.01384700	-2.79268000	0.86575100
H	-1.67457400	-2.58601000	1.70913900
Rh	0.57392100	-0.93863300	-1.14027400
C	-0.93434000	-1.59100000	-4.01268500

H	-1.74876700	-2.04913100	-4.58901500
H	-0.00805500	-2.11620000	-4.25297600
H	-0.84403200	-0.55213700	-4.34165800
P	2.21122200	0.43368200	-0.24946800
C	3.66997200	-0.47797100	0.41018200
C	5.90912500	-1.90489000	1.32572500
C	4.83572900	0.20337300	0.80391800
C	3.64549900	-1.88018300	0.46430100
C	4.76085100	-2.58931100	0.92076500
C	5.94435300	-0.50725000	1.26527600
H	4.88782900	1.28555500	0.74414600
H	2.76002800	-2.41837300	0.14196300
H	4.73412300	-3.67466700	0.94884500
H	6.83896400	0.02944400	1.56633000
H	6.77717700	-2.45579400	1.67507500
C	1.36708100	1.42955100	1.07099100
C	-0.22279300	3.04742800	2.75517000
C	1.32770600	1.17230500	2.46432000
C	0.57377600	2.47501600	0.55445800
C	-0.20796200	3.28033300	1.37988000
C	0.53374700	2.00011800	3.27632400
H	0.57616300	2.67430300	-0.51263900
H	-0.79454100	4.08493800	0.94720800
H	0.51506400	1.81122200	4.34614300
H	-0.81644600	3.67126400	3.41631900
H	-0.57658900	-3.79378100	0.97545800
O	0.03880300	-1.81177400	0.80096300
H	0.44875700	-1.59690500	1.67799900
C	2.97842400	1.68065900	-1.36774600
C	4.32584300	3.45638800	-3.07894400
C	3.42802600	2.92478000	-0.89228700
C	3.21447700	1.33659500	-2.70837100
C	3.88669800	2.21906500	-3.55693000
C	4.09411200	3.80703400	-1.74617700
H	3.25201700	3.21808100	0.13768500
H	2.87407900	0.38159200	-3.09419600
H	4.06173100	1.93999200	-4.59154700
H	4.42979300	4.76789100	-1.36764200
H	4.84259700	4.14441300	-3.74111000
C	2.05918500	0.05280700	3.16902700
H	3.06582000	-0.10949100	2.77628200
H	2.14499600	0.29762100	4.23466800
O	1.30439700	-1.17250300	3.05349500
C	1.85481300	-2.23644900	3.84013800
H	2.87790100	-2.47001500	3.52145300
H	1.21530100	-3.10874500	3.69366100
H	1.85199500	-1.96327400	4.90207700
H	1.61801400	-1.50886100	-2.07306200
H	0.66114300	-0.03997100	-2.37137000

Complex B

C	-1.28790100	-0.75218700	-2.99139500
C	-0.97334500	-2.05544100	-2.69087000
H	-0.35883800	-2.70600600	-3.30452400
C	-2.44238600	-0.32493900	-2.10365100
H	-3.39635800	-0.46838800	-2.63893800
H	-2.38092700	0.70710000	-1.75578400
C	-1.89027200	-2.59029500	-1.60082000
H	-2.77215900	-3.09387300	-2.03043100
N	-2.27723000	-1.27654300	-0.96571000
S	-3.63824500	-1.41447000	0.13007400
O	-4.71353400	-2.13204100	-0.56678100
O	-3.05399100	-1.96699300	1.35985500
C	-4.13766300	0.27549400	0.39499600
C	-4.98206200	2.90394000	0.84564400
C	-3.41536300	1.08485200	1.27829900
C	-5.28032800	0.74890500	-0.25793900
C	-5.69085800	2.06119700	-0.02659500
C	-3.84055000	2.39467500	1.48939300
H	-2.54932400	0.69622900	1.80226000
H	-5.84288200	0.09407800	-0.91477700
H	-6.58174900	2.43274700	-0.52504600
H	-3.28421500	3.02879500	2.17388000
C	-5.45815700	4.30887400	1.11818700
H	-4.62507100	4.97575800	1.35756800
H	-6.14410300	4.32055400	1.97434400
H	-5.99755200	4.72301200	0.26192200
C	-1.17938500	-3.54946600	-0.65735000
H	-1.76837500	-3.75562200	0.23764600
Rh	0.34173700	-0.86752900	-1.21981200
C	-0.91268300	0.02020200	-4.22011100
H	-1.73519700	-0.03539700	-4.94534100
H	-0.01708700	-0.39077600	-4.69088900
H	-0.74030900	1.07675600	-3.99836200
P	1.78668500	-0.11274200	0.44474100
C	3.57204200	-0.42304700	0.13080900
C	6.28697800	-1.00897700	-0.26781800
C	4.56207500	0.45248700	0.60487200
C	3.95383200	-1.59647900	-0.54143500
C	5.30514900	-1.88805700	-0.73596500
C	5.91345200	0.15979200	0.40058900
H	4.28610300	1.36459500	1.12419000
H	3.19894600	-2.28338100	-0.91292800
H	5.58993200	-2.79774700	-1.25600600
H	6.67087200	0.84794400	0.76352800
H	7.33763000	-1.23328500	-0.42551600
C	1.44319700	-1.03891000	2.00686300
C	0.85132800	-2.46451800	4.36031600
C	2.47647600	-1.48871700	2.84517200
C	0.10895100	-1.31770300	2.36185700

C	-0.18538400	-2.02667800	3.53014400
C	2.17816900	-2.19343400	4.01540900
H	-0.71321800	-0.98585900	1.73495000
H	-1.22163500	-2.23357500	3.77957500
H	2.98734000	-2.53360700	4.65465200
H	0.62617000	-3.01664600	5.26771400
H	-0.98457100	-4.48949500	-1.18431100
O	0.09539600	-2.96148100	-0.29608800
H	0.19206400	-2.94227900	0.66886100
C	1.63807600	1.67657200	0.88690100
C	1.36784100	4.36331600	1.67300000
C	1.19809400	2.01257700	2.18059400
C	1.94434000	2.71243200	-0.03054300
C	1.80594300	4.04326100	0.38767900
C	1.06116200	3.34409200	2.57416900
H	0.97531700	1.23167600	2.89778700
H	2.06807900	4.82994400	-0.31085800
H	0.73195800	3.57608500	3.58262000
H	1.27626500	5.40430900	1.96849400
C	2.40451300	2.46578500	-1.45494800
H	2.89725500	1.48997200	-1.55692900
O	3.28786700	3.49847900	-1.84574700
C	3.72506300	3.37535000	-3.19180300
H	4.26807100	2.43234900	-3.35113900
H	4.39757600	4.21310500	-3.38368800
H	2.87811900	3.42350400	-3.89266400
H	1.58546800	-0.93460200	-2.07507300
H	0.43291600	0.55988400	-1.75236900
H	3.51240700	-1.29439300	2.59040000
H	1.52720200	2.45034700	-2.12741800